Quantum Calculation of Proton and Other Charge Transfer Steps in Voltage Sensing in the Kv1.2 Channel

Alisher M Kariev, Michael Green

Submitted date: 10/06/2019 • Posted date: 12/06/2019

Licence: CC BY-NC 4.0

Citation information: Kariev, Alisher M; Green, Michael (2019): Quantum Calculation of Proton and Other Charge Transfer Steps in Voltage Sensing in the Kv1.2 Channel. ChemRxiv. Preprint.

Quantum calculations on 976 atoms of the voltage sensing domain of the K_v1.2 channel, with protons in several positions, give energy, charge transfer, and other properties. Motion of the S4 transmembrane segment that accounts for gating current in standard models is shown not to occur; there is H⁺ transfer instead. The potential at which two proton positions cross in energy approximately corresponds to the gating potential for the channel. The charge displacement seems approximately correct for the gating current. Two mutations are accounted for (Y266F, R300cit, cit =citrulline). The primary conclusion is that voltage sensing depends on H⁺ transfer, not motion of arginine charges.

File list (2)

voltagesenspaper_5.pdf (1.16 MiB)

[view on ChemRxiv](#) • [download file](#)

SUPPORTINGINF_06_07_19.docx (272.06 KiB)

[view on ChemRxiv](#) • [download file](#)

Quantum Calculation of Proton and Other Charge Transfer Steps in Voltage Sensing in the K_v1.2 Channel

Alisher M. Kariev and Michael E. Green*

Department of Chemistry and Biochemistry

City College of New York

New York, NY United States of America

*Corresponding Author: mgreen@ccny.cuny.edu;

Alisher M Kariev: akariev@ccny.cuny.edu

Key Words: Ion Channels, Voltage Gating, Proton Transport, Quantum Calculations

16 ABSTRACT: Ion channels in cell membranes control entry and exit of ions; their gating (opening and
17 closing) is key to their functioning. It is known that protons can pass through the voltage sensing domain
18 (VSD) of channels such as K_v1.2; quantum calculations for a section of the VSD show the steps protons
19 take in responding to voltage, and show no major displacement of the protein backbone with voltage
20 change; 70 amino acids are included, 42 with side chains (9 directly in the proton path), 28 as backbone
21 only, and 24 water molecules. Protons provide much of the gating current, the capacitive current
22 immediately preceding channel opening, with significant additional contributions from charge transfer
23 to other groups. Most gating models, in contrast, require major protein displacement during gating.
24 Energy terms without classical analogues (exchange plus correlation energy, which are greater than
25 thermal energy) show quantum calculations are required. Energy as a function of voltage for a key proton
26 transfer leads to approximately the correct voltage for channel opening. Calculated total charge transfer
27 (not only protons) for gating is reasonable compared to experimental values. We are also able to account,
28 at least qualitatively, for two mutations, one left shifted, one right shifted, and show the alternate proton
29 paths that are required to account for these.

INTRODUCTION:

Ion channels are an extremely important class of proteins; channels of various types are present in all cells, allowing the transport of Na^+ , K^+ , and Ca^{2+} through the cell membrane(1); other channels are responsible for transport of other substances, in particular protons(2, 3). Channels have even been found in viruses(4, 5). Voltage gated ion channels (VGIC) are a particular class of channels, and certain types of these are responsible for the nerve impulse, as well as the properties of other excitable tissue(6-8). VGIC, both for Na^+ and K^+ , have four voltage sensing domains (VSD); for the K^+ channels, these are identical, while for Na^+ they are similar (one having a different function). Here we will be concerned with the way a K^+ channel senses voltage. Each VSD of a Na^+ or K^+ channel has four transmembrane (TM) helical segments, linked by extra- or intracellular loops that extend beyond the membrane. The fourth TM helix (labeled S4) is connected via a linker of several amino acids to a domain with 8 TM helices, 2 extending from each VSD, that together form the pore through which the ion passes. Channels of the type we are discussing are closed when there is a voltage of approximately -70 mV, (minus meaning intracellular side negative with respect to the extracellular side), that holds the channel closed; with 0 mV across the channel, it is open. Fig. 1 shows the complete channel. The channel has extensive intracellular sections, and the section closest to the membrane (called T1) is involved with gating(9). S4 has arginines in every third position (except for one lysine near the intracellular end). Gating is preceded by a capacitative current ("gating current"), in which positive charges move in an extracellular direction in response to membrane depolarization. Negative charges moving in an intracellular direction could produce a similar current, but, in spite of the fact that negative charges do exist on the S2 and S3 TM segments, this possibility is not considered in the standard models of gating. These models are based on the motion of the S4 TM segment in an extracellular direction upon membrane depolarization, when its positive charges, assumed to be on three of the arginines, no longer hold it down.

55 *Fig.1: The complete Kv1.2 channel, reproduced from the*
 56 *(rcsb) pdb structure 3Lut(10); the red and blue planes mark*
 57 *the membrane boundaries, blue intracellular. The entire blue*
 58 *section below the blue membrane boundary is intracellular;*
 59 *the red helices constitute the VSD and pore. There are four*
 60 *voltage sensing domains, each with four transmembrane*
 61 *segments, between these boundaries; the pore is hidden*
 62 *behind the front VSD. Extracellular loops connecting*

63 *alternating transmembrane segments are above the red extracellular membrane boundary. The T1 moiety*
 64 *(arrow) constitutes the upper part of the intracellular section, and is involved in gating(9)*

65 *Standard gating models:* There are variations in the details of the motion proposed in different versions
 66 of the standard model, but as a class, these models are defined by extracellular motion of S4 upon
 67 depolarization. The evidence for this type of model was first based on scanning cysteine accessibility
 68 mutagenesis (SCAM(11)), and has since been supplemented, primarily by molecular dynamics (MD)
 69 (12-16), and FRET (fluorescence quenching) (17, 18). We have discussed this evidence in previous
 70 reviews (19-22), and concluded that it does not rule out an alternative source of gating current,
 71 specifically, proton transport, with S4 remaining stationary. The SCAM method requires the mutation
 72 of an amino acid to cysteine. In this case, it was the arginines on S4 that were mutated first. Arginine
 73 has a very large side chain, cysteine a very short side chain. The large difference in the molecular
 74 volume of these side chains is critical. In the SCAM method, it is assumed that cysteine must move to
 75 the membrane surface (either intracellularly or extracellularly) in order to ionize, because the
 76 membrane dielectric constant is too low to allow ionization; only the ionized form can react with a
 77 methanethiosulfonate (MTS) reagent; the test for whether the cysteine had moved to the membrane
 78 surface was that adding an MTS reagent at the side that reacted killed the channel. If the reaction really
 79 indicated that the S4 had moved enough as a fairly rigid body to make the cysteine accessible, then

one would have evidence for the standard model. However, if the cysteine could react *in situ*, without moving, then the conclusion would have to be that the ability of the MTS reagent to penetrate the membrane had changed, not that the S4 had moved. For the cysteine to ionize, at least two or three water molecules are needed near the cysteine; the presence of water molecules would make the low dielectric assumption no longer valid. The difference in side chain volume is in fact adequate for two or three water molecules. Once ionization occurs, the reactive head of an MTS reagent could replace the water, so that it could react with the ionized cysteine. Therefore, the interpretation of the SCAM data can be reconsidered.

FRET data sometimes show appreciable motion. While we cannot discuss all the data that have been adduced to support the standard model, we note that FRET data showing small S4 motions have also been reported (18, 23-25). FRET data may not have high resolution, as the probe is typically approximately 10 Å, and the orientation of the probe is important and hard to determine. Most of the computational literature on the VGIC uses molecular dynamics (MD), which is strictly classical. We will discuss below reasons for doubting MD simulations of voltage gating can properly describe this phenomenon.

Proton transport: We have proposed proton transport as the main source of gating current, instead of S4 motion, in K_v channels, especially for channels in the *Shaker* and K_v1 families, not only in the reviews just cited, but in earlier work as well (26-28). Gating current includes charge transfer on heavy atoms (oxygen and nitrogen), in addition to the proton transfers. These must be added to get the complete gating current. (Charge transfer from water to ions is known to be large, and to require quantum calculations to determine it (29, 30)) Proton transport is known in a number of systems that are analogous to the K_v voltage gated potassium family of channels. The discovery that the H_v1 proton channel is very similar to the VSD (31-33) helps show that proton transport could exist in the VSD.

Other channels with similarities to the K_v channels also show proton transport through membranes: Woelke et al give MD calculations on cytochrome c (cyt c), in which the analogy to the K_v channel is discussed explicitly (34), shows a very similar sequence to what is present in the K_v VSD (35, 36); this paper shows a tyrosine ionization essentially similar to what we report here. Additional analogous systems, not all protein, include: the M2 channel in the influenza virus (37-40); a guanidinium-ammonium competition with a crown ether(41); an amino acid-polyether/polyamine macrocycle (42); bacteriorhodopsin (a case involving tyrosine) (43); and arginine-carboxylate interactions(44). Han et al have shown how protonation states control function in a $Na^+, K^+, ATPase$ (45), in this case relevant to Na^+ binding. Mutated VSD of a *Shaker* potassium channel (46-48), which is essentially the same channel as we are considering, also transmits protons; the key is an $R \rightarrow H$ mutation at the end of the path, while the section we calculate here is part of the same path the H^+ is expected to follow in that case. In WT, the transfer to the extracellular solution is presumably blocked by arginine. Thus, our calculated proton path is consistent with previous experimental results. A proton current through the VSD has also been measured by Zhao and Blunck (49), who showed that the VSD forms a cation channel, with a preference for protons. This appears distinct from the “omega current” (50, 51). Motion of the S4 segment would seemingly produce approximately the correct gating current (with $K_v1.2$, about 10 charges move across the electric field (52), compared to approximately 13 for *Shaker*); many standard models assume that there were full +1 charges on the arginines. However, given the distribution of charge, this would not be the case, as we show below; charge on the arginines is <1 , while charge shifts on other atoms must add to the overall measured charge shift. There is also the question of why the S2 and S3 helices, with their negative charges, should not move in the opposite direction and contribute to the gating current that way; mutational evidence has generally been accepted as showing that only S4 moves. The only time we are aware of that this has been tested, using the SCAM method, the evidence suggested S3 motion in the *same* direction as the S4 (53); this would be consistent with the cysteine ionizing *in situ*, not moving to the membrane surface; also, that the access to the cavity with the cysteine was being measured within the membrane, which would be the same for positive and negative charges. If so, basic evidence for the standard model must be reinterpreted. It should also be

the case that substituting a positive or a negative charge would have opposite effects on gating current; such an experiment was done and it was found that the two charges had the same effect. Those authors interpreted the result in terms of a version of the standard model (54), although it is not clear how nearly compatible this interpretation is with other versions. If the net effect of charge on proton motion is similar, even if by different mechanisms for different charge, this experiment too appears more compatible with proton motion being largely, but not completely, responsible for gating current; we will see that gating current involves charge transfer on heavy atoms (O, N) as well, together with side chain rotation (Fig. 8 will illustrate this). More details of the evidence for S4 motion could be discussed, but would not add to what we have considered in previous work (19, 21).

There is no crystallographic water in the section of the membrane from just below the membrane extracellular side to the lower end of the helix bundle (by convention, consider the orientation of the channel such that extracellular is “up”, intracellular “down”). Therefore one section of the proton current which is found, for example in the R→H mutation case discussed above, is required to consist of protons transferring among amino acids, without water. Proteins contain salt bridges, with a base (arginine or lysine) paired with an acid (glutamate or aspartate); these exist in the VSD. It is assumed in standard models that the two side chains are ionized, and the S4 motion exchanges salt bridge partners as the segment moves. This need not be the case; in fact, without water, salt bridges generally do not ionize (55); however, in groups of three or more ionizable amino acids, even without water, ionization is possible. In addition, we show that a tyrosine, Y266, can ionize in the VSD. Other cases in which tyrosine ionizes within a protein, albeit in the presence of water, have been shown (56, 57). Proton transfer may involve the arginine NE atom (here we use pdb notation for NE and NH nitrogens on guanidinium, not N ϵ , N η). The role of individual groups or atoms has, with some exceptions, not been considered in standard models, and the ability of the NE nitrogen to act as a base does not appear to be included in any discussion of the standard model.

Calculations show proton transfer: We have carried out quantum calculations starting from the X-ray structure of a 976 atom section of the VSD of the K_v1.2 channel. These show specific proton transfers with voltage. Groups of three to five ionizable amino acids, which may include tyrosine (58), are present in all the analogous channels, cited above, that are known to transfer protons; even salt bridge and hydrogen bond distances are generally similar. There is also a tyrosine dependent voltage sensor in the M2 muscarinic receptor (59). Thus, the results of our calculations are consonant with the properties of a number of proteins well-known to transmit protons; the VSD of a K_v1.2 potassium channel is similar enough to these other channels that it should not be a surprise that the VSD transmits protons. Other charge transfer in response to membrane depolarization can also contribute. Then the motion of S4 must contribute less. If these contributions are sufficient, it is possible for S4 to not move, and thus not contribute at all. Fig. 6 shows that there is enough charge displacement with no S4 motion to account for the entire gating charge displacement.

RESULTS AND DISCUSSION: *Immobility of the S4 backbone:* We carried out computations on a segment of the VSD with 976 atoms, of which 904 were protein, from the 3Lut (pdb) X-ray structure with hydrogens added by normal mode analysis (60), and the remainder were 24 water molecules (not crystallographic) that were added in the extracellular cleft. The water, placed at the extracellular (“up”) side as a single cluster, was added at bulk density, but at random orientations. Most of the computations shown have all four transmembrane helices anchored by several backbone atoms; 62 atoms in all were fixed. The side chains of 42 amino acids were included, and the backbone of all amino acids (total, 70) in the section were also included; thus less than one atom per amino acid was fixed, on average. However, the key question is whether S4 moves under applied voltage with respect to the remainder of the VSD. Therefore, optimizations were done with S4 free to move (no S4 atoms fixed), with the voltage set to the closed (-70 mV) value; the result was compared to the X-ray structure (see Fig. 2), which is considered to be the open state. The S4 backbone does not move in such a way as to provide any gating current; some atoms move about 1 Å, in a very few cases, up to 2 Å. The exception is one isoleucine, the side chain of which pops up

(see Fig. 2), and a somewhat larger movement of the side chain of the first arginine, which rotates to some extent. We also compared the 0 mV (open) optimized fixed and free S4 cases to the X-ray structure, and found that the structures are quite close; it turned out that the S4 fixed (*i.e.*, some backbone atoms fixed) structure was slightly closer to the X-ray structure, so we kept S4 fixed thereafter. There is then the question of how the protons contribute to the gating current, and what other charge movement there is. We have done 29 calculations of wild type VSD, with different fields and proton positions (in other words, ionization of different residues), plus a check calculation, and calculations on the two mutations discussed below. The results do not agree with the standard model, but do agree with the experimental results. We have determined the total charge movement, as this is what would be measured, rather than the movement of the protons alone. We do not assume that any residue or atom has nominal charge, but use Natural Bond Orbital (NBO)(61, 62) calculations to determine charge. Details of the calculation are described below.

Fig. 2: Comparison of the X-ray (red) and S4 free optimized structure (green), for one VSD, with -70 mV applied, hence what must be the closed structure. The S4 does not move down with respect to the X-ray structure, which has the channel open. One amino acid side chain, an isoleucine, pops up. There is practically no displacement of the S4 transmembrane helix backbone, although side chain rotations are extensive, and important for proton transport.

Proton transfer: The calculations show that the entire system acts cooperatively to transfer protons up (closed to open) or down (open to closed). We look primarily at ten amino acids (R297, S184, F222, E183, R300, R303,

E226, Y266, S176, F180) that are directly involved in proton transport (see Table 6 for the complete list of 42 amino acids in the computation with side chains), although the structural elements of the system are also necessary for the VSD to function. The opening and return paths need not be identical, and because hysteresis in gating has been shown, (63) there must be more than one path. We show a primary path, and show that an alternate path (at least one) exists. We focus further on a triad of amino acids located where it is expected that the main voltage drop occurs(64). This said, the entire group of ten must be understood if we are to explain two mutations that we have calculated, and that have been tested experimentally; these are discussed after the wild type (WT) has been described, as to energy and other properties associated with charge transfer. Non-obvious local transitions, such as the rotation of a serine hydroxyl group, turn out to be important in stabilizing intermediate configurations. A trigger type response followed by a proton cascade would be consistent with the initiation of gating by a very small very fast component of gating current (the “piquito”)(65, 66). This may not be the only possible interpretation of the “piquito” but it seems the most straightforward. A single proton transfer could produce this result, and once the initial proton had transferred, the others would follow. However, rather than a trigger/cascade mechanism, the overall proton transfer may be a concerted change of state. There are two conformations of the set of ten amino acids, with and without voltage (closed/open), and the entire system may toggle between them. This calculation cannot distinguish an initial state transfer, followed by a cascade (or followed by a concerted shift), from an entirely concerted mechanism. It is almost certainly not important whether there is a slight delay between the first step and the complete transition, or whether the system moves the proton(s) in a concerted transition. Overall, we are able to distinguish two states, open and closed, and under normal circumstances the system toggles between them, but apparently through intermediate states. Because there is hysteresis, and the return may take longer than opening because of inactivation, the switch need not be simple, and may require time for the reverse step to be completed, so that it may be concerted in the forward direction only. Distinguishing these possibilities is left for future work.

The Y266, E183, R300 triad: The K_v1.2 VSD contains a grouping that includes a tyrosine, a glutamate, and

an arginine; it is one of several similar groups of three to as many as five amino acids that collectively appear to form a section of a proton pathway (in Kv1.2 at least one other triad shares one amino acid, the tyrosine, with this triad, making them together a pentad of amino acids, constituting one section of the VSD). These proton transfers do not need water. Arginine may act as an acid in two ways, either losing a proton from the NE nitrogen, or losing one from the two amine groups on the terminal carbon of the guanidinium (*i.e.*, from NH1 or NH2); obviously, the deprotonated forms of these groups can act as bases. We analyze the Y266, R300, E183 triad of amino acids that transfer a proton in detail, calculating the energy of the possible positions of the proton. In Hv1 there is a very similar triad to the R300, Y266, E183 group in Kv1.2 (for Hv1 in 3WKV pdb numbering, R207, D170, Y157) which also appears to be involved with proton transfer. It appears that similar groupings occur in bacteriorhodopsin (Y57, R82, E194 in the 1P8H structure, where the Y, R, E distances are similar to those in the Kv1.2 VSD structure for its key triad) and in cytochrome c (34). Bacteriorhodopsin and cytochrome c are known to transmit protons.

Table 1:

Total energies of the three WT proton configurations with and without field

FIELD (mV) transition standard	H ⁺ from	Y266 charge	R300 charge	E183 charge	ΔEnergy (kJ/mole)# (kJ)
0: (none)		0	+	-	65.7
-70		0	+	-	63.7
0: R300→E183		0	0	0	88.5
-70		0	0	0	0* (Lowest total energy)
0: Y266→E183		-	+	0	38.3** (Lowest total energy, for the open state)
-70		-	+	0	78.7

*lowest energy; absolute value -25111.7266 Ha; #all other terms are higher energy by the amount shown, translated to kJ/mole. See also Fig. 7 for energy as a function of voltage for the two proton positions that have the lowest energy with -70 mV and with 0 mV. $2.5 \text{ kJ} \approx k_B T$ at 300 K.

There are additional similar triads in K_v1.2 itself (e.g., R303, E226, Y266); the Y266 connects this triad to the grouping discussed above, making a pentad. There are other channels with similar triads for which the distances between key atoms are almost identical, with the same H-bond distances between heavy atoms; one such triad in H_v1, in addition to the triad mentioned above, is its selectivity filter (R201, D108, R204, comparable in dimensions to the K_v1.2 R303, E226, R300, triad (67). Only one case is discussed here, but others are sufficiently similar that the analogy for proton transfer is clear. This result demonstrates the necessity of specifically calculating possible proton transfers, rather than assuming charges based on solution pK values. In addition, water density fluctuations have been suggested as important for the inhibition of the H_v1 channel(39); there is rotation of the water cluster in our calculation (see Fig. 3) so that we also see a role of water in facilitating or blocking proton transfer; hydrogen bonds in the transfer sequence show linkage to one end of the ten amino acid sequence discussed with Fig. 3, and especially Fig. 4..

Table 1 shows how the energy changes with protonation state and field (corresponding to open and closed states) for the Y266, R300, E183 triad. When a proton is transferred among the three amino acids of a triad, the charges on all three of the amino acids necessarily change. The structure can be optimized, and then the energy calculated, for each configuration resulting from an initial proton placement, with and without an electric field added. As always -70 mV is taken as the potential drop across the membrane in the closed state. These cases are calculated for wild type. Fig. 4 shows the configurations of the most important subset of the WT optimized structures under the conditions that were calculated. A Y266F mutation is relevant here; the proposed proton path suggests this mutation must be important, and experimental results, for which we thank Dr. Carlos Bassetto and Professor Francisco Bezanilla, confirm this, with an 8.5 mV right shift in gating current. Fig. 5 includes results for this mutation.

Fig. 3: Overview of the 976 atom system shift between closed and open states: **A: The lowest energy closed state (-70 mV) Gray: backbone plus most side chain protein atoms. Blue: water cluster at the extracellular (top) end; Yellow: S4 arginines and K306, from R297 to R309. Magenta: acids, from top E183, E226, D259. Red: F233. Light blue: Y266, the key tyrosine. The arrows point to the (dark blue) proton on the Y266 –OH which will ionize to go to the open state, bonded to the red oxygen (Nominal charges R300(0), Y266(0), E183(0)); **B**: same groups and colors, arrow to same proton, except the proton is now attached to the R300 NE atom (green, just above the dark blue proton in both A and B), instead of the Y266 oxygen (Nominal charges R300(+), Y266(-), E183(0)). Dotted lines indicate hydrogen bonds, including on backbone. For a detail view of the proton transfer, see Fig. 4.**

Fig. 3 shows the key shift of a proton from Y266 to R300 (NE atom). In both cases shown here

E183 is neutral (carboxyl group protonated). When the energy was calculated with the salt bridge R300-E183 ionized, using the X-ray coordinates instead of optimization, the energy was very high, so that the E183 deprotonated state may be transient (also, optimization may lower the energy somewhat). E183 must transfer a proton to water, and accept a proton from R300. These calculations are not sufficient to demonstrate whether the transition is concerted or sequential, but the concerted transition seems likely to have the lower activation energy, as it avoids the high energy ionized state. Comparison of Fig. 3A and 3B shows a number of shifts of side chains, and water molecules. The latter are obvious, as the water spreads out in the open state, and approaches E183, making it easier for water to accept a proton from E183. The R297 side chain rotates slightly up, leaving less space for water; the water cluster rotates and becomes slightly more compact. E226 slides to the right in Fig. 3B, as the Y266 proton to which it was hydrogen bonded in the closed state moves to R300; the E226 - Y266 distance increases by more than 1 Å, and the carboxyl group rotates away from Y266. At the lower end, F233 rotates downward and, at the bottom, R309 also rotates downward. The location of cavities in the structure shifts somewhat as well. Fig. 4 shows the transfer in detail, with rotations of neighboring groups.

A

B

Fig 4: 145 atom detail from Fig. 3, with the amino acid side chains involved in the proton transfer of the system, here showing the key proton transfer Y266 to R300 (arrows). **A**: closed (cf. Fig. 3A) **B**: open (cf. Fig. 3B). In the closed case, there is a proton on Y266, nominal charge 0. The open case has the proton transferred to R300, NE atom, making the nominal charges Y266(-), R300(+). Carbon is green, nitrogen blue, oxygen red, hydrogen white. Atoms not part of the side chains or water are part of the backbone.

In Fig. 4B, the F180 is behind two H-bonds from R300 to E183, not involved in hydrogen bonding itself, but the rotation of the aromatic group may assist in proton transfer(68). The cation- π interaction is also affected by pH (*i.e.*, protonation state), as can be determined spectroscopically(69, 70); rotation of the aromatic side chains must affect the protonation state. The differences between closed (Fig. 4A) and open configurations (Fig. 4B) include rotation by almost 90° of the R297 guanidinium group, and the inclusion of two waters between R297 and E183, completing a plausible proton path from R300 to R297; in the closed state no such path is possible. A nearly linear arrangement of three waters appears near the R297, but not so close to R297 that it can form a path for H⁺. T184 is hydrogen bonded to R297 in the closed

configuration, but rotates down and hydrogen bonds to water and a backbone carbonyl in the open case. In short, an H^+ can move through the entire section, reaching R297, in the open case, but not in the closed case.

Fig. 5: The main changes between closed (A) and open (B) configurations for the Y266F mutant with the same set of atoms as in Fig. 4. Three proton positions each were optimized for closed and for open, and the lowest energy case for each is shown. F266 replaces Y266 in the mutant. The most obvious difference between open and closed here is in the S176—R303—E226 sequence starting at the lower right. In the closed case R303 does not communicate with E226, nor with S176. The orientation of the protons in E226 and S176 leaves the E226 isolated and without hydrogen bonds relevant to the proton path; the S176 hydroxyl is

oriented down toward the backbone. In the open state, the S176 hydroxyl is hydrogen bonded to R303, which in turn is much closer to E226, in a position to transfer a proton; the S176 hydrogen bond makes this more energetically favorable. From E226 to R300 transfer appears possible in both open and closed configurations, although the voltage may prevent this in the closed case. The F266 ring rotates but does not take part in this transfer. The aromatics (F180 and F222, upper section, not labeled) and the water both move appreciably. A proton path can be found for both open and closed configurations from E226 upward.

The Y266F mutation produces a major rearrangement of side chains in the vicinity of the mutation, as shown by Fig. 5. To the extent that the backbone shifts at all, it is a bit higher in the closed state, the reverse of the standard model. However, the motion is so slight as to be insignificant. In Fig. 5 there is an alternate proton path, via E226, when the tyrosine path is blocked by the Y266F mutation. S176 acts as a switch, which it does not do in WT; in the calculation the –OH from S176 rotates so as to be able to H-bond to R303 when the proton opening transitions start, with R303 becoming neutral. This is very similar to a configuration in bacteriorhodopsin in which a serine (S193) undergoes a rotation when a neighboring glutamate becomes deprotonated (71). Here the path must bypass a break in the proton path that is present in WT. In addition, there exists the possibility of a proton moving along the helical backbone. It was shown by Oliver and Deamer that polyalanine or, better, polyleucine, could conduct protons through a lipid membrane, so it is not possible to rule out steps that include the backbone, even if a much shorter segment than in the Oliver and Deamer case, which brought protons entirely through a membrane (72). In the mutant, the aromatic ring of the phenylalanine (F266) rotates $\approx 90^\circ$ under the influence of the field. Since H^+ -aromatic interactions are generally stronger than $k_B T$ (73), this may allow a proton to pass via yet another path in the mutant. We also observe essentially the opposite E226 rotation to that in the WT, forming an H-bond with R300 in the closed state. The role of a dihedral transition of an aromatic (phenylalanine) in assisting proton transport in the H_v1 channel has been suggested, based on QM/MM calculations, by van Keulen et al (68).

Also, in the mutant, the phenyl ring of F222 shifts approximately 1 Å relative to backbone (alternatively, this could be considered a shift in the phenyl(CG)-C α -C β -N dihedral angle (52.9° open, 75.6° closed), which

in WT remains almost fixed). The F233 phenyl in the Y266F rotation resembles that in Schwaiger et al(74); here it appears to facilitate transition to the open state. That the Y266 (WT) path is preferred is shown by the Q-V curve being right shifted in the mutant. The calculated energy of the configuration with the E226 protonated is, in WT, approximately 19 k_BT greater than that with the Y266 protonated. The sign of the energy change is as needed for a right shifted curve. Although the magnitude is somewhat too large, a fairly small shift would bring it within range.

These shifts make several interatomic distances differ from WT by about 1 Å, in addition to the F266 ring rotation, with its effect on H⁺-π interaction; these are shown in Fig. 5. None of the side chain changes is individually large, but collectively they can easily account for a difference of several k_BT in energy. One expects that a loss of gating charge would accompany disruption of this system, although this calculation cannot directly show that. Standard models would make an opposite prediction; the removal of the –OH should make sliding S4 easier, producing a left shift. Y266 ionization in WT is the only apparent explanation for the effect of the Y266F mutation.

A second mutation is also relevant, in which the putative, standard model, gating charges, R297, R300, and R303, are replaced by isosteric, but uncharged, citrulline. Fig. 6 shows the result of a calculation of R303cit, which helps to understand the experimental left shift in the Q – V curve found for this mutation.

Fig. 6: Two cases of the R303cit mutation, both with the closed proton position (nominal charge Y266(0), R300(0), E226(0)), corresponding to the blue line in Fig. 7). The mutation is marked by the yellow arrow, which points at the carbonyl that replaces the $-NH_2$ of arginine. There are at least three major hydrogen bond shifts marked by blue arrows: T184 rotates (top blue arrow), Y266 switches its hydrogen bond from R300 ($V=-70$ mV) to E226 ($V=0$ mV) (middle blue arrow) and the citrulline carbonyl switches from no H bond to an H-bond with S176 at $V=0$ mV (bottom blue arrow). The largest change is the water cluster at the top, which is pulled up in the $V=-70$ mV state (A), interacting only with R297, but in B, it interacts strongly with the aromatics and with R300 as well.

Also, in the mutant, the phenyl ring of F222 shifts approximately $1 \text{ \AA}$ relative to backbone (alternatively, this

could be considered a shift in the phenyl(CG)-C α -C β -N dihedral angle (52.9° open, 75.6° closed), which in WT remains almost fixed). The F233 phenyl in the Y266F rotation resembles that in Schwaiger et al(74); here it appears to facilitate transition to the open state. That the Y266 (WT) path is preferred is shown by the Q-V curve being right shifted in the mutant. The calculated energy of the configuration with the E226 protonated is, in WT, approximately 19 k_BT greater than that with the Y266 protonated. The sign of the energy change is as needed for a right shifted curve. Although the magnitude is somewhat too large, a fairly small shift would bring it within range.

These shifts make several interatomic distances differ from WT by about 1 Å, in addition to the F266 ring rotation, with its effect on H⁺- π interaction; these are shown in Fig. 5. None of the side chain changes is individually large, but collectively they can easily account for a difference of several k_BT in energy. One expects that a loss of gating charge would accompany disruption of this system, although this calculation cannot directly show that. Standard models would make an opposite prediction; the removal of the -OH should make sliding S4 easier, producing a left shift. Y266 ionization in WT is the only apparent explanation for the effect of the Y266F mutation.

A second mutation is also relevant, in which the putative, standard model, gating charges, R297, R300, and R303, are replaced by isosteric, but uncharged, citrulline. Fig. 6 shows the result of a calculation of R303cit, which helps to understand the experimental left shift in the Q - V curve found for this mutation.

Fig. 6: Two cases of the R303cit mutation, both with the closed proton position (nominal charge Y266(0), R300(0), E226(0)), corresponding to the blue line in Fig. 7). The mutation is marked by the yellow arrow, which points at the carbonyl that replaces the -NH₂ of arginine. There are at least three major hydrogen

bond shifts marked by blue arrows: T184 rotates (top blue arrow), Y266 switches its hydrogen bond from R300 ($V=-70$ mV) to E226 ($V=0$ mV) (middle blue arrow) and the citrulline carbonyl switches from no H bond to an H-bond with S176 at $V=0$ mV (bottom blue arrow). The largest change is the water cluster at the top, which is pulled up in the $V=-70$ mV state (A), interacting only with R297, but in B, it interacts strongly with the aromatics and with R300 as well.

In Fig. 6 we see a number of changes with voltage, without shifting a proton. If we compare with the blue line in Fig. 7, representing the energy of the closed state, we see that the 0 mV energy is pulled down by more than 50 kJ, thus reducing the barrier between closed and open by about 10 kJ (the maximum of the blue curve is pulled down by >50 kJ). Experimentally, the $Q-V$ curve is left shifted by over 40 mV; this suggests that the energy change is not unreasonable.

Summary of mutations: We should expect that if the proton cannot transfer from the Y266, it should make gating more difficult, and it does; the Y266F mutation leaves a still functional channel, right shifted by approximately 8.5 mV for the gating current curve. Fig. 5 showed the missing $-OH$ and the possible alternate paths through which the channel could still function. The discussion that accompanied Fig. 5 showed how plausible alternate proton paths could be found.

The second mutation, R303cit, in which a putative (in standard models) gating charge is replaced by the isosteric, but uncharged, citrulline side chain, showed a left shift (75). The energy for the proton transfer dropped in the mutant by approximately 10 kJ, equivalent to $4k_B T$, so that the calculation is consistent with a left shift, as in the experiment; the >50 kJ drop is the total for 0 mV, while the 10 kJ refers to the change in the barrier, that is, the energy at which the two curves in Fig. 7 would cross. In this case, the magnitude is quite reasonable. In the wild type, the energy at this point rises, so the mutant favors the open state. Fig. 6 shows the mutant, with the relevant shifts in position of the aromatic rings marked. For lack of computer resources, we did not calculate the R297cit mutation, nor the R300cit mutation, which right shifted the $Q-V$ curve. Experimentally, R297cit kills the channel; from Fig. 4 it is fairly easy to see why this should be, as both paths for the proton must go through that arginine, and the citrulline does not have the requisite

NH₂ group to transfer a proton; unlike arginine it is not amphoteric. In addition, that is the location where the largest part of the electric field drops(64). The R300cit mutation right shifts the Q-V curve. Given that R300 is part of the Y266,E183,R300 triad, it is not surprising that R300 behaves like Y266, and removing that path right shifts the curve, similarly to removing Y266; experimentally, it is somewhat larger, but not so much so as to make the interpretation implausible (75). Given that all other mutations and the WT calculations are consistent with the model presented here, the more extensive calculations are left for future work.

Bond orders of hydrogen bonds: The bond orders of certain hydrogen bonds differ in open and closed states. Bond orders were calculated using NBO, and the results for some hydrogen bonds in WT are shown in Table 2. Not surprisingly there is a relation between bond order and bond length. The small side chain displacements strongly affect the bond strength, since 0.2 Å is enough to change the bond strength appreciably, especially in H-bonds.

Table 2:

Bond Orders of Certain Hydrogen Bonds (WT)**

	H shift →	no H shift	no H shift	R300→ E183	R300→ E183	Y266→ E183	Y266→ E183	Y266F mutant	Y266F mutant
H-bond	V(mV)	-70	0	-70	0	-70	0	-70	0
R300- E183	H1-O1	0.16	0.16	0.10	0.13	0.13	0.16	0.16	0.16
	H2-O1	0.24	0.24	0.11	0.09	0.13	0.10	0.21	0.23
R303- E226	H1-O1	---+	--	0.24	--	0.22	0.22	--	0.19
	H2-O2			0.31		0.30	0.29		0.31
Y266#- E226	O-H-O	0.31	0.31	--	0.22	--	--	--	--

Y266- R300(NE)	O ⁻ NE(H)	--	--	--	-0.31*	-0.30*	--	--	--
Y266- R303	O ⁻ - NH	--	--	--	--	0.12	0.11	--	--

*: Note that these are fairly strongly anti-bonding: there is at least one node in the electron density between the two possible positions of the hydrogen atom.

There is also a strong H-bond (0.40** bond order) between the NE of R300 and the –OH of Y266 in one case only: (-70 mV, R300 proton transferred to E183)

--Blanks: there is no H-bond

Where there is a blank in Table 2, there is no interaction, generally because the side chain has rotated in such a way that the relevant heavy atoms are either too far apart to form an H-bond, or oriented so as to make the bond impossible by reason of intervening atoms—examination of Fig. 3 through Fig. 6 also shows this. The strongest H-bond bond order, 0.40, almost covalent, (see footnote, Table 2), is between the NE of R300 and the –OH of Y266, when the proton has shifted from R300 to E183, neutralizing the salt bridge; this practically locks the structure in the closed state, and has the lowest energy (Fig. 7), about 20 k_BT (≈50 kJ) below the crossing point of the two positions, within the error of the calculation and the experimental error of what is found for the activation energy of gating from the temperature dependence of the current. However, this is not so easy to interpret. The fact that individual steps calculated here have different temperature dependences may not be relevant, as the steps from the calculated section to the gate may also be responsible for temperature dependence (76, 77), and other steps may contribute. Removing the voltage allows the proton to transfer so that the R300-Y266 H-bond no longer exists, and the side chains can change their local structure. Second, there are hydrogen bonds with bond order near 0.3 between E226 and Y266, and E226 and R303. There is a net of one extra bond with V= -70 mV. It appears that there are no other particularly remarkable H-bonds in this region. However, there are side chain rotations. Since the closed state

has lower energy than the open state (with the aid of the voltage) it appears that these strong H-bonds are in the range that could contribute to the lower energy of the closed state. The complication of the system, with multiple possibilities, suggests great caution in interpreting temperature dependence as a consequence of individual steps. It is possible for an individual step to require so large an energy step as to be incompatible with observation. Our result is not incompatible with the observed temperature dependence, but we should not go beyond this.

The exchange and correlation energies were also calculated; in general, their differences with voltage, as well as proton position, are on the order of tens of kJ (see Table 3), so that they cannot be neglected.

Table 3:

Exchange and correlation energies (kJ/mole)⁺ for the same six cases as Table 1

Nominal charge and energy →	Y266	R300	E183	Exchange energy	Correlation energy	Sum
-70 mV	0	+	-	0	2.5	2.5
0	0	+	-	0	0	0
-70	0	0	0	75.8	20.2	96.0
0	0	0	0	37.9	22.7	60.6
-70	-	+	0	65.7	37.9	103.6
0	-	+	0	12.6	12.6	25.2

⁺ Absolute value of energy of the lowest energy state (2nd row) is subtracted from each term. The energies shown are the energy differences between this state and the energy of each configuration. 0, +, - in columns 2-4 are the nominal charge states of the amino acid shown for that configuration. To get absolute values of energy, add 6635.04 kJ to exchange energy, 430.78 kJ to correlation energy for all cases.

Translate the exchange + correlation energies into units of k_BT for T=300 K, approximately 2.5 kJ/k_BT, to

understand the physiological significance. For the (0,0,0) cases that total 24 k_BT for 0 field, 38 k_BT for field on, there is a difference of 14 k_BT; for the (-,+,0) cases, the energy is 10 k_BT (0 field) compared to 41.5 k_BT (with field), a difference of approximately 31 k_BT; without the exchange and correlation terms the wrong ionization states would be assigned. The difference of 17 kJ, or about 7 k_BT, makes a considerable difference in the voltage at which the crossing of the two states occurs. These “quantum terms”, those with no classical analogue, (the values of kinetic, etc. energy also are quantum terms in this calculation, although classical values exist for these) also bring the “normal” ionization states somewhat closer to the others, although the sum of potential plus kinetic terms still leave them slightly higher in energy. The nominal charges in Table 3 show the location of the proton, while the actual charges, from NBO calculation, are in Table 4

Table 4a:
Charges on Y266 and glutamates* as determined by NBO calculations(61, 62, 67)

Field, R300 charge**	V=0, R300(+)	V=0, R300(0)	V<0, R300(+)	V<0, R300(0)
Y266	-0.843	-0.247	-0.843	-0.248
E183	-0.014	-0.016	-0.009	-0.013
E226	-0.733	-0.729	-0.732	-0.728

**For Y266, the charge is either that on the oxygen if ionized (columns 2 and 4), or else small and distributed if it is not ionized; for glutamates, charge is the sum of that on the carboxyl oxygens plus the carbon to which they are bound, plus the proton; the E183 proton comes from the tyrosine if the arginine is charged. E226 is ionized, with constant charge of ≈ -0.73 ; none of the charges is close to unity. All these cases have E183 nominally neutral, E226 nominally -1.*

***nominal charge (i.e., H^+ position)*

Table 4b
Charges on arginines

Field, R300 charge** (Number of atoms counted)	V=0, R300(+)	V=0, R300(0)	V<0, R300(+)	V<0, R300(0)
R297(6)	0.158	0.162	0.147	0.16
R297(7)	0.838	0.842	0.835	0.840
R297(9)	0.651	0.653	0.655	0.653
R300(6)	0.091	0.070	0.093	-0.071
R300(7)	0.778	0.572	0.781	0.570
R300(9)	0.622	-0.094	0.624	-0.095
R303(6)	0.116	0.135	0.111	0.134
R303(7)	0.798	0.817	0.793	0.816
R303(9)	0.577	0.599	0.577	0.598

**On each arginine, charges are summed over 6, 7, or 9 atoms: for 6 atoms, the sum is over both NH₂ groups, or NH+NH₂ if one proton has transferred to another group; 7 atoms, add the central carbon; 9 atoms, add the preceding (nearer backbone) N (+H, if present; this is the NE nitrogen). i.e., if the H⁺ from a guanidinium has transferred to another group, the sum over two NH₂ groups becomes the sum over NH + NH₂ and the number of atoms decreases by one to 5, 6, or 8.*

Table 4 shows the calculated charges on side chain functional groups (guanidinium in arginines, carboxyl in acids, oxygen in tyrosine). Note that these results show a small dependence on applied voltage, and a large dependence on proton position. The charges are not close to +1 and -1, but show the distribution of electron density. We earlier (Table 3, and accompanying discussion) emphasized the importance of including the exchange and correlation terms in order to determine the correct order of states, and thus the ionization states with and without field. The charges in Table 4, and the exchange and correlation energies in Table 3, show quantitatively that the charges on groups depend significantly on the external field and protonation state, and, to a lesser extent, on the hydrogen bonds they participate in.

The importance of the NE atom on the arginines: As noted in the Table 4 footnotes, it is the NE atom, more than the guanidinium group amines, that is responsible for most of the charge, when the arginine becomes protonated. When protonated it also forms hydrogen bonds that are stronger than most, as shown by the bond orders listed in Table 2. The combination of the NE and guanidinium is thus amphoteric, able to act simultaneously as base and acid, thereby transmitting a proton. Arginine is the only amino acid with this property, which provides an alternate explanation, not involving carrying charge by physical movement, for its conservation on the S4 helix.

BLUE LINE, closed: R300(0), Y266(0), E183(0); ORANGE LINE, open: R300(+), Y266(-), E183(0)

Fig. 7: Total energy (entire 976 atom group) as a function of voltage for the two relevant proton configurations. Charges are nominal, indicating only proton position. Energy units are kJ, in relative units; for total energy, add 63419.575 MJ. Calculations were done at 35 mV intervals. The green box indicates the approximate range at which channel open probability goes from near zero (negative voltage) to near one, as well as a rough estimate of calculation error. Conclusions would be essentially unchanged if the crossing were anywhere in the green box, corresponding to an error in relative energy of about ± 10 kJ (± 4

$k_B T$), in a range of ± 10 mV, as large as can reasonably be expected.

Fig. 8 shows a calculation of the center of charge in the 976 atom section for an open (*i.e.*, 0 mV) and a closed (-70 mV) configuration, with the proton shifted, as in Fig. 3 and Fig. 4, from Y266 (closed) to R300 (open); the Fig. 8 red line corresponds to the orange line in Fig. 7, the blue line to the blue line. The center of charge, in coordinates that place the VSD between 0 Å and 33 Å, is at 19.5 Å for the open VSD conformation, and 8.2 Å for the closed case, so the center of charge moves 11.3 Å in response to voltage. Because the charges are the sum of *all* charges in successive 3 Å slices, it includes the effects of all charge transfer, side chain rotation, and hydrogen bond shifts.

Fig. 8: The sum of the charges on 3 Å slices parallel to the membrane surface; the curves shown are smooth fits to these values. The charge displacement is approximately 11.3 Å between the lowest energy state with -70 mV and the lowest energy state with 0 mV: “TOP” is the extracellular end, starting with 0 Å. (corresponding Fig 7 curves: blue curve to blue curve, red curve to orange curve),

Thus, gating current includes the proton transfer, plus the rotation of the side chains, together with polarization of all groups, which is the collective response of the VSD, including all its atoms. As can be seen from Table 4, the charges are not +1 on each arginine and zero elsewhere. The same is true for other residues, not in the Table. While most other charges are not large, they add to become non-negligible.

565

566 For the case with the R297 – E183 salt bridge neutral: nominal charge, R297(0), E183(0), and the other two
567 atoms with “normal” nominal charge (R300(+), Y266(0)) in Fig. 5, the energy requirement to transfer a
568 proton from R300 to Y266 is cut by about 15 $k_B T$ (37 kJ) as the transfer lowers the energy when the voltage
569 becomes more positive. That state also showed minimal response to applied electric field, energy changing
570 less than 1 $k_B T$ in the entire range of voltages. So small an effect is somewhat surprising. Without charge
571 on R297 and E183, this state would not be expected to respond strongly to voltage, for practical purposes,
572 so that it would not take part in gating; the fact that it is as small as it is may be partially fortuitous. On
573 examining the terms that add to give the total energy, we see that the variation in nucleus-nucleus repulsion
574 as the structure shifts slightly very nearly cancels the variation in electron-nuclear attraction, While having
575 $\Delta E \leq k_B T$ for this case may be fortuitous, if it were $\pm 4k_B T$, as in the Fig. 7 error estimate, we would still
576 consider this state as not participating in response to voltage, although it is close enough to perhaps offer a
577 secondary path in case of mutation.

578

579 While this set of calculations is not compatible with any model in which S4 moves normal to the membrane
580 sufficiently to contribute to gating current or gating, it is still compatible with an intracellular rotation,
581 turning on a hinge below the region calculated, somewhat like that suggested by the bacterial sodium
582 channels studied by Wallace and coworkers(78). Vertical S4 motion does not appear to play a role in those
583 channels either, but the rotation of the helices at the intracellular end of the VSD is central to gating.
584 However, the intracellular region of the K_v channels is different from that in those channels, so the K_v
585 channels must use a different mechanism to gate. An extended proton path toward the gate would be
586 possible in the K_v channel, and would account for gating. In principle, the section not yet calculated, below
587 the 976 atom section discussed here, and near or below the intracellular membrane surface, could add to
588 gating current, but it is expected to make a negligible contribution. This section is also not expected to
589 contribute significantly to voltage dependence, in either standard models, or our model. Experimentally it is

known that most of the voltage drop across the membrane is localized near R297(64). We expect the continuing proton path to be generated by interaction with the protons that move in response to voltage in the region we have calculated so far. The proton path can be postulated from a position near F233, where these 976 atom calculations end, along the intracellular surface of the membrane, including part of the T1 moiety, to the gate, which is below the transmembrane pore of the channel. There are water molecules in this part of the path. The proton would reach a histidine near the PVPV section at the gate, producing current largely along the membrane surface, rather than perpendicular to it. Protons in this section move in response to the change in protonation state of the section which we have already calculated, hence making little contribution to gating current while still moving protons to (closing) or away from (opening) the gate. The details of the effect of protonating the histidine remain to be calculated. With only a subtle change in the gate diameter required to switch from closed to open, likely as little as 2 to 3 Å for each VSD, the interaction with water at the gate and the interaction with the ion are both crucial. So far, we must restrict ourselves to saying that the protonated histidine will be different from the unprotonated histidine; it would be speculative to go beyond this without doing the calculation, which has just begun.

CALCULATION: All calculations were done using Gaussian09 (D or E versions) (79). The calculations presented here are a section of one domain of the VSD of Kv1.2; all amino acids are referred to with the 3Lut (pdb) numbering; 976 atoms (904 from protein, plus 24 water molecules) were optimized at HF/6-31G* level; Table 6 shows which amino acids had their side chains included in the calculation; others in the range shown had their backbone atoms included, but the side chains (which in all these cases pointed away from the central path) were truncated, terminated with H. The net charge in all cases was +2 for the entire system. In Fig. 2, all atoms of S4 were free to move, and two cases were optimized, at 0 mV, which should correspond to the X-ray structure, and -70 mV, which should show whether S4 can move when closing with respect to the other transmembrane segments. In both cases, there was little motion of S4, and such motion as there was (always <2 Å, rarely >1 Å) in the -70 mV case was in the wrong direction

for standard models—S4 showed a very slight rise, rather than moving toward the intracellular end. After the structure was determined at HF/6-31G* level, the energy was calculated at B3LYP/6-31G** level, which was also used for NBO calculations, as single point calculations. The NBO calculations, which give the charges on the atoms, show that the charges depend on the field and the proton position, which would also affect the Coulomb terms in the Hamiltonian. There is also less symmetry than might be expected; for example, the hydrogens on the NH nitrogens on arginine differ sometimes by as much as 0.02 charges, which is not negligible. Ahmadi et al have provided an extensive and careful review of possible uses of QM calculations in multiscale applications, as well as the ways QM cluster calculations can be advantageous, or not(80). HF was not sufficiently accurate for energy and NBO calculations, (for one thing, HF lacks correlation energy), so B3LYP/6-31G** was used in single point computations on the HF optimized structure. Taking these results together, along with the charge transition in Fig. 8, we can conclude that *Voltage sensing is a collective response; it is not a single charge, or just three charges, that respond.* The possible proton pathways are complex, and alternate pathways exist, involving amino acids that may have only a peripheral role in the lowest energy, hence preferred, path. It is only by including all the relevant amino acids that we can understand the behavior of the channel. This said, it is also true that there are amino acids that play a primarily structural role, and are not directly involved in any proton transfer path. *Validation, with some questions that remain to be resolved.* There are problems with these calculations as well. For one thing they find local minima at 0 K, and do not directly allow for any dynamics. If the local minima were shallow, and the probability were high of a system optimizing into a random and unimportant minimum, the meaning of the calculation would be questionable; however, the minima are not shallow compared to $k_B T$ at 300 K. As a further test, we started the system from two different configurations (proton positions given in column 1 of Table 5, one of them the X-ray configuration). If there were multiple minima, these would be expected to give different results. If the calculation is reliable, the system should reoptimize with the proton in the -70mV position as found starting from the X-ray coordinates; otherwise it will probably give a different minimum. The calculation was done, and the result had the system return to the

640 same position as it found starting from the X-ray coordinates, with the large distances (atoms separated by
641 $> 20 \text{ \AA}$) from one TM segment to another changed by $< 0.01 \text{ \AA}$, and hydrogen bonds also the same within
642 $< 0.01 \text{ \AA}$ (three are shown in Table 5). The energy differed by approximately 0.0007 Ha , $\approx 1.6 \text{ kJ}$, or about
643 $0.7 \text{ k}_B\text{T}$. In essence, the system found the same minimum. This was not a short calculation, taking over two
644 months, but the result did show that at least this key minimum is reliable. Limited computer resources
645 prevented testing multiple starting positions, but this case gave as good a chance as any of finding a different
646 minimum. Table 5 summarizes the results.

647 Table 5
648 Energy and distance comparison of a minimum obtained from different starting coordinates

Energy and distances	Energy (kJ) relative to lowest state	R300/NE to Y266/O Angstroms	Y266/O to E226/O Angstroms	Y266/O to R303/NH1 Angstroms	R297/N to S169/O Angstroms	T184/O to S398/O Angstroms
X-ray structure: R297(+);E183(-); Y266(0)	57.4	3.15	2.66	3.58	24.14	22.58
R297(+);E183(0); R300(+); Y266(-)	80.2	2.74	3.85	2.76	24.74	22.88
R297(+);E183(0); R300(0); Y266(0)*	1.6	2.77	3.69	2.91	24.79	23.73
R297(+);E183(0); R300(0); Y266(0)#	0.0	2.77	3.69	2.91	24.79	23.73

649 *Configuration optimized starting from the 3Lut coordinates (X-ray); #same configuration. In each case,
650 the starting coordinates are the structure shown two lines above. Energy shown is relative to that in the
651 last line. Both of the last two lines are at -70 mV , and show the same optimized state.

652 Testing reversibility is a stringent test for whether the minima that are found represent actual configurations
653 of the system, and are not random local valleys in the energy landscape. (To the best of our knowledge,
654 there do not appear to be any published MD calculations that attempt to return the system to the starting
655 configuration, except for steered MD.)

656

A second problem is that these calculations are limited in the number of atoms that can be included. Here, with 976 atoms, we have a very large QM computation, but it is roughly two orders of magnitude smaller than a MD calculation would be. However, once we have determined that the QM exchange and correlation terms are required, along with charge transfer, and the correct kinetic and potential energy terms differ from their classical analogs by more than $k_B T$ (the changes in charge in an optimization are already large enough to see this—no classical calculation allows for such changes; including polarization helps, but is not only rarely used but insufficient, while other changes remain to be counted in the total difference), we are obligated to find a means of doing the QM calculation, even without including dynamics. To do so, we try as many as possible of the plausible configurations of the voltage sensing section (including the 3 critical arginines) of the VSD; we do not consider some combinations as plausible, such as anything in which Y266 or E183 is positive, or any guanidinium group negative. If we have enough local minima, we can track a path for the proton as a function of voltage. The region we have calculated includes most of the region in which the field drops(64), and is therefore the relevant region for testing the difference between the proton positions with and without voltage.

Finally, cancellation of errors in the *total* energy between calculations with different fields and proton positions is likely, to very good accuracy, as the system changes only in local transfers of protons, leaving most of the system unchanged. The lowest energy proton position is different with and without the field applied. We observe that the configuration (Y(0),R(+),E(-)) is never the lowest energy; the calculation shows that the proton shifts. Neglecting the exchange and correlation energy would generally assign incorrect charges to the main charged groups; in particular, it would lead to an incorrect result in this case. The limit on the size of the system may, in principle, produce a problem with the boundaries. However, for these calculations, the boundaries are identical for all positions of the proton that shifts internal to the protein. Also, the proton transfer is fairly close to being an isodesmic reaction (one in which the total number of bonds of each type is unchanged); this type of reaction will have the reaction energy essentially correct, even if the

absolute value of the total energy is not.(81, 82). If we consider the proton transfer Y266→E183, it is essentially isodesmic, the –OH from the tyrosine being at least similar to the carboxyl from the glutamate, even though the bonds are not actually identical; all other bonds are unchanged. This neglects the intermediate R300, and only considers the overall transfer, but that is what we need. The atoms at the boundaries, frozen or not, are the same in all cases. None of the amino acids with which we are concerned are at the system boundary; the proton transfer affects only internal amino acids, and effects no change at the boundaries. The error in the crossing energy for the two configurations is then estimated as within $10 \text{ kJ} \approx 4 k_B T$. This is a reasonable to generous error estimate; the overall consistency of the results also supports this estimate, as major errors would prevent the independent calculations from giving a coherent result; significant errors would lead to much more scatter, and not a reasonably consistent dependence on voltage, as shown in Fig. 7. We have spent some effort on validation and error estimates as this is a fairly unique calculation, being large for a quantum calculation, and requiring that the errors be within fairly stringent limits. It appears that the results have passed all the tests we were able to subject them to, and the two mutations gave further validation. The conclusions as stated are justified, to the extent possible.

Most amino acids in the calculated region had their side chains included, but those that pointed away were not included. Table 6 shows which side chains were included, representing 42 out of 70 amino acids in the region; those not indicated had their side chains truncated to H atoms (alternatively, these could be considered replaced by glycine). All backbone atoms were included.

Table 6

42 amino acids with side chains included in the calculation (the other 28, backbone atoms only)

S1	S2	S3	S4
A166	T219	M255	I292
S169	F222	N256	I296
V170	V225	I258	R297*

V172	E226*	D259**	V299
I173	T227	A262	R300**
S176	C229	I263	R303
I177	I230	P265	K306***
S179	F233	Y266	L307
F180		T269	S308
C181		L270	R309***
E183*		G271	H310
T184			

*salt bridge; **,***members of apparent triads, or larger group

Frozen atoms: The amino acids with truncated side chains would normally have anchored the amino acid against the surroundings (possibly the membrane lipids, not included in the calculation); to replace this, either the backbone carbon, or nitrogen, or, towards the end of the segment, sometimes both, were fixed; in all, 62 atoms out 904 protein atoms were fixed, except that fewer were fixed in the S4 free case (Fig. 2). All water atoms were free. The frozen atoms provided the equivalent to environmental restraints, to a reasonable approximation. In addition to the S4 free, $V = -70$ mV case, for the sake of completeness one case with S4 free at 0 mV was also run. Both of these were found to not move enough to produce any gating current; the backbone hardly moved at all (< 1 Å). The water in the calculation is not crystallographic water, but is present at the extracellular surface of the protein, where it comes in contact with water; the cleft in the protein makes it unlikely that there is lipid at this position. There is no crystallographic water within the helix bundle; if any water were present it would be expected to be between charged, or at least polar, residues, and to be held rather tightly; hence it would be expected to be crystallographic water. Since none is seen, it is reasonable to use a model in which one does not insert such water; the water at the top is inserted where the cleft in the extracellular surface of the protein strongly suggests there must be water present.

The maximum voltage applied is equivalent to 70 mV across a 70 Å membrane (applied as a field of 0.00002 atomic units, $\approx 10^7$ V m⁻¹; when the field is shown as -70 mV, it is equivalent to the closed state of the VSD; zero and positive voltages correspond to the open state). The intracellular and extracellular loops are omitted, as is the upper end of S4, including R294, which would be expected to be complexed to the phosphate headgroups in the membrane (36-38); for it to move, this complex would have to be broken, which would cost considerable energy. However, the other three arginines (R297, R300, R303) which in the standard model would be the gating charges, are included. The 35 mV cases were needed to determine the voltage at which the energy curves for the proton transfer crossed (Fig. 7), so the relevant cases were also run with the 35 mV potentials.

SUMMARY: 1) *The overall charge transfer in gating is a cooperative transition of at least much of the VSD; proton transfer is a major part of this, with more than one possible proton pathway.*

2) In a calculation in which S4 was free to move, it did not move in response to application of a voltage. (Fig. 2)

3) Proton transfers in response to a change in voltage can be found from a calculation of the energy of several protein configurations with different proton positions as a function of voltage. Two paths in one section of the VSD were found: one through Y266 (preferred), the other through E226; both connect R303 to R300 and then E183 (Fig. 4). All paths then go through R297, which must be able to accept and transfer the proton to the extracellular surface, defined to include the lipid headgroup region, and water in the protein cleft. The energy of the proton transfer as a function of voltage is consistent with the direction of H⁺ motion needed for gating, and with the voltage at which the probability of channel opening increases rapidly. The existence of more than one path is also consistent with hysteresis in gating, which has been shown.

4) The charge displacement in response to the voltage change is consistent with the gating current; it is necessary to include the charges on *all* atoms to account for charge displacement in the VSD. (Fig. 8)

5) A possible explanation for the conservation of the arginines depends on their amphoteric property, in

742 which NE takes part in proton transfer. This is an alternative to accounting for the conservation of the
743 arginines by having them move as positive charges to produce gating current, as in standard models.

744 6) Hydrogen bonds involving serine, and sometimes threonine, make a significant contribution to the
745 stability of the calculated states via hydrogen bonding; the open case here involves S176, and the closed
746 state, S184. The hydrogen bonds may switch (*i.e.*, -OH rotates) when protons switch positions; this is seen
747 very clearly in the Y266F mutation.

748 7) These calculations allow for at least qualitative prediction of the non-obvious effects of two mutations;
749 although insufficient information is in the calculation to make quantitative comparison to experiment
750 possible, even the qualitative prediction is not intuitive.

751 8) It is possible to see a probable continuation of the proton path beyond the region calculated, in the
752 intracellular direction, then along the intracellular surface of the membrane, toward the gate, so that the
753 entire gating transition can be accomplished by proton transfer. It remains to test whether this plausible
754 path is correct.

755 9) In the one case in which it was tested, the calculation found the same optimized structure from two
756 different starting points, one of which was a reversal of the original proton transfer. This helps confirm the
757 validity of the calculation of the energy minima.

758 10) The RYE triad of amino acids in the proton transfer step shown in detail in Fig. 4 is similar to groups
759 found in at least several other cases in which protons are known to transfer, so may be a general part of
760 protein proton transfer mechanisms.

761 **SUPPORTING MATERIAL:** Supporting Material consists of fourteen coordinate files, the results of the
762 optimizations used in Fig. 7, plus the two for each of the two mutations shown in Fig. 5 and Fig. 6.

763 **ACKNOWLEDGMENTS:** We are grateful to Dr. Carlos Bassetto and Professor Francisco Bezanilla
764 for carrying out the experiment with tyrosine mutation, and for permission to use their unpublished data.
765 We thank Miguel Chavez for the calculation of the charge distribution and for providing the accompanying

Fig. 8. This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, and the Scientific Data and Computing Center, a component of the Computational Science Initiative, at Brookhaven National Laboratory under Contract No. DE-SC0012704, and resources at the High Performance Computation facility at City University of New York.

References:

- Hille B. Ion Channels of Excitable Membranes. 3rd ed. Sunderland, MA: Sinauer Associates; 2001.
- DeCoursey TE. Four varieties of voltage-gated proton channels. *Front Biosci.* 1998;3:D477-D82.
- DeCoursey TE. The Voltage-Gated Proton Channel: A Riddle, Wrapped in a Mystery, inside an Enigma. *Biochemistry.* 2015;54(21):3250-68.
- Gazzarrini S, Van EJL, DiFrancesco D, Thiel G, Moroni A. Voltage-dependence of virus-encoded miniature K⁺ channel Kcv. *J Membr Biol.* 2002;187(1):15-25.
- Moroni A, Thiel G. Flip-flopping salt bridges gate an ion-channel. *Nat Chem Biol.* 2006;2:572-3.
- Hodgkin AL, Huxley AF. Currents carried by sodium and potassium ions through the giant membrane of *Loligo*. *J Physiol (Lond).* 1952;116:449-72.
- Hodgkin AL, Huxley AF. The components of membrane conductance in the giant axon of *Loligo*. *J Physiol (Lond).* 1952;116:473-96.
- Hodgkin AL, Huxley AF. The dual effect of membrane potential on sodium conductance in the giant axon of *Loligo*. *J Physiol (Lond).* 1952;116:497-506.
- Minor DL, Jr., Lin Y-F, Mobley BC, Avelar A, Jan YN, Jan LY, et al. The polar T1 interface is linked to conformational changes that open the voltage-gated potassium channel. *Cell (Cambridge, Mass).* 2000;102(5):657-70.
- Chen X, Wang Q, Ni F, Ma J. Structure of the full-length Shaker potassium channel Kv1.2 by normal-mode-based X-ray crystallographic refinement. *Proc Natl Acad Sci U S A.* 2010;107(25):11352-7.
- Karlin A, Akabas MA. Substituted-Cysteine Accessibility Method. In: Conn PM, editor. *Methods in Enzymology.* New York: Academic Press; 1998. p. 123-45.
- Delemotte L, Klein ML, Tarek M. Molecular dynamics simulations of voltage-gated cation channels: insights on voltage-sensor domain function and modulation. *Front Pharmacol Ion Channels Channelopathies.* 2012;3(May):97.
- Delemotte L, Tarek M, Klein ML, Amaral C, Treptow W. Intermediate states of the Kv1.2 voltage sensor from atomistic molecular dynamics simulations. *Proc Natl Acad Sci.* 2011.
- Deyawe A, Kasimova MA, Delemotte L, Tarek M, Loussouarn G, Tarek M. Studying Kv Channels Function using Computational Methods. *Methods Mol Biol.* 2018;1684:321-41.
- Jensen MO, Jogini V, Borhani DW, Leffler AE, Dror RO, Shaw DE. Mechanism of voltage gating in potassium channels. *Science (Washington, DC, U S).* 2012;336(Copyright (C) 2012 American Chemical Society (ACS). All Rights Reserved.):229-33.
- Schow EV, Freites JA, Gogna K, White SH, Tobias DJ. Down-State Model of the Voltage-Sensing Domain of a Potassium Channel. *Biophys J.* 2010;98(Copyright (C) 2012 American Chemical Society (ACS). All Rights Reserved.):2857-66.
- Blunck R, McGuire H, Hyde HC, Bezanilla F. Fluorescence detection of the movement of single KcsA subunits reveals cooperativity. *Proc Nat'l Academy of Sciences.* 2008;105:20263-8.
- Sandtner W, Bezanilla F, Correa AM. In vivo measurement of intramolecular distances using genetically encoded reporters. *Biophys J.* 2007;93:L45-L7.
- Kariev AM, Green ME. Voltage gated ion channel function: gating, conduction, and the role of water and protons. *Int J Mol Sci.* 2012;13:1680-709.
- Kariev AM, Green ME. Caution is required in interpretation of mutations in the voltage sensing domain of voltage gated channels as evidence for gating mechanisms. *Int J Mol Sci.* 2015;16(1):1627-43.

21. Kariev AM, Green ME. Quantum Calculations on the Kv1.2 Channel Voltage Sensing Domain Show H⁺ Transfer Provides the Gating Current. arXiv 2017:1712:02866
22. Kariev AM, Green ME. The role of proton transport in gating current in a voltage gated ion channel, as shown by quantum calculations. *Sensors*. 2018;18(9):3143/1-/29.
23. Cha A, Snyder G, Selvin PR, Bezanilla F. Atomic scale movement of the voltage-sensing region in a potassium channel measured via spectroscopy. *Nature*. 1999;402:809-13.
24. Chanda B, Asamoah OK, Blunck R, Roux B, Bezanilla F. Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. *Nature*. 2005;436:852-6.
25. Posson DJ, Ge P, Miller C, Bezanilla F, Selvin PR. Small vertical movement of a K⁺ channel voltage sensor measured with luminescence energy transfer. *Nature*. 2005;436:848-51.
26. Lu J, Yin J, Green ME. A model for ion channel voltage gating with static S4 segments. *Ferroelectrics*. 1999;220:249-71.
27. Saprova A, Bystrov V, Green ME. Ion channel gating and proton transport. *J Mol Struct: THEOCHEM*. 2003;630:297-307.
28. Saprova AV, Bystrov VS, Green ME. Water, proton transfer, and hydrogen bonding in ion channel gating. *Frontiers in Bioscience*. 2003;8:s1356-s70.
29. Dal Peraro M, Raugei S, Carloni P, Klein ML. Solute-solvent charge transfer in aqueous solution. *ChemPhysChem*. 2005;6(9):1715-8.
30. Yao Y, Kanai Y, Berkowitz ML. Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. *J Phys Chem Lett*. 2014;5(15):2711-6.
31. Ramsey IS, Moran MM, Chong JA, Clapham DE. A voltage-gated proton-selective channel lacking the pore domain. *Nature*. 2006;440:1213-6.
32. Okamura Y, Fujiwara Y, Sakata S. Gating mechanisms of voltage-gated proton channels. *Annu Rev Biochem*. 2015;84:685-709.
33. Decoursey TE. Voltage-gated proton channels. *Compr Physiol*. 2012;2(2):1355-85.
34. Woelke AL, Wagner A, Galstyan G, Meyer T, Knapp E-W. Proton Transfer in the K-Channel Analog of B-Type Cytochrome c Oxidase from *Thermus thermophilus*. *Biophys J*. 2014;107(9):2177-84.
35. Kim YC, Wikstrom M, Hummer G. Kinetic gating of the proton pump in cytochrome c oxidase. *Proc Natl Acad Sci U S A*. 2009;106(33):13707-12, S/1-S/6.
36. Peng Y, Voth GA. Expanding the view of proton pumping in cytochrome c oxidase through computer simulation. *Biochim Biophys Acta, Bioenerg*. 2012;1817(4):518-25.
37. Smondyrev AM, Voth GA. Molecular dynamics simulation of proton transport through the influenza A virus M2 channel. *Biophys J*. 2002;83(4):1987-96.
38. Chen H, Wu Y, Voth GA. Proton transport behavior through the influenza A M2 channel: insights from molecular simulation. *Biophys J*. 2007;93(10):3470-9.
39. Gianti E, Carnevale V, DeGrado WF, Klein ML, Fiorin G. Hydrogen-Bonded Water Molecules in the M2 Channel of the Influenza A Virus Guide the Binding Preferences of Ammonium-Based Inhibitors. *J Phys Chem B*. 2015;119(3):1173-83.
40. Hu J, Fu R, Nishimura K, Zhang L, Zhou H-X, Busath DD, et al. Histidines, heart of the hydrogen ion channel from influenza A virus: Toward an understanding of conductance and proton selectivity. *Proc Natl Acad Sci USA*. 2006;103:6865-70.
41. Aviles-Moreno JR, Berden G, Oomens J, Martinez-Haya B. Guanidinium/ammonium competition and proton transfer in the interaction of the amino acid arginine with the tetracarboxylic 18-crown-6 ionophore. *Phys Chem Chem Phys*. 2018;20(6):4067-73.
42. Aviles-Moreno JR, Berden G, Oomens J, Martinez-Haya B. Isolated complexes of the amino acid arginine with polyether and polyamine macrocycles, the role of proton transfer. *Phys Chem Chem Phys*. 2017;19(46):31345-51.
43. Ma Y, Yu J-G, Sun Q, Li Z, Smith SC. The mechanism of dehydration in chromophore maturation of wild-type green fluorescent protein: A theoretical study. *Chem Phys Lett*. 2015;631-632:42-6.
44. Melo A, Ramos MJ, Floriano WB, Gomes JANF, Leao JFR, Magalhaes AL, et al. Theoretical study of arginine-carboxylate residues. *THEOCHEM*. 1999;463:81-90.
45. Han M, Kopec W, Solov'yov IA, Khandelia H. Glutamate Water Gates in the Ion Binding Pocket of Na⁺ Bound Na⁺, K⁺-ATPase. *Sci Rep*. 2017;7:39829.
46. Starace D, Stefani E, Bezanilla F. Histidine scanning mutagenesis indicates full translocation of two charges of the Shaker K channel voltage sensor. *Biophys J*. 1998;74:A215.

47. Starace DM, Stefani E, Bezanilla F. Voltage-dependent proton transport by the voltage sensor of the *Shaker* K⁺ channel. *Neuron*. 1997;19:1319-27.
48. Starace DM, Bezanilla F. Histidine scanning mutagenesis of uncharged residues of the *Shaker* K⁺ channel S4 segment. *Biophys J*. 2001;80:217a.
49. Zhao J, Blunck R. The isolated voltage sensing domain of the Shaker potassium channel forms a voltage-gated cation channel. *Elife*. 2016;5.
50. El-Din TMG, Heldstab H, Lehmann C, Greeff NG. Double gaps along Shaker S4 demonstrate omega currents at three different closed states *Channels*. 2010;4:93-100.
51. Tarek M, Delemotte L. Omega currents in voltage-gated ion channels: What can we learn from uncovering the voltage-sensing mechanism using MD simulations? *Acc Chem Res*. 2013;46(12):2755-62.
52. Ishida IG, Rangel-Yescas GE, Carrasco-Zanini J, Islas LD. Voltage-dependent gating and gating charge measurements in the Kv1.2 potassium channel. *J Gen Physiol*. 2015;145(4):345-58.
53. Nguyen TP, Horn R. Movement and crevices around a sodium channel S3 segment. *J Gen'l Physiol*. 2002;120:419-36.
54. Gonzalez-Perez V, Stack K, Boric K, Naranjo D. Reduced voltage sensitivity in a K⁺-channel voltage sensor by electric field remodeling. *Proc Natl Acad Sci*. 2010;107:5178-83.
55. Liao S, Green ME. Quantum calculations on salt bridges with water: Potentials, structure, and properties. *Comput Theo Chem*. 2011;963:207-14.
56. Garczarek F, Brown LS, Lanyi JK, Gerwert K. Proton binding within a membrane protein by a protonated water cluster. *Proc Natl Acad Sci U S A*. 2005;102(10):3633-8.
57. Garczarek F, Gerwert K. Functional waters in intraprotein proton transfer monitored by FTIR difference spectroscopy. *Nature (London, U K)*. 2006;439(7072):109-12.
58. Takeda M, Jee JG, Ono AM, Terauchi T, Kainosho M. Hydrogen Exchange Rate of Tyrosine Hydroxyl Groups in Proteins As Studied by the Deuterium Isotope Effect on C ζ Chemical Shifts. *J Am Chem Soc*. 2009;131(51):18556-62.
59. Barchad-Avitzur O, Priest MF, Dekel N, Bezanilla F, Parnas H, Ben-Chaim Y. A Novel Voltage Sensor in the Orthosteric Binding Site of the M2 Muscarinic Receptor. *Biophys J*. 2016;111(7):1396-408.
60. Chen X, Wang Q, Ni F, Ma J. Structure of the full-length Shaker potassium channel Kv1.2 by normal-mode-based X-ray crystallographic refinement. *Proc Natl Acad Sci*. 2010;107:11352-7.
61. Weinhold F. NBO 5.0 Program Manual. Madison, WI: Theoretical Chemistry Institute, U. of Wisconsin; 2001.
62. Weinhold F. Natural Bond Orbital Analysis: A Critical Overview of Relationships to Alternative Bonding Perspectives. *J Comp Chem*. 2012;33:2363-79.
63. Villalba-Galea CA. Hysteresis in voltage-gated channels. *Channels (Austin)*. 2017;11(2):140-55.
64. Asamoah OK, Wuskell JP, Loew LM, Bezanilla F. A Fluorometric Approach to Local Electric Field Measurements in a Voltage-Gated Ion Channel. *Neuron*. 2003;37:85-97.
65. Stefani E, Bezanilla F. Voltage dependence of the early events in voltage gating. *Biophys J*. 1997;72:A131.
66. Stefani E, Sigg D, Bezanilla F. Correlation between the early component of gating current and total gating current in Shaker K channels. *Biophysical Journal*. 2000;78:7A.
67. Dudev T, Musset B, Morgan D, Cherny VV, Smith SME, Mazmanian K, et al. Selectivity Mechanism of the Voltage-gated Proton Channel, HV1. *Sci Rep*. 2015;5:10320.
68. van Keulen SC, Gianti E, Carnevale V, Klein ML, Rothlisberger U, Delemotte L. Does proton conduction in the voltage-gated H⁺ channel hHv1 involve Grotthuss-like hopping via acidic residues? *J Phys Chem B*. 2017;121:3340-51.
69. Eisenberg AS, Juszczak LJ. The Broken Ring: Reduced Aromaticity in Lys-Trp Cations and High pH Tautomer Correlates with Lower Quantum Yield and Shorter Lifetimes. *J Phys Chem B*. 2014;118(25):7059-69.
70. Juszczak LJ, Eisenberg AS. The Color of Cation- π Interactions: Subtleties of Amine-Tryptophan Interaction Energetics Allow for Radical-like Visible Absorbance and Fluorescence. *J Am Chem Soc*. 2017;139(24):8302-11.
71. Wolf S, Freier E, Gerwert K. A Delocalized Proton-Binding Site within a Membrane Protein. *Biophys J*. 2014;107(1):174-84.
72. Oliver AE, Deamer DW. α -Helical hydrophobic polypeptides form proton-selective channels in lipid bilayers. *Biophys J*. 1994;66(5):1364-79.
73. Mohajeri A, Karimi E. AIM and NBO analyses of cation- π interaction. *J Mol Struct: THEOCHEM*. 2006;774(1-3):71-6.
74. Schwaiger CS, Liin SI, Elinder F, Lindahl E. The Conserved Phenylalanine in the K⁺ Channel Voltage-

Sensor Domain Creates a Barrier with Unidirectional Effects. *Biophys J.* 2013;104(Copyright (C) 2013 American Chemical Society (ACS). All Rights Reserved.):75-84.

75. Infield DT, Galpin JD, Galles GD, Ahern CA, Lee EEL, Bezanilla F. Replacing voltage sensor arginines with citrulline provides mechanistic insight into charge versus shape. *J Gen Physiol.* 2018.

76. Chowdhury S, Chanda B. Free-energy relationships in ion channels activated by voltage and ligand. *J Gen Physiol.* 2013;141(1):11-28.

77. Rodriguez BM, Sigg D, Bezanilla F. Voltage gating of Shaker K⁺ channels: the effect of temperature on ionic and gating currents. *J Gen'l Physiol.* 1998;112:223-42.

78. McCusker EC, Bagnris C, E. NC, Cole AR, D'Avanzo N, Nichols CG, et al. Structure of a bacterial voltage-gated sodium channel pore reveals mechanisms of opening and closing. *Nature Communications.* 2012;3(Art. no. 1102).

79. Frisch MJT, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, .; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. . Gaussian09, Rev. E01. 2016.

80. Ahmadi S, Barrios Herrera L, Chehelamirani M, Hostas J, Jalife S, Salahub DR. Multiscale modeling of enzymes: QM-cluster, QM/MM, and QM/MM/MD: A tutorial review. *Int J Quantum Chem.* 2018: Ahead of Print.

81. Dorofeeva OV, Ryzhova ON. Gas-Phase Enthalpies of Formation and Enthalpies of Sublimation of Amino Acids Based on Isodesmic Reaction Calculations. *J Phys Chem A.* 2014;118(19):3490-502.

82. Hudzik JM, Bozzelli JW. Thermochemistry and Bond Dissociation Energies of Ketones. *J Phys Chem A.* 2012;116(23):5707-22.

voltagesenspaper_5.pdf (1.16 MiB)

[view on ChemRxiv](#) • [download file](#)

SUPPORTING INFORMATION: OPTIMIZED COORDINATE FILES

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(0),Y266(0),E183(0)

POTENTIAL: -70mV

N	15.580944	-6.451469	5.391416
H	14.780731	-6.200923	5.939305
C	15.509643	-5.856520	4.054221
C	14.783016	-6.782962	3.060452
O	14.052228	-6.345797	2.186827
C	16.919741	-5.576790	3.520757
H	16.389845	-6.128186	5.884447
H	14.945059	-4.933534	4.050349
H	16.889045	-5.190425	2.508988
H	17.403781	-4.831921	4.142207
H	17.526994	-6.475176	3.529510
N	15.032378	-8.085604	3.186404
H	15.612369	-8.361765	3.949488
C	14.398661	-9.092386	2.333235
H	14.482431	-8.823798	1.292859
H	14.891368	-10.042265	2.492758
C	12.912802	-9.220816	2.671363
O	12.081430	-9.424712	1.825901
N	12.582804	-9.055884	3.966877
H	13.302707	-8.986374	4.648923
C	11.195108	-9.170814	4.421376
H	11.188268	-9.157965	5.503131
H	10.743743	-10.088315	4.077111
C	10.336944	-8.010595	3.900734
O	9.190715	-8.185973	3.584565

N	10.947166	-6.814584	3.855271
C	10.318595	-5.634057	3.317570
C	10.126801	-5.690990	1.799352
O	9.096244	-5.262541	1.337380
C	11.093003	-4.388030	3.776268
O	12.478911	-4.570920	3.769522
H	11.905594	-6.744371	4.106682
H	9.314756	-5.553195	3.701226
H	10.801687	-3.539751	3.167074
H	10.827406	-4.174248	4.801233
H	12.805998	-4.755413	2.897553
N	11.099962	-6.200428	1.023953
C	10.844256	-6.396651	-0.400382
C	9.693378	-7.385344	-0.601380
O	8.944764	-7.279524	-1.544861
C	12.132565	-6.785513	-1.187311
C	12.333415	-8.290910	-1.404097
C	12.159258	-6.060439	-2.534205
H	11.924166	-6.585903	1.431072
H	10.474583	-5.462318	-0.791691
H	12.964681	-6.415407	-0.598905
H	13.287085	-8.454107	-1.895336
H	12.332057	-8.857111	-0.483479
H	11.566150	-8.698123	-2.055406
H	13.053903	-6.324343	-3.087057
H	11.298808	-6.332248	-3.135779
H	12.159266	-4.985220	-2.401000
N	9.570431	-8.340344	0.328319
H	10.315059	-8.474836	0.973641
C	8.593019	-9.421180	0.241223

H	8.934634	-10.218590	0.888835
H	8.533193	-9.803631	-0.766085
C	7.181698	-9.045745	0.642909
O	6.257483	-9.502080	0.010630
N	7.003520	-8.226545	1.685802
C	5.669684	-7.739286	1.954979
C	5.251021	-6.727652	0.893553
O	4.074248	-6.630710	0.617445
C	5.415518	-7.234086	3.389334
C	5.557535	-8.378469	4.397949
C	6.257448	-6.025280	3.802561
H	7.780930	-7.960683	2.250279
H	4.986652	-8.558610	1.792682
H	4.374715	-6.925106	3.382500
H	5.267463	-8.041397	5.387567
H	4.919466	-9.215853	4.134954
H	6.579689	-8.735715	4.453711
H	5.917068	-5.653359	4.763052
H	7.299760	-6.295845	3.909491
H	6.185275	-5.210641	3.090221
N	6.171801	-6.003043	0.249776
C	5.776269	-5.184213	-0.884109
C	5.343447	-6.067678	-2.062536
O	4.319744	-5.815739	-2.653842
C	6.868947	-4.165014	-1.264115
C	7.066958	-3.148300	-0.125802
C	6.498212	-3.454662	-2.570627
C	8.360686	-2.341733	-0.239822
H	7.133074	-6.061030	0.508390
H	4.878561	-4.647265	-0.616972

H	7.798814	-4.706502	-1.411874
H	6.211977	-2.473862	-0.109879
H	7.076657	-3.662085	0.826136
H	7.203684	-2.665133	-2.790646
H	6.498225	-4.129893	-3.416516
H	5.510152	-3.011194	-2.503906
H	8.461932	-1.668112	0.604440
H	9.222078	-2.999285	-0.239564
H	8.396893	-1.742148	-1.142435
N	6.115624	-7.109718	-2.399307
H	7.009706	-7.232401	-1.972530
C	5.773400	-7.949754	-3.527335
H	6.603987	-8.623480	-3.697355
H	5.618446	-7.363666	-4.420900
C	4.504403	-8.778232	-3.325492
O	3.666321	-8.836197	-4.193943
N	4.393375	-9.431857	-2.162281
H	5.131093	-9.388629	-1.491888
C	3.207303	-10.187596	-1.834320
H	2.967719	-10.900050	-2.609395
H	3.399564	-10.730343	-0.917280
C	1.974183	-9.306851	-1.644814
O	0.887188	-9.696141	-2.004685
N	2.187877	-8.107003	-1.107171
C	1.062466	-7.184491	-1.071036
C	0.616982	-6.720560	-2.460413
O	-0.565457	-6.584496	-2.680891
C	1.278265	-5.930431	-0.230694
O	1.413888	-6.189100	1.126776
H	3.087713	-7.817102	-0.798466

H	0.211115	-7.703913	-0.662271
H	2.121256	-5.365061	-0.613768
H	0.384351	-5.341622	-0.351912
H	2.307761	-6.456344	1.293756
N	1.544191	-6.431998	-3.383126
C	1.145560	-6.024187	-4.718096
C	0.378786	-7.146591	-5.411039
O	-0.608559	-6.891422	-6.067885
C	2.355968	-5.521342	-5.538583
C	2.762317	-4.129358	-5.026355
C	2.060425	-5.496360	-7.043553
C	4.087807	-3.618829	-5.589442
H	2.514587	-6.487425	-3.159323
H	0.424503	-5.223000	-4.638776
H	3.176906	-6.211370	-5.367887
H	1.970489	-3.423667	-5.272036
H	2.836027	-4.155457	-3.946763
H	2.918349	-5.124936	-7.589997
H	1.841543	-6.483228	-7.432707
H	1.215561	-4.853593	-7.270059
H	4.381029	-2.705502	-5.082374
H	4.879679	-4.345737	-5.439446
H	4.030768	-3.400397	-6.649947
N	0.820049	-8.397338	-5.251532
H	1.667134	-8.572954	-4.752448
C	0.043277	-9.504951	-5.753923
H	-0.064069	-9.462747	-6.827588
H	0.556407	-10.421435	-5.491701
C	-1.365276	-9.540103	-5.166934
O	-2.319135	-9.771082	-5.874320

N	-1.472639	-9.318869	-3.858022
C	-2.776408	-9.352422	-3.235418
C	-3.692485	-8.216308	-3.692213
O	-4.890821	-8.424043	-3.732787
C	-2.679029	-9.329546	-1.702831
O	-3.923334	-9.599034	-1.118463
H	-0.656825	-9.231529	-3.289008
H	-3.292832	-10.256969	-3.524128
H	-1.996629	-10.103273	-1.379346
H	-2.290277	-8.372770	-1.370431
H	-4.613441	-9.195680	-1.630922
N	-3.143422	-7.035403	-3.971064
C	-3.907948	-5.914822	-4.493113
C	-4.449216	-6.233753	-5.886715
O	-5.613112	-6.041171	-6.155960
C	-3.013316	-4.655286	-4.488139
C	-3.472078	-3.518231	-5.385380
C	-4.792824	-3.082106	-5.426259
C	-2.544447	-2.883423	-6.203112
C	-5.168659	-2.055609	-6.276261
C	-2.913664	-1.844149	-7.041965
C	-4.233507	-1.431282	-7.085985
H	-2.166724	-6.912808	-3.802062
H	-4.776065	-5.749068	-3.875653
H	-2.930369	-4.319418	-3.458829
H	-2.021582	-4.947355	-4.803627
H	-5.537506	-3.560182	-4.818737
H	-1.519848	-3.211204	-6.194444
H	-6.201301	-1.752629	-6.312157
H	-2.174840	-1.370521	-7.663061

H	-4.528535	-0.637244	-7.749953
N	-3.576116	-6.724283	-6.775034
C	-4.019462	-7.062119	-8.108086
C	-5.145266	-8.094859	-8.085430
O	-6.033051	-8.031072	-8.895558
C	-2.870758	-7.593788	-8.968672
S	-1.652356	-6.342773	-9.485001
H	-2.634887	-6.908353	-6.497413
H	-4.443881	-6.190243	-8.582972
H	-2.366820	-8.412362	-8.472689
H	-3.288935	-7.972050	-9.891765
H	-1.047772	-6.179428	-8.318771
N	-5.078558	-9.066913	-7.155619
H	-4.254248	-9.192308	-6.607817
C	-6.085907	-10.115215	-7.183050
H	-6.258813	-10.452766	-8.193234
H	-5.714550	-10.947558	-6.596550
C	-7.459140	-9.722570	-6.613183
O	-8.481540	-10.086905	-7.126858
N	-7.417939	-9.016209	-5.478356
C	-8.641654	-8.653168	-4.788765
C	-9.504927	-7.658196	-5.556657
O	-10.702666	-7.658824	-5.450443
C	-8.361797	-8.103652	-3.378663
C	-7.519565	-6.820350	-3.271137
C	-8.193200	-5.469023	-3.256946
O	-9.495268	-5.469727	-3.327708
H	-9.844193	-4.571910	-3.238798
O	-7.547134	-4.455075	-3.162024
H	-6.535785	-8.774572	-5.078978

H	-9.260681	-9.533426	-4.686412
H	-9.317927	-7.967214	-2.894271
H	-7.836469	-8.883813	-2.838322
H	-6.956763	-6.846764	-2.345164
H	-6.778024	-6.766612	-4.050597
N	-8.837301	-6.733962	-6.273855
C	-9.555196	-5.702617	-7.000840
C	-10.386302	-6.273665	-8.141462
H	-10.409108	-7.356394	-8.248911
O	-10.987947	-5.559205	-8.887919
C	-8.631217	-4.564540	-7.490669
O	-9.434347	-3.442192	-7.832385
C	-7.723201	-4.928742	-8.657701
H	-7.856541	-6.841277	-6.421677
H	-10.268224	-5.253622	-6.319020
H	-8.030048	-4.257022	-6.646351
H	-10.110641	-3.751079	-8.429613
H	-7.045481	-4.104314	-8.851716
H	-7.131392	-5.809814	-8.458451
H	-8.304290	-5.105593	-9.556372
N	-12.952122	-9.022524	3.174171
H	-13.214938	-9.550528	2.367628
C	-11.773531	-8.180020	2.898781
C	-10.789152	-8.123178	4.050099
O	-9.659878	-7.714257	3.857081
C	-12.146694	-6.722637	2.563055
O	-12.716169	-6.204126	3.737580
C	-13.114369	-6.605222	1.390979
H	-13.731500	-8.453468	3.442359
H	-11.222755	-8.599619	2.068278

H	-11.230811	-6.196532	2.328527
H	-12.850275	-5.263293	3.637750
H	-13.281620	-5.557270	1.166354
H	-12.728750	-7.082400	0.497945
H	-14.074828	-7.045224	1.631540
N	-11.197257	-8.533635	5.241900
H	-12.119322	-8.910812	5.275372
C	-10.412532	-8.529004	6.451303
H	-10.336968	-7.533916	6.860733
H	-10.933725	-9.138450	7.180182
C	-8.974764	-9.043519	6.375023
O	-8.140210	-8.478406	7.038097
N	-8.658727	-10.119661	5.632233
H	-9.369329	-10.599092	5.127070
C	-7.270140	-10.552705	5.532084
H	-7.253507	-11.532129	5.071308
H	-6.830742	-10.631426	6.513558
C	-6.387460	-9.608364	4.692694
O	-5.219627	-9.468420	4.949188
N	-7.045394	-9.018012	3.701158
C	-6.302000	-8.005885	2.963248
C	-6.261921	-6.695390	3.744988
O	-5.267278	-6.009548	3.699390
C	-6.611046	-7.876391	1.459456
C	-7.789973	-7.050307	0.991656
C	-7.776294	-5.663150	1.107344
C	-8.850003	-7.647187	0.322326
C	-8.803632	-4.895981	0.584954
C	-9.869113	-6.881098	-0.220160
C	-9.853576	-5.503358	-0.083978

H	-8.039939	-9.013977	3.679635
H	-5.279281	-8.337534	2.997281
H	-5.714131	-7.456725	1.017445
H	-6.688005	-8.886111	1.073921
H	-6.944102	-5.173253	1.579317
H	-8.862559	-8.715641	0.190486
H	-8.766571	-3.824847	0.672310
H	-10.658922	-7.355970	-0.772726
H	-10.635584	-4.909949	-0.520432
N	-7.292893	-6.385747	4.534672
C	-7.221569	-5.273489	5.451656
C	-6.102284	-5.491033	6.469414
O	-5.455956	-4.539151	6.852734
C	-8.598656	-5.101583	6.124751
C	-8.810243	-3.808954	6.883919
C	-8.979045	-2.606893	6.201181
C	-8.906046	-3.804699	8.268743
C	-9.226379	-1.430441	6.886055
C	-9.163887	-2.629068	8.960916
C	-9.323736	-1.438445	8.271779
H	-8.158167	-6.869402	4.428727
H	-6.951315	-4.368588	4.926161
H	-9.342075	-5.168088	5.336903
H	-8.761766	-5.940556	6.787251
H	-8.925242	-2.589088	5.126356
H	-8.781945	-4.722924	8.815886
H	-9.345858	-0.512282	6.340225
H	-9.227190	-2.645511	10.034243
H	-9.506599	-0.522727	8.805758
N	-5.861756	-6.728179	6.898228

H	-6.516417	-7.449843	6.693430
C	-4.785610	-7.023263	7.817870
H	-4.824644	-6.393718	8.694135
H	-4.898019	-8.053223	8.131547
C	-3.389823	-6.846971	7.222572
O	-2.515980	-6.352256	7.894544
N	-3.189413	-7.272080	5.970444
C	-1.911491	-7.092406	5.298841
C	-1.665164	-5.620520	4.938846
O	-0.566782	-5.133818	5.107238
C	-1.829952	-8.027673	4.072110
C	-0.664512	-7.670389	3.147846
C	-1.728546	-9.487857	4.527528
H	-3.922668	-7.753219	5.495583
H	-1.118126	-7.338226	5.989758
H	-2.750581	-7.903937	3.506544
H	-0.600417	-8.397138	2.345039
H	-0.774998	-6.696017	2.693021
H	0.280109	-7.682140	3.682962
H	-1.741719	-10.148433	3.666644
H	-0.794904	-9.654675	5.058852
H	-2.545387	-9.777676	5.175684
N	-2.700639	-4.933584	4.446697
C	-2.569829	-3.551378	4.028841
C	-2.420113	-2.639002	5.244019
O	-1.528605	-1.820135	5.290629
C	-3.758286	-3.090364	3.171672
C	-3.994034	-3.840510	1.850012
C	-2.860081	-3.730762	0.845346
O	-1.747217	-4.135874	1.218613

O	-3.112647	-3.254404	-0.273866
H	-3.564207	-5.403285	4.285141
H	-1.662752	-3.440843	3.465207
H	-4.667153	-3.158040	3.761700
H	-3.604929	-2.035165	2.961915
H	-4.149292	-4.890266	2.048879
H	-4.899444	-3.450472	1.399192
N	-3.309568	-2.774884	6.244298
C	-3.093978	-2.024901	7.456985
C	-1.778252	-2.422295	8.133804
O	-1.106968	-1.582694	8.694212
C	-4.226302	-2.004940	8.493910
O	-4.436303	-3.246513	9.098559
C	-5.507646	-1.387323	7.948154
H	-3.988197	-3.503289	6.218708
H	-2.937574	-0.995415	7.174780
H	-3.851323	-1.365655	9.283504
H	-4.889420	-3.818315	8.490671
H	-6.240042	-1.327303	8.743421
H	-5.322003	-0.384111	7.576784
H	-5.928460	-1.976911	7.144841
N	-1.380397	-3.700457	8.043328
H	-2.031177	-4.418219	7.811975
C	-0.187160	-4.107493	8.739874
H	-0.237332	-3.891849	9.797887
H	-0.075804	-5.175185	8.604000
C	1.064036	-3.420003	8.218010
O	1.940520	-3.076040	8.977882
N	1.153963	-3.258734	6.881772
C	2.332594	-2.660245	6.317782

C	2.291096	-1.138359	6.164142
O	3.359963	-0.574312	6.022983
C	2.830820	-3.345975	5.045590
S	1.922866	-2.976896	3.520328
H	0.422815	-3.612332	6.296775
H	3.116491	-2.797974	7.047090
H	3.840685	-3.007650	4.863293
H	2.853489	-4.415035	5.205088
H	0.859339	-3.741312	3.719541
N	1.140119	-0.470673	6.273050
C	1.204068	0.968497	6.491343
C	1.755726	1.271283	7.870550
O	2.368197	2.289064	8.085588
C	-0.095730	1.741716	6.182264
C	-1.196980	1.568389	7.238506
C	-0.554707	1.440122	4.750694
C	-2.466369	2.370643	6.944548
H	0.271804	-0.965355	6.291883
H	1.951513	1.351097	5.814811
H	0.208520	2.782230	6.222188
H	-1.446000	0.523604	7.355738
H	-0.807789	1.892646	8.199120
H	-1.310124	2.147457	4.431579
H	0.277973	1.520390	4.057207
H	-0.966271	0.444389	4.656851
H	-3.136044	2.340272	7.798665
H	-2.241293	3.414113	6.738921
H	-3.007065	1.973406	6.092389
N	1.549788	0.323258	8.791266
H	0.889828	-0.402217	8.613495

C	1.978276	0.512612	10.160076
H	1.470069	-0.222732	10.771000
H	1.737711	1.502298	10.518179
C	3.482342	0.337369	10.305033
O	4.164480	1.128924	10.896138
N	3.999955	-0.753863	9.695360
H	3.390737	-1.466241	9.351675
C	5.425061	-0.938911	9.667405
H	5.638287	-1.909420	9.234458
H	5.855763	-0.904784	10.657461
C	6.156882	0.119117	8.844832
O	7.291893	0.411950	9.129239
N	5.502078	0.621285	7.799030
C	6.098617	1.759274	7.146315
C	5.514803	3.076764	7.649619
H	5.013135	3.037215	8.615064
O	5.636470	4.094801	7.040848
C	6.003008	1.674981	5.620777
C	6.755411	0.506853	5.017547
C	8.121035	0.322829	5.238389
C	6.095144	-0.401675	4.195769
C	8.807450	-0.722633	4.635688
C	6.779320	-1.444771	3.591585
C	8.139375	-1.605749	3.801627
H	4.575274	0.334619	7.572613
H	7.134062	1.774610	7.451350
H	4.960818	1.610760	5.334266
H	6.381340	2.609398	5.220643
H	8.649059	0.978934	5.909006
H	5.034983	-0.305689	4.057496

H	9.858141	-0.849996	4.831622
H	6.247195	-2.136641	2.963271
H	8.659788	-2.418340	3.328667
N	12.613550	9.596234	-1.248802
H	11.873463	9.913870	-1.846454
C	12.304852	8.264740	-0.719487
C	11.274100	8.450699	0.386872
O	10.265804	7.779082	0.416374
C	13.562726	7.580985	-0.165336
C	14.645038	7.276039	-1.206574
S	14.017038	6.202095	-2.529928
C	15.499712	6.053551	-3.555389
H	13.433688	9.573142	-1.821868
H	11.834462	7.616523	-1.447350
H	14.001313	8.205395	0.607189
H	13.255653	6.653816	0.304804
H	15.045481	8.188485	-1.633895
H	15.470190	6.783597	-0.704576
H	15.248366	5.398907	-4.375947
H	15.798746	7.017618	-3.946054
H	16.318070	5.616646	-2.998124
N	11.504281	9.412877	1.296997
C	10.594285	9.607741	2.408568
C	9.277001	10.274697	2.010348
O	8.280895	10.053125	2.652572
C	11.276205	10.369076	3.552095
C	12.447964	9.564527	4.084498
O	13.582765	9.826353	3.744622
N	12.144410	8.562238	4.918949
H	12.328099	9.967716	1.206347

H	10.295508	8.637691	2.771304
H	11.657189	11.326324	3.218975
H	10.546022	10.537651	4.333516
H	12.888282	7.966933	5.213303
H	11.222912	8.176002	4.954870
N	9.263811	11.067697	0.922328
H	10.110810	11.229654	0.427419
C	8.003502	11.517470	0.368859
H	8.201251	12.260241	-0.393337
H	7.389096	11.966669	1.131932
C	7.186384	10.384439	-0.254324
O	5.986288	10.470076	-0.291498
N	7.862643	9.333319	-0.763272
C	7.170445	8.145634	-1.233957
C	6.634883	7.300728	-0.067335
O	5.534494	6.808351	-0.148247
C	8.048947	7.344296	-2.224251
C	8.343686	8.197252	-3.472933
C	7.379505	6.019216	-2.608174
C	9.428319	7.625157	-4.388995
H	8.823869	9.230816	-0.536812
H	6.279720	8.471711	-1.748418
H	8.987987	7.117876	-1.727335
H	7.421774	8.323284	-4.036274
H	8.645788	9.192886	-3.165432
H	7.996920	5.478892	-3.314375
H	7.228376	5.377920	-1.748363
H	6.409824	6.182873	-3.066713
H	9.622358	8.305747	-5.211606
H	10.363628	7.479590	-3.855310

H	9.148450	6.671115	-4.820162
N	7.387601	7.175215	1.043839
C	6.879055	6.458277	2.201910
C	5.527970	7.039470	2.639634
O	4.575502	6.332974	2.866901
C	7.833208	6.546127	3.403444
C	9.254686	5.997273	3.244152
O	10.145886	6.631293	3.802334
O	9.428294	4.935727	2.595041
H	8.347661	7.444953	1.022551
H	6.682440	5.429463	1.943291
H	7.921267	7.570736	3.733003
H	7.375097	5.992729	4.220654
N	5.489851	8.377405	2.786069
H	6.320917	8.912597	2.648950
C	4.299225	9.045885	3.249968
H	4.538258	10.090241	3.407632
H	3.957292	8.638800	4.188424
C	3.136629	8.987513	2.268583
O	1.995144	9.109701	2.649473
N	3.470176	8.824775	0.985192
H	4.431315	8.829449	0.735279
C	2.517191	8.905260	-0.078305
H	3.059863	9.091715	-0.996305
H	1.843943	9.738046	0.071914
C	1.609133	7.687020	-0.310194
O	0.561833	7.815066	-0.879403
N	2.094474	6.538092	0.201332
C	1.289982	5.364375	0.431021
C	0.472387	5.479549	1.721794

O	-0.722708	5.301804	1.692203
C	2.166758	4.112402	0.445792
H	3.001528	6.575688	0.615931
H	0.559552	5.290356	-0.357506
H	1.566520	3.234004	0.657550
H	2.636496	3.991476	-0.523448
H	2.946380	4.184428	1.196930
N	1.102514	5.751803	2.879294
C	0.364292	5.585250	4.123057
C	-0.756432	6.611697	4.274013
O	-1.792392	6.302325	4.823364
C	1.276011	5.511847	5.372732
C	1.867809	6.857295	5.819745
C	2.362801	4.445288	5.169506
C	2.698994	6.761005	7.101577
H	2.090092	5.889616	2.900944
H	-0.159830	4.642184	4.064825
H	0.615200	5.173522	6.165183
H	2.478118	7.266410	5.021408
H	1.064424	7.567408	5.986930
H	2.732516	4.092368	6.121037
H	1.969615	3.588567	4.631398
H	3.205855	4.834276	4.608937
H	3.004293	7.751938	7.424490
H	2.121237	6.317646	7.907208
H	3.593843	6.165183	6.971697
N	-0.542960	7.847390	3.800966
H	0.341472	8.089930	3.404868
C	-1.513857	8.887768	4.018661
H	-1.103669	9.816493	3.642539

H	-1.724196	9.016468	5.070588
C	-2.866972	8.618762	3.365891
O	-3.871073	8.837212	4.003256
N	-2.902689	8.108966	2.120757
C	-4.239977	8.013753	1.535301
C	-4.984715	6.749522	1.927679
O	-6.195865	6.757018	1.919701
C	-4.021961	8.221377	0.030789
C	-2.766351	9.099777	0.020009
C	-1.907226	8.456184	1.096092
H	-4.854248	8.814662	1.917299
H	-3.842397	7.278855	-0.469760
H	-4.886376	8.684666	-0.427231
H	-2.255711	9.142462	-0.923535
H	-3.027230	10.114461	0.311403
H	-1.420606	7.566072	0.740457
H	-1.151144	9.119009	1.484459
N	-4.269046	5.673779	2.291121
C	-4.938190	4.512574	2.850520
C	-5.638483	4.853566	4.168965
O	-6.741401	4.413645	4.408446
C	-3.973826	3.331470	3.086429
C	-3.635815	2.505644	1.861076
C	-4.332918	1.334795	1.576597
C	-2.597742	2.864590	1.013744
C	-4.007257	0.547987	0.482013
C	-2.270778	2.094060	-0.087910
C	-2.970648	0.931871	-0.361397
O	-2.617894	0.205846	-1.447897
H	-3.414708	-0.117636	-1.907891

H	-3.275163	5.750834	2.345475
H	-5.725584	4.209370	2.178854
H	-3.068141	3.711073	3.548038
H	-4.443505	2.682244	3.816470
H	-5.141527	1.028394	2.216937
H	-2.032818	3.752495	1.204511
H	-4.536059	-0.366907	0.289642
H	-1.479397	2.397067	-0.750378
N	-4.970841	5.618292	5.048293
H	-4.034958	5.911381	4.856514
C	-5.582761	6.005336	6.299177
H	-4.805951	6.385456	6.951028
H	-6.052296	5.158934	6.774233
C	-6.651500	7.084436	6.135928
O	-7.706439	7.027961	6.726190
N	-6.342147	8.091247	5.313906
H	-5.445011	8.139362	4.880103
C	-7.257687	9.220267	5.085304
H	-6.781273	9.871884	4.364233
H	-7.419732	9.775731	5.997427
C	-8.632474	8.840758	4.569496
O	-9.611456	9.429009	4.959389
N	-8.690353	7.854323	3.658142
C	-9.953936	7.451763	3.088772
C	-10.766367	6.542276	3.995474
O	-11.807718	6.069059	3.559312
C	-9.761225	6.816107	1.689871
O	-10.954474	6.903389	0.953235
C	-9.239336	5.382290	1.729344
H	-7.846104	7.427544	3.334380

H	-10.571605	8.331054	2.962637
H	-9.046138	7.439464	1.169803
H	-11.641616	6.500567	1.473253
H	-8.968511	5.061323	0.731363
H	-8.362386	5.288810	2.354441
H	-10.001049	4.705882	2.098831
N	-10.353337	6.327943	5.240900
C	-11.259067	5.732432	6.212920
C	-12.445055	6.655970	6.501978
O	-13.529692	6.188238	6.758346
C	-10.538004	5.397364	7.526365
C	-9.534250	4.235087	7.447170
C	-8.716902	4.184513	8.741571
C	-10.219887	2.887550	7.196651
H	-9.462967	6.657426	5.550927
H	-11.696982	4.842273	5.794089
H	-10.028467	6.287234	7.878934
H	-11.302465	5.156738	8.260029
H	-8.847363	4.423679	6.629000
H	-7.988780	3.378765	8.709922
H	-8.181943	5.114221	8.898199
H	-9.358073	4.014626	9.603746
H	-9.479693	2.092166	7.178789
H	-10.931085	2.662089	7.989148
H	-10.750009	2.858102	6.251782
N	-12.200522	7.978949	6.518744
C	-13.273039	8.917896	6.674532
C	-14.049258	9.175384	5.400083
H	-14.889087	9.868465	5.516222
O	-13.795693	8.696578	4.344326

H	-11.339629	8.323361	6.149409
H	-13.965271	8.567023	7.429623
H	-12.873459	9.866487	7.019929
N	-11.399969	10.603551	-3.013216
H	-11.150848	10.793386	-2.062913
C	-11.816457	9.206991	-3.172692
C	-11.420851	8.859935	-4.600828
O	-10.381233	8.297434	-4.846936
C	-13.274734	8.886640	-2.781030
C	-13.514063	9.244538	-1.302422
C	-13.600995	7.414363	-3.063721
C	-14.953793	9.046013	-0.824864
H	-12.140699	11.235339	-3.252888
H	-11.162961	8.606955	-2.555415
H	-13.942021	9.511372	-3.379459
H	-12.841528	8.656467	-0.682305
H	-13.250014	10.285347	-1.142897
H	-14.652333	7.209527	-2.907474
H	-13.370472	7.129681	-4.086153
H	-13.034591	6.765561	-2.402933
H	-15.063023	9.412864	0.189451
H	-15.657185	9.588738	-1.450951
H	-15.244933	8.002168	-0.821506
N	-12.217787	9.294727	-5.606272
H	-13.139288	9.595964	-5.384742
C	-11.972872	8.843880	-6.959258
H	-12.033869	7.767144	-7.039983
H	-12.729040	9.278162	-7.601904
C	-10.601635	9.233244	-7.517693
O	-9.996993	8.496745	-8.241578

N	-10.162849	10.477782	-7.182627
H	-10.710967	11.007726	-6.544640
C	-8.894341	11.023967	-7.637100
H	-8.789701	10.891253	-8.702753
H	-8.878587	12.081461	-7.407588
C	-7.672564	10.359017	-6.988311
O	-6.753288	9.935059	-7.630848
N	-7.659101	10.352152	-5.619641
H	-8.482401	10.628144	-5.133559
C	-6.495253	9.961264	-4.832348
H	-5.599190	10.377760	-5.264327
H	-6.616272	10.359353	-3.832338
C	-6.268292	8.463912	-4.714277
O	-5.133741	8.047355	-4.711552
N	-7.321035	7.642772	-4.555883
C	-7.043209	6.284748	-4.116210
C	-6.395979	5.449108	-5.213283
O	-5.518963	4.674302	-4.918169
C	-8.232873	5.569489	-3.436346
C	-9.368536	5.183245	-4.399222
C	-8.697051	6.392810	-2.229037
C	-10.549916	4.494220	-3.715501
H	-8.255734	7.997394	-4.570135
H	-6.261740	6.342785	-3.373841
H	-7.807333	4.647372	-3.048883
H	-9.726245	6.052590	-4.935411
H	-8.960384	4.506207	-5.145609
H	-9.400969	5.838945	-1.623718
H	-7.854514	6.643390	-1.592420
H	-9.177968	7.313947	-2.533284

H	-11.255488	4.128223	-4.455611
H	-10.227310	3.646433	-3.122056
H	-11.086931	5.173571	-3.065645
N	-6.814696	5.564734	-6.493518
C	-6.106090	4.822427	-7.516751
C	-4.760271	5.444493	-7.899241
O	-3.890185	4.715921	-8.316589
C	-6.966879	4.499655	-8.746711
C	-8.036858	3.417976	-8.510429
C	-7.450679	2.076806	-8.041102
N	-8.388348	0.950372	-8.074819
C	-9.198500	0.573081	-7.082223
N	-9.461714	1.417389	-6.096291
N	-9.735184	-0.627041	-7.081494
H	-7.489226	6.258287	-6.735688
H	-5.795827	3.898635	-7.061643
H	-7.450821	5.399941	-9.113901
H	-6.295934	4.164635	-9.530188
H	-8.777741	3.779653	-7.803319
H	-8.564457	3.255563	-9.444503
H	-6.625621	1.798488	-8.683815
H	-7.050857	2.146512	-7.038324
H	-8.318670	0.320537	-8.843177
H	-9.209212	2.374113	-6.170856
H	-9.975771	1.152008	-5.272487
H	-9.386628	-1.392606	-7.629608
H	-10.455373	-0.868109	-6.419059
N	-4.571383	6.757521	-7.721942
H	-5.312315	7.350933	-7.425900
C	-3.257811	7.352384	-8.011367

H	-2.933574	7.093301	-9.006671
H	-3.359217	8.427153	-7.938226
C	-2.194224	6.878592	-7.032969
O	-1.067347	6.644049	-7.392535
N	-2.610525	6.772889	-5.765796
C	-1.723015	6.464254	-4.671163
C	-1.444922	4.978007	-4.544804
O	-0.316679	4.592094	-4.340327
C	-2.307517	7.057597	-3.382763
C	-1.724815	6.352660	-2.158849
C	-2.065393	8.573596	-3.416044
H	-3.535125	7.069357	-5.539459
H	-0.755120	6.905332	-4.861635
H	-3.376238	6.879910	-3.397953
H	-1.939327	6.893010	-1.256063
H	-2.140827	5.355759	-2.055908
H	-0.652629	6.275441	-2.228523
H	-2.802863	9.103968	-2.830568
H	-1.077849	8.814563	-3.037015
H	-2.144576	8.956417	-4.426975
N	-2.474279	4.124764	-4.663732
C	-2.164153	2.717524	-4.734152
C	-1.265570	2.444041	-5.932826
O	-0.396160	1.606643	-5.875480
C	-3.408746	1.806689	-4.774910
C	-4.360548	1.970537	-3.579979
C	-5.448860	0.884498	-3.485581
N	-5.007994	-0.292803	-2.757323
C	-5.828029	-1.254631	-2.564076
N	-7.132262	-1.285043	-3.042009

N	-5.529317	-2.307063	-1.768386
H	-3.401452	4.451776	-4.832759
H	-1.576330	2.442308	-3.871014
H	-3.956468	1.985261	-5.698705
H	-3.044992	0.786285	-4.822080
H	-3.794850	1.985348	-2.660536
H	-4.853445	2.927338	-3.654639
H	-6.318442	1.325235	-2.997340
H	-5.765388	0.631232	-4.501235
H	-7.269977	-0.782391	-3.890775
H	-7.547087	-2.198151	-3.082629
H	-4.606193	-2.417209	-1.394936
H	-6.033447	-3.156481	-1.906178
N	-1.459759	3.193337	-7.035104
H	-2.264461	3.769652	-7.144117
C	-0.595841	2.983570	-8.179101
H	-0.940101	3.626229	-8.979236
H	-0.614301	1.957456	-8.516738
C	0.858326	3.326035	-7.861317
O	1.786260	2.682485	-8.284293
N	1.007445	4.395989	-7.064151
H	0.213483	4.959514	-6.860698
C	2.282309	4.880648	-6.640293
H	2.918466	5.143119	-7.476200
H	2.121619	5.773634	-6.050398
C	3.094242	3.926519	-5.780065
O	4.300265	4.045735	-5.701433
N	2.428061	2.983367	-5.101940
C	3.101620	2.134935	-4.154869
C	4.282205	1.343779	-4.722365

O	5.201482	1.052542	-3.983650
C	2.031171	1.219401	-3.563977
C	2.428250	0.354637	-2.373360
C	1.133384	-0.209485	-1.811071
N	1.349158	-1.211023	-0.786673
C	0.367638	-2.053383	-0.419188
N	-0.791056	-2.021281	-1.034301
N	0.596532	-2.937674	0.523852
H	1.433630	2.938723	-5.174896
H	3.548660	2.735576	-3.371638
H	1.222627	1.874467	-3.257090
H	1.623761	0.598106	-4.353093
H	3.090803	-0.451472	-2.668464
H	2.949613	0.944398	-1.622858
H	0.514109	0.599037	-1.434189
H	0.590668	-0.683203	-2.616428
H	2.061201	-1.044576	-0.110880
H	-1.129890	-1.169180	-1.431149
H	-1.541493	-2.653972	-0.762209
H	1.513554	-3.109966	0.865333
H	-0.183117	-3.502400	0.855326
N	4.281487	0.944899	-6.004135
H	3.540425	1.225017	-6.613436
C	5.363433	0.116651	-6.504612
H	5.138940	-0.142416	-7.531832
H	5.441318	-0.797906	-5.938283
C	6.736189	0.756137	-6.475992
O	7.738501	0.089706	-6.364641
N	6.766107	2.085332	-6.608300
H	5.912164	2.604987	-6.573201

C	8.005490	2.823550	-6.551058
H	8.709874	2.439443	-7.275292
H	7.800317	3.854257	-6.807692
C	8.748767	2.826982	-5.213265
O	9.889900	3.236396	-5.161819
N	8.104020	2.338761	-4.145791
C	8.686068	2.174994	-2.824665
C	9.950624	1.305640	-2.832450
O	10.769444	1.388760	-1.931350
C	7.582249	1.508360	-1.973451
C	7.781315	1.384520	-0.462949
C	7.442009	2.654382	0.326956
C	7.332442	2.387275	1.824347
N	8.672831	2.353850	2.481175
O	11.043759	1.617662	0.892575
H	10.893507	1.828893	-0.029265
H	11.522402	0.791091	0.841458
H	7.158111	2.035733	-4.258492
H	8.985609	3.132478	-2.419373
H	6.666397	2.054216	-2.156485
H	7.412186	0.521668	-2.388594
H	7.101435	0.605609	-0.131487
H	8.776633	1.030649	-0.229089
H	8.155686	3.454433	0.151271
H	6.477032	3.027453	-0.000996
H	6.772474	3.159663	2.328139
H	6.851243	1.441279	2.019126
H	9.383412	1.890053	1.923632
H	8.992797	3.324044	2.635486
H	8.619521	1.875958	3.368834

N	10.062466	0.448215	-3.837530
C	11.109254	-0.537626	-4.069489
C	12.486198	0.023151	-4.427404
O	13.443814	-0.705721	-4.301297
C	10.700747	-1.444010	-5.252697
C	9.562911	-2.442684	-4.997425
C	9.130917	-3.067132	-6.327922
C	9.990732	-3.533414	-4.015314
H	9.324095	0.446353	-4.510534
H	11.264786	-1.125192	-3.176512
H	10.433793	-0.798369	-6.084028
H	11.583581	-1.996252	-5.551753
H	8.706525	-1.911855	-4.593193
H	8.329833	-3.783547	-6.173252
H	8.773306	-2.310222	-7.014278
H	9.957889	-3.595023	-6.796351
H	9.201125	-4.263650	-3.875431
H	10.860862	-4.059408	-4.394208
H	10.243855	-3.136731	-3.036861
N	12.574050	1.261829	-4.919244
C	13.814631	1.844748	-5.393664
C	14.958652	2.033747	-4.379133
O	16.013009	2.415248	-4.811960
C	13.497155	3.171312	-6.087132
O	12.917856	4.088294	-5.202925
H	11.756474	1.833638	-4.917124
H	14.248647	1.177688	-6.129059
H	14.420302	3.590289	-6.455810
H	12.846475	2.977264	-6.933908
H	11.970501	4.079249	-5.267949

N	14.792295	1.722326	-3.074279
C	15.928389	1.647509	-2.176950
C	16.804567	0.409888	-2.402431
O	17.934351	0.393805	-1.987788
C	15.495714	1.578526	-0.707339
C	14.639621	2.736041	-0.198122
C	14.286898	2.490214	1.269214
N	13.261669	3.385117	1.791185
C	13.439234	4.535908	2.419308
N	14.656891	5.011309	2.656558
O	15.028868	7.467212	4.211320
H	14.745472	8.353707	3.972084
H	15.747678	7.573264	4.821449
N	12.389203	5.224410	2.815850
H	13.901122	1.419326	-2.758405
H	16.562104	2.504313	-2.346960
H	14.954936	0.650825	-0.551362
H	16.407795	1.509207	-0.124733
H	15.157465	3.683640	-0.315118
H	13.720191	2.817208	-0.766111
H	13.890572	1.490897	1.376863
H	15.166566	2.533534	1.900576
H	12.321594	3.089418	1.619820
H	15.464852	4.518742	2.358635
H	14.792087	5.866171	3.168376
H	11.433766	4.944541	2.657797
H	12.481544	6.067381	3.336224
N	16.200238	-0.648980	-2.967241
C	16.870746	-1.911547	-3.168273
C	17.669182	-1.889188	-4.468289

H	18.064101	-0.909799	-4.747558
O	17.874238	-2.852596	-5.131737
C	15.867974	-3.070182	-3.149443
C	15.324792	-3.399919	-1.791907
N	14.403950	-2.627679	-1.111941
O	12.508282	-0.434546	-0.465242
H	13.146230	-1.037812	-0.850717
H	12.028284	-0.039090	-1.184792
C	15.620109	-4.490418	-1.049700
C	14.173035	-3.251908	-0.003455
N	14.883490	-4.381979	0.103203
H	15.285820	-0.550151	-3.353081
H	17.596166	-2.030815	-2.371151
H	15.050388	-2.842211	-3.824572
H	16.368621	-3.944015	-3.544099
H	16.275589	-5.314100	-1.235269
H	13.494850	-2.922513	0.757658
H	14.783037	-5.064865	0.821930
O	-14.929722	-2.440555	5.284115
H	-15.070645	-1.570308	4.920278
H	-14.426611	-2.308294	6.080648
O	-12.772073	-1.570060	7.335180
H	-12.082833	-2.061380	7.768270
H	-12.982013	-0.850239	7.917504
O	-11.882781	-0.958346	4.587550
H	-11.986054	-1.109474	5.523663
H	-12.698956	-0.533300	4.317258
O	-13.470918	-1.497777	1.153079
H	-12.611455	-1.069906	1.129696
H	-13.392863	-2.234513	1.762452

O	-7.423101	2.196895	-0.103248
H	-7.555141	2.263076	0.846437
H	-6.505869	1.972041	-0.203877
O	-7.633194	2.149865	2.721403
H	-8.411248	1.691243	3.031058
H	-7.483551	2.881695	3.315408
O	-9.180003	0.348640	-1.275893
H	-8.589395	1.014137	-0.904100
H	-8.610225	-0.340588	-1.612839
O	-13.000615	-1.922159	-1.654690
H	-13.314073	-1.992348	-0.752737
H	-13.713766	-2.168422	-2.234912
O	-13.813123	1.513256	0.356362
H	-14.241874	0.686036	0.545542
H	-12.888966	1.336987	0.542750
O	-14.680102	5.246503	4.124659
H	-14.014772	5.838141	3.788336
H	-14.614055	5.349535	5.069799
O	-14.703140	2.662480	2.986863
H	-14.903586	3.540852	3.322938
H	-14.603806	2.715437	2.041412
O	-13.336314	0.833938	-2.396199
H	-13.632472	1.332355	-1.635709
H	-13.077163	-0.016978	-2.039838
O	-14.474249	-1.109944	-4.141616
H	-14.414024	-0.260518	-3.708060
H	-15.298233	-1.129403	-4.610488
O	-10.572576	-2.940057	-3.030987
H	-10.892165	-2.579067	-3.854251
H	-11.254346	-2.730956	-2.398086

O	-11.266363	0.240360	0.789619
H	-10.601802	0.163027	0.104301
H	-10.806630	0.507530	1.590718
O	-10.209266	0.992222	3.285589
H	-10.577648	0.309838	3.844682
H	-10.727928	1.781921	3.462077
O	-11.957294	3.113818	3.705388
H	-11.912013	4.064500	3.654371
H	-12.872601	2.889280	3.553491
O	-10.746130	0.954414	-3.524643
H	-11.593027	1.223341	-3.167919
H	-10.181390	0.783597	-2.763551
O	-14.430978	-0.068486	3.680545
H	-14.660585	0.857060	3.580157
H	-14.387286	-0.433740	2.802022
O	-13.081754	-3.334161	3.367518
H	-13.830590	-3.189757	3.954727
H	-12.406096	-2.767751	3.737159
O	-11.696982	-1.220164	-5.030317
H	-12.648753	-1.298531	-4.990898
H	-11.457902	-0.551984	-4.388114

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(0),Y266(0),E183(0)

POTENTIAL:-35mV

N	15.580944	-6.451469	5.391416
H	14.780605	-6.201176	5.939239
C	15.509567	-5.856494	4.054239
C	14.783016	-6.782962	3.060452

O	14.052292	-6.345799	2.186782
C	16.919631	-5.576623	3.520772
H	16.389693	-6.127924	5.884523
H	14.944896	-4.933563	4.050387
H	16.888874	-5.190224	2.509018
H	17.403616	-4.831732	4.142242
H	17.526957	-6.474962	3.529482
N	15.032378	-8.085604	3.186404
H	15.612322	-8.361768	3.949519
C	14.398661	-9.092386	2.333235
H	14.482433	-8.823803	1.292858
H	14.891371	-10.042262	2.492770
C	12.912807	-9.220830	2.671366
O	12.081463	-9.424755	1.825889
N	12.582804	-9.055884	3.966877
H	13.302703	-8.986414	4.648929
C	11.195108	-9.170814	4.421376
H	11.188270	-9.157957	5.503131
H	10.743739	-10.088316	4.077120
C	10.336944	-8.010595	3.900734
O	9.190736	-8.186000	3.584535
N	10.947160	-6.814579	3.855252
C	10.318570	-5.634049	3.317564
C	10.126840	-5.690931	1.799336
O	9.096371	-5.262336	1.337324
C	11.092959	-4.388035	3.776306
O	12.478878	-4.570872	3.769343
H	11.905570	-6.744345	4.106716
H	9.314721	-5.553204	3.701198
H	10.801517	-3.539712	3.167236

H	10.827475	-4.174374	4.801325
H	12.805795	-4.755324	2.897303
N	11.099999	-6.200434	1.023965
C	10.844305	-6.396689	-0.400370
C	9.693436	-7.385377	-0.601404
O	8.944937	-7.279603	-1.544975
C	12.132613	-6.785588	-1.187278
C	12.333425	-8.290993	-1.404044
C	12.159325	-6.060542	-2.534189
H	11.924065	-6.586137	1.431140
H	10.474649	-5.462356	-0.791691
H	12.964734	-6.415498	-0.598871
H	13.287101	-8.454227	-1.895265
H	12.332025	-8.857181	-0.483417
H	11.566158	-8.698188	-2.055359
H	13.053968	-6.324471	-3.087038
H	11.298871	-6.332352	-3.135753
H	12.159341	-4.985320	-2.401010
N	9.570431	-8.340344	0.328319
H	10.314998	-8.474790	0.973714
C	8.593019	-9.421180	0.241223
H	8.934621	-10.218583	0.888853
H	8.533220	-9.803641	-0.766081
C	7.181685	-9.045756	0.642870
O	6.257522	-9.502155	0.010573
N	7.003461	-8.226499	1.685712
C	5.669615	-7.739212	1.954813
C	5.251037	-6.727566	0.893366
O	4.074289	-6.630604	0.617199
C	5.415370	-7.234001	3.389149

C	5.557241	-8.378393	4.397775
C	6.257332	-6.025242	3.802446
H	7.780838	-7.960621	2.250218
H	4.986577	-8.558522	1.792481
H	4.374586	-6.924964	3.382236
H	5.267122	-8.041301	5.387372
H	4.919129	-9.215730	4.134739
H	6.579369	-8.735711	4.453607
H	5.916866	-5.653281	4.762890
H	7.299619	-6.295871	3.909499
H	6.185287	-5.210612	3.090082
N	6.171856	-6.002978	0.249613
C	5.776344	-5.184142	-0.884278
C	5.343491	-6.067588	-2.062706
O	4.319796	-5.815624	-2.653994
C	6.869047	-4.164972	-1.264289
C	7.067139	-3.148304	-0.125951
C	6.498301	-3.454558	-2.570765
C	8.360934	-2.341843	-0.239949
H	7.133119	-6.060987	0.508240
H	4.878652	-4.647170	-0.617137
H	7.798892	-4.706491	-1.412092
H	6.212216	-2.473797	-0.110016
H	7.076791	-3.662111	0.825975
H	7.203790	-2.665038	-2.790771
H	6.498266	-4.129757	-3.416679
H	5.510258	-3.011068	-2.504004
H	8.462235	-1.668249	0.604329
H	9.222273	-2.999469	-0.239707
H	8.397192	-1.742241	-1.142551

N	6.115623	-7.109673	-2.399467
H	7.009719	-7.232356	-1.972736
C	5.773357	-7.949703	-3.527488
H	6.603932	-8.623441	-3.697534
H	5.618384	-7.363603	-4.421041
C	4.504357	-8.778168	-3.325618
O	3.666280	-8.836135	-4.194066
N	4.393359	-9.431802	-2.162407
H	5.131091	-9.388570	-1.492038
C	3.207309	-10.187565	-1.834412
H	2.967702	-10.899995	-2.609501
H	3.399615	-10.730343	-0.917398
C	1.974183	-9.306851	-1.644814
O	0.887188	-9.696194	-2.004603
N	2.187877	-8.107003	-1.107171
C	1.062409	-7.184556	-1.070943
C	0.616899	-6.720548	-2.460282
O	-0.565535	-6.584413	-2.680697
C	1.278111	-5.930572	-0.230466
O	1.413950	-6.189414	1.126952
H	3.087725	-7.817064	-0.798549
H	0.211098	-7.704080	-0.662224
H	2.120966	-5.365010	-0.613564
H	0.384092	-5.341882	-0.351483
H	2.307864	-6.456596	1.293773
N	1.544084	-6.431961	-3.383021
C	1.145401	-6.024110	-4.717962
C	0.378713	-7.146528	-5.410977
O	-0.608617	-6.891359	-6.067831
C	2.355745	-5.521072	-5.538423

C	2.761868	-4.129042	-5.026137
C	2.060227	-5.496091	-7.043398
C	4.087304	-3.618286	-5.589143
H	2.514483	-6.487418	-3.159265
H	0.424266	-5.223003	-4.638574
H	3.176787	-6.210979	-5.367731
H	1.969949	-3.423461	-5.271828
H	2.835530	-4.155166	-3.946542
H	2.918116	-5.124544	-7.589820
H	1.841475	-6.482977	-7.432575
H	1.215284	-4.853434	-7.269908
H	4.380365	-2.704936	-5.082017
H	4.879282	-4.345086	-5.439155
H	4.030270	-3.399810	-6.649639
N	0.820021	-8.397267	-5.251521
H	1.667088	-8.572880	-4.752418
C	0.043272	-9.504886	-5.753937
H	-0.064086	-9.462635	-6.827599
H	0.556435	-10.421367	-5.491762
C	-1.365276	-9.540103	-5.166934
O	-2.319108	-9.771152	-5.874321
N	-1.472639	-9.318869	-3.858022
C	-2.776401	-9.352477	-3.235399
C	-3.692486	-8.216370	-3.692178
O	-4.890811	-8.424118	-3.732703
C	-2.679003	-9.329616	-1.702814
O	-3.923262	-9.599234	-1.118426
H	-0.656826	-9.231548	-3.289012
H	-3.292805	-10.257033	-3.524111
H	-1.996532	-10.103288	-1.379346

H	-2.290336	-8.372808	-1.370401
H	-4.613427	-9.195876	-1.630806
N	-3.143423	-7.035461	-3.971032
C	-3.907940	-5.914860	-4.493056
C	-4.449187	-6.233746	-5.886671
O	-5.613068	-6.041126	-6.155912
C	-3.013296	-4.655333	-4.488046
C	-3.472029	-3.518247	-5.385264
C	-4.792743	-3.082017	-5.426058
C	-2.544404	-2.883530	-6.203072
C	-5.168555	-2.055510	-6.276057
C	-2.913599	-1.844251	-7.041929
C	-4.233412	-1.431280	-7.085866
H	-2.166731	-6.912867	-3.802026
H	-4.776058	-5.749113	-3.875597
H	-2.930343	-4.319494	-3.458727
H	-2.021567	-4.947411	-4.803548
H	-5.537422	-3.560018	-4.818474
H	-1.519831	-3.211402	-6.194476
H	-6.201174	-1.752456	-6.311892
H	-2.174785	-1.370705	-7.663102
H	-4.528428	-0.637244	-7.749839
N	-3.576093	-6.724267	-6.775011
C	-4.019466	-7.062103	-8.108057
C	-5.145297	-8.094816	-8.085388
O	-6.033114	-8.030967	-8.895470
C	-2.870780	-7.593811	-8.968643
S	-1.652311	-6.342848	-9.484955
H	-2.634890	-6.908431	-6.497377
H	-4.443858	-6.190215	-8.582945

H	-2.366882	-8.412419	-8.472675
H	-3.288966	-7.972037	-9.891749
H	-1.047846	-6.179409	-8.318677
N	-5.078558	-9.066913	-7.155619
H	-4.254248	-9.192320	-6.607830
C	-6.085910	-10.115215	-7.183049
H	-6.258812	-10.452778	-8.193230
H	-5.714556	-10.947552	-6.596537
C	-7.459140	-9.722570	-6.613183
O	-8.481524	-10.086878	-7.126898
N	-7.417939	-9.016209	-5.478356
C	-8.641654	-8.653167	-4.788754
C	-9.504928	-7.658159	-5.556595
O	-10.702650	-7.658734	-5.450267
C	-8.361790	-8.103681	-3.378645
C	-7.519477	-6.820431	-3.271096
C	-8.193038	-5.469071	-3.256679
O	-9.495079	-5.469695	-3.327671
H	-9.844036	-4.571891	-3.238586
O	-7.546903	-4.455184	-3.161451
H	-6.535789	-8.774594	-5.078968
H	-9.260690	-9.533420	-4.686410
H	-9.317922	-7.967172	-2.894287
H	-7.836541	-8.883885	-2.838288
H	-6.956541	-6.846961	-2.345210
H	-6.778057	-6.766643	-4.050670
N	-8.837301	-6.733962	-6.273855
C	-9.555196	-5.702617	-7.000840
C	-10.386046	-6.273602	-8.141689
H	-10.409089	-7.356342	-8.248993

O	-10.987293	-5.559103	-8.888423
C	-8.631312	-4.564298	-7.490284
O	-9.434533	-3.441998	-7.831927
C	-7.723015	-4.928132	-8.657220
H	-7.856607	-6.841481	-6.421929
H	-10.268410	-5.253865	-6.319060
H	-8.030343	-4.256844	-6.645801
H	-10.110596	-3.750863	-8.429428
H	-7.045359	-4.103576	-8.850925
H	-7.131131	-5.809168	-8.458024
H	-8.303897	-5.104881	-9.556039
N	-12.952122	-9.022524	3.174171
H	-13.215000	-9.550467	2.367604
C	-11.773531	-8.180020	2.898781
C	-10.789122	-8.123249	4.050087
O	-9.659793	-7.714465	3.857064
C	-12.146619	-6.722601	2.563120
O	-12.715837	-6.204029	3.737738
C	-13.114462	-6.605062	1.391196
H	-13.731488	-8.453499	3.442454
H	-11.222783	-8.599613	2.068258
H	-11.230715	-6.196590	2.328454
H	-12.850019	-5.263217	3.637899
H	-13.281661	-5.557085	1.166643
H	-12.729025	-7.082233	0.498078
H	-14.074921	-7.044986	1.631883
N	-11.197257	-8.533635	5.241900
H	-12.119355	-8.910736	5.275381
C	-10.412545	-8.529115	6.451311
H	-10.337037	-7.534078	6.860877

H	-10.933713	-9.138687	7.180104
C	-8.974757	-9.043554	6.374947
O	-8.140154	-8.478376	7.037913
N	-8.658722	-10.119724	5.632203
H	-9.369346	-10.599264	5.127171
C	-7.270130	-10.552738	5.532057
H	-7.253485	-11.532149	5.071252
H	-6.830728	-10.631478	6.513529
C	-6.387460	-9.608364	4.692694
O	-5.219619	-9.468422	4.949191
N	-7.045394	-9.018012	3.701158
C	-6.301973	-8.005930	2.963216
C	-6.261971	-6.695345	3.744811
O	-5.267301	-6.009523	3.699222
C	-6.610841	-7.876580	1.459383
C	-7.789996	-7.050923	0.991428
C	-7.776654	-5.663737	1.106805
C	-8.849933	-7.648230	0.322340
C	-8.804228	-4.896947	0.584329
C	-9.869293	-6.882523	-0.220215
C	-9.854080	-5.504749	-0.084365
H	-8.039943	-9.014006	3.679598
H	-5.279248	-8.337545	2.997382
H	-5.714001	-7.456606	1.017512
H	-6.687392	-8.886335	1.073854
H	-6.944552	-5.173537	1.578631
H	-8.862239	-8.716719	0.190761
H	-8.767446	-3.825784	0.671445
H	-10.659064	-7.357730	-0.772552
H	-10.636287	-4.911642	-0.520867

N	-7.293002	-6.385610	4.534364
C	-7.221730	-5.273353	5.451352
C	-6.102461	-5.490852	6.469145
O	-5.456099	-4.538968	6.852411
C	-8.598843	-5.101510	6.124410
C	-8.810397	-3.809065	6.883898
C	-8.979288	-2.606845	6.201470
C	-8.906107	-3.805157	8.268734
C	-9.226647	-1.430576	6.886655
C	-9.163955	-2.629711	8.961213
C	-9.323917	-1.438928	8.272379
H	-8.158220	-6.869398	4.428525
H	-6.951490	-4.368444	4.925868
H	-9.342225	-5.167801	5.336512
H	-8.762024	-5.940633	6.786700
H	-8.925588	-2.588776	5.126645
H	-8.781967	-4.723519	8.815638
H	-9.346256	-0.512296	6.341059
H	-9.227231	-2.646428	10.034539
H	-9.506863	-0.523364	8.806590
N	-5.861975	-6.727968	6.898076
H	-6.516693	-7.449620	6.693395
C	-4.785924	-7.022971	7.817853
H	-4.825001	-6.393313	8.694036
H	-4.898403	-8.052884	8.131654
C	-3.390082	-6.846814	7.222645
O	-2.516229	-6.352123	7.894630
N	-3.189628	-7.271995	5.970549
C	-1.911667	-7.092411	5.299011
C	-1.665261	-5.620551	4.938950

O	-0.566846	-5.133893	5.107319
C	-1.830104	-8.027759	4.072347
C	-0.664591	-7.670603	3.148131
C	-1.728812	-9.487918	4.527864
H	-3.922885	-7.753130	5.495678
H	-1.118350	-7.338224	5.989987
H	-2.750689	-7.904009	3.506718
H	-0.600501	-8.397395	2.345361
H	-0.774988	-6.696245	2.693253
H	0.280001	-7.682386	3.683300
H	-1.741975	-10.148550	3.667022
H	-0.795210	-9.654755	5.059259
H	-2.545713	-9.777642	5.175983
N	-2.700683	-4.933602	4.446723
C	-2.569791	-3.551413	4.028848
C	-2.420055	-2.639035	5.244026
O	-1.528454	-1.820255	5.290671
C	-3.758179	-3.090370	3.171592
C	-3.993855	-3.840527	1.849922
C	-2.859849	-3.730828	0.845315
O	-1.746949	-4.135755	1.218717
O	-3.112387	-3.254706	-0.274000
H	-3.564290	-5.403253	4.285196
H	-1.662684	-3.440938	3.465257
H	-4.667090	-3.158025	3.761551
H	-3.604787	-2.035175	2.961839
H	-4.149166	-4.890275	2.048787
H	-4.899225	-3.450481	1.399036
N	-3.309527	-2.774871	6.244281
C	-3.093978	-2.024901	7.456985

C	-1.778227	-2.422283	8.133769
O	-1.106870	-1.582682	8.694100
C	-4.226306	-2.005092	8.493911
O	-4.436264	-3.246772	9.098351
C	-5.507665	-1.387418	7.948248
H	-3.988319	-3.503125	6.218592
H	-2.937615	-0.995394	7.174834
H	-3.851340	-1.365921	9.283604
H	-4.889516	-3.818426	8.490419
H	-6.240075	-1.327579	8.743512
H	-5.322056	-0.384126	7.577075
H	-5.928451	-1.976867	7.144820
N	-1.380397	-3.700457	8.043328
H	-2.031219	-4.418216	7.812066
C	-0.187162	-4.107473	8.739880
H	-0.237315	-3.891790	9.797886
H	-0.075815	-5.175172	8.604040
C	1.064024	-3.420008	8.217958
O	1.940562	-3.076028	8.977771
N	1.153879	-3.258765	6.881711
C	2.332480	-2.660282	6.317666
C	2.291031	-1.138383	6.164108
O	3.359924	-0.574352	6.023012
C	2.830599	-3.345982	5.045415
S	1.922615	-2.976798	3.520199
H	0.422681	-3.612342	6.296759
H	3.116420	-2.798068	7.046915
H	3.840481	-3.007717	4.863090
H	2.853201	-4.415051	5.204870
H	0.859018	-3.741107	3.719458

N	1.140073	-0.470671	6.273042
C	1.204068	0.968497	6.491343
C	1.755867	1.271210	7.870506
O	2.368584	2.288860	8.085489
C	-0.095735	1.741771	6.182377
C	-1.196941	1.568454	7.238669
C	-0.554806	1.440244	4.750822
C	-2.466310	2.370770	6.944793
H	0.271734	-0.965324	6.291801
H	1.951475	1.351091	5.814764
H	0.208555	2.782274	6.222312
H	-1.446001	0.523677	7.355885
H	-0.807694	1.892671	8.199275
H	-1.310205	2.147625	4.431774
H	0.277840	1.520488	4.057287
H	-0.966433	0.444537	4.656977
H	-3.135946	2.340396	7.798938
H	-2.241207	3.414239	6.739191
H	-3.007062	1.973583	6.092649
N	1.549788	0.323258	8.791266
H	0.889674	-0.402097	8.613548
C	1.978259	0.512664	10.160074
H	1.470031	-0.222645	10.771021
H	1.737710	1.502369	10.518137
C	3.482320	0.337408	10.305053
O	4.164481	1.128932	10.896182
N	3.999933	-0.753835	9.695408
H	3.390718	-1.466103	9.351485
C	5.425034	-0.938857	9.667453
H	5.638280	-1.909399	9.234591

H	5.855716	-0.904647	10.657516
C	6.156882	0.119117	8.844832
O	7.291930	0.411889	9.129191
N	5.502078	0.621285	7.799030
C	6.098617	1.759274	7.146315
C	5.514930	3.076794	7.649682
H	5.013174	3.037228	8.615080
O	5.636959	4.094891	7.041084
C	6.002880	1.675018	5.620789
C	6.755249	0.506917	5.017467
C	8.120897	0.322917	5.238163
C	6.094905	-0.401623	4.195757
C	8.807270	-0.722520	4.635365
C	6.779038	-1.444694	3.591485
C	8.139125	-1.605637	3.801366
H	4.575199	0.334750	7.572736
H	7.134082	1.774541	7.451288
H	4.960665	1.610784	5.334377
H	6.381157	2.609453	5.220641
H	8.648975	0.979017	5.908743
H	5.034721	-0.305680	4.057633
H	9.857989	-0.849857	4.831180
H	6.246852	-2.136576	2.963236
H	8.659502	-2.418213	3.328337
N	12.613550	9.596234	-1.248802
H	11.873251	9.914036	-1.846107
C	12.304852	8.264740	-0.719487
C	11.274139	8.450687	0.386897
O	10.265877	7.779033	0.416424
C	13.562740	7.581006	-0.165338

C	14.645071	7.276096	-1.206565
S	14.017112	6.202108	-2.529901
C	15.499794	6.053606	-3.555345
H	13.433413	9.573022	-1.822259
H	11.834450	7.616518	-1.447338
H	14.001304	8.205423	0.607192
H	13.255687	6.653825	0.304791
H	15.045468	8.188561	-1.633889
H	15.470243	6.783690	-0.704559
H	15.248468	5.398939	-4.375892
H	15.798798	7.017676	-3.946031
H	16.318169	5.616741	-2.998068
N	11.504319	9.412913	1.296974
C	10.594348	9.607808	2.408562
C	9.277067	10.274789	2.010382
O	8.281020	10.053301	2.652714
C	11.276314	10.369119	3.552080
C	12.448034	9.564515	4.084489
O	13.582868	9.826309	3.744685
N	12.144421	8.562209	4.918899
H	12.328109	9.967780	1.206258
H	10.295558	8.637760	2.771295
H	11.657342	11.326350	3.218957
H	10.546139	10.537733	4.333500
H	12.888265	7.966850	5.213200
H	11.222925	8.175946	4.954709
N	9.263831	11.067722	0.922310
H	10.110797	11.229597	0.427324
C	8.003502	11.517470	0.368859
H	8.201222	12.260245	-0.393341

H	7.389103	11.966665	1.131940
C	7.186384	10.384439	-0.254324
O	5.986296	10.470082	-0.291509
N	7.862661	9.333318	-0.763260
C	7.170486	8.145603	-1.233909
C	6.634992	7.300679	-0.067270
O	5.534682	6.808152	-0.148207
C	8.048994	7.344301	-2.224229
C	8.343645	8.197264	-3.472928
C	7.379617	6.019178	-2.608125
C	9.428312	7.625246	-4.388996
H	8.823868	9.230810	-0.536735
H	6.279734	8.471644	-1.748344
H	8.988067	7.117937	-1.727344
H	7.421718	8.323212	-4.036260
H	8.645669	9.192928	-3.165447
H	7.997037	5.478886	-3.314349
H	7.228554	5.377877	-1.748308
H	6.409910	6.182774	-3.066625
H	9.622269	8.305829	-5.211634
H	10.363646	7.479783	-3.855321
H	9.148522	6.671165	-4.820127
N	7.387690	7.175308	1.043947
C	6.879166	6.458329	2.201997
C	5.528064	7.039473	2.639720
O	4.575678	6.332911	2.867084
C	7.833311	6.546165	3.403537
C	9.254785	5.997325	3.244210
O	10.146034	6.631439	3.802226
O	9.428387	4.935707	2.595214

H	8.347749	7.445033	1.022646
H	6.682584	5.429517	1.943351
H	7.921361	7.570767	3.733117
H	7.375197	5.992739	4.220726
N	5.489887	8.377412	2.786093
H	6.320922	8.912627	2.648912
C	4.299247	9.045888	3.249974
H	4.538272	10.090246	3.407640
H	3.957307	8.638803	4.188427
C	3.136661	8.987517	2.268580
O	1.995196	9.109753	2.649482
N	3.470198	8.824750	0.985184
H	4.431331	8.829481	0.735262
C	2.517191	8.905260	-0.078305
H	3.059845	9.091730	-0.996314
H	1.843947	9.738043	0.071942
C	1.609133	7.687020	-0.310194
O	0.561873	7.815080	-0.879456
N	2.094450	6.538077	0.201341
C	1.289915	5.364391	0.431052
C	0.472366	5.479579	1.721851
O	-0.722723	5.301849	1.692290
C	2.166640	4.112382	0.445787
H	3.001458	6.575677	0.616027
H	0.559459	5.290403	-0.357453
H	1.566371	3.234011	0.657559
H	2.636342	3.991439	-0.523469
H	2.946287	4.184370	1.196906
N	1.102526	5.751848	2.879338
C	0.364319	5.585295	4.123115

C	-0.756395	6.611745	4.274095
O	-1.792311	6.302365	4.823511
C	1.276044	5.511889	5.372777
C	1.867890	6.857325	5.819756
C	2.362792	4.445281	5.169577
C	2.699032	6.761047	7.101617
H	2.090115	5.889556	2.900976
H	-0.159805	4.642232	4.064891
H	0.615224	5.173609	6.165237
H	2.478240	7.266383	5.021419
H	1.064534	7.567480	5.986889
H	2.732497	4.092365	6.121113
H	1.969567	3.588565	4.631492
H	3.205860	4.834223	4.608992
H	3.004371	7.751979	7.424500
H	2.121225	6.317754	7.907248
H	3.593851	6.165168	6.971790
N	-0.542944	7.847430	3.801020
H	0.341450	8.089943	3.404838
C	-1.513861	8.887808	4.018652
H	-1.103685	9.816518	3.642483
H	-1.724196	9.016557	5.070574
C	-2.866972	8.618762	3.365891
O	-3.871054	8.837162	4.003288
N	-2.902689	8.108966	2.120757
C	-4.239994	8.013726	1.535324
C	-4.984708	6.749465	1.927653
O	-6.195848	6.756948	1.919618
C	-4.022033	8.221434	0.030819
C	-2.766445	9.099865	0.020044

C	-1.907276	8.456243	1.096073
H	-4.854277	8.814601	1.917373
H	-3.842473	7.278944	-0.469789
H	-4.886472	8.684732	-0.427141
H	-2.255835	9.142614	-0.923514
H	-3.027341	10.114526	0.311498
H	-1.420659	7.566150	0.740384
H	-1.151189	9.119065	1.484439
N	-4.269045	5.673722	2.291129
C	-4.938229	4.512552	2.850562
C	-5.638496	4.853563	4.169019
O	-6.741410	4.413657	4.408508
C	-3.973914	3.331409	3.086460
C	-3.635868	2.505617	1.861093
C	-4.333057	1.334853	1.576479
C	-2.597692	2.864521	1.013868
C	-4.007367	0.548080	0.481876
C	-2.270704	2.094030	-0.087806
C	-2.970649	0.931914	-0.361421
O	-2.617869	0.205930	-1.447938
H	-3.414679	-0.117521	-1.907982
H	-3.275174	5.750810	2.345605
H	-5.725643	4.209378	2.178910
H	-3.068234	3.710965	3.548120
H	-4.443647	2.682173	3.816457
H	-5.141779	1.028511	2.216703
H	-2.032745	3.752393	1.204716
H	-4.536277	-0.366724	0.289378
H	-1.479270	2.397027	-0.750216
N	-4.970839	5.618277	5.048350

H	-4.034974	5.911393	4.856556
C	-5.582770	6.005349	6.299222
H	-4.805964	6.385465	6.951082
H	-6.052320	5.158954	6.774277
C	-6.651496	7.084455	6.135958
O	-7.706406	7.028002	6.726261
N	-6.342147	8.091247	5.313906
H	-5.445016	8.139354	4.880110
C	-7.257687	9.220267	5.085304
H	-6.781278	9.871869	4.364214
H	-7.419712	9.775739	5.997421
C	-8.632477	8.840767	4.569520
O	-9.611434	9.429008	4.959464
N	-8.690359	7.854349	3.658146
C	-9.953936	7.451763	3.088772
C	-10.766323	6.542229	3.995444
O	-11.807588	6.068902	3.559164
C	-9.761142	6.816141	1.689857
O	-10.954305	6.903463	0.953096
C	-9.239228	5.382323	1.729283
H	-7.846118	7.427536	3.334427
H	-10.571638	8.331037	2.962658
H	-9.046018	7.439524	1.169869
H	-11.641554	6.500755	1.473063
H	-8.968246	5.061445	0.731314
H	-8.362371	5.288787	2.354506
H	-10.000981	4.705865	2.098583
N	-10.353337	6.327943	5.240900
C	-11.259093	5.732447	6.212924
C	-12.445055	6.656022	6.502021

O	-13.529726	6.188271	6.758159
C	-10.538025	5.397307	7.526339
C	-9.534251	4.235052	7.447051
C	-8.716965	4.184331	8.741485
C	-10.219852	2.887533	7.196333
H	-9.463052	6.657570	5.550986
H	-11.697039	4.842319	5.794053
H	-10.028513	6.287162	7.878980
H	-11.302479	5.156613	8.259987
H	-8.847326	4.423758	6.628936
H	-7.988825	3.378599	8.709769
H	-8.182037	5.114034	8.898260
H	-9.358174	4.014320	9.603606
H	-9.479647	2.092158	7.178431
H	-10.931103	2.661970	7.988749
H	-10.749907	2.858178	6.251424
N	-12.200391	7.978986	6.519086
C	-13.272865	8.918063	6.674440
C	-14.047138	9.177161	5.399140
H	-14.886714	9.870642	5.514692
O	-13.792339	8.699104	4.343338
H	-11.339485	8.323326	6.149711
H	-13.966260	8.566385	7.428079
H	-12.873616	9.866157	7.021585
N	-11.400139	10.603601	-3.013218
H	-11.151156	10.793474	-2.062887
C	-11.816457	9.206991	-3.172692
C	-11.420798	8.859979	-4.600829
O	-10.381146	8.297520	-4.846936
C	-13.274697	8.886451	-2.781041

C	-13.514119	9.244426	-1.302467
C	-13.600730	7.414103	-3.063630
C	-14.953833	9.045731	-0.824926
H	-12.140937	11.235286	-3.252954
H	-11.162892	8.607041	-2.555403
H	-13.942062	9.511037	-3.379532
H	-12.841512	8.656501	-0.682289
H	-13.250226	10.285287	-1.143016
H	-14.652033	7.209116	-2.907368
H	-13.370171	7.129386	-4.086046
H	-13.034226	6.765433	-2.402795
H	-15.063132	9.412642	0.189358
H	-15.657291	9.588307	-1.451064
H	-15.244825	8.001845	-0.821495
N	-12.217767	9.294713	-5.606266
H	-13.139261	9.595970	-5.384728
C	-11.972872	8.843880	-6.959258
H	-12.033858	7.767145	-7.039985
H	-12.729057	9.278149	-7.601893
C	-10.601635	9.233244	-7.517693
O	-9.996941	8.496732	-8.241527
N	-10.162845	10.477780	-7.182625
H	-10.711033	11.007782	-6.544746
C	-8.894341	11.023967	-7.637100
H	-8.789698	10.891248	-8.702753
H	-8.878586	12.081461	-7.407589
C	-7.672564	10.359017	-6.988311
O	-6.753256	9.935092	-7.630831
N	-7.659106	10.352139	-5.619638
H	-8.482447	10.628022	-5.133559

C	-6.495253	9.961264	-4.832348
H	-5.599197	10.377765	-5.264338
H	-6.616278	10.359356	-3.832341
C	-6.268292	8.463912	-4.714277
O	-5.133740	8.047342	-4.711620
N	-7.321026	7.642803	-4.555739
C	-7.043152	6.284788	-4.116082
C	-6.395851	5.449242	-5.213188
O	-5.518651	4.674607	-4.918154
C	-8.232787	5.569469	-3.436228
C	-9.368455	5.183222	-4.399094
C	-8.696989	6.392754	-2.228906
C	-10.549754	4.494052	-3.715373
H	-8.255737	7.997406	-4.569992
H	-6.261691	6.342851	-3.373705
H	-7.807220	4.647354	-3.048787
H	-9.726255	6.052590	-4.935186
H	-8.960269	4.506274	-5.145546
H	-9.400871	5.838844	-1.623588
H	-7.854458	6.643370	-1.592293
H	-9.177962	7.313866	-2.533136
H	-11.255362	4.128107	-4.455475
H	-10.227063	3.646217	-3.122038
H	-11.086774	5.173295	-3.065412
N	-6.814645	5.564832	-6.493391
C	-6.106146	4.822474	-7.516656
C	-4.760276	5.444472	-7.899124
O	-3.890142	4.715858	-8.316310
C	-6.967005	4.499892	-8.746620
C	-8.037268	3.418486	-8.510343

C	-7.451480	2.077185	-8.040920
N	-8.389453	0.950985	-8.074694
C	-9.199263	0.573556	-7.081841
N	-9.462412	1.417955	-6.095954
N	-9.735558	-0.626717	-7.080755
H	-7.489451	6.258135	-6.735507
H	-5.795978	3.898611	-7.061617
H	-7.450710	5.400293	-9.113841
H	-6.296125	4.164688	-9.530075
H	-8.778088	3.780379	-7.803276
H	-8.564870	3.256187	-9.444433
H	-6.626428	1.798640	-8.683547
H	-7.051772	2.146842	-7.038095
H	-8.319794	0.321084	-8.843001
H	-9.210871	2.374884	-6.171143
H	-9.976329	1.152578	-5.272038
H	-9.387084	-1.392206	-7.629023
H	-10.455807	-0.867823	-6.418365
N	-4.571383	6.757521	-7.721942
H	-5.312316	7.350933	-7.425893
C	-3.257811	7.352384	-8.011367
H	-2.933574	7.093271	-9.006665
H	-3.359220	8.427155	-7.938262
C	-2.194217	6.878612	-7.032962
O	-1.067310	6.644126	-7.392501
N	-2.610531	6.772888	-5.765801
C	-1.723040	6.464253	-4.671160
C	-1.444918	4.978008	-4.544815
O	-0.316663	4.592108	-4.340345
C	-2.307585	7.057556	-3.382764

C	-1.724829	6.352659	-2.158853
C	-2.065567	8.573569	-3.416052
H	-3.535171	7.069255	-5.539484
H	-0.755152	6.905360	-4.861604
H	-3.376293	6.879800	-3.397955
H	-1.939342	6.893014	-1.256070
H	-2.140806	5.355748	-2.055884
H	-0.652641	6.275472	-2.228560
H	-2.803049	9.103886	-2.830544
H	-1.078020	8.814606	-3.037070
H	-2.144829	8.956383	-4.426977
N	-2.474273	4.124764	-4.663714
C	-2.164153	2.717524	-4.734152
C	-1.265510	2.444099	-5.932795
O	-0.395981	1.606821	-5.875409
C	-3.408743	1.806684	-4.774960
C	-4.360591	1.970565	-3.580069
C	-5.448858	0.884496	-3.485617
N	-5.007890	-0.292811	-2.757433
C	-5.827923	-1.254618	-2.564041
N	-7.132237	-1.284998	-3.041769
N	-5.529119	-2.307063	-1.768413
H	-3.401435	4.451781	-4.832822
H	-1.576351	2.442291	-3.871004
H	-3.956426	1.985242	-5.698780
H	-3.044991	0.786278	-4.822098
H	-3.794925	1.985472	-2.660604
H	-4.853529	2.927337	-3.654816
H	-6.318404	1.325198	-2.997289
H	-5.765468	0.631256	-4.501251

H	-7.270081	-0.782411	-3.890557
H	-7.547128	-2.198086	-3.082229
H	-4.605959	-2.417238	-1.395079
H	-6.033341	-3.156447	-1.906095
N	-1.459759	3.193337	-7.035104
H	-2.264571	3.769495	-7.144196
C	-0.595832	2.983550	-8.179089
H	-0.940093	3.626187	-8.979240
H	-0.614272	1.957428	-8.516706
C	0.858332	3.326033	-7.861294
O	1.786295	2.682497	-8.284242
N	1.007444	4.396007	-7.064155
H	0.213477	4.959530	-6.860689
C	2.282309	4.880648	-6.640293
H	2.918466	5.143147	-7.476195
H	2.121614	5.773614	-6.050368
C	3.094243	3.926494	-5.780092
O	4.300279	4.045687	-5.701465
N	2.428061	2.983367	-5.101940
C	3.101641	2.134963	-4.154867
C	4.282232	1.343822	-4.722385
O	5.201595	1.052678	-3.983728
C	2.031200	1.219459	-3.563912
C	2.428279	0.354765	-2.373247
C	1.133390	-0.209096	-1.810740
N	1.349169	-1.210787	-0.786501
C	0.367647	-2.053261	-0.419186
N	-0.791012	-2.021153	-1.034330
N	0.596603	-2.937678	0.523714
H	1.433627	2.938694	-5.174913

H	3.548704	2.735628	-3.371667
H	1.222666	1.874552	-3.257062
H	1.623769	0.598124	-4.352985
H	3.090659	-0.451492	-2.668342
H	2.949837	0.944516	-1.622870
H	0.514363	0.599529	-1.433668
H	0.590414	-0.682622	-2.616027
H	2.060887	-1.044140	-0.110411
H	-1.129920	-1.169038	-1.431095
H	-1.541386	-2.654010	-0.762410
H	1.513623	-3.109826	0.865267
H	-0.183083	-3.502307	0.855343
N	4.281487	0.944901	-6.004141
H	3.540371	1.224938	-6.613418
C	5.363433	0.116651	-6.504612
H	5.138944	-0.142419	-7.531832
H	5.441320	-0.797906	-5.938283
C	6.736191	0.756138	-6.475981
O	7.738526	0.089729	-6.364633
N	6.766107	2.085332	-6.608300
H	5.912156	2.604985	-6.573201
C	8.005486	2.823552	-6.551065
H	8.709854	2.439480	-7.275335
H	7.800291	3.854267	-6.807648
C	8.748798	2.826930	-5.213288
O	9.889951	3.236315	-5.161832
N	8.104016	2.338735	-4.145826
C	8.685994	2.174934	-2.824675
C	9.950570	1.305606	-2.832425
O	10.769365	1.388724	-1.931295

C	7.582130	1.508244	-1.973555
C	7.780996	1.384533	-0.463019
C	7.441450	2.654429	0.326731
C	7.331647	2.387428	1.824123
N	8.671949	2.354031	2.481140
O	11.043286	1.617612	0.892719
H	10.893052	1.828799	-0.029133
H	11.521828	0.790985	0.841668
H	7.158097	2.035734	-4.258562
H	8.985493	3.132409	-2.419326
H	6.666251	2.053993	-2.156744
H	7.412207	0.521513	-2.388659
H	7.101135	0.605589	-0.131601
H	8.776310	1.030766	-0.228981
H	8.155104	3.454515	0.151101
H	6.476503	3.027407	-0.001413
H	6.771589	3.159838	2.327782
H	6.850425	1.441442	2.018892
H	9.382571	1.890136	1.923742
H	8.991993	3.324207	2.635424
H	8.618503	1.876206	3.368828
N	10.062466	0.448215	-3.837530
C	11.109251	-0.537627	-4.069489
C	12.486201	0.023149	-4.427400
O	13.443843	-0.705691	-4.301267
C	10.700734	-1.443986	-5.252716
C	9.562929	-2.442696	-4.997444
C	9.130895	-3.067095	-6.327950
C	9.990812	-3.533456	-4.015394
H	9.324093	0.446344	-4.510536

H	11.264778	-1.125208	-3.176521
H	10.433734	-0.798323	-6.084015
H	11.583574	-1.996197	-5.551819
H	8.706548	-1.911906	-4.593160
H	8.329842	-3.783539	-6.173274
H	8.773221	-2.310164	-7.014248
H	9.957864	-3.594938	-6.796442
H	9.201223	-4.263707	-3.875504
H	10.860934	-4.059422	-4.394350
H	10.243969	-3.136808	-3.036935
N	12.574050	1.261829	-4.919244
C	13.814624	1.844749	-5.393663
C	14.958706	2.033567	-4.379164
O	16.013158	2.414783	-4.812030
C	13.497165	3.171410	-6.086959
O	12.917964	4.088335	-5.202640
H	11.756425	1.833577	-4.917248
H	14.248583	1.177768	-6.129163
H	14.420310	3.590389	-6.455646
H	12.846429	2.977487	-6.933720
H	11.970594	4.079224	-5.267509
N	14.792295	1.722326	-3.074279
C	15.928362	1.647498	-2.176930
C	16.804572	0.409919	-2.402499
O	17.934404	0.393867	-1.987966
C	15.495618	1.578402	-0.707341
C	14.639479	2.735871	-0.198089
C	14.286573	2.489893	1.269178
N	13.261352	3.384797	1.791148
C	13.438934	4.535615	2.419219

N	14.656613	5.010999	2.656427
O	15.029030	7.467122	4.210782
H	14.745418	8.353611	3.971764
H	15.747617	7.573218	4.821163
N	12.388927	5.224132	2.815771
H	13.901038	1.419628	-2.758344
H	16.562064	2.504331	-2.346854
H	14.954846	0.650683	-0.551461
H	16.407670	1.509060	-0.124688
H	15.157351	3.683476	-0.314932
H	13.720110	2.817115	-0.766163
H	13.890152	1.490595	1.376643
H	15.166171	2.533074	1.900653
H	12.321274	3.089093	1.619810
H	15.464549	4.518437	2.358435
H	14.791850	5.865912	3.168142
H	11.433471	4.944259	2.657765
H	12.481277	6.067154	3.336059
N	16.200238	-0.648980	-2.967241
C	16.870796	-1.911508	-3.168197
C	17.669503	-1.889228	-4.468054
H	18.063310	-0.909605	-4.748073
O	17.875929	-2.852970	-5.130598
C	15.868043	-3.070177	-3.149486
C	15.324788	-3.399916	-1.791982
N	14.403993	-2.627607	-1.112039
O	12.508231	-0.434478	-0.465182
H	13.146153	-1.037701	-0.850756
H	12.028078	-0.039074	-1.184664
C	15.619975	-4.490463	-1.049798

C	14.172980	-3.251840	-0.003576
N	14.883327	-4.381982	0.103080
H	15.285740	-0.550231	-3.352920
H	17.596095	-2.030812	-2.370971
H	15.050489	-2.842195	-3.824652
H	16.368753	-3.943989	-3.544107
H	16.275364	-5.314216	-1.235376
H	13.494777	-2.922413	0.757508
H	14.782798	-5.064870	0.821794
O	-14.930263	-2.440032	5.283656
H	-15.070599	-1.569671	4.919845
H	-14.427377	-2.308097	6.080381
O	-12.772909	-1.570133	7.335218
H	-12.084057	-2.061818	7.768504
H	-12.983745	-0.851100	7.918196
O	-11.882749	-0.958225	4.588006
H	-11.986359	-1.108925	5.524154
H	-12.698520	-0.532607	4.317364
O	-13.470540	-1.498157	1.152937
H	-12.611059	-1.070319	1.129708
H	-13.392767	-2.234664	1.762625
O	-7.422954	2.197725	-0.103554
H	-7.555241	2.263681	0.846107
H	-6.505638	1.973138	-0.203986
O	-7.633101	2.150031	2.721242
H	-8.410996	1.691130	3.030900
H	-7.483601	2.881792	3.315363
O	-9.179938	0.349107	-1.275921
H	-8.589391	1.014686	-0.904213
H	-8.610112	-0.340096	-1.612837

O	-13.000534	-1.922754	-1.654893
H	-13.314173	-1.992742	-0.752983
H	-13.713485	-2.169468	-2.235174
O	-13.813492	1.512328	0.356300
H	-14.241974	0.684947	0.545414
H	-12.889308	1.336384	0.542820
O	-14.679677	5.246409	4.124678
H	-14.013136	5.837092	3.789073
H	-14.614470	5.349385	5.069876
O	-14.702604	2.662671	2.986968
H	-14.903288	3.540962	3.323119
H	-14.603995	2.715563	2.041436
O	-13.336717	0.833135	-2.396289
H	-13.633173	1.331508	-1.635880
H	-13.077609	-0.017755	-2.039831
O	-14.474167	-1.111029	-4.142076
H	-14.414266	-0.261514	-3.708659
H	-15.298045	-1.130810	-4.611127
O	-10.572453	-2.940303	-3.030550
H	-10.892042	-2.579323	-3.853822
H	-11.254298	-2.731306	-2.397683
O	-11.266099	0.240199	0.789947
H	-10.601653	0.163090	0.104503
H	-10.806266	0.507340	1.591006
O	-10.208600	0.991664	3.285826
H	-10.576781	0.309085	3.844813
H	-10.727483	1.781199	3.462469
O	-11.956667	3.113274	3.704819
H	-11.911088	4.063934	3.653883
H	-12.872018	2.889008	3.552708

O	-10.746486	0.954037	-3.524517
H	-11.593341	1.223036	-3.167728
H	-10.181604	0.783524	-2.763460
O	-14.430372	-0.068004	3.680697
H	-14.660205	0.857483	3.580218
H	-14.386823	-0.433381	2.802221
O	-13.081569	-3.333714	3.367965
H	-13.830636	-3.189182	3.954855
H	-12.406101	-2.767136	3.737728
O	-11.697057	-1.220663	-5.029854
H	-12.648835	-1.299146	-4.990487
H	-11.458123	-0.552442	-4.387631

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(0),Y266(0),E183(0)

POTENTIAL: 0 mV

N	15.802748	-6.133741	5.261069
H	15.000474	-5.906329	5.815964
C	15.709624	-5.529811	3.929295
C	15.001670	-6.466409	2.931375
O	14.254140	-6.041260	2.065796
C	17.109416	-5.209681	3.391311
H	16.607142	-5.796305	5.751991
H	15.121687	-4.621509	3.935920
H	17.063954	-4.816033	2.382904
H	17.577240	-4.457711	4.016567
H	17.739550	-6.092207	3.389811
N	15.285550	-7.763112	3.044991
H	15.877215	-8.030363	3.802303

C	14.673853	-8.778914	2.186456
H	14.746006	-8.500238	1.147858
H	15.190942	-9.717305	2.336458
C	13.193214	-8.946854	2.530571
O	12.362027	-9.161640	1.687330
N	12.866158	-8.803500	3.829326
H	13.587727	-8.723517	4.508537
C	11.484286	-8.958399	4.289736
H	11.482590	-8.954602	5.371574
H	11.055077	-9.884466	3.940086
C	10.593529	-7.816666	3.783179
O	9.450421	-8.019874	3.471227
N	11.170827	-6.604632	3.745066
C	10.507953	-5.436464	3.221573
C	10.309540	-5.486674	1.704078
O	9.264435	-5.084642	1.249788
C	11.252668	-4.174356	3.686533
O	12.642423	-4.322692	3.673183
H	12.127772	-6.510127	3.994548
H	9.504595	-5.385282	3.611648
H	10.937622	-3.329139	3.084844
H	10.985755	-3.974887	4.713991
H	12.971644	-4.488421	2.798266
N	11.292688	-5.962586	0.920590
C	11.037128	-6.153732	-0.504232
C	9.910206	-7.168917	-0.707747
O	9.151731	-7.071253	-1.644702
C	12.331963	-6.504276	-1.299021
C	12.565671	-8.002012	-1.535208
C	12.339033	-5.762081	-2.636815

H	12.130428	-6.325788	1.320764
H	10.642682	-5.226036	-0.887172
H	13.157179	-6.123167	-0.707998
H	13.520521	-8.137387	-2.032441
H	12.581601	-8.579208	-0.621618
H	11.805032	-8.418528	-2.188472
H	13.238657	-5.997828	-3.194163
H	11.484320	-6.047105	-3.240534
H	12.313833	-4.688852	-2.490505
N	9.817331	-8.136373	0.212020
H	10.569257	-8.257922	0.851718
C	8.868022	-9.241609	0.120497
H	9.237689	-10.037783	0.754129
H	8.809266	-9.613071	-0.890983
C	7.451044	-8.911795	0.540059
O	6.533445	-9.381790	-0.092114
N	7.258889	-8.114639	1.597322
C	5.914032	-7.670855	1.882615
C	5.458354	-6.661318	0.834886
O	4.274943	-6.583092	0.580055
C	5.655596	-7.187100	3.323779
C	5.841147	-8.335144	4.321046
C	6.461916	-5.955941	3.742489
H	8.032219	-7.837947	2.162579
H	5.253503	-8.507948	1.717107
H	4.605128	-6.912388	3.327921
H	5.548252	-8.015614	5.315475
H	5.227594	-9.189776	4.055306
H	6.874357	-8.660447	4.365866
H	6.110686	-5.597222	4.704005

H	7.511554	-6.196499	3.848301
H	6.368667	-5.140781	3.032580
N	6.354726	-5.914430	0.181730
C	5.931727	-5.102530	-0.947122
C	5.527744	-5.988931	-2.133641
O	4.492212	-5.764840	-2.716587
C	6.987312	-4.041396	-1.317312
C	7.147864	-3.028089	-0.170286
C	6.594155	-3.335295	-2.619478
C	8.408132	-2.169551	-0.276491
H	7.320806	-5.958333	0.425317
H	5.013931	-4.602217	-0.677309
H	7.936597	-4.546701	-1.467448
H	6.267486	-2.384975	-0.148062
H	7.177721	-3.549449	0.777112
H	7.269413	-2.518046	-2.832373
H	6.620301	-4.003373	-3.470330
H	5.588856	-2.930740	-2.553669
H	8.482391	-1.500994	0.574242
H	9.293835	-2.793589	-0.281833
H	8.420624	-1.561022	-1.173564
N	6.331194	-7.000322	-2.485061
H	7.231876	-7.098295	-2.065280
C	6.006648	-7.842851	-3.616850
H	6.851172	-8.498178	-3.789603
H	5.839077	-7.256977	-4.508291
C	4.755158	-8.697411	-3.415597
O	3.916274	-8.770019	-4.282039
N	4.658416	-9.353786	-2.252550
H	5.399685	-9.303325	-1.586413

C	3.490006	-10.137156	-1.926906
H	3.264766	-10.851309	-2.704675
H	3.694665	-10.679454	-1.012301
C	2.238767	-9.284259	-1.731649
O	1.159870	-9.694837	-2.091310
N	2.423893	-8.083818	-1.184805
C	1.273961	-7.190680	-1.156699
C	0.821010	-6.740694	-2.548666
O	-0.363806	-6.622665	-2.764319
C	1.484533	-5.917358	-0.353069
O	1.626429	-6.121778	1.018217
H	3.320025	-7.766764	-0.892777
H	0.434883	-7.723825	-0.740868
H	2.328249	-5.376915	-0.756689
H	0.592172	-5.322698	-0.482288
H	2.493379	-6.471572	1.180093
N	1.741980	-6.433439	-3.470856
C	1.337628	-6.029174	-4.806418
C	0.583618	-7.161829	-5.495852
O	-0.414651	-6.924998	-6.142244
C	2.542054	-5.518012	-5.630954
C	2.941030	-4.121456	-5.125238
C	2.240675	-5.499481	-7.135097
C	4.263526	-3.607619	-5.693153
H	2.713252	-6.475322	-3.248263
H	0.609644	-5.234427	-4.726866
H	3.368439	-6.201764	-5.461649
H	2.145325	-3.420994	-5.372929
H	3.016607	-4.143456	-4.045455
H	3.093572	-5.123035	-7.685782

H	2.028242	-6.489108	-7.520646
H	1.390108	-4.863974	-7.360555
H	4.553952	-2.689064	-5.193861
H	5.059399	-4.329581	-5.539671
H	4.204307	-3.396494	-6.754782
N	1.052900	-8.403395	-5.341579
H	1.906718	-8.561590	-4.848372
C	0.292540	-9.526508	-5.833032
H	0.178789	-9.493322	-6.906357
H	0.820525	-10.433212	-5.566498
C	-1.111732	-9.575076	-5.239009
O	-2.067570	-9.804500	-5.945007
N	-1.217901	-9.367827	-3.927608
C	-2.522875	-9.413595	-3.306249
C	-3.454420	-8.284898	-3.755120
O	-4.649155	-8.508635	-3.796956
C	-2.424017	-9.396615	-1.773672
O	-3.663373	-9.680314	-1.186800
H	-0.402368	-9.276158	-3.358981
H	-3.030589	-10.321873	-3.598442
H	-1.733119	-10.164896	-1.454967
H	-2.043728	-8.437411	-1.438209
H	-4.360911	-9.288971	-1.698526
N	-2.922992	-7.092240	-4.019939
C	-3.699120	-5.963151	-4.507090
C	-4.266581	-6.254021	-5.894860
O	-5.431084	-6.023322	-6.151709
C	-2.797331	-4.703446	-4.499222
C	-3.209253	-3.587394	-5.442368
C	-4.494906	-3.057994	-5.451093

C	-2.278404	-3.070113	-6.334911
C	-4.840068	-2.054184	-6.339080
C	-2.613330	-2.051179	-7.212352
C	-3.900316	-1.543837	-7.220504
H	-1.947778	-6.960565	-3.851005
H	-4.557863	-5.807294	-3.872755
H	-2.750007	-4.341042	-3.477091
H	-1.797726	-5.011419	-4.768673
H	-5.237413	-3.445645	-4.779343
H	-1.281404	-3.473773	-6.353442
H	-5.848912	-1.682233	-6.350090
H	-1.874235	-1.666058	-7.891564
H	-4.168910	-0.763907	-7.911241
N	-3.424976	-6.765524	-6.794730
C	-3.901721	-7.102960	-8.117293
C	-5.015665	-8.146642	-8.051272
O	-5.986586	-8.038891	-8.755275
C	-2.770058	-7.620611	-9.008468
S	-1.576341	-6.355968	-9.547156
H	-2.484376	-6.973635	-6.530493
H	-4.350060	-6.233736	-8.573782
H	-2.246139	-8.436966	-8.529932
H	-3.206103	-7.999536	-9.923341
H	-0.946915	-6.192580	-8.393968
N	-4.846012	-9.182107	-7.204948
H	-3.988537	-9.313012	-6.711513
C	-5.828424	-10.255158	-7.239410
H	-6.001956	-10.584056	-8.252976
H	-5.430288	-11.085676	-6.668447
C	-7.207602	-9.905697	-6.656110

O	-8.221584	-10.297350	-7.164233
N	-7.176471	-9.204614	-5.516534
C	-8.405087	-8.888694	-4.813583
C	-9.295053	-7.892144	-5.549413
O	-10.487679	-7.899805	-5.403543
C	-8.123801	-8.374777	-3.392059
C	-7.335396	-7.061709	-3.261420
C	-8.076275	-5.748480	-3.272464
O	-9.376603	-5.830778	-3.312950
H	-9.777446	-4.958579	-3.223018
O	-7.492178	-4.695781	-3.211041
H	-6.297958	-8.952920	-5.115385
H	-9.002589	-9.785822	-4.732765
H	-9.073941	-8.290667	-2.885504
H	-7.556829	-9.148504	-2.885423
H	-6.809518	-7.062844	-2.312834
H	-6.568258	-6.978572	-4.012532
N	-8.659483	-6.956499	-6.285211
C	-9.413283	-5.938871	-6.996586
C	-10.435645	-6.574016	-7.933625
H	-10.226589	-7.596577	-8.250185
O	-11.392722	-5.979786	-8.314266
C	-8.412166	-5.020115	-7.727878
O	-7.712074	-4.259095	-6.766165
C	-9.057410	-4.040272	-8.697726
H	-7.703276	-7.105189	-6.523395
H	-9.976016	-5.342482	-6.289748
H	-7.706396	-5.637513	-8.273658
H	-6.962397	-4.744461	-6.429734
H	-8.292053	-3.357331	-9.048877

H	-9.491093	-4.546015	-9.549108
H	-9.844202	-3.472736	-8.213192
N	-12.664563	-9.429889	3.164222
H	-12.922766	-9.946953	2.349065
C	-11.516487	-8.546511	2.893191
C	-10.519175	-8.500792	4.031525
O	-9.392645	-8.085782	3.829688
C	-11.932060	-7.082274	2.633439
O	-12.474845	-6.633573	3.848899
C	-12.935884	-6.926080	1.497481
H	-13.458516	-8.892653	3.454407
H	-10.971693	-8.917900	2.037330
H	-11.033097	-6.527056	2.397600
H	-12.541560	-5.680343	3.845233
H	-13.128231	-5.872036	1.327427
H	-12.569422	-7.352180	0.570999
H	-13.881137	-7.394637	1.743802
N	-10.912409	-8.912490	5.227241
H	-11.836108	-9.282675	5.278305
C	-10.117759	-8.874740	6.429074
H	-10.065494	-7.874086	6.829758
H	-10.611782	-9.494111	7.168415
C	-8.667437	-9.345701	6.335156
O	-7.838228	-8.745009	6.973389
N	-8.330303	-10.424052	5.604750
H	-9.032680	-10.929901	5.114057
C	-6.931824	-10.817710	5.495285
H	-6.890673	-11.799038	5.039984
H	-6.481718	-10.878653	6.473277
C	-6.079123	-9.857234	4.644362

O	-4.909138	-9.699485	4.884645
N	-6.757552	-9.275458	3.661449
C	-6.038043	-8.278086	2.880352
C	-6.032951	-6.932366	3.598651
O	-5.071207	-6.205153	3.495938
C	-6.365409	-8.211815	1.375404
C	-7.563889	-7.414372	0.907779
C	-7.554388	-6.022942	0.960824
C	-8.650173	-8.045961	0.317469
C	-8.615467	-5.285316	0.463498
C	-9.703604	-7.310186	-0.200852
C	-9.695539	-5.927888	-0.119682
H	-7.751975	-9.304257	3.637764
H	-5.007752	-8.584803	2.922330
H	-5.479883	-7.798417	0.905878
H	-6.438147	-9.235389	1.027308
H	-6.703622	-5.508566	1.370048
H	-8.660485	-9.119306	0.232669
H	-8.582834	-4.211204	0.502953
H	-10.517229	-7.813391	-0.690783
H	-10.505638	-5.358031	-0.535137
N	-7.068614	-6.639245	4.386842
C	-7.049148	-5.501546	5.271473
C	-5.961075	-5.671111	6.331199
O	-5.372862	-4.692340	6.740093
C	-8.450381	-5.333199	5.899359
C	-8.751341	-3.960707	6.461252
C	-8.965609	-2.885350	5.600933
C	-8.874792	-3.754368	7.827316
C	-9.286704	-1.632532	6.093501

C	-9.195603	-2.500391	8.327972
C	-9.398100	-1.436530	7.465149
H	-7.903950	-7.178532	4.319669
H	-6.779097	-4.608454	4.727083
H	-9.172151	-5.551465	5.119998
H	-8.582433	-6.083469	6.668561
H	-8.872206	-3.025792	4.536719
H	-8.718599	-4.572081	8.508817
H	-9.448415	-0.817091	5.412546
H	-9.275206	-2.356397	9.390682
H	-9.617167	-0.457767	7.853658
N	-5.685488	-6.900498	6.761219
H	-6.315177	-7.639717	6.543351
C	-4.631720	-7.174764	7.711953
H	-4.686018	-6.524319	8.571651
H	-4.754942	-8.196190	8.048555
C	-3.227715	-7.014292	7.133762
O	-2.367537	-6.481107	7.793480
N	-3.003625	-7.484309	5.900788
C	-1.725803	-7.275557	5.240277
C	-1.513059	-5.794499	4.908379
O	-0.427999	-5.287363	5.091746
C	-1.611442	-8.184485	3.996883
C	-0.441793	-7.783753	3.093626
C	-1.478461	-9.650672	4.424243
H	-3.713061	-8.010858	5.437440
H	-0.929713	-7.514148	5.930938
H	-2.527989	-8.070681	3.423080
H	-0.359090	-8.489264	2.273441
H	-0.559254	-6.798317	2.663451

H	0.496694	-7.796616	3.639845
H	-1.469878	-10.294669	3.550747
H	-0.544786	-9.805130	4.959131
H	-2.292382	-9.972110	5.060412
N	-2.558118	-5.116075	4.420471
C	-2.426588	-3.732439	4.010585
C	-2.324387	-2.803144	5.221773
O	-1.475246	-1.932802	5.235110
C	-3.575238	-3.292506	3.091832
C	-3.628136	-3.979870	1.713639
C	-2.479503	-3.590899	0.790552
O	-1.342591	-3.954180	1.143503
O	-2.739628	-2.938473	-0.234984
H	-3.410076	-5.596120	4.225320
H	-1.497605	-3.622503	3.481084
H	-4.519995	-3.463047	3.596899
H	-3.484559	-2.219278	2.954851
H	-3.614135	-5.053802	1.840203
H	-4.563888	-3.711327	1.237959
N	-3.177610	-2.969248	6.241614
C	-2.974605	-2.214912	7.461881
C	-1.640742	-2.582382	8.119778
O	-0.980839	-1.722762	8.662099
C	-4.109964	-2.244122	8.495206
O	-4.313550	-3.515362	9.037236
C	-5.394365	-1.610222	7.972251
H	-3.839910	-3.713084	6.219782
H	-2.847728	-1.180019	7.184399
H	-3.742723	-1.638615	9.314637
H	-4.785192	-4.049063	8.409040

H	-6.133761	-1.601223	8.763995
H	-5.216438	-0.585765	7.660682
H	-5.803610	-2.157134	7.133035
N	-1.210544	-3.848625	8.020389
H	-1.843776	-4.589353	7.811082
C	0.050815	-4.201498	8.622318
H	0.083492	-3.965337	9.676576
H	0.189537	-5.267439	8.496148
C	1.221575	-3.477235	7.972298
O	2.158276	-3.080226	8.626546
N	1.159934	-3.329648	6.637167
C	2.250933	-2.710311	5.932569
C	2.307638	-1.197139	6.114518
O	3.391932	-0.651233	6.088007
C	2.246399	-3.076065	4.437518
S	1.378895	-1.930579	3.318776
H	0.431044	-3.787567	6.128394
H	3.178921	-3.066031	6.357491
H	3.270579	-3.062558	4.087529
H	1.859735	-4.077278	4.311634
H	0.164234	-1.986988	3.842867
N	1.164542	-0.526618	6.278802
C	1.235250	0.904035	6.497816
C	1.821366	1.192585	7.867627
O	2.444194	2.205491	8.080769
C	-0.076753	1.680972	6.250513
C	-1.140346	1.495259	7.344063
C	-0.598007	1.407534	4.835329
C	-2.418168	2.302508	7.103229
H	0.290780	-1.009638	6.259376

H	1.960746	1.295620	5.801259
H	0.231373	2.719880	6.294890
H	-1.387546	0.448886	7.459256
H	-0.718301	1.808024	8.294147
H	-1.340271	2.142554	4.552689
H	0.207234	1.461563	4.108774
H	-1.053415	0.429760	4.751920
H	-3.057469	2.263117	7.979825
H	-2.199018	3.347843	6.901398
H	-2.989606	1.916613	6.265996
N	1.617625	0.243785	8.787960
H	0.981755	-0.499819	8.600173
C	2.050768	0.429130	10.154569
H	1.549636	-0.311413	10.765252
H	1.802070	1.414861	10.518231
C	3.555361	0.267358	10.306953
O	4.214056	1.036300	10.953169
N	4.098247	-0.786619	9.658822
H	3.511996	-1.446043	9.192314
C	5.527090	-0.933177	9.619740
H	5.763342	-1.888623	9.166057
H	5.955740	-0.908823	10.610386
C	6.228689	0.159508	8.816932
O	7.355392	0.482952	9.101689
N	5.555629	0.653155	7.778697
C	6.120025	1.811755	7.133439
C	5.515616	3.112176	7.655833
H	5.026430	3.053767	8.626533
O	5.611046	4.137864	7.055268
C	6.008296	1.737836	5.608566

C	6.784554	0.591938	4.994027
C	8.162248	0.463588	5.177200
C	6.135465	-0.354819	4.207908
C	8.871836	-0.563028	4.569974
C	6.843548	-1.379535	3.599952
C	8.214360	-1.484291	3.769247
H	4.630602	0.352148	7.562127
H	7.158632	1.845458	7.426406
H	4.964569	1.648830	5.333407
H	6.358299	2.683683	5.209822
H	8.682240	1.149650	5.824100
H	5.068106	-0.303880	4.103691
H	9.931830	-0.647230	4.736986
H	6.321910	-2.105105	3.001245
H	8.752085	-2.283556	3.292809
N	12.383857	9.886082	-1.227636
H	11.630001	10.191693	-1.814265
C	12.112715	8.542590	-0.708150
C	11.085237	8.693381	0.406429
O	10.095792	7.994430	0.438015
C	13.391383	7.886848	-0.167975
C	14.475049	7.620190	-1.218230
S	13.868045	6.540985	-2.547125
C	15.347148	6.442829	-3.583754
H	13.198078	9.888251	-1.809547
H	11.654092	7.888713	-1.438492
H	13.818114	8.515339	0.607837
H	13.111438	6.947613	0.295098
H	14.847990	8.546716	-1.640023
H	15.316364	7.145977	-0.725587

H	15.107796	5.789869	-4.409240
H	15.617264	7.418448	-3.966705
H	16.180919	6.022870	-3.036382
N	11.295982	9.655610	1.320992
C	10.388487	9.820145	2.439510
C	9.050916	10.452758	2.053155
O	8.065149	10.198791	2.699204
C	11.057152	10.594026	3.582483
C	12.252313	9.817485	4.104239
O	13.377804	10.107592	3.756372
N	11.979720	8.806247	4.938560
H	12.103934	10.232935	1.227910
H	10.118612	8.840609	2.799267
H	11.411283	11.562274	3.251529
H	10.327490	10.740272	4.368871
H	12.739835	8.228462	5.226151
H	11.068087	8.398111	4.980888
N	9.009229	11.252354	0.970760
H	9.848677	11.443606	0.473489
C	7.733763	11.672740	0.429119
H	7.906541	12.427355	-0.327496
H	7.112401	12.098598	1.199931
C	6.943222	10.524008	-0.199576
O	5.741296	10.577846	-0.230249
N	7.645152	9.495791	-0.720961
C	6.983405	8.293529	-1.197890
C	6.479952	7.422750	-0.035888
O	5.395673	6.896153	-0.116478
C	7.877311	7.526978	-2.201847
C	8.140504	8.400451	-3.443380

C	7.242399	6.187890	-2.595638
C	9.233707	7.867386	-4.372701
H	8.609818	9.417835	-0.499519
H	6.080261	8.599108	-1.703230
H	8.825439	7.321574	-1.712961
H	7.211700	8.507628	-3.999226
H	8.417932	9.400511	-3.127307
H	7.870034	5.672220	-3.311277
H	7.114159	5.534008	-1.741643
H	6.265695	6.329547	-3.046508
H	9.404524	8.562101	-5.188613
H	10.175992	7.740289	-3.846574
H	8.975894	6.911343	-4.813183
N	7.241240	7.312631	1.071146
C	6.758910	6.575094	2.227283
C	5.394786	7.116569	2.675935
O	4.464116	6.382429	2.904781
C	7.717131	6.680898	3.424162
C	9.152789	6.174196	3.253817
O	10.028205	6.826612	3.815162
O	9.354669	5.124504	2.592663
H	8.192235	7.612284	1.048095
H	6.588370	5.543074	1.962990
H	7.778016	7.705052	3.761116
H	7.279348	6.108991	4.239792
N	5.320965	8.452235	2.829043
H	6.136771	9.010091	2.691104
C	4.116095	9.086744	3.304149
H	4.329186	10.135870	3.467203
H	3.790535	8.665205	4.241985

C	2.949105	9.005195	2.329710
O	1.807928	9.098765	2.718544
N	3.277772	8.856085	1.043021
H	4.236666	8.887923	0.786687
C	2.315110	8.922066	-0.012995
H	2.845449	9.132165	-0.933090
H	1.621128	9.734982	0.150817
C	1.437959	7.682495	-0.250768
O	0.387946	7.788238	-0.819563
N	1.951160	6.542334	0.253240
C	1.171912	5.351145	0.482825
C	0.361371	5.446887	1.779559
O	-0.831956	5.257420	1.757791
C	2.073747	4.117060	0.486749
H	2.855588	6.600485	0.670987
H	0.438235	5.266224	-0.301549
H	1.494563	3.225435	0.701115
H	2.537735	4.009248	-0.486920
H	2.858441	4.202792	1.231184
N	0.998212	5.717252	2.934108
C	0.275445	5.525141	4.183080
C	-0.868864	6.522241	4.349713
O	-1.890221	6.183620	4.908404
C	1.199852	5.466570	5.423842
C	1.765598	6.822965	5.871129
C	2.308303	4.425232	5.206004
C	2.607500	6.740673	7.146901
H	1.984395	5.864619	2.948433
H	-0.225898	4.569811	4.123881
H	0.553566	5.110669	6.220525

H	2.361547	7.246916	5.069795
H	0.948472	7.515283	6.045784
H	2.693298	4.073751	6.152106
H	1.930509	3.563554	4.664756
H	3.138550	4.836578	4.642139
H	2.895374	7.736762	7.469958
H	2.044140	6.284611	7.955656
H	3.513073	6.162905	7.009565
N	-0.692923	7.764629	3.879136
H	0.180600	8.032433	3.475516
C	-1.694154	8.774355	4.102975
H	-1.314008	9.716363	3.728426
H	-1.904515	8.893212	5.155959
C	-3.041855	8.466288	3.455299
O	-4.047221	8.649548	4.101027
N	-3.070667	7.966250	2.206026
C	-4.406233	7.836078	1.623995
C	-5.094550	6.531640	1.984415
O	-6.304689	6.488564	1.983499
C	-4.208045	8.094939	0.123981
C	-2.974220	9.003829	0.124771
C	-2.092246	8.357384	1.180601
H	-5.048940	8.599905	2.033488
H	-4.012536	7.172667	-0.407075
H	-5.088412	8.550702	-0.310665
H	-2.471857	9.079763	-0.821686
H	-3.257158	10.005150	0.440630
H	-1.588773	7.486191	0.802424
H	-1.347523	9.028405	1.576536
N	-4.330088	5.480246	2.318004

C	-4.939773	4.287578	2.879019
C	-5.662807	4.598426	4.194002
O	-6.734970	4.091019	4.436276
C	-3.908856	3.172631	3.151819
C	-3.498995	2.288368	1.988751
C	-4.070440	1.031025	1.821627
C	-2.471099	2.643734	1.124587
C	-3.608548	0.142446	0.863177
C	-1.993049	1.765001	0.169450
C	-2.533348	0.493957	0.054352
O	-1.980588	-0.355925	-0.831761
H	-3.339965	5.599635	2.365121
H	-5.702994	3.930468	2.205395
H	-3.030555	3.626387	3.598977
H	-4.338682	2.532664	3.914101
H	-4.883486	0.726258	2.458948
H	-2.011482	3.605910	1.209833
H	-4.057421	-0.825899	0.753641
H	-1.186879	2.052809	-0.482149
H	-2.410248	-1.214754	-0.789572
N	-5.041506	5.405707	5.070182
H	-4.118312	5.738167	4.882226
C	-5.658300	5.744123	6.333700
H	-4.888942	6.133471	6.989071
H	-6.095539	4.871295	6.791254
C	-6.764388	6.791694	6.209783
O	-7.810298	6.680503	6.806277
N	-6.491976	7.831950	5.415786
H	-5.600377	7.910776	4.975696
C	-7.437641	8.938719	5.201742

H	-6.977888	9.611436	4.489175
H	-7.611958	9.479724	6.120432
C	-8.800673	8.534415	4.682785
O	-9.791069	9.104447	5.066729
N	-8.835835	7.546389	3.772404
C	-10.092268	7.121937	3.209379
C	-10.929987	6.249957	4.136488
O	-12.007398	5.854152	3.729266
C	-9.867420	6.401904	1.860625
O	-11.079957	6.338429	1.139119
C	-9.255115	5.015759	2.015190
H	-7.982515	7.141712	3.446454
H	-10.703100	7.995526	3.023360
H	-9.200640	7.024912	1.279211
H	-11.780557	6.166429	1.764307
H	-9.038669	4.594942	1.039850
H	-8.328106	5.042938	2.566355
H	-9.940372	4.350556	2.524124
N	-10.456258	5.965807	5.348047
C	-11.302903	5.322569	6.337304
C	-12.343941	6.267083	6.945964
O	-13.316478	5.802174	7.481217
C	-10.474461	4.700681	7.469339
C	-9.476803	3.616299	7.037939
C	-8.687130	3.140127	8.261023
C	-10.151012	2.434062	6.338097
H	-9.553545	6.284560	5.629687
H	-11.883924	4.561948	5.842119
H	-9.932887	5.490667	7.979045
H	-11.180362	4.285920	8.181983

H	-8.769630	4.051118	6.342279
H	-7.940700	2.402325	7.980096
H	-8.173974	3.968077	8.739364
H	-9.342523	2.685460	9.001295
H	-9.412913	1.679941	6.082584
H	-10.901186	1.971142	6.977240
H	-10.637981	2.725219	5.414616
N	-12.075339	7.588921	6.914073
C	-13.044269	8.545836	7.358486
C	-13.963462	9.038987	6.261640
H	-14.736248	9.737014	6.603628
O	-13.879623	8.735855	5.118199
H	-11.334800	7.927312	6.339070
H	-13.647074	8.109472	8.143917
H	-12.541807	9.412364	7.780728
N	-11.774269	10.301570	-2.867425
H	-11.550479	10.511687	-1.915085
C	-12.057381	8.873136	-3.031538
C	-11.637701	8.561088	-4.461752
O	-10.573975	8.047280	-4.711819
C	-13.477255	8.411683	-2.638576
C	-13.738860	8.720923	-1.152848
C	-13.669542	6.921041	-2.946100
C	-15.150582	8.382236	-0.670443
H	-12.569189	10.862537	-3.109816
H	-11.346835	8.335175	-2.419433
H	-14.202226	8.982667	-3.223557
H	-13.012665	8.183499	-0.547093
H	-13.568194	9.778381	-0.975725
H	-14.695271	6.617766	-2.780854

H	-13.428081	6.677733	-3.976698
H	-13.037964	6.313969	-2.305421
H	-15.290557	8.734224	0.345229
H	-15.905575	8.856387	-1.292304
H	-15.336959	7.314989	-0.667488
N	-12.454351	8.971177	-5.463497
H	-13.386990	9.230152	-5.234506
C	-12.203840	8.540113	-6.822271
H	-12.239052	7.462990	-6.914349
H	-12.972240	8.963496	-7.457590
C	-10.843941	8.968308	-7.379885
O	-10.218054	8.251090	-8.106106
N	-10.441202	10.224953	-7.045037
H	-11.000653	10.735764	-6.401013
C	-9.186693	10.805485	-7.496849
H	-9.082878	10.689732	-8.564582
H	-9.192905	11.859428	-7.251726
C	-7.950004	10.154849	-6.859773
O	-7.030748	9.742790	-7.510898
N	-7.924642	10.148202	-5.491991
H	-8.750879	10.403576	-4.999946
C	-6.746635	9.782074	-4.713273
H	-5.864645	10.225397	-5.147240
H	-6.874295	10.170116	-3.710183
C	-6.476702	8.292089	-4.610371
O	-5.330600	7.909733	-4.664048
N	-7.492467	7.436523	-4.399787
C	-7.153435	6.077348	-3.999693
C	-6.570537	5.265334	-5.149732
O	-5.743984	4.414192	-4.923375

C	-8.275357	5.318294	-3.252192
C	-9.452254	4.883170	-4.142003
C	-8.705067	6.123713	-2.020850
C	-10.516487	4.070834	-3.400982
H	-8.439857	7.756500	-4.382877
H	-6.326213	6.147364	-3.309479
H	-7.789055	4.415569	-2.893135
H	-9.915572	5.746170	-4.604973
H	-9.065322	4.267012	-4.949600
H	-9.336642	5.531938	-1.373288
H	-7.842089	6.427344	-1.436729
H	-9.259547	7.013582	-2.296123
H	-11.254875	3.692881	-4.100414
H	-10.083257	3.214659	-2.897101
H	-11.040818	4.667261	-2.664049
N	-6.998006	5.503105	-6.407942
C	-6.362224	4.816119	-7.512847
C	-4.962937	5.348416	-7.824774
O	-4.110131	4.591822	-8.224643
C	-7.258994	4.807640	-8.759840
C	-8.375610	3.758623	-8.670076
C	-7.828880	2.341058	-8.860548
N	-8.821775	1.285910	-8.671057
C	-9.140480	0.701623	-7.518305
N	-8.653572	1.117996	-6.365612
N	-9.980252	-0.325030	-7.514862
H	-7.655215	6.233623	-6.576107
H	-6.167801	3.806302	-7.192415
H	-7.691418	5.791967	-8.909186
H	-6.641402	4.606136	-9.629449

H	-8.889923	3.841983	-7.717773
H	-9.118264	3.951122	-9.436925
H	-7.456656	2.226713	-9.869675
H	-6.987218	2.139202	-8.211451
H	-9.195402	0.868814	-9.493519
H	-8.081304	1.928561	-6.314791
H	-9.071247	0.799664	-5.496124
H	-10.263431	-0.722632	-8.382475
H	-9.927012	-0.971018	-6.738523
N	-4.754067	6.653678	-7.639028
H	-5.497497	7.241151	-7.336808
C	-3.458658	7.285624	-7.930073
H	-3.131748	7.045217	-8.929764
H	-3.589236	8.356009	-7.845070
C	-2.379194	6.827494	-6.960669
O	-1.247966	6.625809	-7.326991
N	-2.790477	6.693948	-5.694638
C	-1.893827	6.400219	-4.603203
C	-1.572135	4.921459	-4.490809
O	-0.430339	4.569941	-4.297964
C	-2.493377	6.963548	-3.308186
C	-1.882206	6.271030	-2.091065
C	-2.303139	8.486730	-3.327439
H	-3.721010	6.968701	-5.464970
H	-0.939124	6.870919	-4.789568
H	-3.555952	6.750370	-3.321073
H	-2.113193	6.798492	-1.184326
H	-2.261283	5.259152	-1.992765
H	-0.808109	6.233310	-2.164805
H	-3.049481	8.984000	-2.724442

H	-1.319034	8.756132	-2.958611
H	-2.409773	8.878835	-4.332153
N	-2.575259	4.037305	-4.605964
C	-2.222951	2.639263	-4.694383
C	-1.324197	2.410477	-5.902598
O	-0.418234	1.611602	-5.856302
C	-3.442005	1.700715	-4.705460
C	-4.272908	1.753024	-3.415302
C	-5.392390	0.695236	-3.355790
N	-4.964371	-0.487506	-2.638029
C	-5.736553	-1.483163	-2.534551
N	-7.015059	-1.592161	-3.091903
N	-5.426364	-2.549541	-1.735825
H	-3.511859	4.333369	-4.781694
H	-1.608930	2.380591	-3.844315
H	-4.073469	1.938191	-5.559538
H	-3.068722	0.693524	-4.856035
H	-3.627602	1.600034	-2.559519
H	-4.713334	2.737240	-3.320084
H	-6.258872	1.141773	-2.868512
H	-5.707339	0.465385	-4.378258
H	-7.156105	-1.056987	-3.921307
H	-7.328802	-2.535277	-3.219982
H	-4.495864	-2.589562	-1.369950
H	-5.831305	-3.430454	-1.968264
N	-1.546899	3.166383	-6.996490
H	-2.384008	3.695807	-7.104179
C	-0.684621	2.988588	-8.146855
H	-1.048786	3.629593	-8.939611
H	-0.677718	1.965414	-8.494111

C	0.761414	3.366436	-7.833196
O	1.704631	2.751445	-8.266111
N	0.886570	4.434447	-7.030068
H	0.077947	4.970822	-6.811251
C	2.150711	4.947380	-6.607804
H	2.774349	5.237305	-7.444073
H	1.969938	5.828493	-6.005802
C	2.988861	4.006517	-5.765766
O	4.192980	4.151955	-5.695960
N	2.354379	3.042206	-5.086466
C	3.081572	2.233818	-4.149153
C	4.274256	1.480442	-4.743854
O	5.224074	1.228848	-4.027510
C	2.091308	1.277985	-3.483307
C	2.701082	0.445943	-2.366101
C	1.630090	-0.376493	-1.677118
N	2.267514	-1.276559	-0.727735
C	1.605599	-2.275340	-0.135155
N	0.319277	-2.373148	-0.211845
N	2.349633	-3.204568	0.493186
H	1.359993	2.965328	-5.140961
H	3.535366	2.865429	-3.394631
H	1.287387	1.888614	-3.085004
H	1.642934	0.639218	-4.236031
H	3.460178	-0.218313	-2.766251
H	3.194403	1.086214	-1.640124
H	0.929690	0.260970	-1.154057
H	1.071727	-0.947326	-2.412459
H	3.242728	-1.428775	-0.853500
H	-0.224512	-1.676438	-0.678853

H	-0.238034	-3.061896	0.324159
H	3.185036	-2.867870	0.917627
H	1.859640	-3.863432	1.066685
N	4.255160	1.062184	-6.017655
H	3.495761	1.315850	-6.616364
C	5.356056	0.264885	-6.527831
H	5.134253	0.006589	-7.555780
H	5.460038	-0.651013	-5.967442
C	6.711559	0.940334	-6.498776
O	7.730666	0.298281	-6.395134
N	6.706442	2.270224	-6.621776
H	5.839990	2.768362	-6.583816
C	7.927348	3.039685	-6.568360
H	8.635467	2.679711	-7.301300
H	7.693344	4.066636	-6.815194
C	8.681407	3.052067	-5.236507
O	9.813889	3.485641	-5.192020
N	8.055645	2.544411	-4.166993
C	8.650716	2.387740	-2.850913
C	9.934176	1.546812	-2.871461
O	10.756469	1.643148	-1.974849
C	7.568167	1.691852	-1.995590
C	7.779636	1.560365	-0.487081
C	7.404784	2.811082	0.317200
C	7.314321	2.526708	1.812828
N	8.659764	2.532590	2.459248
O	11.041439	1.863703	0.850900
H	10.883284	2.079267	-0.068494
H	11.538746	1.048805	0.791572
H	7.115177	2.222033	-4.274544

H	8.931345	3.349542	-2.442288
H	6.639722	2.219138	-2.168699
H	7.417572	0.704827	-2.417773
H	7.125707	0.758072	-0.158624
H	8.786470	1.234814	-0.261518
H	8.091564	3.634946	0.144614
H	6.426425	3.156445	-0.001087
H	6.732013	3.275340	2.327000
H	6.865679	1.563523	2.002905
H	9.380389	2.094429	1.894021
H	8.951158	3.512073	2.617746
H	8.627893	2.047850	3.343990
N	10.058650	0.696606	-3.881387
C	11.129472	-0.259667	-4.125770
C	12.489143	0.339165	-4.489112
O	13.465331	-0.366932	-4.376726
C	10.735989	-1.171172	-5.309690
C	9.624889	-2.198394	-5.049916
C	9.198826	-2.829031	-6.379392
C	10.086508	-3.281167	-4.074183
H	9.318266	0.683740	-4.552079
H	11.306775	-0.846992	-3.236697
H	10.447111	-0.529551	-6.136758
H	11.630117	-1.700232	-5.616872
H	8.758645	-1.689694	-4.637881
H	8.416909	-3.565845	-6.221833
H	8.817637	-2.078794	-7.060355
H	10.035197	-3.334490	-6.855692
H	9.317612	-4.033170	-3.933316
H	10.968253	-3.782358	-4.459495

H	10.334401	-2.881562	-3.095488
N	12.542524	1.584484	-4.968577
C	13.765787	2.202097	-5.444716
C	14.910696	2.409630	-4.434670
O	15.954544	2.815639	-4.870377
C	13.411961	3.526644	-6.124218
O	12.813856	4.419940	-5.228417
H	11.710868	2.135565	-4.957977
H	14.211829	1.552525	-6.188459
H	14.322623	3.972013	-6.493133
H	12.762343	3.324321	-6.969834
H	11.866893	4.390685	-5.292755
N	14.757554	2.087271	-3.130783
C	15.898589	2.034411	-2.238236
C	16.805271	0.821235	-2.476649
O	17.935779	0.830173	-2.063942
C	15.472907	1.943926	-0.767740
C	14.595386	3.079522	-0.245368
C	14.258499	2.817660	1.223026
N	13.216154	3.685176	1.757003
C	13.370553	4.832917	2.397392
N	14.577967	5.334231	2.632910
O	14.887347	7.785931	4.204727
H	14.578776	8.665622	3.971311
H	15.604143	7.908461	4.814163
N	12.306995	5.491581	2.807899
H	13.873120	1.768387	-2.811523
H	16.510192	2.908101	-2.403639
H	14.952133	1.003743	-0.617587
H	16.388419	1.888623	-0.189083

H	15.091918	4.038693	-0.360045
H	13.670505	3.144588	-0.806631
H	13.886981	1.808507	1.328228
H	15.141340	2.878477	1.848384
H	12.282184	3.369420	1.588875
H	15.395644	4.865869	2.322748
H	14.695290	6.187779	3.151491
H	11.357379	5.190863	2.652281
H	12.383061	6.331278	3.336222
N	16.227348	-0.247290	-3.050912
C	16.929294	-1.490185	-3.266240
C	17.718560	-1.436230	-4.570917
H	18.090134	-0.445400	-4.841683
O	17.940201	-2.387623	-5.246250
C	15.957168	-2.674677	-3.251207
C	15.430677	-3.029401	-1.893381
N	14.492872	-2.287890	-1.202385
O	12.530502	-0.160862	-0.526063
H	13.189211	-0.736126	-0.919235
H	12.046009	0.237110	-1.241214
C	15.759939	-4.117039	-1.161279
C	14.285604	-2.926542	-0.097458
N	15.027110	-4.037674	-0.003582
H	15.309545	-0.168152	-3.433238
H	17.662417	-1.596689	-2.474392
H	15.130048	-2.462611	-3.919868
H	16.477984	-3.531995	-3.655863
H	16.436989	-4.920770	-1.356654
H	13.603393	-2.621376	0.670151
H	14.950024	-4.728121	0.710725

O	-14.438086	-2.383573	5.091980
H	-14.767973	-1.787825	4.422158
H	-14.099199	-1.827430	5.786474
O	-12.890300	-0.584917	6.951697
H	-12.132422	-1.045627	7.292992
H	-13.246819	-0.080253	7.672366
O	-12.135746	0.209585	4.158463
H	-12.314066	0.221434	5.092147
H	-12.957235	-0.047264	3.739165
O	-12.837848	-2.314602	1.292744
H	-12.098380	-1.737748	1.093041
H	-12.582524	-2.869011	2.028398
O	-7.036657	1.814962	-0.038654
H	-7.225215	1.880872	0.900906
H	-6.141776	1.502057	-0.098539
O	-7.717176	1.874269	2.715620
H	-8.670871	1.824102	2.688340
H	-7.496990	2.582716	3.315511
O	-8.793847	0.063963	-1.356228
H	-8.229756	0.699752	-0.902017
H	-8.202043	-0.592126	-1.723694
O	-13.028528	-2.718408	-1.533118
H	-13.194345	-2.680124	-0.593613
H	-12.154913	-3.082244	-1.625007
O	-13.061449	1.290371	-0.778209
H	-12.441591	0.650155	-0.422362
H	-12.639838	2.134677	-0.618408
O	-14.098216	4.428300	2.099492
H	-13.767483	4.776763	2.922080
H	-14.582774	3.631437	2.285102

O	-15.111912	1.660826	1.203236
H	-15.948448	1.770159	0.769981
H	-14.468988	1.521245	0.502477
O	-12.668751	-0.443425	-3.150057
H	-12.982382	0.332983	-2.692212
H	-12.818264	-1.162455	-2.528201
O	-12.299681	-2.511599	-5.076945
H	-12.624584	-1.709556	-4.666812
H	-13.058730	-3.041389	-5.287997
O	-10.592271	-3.361633	-2.937916
H	-9.930690	-2.692983	-3.079320
H	-11.253597	-3.197991	-3.610429
O	-11.005167	-0.364898	0.396741
H	-10.270494	-0.380491	-0.219277
H	-10.747130	0.248030	1.089289
O	-10.582475	1.634128	2.322356
H	-11.130577	1.312913	3.041652
H	-11.058205	2.324770	1.862869
O	-11.974884	3.550962	0.543654
H	-12.747957	3.850999	1.031936
H	-11.464680	4.343137	0.405926
O	-9.971490	0.540979	-3.903732
H	-10.851526	0.198577	-3.758063
H	-9.549248	0.514014	-3.044481
O	-14.525230	-0.619052	2.842211
H	-14.890310	0.126340	2.366871
H	-14.119313	-1.189423	2.188264
O	-12.385611	-3.733866	3.807224
H	-13.142009	-3.345255	4.266564
H	-11.623186	-3.381574	4.250543

O	-9.420324	-2.321268	-5.567122
H	-10.278427	-2.728276	-5.512558
H	-8.803969	-2.991078	-5.871417

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(0),Y266(0),E183(0)

POTENTIAL:mV

N	15.580942	-6.451471	5.391415
H	14.780479	-6.201511	5.939215
C	15.509435	-5.856447	4.054287
C	14.783016	-6.782958	3.060460
O	14.052429	-6.345779	2.186689
C	16.919450	-5.576363	3.520804
H	16.389532	-6.127655	5.884604
H	14.944632	-4.933596	4.050480
H	16.888621	-5.189909	2.509075
H	17.403352	-4.831448	4.142312
H	17.526880	-6.474634	3.529458
N	15.032384	-8.085605	3.186393
H	15.612145	-8.361766	3.949651
C	14.398655	-9.092385	2.333235
H	14.482424	-8.823789	1.292862
H	14.891358	-10.042266	2.492764
C	12.912790	-9.220804	2.671360
O	12.081437	-9.424628	1.825872
N	12.582805	-9.055889	3.966871
H	13.302707	-8.986601	4.648937
C	11.195100	-9.170804	4.421405
H	11.188266	-9.157888	5.503158

H	10.743721	-10.088321	4.077202
C	10.336963	-8.010603	3.900697
O	9.190766	-8.186036	3.584551
N	10.947138	-6.814584	3.855238
C	10.318531	-5.634101	3.317471
C	10.126974	-5.691219	1.799240
O	9.096466	-5.262968	1.337009
C	11.092846	-4.388030	3.776178
O	12.478788	-4.570848	3.769250
H	11.905504	-6.744284	4.106854
H	9.314641	-5.553287	3.701015
H	10.801417	-3.539736	3.167069
H	10.827334	-4.174335	4.801180
H	12.805733	-4.755148	2.897195
N	11.100353	-6.200682	1.024103
C	10.845034	-6.397096	-0.400261
C	9.694185	-7.385714	-0.601587
O	8.946438	-7.280155	-1.545785
C	12.133522	-6.786225	-1.186799
C	12.333825	-8.291648	-1.403956
C	12.161035	-6.060793	-2.533486
H	11.924441	-6.586132	1.431466
H	10.475519	-5.462799	-0.791815
H	12.965563	-6.416658	-0.597953
H	13.287629	-8.455103	-1.894858
H	12.331845	-8.858100	-0.483496
H	11.566654	-8.698326	-2.055702
H	13.055861	-6.324799	-3.086002
H	11.300786	-6.332239	-3.135504
H	12.161253	-4.985603	-2.400022

N	9.570408	-8.340330	0.328361
H	10.314554	-8.474508	0.974296
C	8.593032	-9.421193	0.241195
H	8.935836	-10.219581	0.886993
H	8.532029	-9.802164	-0.766590
C	7.181949	-9.047511	0.645327
O	6.257502	-9.505198	0.014371
N	7.004066	-8.228535	1.688395
C	5.670100	-7.742121	1.958461
C	5.250597	-6.730659	0.897218
O	4.073671	-6.634113	0.621668
C	5.416252	-7.237171	3.392948
C	5.559846	-8.381368	4.401542
C	6.257073	-6.027437	3.805773
H	7.781739	-7.961854	2.252086
H	4.987440	-8.561786	1.796420
H	4.375092	-6.929353	3.386541
H	5.269940	-8.044537	5.391283
H	4.922452	-9.219365	4.138886
H	6.582366	-8.737628	4.456781
H	5.916524	-5.655616	4.766245
H	7.299674	-6.296965	3.912576
H	6.184061	-5.213007	3.093247
N	6.171141	-6.006024	0.253015
C	5.775821	-5.188189	-0.881627
C	5.344902	-6.072718	-2.059952
O	4.321527	-5.821692	-2.652240
C	6.867622	-4.167921	-1.261341
C	7.064018	-3.150665	-0.123252
C	6.496716	-3.458381	-2.568268

C	8.356690	-2.342411	-0.237303
H	7.132427	-6.063826	0.511597
H	4.877378	-4.652001	-0.615495
H	7.798150	-4.708422	-1.408517
H	6.208140	-2.477374	-0.107600
H	7.074268	-3.664218	0.828805
H	7.201530	-2.668254	-2.788286
H	6.497673	-4.133880	-3.413917
H	5.508189	-3.015822	-2.502062
H	8.456989	-1.668587	0.606900
H	9.218939	-2.998846	-0.236964
H	8.392128	-1.742864	-1.139973
N	6.117667	-7.114687	-2.395326
H	7.012122	-7.235793	-1.968905
C	5.776732	-7.955836	-3.522959
H	6.607343	-8.630035	-3.690966
H	5.623352	-7.370778	-4.417476
C	4.507108	-8.783602	-3.322011
O	3.670412	-8.842385	-4.191720
N	4.393861	-9.435378	-2.157989
H	5.130915	-9.392171	-1.486873
C	3.206588	-10.189414	-1.830430
H	2.967436	-10.903132	-2.604468
H	3.396868	-10.730498	-0.911998
C	1.974201	-9.306854	-1.644807
O	0.887577	-9.694694	-2.007244
N	2.187865	-8.107004	-1.107166
C	1.065926	-7.180031	-1.078543
C	0.623280	-6.721154	-2.470727
O	-0.558603	-6.582579	-2.692724

C	1.286930	-5.920607	-0.247529
O	1.414503	-6.167183	1.112812
H	3.087790	-7.818090	-0.797813
H	0.211762	-7.692804	-0.667171
H	2.135110	-5.363953	-0.632026
H	0.397794	-5.326624	-0.378159
H	2.304989	-6.441424	1.286538
N	1.552222	-6.437210	-3.393005
C	1.156378	-6.032032	-4.729704
C	0.385351	-7.153770	-5.418695
O	-0.601544	-6.897828	-6.075722
C	2.369642	-5.538780	-5.551809
C	2.784754	-4.147329	-5.045158
C	2.073800	-5.517412	-7.056823
C	4.115057	-3.649297	-5.608316
H	2.522139	-6.493774	-3.167551
H	0.439087	-5.227080	-4.653887
H	3.186448	-6.233131	-5.378830
H	1.998478	-3.437158	-5.295842
H	2.856259	-4.168626	-3.965333
H	2.933338	-5.151974	-7.604763
H	1.849929	-6.504431	-7.442677
H	1.231979	-4.871320	-7.285177
H	4.414579	-2.735892	-5.105135
H	4.901158	-4.381480	-5.453470
H	4.061695	-3.435596	-6.669960
N	0.823537	-8.405147	-5.255465
H	1.669692	-8.581375	-4.755081
C	0.043375	-9.512147	-5.753635
H	-0.063611	-9.473771	-6.827473

H	0.553342	-10.429288	-5.487588
C	-1.365316	-9.540114	-5.166944
O	-2.319964	-9.767304	-5.874452
N	-1.472594	-9.318871	-3.858013
C	-2.776797	-9.346644	-3.236459
C	-3.690587	-8.211648	-3.700405
O	-4.888661	-8.419507	-3.743653
C	-2.680550	-9.315430	-1.703970
O	-3.925580	-9.579847	-1.118911
H	-0.656813	-9.233311	-3.288688
H	-3.294811	-10.251763	-3.520575
H	-1.999603	-10.088451	-1.375710
H	-2.290578	-8.357443	-1.376562
H	-4.614968	-9.178369	-1.633771
N	-3.140655	-7.031662	-3.981788
C	-3.902769	-5.911621	-4.509797
C	-4.444447	-6.236110	-5.902240
O	-5.608389	-6.045075	-6.172188
C	-3.003095	-4.655420	-4.508645
C	-3.446380	-3.519790	-5.415705
C	-4.768321	-3.093150	-5.495271
C	-2.499073	-2.874260	-6.202304
C	-5.125934	-2.067125	-6.354129
C	-2.850183	-1.834735	-7.048233
C	-4.171537	-1.432443	-7.132354
H	-2.163927	-6.909817	-3.812392
H	-4.770871	-5.740594	-3.893622
H	-2.925229	-4.313042	-3.481049
H	-2.010643	-4.954531	-4.814990
H	-5.527473	-3.578761	-4.912377

H	-1.472579	-3.193931	-6.163025
H	-6.159656	-1.773327	-6.422551
H	-2.096146	-1.352477	-7.643889
H	-4.452436	-0.638994	-7.803045
N	-3.570652	-6.729299	-6.788369
C	-4.012526	-7.071457	-8.120709
C	-5.136406	-8.106133	-8.097629
O	-6.015097	-8.052808	-8.918295
C	-2.862124	-7.602866	-8.979106
S	-1.645366	-6.350795	-9.496697
H	-2.629940	-6.913399	-6.509064
H	-4.438351	-6.201492	-8.597927
H	-2.357426	-8.419574	-8.480780
H	-3.278871	-7.983616	-9.901770
H	-1.045043	-6.180632	-8.329226
N	-5.078532	-9.066905	-7.155631
H	-4.257160	-9.188229	-6.602657
C	-6.085167	-10.116169	-7.180925
H	-6.256477	-10.456664	-8.190310
H	-5.713987	-10.946522	-6.591454
C	-7.459147	-9.722831	-6.613014
O	-8.481320	-10.087395	-7.126865
N	-7.418017	-9.015655	-5.478475
C	-8.641670	-8.655601	-4.788458
C	-9.503017	-7.657777	-5.554102
O	-10.700968	-7.657543	-5.447825
C	-8.362855	-8.115633	-3.374865
C	-7.517860	-6.836014	-3.258320
C	-8.186753	-5.483364	-3.283175
O	-9.487551	-5.484227	-3.352543

H	-9.837256	-4.582248	-3.306502
O	-7.537304	-4.468857	-3.215812
H	-6.535762	-8.773452	-5.079871
H	-9.261405	-9.536031	-4.692017
H	-9.318911	-7.979418	-2.890214
H	-7.839687	-8.900248	-2.838717
H	-6.984941	-6.853282	-2.314174
H	-6.752283	-6.796836	-4.014541
N	-8.837317	-6.734064	-6.273863
C	-9.562353	-5.706192	-6.995284
C	-10.429122	-6.285710	-8.105065
H	-10.447462	-7.368398	-8.211424
O	-11.058251	-5.576097	-8.833344
C	-8.635007	-4.592758	-7.533829
O	-9.429395	-3.468152	-7.883445
C	-7.759880	-4.998445	-8.712315
H	-7.855288	-6.834373	-6.418161
H	-10.250398	-5.232968	-6.304218
H	-8.009309	-4.274530	-6.711386
H	-10.132133	-3.782359	-8.446361
H	-7.080861	-4.185601	-8.946726
H	-7.169989	-5.878957	-8.504625
H	-8.364799	-5.194171	-9.591307
N	-12.952321	-9.022071	3.174379
H	-13.222146	-9.545387	2.367154
C	-11.777508	-8.184389	2.899330
C	-10.788057	-8.138211	4.046012
O	-9.654089	-7.745134	3.846077
C	-12.130679	-6.717804	2.577699
O	-12.657772	-6.188815	3.767602

C	-13.123009	-6.574425	1.429801
H	-13.731297	-8.457322	3.452923
H	-11.232578	-8.601504	2.063676
H	-11.209169	-6.212258	2.322468
H	-12.680856	-5.236061	3.711671
H	-13.268370	-5.522651	1.207567
H	-12.771076	-7.061543	0.527784
H	-14.088587	-6.989138	1.693548
N	-11.197267	-8.533701	5.241859
H	-12.124297	-8.897000	5.283782
C	-10.409179	-8.524195	6.449430
H	-10.331005	-7.527003	6.853274
H	-10.928917	-9.129397	7.182851
C	-8.972216	-9.040204	6.371429
O	-8.135522	-8.471439	7.028538
N	-8.657864	-10.121159	5.634789
H	-9.368751	-10.601812	5.131275
C	-7.269066	-10.552649	5.533214
H	-7.251942	-11.532377	5.073068
H	-6.828289	-10.630327	6.514174
C	-6.387526	-9.608322	4.692701
O	-5.219513	-9.466974	4.948500
N	-7.045373	-9.017976	3.701159
C	-6.304936	-8.012553	2.952685
C	-6.268136	-6.697733	3.725430
O	-5.276217	-6.007839	3.677062
C	-6.623050	-7.894358	1.449040
C	-7.795906	-7.059156	0.980215
C	-7.766186	-5.671085	1.083039
C	-8.866659	-7.649456	0.322003

C	-8.788086	-4.896873	0.560016
C	-9.880568	-6.876670	-0.221238
C	-9.849027	-5.497956	-0.097356
H	-8.039864	-9.019892	3.675724
H	-5.281581	-8.342668	2.985222
H	-5.724586	-7.489365	0.996656
H	-6.714094	-8.906804	1.073831
H	-6.926224	-5.186208	1.546229
H	-8.892439	-8.718846	0.200032
H	-8.738598	-3.825486	0.637859
H	-10.679453	-7.347689	-0.764169
H	-10.627349	-4.898939	-0.533061
N	-7.302432	-6.389941	4.510455
C	-7.241876	-5.272633	5.420616
C	-6.127028	-5.479086	6.445287
O	-5.497120	-4.519354	6.836475
C	-8.622432	-5.098381	6.088825
C	-8.872758	-3.754050	6.737521
C	-9.064858	-2.621777	5.950879
C	-8.980392	-3.631623	8.116053
C	-9.345681	-1.395909	6.527569
C	-9.269866	-2.406899	8.700123
C	-9.450149	-1.284429	7.908656
H	-8.162406	-6.883368	4.408389
H	-6.972227	-4.370832	4.889855
H	-9.367772	-5.249049	5.314885
H	-8.757597	-5.887147	6.816788
H	-8.996785	-2.697078	4.879017
H	-8.840090	-4.495318	8.742128
H	-9.481069	-0.533084	5.901567

H	-9.342478	-2.330740	9.770197
H	-9.648834	-0.328309	8.360311
N	-5.873230	-6.714979	6.870111
H	-6.521864	-7.441240	6.663048
C	-4.799079	-7.005524	7.793367
H	-4.839922	-6.373376	8.667599
H	-4.911843	-8.034232	8.110938
C	-3.402203	-6.831989	7.199980
O	-2.527231	-6.342434	7.874409
N	-3.202368	-7.252154	5.946254
C	-1.926484	-7.066532	5.272865
C	-1.685057	-5.591986	4.920271
O	-0.587038	-5.103739	5.087820
C	-1.845247	-7.995910	4.041724
C	-0.684044	-7.630164	3.115619
C	-1.736978	-9.457662	4.490480
H	-3.935846	-7.731711	5.470360
H	-1.130903	-7.313510	5.960817
H	-2.767910	-7.872757	3.479479
H	-0.619196	-8.353490	2.309793
H	-0.800420	-6.654424	2.665166
H	0.262242	-7.639889	3.647725
H	-1.751175	-10.114617	3.626812
H	-0.800585	-9.623373	5.017337
H	-2.550182	-9.753032	5.140610
N	-2.723927	-4.903732	4.437466
C	-2.597893	-3.516499	4.035543
C	-2.446034	-2.619079	5.261650
O	-1.559470	-1.794995	5.313931
C	-3.790408	-3.045701	3.189295

C	-4.037981	-3.782445	1.862420
C	-2.904492	-3.687105	0.855819
O	-1.795440	-4.103132	1.227785
O	-3.154514	-3.213727	-0.265368
H	-3.585464	-5.375494	4.270725
H	-1.693303	-3.396975	3.469887
H	-4.695986	-3.115585	3.784333
H	-3.635064	-1.989098	2.988351
H	-4.209536	-4.830885	2.054288
H	-4.937934	-3.375541	1.415391
N	-3.328777	-2.774748	6.264400
C	-3.116859	-2.037315	7.484959
C	-1.791667	-2.427115	8.149577
O	-1.125609	-1.586204	8.713719
C	-4.245943	-2.040807	8.526022
O	-4.452008	-3.295287	9.104614
C	-5.530736	-1.412400	7.998357
H	-4.008785	-3.501260	6.228593
H	-2.972317	-1.002434	7.215561
H	-3.869434	-1.417281	9.327417
H	-4.908584	-3.852181	8.485616
H	-6.261222	-1.373425	8.797095
H	-5.347553	-0.399450	7.653245
H	-5.953407	-1.981174	7.180933
N	-1.380408	-3.700466	8.043355
H	-2.027708	-4.421554	7.811933
C	-0.184091	-4.103747	8.736407
H	-0.230724	-3.886177	9.794168
H	-0.071074	-5.171591	8.602276
C	1.063838	-3.415919	8.208175

O	1.943307	-3.068518	8.963123
N	1.148181	-3.258361	6.871275
C	2.325631	-2.662470	6.301979
C	2.289707	-1.139358	6.162426
O	3.359923	-0.576622	6.026584
C	2.805207	-3.337765	5.017039
S	1.888426	-2.938262	3.504732
H	0.413889	-3.611959	6.290052
H	3.116264	-2.811866	7.021712
H	3.817303	-3.008412	4.830443
H	2.817064	-4.409033	5.162202
H	0.819662	-3.695520	3.703153
N	1.139734	-0.470510	6.273420
C	1.204805	0.968264	6.492091
C	1.755965	1.271304	7.871007
O	2.368723	2.288945	8.086022
C	-0.095215	1.740145	6.181627
C	-1.202794	1.552827	7.228616
C	-0.544654	1.447358	4.745150
C	-2.470463	2.358748	6.937163
H	0.270186	-0.963421	6.287491
H	1.952683	1.350982	5.815981
H	0.205170	2.781457	6.231659
H	-1.452823	0.506505	7.328410
H	-0.820147	1.863386	8.196292
H	-1.301520	2.153743	4.427573
H	0.291333	1.536440	4.056705
H	-0.951844	0.450705	4.642208
H	-3.144870	2.318451	7.787086
H	-2.244335	3.404566	6.744903

H	-3.006485	1.971194	6.077663
N	1.549780	0.323275	8.791255
H	0.890658	-0.402710	8.612969
C	1.977859	0.512213	10.160290
H	1.469235	-0.223036	10.770952
H	1.737340	1.501890	10.518399
C	3.481799	0.336565	10.305798
O	4.163615	1.126810	10.899127
N	3.999641	-0.753619	9.694705
H	3.390695	-1.463403	9.345242
C	5.424653	-0.938721	9.667238
H	5.638022	-1.909234	9.234361
H	5.854686	-0.904700	10.657563
C	6.156890	0.119123	8.844832
O	7.292087	0.411119	9.129513
N	5.502074	0.621268	7.799018
C	6.105378	1.756770	7.150115
C	5.525641	3.075937	7.654194
H	5.023288	3.036911	8.619393
O	5.649980	4.094244	7.046402
C	6.011878	1.676263	5.624076
C	6.760826	0.506536	5.019756
C	8.126630	0.320636	5.237924
C	6.097432	-0.401574	4.200043
C	8.810266	-0.726233	4.634553
C	6.778853	-1.446088	3.595216
C	8.139103	-1.608939	3.802541
H	4.574672	0.337152	7.571829
H	7.140254	1.766956	7.456616
H	4.969867	1.616766	5.335682

H	6.394472	2.610041	5.226532
H	8.656907	0.976659	5.906885
H	5.037127	-0.304115	4.063932
H	9.861208	-0.854931	4.828272
H	6.244460	-2.137561	2.968384
H	8.657307	-2.422587	3.328959
N	12.613548	9.596235	-1.248797
H	11.873073	9.914179	-1.845810
C	12.304855	8.264733	-0.719494
C	11.274028	8.450598	0.386818
O	10.265751	7.778972	0.416160
C	13.562725	7.581082	-0.165205
C	14.645173	7.276181	-1.206308
S	14.017431	6.202019	-2.529609
C	15.500221	6.053543	-3.554886
H	13.433195	9.572927	-1.822563
H	11.834545	7.616477	-1.447377
H	14.001191	8.205558	0.607330
H	13.255689	6.653907	0.304954
H	15.045510	8.188653	-1.633679
H	15.470345	6.783887	-0.704191
H	15.249053	5.398756	-4.375389
H	15.799178	7.017593	-3.945666
H	16.318592	5.616834	-2.997477
N	11.504154	9.412695	1.297047
C	10.594052	9.607451	2.408568
C	9.276854	10.274549	2.010327
O	8.280717	10.052953	2.652477
C	11.275896	10.368514	3.552323
C	12.447318	9.563602	4.084891

O	13.582290	9.825107	3.745252
N	12.143320	8.561357	4.919198
H	12.327994	9.967518	1.206545
H	10.295156	8.637352	2.771082
H	11.657172	11.325715	3.219399
H	10.545575	10.537170	4.333596
H	12.886915	7.965736	5.213588
H	11.221689	8.175412	4.954942
N	9.263775	11.067655	0.922390
H	10.110811	11.229659	0.427571
C	8.003507	11.517472	0.368847
H	8.201320	12.260188	-0.393384
H	7.389092	11.966751	1.131867
C	7.186380	10.384432	-0.254307
O	5.986305	10.470120	-0.291584
N	7.862638	9.333265	-0.763205
C	7.170367	8.145651	-1.233959
C	6.634520	7.300821	-0.067416
O	5.534028	6.808746	-0.148451
C	8.048860	7.344203	-2.224163
C	8.343758	8.197099	-3.472847
C	7.379302	6.019178	-2.608086
C	9.428431	7.624913	-4.388803
H	8.823805	9.230641	-0.536565
H	6.279740	8.471836	-1.748518
H	8.987847	7.117705	-1.727184
H	7.421907	8.323173	-4.036275
H	8.645895	9.192725	-3.165352
H	7.996709	5.478750	-3.314220
H	7.228034	5.377937	-1.748260

H	6.409672	6.182905	-3.066700
H	9.622568	8.305455	-5.211433
H	10.363692	7.479321	-3.855031
H	9.148543	6.670865	-4.819945
N	7.387113	7.175020	1.043841
C	6.878130	6.458284	2.201865
C	5.527274	7.040164	2.639452
O	4.574360	6.334191	2.866542
C	7.832261	6.545612	3.403471
C	9.253675	5.996725	3.243850
O	10.145147	6.631019	3.801318
O	9.427075	4.934907	2.595110
H	8.347195	7.444671	1.022750
H	6.681020	5.429582	1.943173
H	7.920449	7.570104	3.733357
H	7.374114	5.991983	4.220501
N	5.489857	8.378108	2.785881
H	6.321223	8.912873	2.648924
C	4.299553	9.047240	3.249676
H	4.538928	10.091629	3.406586
H	3.957729	8.640894	4.188486
C	3.136800	8.988549	2.268521
O	1.995347	9.111078	2.649457
N	3.470143	8.825044	0.985192
H	4.431256	8.829047	0.735185
C	2.517174	8.905264	-0.078282
H	3.059647	9.091911	-0.996340
H	1.843672	9.737837	0.071976
C	1.609145	7.687007	-0.310220
O	0.563844	7.814918	-0.883302

N	2.090551	6.538698	0.206399
C	1.283461	5.366493	0.435216
C	0.467909	5.480602	1.727559
O	-0.727375	5.301066	1.700446
C	2.156825	4.112013	0.446620
H	2.996944	6.575258	0.622557
H	0.552025	5.295917	-0.352648
H	1.554542	3.234765	0.657298
H	2.625134	3.991727	-0.523375
H	2.937416	4.180555	1.197084
N	1.100153	5.752901	2.883514
C	0.363855	5.588889	4.128797
C	-0.756499	6.616005	4.277630
O	-1.793405	6.307721	4.825433
C	1.276925	5.517244	5.377594
C	1.869158	6.863261	5.822215
C	2.363409	4.450295	5.174675
C	2.702750	6.768435	7.102599
H	2.087537	5.892449	2.903121
H	-0.160444	4.645841	4.073045
H	0.616881	5.179865	6.171099
H	2.477873	7.271798	5.022356
H	1.065866	7.573300	5.990218
H	2.734254	4.098677	6.126275
H	1.969468	3.592745	4.638542
H	3.205721	4.838364	4.612320
H	3.008373	7.759737	7.424027
H	2.126664	6.325645	7.909712
H	3.597555	6.172743	6.971574
N	-0.542379	7.851102	3.802898

H	0.342671	8.093786	3.408281
C	-1.514248	8.891015	4.018121
H	-1.105089	9.819419	3.640139
H	-1.725162	9.021732	5.069675
C	-2.867021	8.618723	3.365915
O	-3.871201	8.835194	4.003704
N	-2.902653	8.109029	2.120712
C	-4.238304	8.007140	1.534087
C	-4.968813	6.730657	1.912238
O	-6.180395	6.724062	1.899541
C	-4.023360	8.231437	0.030870
C	-2.767508	9.109534	0.024558
C	-1.907940	8.459272	1.096327
H	-4.860614	8.797324	1.924965
H	-3.845773	7.294410	-0.480499
H	-4.888841	8.699932	-0.419823
H	-2.258022	9.157414	-0.919586
H	-3.027490	10.122568	0.322266
H	-1.423282	7.569977	0.735735
H	-1.149998	9.118592	1.486782
N	-4.242062	5.660723	2.268993
C	-4.898274	4.489751	2.822160
C	-5.601877	4.809738	4.143779
O	-6.682132	4.319340	4.387400
C	-3.922450	3.315696	3.044939
C	-3.602503	2.490692	1.814569
C	-4.319708	1.332976	1.526721
C	-2.563174	2.838102	0.963972
C	-4.010612	0.545503	0.427976
C	-2.253167	2.067810	-0.142660

C	-2.971075	0.916975	-0.417876
O	-2.631644	0.190555	-1.507482
H	-3.433245	-0.132650	-1.959688
H	-3.248636	5.746562	2.321847
H	-5.684950	4.182806	2.150951
H	-3.011371	3.702003	3.489514
H	-4.374445	2.664801	3.784727
H	-5.129104	1.032648	2.170014
H	-1.985680	3.717778	1.156763
H	-4.552287	-0.361740	0.235736
H	-1.460646	2.361894	-0.807782
N	-4.963871	5.610892	5.012293
H	-4.035546	5.925060	4.817543
C	-5.577344	5.988661	6.265812
H	-4.801079	6.365747	6.920127
H	-6.043692	5.137099	6.734369
C	-6.651448	7.065798	6.114413
O	-7.709569	6.987260	6.695029
N	-6.341993	8.091462	5.314137
H	-5.441180	8.148207	4.889102
C	-7.257699	9.220084	5.085090
H	-6.773822	9.881153	4.377801
H	-7.436849	9.765732	5.999939
C	-8.620671	8.834785	4.545740
O	-9.605844	9.430471	4.903626
N	-8.666119	7.828890	3.652672
C	-9.928735	7.427001	3.085873
C	-10.814208	6.631357	4.032647
O	-11.920018	6.304751	3.637635
C	-9.727470	6.646850	1.766838

O	-10.949281	6.583909	1.057384
C	-9.151222	5.252050	1.967219
H	-7.818177	7.408817	3.331702
H	-10.503055	8.315241	2.856243
H	-9.047561	7.228395	1.158214
H	-11.656044	6.539440	1.697476
H	-8.976819	4.784915	1.004375
H	-8.208806	5.278256	2.490847
H	-9.838715	4.627531	2.524461
N	-10.353503	6.328342	5.241144
C	-11.230801	5.723599	6.228936
C	-12.252343	6.706083	6.809021
O	-13.255900	6.278141	7.316874
C	-10.435120	5.093126	7.379532
C	-9.488846	3.950511	6.981945
C	-8.704722	3.491845	8.215332
C	-10.221807	2.767264	6.343005
H	-9.434313	6.600061	5.520595
H	-11.827697	4.972732	5.737374
H	-9.858702	5.870268	7.869945
H	-11.161036	4.730162	8.100289
H	-8.772377	4.325185	6.260399
H	-7.994884	2.710804	7.958003
H	-8.150028	4.315991	8.651707
H	-9.369896	3.098314	8.981175
H	-9.518995	1.971602	6.115290
H	-10.981145	2.365577	7.011897
H	-10.707761	3.037695	5.411874
N	-11.934887	8.016946	6.787785
C	-12.883747	9.001314	7.216481

C	-13.851804	9.433132	6.135411
H	-14.611514	10.147443	6.472740
O	-13.817023	9.067938	5.007695
H	-11.174354	8.331188	6.225258
H	-13.453358	8.617522	8.052914
H	-12.358801	9.887276	7.563048
N	-11.450257	10.622822	-3.030063
H	-11.209401	10.836207	-2.082680
C	-11.805542	9.208255	-3.171992
C	-11.410578	8.856581	-4.599606
O	-10.372866	8.290255	-4.846274
C	-13.244634	8.824411	-2.765598
C	-13.482045	9.162735	-1.282253
C	-13.513530	7.341796	-3.054282
C	-14.912049	8.922018	-0.794870
H	-12.216615	11.220134	-3.277471
H	-11.119531	8.644244	-2.555653
H	-13.943185	9.424308	-3.353434
H	-12.790636	8.583990	-0.673589
H	-13.242353	10.208066	-1.113989
H	-14.550493	7.090409	-2.872697
H	-13.297926	7.076618	-4.085117
H	-12.902994	6.712089	-2.414610
H	-15.024746	9.283026	0.221026
H	-15.634259	9.446908	-1.414658
H	-15.172536	7.870289	-0.791612
N	-12.211998	9.288077	-5.602655
H	-13.130162	9.596732	-5.377231
C	-11.972873	8.843875	-6.959238
H	-12.037085	7.767788	-7.045622

H	-12.729643	9.284213	-7.596911
C	-10.601375	9.232961	-7.517198
O	-9.996310	8.496530	-8.240798
N	-10.162436	10.477354	-7.181606
H	-10.711595	11.008624	-6.545545
C	-8.894348	11.024005	-7.637086
H	-8.790095	10.891080	-8.702745
H	-8.878879	12.081542	-7.407784
C	-7.672362	10.359334	-6.988510
O	-6.752675	9.936618	-7.631252
N	-7.659715	10.350056	-5.619875
H	-8.482644	10.627868	-5.134444
C	-6.495283	9.961236	-4.832291
H	-5.599767	10.376146	-5.266668
H	-6.615421	10.362681	-3.833478
C	-6.266714	8.464815	-4.710673
O	-5.130749	8.052024	-4.722058
N	-7.313248	7.638944	-4.532851
C	-7.014154	6.281817	-4.104237
C	-6.385456	5.453663	-5.218210
O	-5.500989	4.680577	-4.941478
C	-8.169246	5.547930	-3.385353
C	-9.334491	5.136850	-4.300200
C	-8.608671	6.363499	-2.163462
C	-10.433624	4.357136	-3.576042
H	-8.251731	7.983895	-4.545473
H	-6.212394	6.347979	-3.384898
H	-7.712488	4.634768	-3.012760
H	-9.766675	6.006171	-4.779698
H	-8.937059	4.509640	-5.094556

H	-9.268033	5.788314	-1.527947
H	-7.750844	6.646609	-1.561923
H	-9.133340	7.266292	-2.452937
H	-11.164286	3.980870	-4.285180
H	-10.029718	3.505141	-3.040149
H	-10.964625	4.978458	-2.865183
N	-6.821804	5.574681	-6.491828
C	-6.122650	4.837516	-7.526359
C	-4.766933	5.445622	-7.897427
O	-3.900287	4.709945	-8.309122
C	-6.985446	4.553700	-8.764525
C	-8.063468	3.474445	-8.557259
C	-7.485599	2.123282	-8.106835
N	-8.413266	0.992326	-8.200115
C	-9.246595	0.580570	-7.239923
N	-9.565574	1.404866	-6.254236
N	-9.750218	-0.632824	-7.273985
H	-7.500345	6.268083	-6.723064
H	-5.828110	3.900653	-7.087703
H	-7.460724	5.467152	-9.109803
H	-6.316866	4.232021	-9.555641
H	-8.808023	3.827661	-7.849474
H	-8.583770	3.331754	-9.498531
H	-6.639228	1.867242	-8.730931
H	-7.117893	2.168777	-7.090395
H	-8.305494	0.376873	-8.975587
H	-9.343070	2.370149	-6.313647
H	-10.096875	1.113067	-5.449591
H	-9.353943	-1.381802	-7.810369
H	-10.478063	-0.911624	-6.634207

N	-4.571397	6.757500	-7.722194
H	-5.311839	7.353646	-7.430197
C	-3.257798	7.352383	-8.011132
H	-2.933328	7.094293	-9.006716
H	-3.359263	8.427000	-7.936787
C	-2.193925	6.877266	-7.033153
O	-1.066831	6.644365	-7.393204
N	-2.610444	6.768791	-5.766313
C	-1.723879	6.459944	-4.670821
C	-1.446884	4.973443	-4.542387
O	-0.318980	4.587434	-4.335975
C	-2.308725	7.054951	-3.383215
C	-1.727750	6.351465	-2.157691
C	-2.065842	8.570665	-3.416545
H	-3.535779	7.063300	-5.540733
H	-0.755531	6.900104	-4.861077
H	-3.377571	6.877876	-3.399277
H	-1.942860	6.894108	-1.256264
H	-2.144386	5.355004	-2.053182
H	-0.655538	6.273649	-2.226193
H	-2.801574	9.100883	-2.828668
H	-1.077337	8.810805	-3.039524
H	-2.147406	8.954165	-4.426999
N	-2.476495	4.120597	-4.661333
C	-2.166304	2.713538	-4.735604
C	-1.263088	2.445083	-5.932189
O	-0.390986	1.610467	-5.875037
C	-3.409265	1.801838	-4.796464
C	-4.384645	1.957318	-3.620059
C	-5.461595	0.858245	-3.551953

N	-5.024496	-0.309681	-2.806600
C	-5.834253	-1.285002	-2.637217
N	-7.120260	-1.337914	-3.162348
N	-5.545493	-2.328910	-1.829167
H	-3.402222	4.448079	-4.837172
H	-1.584944	2.432904	-3.869959
H	-3.941466	1.981175	-5.729108
H	-3.042275	0.782435	-4.840131
H	-3.838600	1.977226	-2.688909
H	-4.885377	2.909031	-3.704561
H	-6.351110	1.287881	-3.090705
H	-5.745251	0.597613	-4.575295
H	-7.226831	-0.855575	-4.027498
H	-7.521314	-2.257482	-3.202541
H	-4.636504	-2.422368	-1.418150
H	-6.040973	-3.182962	-1.968369
N	-1.459772	3.193335	-7.035054
H	-2.267073	3.766053	-7.144654
C	-0.596025	2.984495	-8.179304
H	-0.940339	3.627838	-8.978877
H	-0.614408	1.958680	-8.517967
C	0.858091	3.326704	-7.861354
O	1.786002	2.683366	-8.284673
N	1.007247	4.396226	-7.063566
H	0.213454	4.960291	-6.860760
C	2.282316	4.880650	-6.640295
H	2.918451	5.142291	-7.476484
H	2.122218	5.774110	-6.050950
C	3.094585	3.926538	-5.779514
O	4.300619	4.045709	-5.700965

N	2.428034	2.983354	-5.101941
C	3.098463	2.130525	-4.156529
C	4.281958	1.344186	-4.723576
O	5.201586	1.054233	-3.984871
C	2.026251	1.207917	-3.579545
C	2.417358	0.331843	-2.395340
C	1.121318	-0.252054	-1.856988
N	1.333465	-1.247445	-0.825635
C	0.341907	-2.073104	-0.445731
N	-0.814703	-2.039920	-1.064747
N	0.558570	-2.942123	0.514014
H	1.433644	2.939389	-5.176189
H	3.540141	2.726312	-3.366558
H	1.214753	1.858392	-3.271114
H	1.624538	0.593943	-4.377136
H	3.092421	-0.463484	-2.691511
H	2.922225	0.917788	-1.630589
H	0.483874	0.548064	-1.492865
H	0.600009	-0.735144	-2.671209
H	2.042994	-1.075112	-0.148596
H	-1.141136	-1.193131	-1.482368
H	-1.575371	-2.653224	-0.776534
H	1.472959	-3.119916	0.859965
H	-0.227421	-3.495280	0.850676
N	4.281635	0.945291	-6.005325
H	3.540573	1.224875	-6.614868
C	5.363426	0.116658	-6.504603
H	5.139409	-0.143537	-7.531646
H	5.441115	-0.797352	-5.937286
C	6.736239	0.756118	-6.476126

O	7.738555	0.089656	-6.364875
N	6.766121	2.085332	-6.608323
H	5.912181	2.604987	-6.573038
C	8.005506	2.823554	-6.551101
H	8.709856	2.439513	-7.275404
H	7.800297	3.854280	-6.807629
C	8.748820	2.826845	-5.213322
O	9.890039	3.236074	-5.161844
N	8.103915	2.338674	-4.145947
C	8.685626	2.174737	-2.824696
C	9.950262	1.305501	-2.832336
O	10.768881	1.388557	-1.931030
C	7.581575	1.507829	-1.973953
C	7.779817	1.384037	-0.463337
C	7.439605	2.653774	0.326391
C	7.329383	2.386651	1.823737
N	8.669523	2.353504	2.481094
O	11.041612	1.616871	0.893228
H	10.891632	1.828025	-0.028672
H	11.520020	0.790173	0.842419
H	7.157877	2.036062	-4.258768
H	8.984963	3.132165	-2.419114
H	6.665683	2.053445	-2.157437
H	7.411974	0.521088	-2.389189
H	7.099968	0.604930	-0.132299
H	8.775100	1.030447	-0.228885
H	8.153081	3.454089	0.151070
H	6.474658	3.026456	-0.002074
H	6.769015	3.158916	2.327285
H	6.848286	1.440553	2.018338

H	9.380292	1.889581	1.923937
H	8.989521	3.323710	2.635327
H	8.615971	1.875762	3.368830
N	10.062478	0.448235	-3.837531
C	11.109302	-0.537622	-4.069126
C	12.486186	0.023064	-4.427545
O	13.443828	-0.705843	-4.301729
C	10.700491	-1.444770	-5.251616
C	9.562626	-2.443148	-4.995255
C	9.130006	-3.068388	-6.325173
C	9.990725	-3.533279	-4.012591
H	9.324254	0.446347	-4.510701
H	11.265043	-1.124641	-3.175827
H	10.433337	-0.799693	-6.083324
H	11.583200	-1.997286	-5.550529
H	8.706467	-1.911957	-4.590989
H	8.328910	-3.784615	-6.169730
H	8.772190	-2.311859	-7.011845
H	9.956732	-3.596651	-6.793621
H	9.201166	-4.263427	-3.872016
H	10.860730	-4.059506	-4.391441
H	10.244155	-3.135993	-3.034455
N	12.574038	1.261815	-4.919239
C	13.814611	1.844699	-5.393667
C	14.958796	2.033213	-4.379222
O	16.013406	2.413914	-4.812180
C	13.497216	3.171519	-6.086692
O	12.918143	4.088316	-5.202169
H	11.756430	1.833595	-4.917107
H	14.248463	1.177819	-6.129320

H	14.420374	3.590493	-6.455363
H	12.846416	2.977796	-6.933449
H	11.970767	4.079321	-5.267015
N	14.792294	1.722322	-3.074271
C	15.928290	1.647471	-2.176854
C	16.804559	0.409966	-2.402567
O	17.934463	0.393973	-1.988198
C	15.495410	1.578098	-0.707307
C	14.638887	2.735265	-0.197980
C	14.285572	2.488812	1.269118
N	13.260121	3.383439	1.791074
C	13.437415	4.534331	2.419116
N	14.655014	5.009909	2.656431
O	15.027888	7.465698	4.211033
H	14.744161	8.352217	3.972230
H	15.746003	7.571727	4.821972
N	12.387261	5.222685	2.815466
H	13.900860	1.420265	-2.758213
H	16.561977	2.504360	-2.346580
H	14.954873	0.650222	-0.551603
H	16.407420	1.508933	-0.124562
H	15.156582	3.683014	-0.314429
H	13.719649	2.816474	-0.766270
H	13.889203	1.489447	1.376121
H	15.164998	2.531855	1.900852
H	12.320099	3.087488	1.619789
H	15.463034	4.517248	2.358844
H	14.790124	5.864747	3.168310
H	11.431842	4.942742	2.657259
H	12.479311	6.065747	3.335753

N	16.200243	-0.648980	-2.967249
C	16.870870	-1.911472	-3.168108
C	17.669797	-1.889273	-4.467827
H	18.062651	-0.909448	-4.748489
O	17.877414	-2.853311	-5.129576
C	15.868175	-3.070204	-3.149457
C	15.324743	-3.399835	-1.791995
N	14.403816	-2.627471	-1.112311
O	12.508299	-0.434059	-0.465262
H	13.145756	-1.037495	-0.851236
H	12.027967	-0.038276	-1.184423
C	15.619899	-4.490240	-1.049586
C	14.172673	-3.251535	-0.003779
N	14.883079	-4.381616	0.103171
H	15.285669	-0.550324	-3.352780
H	17.596080	-2.030752	-2.370797
H	15.050696	-2.842318	-3.824751
H	16.369011	-3.944015	-3.543925
H	16.275354	-5.313992	-1.234936
H	13.494351	-2.922007	0.757153
H	14.782435	-5.064439	0.821938
O	-14.798044	-2.305754	5.077409
H	-15.090905	-1.616880	4.485558
H	-14.377340	-1.863123	5.807280
O	-12.885843	-0.761308	6.903392
H	-12.159022	-1.250959	7.273172
H	-13.152096	-0.138636	7.568679
O	-12.140923	-0.228943	4.090862
H	-12.285262	-0.224152	5.032934
H	-13.017632	-0.218848	3.703235

O	-13.359540	-2.023823	0.907578
H	-12.590514	-1.456197	0.826825
H	-13.169463	-2.625755	1.627177
O	-7.462981	2.078119	-0.250589
H	-7.582864	2.166507	0.698314
H	-6.548782	1.844730	-0.359079
O	-7.781876	2.148195	2.588044
H	-8.712592	1.982084	2.721336
H	-7.530711	2.835493	3.200300
O	-9.219699	0.267820	-1.542912
H	-8.654544	0.920588	-1.115801
H	-8.625703	-0.395486	-1.892490
O	-13.105016	-2.225681	-1.907724
H	-13.351473	-2.375355	-0.993383
H	-13.802370	-2.556482	-2.463211
O	-13.484751	1.744874	-0.190583
H	-12.857725	1.055718	0.037437
H	-12.999711	2.554839	-0.018400
O	-14.181219	4.914623	2.450307
H	-13.801617	5.401629	3.176341
H	-14.711518	4.211966	2.807283
O	-15.446010	2.146062	1.862203
H	-16.298712	2.345649	1.498153
H	-14.850012	2.052006	1.116081
O	-13.497394	0.499191	-2.728085
H	-13.706526	1.081279	-1.997199
H	-13.279600	-0.342387	-2.323820
O	-14.513808	-1.463214	-4.510948
H	-14.515842	-0.619392	-4.063504
H	-15.310723	-1.512896	-5.022209

O	-10.574806	-2.969291	-3.202223
H	-10.866863	-2.657694	-4.055438
H	-11.319224	-2.817613	-2.624595
O	-11.340807	-0.095887	0.389376
H	-10.664017	-0.135631	-0.288250
H	-10.954649	0.397056	1.116747
O	-10.645993	1.634979	2.510579
H	-11.151044	1.180499	3.185947
H	-11.153168	2.384140	2.200282
O	-12.086443	3.782053	1.051736
H	-12.806674	4.185137	1.549897
H	-11.540687	4.511513	0.773464
O	-10.887995	0.832534	-3.747225
H	-11.765775	0.977393	-3.390389
H	-10.308430	0.682653	-2.994348
O	-14.735692	-0.392839	2.923980
H	-15.121422	0.439458	2.650263
H	-14.531649	-0.883577	2.129567
O	-12.750308	-3.277875	3.454294
H	-13.513474	-3.074762	4.007107
H	-12.113285	-2.610857	3.692400
O	-11.716682	-1.375674	-5.293692
H	-12.662486	-1.515867	-5.271991
H	-11.531033	-0.699389	-4.643671

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(0),Y266(0),E183(0)

POTENTIAL:+70mV

N	15.580942	-6.451471	5.391415
---	-----------	-----------	----------

H	14.780349	-6.201766	5.939146
C	15.509367	-5.856426	4.054303
C	14.783016	-6.782958	3.060460
O	14.052521	-6.345772	2.186629
C	16.919361	-5.576248	3.520821
H	16.389372	-6.127384	5.884687
H	14.944498	-4.933617	4.050508
H	16.888494	-5.189753	2.509108
H	17.403232	-4.831330	4.142353
H	17.526831	-6.474492	3.529436
N	15.032384	-8.085605	3.186393
H	15.612054	-8.361765	3.949721
C	14.398655	-9.092385	2.333235
H	14.482396	-8.823759	1.292869
H	14.891390	-10.042255	2.492729
C	12.912798	-9.220863	2.671372
O	12.081474	-9.424771	1.825885
N	12.582805	-9.055889	3.966871
H	13.302698	-8.986571	4.648940
C	11.195100	-9.170804	4.421405
H	11.188267	-9.157896	5.503158
H	10.743722	-10.088319	4.077196
C	10.336963	-8.010603	3.900697
O	9.190772	-8.186042	3.584573
N	10.947108	-6.814557	3.855284
C	10.318434	-5.634083	3.317568
C	10.126894	-5.691133	1.799331
O	9.096452	-5.262764	1.337093
C	11.092693	-4.388012	3.776312
O	12.478661	-4.570737	3.769134

H	11.905473	-6.744232	4.106887
H	9.314542	-5.553322	3.701121
H	10.801112	-3.539672	3.167344
H	10.827326	-4.174458	4.801380
H	12.805421	-4.755040	2.897012
N	11.100275	-6.200613	1.024177
C	10.844930	-6.396984	-0.400192
C	9.694191	-7.385718	-0.601590
O	8.946504	-7.280192	-1.545833
C	12.133418	-6.785894	-1.186814
C	12.333972	-8.291280	-1.403984
C	12.160705	-6.060462	-2.533508
H	11.924268	-6.586240	1.431556
H	10.475301	-5.462697	-0.791660
H	12.965434	-6.416169	-0.598032
H	13.287800	-8.454577	-1.894898
H	12.332078	-8.857756	-0.483538
H	11.566859	-8.698071	-2.055726
H	13.055508	-6.324363	-3.086116
H	11.300428	-6.332005	-3.135436
H	12.160806	-4.985273	-2.400041
N	9.570408	-8.340330	0.328361
H	10.314480	-8.474432	0.974388
C	8.593032	-9.421193	0.241195
H	8.935861	-10.219590	0.886968
H	8.532017	-9.802139	-0.766597
C	7.181944	-9.047549	0.645357
O	6.257521	-9.505331	0.014451
N	7.004056	-8.228491	1.688362
C	5.670081	-7.742066	1.958390

C	5.250599	-6.730681	0.897072
O	4.073692	-6.634174	0.621488
C	5.416214	-7.237024	3.392842
C	5.559791	-8.381152	4.401516
C	6.257028	-6.027261	3.805597
H	7.781723	-7.961726	2.252011
H	4.987432	-8.561748	1.796393
H	4.375059	-6.929201	3.386405
H	5.269882	-8.044251	5.391231
H	4.922390	-9.219159	4.138918
H	6.582310	-8.737422	4.456785
H	5.916438	-5.655352	4.766019
H	7.299625	-6.296792	3.912474
H	6.184055	-5.212892	3.092997
N	6.171151	-6.006054	0.252849
C	5.775815	-5.188296	-0.881848
C	5.344935	-6.072896	-2.060131
O	4.321599	-5.821913	-2.652478
C	6.867606	-4.168045	-1.261631
C	7.064145	-3.150823	-0.123538
C	6.496595	-3.458456	-2.568499
C	8.356860	-2.342647	-0.237676
H	7.132427	-6.063805	0.511463
H	4.877360	-4.652106	-0.615760
H	7.798107	-4.708570	-1.408911
H	6.208311	-2.477482	-0.107810
H	7.074430	-3.664394	0.828510
H	7.201410	-2.668340	-2.788559
H	6.497445	-4.133933	-3.414165
H	5.508088	-3.015876	-2.502185

H	8.457266	-1.668840	0.606528
H	9.219071	-2.999136	-0.237414
H	8.392266	-1.743091	-1.140341
N	6.117711	-7.114918	-2.395362
H	7.012137	-7.235987	-1.968883
C	5.776849	-7.956143	-3.522959
H	6.607482	-8.630335	-3.690883
H	5.623490	-7.371145	-4.417519
C	4.507232	-8.783923	-3.322025
O	3.670649	-8.842852	-4.191822
N	4.393877	-9.435505	-2.157905
H	5.130851	-9.392153	-1.486720
C	3.206567	-10.189471	-1.830312
H	2.967419	-10.903250	-2.604295
H	3.396800	-10.730478	-0.911826
C	1.974201	-9.306854	-1.644807
O	0.887592	-9.694727	-2.007218
N	2.187865	-8.107004	-1.107166
C	1.065875	-7.180082	-1.078547
C	0.623278	-6.721166	-2.470731
O	-0.558585	-6.582566	-2.692751
C	1.286703	-5.920711	-0.247405
O	1.414449	-6.167423	1.112892
H	3.087781	-7.818076	-0.797810
H	0.211730	-7.692961	-0.667269
H	2.134735	-5.363828	-0.631909
H	0.397434	-5.326895	-0.377869
H	2.304978	-6.441587	1.286480
N	1.552246	-6.437224	-3.393002
C	1.156398	-6.032021	-4.729693

C	0.385423	-7.153760	-5.418744
O	-0.601390	-6.897794	-6.075867
C	2.369640	-5.538668	-5.551767
C	2.784659	-4.147221	-5.045031
C	2.073813	-5.517231	-7.056783
C	4.114937	-3.649070	-5.608139
H	2.522156	-6.493743	-3.167532
H	0.439066	-5.227110	-4.653854
H	3.186486	-6.232980	-5.378815
H	1.998346	-3.437083	-5.295685
H	2.856144	-4.168576	-3.965206
H	2.933347	-5.151736	-7.604695
H	1.849975	-6.504239	-7.442685
H	1.231972	-4.871160	-7.285116
H	4.414406	-2.735690	-5.104875
H	4.901076	-4.381227	-5.453355
H	4.061563	-3.435277	-6.669765
N	0.823559	-8.405150	-5.255441
H	1.669666	-8.581384	-4.754991
C	0.043390	-9.512153	-5.753610
H	-0.063568	-9.473792	-6.827452
H	0.553346	-10.429292	-5.487533
C	-1.365316	-9.540114	-5.166944
O	-2.319938	-9.767288	-5.874474
N	-1.472594	-9.318871	-3.858013
C	-2.776806	-9.346623	-3.236465
C	-3.690591	-8.211640	-3.700453
O	-4.888648	-8.419516	-3.743742
C	-2.680572	-9.315384	-1.703977
O	-3.925575	-9.579870	-1.118921

H	-0.656820	-9.233313	-3.288687
H	-3.294817	-10.251748	-3.520567
H	-1.999587	-10.088365	-1.375700
H	-2.290650	-8.357371	-1.376577
H	-4.614992	-9.178316	-1.633687
N	-3.140671	-7.031631	-3.981802
C	-3.902800	-5.911611	-4.509848
C	-4.444401	-6.236116	-5.902315
O	-5.608320	-6.045095	-6.172322
C	-3.003179	-4.655368	-4.508644
C	-3.446430	-3.519778	-5.415770
C	-4.768369	-3.093147	-5.495387
C	-2.499107	-2.874292	-6.202386
C	-5.125967	-2.067161	-6.354301
C	-2.850203	-1.834810	-7.048372
C	-4.171554	-1.432517	-7.132535
H	-2.163960	-6.909757	-3.812366
H	-4.770939	-5.740614	-3.893718
H	-2.925428	-4.312966	-3.481048
H	-2.010683	-4.954438	-4.814888
H	-5.527531	-3.578735	-4.912488
H	-1.472615	-3.193968	-6.163074
H	-6.159685	-1.773371	-6.422763
H	-2.096161	-1.352588	-7.644053
H	-4.452444	-0.639105	-7.803271
N	-3.570568	-6.729386	-6.788376
C	-4.012389	-7.071542	-8.120729
C	-5.136283	-8.106206	-8.097705
O	-6.014865	-8.052897	-8.918488
C	-2.861979	-7.603003	-8.979078

S	-1.645138	-6.351001	-9.496656
H	-2.629879	-6.913493	-6.509016
H	-4.438183	-6.201578	-8.597974
H	-2.357333	-8.419729	-8.480725
H	-3.278715	-7.983739	-9.901750
H	-1.045060	-6.180606	-8.329095
N	-5.078532	-9.066905	-7.155631
H	-4.257250	-9.188153	-6.602517
C	-6.085178	-10.116164	-7.180937
H	-6.256484	-10.456631	-8.190330
H	-5.714002	-10.946528	-6.591481
C	-7.459147	-9.722831	-6.613014
O	-8.481305	-10.087403	-7.126876
N	-7.418017	-9.015655	-5.478475
C	-8.641664	-8.655583	-4.788433
C	-9.503025	-7.657707	-5.553989
O	-10.700950	-7.657359	-5.447580
C	-8.362789	-8.115649	-3.374852
C	-7.517819	-6.836019	-3.258320
C	-8.186702	-5.483367	-3.283259
O	-9.487484	-5.484213	-3.352610
H	-9.837195	-4.582227	-3.306516
O	-7.537218	-4.468877	-3.215821
H	-6.535760	-8.773291	-5.079991
H	-9.261399	-9.536011	-4.691970
H	-9.318829	-7.979455	-2.890166
H	-7.839592	-8.900272	-2.838741
H	-6.984949	-6.853250	-2.314144
H	-6.752209	-6.796859	-4.014506
N	-8.837317	-6.734064	-6.273863

C	-9.562353	-5.706192	-6.995284
C	-10.429282	-6.285649	-8.104962
H	-10.447834	-7.368339	-8.211261
O	-11.058382	-5.575959	-8.833188
C	-8.634934	-4.592890	-7.533973
O	-9.429234	-3.468192	-7.883582
C	-7.760018	-4.998713	-8.712559
H	-7.855346	-6.834553	-6.418399
H	-10.250263	-5.232842	-6.304175
H	-8.009124	-4.274700	-6.711601
H	-10.132138	-3.782364	-8.446313
H	-7.080829	-4.186024	-8.947006
H	-7.170316	-5.879379	-8.504966
H	-8.365083	-5.194266	-9.591490
N	-12.952321	-9.022071	3.174379
H	-13.222242	-9.545279	2.367114
C	-11.777508	-8.184389	2.899330
C	-10.788044	-8.138268	4.046003
O	-9.654030	-7.745285	3.846063
C	-12.130734	-6.717775	2.577797
O	-12.657555	-6.188825	3.767839
C	-13.123326	-6.574357	1.430132
H	-13.731255	-8.457326	3.453056
H	-11.232605	-8.601484	2.063655
H	-11.209285	-6.212204	2.322373
H	-12.680798	-5.236074	3.711916
H	-13.268773	-5.522576	1.207991
H	-12.771579	-7.061413	0.528011
H	-14.088830	-6.989115	1.694065
N	-11.197267	-8.533701	5.241859

H	-12.124328	-8.896923	5.283816
C	-10.409167	-8.524250	6.449423
H	-10.331035	-7.527086	6.853346
H	-10.928864	-9.129539	7.182800
C	-8.972188	-9.040182	6.371330
O	-8.135436	-8.471324	7.028298
N	-8.657852	-10.121190	5.634760
H	-9.368763	-10.601945	5.131375
C	-7.269059	-10.552673	5.533184
H	-7.251934	-11.532386	5.073001
H	-6.828276	-10.630382	6.514139
C	-6.387526	-9.608322	4.692701
O	-5.219497	-9.466997	4.948475
N	-7.045373	-9.017976	3.701159
C	-6.304931	-8.012558	2.952689
C	-6.268090	-6.697759	3.725473
O	-5.276112	-6.007922	3.677171
C	-6.623074	-7.894316	1.449060
C	-7.795882	-7.059029	0.980280
C	-7.766000	-5.670957	1.082999
C	-8.866773	-7.649269	0.322235
C	-8.787869	-4.896672	0.560020
C	-9.880657	-6.876416	-0.220950
C	-9.848945	-5.497693	-0.097189
H	-8.039868	-9.019905	3.675706
H	-5.281581	-8.342691	2.985193
H	-5.724588	-7.489368	0.996675
H	-6.714187	-8.906752	1.073838
H	-6.925939	-5.186139	1.546078
H	-8.892693	-8.718667	0.200367

H	-8.738272	-3.825285	0.637789
H	-10.679672	-7.347393	-0.763725
H	-10.627261	-4.898628	-0.532836
N	-7.302440	-6.389884	4.510376
C	-7.241904	-5.272589	5.420553
C	-6.127059	-5.479045	6.445228
O	-5.497086	-4.519332	6.836380
C	-8.622454	-5.098367	6.088776
C	-8.872837	-3.753989	6.737360
C	-9.064940	-2.621771	5.950646
C	-8.980564	-3.631491	8.115883
C	-9.345869	-1.395886	6.527256
C	-9.270126	-2.406751	8.699869
C	-9.450419	-1.284332	7.908326
H	-8.162416	-6.883321	4.408297
H	-6.972272	-4.370777	4.889804
H	-9.367819	-5.249171	5.314884
H	-8.757533	-5.887072	6.816818
H	-8.996843	-2.697121	4.878790
H	-8.840289	-4.495153	8.742009
H	-9.481307	-0.533112	5.901194
H	-9.342837	-2.330540	9.769933
H	-9.649214	-0.328205	8.359915
N	-5.873327	-6.714919	6.870140
H	-6.522006	-7.441169	6.663147
C	-4.799226	-7.005427	7.793460
H	-4.840126	-6.373275	8.667686
H	-4.911987	-8.034134	8.111036
C	-3.402321	-6.831884	7.200144
O	-2.527365	-6.342320	7.874602

N	-3.202406	-7.252132	5.946462
C	-1.926492	-7.066544	5.273132
C	-1.685041	-5.592029	4.920417
O	-0.587000	-5.103790	5.087924
C	-1.845186	-7.996026	4.042074
C	-0.683925	-7.630368	3.116008
C	-1.736960	-9.457739	4.490962
H	-3.935891	-7.731633	5.470520
H	-1.130946	-7.313462	5.961147
H	-2.767813	-7.872914	3.479766
H	-0.619047	-8.353756	2.310238
H	-0.800258	-6.654658	2.665480
H	0.262332	-7.640071	3.648170
H	-1.751106	-10.114767	3.627348
H	-0.800602	-9.623412	5.017899
H	-2.550214	-9.753041	5.141056
N	-2.723898	-4.903800	4.437579
C	-2.597873	-3.516586	4.035586
C	-2.446008	-2.619124	5.261663
O	-1.559369	-1.795104	5.313952
C	-3.790373	-3.045871	3.189272
C	-4.037835	-3.782688	1.862411
C	-2.904281	-3.687319	0.855894
O	-1.795219	-4.103278	1.227963
O	-3.154229	-3.214010	-0.265332
H	-3.585472	-5.375546	4.270945
H	-1.693274	-3.397091	3.469942
H	-4.695979	-3.115782	3.784263
H	-3.635079	-1.989268	2.988289
H	-4.209364	-4.831126	2.054315

H	-4.937775	-3.375838	1.415311
N	-3.328770	-2.774724	6.264389
C	-3.116859	-2.037315	7.484959
C	-1.791620	-2.427091	8.149505
O	-1.125457	-1.586158	8.713508
C	-4.245902	-2.040988	8.526077
O	-4.451830	-3.295548	9.104538
C	-5.530771	-1.412628	7.998546
H	-4.008877	-3.501147	6.228544
H	-2.972408	-1.002401	7.215625
H	-3.869398	-1.417516	9.327519
H	-4.908463	-3.852384	8.485526
H	-6.261226	-1.373828	8.797319
H	-5.347703	-0.399615	7.653558
H	-5.953429	-1.981335	7.181070
N	-1.380408	-3.700466	8.043355
H	-2.027778	-4.421552	7.812090
C	-0.184104	-4.103740	8.736422
H	-0.230722	-3.886129	9.794177
H	-0.071111	-5.171594	8.602335
C	1.063837	-3.415977	8.208148
O	1.943392	-3.068667	8.963047
N	1.148099	-3.258383	6.871248
C	2.325512	-2.662498	6.301899
C	2.289608	-1.139382	6.162378
O	3.359845	-0.576666	6.026494
C	2.805039	-3.337807	5.016948
S	1.888257	-2.938296	3.504645
H	0.413717	-3.611876	6.290069
H	3.116173	-2.811897	7.021600

H	3.817145	-3.008490	4.830336
H	2.816852	-4.409073	5.162126
H	0.819535	-3.695637	3.703000
N	1.139670	-0.470506	6.273406
C	1.204805	0.968264	6.492091
C	1.756128	1.271223	7.870957
O	2.369161	2.288717	8.085908
C	-0.095209	1.740211	6.181737
C	-1.202670	1.553130	7.228888
C	-0.544879	1.447272	4.745363
C	-2.470298	2.359126	6.937464
H	0.270099	-0.963389	6.287514
H	1.952635	1.350962	5.815916
H	0.205266	2.781508	6.231591
H	-1.452777	0.506845	7.328849
H	-0.819884	1.863788	8.196479
H	-1.301750	2.153662	4.427816
H	0.291009	1.536211	4.056776
H	-0.952151	0.450631	4.642613
H	-3.144614	2.318997	7.787465
H	-2.244102	3.404899	6.745042
H	-3.006451	1.971509	6.078076
N	1.549780	0.323275	8.791255
H	0.890444	-0.402546	8.613047
C	1.977874	0.512251	10.160280
H	1.469252	-0.222981	10.770964
H	1.737371	1.501937	10.518378
C	3.481809	0.336581	10.305781
O	4.163662	1.126803	10.899107
N	3.999635	-0.753621	9.694705

H	3.390680	-1.463356	9.345149
C	5.424640	-0.938719	9.667230
H	5.638010	-1.909229	9.234347
H	5.854673	-0.904705	10.657557
C	6.156890	0.119123	8.844832
O	7.292104	0.411098	9.129501
N	5.502074	0.621268	7.799018
C	6.105378	1.756770	7.150115
C	5.525754	3.075976	7.654228
H	5.023096	3.036937	8.619263
O	5.650481	4.094321	7.046575
C	6.011748	1.676271	5.624080
C	6.760831	0.506655	5.019708
C	8.126684	0.320974	5.237773
C	6.097513	-0.401591	4.200082
C	8.810437	-0.725805	4.634383
C	6.779052	-1.446022	3.595243
C	8.139346	-1.608653	3.802465
H	4.574642	0.337206	7.571870
H	7.140280	1.766917	7.456520
H	4.969721	1.616607	5.335781
H	6.394175	2.610107	5.226508
H	8.656905	0.977099	5.906681
H	5.037177	-0.304328	4.064082
H	9.861415	-0.854335	4.828031
H	6.244709	-2.137611	2.968497
H	8.657635	-2.422252	3.328888
N	12.613548	9.596235	-1.248797
H	11.872888	9.914331	-1.845504
C	12.304855	8.264733	-0.719494

C	11.274118	8.450599	0.386898
O	10.265933	7.778869	0.416405
C	13.562743	7.581057	-0.165268
C	14.645171	7.276174	-1.206399
S	14.017413	6.202010	-2.529687
C	15.500160	6.053615	-3.555024
H	13.432955	9.572824	-1.822901
H	11.834482	7.616492	-1.447350
H	14.001230	8.205515	0.607268
H	13.255717	6.653873	0.304879
H	15.045479	8.188658	-1.633772
H	15.470364	6.783888	-0.704308
H	15.248997	5.398790	-4.375499
H	15.799031	7.017675	-3.945849
H	16.318596	5.616979	-2.997646
N	11.504255	9.412828	1.296996
C	10.594230	9.607677	2.408576
C	9.277006	10.274769	2.010397
O	8.280961	10.053319	2.652723
C	11.276203	10.368772	3.552226
C	12.447520	9.563777	4.084885
O	13.582550	9.825193	3.745343
N	12.143330	8.561481	4.919061
H	12.328022	9.967725	1.206308
H	10.295334	8.637602	2.771156
H	11.657595	11.325890	3.219193
H	10.545941	10.537611	4.333516
H	12.886830	7.965718	5.213395
H	11.221666	8.175583	4.954638
N	9.263820	11.067708	0.922336

H	10.110806	11.229613	0.427402
C	8.003507	11.517472	0.368847
H	8.201268	12.260205	-0.393381
H	7.389112	11.966735	1.131893
C	7.186380	10.384432	-0.254307
O	5.986325	10.470163	-0.291674
N	7.862646	9.333243	-0.763184
C	7.170360	8.145621	-1.233907
C	6.634551	7.300767	-0.067358
O	5.534115	6.808599	-0.148417
C	8.048803	7.344196	-2.224169
C	8.343623	8.197115	-3.472857
C	7.379229	6.019179	-2.608087
C	9.428272	7.624966	-4.388863
H	8.823800	9.230617	-0.536510
H	6.279715	8.471812	-1.748434
H	8.987821	7.117690	-1.727244
H	7.421746	8.323158	-4.036246
H	8.645736	9.192750	-3.165369
H	7.996585	5.478783	-3.314292
H	7.228035	5.377911	-1.748270
H	6.409560	6.182911	-3.066614
H	9.622315	8.305493	-5.211529
H	10.363575	7.479448	-3.855143
H	9.148417	6.670885	-4.819956
N	7.387121	7.175059	1.043940
C	6.878148	6.458328	2.201978
C	5.527294	7.040202	2.639577
O	4.574441	6.334199	2.866783
C	7.832292	6.545691	3.403562

C	9.253664	5.996720	3.243963
O	10.145200	6.631053	3.801319
O	9.427037	4.934897	2.595238
H	8.347205	7.444682	1.022838
H	6.681042	5.429620	1.943308
H	7.920530	7.570200	3.733380
H	7.374144	5.992143	4.220647
N	5.489861	8.378154	2.785912
H	6.321206	8.912914	2.648845
C	4.299565	9.047333	3.249675
H	4.538969	10.091718	3.406566
H	3.957722	8.641020	4.188490
C	3.136817	8.988654	2.268517
O	1.995394	9.111339	2.649451
N	3.470151	8.825006	0.985194
H	4.431261	8.828978	0.735190
C	2.517174	8.905264	-0.078282
H	3.059635	9.091925	-0.996343
H	1.843680	9.737834	0.072013
C	1.609145	7.687007	-0.310220
O	0.563858	7.814945	-0.883301
N	2.090528	6.538674	0.206384
C	1.283381	5.366494	0.435195
C	0.467875	5.480594	1.727562
O	-0.727393	5.301042	1.700501
C	2.156685	4.111974	0.446513
H	2.996864	6.575239	0.622653
H	0.551923	5.295989	-0.352655
H	1.554370	3.234745	0.657176
H	2.624951	3.991708	-0.523505

H	2.937305	4.180443	1.196957
N	1.100166	5.752938	2.883496
C	0.363908	5.588936	4.128803
C	-0.756441	6.616054	4.277688
O	-1.793301	6.307749	4.825540
C	1.277017	5.517294	5.377563
C	1.869171	6.863332	5.822217
C	2.363575	4.450435	5.174566
C	2.702782	6.768521	7.102590
H	2.087549	5.892476	2.903068
H	-0.160392	4.645887	4.073071
H	0.617019	5.179838	6.171072
H	2.477859	7.271919	5.022362
H	1.065842	7.573320	5.990239
H	2.734478	4.098798	6.126137
H	1.969683	3.592879	4.638409
H	3.205836	4.838596	4.612193
H	3.008334	7.759834	7.424055
H	2.126734	6.325663	7.909692
H	3.597632	6.172900	6.971536
N	-0.542353	7.851148	3.802925
H	0.342661	8.093820	3.408237
C	-1.514248	8.891052	4.018116
H	-1.105100	9.819454	3.640120
H	-1.725168	9.021780	5.069665
C	-2.867021	8.618723	3.365915
O	-3.871177	8.835136	4.003743
N	-2.902653	8.109029	2.120712
C	-4.238324	8.007130	1.534100
C	-4.968810	6.730607	1.912165

O	-6.180377	6.723992	1.899404
C	-4.023439	8.231576	0.030898
C	-2.767606	9.109700	0.024624
C	-1.907994	8.459364	1.096316
H	-4.860642	8.797264	1.925061
H	-3.845864	7.294605	-0.480577
H	-4.888944	8.700104	-0.419709
H	-2.258156	9.157674	-0.919537
H	-3.027601	10.122702	0.322427
H	-1.423342	7.570099	0.735637
H	-1.150039	9.118658	1.486793
N	-4.242059	5.660668	2.268948
C	-4.898311	4.489696	2.822075
C	-5.601942	4.809620	4.143697
O	-6.682156	4.319140	4.387286
C	-3.922513	3.315617	3.044840
C	-3.602555	2.490632	1.814460
C	-4.319968	1.333086	1.526420
C	-2.563037	2.837884	0.964040
C	-4.010876	0.545635	0.427664
C	-2.253031	2.067610	-0.142613
C	-2.971130	0.916942	-0.418016
O	-2.631708	0.190538	-1.507631
H	-3.433330	-0.132565	-1.959934
H	-3.248637	5.746501	2.321824
H	-5.684982	4.182788	2.150843
H	-3.011435	3.701906	3.489434
H	-4.374530	2.664717	3.784611
H	-5.129536	1.032893	2.169558
H	-1.985421	3.717452	1.156964

H	-4.552745	-0.361458	0.235267
H	-1.460382	2.361604	-0.807624
N	-4.963985	5.610804	5.012229
H	-4.035727	5.925115	4.817424
C	-5.577479	5.988549	6.265746
H	-4.801211	6.365451	6.920165
H	-6.043964	5.136989	6.734166
C	-6.651474	7.065805	6.114413
O	-7.709535	6.987358	6.695136
N	-6.341993	8.091462	5.314137
H	-5.441195	8.148173	4.889085
C	-7.257699	9.220084	5.085090
H	-6.773806	9.881174	4.377832
H	-7.436862	9.765711	5.999948
C	-8.620673	8.834837	4.545706
O	-9.605806	9.430594	4.903538
N	-8.666130	7.828883	3.652697
C	-9.928735	7.427001	3.085873
C	-10.814144	6.631211	4.032578
O	-11.919862	6.304410	3.637505
C	-9.727464	6.646934	1.766796
O	-10.949256	6.584046	1.057330
C	-9.151248	5.252108	1.967152
H	-7.818197	7.408776	3.331769
H	-10.503099	8.315235	2.856328
H	-9.047528	7.228489	1.158208
H	-11.656023	6.539435	1.697411
H	-8.976723	4.785046	1.004296
H	-8.208905	5.278259	2.490920
H	-9.838835	4.627571	2.524251

N	-10.353503	6.328342	5.241144
C	-11.230850	5.723473	6.228817
C	-12.252751	6.705790	6.808551
O	-13.256428	6.277675	7.316005
C	-10.435281	5.093264	7.379626
C	-9.488829	3.950679	6.982356
C	-8.704761	3.492370	8.215910
C	-10.221569	2.767193	6.343598
H	-9.434347	6.600099	5.520645
H	-11.827490	4.972438	5.737201
H	-9.859024	5.870540	7.870016
H	-11.161263	4.730326	8.100330
H	-8.772341	4.325287	6.260793
H	-7.994812	2.711349	7.958815
H	-8.150205	4.316678	8.652154
H	-9.369959	3.098927	8.981775
H	-9.518635	1.971544	6.116205
H	-10.980974	2.365598	7.012467
H	-10.707399	3.037330	5.412318
N	-11.935445	8.016698	6.787516
C	-12.884695	9.000950	7.215647
C	-13.851947	9.432812	6.133866
H	-14.612175	10.146788	6.470712
O	-13.816147	9.067787	5.006124
H	-11.174724	8.331014	6.225290
H	-13.454872	8.617012	8.051621
H	-12.360078	9.886922	7.562692
N	-11.450004	10.622759	-3.030048
H	-11.209347	10.836129	-2.082610
C	-11.805542	9.208255	-3.171992

C	-11.410598	8.856561	-4.599609
O	-10.372854	8.290278	-4.846281
C	-13.244706	8.824652	-2.765620
C	-13.482122	9.163105	-1.282303
C	-13.513810	7.342058	-3.054218
C	-14.912145	8.922492	-0.794921
H	-12.216211	11.220192	-3.277637
H	-11.119634	8.644120	-2.555652
H	-13.943154	9.424616	-3.353506
H	-12.790744	8.584378	-0.673583
H	-13.242391	10.208439	-1.114120
H	-14.550839	7.090861	-2.872760
H	-13.298105	7.076750	-4.084999
H	-12.903473	6.712301	-2.414402
H	-15.024839	9.283592	0.220942
H	-15.634322	9.447362	-1.414760
H	-15.172680	7.870776	-0.791579
N	-12.211997	9.288083	-5.602657
H	-13.130153	9.596772	-5.377247
C	-11.972873	8.843875	-6.959238
H	-12.037064	7.767786	-7.045600
H	-12.729661	9.284178	-7.596912
C	-10.601375	9.232961	-7.517198
O	-9.996255	8.496520	-8.240744
N	-10.162429	10.477356	-7.181602
H	-10.711675	11.008704	-6.545682
C	-8.894348	11.024005	-7.637086
H	-8.790089	10.891089	-8.702746
H	-8.878869	12.081540	-7.407775
C	-7.672362	10.359334	-6.988510

O	-6.752644	9.936648	-7.631237
N	-7.659719	10.350048	-5.619869
H	-8.482692	10.627738	-5.134437
C	-6.495283	9.961236	-4.832291
H	-5.599773	10.376146	-5.266681
H	-6.615414	10.362680	-3.833476
C	-6.266714	8.464815	-4.710673
O	-5.130741	8.052021	-4.722029
N	-7.313250	7.638968	-4.532827
C	-7.014200	6.281823	-4.104247
C	-6.385416	5.453733	-5.218218
O	-5.500749	4.680846	-4.941532
C	-8.169386	5.547942	-3.385495
C	-9.334503	5.136864	-4.300510
C	-8.608947	6.363530	-2.163665
C	-10.433979	4.357572	-3.576425
H	-8.251741	7.983907	-4.545552
H	-6.212499	6.347950	-3.384840
H	-7.712696	4.634775	-3.012828
H	-9.766409	6.006148	-4.780323
H	-8.936982	4.509370	-5.094599
H	-9.268349	5.788334	-1.528201
H	-7.751178	6.646670	-1.562057
H	-9.133613	7.266301	-2.453200
H	-11.164557	3.981301	-4.285647
H	-10.030402	3.505615	-3.040225
H	-10.965010	4.979204	-2.865860
N	-6.821822	5.574666	-6.491817
C	-6.122655	4.837517	-7.526349
C	-4.766885	5.445593	-7.897275

O	-3.900145	4.709900	-8.308774
C	-6.985394	4.553869	-8.764595
C	-8.063608	3.474780	-8.557474
C	-7.486040	2.123528	-8.106951
N	-8.413891	0.992753	-8.200354
C	-9.247023	0.580826	-7.240055
N	-9.565917	1.405081	-6.254299
N	-9.750419	-0.632651	-7.274070
H	-7.500531	6.267906	-6.723047
H	-5.828205	3.900592	-7.087760
H	-7.460499	5.467402	-9.109894
H	-6.316779	4.232109	-9.555651
H	-8.808220	3.828074	-7.849781
H	-8.583797	3.332195	-9.498826
H	-6.639544	1.867317	-8.730819
H	-7.118616	2.168991	-7.090414
H	-8.306663	0.377692	-8.976215
H	-9.344245	2.370532	-6.314187
H	-10.097070	1.113256	-5.449550
H	-9.353985	-1.381590	-7.810395
H	-10.478295	-0.911510	-6.634346
N	-4.571397	6.757500	-7.722194
H	-5.311895	7.353674	-7.430382
C	-3.257798	7.352383	-8.011132
H	-2.933305	7.094249	-9.006697
H	-3.359275	8.427002	-7.936831
C	-2.193936	6.877304	-7.033115
O	-1.066806	6.644459	-7.393122
N	-2.610473	6.768838	-5.766290
C	-1.723951	6.459952	-4.670781

C	-1.446916	4.973453	-4.542400
O	-0.318988	4.587468	-4.336016
C	-2.308861	7.054869	-3.383162
C	-1.727790	6.351443	-2.157648
C	-2.066160	8.570611	-3.416451
H	-3.535867	7.063198	-5.540745
H	-0.755605	6.900148	-4.860973
H	-3.377683	6.877671	-3.399219
H	-1.942950	6.894074	-1.256222
H	-2.144316	5.354939	-2.053116
H	-0.655569	6.273740	-2.226170
H	-2.801922	9.100706	-2.828503
H	-1.077657	8.810853	-3.039486
H	-2.147842	8.954143	-4.426881
N	-2.476509	4.120594	-4.661332
C	-2.166304	2.713538	-4.735604
C	-1.263021	2.445154	-5.932153
O	-0.390765	1.610691	-5.874936
C	-3.409253	1.801827	-4.796543
C	-4.384750	1.957396	-3.620250
C	-5.461605	0.858243	-3.552073
N	-5.024352	-0.309686	-2.806819
C	-5.834088	-1.285026	-2.637352
N	-7.120142	-1.337912	-3.162328
N	-5.545208	-2.328950	-1.829388
H	-3.402241	4.448062	-4.837198
H	-1.584983	2.432899	-3.869933
H	-3.941363	1.981098	-5.729249
H	-3.042255	0.782421	-4.840102
H	-3.838795	1.977506	-2.689048

H	-4.885565	2.909052	-3.704949
H	-6.351102	1.287798	-3.090722
H	-5.745348	0.597643	-4.575397
H	-7.226829	-0.855583	-4.027469
H	-7.521277	-2.257450	-3.202406
H	-4.636224	-2.422398	-1.418379
H	-6.040804	-3.182966	-1.968389
N	-1.459772	3.193335	-7.035054
H	-2.267192	3.765881	-7.144744
C	-0.596016	2.984490	-8.179296
H	-0.940318	3.627846	-8.978864
H	-0.614398	1.958679	-8.517973
C	0.858094	3.326702	-7.861330
O	1.786035	2.683375	-8.284624
N	1.007247	4.396249	-7.063579
H	0.213446	4.960297	-6.860737
C	2.282316	4.880650	-6.640295
H	2.918456	5.142312	-7.476474
H	2.122221	5.774091	-6.050920
C	3.094582	3.926515	-5.779533
O	4.300635	4.045656	-5.701005
N	2.428034	2.983354	-5.101941
C	3.098460	2.130521	-4.156539
C	4.281984	1.344235	-4.723594
O	5.201684	1.054362	-3.984935
C	2.026255	1.207884	-3.579586
C	2.417310	0.331931	-2.395276
C	1.121230	-0.251754	-1.856780
N	1.333350	-1.247206	-0.825494
C	0.341807	-2.072958	-0.445718

N	-0.814787	-2.039801	-1.064745
N	0.558512	-2.942064	0.513940
H	1.433643	2.939341	-5.176232
H	3.540110	2.726300	-3.366546
H	1.214694	1.858336	-3.271280
H	1.624632	0.593830	-4.377160
H	3.092263	-0.463522	-2.691370
H	2.922286	0.917915	-1.630625
H	0.483946	0.548459	-1.492586
H	0.599758	-0.734748	-2.670949
H	2.042725	-1.074796	-0.148314
H	-1.141342	-1.192989	-1.482243
H	-1.575377	-2.653242	-0.776559
H	1.472900	-3.119781	0.859926
H	-0.227485	-3.495225	0.850629
N	4.281642	0.945295	-6.005331
H	3.540514	1.224776	-6.614846
C	5.363426	0.116658	-6.504603
H	5.139423	-0.143515	-7.531654
H	5.441111	-0.797366	-5.937306
C	6.736237	0.756120	-6.476105
O	7.738575	0.089675	-6.364842
N	6.766121	2.085332	-6.608323
H	5.912179	2.604995	-6.573019
C	8.005509	2.823538	-6.551101
H	8.709834	2.439534	-7.275449
H	7.800300	3.854283	-6.807558
C	8.748871	2.826732	-5.213347
O	9.890154	3.235828	-5.161891
N	8.103920	2.338653	-4.145971

C	8.685569	2.174685	-2.824698
C	9.950210	1.305456	-2.832305
O	10.768807	1.388487	-1.930967
C	7.581462	1.507752	-1.974036
C	7.779545	1.384045	-0.463395
C	7.439220	2.653824	0.326219
C	7.328841	2.386785	1.823564
N	8.668931	2.353589	2.481038
O	11.041280	1.616744	0.893292
H	10.891336	1.827886	-0.028619
H	11.519641	0.790022	0.842503
H	7.157843	2.036144	-4.258798
H	8.984887	3.132101	-2.419072
H	6.665568	2.053317	-2.157635
H	7.411935	0.520992	-2.389253
H	7.099674	0.604947	-0.132388
H	8.774806	1.030482	-0.228813
H	8.152705	3.454140	0.150925
H	6.474304	3.026469	-0.002372
H	6.768461	3.159097	2.327029
H	6.847680	1.440721	2.018165
H	9.379709	1.889596	1.923959
H	8.989016	3.323756	2.635285
H	8.615271	1.875867	3.368782
N	10.062478	0.448235	-3.837531
C	11.109288	-0.537620	-4.069164
C	12.486185	0.023066	-4.427535
O	13.443856	-0.705807	-4.301670
C	10.700469	-1.444643	-5.251751
C	9.562495	-2.442934	-4.995550

C	9.129826	-3.067907	-6.325579
C	9.990453	-3.533264	-4.013046
H	9.324245	0.446354	-4.510697
H	11.265001	-1.124722	-3.175914
H	10.433405	-0.799467	-6.083409
H	11.583144	-1.997215	-5.550670
H	8.706388	-1.911705	-4.591231
H	8.328652	-3.784069	-6.170262
H	8.772094	-2.311226	-7.012127
H	9.956502	-3.596183	-6.794105
H	9.200793	-4.263319	-3.872571
H	10.860385	-4.059559	-4.391976
H	10.243938	-3.136158	-3.034849
N	12.574038	1.261815	-4.919239
C	13.814598	1.844700	-5.393665
C	14.958833	2.033070	-4.379249
O	16.013518	2.413551	-4.812238
C	13.497199	3.171601	-6.086541
O	12.918242	4.088351	-5.201903
H	11.756392	1.833549	-4.917202
H	14.248406	1.177890	-6.129408
H	14.420350	3.590566	-6.455251
H	12.846329	2.977977	-6.933265
H	11.970851	4.079335	-5.266599
N	14.792294	1.722322	-3.074271
C	15.928267	1.647463	-2.176843
C	16.804560	0.409991	-2.402623
O	17.934510	0.394028	-1.988350
C	15.495334	1.578022	-0.707310
C	14.638736	2.735142	-0.197993

C	14.285265	2.488615	1.269059
N	13.259778	3.383220	1.790963
C	13.437031	4.534134	2.418972
N	14.654643	5.009739	2.656236
O	15.027936	7.465602	4.210742
H	14.744204	8.352164	3.972083
H	15.745893	7.571535	4.821879
N	12.386879	5.222483	2.815285
H	13.900806	1.420456	-2.758176
H	16.561947	2.504372	-2.346507
H	14.954826	0.650121	-0.551663
H	16.407320	1.508875	-0.124521
H	15.156423	3.682909	-0.314349
H	13.719550	2.816364	-0.766363
H	13.888865	1.489253	1.375952
H	15.164630	2.531614	1.900891
H	12.319759	3.087225	1.619716
H	15.462651	4.517082	2.358613
H	14.789755	5.864579	3.168103
H	11.431450	4.942520	2.657106
H	12.478890	6.065589	3.335508
N	16.200243	-0.648980	-2.967249
C	16.870911	-1.911444	-3.168063
C	17.670040	-1.889279	-4.467661
H	18.062080	-0.909278	-4.748851
O	17.878681	-2.853544	-5.128762
C	15.868239	-3.070209	-3.149497
C	15.324776	-3.399867	-1.792053
N	14.403859	-2.627488	-1.112382
O	12.508213	-0.434098	-0.465247

H	13.145673	-1.037493	-0.851266
H	12.027814	-0.038330	-1.184376
C	15.619918	-4.490272	-1.049640
C	14.172683	-3.251551	-0.003857
N	14.883081	-4.381637	0.103104
H	15.285615	-0.550381	-3.352678
H	17.596037	-2.030736	-2.370677
H	15.050771	-2.842318	-3.824804
H	16.369122	-3.943997	-3.543957
H	16.275343	-5.314047	-1.234992
H	13.494340	-2.922022	0.757056
H	14.782430	-5.064459	0.821874
O	-14.798003	-2.305642	5.077112
H	-15.090888	-1.616867	4.485156
H	-14.377476	-1.862811	5.806964
O	-12.886313	-0.760382	6.902943
H	-12.159802	-1.250025	7.273334
H	-13.153007	-0.137559	7.567914
O	-12.140772	-0.228791	4.090461
H	-12.285224	-0.223791	5.032520
H	-13.017444	-0.218849	3.702739
O	-13.359306	-2.024100	0.907285
H	-12.590290	-1.456457	0.826721
H	-13.169281	-2.625977	1.626936
O	-7.462894	2.078515	-0.250981
H	-7.582969	2.166579	0.697926
H	-6.548672	1.845155	-0.359334
O	-7.781878	2.147925	2.587834
H	-8.712664	1.982022	2.720968
H	-7.530710	2.835293	3.200006

O	-9.219556	0.268046	-1.543300
H	-8.654417	0.920861	-1.116260
H	-8.625594	-0.395291	-1.892853
O	-13.104983	-2.225893	-1.908178
H	-13.351355	-2.375510	-0.993819
H	-13.802447	-2.556578	-2.463598
O	-13.484588	1.744872	-0.191105
H	-12.857556	1.055739	0.036926
H	-12.999598	2.554874	-0.018958
O	-14.181231	4.914670	2.449534
H	-13.801872	5.401488	3.175814
H	-14.711660	4.211922	2.806152
O	-15.446011	2.145884	1.861697
H	-16.298797	2.345407	1.497799
H	-14.850135	2.051818	1.115481
O	-13.497749	0.498958	-2.728436
H	-13.706908	1.081122	-1.997612
H	-13.279855	-0.342565	-2.324130
O	-14.513559	-1.463913	-4.511132
H	-14.515837	-0.619962	-4.063929
H	-15.310446	-1.513964	-5.022410
O	-10.574390	-2.969205	-3.202248
H	-10.866490	-2.657676	-4.055481
H	-11.318892	-2.817667	-2.624688
O	-11.340505	-0.095921	0.389263
H	-10.663811	-0.135502	-0.288446
H	-10.954446	0.397240	1.116547
O	-10.645926	1.635178	2.510120
H	-11.151041	1.180674	3.185435
H	-11.153101	2.384321	2.199776

O	-12.086338	3.782159	1.051177
H	-12.806634	4.185138	1.549342
H	-11.540705	4.511703	0.772887
O	-10.888322	0.832962	-3.747451
H	-11.766127	0.977606	-3.390586
H	-10.308683	0.683062	-2.994652
O	-14.735511	-0.392918	2.923478
H	-15.121325	0.439349	2.649763
H	-14.531491	-0.883649	2.129065
O	-12.750242	-3.277893	3.454330
H	-13.513525	-3.074626	4.006952
H	-12.113276	-2.610803	3.692382
O	-11.716553	-1.375614	-5.293525
H	-12.662337	-1.516011	-5.271893
H	-11.531061	-0.699335	-4.643453

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(+),Y266(-),E183(0)

POTENTIAL:-70mV

N	15.580944	-6.451469	5.391416
H	14.780173	-6.202168	5.939086
C	15.508993	-5.856291	4.054355
C	14.783016	-6.782962	3.060452
O	14.052852	-6.345866	2.186400
C	16.918802	-5.575378	3.520809
H	16.389097	-6.126718	5.884712
H	14.943644	-4.933781	4.050735
H	16.887619	-5.188754	2.509159
H	17.402401	-4.830320	4.142393
H	17.526676	-6.473359	3.529226

N	15.032378	-8.085605	3.186405
H	15.611823	-8.361771	3.949887
C	14.398660	-9.092385	2.333233
H	14.482014	-8.823398	1.292932
H	14.891843	-10.042103	2.492271
C	12.912965	-9.221837	2.671557
O	12.082056	-9.427871	1.826217
N	12.582804	-9.055884	3.966878
H	13.302600	-8.983985	4.648750
C	11.195108	-9.170814	4.421375
H	11.188284	-9.158108	5.503134
H	10.743835	-10.088273	4.076932
C	10.336943	-8.010596	3.900736
O	9.191046	-8.186327	3.583715
N	10.946934	-6.814391	3.855551
C	10.317888	-5.633853	3.318203
C	10.125898	-5.690235	1.799945
O	9.095707	-5.261140	1.338159
C	11.092037	-4.387866	3.777168
O	12.478184	-4.570170	3.768239
H	11.905264	-6.743798	4.107138
H	9.314131	-5.553344	3.702087
H	10.799505	-3.539122	3.169275
H	10.827762	-4.175240	4.802705
H	12.803731	-4.753415	2.895470
N	11.098972	-6.199760	1.024173
C	10.842818	-6.395674	-0.400144
C	9.692691	-7.385274	-0.601544
O	8.944478	-7.280481	-1.545340
C	12.131172	-6.783268	-1.187427

C	12.334410	-8.288589	-1.402440
C	12.155830	-6.059826	-2.535219
H	11.922742	-6.586169	1.431210
H	10.472399	-5.461424	-0.790919
H	12.963052	-6.411050	-0.600020
H	13.288349	-8.450898	-1.893511
H	12.333844	-8.853758	-0.481177
H	11.567700	-8.697764	-2.053167
H	13.050308	-6.323364	-3.088571
H	11.295100	-6.333226	-3.135653
H	12.154727	-4.984474	-2.403241
N	9.570430	-8.340342	0.328312
H	10.314649	-8.474146	0.974145
C	8.593019	-9.421182	0.241228
H	8.932305	-10.216770	0.892269
H	8.535637	-9.806255	-0.765234
C	7.181203	-9.042464	0.638009
O	6.257797	-9.497564	0.003641
N	7.002492	-8.221880	1.679685
C	5.669019	-7.732021	1.946137
C	5.252621	-6.721873	0.882411
O	4.076751	-6.627532	0.602378
C	5.413666	-7.224142	3.379357
C	5.551149	-8.367537	4.389728
C	6.257926	-6.016989	3.792493
H	7.779501	-7.956116	2.244709
H	4.985221	-8.550829	1.784424
H	4.373722	-6.912400	3.370605
H	5.260481	-8.028316	5.378435
H	4.911189	-9.203555	4.126944

H	6.572303	-8.727453	4.447510
H	5.916474	-5.642739	4.751679
H	7.299292	-6.290260	3.902023
H	6.189352	-5.203276	3.078847
N	6.173165	-5.995446	0.240637
C	5.775650	-5.174300	-0.891224
C	5.339778	-6.055846	-2.069924
O	4.316554	-5.802555	-2.661062
C	6.869646	-4.156740	-1.271726
C	7.070893	-3.141320	-0.132717
C	6.498936	-3.444256	-2.577032
C	8.367774	-2.339676	-0.245832
H	7.134029	-6.050096	0.501393
H	4.879069	-4.636632	-0.621597
H	7.798320	-4.700086	-1.420947
H	6.218484	-2.463887	-0.116855
H	7.078334	-3.655467	0.819086
H	7.205586	-2.655636	-2.796593
H	6.497377	-4.118719	-3.423668
H	5.511966	-2.998986	-2.509092
H	8.470914	-1.666203	0.598331
H	9.226825	-3.000371	-0.244817
H	8.406844	-1.740406	-1.148542
N	6.110937	-7.098823	-2.408166
H	7.004041	-7.224504	-1.980349
C	5.766224	-7.936500	-3.536910
H	6.596769	-8.609256	-3.711161
H	5.607735	-7.348312	-4.428476
C	4.498689	-8.766736	-3.333203
O	3.658210	-8.824187	-4.199480

N	4.392527	-9.424027	-2.171602
H	5.130655	-9.378505	-1.501821
C	3.209146	-10.183380	-1.842411
H	2.968932	-10.893506	-2.619442
H	3.405813	-10.729233	-0.928135
C	1.974189	-9.306856	-1.644805
O	0.886786	-9.700155	-2.000101
N	2.187869	-8.107001	-1.107183
C	1.052634	-7.196951	-1.048103
C	0.601552	-6.713526	-2.428651
O	-0.582310	-6.579102	-2.644204
C	1.251457	-5.970574	-0.162525
O	1.412772	-6.294255	1.178745
H	3.086709	-7.815605	-0.796908
H	0.208799	-7.739346	-0.654199
H	2.078030	-5.371688	-0.529123
H	0.344443	-5.394923	-0.244733
H	2.319777	-6.527902	1.321835
N	1.523733	-6.420954	-3.355538
C	1.118171	-6.006582	-4.686094
C	0.366591	-7.131210	-5.393853
O	-0.616579	-6.878354	-6.058668
C	2.319655	-5.472227	-5.499986
C	2.696594	-4.078811	-4.969418
C	2.025603	-5.435939	-7.004976
C	4.006520	-3.527492	-5.529793
H	2.495346	-6.472438	-3.135669
H	0.385122	-5.217788	-4.597028
H	3.153949	-6.147638	-5.335701
H	1.887508	-3.387959	-5.200378

H	2.775597	-4.119379	-3.890688
H	2.876429	-5.040229	-7.545503
H	1.828531	-6.423019	-7.405382
H	1.167262	-4.809177	-7.225534
H	4.277310	-2.614058	-5.010545
H	4.817030	-4.236127	-5.392936
H	3.939404	-3.295428	-6.586923
N	0.812661	-8.380776	-5.239064
H	1.658723	-8.555543	-4.737799
C	0.043838	-9.489011	-5.752955
H	-0.063094	-9.437045	-6.826236
H	0.563431	-10.404330	-5.499466
C	-1.365267	-9.540096	-5.166931
O	-2.317049	-9.778914	-5.874508
N	-1.472644	-9.318876	-3.858022
C	-2.773861	-9.358770	-3.234318
C	-3.688320	-8.224570	-3.694876
O	-4.883588	-8.440681	-3.757278
C	-2.678486	-9.337286	-1.701918
O	-3.924134	-9.612073	-1.121424
H	-0.656065	-9.230217	-3.289993
H	-3.288400	-10.263844	-3.524706
H	-1.994466	-10.109348	-1.378045
H	-2.294276	-8.379929	-1.366622
H	-4.614315	-9.215993	-1.638945
N	-3.140832	-7.038300	-3.955706
C	-3.899323	-5.915086	-4.482726
C	-4.451814	-6.249649	-5.867267
O	-5.624687	-6.088408	-6.120172
C	-2.987397	-4.668975	-4.499857

C	-3.418161	-3.519203	-5.398608
C	-4.746416	-3.185602	-5.638959
C	-2.430755	-2.759753	-6.021257
C	-5.071658	-2.147370	-6.500352
C	-2.750066	-1.710393	-6.864747
C	-4.078759	-1.406114	-7.116393
H	-2.168236	-6.911483	-3.766018
H	-4.761149	-5.732637	-3.860641
H	-2.882581	-4.329553	-3.473769
H	-2.005629	-4.982126	-4.824976
H	-5.540598	-3.751901	-5.194369
H	-1.395513	-2.998702	-5.851834
H	-6.110294	-1.946391	-6.699659
H	-1.964466	-1.141973	-7.329659
H	-4.330924	-0.608516	-7.793667
N	-3.582681	-6.715106	-6.770418
C	-4.048127	-7.046157	-8.097915
C	-5.186090	-8.063944	-8.050111
O	-6.114137	-7.965980	-8.809499
C	-2.916689	-7.590810	-8.972520
S	-1.688348	-6.353753	-9.500059
H	-2.632397	-6.879591	-6.510637
H	-4.472223	-6.170046	-8.565992
H	-2.417255	-8.416480	-8.483860
H	-3.349076	-7.962399	-9.891961
H	-1.067496	-6.199102	-8.340924
N	-5.078560	-9.066910	-7.155609
H	-4.238851	-9.204214	-6.634586
C	-6.086025	-10.114377	-7.182687
H	-6.261083	-10.452751	-8.192667

H	-5.714273	-10.946867	-6.596749
C	-7.459139	-9.722627	-6.613157
O	-8.480633	-10.092015	-7.125244
N	-7.417940	-9.016150	-5.478415
C	-8.636115	-8.653971	-4.781504
C	-9.495657	-7.633536	-5.521422
O	-10.688492	-7.607651	-5.361495
C	-8.345059	-8.144470	-3.358873
C	-7.426847	-6.915813	-3.231955
C	-8.012652	-5.535819	-3.104155
O	-9.305154	-5.428966	-3.235643
H	-9.566081	-4.511826	-3.102773
O	-7.307092	-4.582490	-2.878392
H	-6.532786	-8.774357	-5.086263
H	-9.265048	-9.529213	-4.698554
H	-9.298086	-7.962025	-2.882575
H	-7.870967	-8.961678	-2.826041
H	-6.797836	-7.023546	-2.358218
H	-6.742023	-6.849089	-4.060794
N	-8.837281	-6.733946	-6.273830
C	-9.555208	-5.702634	-7.000846
C	-10.241246	-6.303328	-8.225725
H	-9.886965	-7.288064	-8.536094
O	-11.123214	-5.743558	-8.795675
C	-8.611510	-4.505222	-7.297455
O	-8.597017	-3.622202	-6.192752
C	-8.932695	-3.726903	-8.570353
H	-7.859762	-6.848467	-6.436592
H	-10.361686	-5.346750	-6.373685
H	-7.600579	-4.876156	-7.370234

H	-9.438003	-3.183621	-6.139031
H	-8.252828	-2.882799	-8.630093
H	-8.801458	-4.331156	-9.458851
H	-9.956879	-3.366625	-8.569319
N	-12.952099	-9.022565	3.174142
H	-13.213067	-9.553349	2.368879
C	-11.773563	-8.180068	2.898826
C	-10.790797	-8.116813	4.051837
O	-9.663991	-7.701334	3.858866
C	-12.146833	-6.729545	2.544429
O	-12.732347	-6.198257	3.704599
C	-13.100838	-6.633808	1.358713
H	-13.732180	-8.453398	3.440187
H	-11.218895	-8.607381	2.074186
H	-11.231022	-6.202436	2.314759
H	-12.851647	-5.257655	3.590089
H	-13.263333	-5.590693	1.110282
H	-12.705959	-7.131727	0.480806
H	-14.064686	-7.067140	1.597799
N	-11.197245	-8.533612	5.241880
H	-12.116436	-8.918186	5.272036
C	-10.412669	-8.535205	6.452135
H	-10.331223	-7.540879	6.861664
H	-10.939610	-9.140480	7.180255
C	-8.977467	-9.059643	6.382018
O	-8.146753	-8.509831	7.062118
N	-8.659576	-10.125588	5.624873
H	-9.368442	-10.596078	5.109017
C	-7.270783	-10.559509	5.524535
H	-7.254061	-11.535705	5.056973

H	-6.833680	-10.645053	6.506363
C	-6.387435	-9.608346	4.692696
O	-5.221533	-9.463486	4.952964
N	-7.045410	-9.018041	3.701147
C	-6.310791	-7.982307	2.986439
C	-6.265892	-6.696323	3.808100
O	-5.273688	-6.006844	3.776808
C	-6.639029	-7.804216	1.490455
C	-7.802289	-6.937044	1.054349
C	-7.783366	-5.559917	1.256384
C	-8.849303	-7.481404	0.321962
C	-8.793900	-4.754281	0.759851
C	-9.849025	-6.675063	-0.197929
C	-9.829848	-5.309104	0.027269
H	-8.039932	-9.013245	3.684374
H	-5.287260	-8.313220	2.998176
H	-5.738656	-7.393325	1.047002
H	-6.744883	-8.800772	1.078490
H	-6.960450	-5.105017	1.776080
H	-8.866993	-8.539436	0.124331
H	-8.754232	-3.691639	0.921090
H	-10.626298	-7.108815	-0.799445
H	-10.600457	-4.682964	-0.384771
N	-7.294316	-6.408986	4.609639
C	-7.227561	-5.302045	5.534434
C	-6.096903	-5.516946	6.539673
O	-5.444831	-4.565812	6.913838
C	-8.600103	-5.148622	6.222600
C	-8.841720	-3.835506	6.935796
C	-9.097852	-2.677055	6.207847

C	-8.880551	-3.771106	8.322263
C	-9.376988	-1.483019	6.849914
C	-9.169184	-2.579369	8.971176
C	-9.417835	-1.431224	8.237381
H	-8.162423	-6.882997	4.485443
H	-6.971403	-4.390630	5.012884
H	-9.352249	-5.262344	5.448756
H	-8.730460	-5.968286	6.915933
H	-9.085555	-2.706831	5.131767
H	-8.689596	-4.656063	8.903829
H	-9.561263	-0.597156	6.269776
H	-9.190687	-2.548983	10.045647
H	-9.622741	-0.501325	8.737904
N	-5.855191	-6.753756	6.970338
H	-6.508096	-7.477079	6.765111
C	-4.773232	-7.044576	7.884499
H	-4.809152	-6.412003	8.758724
H	-4.881918	-8.073724	8.202392
C	-3.380280	-6.867559	7.282620
O	-2.505144	-6.368755	7.949534
N	-3.183362	-7.298853	6.031826
C	-1.904254	-7.129798	5.359139
C	-1.649722	-5.662443	4.986657
O	-0.548371	-5.181647	5.149540
C	-1.826576	-8.075697	4.140312
C	-0.660442	-7.730824	3.212267
C	-1.730441	-9.532267	4.608212
H	-3.919237	-7.777663	5.558602
H	-1.112616	-7.373855	6.052609
H	-2.747525	-7.954226	3.574625

H	-0.600446	-8.463360	2.414463
H	-0.765634	-6.759153	2.750581
H	0.284622	-7.743232	3.746384
H	-1.747066	-10.200284	3.753147
H	-0.796988	-9.698143	5.140118
H	-2.547872	-9.813172	5.259657
N	-2.681891	-4.974529	4.488449
C	-2.544729	-3.598248	4.052412
C	-2.409400	-2.667629	5.255735
O	-1.517012	-1.850248	5.300323
C	-3.719613	-3.148952	3.171265
C	-3.946461	-3.930458	1.866772
C	-2.815028	-3.839906	0.855659
O	-1.692692	-4.192297	1.246563
O	-3.087204	-3.435732	-0.288369
H	-3.550456	-5.439000	4.341003
H	-1.630408	-3.497602	3.498921
H	-4.635599	-3.195680	3.752390
H	-3.554492	-2.100768	2.937811
H	-4.095971	-4.976696	2.089065
H	-4.855834	-3.559717	1.407102
N	-3.309499	-2.786699	6.250263
C	-3.093962	-2.024874	7.456968
C	-1.781427	-2.422854	8.139373
O	-1.112920	-1.584727	8.704382
C	-4.230130	-1.984010	8.489110
O	-4.436969	-3.210485	9.125309
C	-5.512456	-1.384185	7.924365
H	-3.985337	-3.517943	6.232720
H	-2.930707	-0.999966	7.162568

H	-3.859592	-1.324027	9.263496
H	-4.880343	-3.802171	8.529640
H	-6.246415	-1.303123	8.716555
H	-5.327951	-0.391537	7.525320
H	-5.931295	-1.996477	7.136884
N	-1.380404	-3.700488	8.043333
H	-2.031405	-4.418664	7.815121
C	-0.187103	-4.107119	8.740481
H	-0.237745	-3.891376	9.798432
H	-0.075398	-5.174668	8.604493
C	1.064398	-3.419527	8.218984
O	1.940509	-3.075711	8.979614
N	1.154868	-3.258584	6.883072
C	2.333323	-2.661209	6.317654
C	2.291863	-1.139270	6.162009
O	3.361073	-0.575733	6.019687
C	2.833850	-3.351996	5.048951
S	1.917574	-3.010657	3.521828
H	0.424128	-3.613200	6.298452
H	3.116994	-2.796536	7.047750
H	3.839399	-3.004126	4.860731
H	2.869582	-4.419143	5.218859
H	0.871393	-3.797789	3.723145
N	1.141585	-0.471381	6.273705
C	1.204073	0.968482	6.491382
C	1.754778	1.271816	7.870572
O	2.367382	2.289418	8.086251
C	-0.097125	1.738345	6.177633
C	-1.199708	1.569150	7.233116
C	-0.554722	1.428947	4.747046

C	-2.468607	2.370110	6.932475
H	0.273305	-0.966275	6.289291
H	1.951674	1.351075	5.815093
H	0.205235	2.779403	6.212995
H	-1.448695	0.524663	7.354476
H	-0.812453	1.897582	8.193255
H	-1.310148	2.133330	4.421954
H	0.278296	1.505066	4.053675
H	-0.965854	0.432503	4.657950
H	-3.141183	2.341901	7.784491
H	-2.243043	3.412937	6.724540
H	-3.006175	1.971272	6.079117
N	1.549774	0.323287	8.791241
H	0.889446	-0.401834	8.613645
C	1.977963	0.512992	10.159942
H	1.469328	-0.221878	10.771109
H	1.737815	1.502921	10.517661
C	3.481890	0.337003	10.305708
O	4.163989	1.127275	10.898753
N	3.999613	-0.753731	9.695240
H	3.390273	-1.464888	9.349179
C	5.424647	-0.938945	9.667146
H	5.637679	-1.909414	9.233983
H	5.855301	-0.905126	10.657241
C	6.156885	0.119116	8.844830
O	7.291893	0.411921	9.129599
N	5.502087	0.621274	7.799020
C	6.098611	1.759282	7.146322
C	5.516989	3.077428	7.650625
H	5.008623	3.037109	8.612516

O	5.647525	4.096724	7.045855
C	6.000490	1.675605	5.620851
C	6.752868	0.508291	5.015840
C	8.118857	0.324860	5.234851
C	6.092155	-0.399758	4.193756
C	8.805238	-0.719444	4.630036
C	6.776271	-1.441664	3.587522
C	8.136741	-1.601990	3.795788
H	4.575437	0.334273	7.572148
H	7.134546	1.773642	7.449604
H	4.957923	1.610670	5.335968
H	6.377511	2.610542	5.220655
H	8.647345	0.980755	5.905308
H	5.031812	-0.304257	4.056810
H	9.856335	-0.846128	4.824330
H	6.243756	-2.132916	2.958885
H	8.657125	-2.413641	3.321104
N	12.613550	9.596234	-1.248801
H	11.871931	9.914842	-1.844065
C	12.304852	8.264740	-0.719487
C	11.274074	8.450488	0.386932
O	10.266460	7.778079	0.416885
C	13.562635	7.581254	-0.164773
C	14.645809	7.276762	-1.205210
S	14.019107	6.202959	-2.529293
C	15.503560	6.052522	-3.551813
H	13.431761	9.572127	-1.824612
H	11.834595	7.616402	-1.447338
H	14.000549	8.205693	0.608096
H	13.255556	6.653940	0.305079

H	15.046417	8.189438	-1.631929
H	15.470590	6.784241	-0.702674
H	15.253538	5.397039	-4.372129
H	15.803961	7.015967	-3.943018
H	16.320662	5.615815	-2.992518
N	11.503854	9.413387	1.296494
C	10.594376	9.608173	2.408605
C	9.277505	10.276976	2.011975
O	8.282490	10.058380	2.656594
C	11.277548	10.367649	3.552607
C	12.448646	9.561571	4.084067
O	13.583823	9.823178	3.744914
N	12.144241	8.558465	4.917144
H	12.327517	9.968356	1.205447
H	10.294804	8.638030	2.770465
H	11.659335	11.324850	3.220226
H	10.547717	10.536155	4.334353
H	12.887664	7.961865	5.209970
H	11.222682	8.171961	4.951082
N	9.263954	11.068441	0.922631
H	10.110243	11.226365	0.425284
C	8.003503	11.517472	0.368854
H	8.201018	12.260056	-0.393596
H	7.389140	11.966802	1.131876
C	7.186384	10.384437	-0.254318
O	5.986775	10.472231	-0.295113
N	7.862978	9.332464	-0.761465
C	7.170138	8.144936	-1.231517
C	6.633636	7.301781	-0.064246
O	5.533035	6.810543	-0.144947

C	8.047996	7.341936	-2.220961
C	8.344874	8.194047	-3.469685
C	7.376586	6.017832	-2.604920
C	9.428444	7.619508	-4.385483
H	8.823031	9.228200	-0.530946
H	6.279797	8.471393	-1.746362
H	8.986449	7.114217	-1.723515
H	7.423341	8.321927	-4.033247
H	8.649049	9.189073	-3.162211
H	7.994109	5.475714	-3.309702
H	7.222745	5.377564	-1.744888
H	6.407909	6.182798	-3.065074
H	9.624223	8.299583	-5.208170
H	10.363320	7.471946	-3.851578
H	9.146586	6.666005	-4.816531
N	7.386090	7.177064	1.047533
C	6.878058	6.458044	2.204615
C	5.525417	7.035242	2.642676
O	4.575698	6.325710	2.869639
C	7.831823	6.546133	3.406336
C	9.253242	5.997872	3.245998
O	10.145552	6.633626	3.800850
O	9.426538	4.934993	2.599048
H	8.346713	7.444503	1.025500
H	6.683575	5.429172	1.944750
H	7.919361	7.570733	3.736175
H	7.374017	5.992117	4.223285
N	5.483175	8.373301	2.790396
H	6.312418	8.911141	2.653236
C	4.290495	9.037052	3.256214

H	4.528240	10.079997	3.424687
H	3.946128	8.620644	4.189680
C	3.130157	8.987765	2.271344
O	1.988696	9.117162	2.649945
N	3.466368	8.825158	0.988734
H	4.428136	8.815095	0.742262
C	2.517188	8.905263	-0.078309
H	3.062191	9.089692	-0.995140
H	1.843547	9.738082	0.069355
C	1.609135	7.687017	-0.310189
O	0.576528	7.817136	-0.907598
N	2.067321	6.540452	0.227893
C	1.247478	5.370795	0.435183
C	0.429320	5.471011	1.727210
O	-0.764889	5.294461	1.701385
C	2.105543	4.106074	0.428589
H	2.967725	6.569127	0.657195
H	0.519337	5.320351	-0.356785
H	1.488821	3.234769	0.619684
H	2.577659	3.996865	-0.540870
H	2.882861	4.150965	1.184548
N	1.068144	5.733430	2.884289
C	0.338240	5.567665	4.132151
C	-0.773547	6.602325	4.288484
O	-1.809091	6.306242	4.844108
C	1.259390	5.493095	5.375049
C	1.849954	6.839293	5.821976
C	2.348874	4.431293	5.161096
C	2.694150	6.741593	7.095152
H	2.056666	5.861681	2.900722

H	-0.191263	4.627355	4.077572
H	0.606028	5.150646	6.171767
H	2.450286	7.255113	5.019340
H	1.045016	7.544810	6.000464
H	2.725099	4.075955	6.109256
H	1.956046	3.575736	4.621135
H	3.187566	4.825930	4.597762
H	2.997228	7.732711	7.419839
H	2.126660	6.291255	7.904203
H	3.590948	6.151261	6.954100
N	-0.550448	7.835331	3.810099
H	0.334165	8.069694	3.410291
C	-1.514985	8.881093	4.023532
H	-1.098684	9.807618	3.648530
H	-1.729449	9.011353	5.074384
C	-2.866971	8.618756	3.365893
O	-3.871298	8.845797	4.000033
N	-2.902686	8.108974	2.120752
C	-4.238908	8.033144	1.526312
C	-4.983016	6.752713	1.867113
O	-6.195326	6.753512	1.841256
C	-4.018977	8.294981	0.029374
C	-2.743956	9.145315	0.042208
C	-1.900516	8.455929	1.102605
H	-4.854125	8.818720	1.936371
H	-3.864510	7.368756	-0.508147
H	-4.874696	8.795099	-0.406124
H	-2.231365	9.201413	-0.900536
H	-2.982282	10.157674	0.359873
H	-1.435726	7.562413	0.726469

H	-1.127588	9.090184	1.504427
N	-4.262083	5.675638	2.205270
C	-4.913756	4.487561	2.728202
C	-5.629669	4.783442	4.049083
O	-6.704184	4.276882	4.284658
C	-3.920509	3.321935	2.930975
C	-3.593074	2.501948	1.699298
C	-4.103263	1.217462	1.542430
C	-2.725310	2.957968	0.709553
C	-3.773125	0.420881	0.456677
C	-2.385976	2.179111	-0.376871
C	-2.891591	0.873949	-0.548713
O	-2.575077	0.154040	-1.578985
H	-3.268415	5.756907	2.260692
H	-5.692121	4.185194	2.045196
H	-3.015997	3.722001	3.380431
H	-4.359600	2.660499	3.669923
H	-4.769433	0.819062	2.291192
H	-2.286245	3.931681	0.795370
H	-4.149608	-0.585843	0.393077
H	-1.708846	2.562527	-1.121988
N	-5.003831	5.588445	4.927061
H	-4.072496	5.898401	4.741623
C	-5.608129	5.941694	6.191342
H	-4.823434	6.281171	6.856408
H	-6.091579	5.085964	6.633940
C	-6.660989	7.045619	6.082282
O	-7.715594	6.968719	6.671221
N	-6.342145	8.091259	5.313948
H	-5.447584	8.140444	4.874543

C	-7.257648	9.220183	5.085240
H	-6.772996	9.882451	4.379837
H	-7.440908	9.763387	6.000489
C	-8.621434	8.828988	4.542963
O	-9.606154	9.421356	4.911824
N	-8.673304	7.827129	3.645035
C	-9.943657	7.435616	3.076809
C	-10.836112	6.654154	4.038280
O	-11.951366	6.350768	3.656646
C	-9.775355	6.671601	1.743354
O	-10.966221	6.755487	0.999702
C	-9.335359	5.222831	1.911865
H	-7.828428	7.411577	3.308851
H	-10.508949	8.330803	2.856257
H	-9.027794	7.206342	1.172417
H	-11.678807	6.479207	1.568244
H	-9.141346	4.784207	0.940478
H	-8.432174	5.142045	2.500323
H	-10.115390	4.638921	2.389369
N	-10.364858	6.344445	5.246952
C	-11.209900	5.754972	6.261796
C	-12.250233	6.739905	6.800707
O	-13.299761	6.324066	7.234959
C	-10.393766	5.201063	7.438215
C	-9.459862	4.028309	7.101350
C	-8.608341	3.695033	8.330318
C	-10.218984	2.785840	6.625799
H	-9.431732	6.593809	5.498784
H	-11.788480	4.964027	5.813640
H	-9.808421	6.007047	7.865124

H	-11.106374	4.885791	8.194963
H	-8.787056	4.333148	6.307967
H	-7.910733	2.890830	8.114203
H	-8.035275	4.558331	8.650941
H	-9.230083	3.379019	9.165326
H	-9.522406	1.974178	6.436950
H	-10.930118	2.450629	7.378911
H	-10.765335	2.958213	5.705507
N	-11.913914	8.040303	6.829253
C	-12.864986	9.029249	7.245767
C	-13.878678	9.396399	6.182266
H	-14.628944	10.123921	6.511973
O	-13.888666	8.967770	5.077159
H	-11.120801	8.352755	6.310483
H	-13.401643	8.681093	8.119589
H	-12.337839	9.934594	7.531090
N	-11.495258	10.629858	-3.034777
H	-11.248077	10.848333	-2.090127
C	-11.816457	9.206991	-3.172691
C	-11.414026	8.858194	-4.598774
O	-10.375345	8.293058	-4.845137
C	-13.245719	8.788261	-2.767124
C	-13.495134	9.129862	-1.286499
C	-13.470822	7.296728	-3.047345
C	-14.921044	8.858600	-0.803354
H	-12.278577	11.208827	-3.272327
H	-11.118046	8.661113	-2.553749
H	-13.958980	9.364155	-3.361464
H	-12.791593	8.573797	-0.671323
H	-13.282903	10.182143	-1.125066

H	-14.499942	7.015742	-2.863719
H	-13.248956	7.033394	-4.077557
H	-12.840088	6.689705	-2.405270
H	-15.044255	9.216650	0.212390
H	-15.653383	9.367357	-1.424742
H	-15.159411	7.801297	-0.802281
N	-12.214010	9.288635	-5.604063
H	-13.131104	9.601756	-5.380554
C	-11.972873	8.843878	-6.959262
H	-12.035595	7.767552	-7.044834
H	-12.729370	9.282577	-7.598478
C	-10.601634	9.233249	-7.517685
O	-9.997336	8.495992	-8.242649
N	-10.162498	10.476538	-7.182377
H	-10.709239	11.005111	-6.541746
C	-8.894338	11.023969	-7.637102
H	-8.790001	10.891226	-8.702742
H	-8.880302	12.081585	-7.408178
C	-7.672571	10.358998	-6.988330
O	-6.759069	9.923372	-7.632194
N	-7.657768	10.354083	-5.620722
H	-8.475389	10.646641	-5.135096
C	-6.495249	9.961279	-4.832307
H	-5.598013	10.374782	-5.264527
H	-6.616236	10.361980	-3.833380
C	-6.268288	8.463922	-4.714299
O	-5.135168	8.046485	-4.751247
N	-7.314744	7.639629	-4.521267
C	-7.020319	6.271198	-4.124299
C	-6.465820	5.440474	-5.275172

O	-5.668775	4.563531	-5.043674
C	-8.156724	5.541156	-3.368995
C	-9.345704	5.122690	-4.249903
C	-8.567333	6.358545	-2.138727
C	-10.386214	4.279190	-3.509429
H	-8.251834	7.988603	-4.514215
H	-6.188423	6.314123	-3.437886
H	-7.685830	4.629992	-3.010188
H	-9.825096	5.993879	-4.678492
H	-8.968657	4.536094	-5.084857
H	-9.222673	5.791693	-1.491862
H	-7.697748	6.634611	-1.551106
H	-9.089360	7.266113	-2.418740
H	-11.138813	3.914238	-4.202010
H	-9.930522	3.416713	-3.033396
H	-10.898388	4.848340	-2.743523
N	-6.882017	5.679794	-6.537956
C	-6.242877	4.969527	-7.628380
C	-4.821659	5.460691	-7.917387
O	-3.990473	4.676202	-8.307804
C	-7.108198	4.971753	-8.897586
C	-8.277947	3.978321	-8.838637
C	-7.800139	2.523672	-8.902302
N	-8.881613	1.534874	-8.891460
C	-9.434749	0.982245	-7.816715
N	-9.166716	1.438150	-6.605629
N	-10.274741	-0.031477	-7.966914
H	-7.493953	6.446051	-6.719521
H	-6.080804	3.958127	-7.296394
H	-7.494577	5.969805	-9.079059

H	-6.473446	4.727161	-9.743172
H	-8.868341	4.149107	-7.943185
H	-8.939450	4.160827	-9.678931
H	-7.254451	2.358428	-9.821294
H	-7.115529	2.281763	-8.100881
H	-9.153769	1.158705	-9.772140
H	-8.640528	2.272789	-6.487212
H	-9.639822	1.093020	-5.784688
H	-10.333485	-0.492681	-8.847730
H	-10.589868	-0.568969	-7.173564
N	-4.571419	6.757537	-7.721986
H	-5.302822	7.370440	-7.441701
C	-3.257792	7.352338	-8.011302
H	-2.929120	7.090538	-9.004951
H	-3.360599	8.426642	-7.939669
C	-2.202314	6.874116	-7.024551
O	-1.073683	6.639153	-7.377141
N	-2.634097	6.758718	-5.763275
C	-1.761616	6.448145	-4.656398
C	-1.491280	4.960888	-4.524187
O	-0.363855	4.577069	-4.319321
C	-2.350380	7.048033	-3.373471
C	-1.763409	6.354104	-2.145479
C	-2.113584	8.563997	-3.410440
H	-3.557786	7.064290	-5.547223
H	-0.788704	6.881447	-4.838418
H	-3.418831	6.866648	-3.387816
H	-1.980538	6.901562	-1.247451
H	-2.173217	5.356047	-2.033377
H	-0.690739	6.283819	-2.215385

H	-2.838959	9.089537	-2.805586
H	-1.118867	8.805764	-3.051243
H	-2.215567	8.949902	-4.418163
N	-2.517791	4.099989	-4.645961
C	-2.183943	2.693865	-4.750294
C	-1.220401	2.507869	-5.924342
O	-0.293656	1.732576	-5.842545
C	-3.407935	1.776689	-4.871585
C	-4.365142	1.887237	-3.676898
C	-5.406639	0.763185	-3.611684
N	-4.878991	-0.427510	-2.949865
C	-5.583335	-1.519506	-2.748470
N	-6.812937	-1.655781	-3.294816
N	-5.154037	-2.493880	-1.972978
H	-3.439509	4.421220	-4.850424
H	-1.629168	2.394292	-3.874460
H	-3.944310	1.990555	-5.794151
H	-3.028749	0.764647	-4.951019
H	-3.802460	1.900235	-2.756953
H	-4.904655	2.820111	-3.734796
H	-6.276650	1.112905	-3.065381
H	-5.727669	0.511016	-4.619263
H	-3.984166	-0.324710	-2.456363
H	-6.974347	-1.177487	-4.151327
H	-7.208358	-2.578475	-3.266250
H	-4.300366	-2.472857	-1.440328
H	-5.664429	-3.351690	-1.949454
N	-1.459790	3.193298	-7.035093
H	-2.285219	3.739318	-7.148812
C	-0.596550	2.997474	-8.183376

H	-0.949630	3.640655	-8.979121
H	-0.611029	1.972250	-8.524591
C	0.855931	3.344672	-7.871776
O	1.781598	2.711140	-8.313085
N	1.005371	4.405090	-7.063925
H	0.212146	4.964338	-6.846605
C	2.282350	4.880661	-6.640316
H	2.919001	5.137295	-7.477590
H	2.128458	5.777142	-6.053742
C	3.092840	3.928367	-5.775178
O	4.297669	4.059457	-5.688187
N	2.428015	2.983364	-5.101894
C	3.096572	2.136985	-4.148066
C	4.270175	1.327688	-4.711094
O	5.184059	1.025872	-3.970246
C	2.008341	1.259942	-3.526779
C	2.372020	0.441550	-2.293976
C	1.055758	0.031691	-1.642286
N	1.235378	-1.004799	-0.647430
C	0.298798	-1.926790	-0.373999
N	-0.855083	-1.920612	-0.991963
N	0.588351	-2.879746	0.489881
H	1.438713	2.900979	-5.211350
H	3.557525	2.746655	-3.380324
H	1.210708	1.943596	-3.257011
H	1.592591	0.612085	-4.289465
H	2.946770	-0.439481	-2.558613
H	2.977062	1.024247	-1.603012
H	0.561443	0.897278	-1.214220
H	0.398150	-0.361469	-2.402202

H	1.939830	-0.874312	0.043445
H	-1.298717	-1.062577	-1.309484
H	-1.527138	-2.646256	-0.776918
H	1.506800	-2.990418	0.850720
H	-0.161269	-3.479286	0.821989
N	4.280002	0.941732	-5.998662
H	3.540833	1.225199	-6.608051
C	5.363424	0.116638	-6.504622
H	5.137151	-0.137697	-7.532686
H	5.442866	-0.800473	-5.942810
C	6.736121	0.755923	-6.476823
O	7.738867	0.089514	-6.368823
N	6.766124	2.085339	-6.608293
H	5.911903	2.604351	-6.566390
C	8.004993	2.823920	-6.549089
H	8.710109	2.440732	-7.273087
H	7.799709	3.854876	-6.804647
C	8.746900	2.826001	-5.210612
O	9.887685	3.236397	-5.157394
N	8.101358	2.335228	-4.144928
C	8.680903	2.169883	-2.822859
C	9.947179	1.302961	-2.830367
O	10.764503	1.385616	-1.927871
C	7.576267	1.499495	-1.975518
C	7.769338	1.380008	-0.464046
C	7.422858	2.651184	0.320627
C	7.309505	2.388446	1.818384
N	8.648575	2.358116	2.478467
O	11.029331	1.615187	0.898018
H	10.881146	1.825071	-0.024448

H	11.506317	0.787662	0.849543
H	7.155638	2.032457	-4.259047
H	8.977804	3.127170	-2.415175
H	6.658632	2.040632	-2.163162
H	7.411904	0.511411	-2.389546
H	7.090270	0.600060	-0.133568
H	8.764776	1.029803	-0.225093
H	8.134561	3.453008	0.144581
H	6.457656	3.019727	-0.011584
H	6.747001	3.161349	2.318600
H	6.829051	1.442376	2.014474
H	9.360209	1.892163	1.924320
H	8.969585	3.328263	2.631120
H	8.593559	1.882790	3.367436
N	10.062468	0.448216	-3.837538
C	11.109355	-0.537517	-4.069387
C	12.486379	0.023157	-4.427133
O	13.444198	-0.705546	-4.301401
C	10.701431	-1.443076	-5.253560
C	9.563249	-2.441793	-5.000147
C	9.132350	-3.064984	-6.331588
C	9.990084	-3.533487	-4.018744
H	9.324190	0.445767	-4.510612
H	11.264635	-1.125579	-3.176687
H	10.435176	-0.796633	-6.084514
H	11.584405	-1.995209	-5.552449
H	8.706564	-1.911333	-4.596274
H	8.331207	-3.781573	-6.178100
H	8.775123	-2.307430	-7.017426
H	9.959751	-3.592416	-6.799865

H	9.199967	-4.263282	-3.879665
H	10.860108	-4.059658	-4.397726
H	10.242959	-3.137666	-3.039915
N	12.574050	1.261829	-4.919242
C	13.814406	1.845262	-5.393366
C	14.958878	2.033284	-4.379087
O	16.013534	2.413871	-4.812175
C	13.496569	3.172498	-6.085440
O	12.918096	4.089114	-5.200443
H	11.756268	1.833402	-4.916258
H	14.248272	1.179028	-6.129607
H	14.419539	3.591691	-6.454352
H	12.845354	2.979136	-6.931993
H	11.970528	4.078373	-5.262637
N	14.792294	1.722326	-3.074279
C	15.927713	1.647124	-2.176233
C	16.804430	0.410056	-2.402579
O	17.934558	0.394323	-1.988747
C	15.493359	1.575964	-0.707144
C	14.634954	2.731677	-0.197567
C	14.278275	2.482164	1.268234
N	13.252919	3.376635	1.790435
C	13.430800	4.528269	2.417003
N	14.648910	5.003840	2.652460
O	15.028274	7.461559	4.203992
H	14.743853	8.348419	3.967260
H	15.746592	7.566788	4.814797
N	12.381272	5.217168	2.813488
H	13.900680	1.420521	-2.758456
H	16.561246	2.504414	-2.344561

H	14.953644	0.647366	-0.552984
H	16.404775	1.507146	-0.123410
H	15.152401	3.679935	-0.311134
H	13.716902	2.813455	-0.767682
H	13.880352	1.483080	1.371699
H	15.156521	2.522513	1.901889
H	12.312653	3.080244	1.620849
H	15.456406	4.510167	2.355170
H	14.784908	5.859087	3.163319
H	11.425389	4.937390	2.656475
H	12.473703	6.061002	3.332453
N	16.200238	-0.648980	-2.967242
C	16.870752	-1.911587	-3.167518
C	17.670006	-1.889781	-4.467008
H	18.062386	-0.909889	-4.748118
O	17.878402	-2.854052	-5.128230
C	15.867932	-3.070228	-3.148719
C	15.323739	-3.398988	-1.791343
N	14.402798	-2.625854	-1.112620
O	12.505039	-0.433470	-0.461488
H	13.142221	-1.035718	-0.849492
H	12.022768	-0.037399	-1.179250
C	15.618082	-4.489097	-1.048180
C	14.170786	-3.249195	-0.003865
N	14.880727	-4.379499	0.104143
H	15.285196	-0.550771	-3.351807
H	17.595790	-2.030750	-2.370018
H	15.050801	-2.842595	-3.824522
H	16.368880	-3.944319	-3.542447
H	16.273237	-5.313268	-1.232733

H	13.492091	-2.918983	0.756432
H	14.779374	-5.062039	0.823108
O	-15.022332	-2.472904	4.971587
H	-15.215300	-1.663969	4.504968
H	-14.530546	-2.214795	5.744220
O	-12.909024	-1.269273	6.930563
H	-12.222363	-1.721546	7.408263
H	-13.143100	-0.515308	7.458159
O	-12.057046	-0.850324	4.159021
H	-12.178973	-0.901868	5.104213
H	-12.869358	-0.460195	3.833426
O	-13.394460	-1.861170	0.708884
H	-12.619910	-1.296729	0.765568
H	-13.316722	-2.508005	1.414714
O	-7.286814	1.298494	-0.241241
H	-7.499537	1.634533	0.633103
H	-6.357823	1.097608	-0.204946
O	-7.887148	2.075832	2.453266
H	-8.798915	1.921491	2.688293
H	-7.560872	2.752423	3.040734
O	-9.343424	-0.025500	-1.609512
H	-8.581061	0.392263	-1.188839
H	-9.094469	-0.923898	-1.806345
O	-12.844866	-2.342602	-2.020416
H	-13.121070	-2.378383	-1.101268
H	-13.457236	-2.853965	-2.536527
O	-14.033873	0.923434	-0.583660
H	-14.378102	0.061001	-0.376872
H	-13.123337	0.882180	-0.275039
O	-14.251532	4.927624	4.735036

H	-13.682965	5.569178	4.315612
H	-14.290144	5.212331	5.643516
O	-15.231526	2.152017	1.699077
H	-15.858627	2.863324	1.685254
H	-14.946794	1.987269	0.801499
O	-13.156822	0.240589	-3.245781
H	-13.606222	0.770980	-2.590586
H	-12.938664	-0.563428	-2.772435
O	-13.770736	-1.932656	-4.984021
H	-13.939482	-1.069812	-4.612480
H	-14.497007	-2.146080	-5.555548
O	-10.158816	-2.763951	-2.954684
H	-10.300592	-2.610371	-3.882439
H	-11.021513	-2.687230	-2.548996
O	-11.486467	0.211533	0.369975
H	-10.759889	0.130538	-0.249436
H	-11.146307	0.652745	1.155701
O	-10.714271	1.340138	2.829264
H	-10.880652	0.580670	3.384821
H	-11.395603	1.966258	3.090879
O	-13.057024	2.613282	3.631853
H	-13.358808	3.352220	4.162904
H	-13.713452	2.533207	2.947629
O	-10.472382	0.624522	-4.111174
H	-11.377476	0.788837	-3.840270
H	-9.985111	0.491478	-3.290428
O	-14.689701	-0.343782	3.041473
H	-15.011369	0.525584	2.812373
H	-14.564724	-0.802618	2.217301
O	-13.086346	-3.361956	3.148089

H	-13.858824	-3.221180	3.705238
H	-12.460173	-2.723946	3.489388
O	-11.006560	-1.654552	-5.649329
H	-11.936215	-1.878970	-5.566085
H	-10.849057	-0.947846	-5.019580

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(+),Y266(-),E183(0)

POTENTIAL:-35mV

N	15.580944	-6.451469	5.391416
H	14.781091	-6.200103	5.939456
C	15.509751	-5.856564	4.054164
C	14.783016	-6.782962	3.060452
O	14.052231	-6.345849	2.186818
C	16.919877	-5.577004	3.520677
H	16.390237	-6.128756	5.884185
H	14.945257	-4.933528	4.050277
H	16.889205	-5.190740	2.508870
H	17.403974	-4.832107	4.142045
H	17.527065	-6.475436	3.529506
N	15.032378	-8.085605	3.186405
H	15.612411	-8.361775	3.949450
C	14.398660	-9.092385	2.333233
H	14.482160	-8.823545	1.292899
H	14.891694	-10.042153	2.492416
C	12.912930	-9.221560	2.671507
O	12.081797	-9.427103	1.826194
N	12.582804	-9.055884	3.966878
H	13.302624	-8.984073	4.648759

C	11.195108	-9.170814	4.421375
H	11.188291	-9.158045	5.503134
H	10.743837	-10.088296	4.076981
C	10.336943	-8.010596	3.900736
O	9.190873	-8.186196	3.583978
N	10.946985	-6.814479	3.855537
C	10.318198	-5.633870	3.318106
C	10.125791	-5.690670	1.799932
O	9.095030	-5.262426	1.338387
C	11.092794	-4.387934	3.776743
O	12.478717	-4.571005	3.769569
H	11.905387	-6.744053	4.106970
H	9.314538	-5.552986	3.702167
H	10.801350	-3.539534	3.167806
H	10.827492	-4.174283	4.801806
H	12.805484	-4.754836	2.897355
N	11.098814	-6.199773	1.024010
C	10.842605	-6.395616	-0.400299
C	9.692264	-7.385027	-0.601336
O	8.943209	-7.279826	-1.544493
C	12.130941	-6.783382	-1.187602
C	12.333878	-8.288693	-1.402909
C	12.155886	-6.059627	-2.535221
H	11.923312	-6.585041	1.430728
H	10.472291	-5.461328	-0.791112
H	12.962862	-6.411440	-0.600078
H	13.287694	-8.451074	-1.894160
H	12.333414	-8.854024	-0.481751
H	11.567004	-8.697623	-2.053617
H	13.050400	-6.323168	-3.088487

H	11.295217	-6.332776	-3.135875
H	12.154970	-4.984307	-2.402985
N	9.570430	-8.340342	0.328312
H	10.315146	-8.474590	0.973538
C	8.593019	-9.421182	0.241228
H	8.932376	-10.216809	0.892183
H	8.535552	-9.806223	-0.765248
C	7.181275	-9.042549	0.638193
O	6.257642	-9.497245	0.003736
N	7.002656	-8.222457	1.680250
C	5.669209	-7.732900	1.947061
C	5.252360	-6.722864	0.883408
O	4.076325	-6.628877	0.603483
C	5.414160	-7.225036	3.380337
C	5.552431	-8.368373	4.390677
C	6.258144	-6.017592	3.793165
H	7.779778	-7.956827	2.245245
H	4.985483	-8.551816	1.785555
H	4.374079	-6.913683	3.371905
H	5.261938	-8.029263	5.379481
H	4.912756	-9.204679	4.128075
H	6.573742	-8.727837	4.448151
H	5.917098	-5.643641	4.752620
H	7.299669	-6.290423	3.902014
H	6.188808	-5.203807	3.079677
N	6.172629	-5.996260	0.241633
C	5.775138	-5.175126	-0.890224
C	5.339353	-6.056734	-2.068895
O	4.315679	-5.803894	-2.659636
C	6.869138	-4.157520	-1.270669

C	7.070399	-3.142261	-0.131528
C	6.498412	-3.444914	-2.575899
C	8.367244	-2.340569	-0.244584
H	7.133553	-6.050773	0.502348
H	4.878541	-4.637464	-0.620622
H	7.797785	-4.700839	-1.419964
H	6.217942	-2.464864	-0.115509
H	7.077954	-3.656580	0.820178
H	7.205179	-2.656424	-2.795501
H	6.496710	-4.119325	-3.422578
H	5.511513	-2.999455	-2.507823
H	8.470448	-1.667319	0.599745
H	9.226289	-3.001250	-0.243796
H	8.406234	-1.741067	-1.147137
N	6.110770	-7.099307	-2.407461
H	7.004114	-7.224662	-1.979936
C	5.766130	-7.937018	-3.536188
H	6.596660	-8.609801	-3.710364
H	5.607740	-7.348885	-4.427809
C	4.498577	-8.767159	-3.332400
O	3.657706	-8.824310	-4.198409
N	4.392510	-9.424584	-2.170883
H	5.130817	-9.379417	-1.501210
C	3.209017	-10.183686	-1.841694
H	2.968869	-10.894126	-2.618465
H	3.405377	-10.729151	-0.927119
C	1.974189	-9.306856	-1.644805
O	0.886706	-9.699804	-2.000519
N	2.187869	-8.107001	-1.107183
C	1.053184	-7.196290	-1.049133

C	0.602296	-6.713916	-2.430128
O	-0.581645	-6.579853	-2.645997
C	1.252922	-5.968692	-0.165429
O	1.412852	-6.289994	1.176558
H	3.086662	-7.815834	-0.796443
H	0.208948	-7.737541	-0.654474
H	2.080444	-5.371463	-0.532552
H	0.346632	-5.392140	-0.249368
H	2.319532	-6.524414	1.320781
N	1.524545	-6.421357	-3.356796
C	1.119340	-6.007312	-4.687560
C	0.366941	-7.131822	-5.394547
O	-0.616594	-6.878978	-6.058973
C	2.321339	-5.474700	-5.501861
C	2.700149	-4.081492	-4.972089
C	2.027002	-5.438763	-7.006801
C	4.010930	-3.532444	-5.532708
H	2.496147	-6.472601	-3.136624
H	0.386994	-5.217779	-4.599022
H	3.154808	-6.151073	-5.337426
H	1.892034	-3.389647	-5.203569
H	2.779037	-4.121497	-3.893337
H	2.878141	-5.044252	-7.547683
H	1.828756	-6.425797	-7.406757
H	1.169328	-4.811086	-7.227436
H	4.283091	-2.619153	-5.013969
H	4.820371	-4.242192	-5.395364
H	3.944286	-3.300907	-6.589979
N	0.812833	-8.381381	-5.239583
H	1.659106	-8.556154	-4.738586

C	0.043777	-9.489598	-5.753025
H	-0.063177	-9.438059	-6.826330
H	0.563129	-10.404949	-5.499179
C	-1.365267	-9.540096	-5.166931
O	-2.317300	-9.778481	-5.874449
N	-1.472644	-9.318876	-3.858022
C	-2.773824	-9.358721	-3.234357
C	-3.688263	-8.224473	-3.694805
O	-4.883636	-8.440525	-3.757268
C	-2.678523	-9.337272	-1.701948
O	-3.924501	-9.611371	-1.121610
H	-0.656034	-9.230247	-3.289963
H	-3.288434	-10.263746	-3.524794
H	-1.994932	-10.109663	-1.377982
H	-2.293917	-8.380107	-1.366616
H	-4.614336	-9.215571	-1.639796
N	-3.140792	-7.038199	-3.955302
C	-3.899230	-5.914910	-4.482136
C	-4.452023	-6.249501	-5.866547
O	-5.625075	-6.088448	-6.119169
C	-2.987087	-4.668947	-4.499399
C	-3.417506	-3.519152	-5.398291
C	-4.745639	-3.185576	-5.639365
C	-2.429784	-2.759580	-6.020311
C	-5.070431	-2.147296	-6.500877
C	-2.748658	-1.710165	-6.863894
C	-4.077226	-1.405944	-7.116296
H	-2.168081	-6.911521	-3.765855
H	-4.760930	-5.732366	-3.859883
H	-2.882251	-4.329419	-3.473346

H	-2.005354	-4.982331	-4.824377
H	-5.540022	-3.751971	-5.195256
H	-1.394633	-2.998469	-5.850315
H	-6.108971	-1.946338	-6.700821
H	-1.962807	-1.141650	-7.328248
H	-4.329005	-0.608301	-7.793668
N	-3.583096	-6.714759	-6.769885
C	-4.048698	-7.045628	-8.097358
C	-5.186661	-8.063368	-8.049386
O	-6.115432	-7.964920	-8.807918
C	-2.917288	-7.590043	-8.972181
S	-1.689356	-6.352640	-9.499737
H	-2.632651	-6.879001	-6.510381
H	-4.472881	-6.169452	-8.565247
H	-2.417606	-8.415632	-8.483638
H	-3.349733	-7.961716	-9.891567
H	-1.067005	-6.199593	-8.341190
N	-5.078560	-9.066910	-7.155609
H	-4.238567	-9.204541	-6.635057
C	-6.086052	-10.114294	-7.182808
H	-6.261190	-10.452571	-8.192815
H	-5.714335	-10.946880	-6.596984
C	-7.459139	-9.722627	-6.613157
O	-8.480744	-10.092011	-7.125161
N	-7.417940	-9.016150	-5.478415
C	-8.636054	-8.653965	-4.781521
C	-9.495623	-7.633624	-5.521555
O	-10.688582	-7.608002	-5.362047
C	-8.344878	-8.144478	-3.358911
C	-7.426713	-6.915793	-3.232024

C	-8.012745	-5.535991	-3.103580
O	-9.305367	-5.429296	-3.235178
H	-9.566295	-4.512283	-3.101628
O	-7.307557	-4.582583	-2.877283
H	-6.532739	-8.774317	-5.086305
H	-9.265015	-9.529190	-4.698509
H	-9.297852	-7.962122	-2.882458
H	-7.870667	-8.961722	-2.826246
H	-6.797312	-7.023712	-2.358611
H	-6.742167	-6.848728	-4.061081
N	-8.837281	-6.733946	-6.273830
C	-9.555208	-5.702634	-7.000846
C	-10.241444	-6.303436	-8.225512
H	-9.886122	-7.287502	-8.536798
O	-11.124482	-5.744364	-8.794575
C	-8.611262	-4.505520	-7.297856
O	-8.596367	-3.622330	-6.193337
C	-8.932608	-3.727460	-8.570875
H	-7.859620	-6.848089	-6.436168
H	-10.361529	-5.346458	-6.373644
H	-7.600419	-4.876651	-7.370771
H	-9.437618	-3.184416	-6.138697
H	-8.252636	-2.883477	-8.630984
H	-8.801590	-4.331958	-9.459248
H	-9.956788	-3.367087	-8.569729
N	-12.952099	-9.022565	3.174142
H	-13.212983	-9.553275	2.368796
C	-11.773563	-8.180068	2.898826
C	-10.790963	-8.116278	4.051923
O	-9.664563	-7.699910	3.859086

C	-12.147103	-6.729778	2.543795
O	-12.733777	-6.198346	3.703356
C	-13.100358	-6.634674	1.357417
H	-13.732123	-8.453221	3.439978
H	-11.218696	-8.607536	2.074398
H	-11.231354	-6.202371	2.314642
H	-12.852378	-5.257660	3.588813
H	-13.263234	-5.591661	1.108782
H	-12.704662	-7.132439	0.479807
H	-14.064139	-7.068482	1.595973
N	-11.197245	-8.533612	5.241880
H	-12.116114	-8.918914	5.271876
C	-10.412641	-8.534803	6.452134
H	-10.330954	-7.540281	6.861132
H	-10.939748	-9.139572	7.180551
C	-8.977528	-9.059639	6.382431
O	-8.147112	-8.510269	7.063166
N	-8.659647	-10.125342	5.624950
H	-9.368430	-10.595275	5.108491
C	-7.270846	-10.559425	5.524585
H	-7.254236	-11.535653	5.057095
H	-6.833782	-10.644954	6.506426
C	-6.387435	-9.608346	4.692696
O	-5.221622	-9.463504	4.953059
N	-7.045410	-9.018041	3.701147
C	-6.310644	-7.982221	2.986667
C	-6.265755	-6.696391	3.808545
O	-5.273914	-6.006573	3.776925
C	-6.638572	-7.803893	1.490680
C	-7.801944	-6.936852	1.054646

C	-7.783273	-5.559758	1.256976
C	-8.848770	-7.481221	0.321991
C	-8.793848	-4.754182	0.760441
C	-9.848520	-6.674923	-0.197906
C	-9.829590	-5.309009	0.027572
H	-8.039897	-9.013221	3.684354
H	-5.287134	-8.313207	2.998513
H	-5.738222	-7.392705	1.047483
H	-6.744121	-8.800366	1.078440
H	-6.960446	-5.104826	1.776764
H	-8.866169	-8.539197	0.124031
H	-8.754263	-3.691552	0.921788
H	-10.625514	-7.108648	-0.799807
H	-10.600112	-4.682866	-0.384637
N	-7.293899	-6.409573	4.610793
C	-7.226774	-5.302748	5.535658
C	-6.096069	-5.517837	6.540834
O	-5.444773	-4.566561	6.915796
C	-8.599152	-5.148978	6.224076
C	-8.840646	-3.835326	6.936330
C	-9.095369	-2.677111	6.207499
C	-8.880576	-3.770076	8.322719
C	-9.374103	-1.482488	6.848635
C	-9.168904	-2.577761	8.970707
C	-9.416084	-1.429845	8.236054
H	-8.162020	-6.883468	4.486674
H	-6.970431	-4.391381	5.014129
H	-9.351528	-5.263245	5.450526
H	-8.729316	-5.968136	6.918061
H	-9.081971	-2.707479	5.131451

H	-8.690468	-4.654767	8.904957
H	-9.556950	-0.596768	6.267818
H	-9.191023	-2.546691	10.045147
H	-9.620419	-0.499437	8.735873
N	-5.853788	-6.754869	6.970525
H	-6.506301	-7.478288	6.764593
C	-4.771469	-7.046114	7.884182
H	-4.807238	-6.414045	8.758773
H	-4.879903	-8.075481	8.201436
C	-3.378763	-6.868401	7.281895
O	-2.503741	-6.369400	7.948712
N	-3.182169	-7.299127	6.030851
C	-1.903339	-7.129367	5.357699
C	-1.649485	-5.661756	4.985820
O	-0.548494	-5.180483	5.149104
C	-1.825810	-8.074680	4.138419
C	-0.659949	-7.729133	3.210260
C	-1.729287	-9.531460	4.605591
H	-3.917955	-7.778217	5.557820
H	-1.111378	-7.373486	6.050772
H	-2.746930	-7.953082	3.572991
H	-0.599900	-8.461363	2.412187
H	-0.765505	-6.757335	2.748919
H	0.285210	-7.741500	3.744188
H	-1.745998	-10.199062	3.750208
H	-0.795673	-9.697428	5.137152
H	-2.546467	-9.812858	5.257167
N	-2.682005	-4.974019	4.487882
C	-2.545164	-3.597631	4.052069
C	-2.409867	-2.667118	5.255465

O	-1.518125	-1.849152	5.299780
C	-3.720352	-3.148186	3.171366
C	-3.947925	-3.929451	1.866852
C	-2.816703	-3.839267	0.855428
O	-1.694637	-4.192671	1.245875
O	-3.088981	-3.434340	-0.288347
H	-3.550187	-5.438910	4.339790
H	-1.630955	-3.496690	3.498427
H	-4.636093	-3.194818	3.752918
H	-3.555192	-2.100004	2.937947
H	-4.097726	-4.975661	2.089032
H	-4.857302	-3.558258	1.407512
N	-3.309689	-2.786764	6.250329
C	-3.093962	-2.024874	7.456968
C	-1.781672	-2.422988	8.139766
O	-1.113697	-1.584913	8.705368
C	-4.230241	-1.983044	8.488898
O	-4.437644	-3.208907	9.126153
C	-5.512339	-1.383379	7.923457
H	-3.984636	-3.518795	6.233181
H	-2.930236	-1.000161	7.162253
H	-3.859682	-1.322574	9.262834
H	-4.879909	-3.801439	8.530532
H	-6.246381	-1.301433	8.715494
H	-5.327528	-0.391141	7.523527
H	-5.931168	-1.996298	7.136449
N	-1.380404	-3.700488	8.043333
H	-2.031003	-4.418665	7.814160
C	-0.186948	-4.107261	8.740209
H	-0.237554	-3.891848	9.798220

H	-0.075182	-5.174752	8.603858
C	1.064490	-3.419348	8.218883
O	1.940102	-3.075052	8.979783
N	1.155313	-3.258516	6.882966
C	2.333919	-2.661015	6.317786
C	2.292315	-1.139101	6.162096
O	3.361308	-0.575434	6.019565
C	2.834703	-3.351539	5.049051
S	1.918436	-3.009871	3.521955
H	0.424945	-3.613498	6.298139
H	3.117469	-2.796350	7.048011
H	3.840189	-3.003438	4.861002
H	2.870646	-4.418722	5.218663
H	0.872619	-3.797578	3.722815
N	1.141841	-0.471357	6.273787
C	1.204073	0.968482	6.491382
C	1.753690	1.272376	7.870910
O	2.364358	2.290991	8.087017
C	-0.097046	1.738100	6.176832
C	-1.200206	1.568193	7.231597
C	-0.553630	1.428961	4.745869
C	-2.469273	2.368698	6.930463
H	0.273681	-0.966378	6.289418
H	1.952058	1.351106	5.815539
H	0.204996	2.779216	6.212705
H	-1.448849	0.523567	7.352494
H	-0.813653	1.896478	8.192054
H	-1.309057	2.133214	4.420446
H	0.279830	1.505532	4.053097
H	-0.964394	0.432418	4.656221

H	-3.142326	2.340022	7.782109
H	-2.243999	3.411664	6.722902
H	-3.006174	1.969830	6.076689
N	1.549774	0.323287	8.791241
H	0.890691	-0.402779	8.613169
C	1.977802	0.512702	10.160033
H	1.469272	-0.222454	10.770953
H	1.737385	1.502491	10.517938
C	3.481795	0.337028	10.305837
O	4.163620	1.127585	10.898746
N	3.999649	-0.753675	9.695463
H	3.390372	-1.464979	9.349663
C	5.424736	-0.938883	9.667283
H	5.637718	-1.909422	9.234270
H	5.855436	-0.904929	10.657348
C	6.156885	0.119116	8.844830
O	7.291754	0.412091	9.129721
N	5.502087	0.621274	7.799020
C	6.098611	1.759282	7.146322
C	5.515755	3.077093	7.649950
H	5.009274	3.036938	8.612868
O	5.642887	4.095919	7.043695
C	6.001799	1.675241	5.620806
C	6.754289	0.507592	5.016621
C	8.119984	0.323554	5.236933
C	6.093947	-0.400178	4.193981
C	8.806411	-0.721137	4.632864
C	6.778104	-1.442485	3.588462
C	8.138271	-1.603448	3.798047
H	4.575710	0.333815	7.571699

H	7.134274	1.774212	7.450535
H	4.959444	1.610593	5.335055
H	6.379367	2.609976	5.220685
H	8.648202	0.979222	5.907817
H	5.033800	-0.304076	4.055849
H	9.857250	-0.848320	4.828159
H	6.245884	-2.133503	2.959315
H	8.658738	-2.415364	3.323940
N	12.613550	9.596234	-1.248801
H	11.873304	9.913777	-1.846311
C	12.304852	8.264740	-0.719487
C	11.273689	8.450546	0.386591
O	10.265530	7.778767	0.415804
C	13.562549	7.581221	-0.164596
C	14.645707	7.276548	-1.205017
S	14.018810	6.203150	-2.529344
C	15.503354	6.052419	-3.551773
H	13.433529	9.572929	-1.822100
H	11.834820	7.616386	-1.447461
H	14.000496	8.205656	0.608263
H	13.255359	6.653971	0.305291
H	15.046679	8.189118	-1.631593
H	15.470297	6.783724	-0.702487
H	15.253298	5.397008	-4.372129
H	15.803968	7.015827	-3.942864
H	16.320271	5.615506	-2.992399
N	11.503479	9.412865	1.296722
C	10.593734	9.607380	2.408635
C	9.276928	10.276086	2.011659
O	8.281457	10.056921	2.655491

C	11.276507	10.366957	3.552816
C	12.448227	9.561470	4.083903
O	13.582992	9.823427	3.743914
N	12.144690	8.558477	4.917500
H	12.327486	9.967466	1.206418
H	10.294206	8.637194	2.770427
H	11.657728	11.324458	3.220662
H	10.546636	10.534855	4.334660
H	12.888577	7.962509	5.210493
H	11.223226	8.171947	4.952502
N	9.263775	11.068227	0.922800
H	10.110275	11.226553	0.425903
C	8.003503	11.517472	0.368854
H	8.201268	12.259938	-0.393645
H	7.389040	11.966937	1.131722
C	7.186384	10.384437	-0.254318
O	5.986674	10.472166	-0.294965
N	7.862838	9.332497	-0.761515
C	7.169921	8.145082	-1.231698
C	6.632700	7.302320	-0.064480
O	5.531496	6.812191	-0.145111
C	8.048023	7.341579	-2.220518
C	8.345826	8.193291	-3.469295
C	7.376281	6.017628	-2.604436
C	9.429443	7.618030	-4.384588
H	8.822974	9.228191	-0.531268
H	6.279891	8.471639	-1.747020
H	8.986130	7.113644	-1.722574
H	7.424555	8.321605	-4.033217
H	8.650434	9.188198	-3.161869

H	7.993928	5.475068	-3.308756
H	7.221789	5.377635	-1.744299
H	6.407889	6.182861	-3.065124
H	9.625971	8.297919	-5.207242
H	10.364005	7.469971	-3.850308
H	9.147214	6.664653	-4.815676
N	7.385225	7.176512	1.047012
C	6.877042	6.457524	2.204057
C	5.524559	7.035060	2.642101
O	4.574308	6.325967	2.868652
C	7.830848	6.545496	3.405779
C	9.252392	5.997242	3.245545
O	10.144252	6.632337	3.801686
O	9.425757	4.935103	2.597434
H	8.346014	7.443499	1.024955
H	6.682390	5.428675	1.944175
H	7.918404	7.570066	3.735686
H	7.373052	5.991421	4.222696
N	5.482753	8.373085	2.790280
H	6.312206	8.910754	2.653481
C	4.290219	9.036913	3.256193
H	4.527987	10.079896	3.424426
H	3.945919	8.620697	4.189781
C	3.129854	8.987455	2.271387
O	1.988204	9.116366	2.649901
N	3.466171	8.825313	0.988812
H	4.427981	8.815249	0.742385
C	2.517188	8.905263	-0.078309
H	3.062362	9.089581	-0.995062
H	1.843510	9.738111	0.069104

C	1.609135	7.687017	-0.310189
O	0.575988	7.817118	-0.906827
N	2.067776	6.540439	0.227359
C	1.248377	5.370549	0.434794
C	0.429813	5.470884	1.726571
O	-0.764475	5.294262	1.700373
C	2.107097	4.106256	0.428929
H	2.968602	6.569054	0.655859
H	0.520431	5.319457	-0.357322
H	1.490830	3.234670	0.620250
H	2.579505	3.996917	-0.540369
H	2.884237	4.151893	1.184999
N	1.068191	5.733375	2.883787
C	0.338029	5.567457	4.131461
C	-0.773870	6.602006	4.287546
O	-1.809965	6.305745	4.842241
C	1.258920	5.492817	5.374590
C	1.849360	6.838951	5.821881
C	2.348493	4.431102	5.160687
C	2.693295	6.740957	7.095211
H	2.056692	5.862019	2.900468
H	-0.191362	4.627095	4.076667
H	0.605403	5.150203	6.171125
H	2.449867	7.254926	5.019470
H	1.044378	7.544444	6.000363
H	2.724610	4.075758	6.108871
H	1.955797	3.575567	4.620583
H	3.187257	4.825824	4.597549
H	2.996390	7.731996	7.420105
H	2.125610	6.290510	7.904070

H	3.590054	6.150574	6.954232
N	-0.550527	7.835200	3.809811
H	0.334405	8.069848	3.410757
C	-1.515000	8.880907	4.023560
H	-1.098733	9.807511	3.648703
H	-1.729412	9.010996	5.074454
C	-2.866971	8.618756	3.365893
O	-3.871476	8.845921	3.999867
N	-2.902686	8.108974	2.120752
C	-4.238787	8.033194	1.526231
C	-4.983202	6.753155	1.867818
O	-6.195626	6.754318	1.842582
C	-4.018520	8.294005	0.029162
C	-2.743446	9.144276	0.041792
C	-1.900223	8.455342	1.102623
H	-4.853889	8.819190	1.935695
H	-3.863914	7.367408	-0.507685
H	-4.874122	8.793873	-0.406893
H	-2.230657	9.199871	-0.900853
H	-2.981774	10.156806	0.358919
H	-1.435443	7.561610	0.727030
H	-1.127335	9.089719	1.504288
N	-4.262497	5.675999	2.205931
C	-4.914197	4.488141	2.729283
C	-5.629842	4.784577	4.050116
O	-6.704975	4.279094	4.285713
C	-3.921052	3.322434	2.932266
C	-3.594390	2.501999	1.700733
C	-4.106842	1.218509	1.543310
C	-2.725103	2.956670	0.711682

C	-3.777512	0.421568	0.457558
C	-2.386559	2.177468	-0.374700
C	-2.894361	0.873216	-0.547092
O	-2.578338	0.152933	-1.577154
H	-3.268757	5.756994	2.260898
H	-5.692673	4.185650	2.046458
H	-3.016284	3.722511	3.381139
H	-4.359935	2.661397	3.671706
H	-4.774113	0.821132	2.291646
H	-2.284183	3.929499	0.798091
H	-4.155513	-0.584569	0.393644
H	-1.708100	2.559722	-1.119194
N	-5.003331	5.588851	4.928170
H	-4.071671	5.898081	4.742882
C	-5.607624	5.942419	6.192324
H	-4.823026	6.282676	6.857091
H	-6.090651	5.086742	6.635504
C	-6.660906	7.045825	6.082512
O	-7.715840	6.968813	6.671022
N	-6.342145	8.091259	5.313948
H	-5.447376	8.140725	4.874874
C	-7.257648	9.220183	5.085240
H	-6.773142	9.882285	4.379589
H	-7.440761	9.763554	6.000424
C	-8.621452	8.828637	4.543285
O	-9.606440	9.420459	4.912576
N	-8.673257	7.827086	3.645025
C	-9.943614	7.435666	3.076848
C	-10.836112	6.654154	4.038280
O	-11.951735	6.351439	3.656934

C	-9.775573	6.671908	1.743215
O	-10.966834	6.755852	1.000025
C	-9.335384	5.223187	1.911330
H	-7.828303	7.411929	3.308412
H	-10.508955	8.330879	2.856496
H	-9.028293	7.206830	1.172109
H	-11.679080	6.479466	1.568919
H	-9.141858	4.784639	0.939817
H	-8.431870	5.142469	2.499257
H	-10.115082	4.639142	2.389249
N	-10.364715	6.343808	5.246677
C	-11.209900	5.754972	6.261796
C	-12.249540	6.740696	6.800523
O	-13.299314	6.325844	7.235299
C	-10.393773	5.201421	7.438426
C	-9.459963	4.028445	7.102085
C	-8.608442	3.695712	8.331194
C	-10.219219	2.785819	6.627183
H	-9.431308	6.592549	5.498266
H	-11.788811	4.964004	5.814091
H	-9.808306	6.007527	7.864915
H	-11.106388	4.886558	8.195353
H	-8.787143	4.332846	6.308556
H	-7.910898	2.891370	8.115457
H	-8.035281	4.559110	8.651339
H	-9.230183	3.380162	9.166390
H	-9.522693	1.974053	6.438632
H	-10.930266	2.450990	7.380572
H	-10.765692	2.957793	5.706887
N	-11.912361	8.040824	6.828433

C	-12.861882	9.030441	7.246619
C	-13.878980	9.396814	6.186155
H	-14.627930	10.124808	6.517977
O	-13.893172	8.967294	5.081459
H	-11.118791	8.352760	6.310016
H	-13.395984	8.683690	8.122608
H	-12.333526	9.935970	7.529092
N	-11.496190	10.630062	-3.035009
H	-11.247733	10.848697	-2.090743
C	-11.816457	9.206991	-3.172691
C	-11.414235	8.858125	-4.598813
O	-10.375790	8.292762	-4.845254
C	-13.245339	8.787459	-2.766642
C	-13.494301	9.128697	-1.285863
C	-13.469848	7.295863	-3.047016
C	-14.919980	8.857049	-0.802254
H	-12.280122	11.208570	-3.271591
H	-11.117532	8.661615	-2.553899
H	-13.959090	9.363117	-3.360659
H	-12.790450	8.572654	-0.671044
H	-13.282206	10.180979	-1.124282
H	-14.498742	7.014321	-2.862893
H	-13.248375	7.032851	-4.077384
H	-12.838464	6.689036	-2.405414
H	-15.042877	9.214780	0.213647
H	-15.652653	9.365844	-1.423251
H	-15.158148	7.799696	-0.801399
N	-12.214200	9.288719	-5.604122
H	-13.131169	9.602190	-5.380670
C	-11.972873	8.843878	-6.959262

H	-12.035531	7.767542	-7.044753
H	-12.729290	9.282532	-7.598613
C	-10.601634	9.233249	-7.517685
O	-9.997808	8.496125	-8.243133
N	-10.162516	10.476492	-7.182350
H	-10.708599	11.004447	-6.540654
C	-8.894338	11.023969	-7.637102
H	-8.790084	10.891100	-8.702725
H	-8.880399	12.081618	-7.408308
C	-7.672571	10.358998	-6.988330
O	-6.759378	9.922967	-7.632279
N	-7.657747	10.354147	-5.620749
H	-8.474939	10.647805	-5.135105
C	-6.495249	9.961279	-4.832307
H	-5.597967	10.374767	-5.264456
H	-6.616235	10.362002	-3.833391
C	-6.268288	8.463922	-4.714299
O	-5.135244	8.046505	-4.751044
N	-7.314867	7.639575	-4.521584
C	-7.020622	6.271133	-4.124525
C	-6.467326	5.439528	-5.275336
O	-5.672345	4.560888	-5.043417
C	-8.156626	5.541630	-3.368127
C	-9.346222	5.122976	-4.248120
C	-8.566288	6.359529	-2.137897
C	-10.386105	4.279503	-3.506728
H	-8.251879	7.988654	-4.514505
H	-6.188186	6.314002	-3.438769
H	-7.685647	4.630542	-3.009289
H	-9.825976	5.994079	-4.676481

H	-8.969838	4.536264	-5.083273
H	-9.221411	5.793059	-1.490471
H	-7.696283	6.635527	-1.550876
H	-9.088194	7.267188	-2.417891
H	-11.139265	3.914479	-4.198687
H	-9.929940	3.417091	-3.031033
H	-10.897643	4.848657	-2.740383
N	-6.882379	5.679822	-6.538388
C	-6.242751	4.969450	-7.628480
C	-4.821713	5.460812	-7.917777
O	-3.990853	4.676350	-8.308830
C	-7.107766	4.970248	-8.897881
C	-8.275025	3.973956	-8.839301
C	-7.793513	2.520527	-8.903265
N	-8.872639	1.529185	-8.891127
C	-9.426215	0.978437	-7.815749
N	-9.158400	1.435841	-6.605222
N	-10.266984	-0.034923	-7.964820
H	-7.492448	6.447501	-6.720172
H	-6.080259	3.958401	-7.295770
H	-7.496482	5.967443	-9.079069
H	-6.472335	4.727412	-9.743447
H	-8.865782	4.143041	-7.943760
H	-8.937018	4.154881	-9.679564
H	-7.248442	2.356428	-9.822809
H	-7.107343	2.280401	-8.102644
H	-9.143815	1.151075	-9.771265
H	-8.629247	2.268681	-6.487321
H	-9.631602	1.091880	-5.783876
H	-10.325757	-0.497121	-8.845103

H	-10.582363	-0.571456	-7.170949
N	-4.571419	6.757537	-7.721986
H	-5.302695	7.370349	-7.441242
C	-3.257792	7.352338	-8.011302
H	-2.929240	7.090628	-9.005007
H	-3.360549	8.426645	-7.939570
C	-2.202231	6.873958	-7.024718
O	-1.073852	6.638604	-7.377578
N	-2.633783	6.758811	-5.763283
C	-1.761007	6.448293	-4.656574
C	-1.491000	4.961024	-4.524131
O	-0.363792	4.576977	-4.319024
C	-2.349255	7.048560	-3.373588
C	-1.762508	6.354340	-2.145654
C	-2.111635	8.564410	-3.410714
H	-3.557144	7.065119	-5.546989
H	-0.788051	6.881331	-4.838967
H	-3.417824	6.867712	-3.387781
H	-1.979380	6.901791	-1.247581
H	-2.172663	5.356412	-2.033629
H	-0.689873	6.283703	-2.215540
H	-2.836841	9.090480	-2.806099
H	-1.116882	8.805684	-3.051328
H	-2.213132	8.950231	-4.418533
N	-2.517723	4.100220	-4.645904
C	-2.183874	2.694098	-4.750258
C	-1.220401	2.507869	-5.924342
O	-0.294163	1.732064	-5.842626
C	-3.407847	1.776927	-4.871499
C	-4.364888	1.887265	-3.676696

C	-5.406675	0.763417	-3.611904
N	-4.879475	-0.427261	-2.949793
C	-5.583840	-1.519150	-2.748491
N	-6.813258	-1.655527	-3.295771
N	-5.155159	-2.493137	-1.972250
H	-3.439230	4.421566	-4.850950
H	-1.629052	2.394610	-3.874428
H	-3.944330	1.990896	-5.793998
H	-3.028660	0.764904	-4.951115
H	-3.802055	1.899610	-2.756841
H	-4.904106	2.820331	-3.734069
H	-6.276908	1.113315	-3.066024
H	-5.727354	0.511292	-4.619620
H	-3.984955	-0.324272	-2.455368
H	-6.972757	-1.178773	-4.153531
H	-7.208521	-2.578273	-3.267051
H	-4.301483	-2.472079	-1.439477
H	-5.665078	-3.351236	-1.949303
N	-1.459790	3.193298	-7.035093
H	-2.284850	3.739868	-7.148495
C	-0.596621	2.997529	-8.183469
H	-0.949748	3.640778	-8.979139
H	-0.611196	1.972323	-8.524722
C	0.855924	3.344619	-7.871933
O	1.781357	2.710999	-8.313423
N	1.005385	4.404934	-7.063953
H	0.212185	4.964248	-6.846845
C	2.282350	4.880661	-6.640316
H	2.918995	5.137222	-7.477606
H	2.128365	5.777235	-6.053918

C	3.092850	3.928537	-5.775022
O	4.297527	4.059879	-5.687843
N	2.428015	2.983364	-5.101894
C	3.096637	2.136984	-4.148030
C	4.270120	1.327443	-4.710931
O	5.183441	1.025017	-3.969758
C	2.008539	1.259742	-3.526825
C	2.372558	0.440796	-2.294456
C	1.056393	0.029098	-1.643842
N	1.236414	-1.007170	-0.648781
C	0.299013	-1.927750	-0.373780
N	-0.855343	-1.920458	-0.991016
N	0.587706	-2.880258	0.490821
H	1.438768	2.900947	-5.211376
H	3.557572	2.746662	-3.380300
H	1.210866	1.943186	-3.256602
H	1.592799	0.612104	-4.289713
H	2.948408	-0.439377	-2.559505
H	2.976597	1.023650	-1.602782
H	0.560578	0.894051	-1.216187
H	0.400052	-0.365038	-2.404392
H	1.942194	-0.877371	0.040877
H	-1.297768	-1.062276	-1.309198
H	-1.528394	-2.645016	-0.775507
H	1.506491	-2.992819	0.850273
H	-0.162067	-3.479780	0.822424
N	4.280031	0.941778	-5.998578
H	3.541252	1.225888	-6.608101
C	5.363424	0.116638	-6.504622
H	5.137067	-0.137711	-7.532661

H	5.442848	-0.800432	-5.942754
C	6.736144	0.755908	-6.476882
O	7.738718	0.089366	-6.368969
N	6.766124	2.085339	-6.608293
H	5.911948	2.604339	-6.566385
C	8.005021	2.823956	-6.549017
H	8.710228	2.440517	-7.272781
H	7.799820	3.854828	-6.804955
C	8.746724	2.826456	-5.210435
O	9.887175	3.237466	-5.157199
N	8.101429	2.335406	-4.144636
C	8.681535	2.170358	-2.822752
C	9.947628	1.303165	-2.830509
O	10.765101	1.385821	-1.928230
C	7.577232	1.500558	-1.974588
C	7.771989	1.380062	-0.463379
C	7.427640	2.651039	0.322537
C	7.315792	2.387413	1.820281
N	8.655413	2.356332	2.479120
O	11.033153	1.615196	0.896933
H	10.884685	1.825393	-0.025412
H	11.511050	0.788172	0.847886
H	7.155893	2.032135	-4.258577
H	8.978832	3.127729	-2.415574
H	6.659843	2.042620	-2.160986
H	7.411669	0.512780	-2.388883
H	7.092628	0.600517	-0.132528
H	8.767415	1.028857	-0.225864
H	8.139802	3.452371	0.146214
H	6.462347	3.020645	-0.008273

H	6.754126	3.160288	2.321462
H	6.835166	1.441414	2.016282
H	9.366719	1.891048	1.923897
H	8.976059	3.326528	2.632108
H	8.601182	1.880366	3.367772
N	10.062468	0.448216	-3.837538
C	11.109366	-0.537544	-4.069419
C	12.486372	0.023143	-4.427254
O	13.444004	-0.705739	-4.301638
C	10.701363	-1.443263	-5.253397
C	9.563117	-2.441846	-4.999769
C	9.132182	-3.065331	-6.331061
C	9.989883	-3.533367	-4.018140
H	9.324246	0.445928	-4.510632
H	11.264674	-1.125458	-3.176633
H	10.435185	-0.796967	-6.084494
H	11.584298	-1.995497	-5.552179
H	8.706457	-1.911239	-4.595973
H	8.330940	-3.781801	-6.177422
H	8.775111	-2.307920	-7.017149
H	9.959527	-3.592977	-6.799164
H	9.199757	-4.263157	-3.878961
H	10.859908	-4.059608	-4.396973
H	10.242747	-3.137364	-3.039386
N	12.574050	1.261829	-4.919242
C	13.814453	1.845370	-5.393357
C	14.958485	2.034739	-4.378827
O	16.012412	2.417529	-4.811576
C	13.496419	3.171929	-6.086597
O	12.917141	4.088890	-5.202404

H	11.756570	1.833767	-4.915474
H	14.248723	1.178604	-6.128872
H	14.419368	3.591232	-6.455377
H	12.845628	2.977723	-6.933290
H	11.969675	4.078408	-5.265672
N	14.792294	1.722326	-3.074279
C	15.927992	1.647230	-2.176435
C	16.804495	0.409874	-2.402229
O	17.934274	0.393859	-1.987681
C	15.494230	1.576952	-0.707148
C	14.636405	2.733139	-0.197767
C	14.280846	2.484613	1.268455
N	13.255547	3.379242	1.790687
C	13.433452	4.530654	2.417606
N	14.651388	5.006220	2.653408
O	15.028043	7.462722	4.207124
H	14.745070	8.349635	3.968965
H	15.748001	7.567698	4.816085
N	12.383758	5.219596	2.814043
H	13.901416	1.417906	-2.758955
H	16.561534	2.504336	-2.345514
H	14.954330	0.648557	-0.552268
H	16.405896	1.508159	-0.123829
H	15.153949	3.681221	-0.312268
H	13.717995	2.814690	-0.767353
H	13.883321	1.485481	1.373081
H	15.159484	2.525723	1.901468
H	12.315325	3.083056	1.620748
H	15.459068	4.512343	2.356887
H	14.787188	5.861152	3.164897

H	11.428069	4.939741	2.656779
H	12.476311	6.063013	3.333653
N	16.200238	-0.648980	-2.967242
C	16.870485	-1.911748	-3.168205
C	17.667865	-1.889273	-4.468826
H	18.067003	-0.910804	-4.745289
O	17.867599	-2.851332	-5.135873
C	15.867590	-3.070231	-3.148676
C	15.324123	-3.399076	-1.791036
N	14.402671	-2.626651	-1.112116
O	12.506042	-0.433892	-0.462206
H	13.143122	-1.036871	-0.849396
H	12.024862	-0.037603	-1.180542
C	15.619497	-4.488899	-1.047858
C	14.171505	-3.250081	-0.003229
N	14.882335	-4.379818	0.104639
H	15.285715	-0.550257	-3.352830
H	17.596346	-2.030782	-2.371442
H	15.050132	-2.842573	-3.824055
H	16.368086	-3.944387	-3.542813
H	16.275389	-5.312474	-1.232455
H	13.492857	-2.920320	0.757312
H	14.781793	-5.062261	0.823783
O	-15.020213	-2.471018	4.973947
H	-15.212269	-1.661971	4.507127
H	-14.526681	-2.213501	5.745680
O	-12.902805	-1.270687	6.931187
H	-12.213112	-1.722239	7.405267
H	-13.132674	-0.515337	7.458650
O	-12.055753	-0.850867	4.158774

H	-12.176337	-0.902832	5.104108
H	-12.868116	-0.459842	3.834508
O	-13.393747	-1.856946	0.710307
H	-12.618284	-1.293680	0.766814
H	-13.315966	-2.505070	1.414951
O	-7.286578	1.302460	-0.239832
H	-7.498670	1.637792	0.634927
H	-6.357470	1.101754	-0.204429
O	-7.886340	2.078825	2.455260
H	-8.797907	1.924358	2.690781
H	-7.559723	2.755410	3.042588
O	-9.340583	-0.024714	-1.607137
H	-8.578916	0.394601	-1.186585
H	-9.089673	-0.922547	-1.804081
O	-12.844468	-2.336472	-2.019732
H	-13.120890	-2.372994	-1.100710
H	-13.457233	-2.846557	-2.536626
O	-14.029220	0.929631	-0.581729
H	-14.374084	0.067218	-0.375890
H	-13.118598	0.887120	-0.273370
O	-14.252289	4.929717	4.735637
H	-13.682720	5.570161	4.315809
H	-14.289917	5.214909	5.644026
O	-15.228230	2.155337	1.701339
H	-15.850248	2.871084	1.687644
H	-14.941090	1.991837	0.804275
O	-13.151682	0.247400	-3.244027
H	-13.600362	0.778017	-2.588539
H	-12.933673	-0.556693	-2.770726
O	-13.770241	-1.924623	-4.981136

H	-13.935128	-1.061137	-4.609276
H	-14.496296	-2.133600	-5.554536
O	-10.158517	-2.764133	-2.953315
H	-10.299828	-2.610238	-3.881079
H	-11.020981	-2.685373	-2.547665
O	-11.483664	0.213499	0.371431
H	-10.756842	0.131628	-0.247651
H	-11.143523	0.654620	1.157231
O	-10.713541	1.341352	2.831460
H	-10.879054	0.581125	3.386200
H	-11.394559	1.967053	3.094746
O	-13.056431	2.612688	3.638284
H	-13.358288	3.352888	4.167517
H	-13.711662	2.532419	2.952964
O	-10.465899	0.624989	-4.110407
H	-11.370355	0.792546	-3.839565
H	-9.979019	0.491443	-3.289473
O	-14.689453	-0.342247	3.042901
H	-15.010244	0.527555	2.814387
H	-14.562674	-0.799930	2.218332
O	-13.086321	-3.361499	3.147701
H	-13.858109	-3.220234	3.705614
H	-12.459215	-2.724240	3.488715
O	-11.004346	-1.654020	-5.646469
H	-11.934456	-1.876332	-5.563288
H	-10.845416	-0.947014	-5.017375

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(+),Y266(-),E183(0)

POTENTIAL:0 mV

N	15.815911	-6.171507	5.162723
H	15.012115	-5.956338	5.720342
C	15.718932	-5.550103	3.839266
C	15.012365	-6.475093	2.829898
O	14.264709	-6.039831	1.969796
C	17.116994	-5.218940	3.303618
H	16.617975	-5.835149	5.658171
H	15.128406	-4.643710	3.858853
H	17.068657	-4.811800	2.300728
H	17.583876	-4.474228	3.938259
H	17.749422	-6.099719	3.289140
N	15.298602	-7.772676	2.926189
H	15.890371	-8.048875	3.680154
C	14.687521	-8.778222	2.055239
H	14.756666	-8.484825	1.020508
H	15.207847	-9.717029	2.190850
C	13.208188	-8.956166	2.399416
O	12.377761	-9.166801	1.554734
N	12.882012	-8.827389	3.699958
H	13.603979	-8.750648	4.379008
C	11.501007	-8.990668	4.160085
H	11.500864	-9.001261	5.241886
H	11.073110	-9.912783	3.798654
C	10.607647	-7.843954	3.669621
O	9.465056	-8.044802	3.355847
N	11.183937	-6.630558	3.646549
C	10.519402	-5.456882	3.137645
C	10.320011	-5.486917	1.619588

O	9.275433	-5.077566	1.172390
C	11.261767	-4.199859	3.618586
O	12.652266	-4.343916	3.599424
H	12.141561	-6.538812	3.893979
H	9.516113	-5.412177	3.528535
H	10.943084	-3.347172	3.029667
H	10.997165	-4.015588	4.649510
H	12.978203	-4.499861	2.721504
N	11.302309	-5.952837	0.828231
C	11.043830	-6.125794	-0.598581
C	9.920193	-7.142080	-0.815398
O	9.166260	-7.039064	-1.754875
C	12.337943	-6.461504	-1.400249
C	12.579909	-7.955836	-1.649226
C	12.336292	-5.708423	-2.731942
H	12.139273	-6.323653	1.222652
H	10.645791	-5.194130	-0.967833
H	13.162736	-6.080200	-0.808697
H	13.535225	-8.081946	-2.148189
H	12.599157	-8.540735	-0.740568
H	11.820913	-8.370919	-2.305224
H	13.234740	-5.935553	-3.294916
H	11.480231	-5.991949	-3.334339
H	12.306844	-4.636609	-2.576471
N	9.827345	-8.118301	0.095592
H	10.577542	-8.244162	0.736091
C	8.879798	-9.223877	-0.009149
H	9.249095	-10.026356	0.616674
H	8.822607	-9.584183	-1.024712
C	7.461395	-8.899175	0.411818

O	6.546433	-9.371842	-0.222127
N	7.267304	-8.106214	1.471719
C	5.922028	-7.662010	1.759189
C	5.467797	-6.643661	0.719015
O	4.288010	-6.579464	0.447490
C	5.664027	-7.190546	3.204285
C	5.843202	-8.349467	4.190133
C	6.476248	-5.967681	3.634998
H	8.041084	-7.827455	2.034821
H	5.261471	-8.497403	1.586382
H	4.615521	-6.908950	3.209784
H	5.551122	-8.038826	5.187782
H	5.225578	-9.198378	3.915493
H	6.874807	-8.680547	4.232569
H	6.133470	-5.624046	4.605080
H	7.526348	-6.211817	3.728883
H	6.375877	-5.141572	2.939627
N	6.363071	-5.877460	0.087204
C	5.936976	-5.048159	-1.027868
C	5.525631	-5.920726	-2.221910
O	4.493851	-5.686874	-2.806180
C	6.996928	-3.989225	-1.391640
C	7.172004	-2.991739	-0.232712
C	6.598023	-3.262041	-2.680452
C	8.441738	-2.146489	-0.335961
H	7.326475	-5.909064	0.342282
H	5.024579	-4.544371	-0.746201
H	7.941423	-4.499968	-1.555842
H	6.298333	-2.342640	-0.198191
H	7.201641	-3.525092	0.708021

H	7.279065	-2.447758	-2.886933
H	6.612884	-3.918794	-3.540651
H	5.598150	-2.848743	-2.599071
H	8.528653	-1.488305	0.521968
H	9.321457	-2.779131	-0.354172
H	8.455705	-1.527074	-1.225707
N	6.325141	-6.934911	-2.580644
H	7.225240	-7.038912	-2.161767
C	6.001247	-7.762011	-3.723308
H	6.848899	-8.409883	-3.909055
H	5.826972	-7.163637	-4.605121
C	4.755989	-8.628406	-3.532713
O	3.916813	-8.694495	-4.399884
N	4.667477	-9.305886	-2.381526
H	5.405486	-9.252845	-1.712100
C	3.503229	-10.098282	-2.062547
H	3.279708	-10.803426	-2.849034
H	3.713572	-10.651382	-1.155703
C	2.248189	-9.253726	-1.853224
O	1.171058	-9.664212	-2.221428
N	2.432037	-8.060222	-1.290929
C	1.278730	-7.174304	-1.222456
C	0.821087	-6.680836	-2.597439
O	-0.365668	-6.562916	-2.809270
C	1.450110	-5.958168	-0.316435
O	1.609903	-6.302678	1.019995
H	3.322655	-7.755572	-0.969563
H	0.444643	-7.739153	-0.839360
H	2.267481	-5.338639	-0.668220
H	0.533492	-5.397167	-0.393286

H	2.521394	-6.515636	1.166869
N	1.735690	-6.364452	-3.523254
C	1.322748	-5.943973	-4.850174
C	0.580855	-7.071626	-5.563151
O	-0.413139	-6.829197	-6.216064
C	2.517962	-5.398415	-5.666596
C	2.889693	-4.003825	-5.135603
C	2.218321	-5.360277	-7.170647
C	4.199134	-3.450508	-5.695892
H	2.708044	-6.396674	-3.303160
H	0.584750	-5.160708	-4.754566
H	3.356524	-6.069514	-5.507594
H	2.079121	-3.315016	-5.367377
H	2.968073	-4.043740	-4.056935
H	3.064376	-4.956828	-7.712833
H	2.027063	-6.347486	-7.573536
H	1.354974	-4.738850	-7.386983
H	4.471026	-2.538718	-5.174713
H	5.009933	-4.159439	-5.561594
H	4.131718	-3.215916	-6.752424
N	1.051637	-8.314455	-5.427477
H	1.903118	-8.479454	-4.931906
C	0.299633	-9.430045	-5.949333
H	0.188985	-9.370557	-7.021905
H	0.833390	-10.339442	-5.704314
C	-1.106360	-9.504557	-5.359776
O	-2.060501	-9.732088	-6.069224
N	-1.211208	-9.314421	-4.045751
C	-2.512865	-9.372129	-3.423385
C	-3.439843	-8.244078	-3.877452

O	-4.629907	-8.477155	-3.965478
C	-2.417153	-9.359004	-1.890916
O	-3.658129	-9.655855	-1.311407
H	-0.393945	-9.226632	-3.477870
H	-3.017615	-10.280884	-3.719320
H	-1.723131	-10.124238	-1.572312
H	-2.045592	-8.399100	-1.549005
H	-4.354114	-9.250711	-1.813396
N	-2.907816	-7.043418	-4.102035
C	-3.672128	-5.903629	-4.584533
C	-4.250155	-6.189476	-5.969087
O	-5.419612	-5.966818	-6.216103
C	-2.740833	-4.667344	-4.583016
C	-3.140595	-3.505856	-5.477645
C	-4.452640	-3.068153	-5.613869
C	-2.151970	-2.841425	-6.196663
C	-4.768087	-2.019308	-6.463105
C	-2.457839	-1.778325	-7.029332
C	-3.773179	-1.369202	-7.173458
H	-1.940464	-6.907594	-3.891406
H	-4.523322	-5.730873	-3.944494
H	-2.642331	-4.339305	-3.553063
H	-1.762702	-4.996428	-4.899528
H	-5.238883	-3.562430	-5.077952
H	-1.129356	-3.164030	-6.111914
H	-5.797626	-1.730485	-6.582119
H	-1.672976	-1.280946	-7.570224
H	-4.017539	-0.559636	-7.838649
N	-3.413087	-6.685176	-6.880158
C	-3.897966	-7.005665	-8.204042

C	-5.017455	-8.043767	-8.143195
O	-5.995957	-7.920163	-8.835136
C	-2.771445	-7.517283	-9.105095
S	-1.573702	-6.249553	-9.627714
H	-2.467960	-6.887333	-6.625516
H	-4.344116	-6.129229	-8.649026
H	-2.250491	-8.342440	-8.638619
H	-3.211211	-7.881628	-10.024132
H	-0.934757	-6.111133	-8.476292
N	-4.844098	-9.092525	-7.315832
H	-3.986326	-9.228331	-6.823724
C	-5.823744	-10.166269	-7.361259
H	-5.998837	-10.483794	-8.378229
H	-5.423212	-11.002472	-6.800525
C	-7.201995	-9.825979	-6.773518
O	-8.216432	-10.208508	-7.288888
N	-7.173193	-9.142581	-5.624140
C	-8.391642	-8.823245	-4.901199
C	-9.283781	-7.797061	-5.591752
O	-10.466389	-7.765069	-5.375929
C	-8.096228	-8.332563	-3.471062
C	-7.205135	-7.086206	-3.329419
C	-7.800066	-5.706614	-3.216403
O	-9.097387	-5.610557	-3.211020
H	-9.355896	-4.698419	-3.016040
O	-7.078197	-4.742800	-3.109370
H	-6.290394	-8.899911	-5.226338
H	-9.000226	-9.713712	-4.828684
H	-9.047620	-8.180115	-2.980848
H	-7.596964	-9.147277	-2.957528

H	-6.608600	-7.182011	-2.429863
H	-6.487896	-7.019283	-4.128150
N	-8.660391	-6.884845	-6.361752
C	-9.415942	-5.859912	-7.059435
C	-10.431904	-6.481777	-8.011729
H	-10.231784	-7.508021	-8.323554
O	-11.380705	-5.879493	-8.400540
C	-8.417634	-4.915254	-7.759585
O	-7.705796	-4.201511	-6.767873
C	-9.062589	-3.889129	-8.679890
H	-7.723338	-7.068918	-6.648105
H	-9.984924	-5.285577	-6.339541
H	-7.716845	-5.510514	-8.335664
H	-6.960535	-4.713374	-6.461190
H	-8.291656	-3.209303	-9.024310
H	-9.524748	-4.355751	-9.538420
H	-9.826674	-3.318814	-8.162469
N	-12.648687	-9.488839	3.058955
H	-12.898815	-10.006846	2.242047
C	-11.501708	-8.600016	2.799741
C	-10.502043	-8.566087	3.937168
O	-9.378989	-8.139091	3.740185
C	-11.938870	-7.137400	2.575382
O	-12.528045	-6.745581	3.788926
C	-12.915009	-6.968443	1.416922
H	-13.445335	-8.955729	3.348272
H	-10.957018	-8.950087	1.934190
H	-11.048317	-6.553161	2.384466
H	-12.575610	-5.792938	3.839620
H	-13.114900	-5.913419	1.263050

H	-12.519116	-7.371986	0.492343
H	-13.859641	-7.454439	1.629614
N	-10.894750	-8.995872	5.126307
H	-11.816196	-9.373014	5.168304
C	-10.099020	-8.986222	6.329155
H	-10.040548	-7.993589	6.747950
H	-10.599214	-9.614499	7.056662
C	-8.649982	-9.465316	6.235949
O	-7.827061	-8.892465	6.906533
N	-8.309789	-10.518610	5.470870
H	-9.009768	-11.003230	4.955995
C	-6.910425	-10.909733	5.351390
H	-6.869764	-11.878907	4.870802
H	-6.461186	-10.995747	6.327774
C	-6.060457	-9.924029	4.525509
O	-4.895128	-9.755453	4.776420
N	-6.740983	-9.331139	3.550898
C	-6.033225	-8.278275	2.833869
C	-6.007952	-7.002819	3.669651
O	-5.030775	-6.291139	3.650802
C	-6.396261	-8.084692	1.346360
C	-7.568891	-7.207952	0.955169
C	-7.543264	-5.834533	1.182797
C	-8.642130	-7.737862	0.251122
C	-8.578963	-5.022811	0.752165
C	-9.666735	-6.923897	-0.205355
C	-9.647577	-5.564417	0.056905
H	-7.735512	-9.354337	3.536299
H	-5.003903	-8.591058	2.825407
H	-5.505074	-7.672503	0.885742

H	-6.517106	-9.076108	0.926010
H	-6.700272	-5.388422	1.677479
H	-8.665919	-8.791570	0.031549
H	-8.537277	-3.963588	0.934797
H	-10.466721	-7.347268	-0.784215
H	-10.442741	-4.930731	-0.290120
N	-7.049127	-6.748929	4.464945
C	-7.024620	-5.641532	5.388471
C	-5.905281	-5.827862	6.411844
O	-5.303885	-4.855587	6.816474
C	-8.412228	-5.508044	6.057831
C	-8.770988	-4.119843	6.543022
C	-9.060277	-3.113744	5.622108
C	-8.880458	-3.833445	7.895282
C	-9.444169	-1.852038	6.042019
C	-9.264792	-2.569863	8.323131
C	-9.545565	-1.577011	7.400791
H	-7.898873	-7.253945	4.337922
H	-6.778110	-4.727777	4.867053
H	-9.148563	-5.804355	5.319014
H	-8.483927	-6.216503	6.873131
H	-8.976501	-3.317597	4.567203
H	-8.664250	-4.595398	8.623286
H	-9.661181	-1.090200	5.315373
H	-9.334441	-2.363724	9.376175
H	-9.816783	-0.590633	7.732615
N	-5.619961	-7.062417	6.820643
H	-6.245690	-7.803215	6.594606
C	-4.545704	-7.337510	7.748180
H	-4.601650	-6.706879	8.622582

H	-4.643967	-8.368186	8.064548
C	-3.148347	-7.140437	7.163329
O	-2.289709	-6.625997	7.839962
N	-2.927161	-7.568375	5.915304
C	-1.644480	-7.363947	5.259385
C	-1.417029	-5.885553	4.915951
O	-0.325947	-5.386531	5.090879
C	-1.534355	-8.285086	4.024036
C	-0.365100	-7.899908	3.114967
C	-1.412866	-9.747757	4.466376
H	-3.647561	-8.058372	5.429539
H	-0.854950	-7.604622	5.956511
H	-2.451610	-8.172182	3.450721
H	-0.282651	-8.616523	2.304696
H	-0.483529	-6.922214	2.669145
H	0.574127	-7.904811	3.659889
H	-1.406955	-10.400258	3.599250
H	-0.481722	-9.904223	5.005130
H	-2.231111	-10.057025	5.103644
N	-2.462416	-5.209014	4.428393
C	-2.351452	-3.823587	4.014602
C	-2.255259	-2.904640	5.230666
O	-1.384995	-2.064571	5.292789
C	-3.523300	-3.394152	3.120749
C	-3.698811	-4.161346	1.800074
C	-2.559594	-4.000107	0.806157
O	-1.425530	-4.298592	1.205748
O	-2.839077	-3.594287	-0.336331
H	-3.319862	-5.689625	4.266155
H	-1.431504	-3.693230	3.476674

H	-4.447910	-3.478920	3.683518
H	-3.385731	-2.337629	2.908573
H	-3.805050	-5.217214	2.001896
H	-4.617668	-3.823819	1.333817
N	-3.159420	-3.058434	6.216537
C	-2.965211	-2.314132	7.438570
C	-1.638603	-2.690243	8.107663
O	-0.994708	-1.847714	8.694142
C	-4.101043	-2.331440	8.472183
O	-4.279417	-3.583414	9.065579
C	-5.398045	-1.740572	7.929362
H	-3.822660	-3.800511	6.181485
H	-2.832323	-1.278631	7.166347
H	-3.744373	-1.689655	9.268072
H	-4.713583	-4.161683	8.450169
H	-6.135168	-1.712113	8.723086
H	-5.238320	-0.726688	7.575824
H	-5.800833	-2.327256	7.114479
N	-1.197653	-3.951979	7.973464
H	-1.830960	-4.682641	7.734735
C	0.003080	-4.342738	8.667209
H	-0.059057	-4.157051	9.730255
H	0.146161	-5.402676	8.503573
C	1.237435	-3.607536	8.171552
O	2.102829	-3.265860	8.945185
N	1.325146	-3.403013	6.841039
C	2.486714	-2.759176	6.293230
C	2.387884	-1.240921	6.125658
O	3.434717	-0.641171	5.966455
C	3.049315	-3.443415	5.048091

S	2.128357	-3.210935	3.503743
H	0.602257	-3.757359	6.246744
H	3.257834	-2.853466	7.042792
H	4.030048	-3.030993	4.859988
H	3.158248	-4.500369	5.248178
H	1.129924	-4.055273	3.717552
N	1.217735	-0.611864	6.259419
C	1.238052	0.824396	6.510019
C	1.794097	1.110658	7.890819
O	2.380680	2.139145	8.125306
C	-0.090012	1.560084	6.229855
C	-1.170786	1.337480	7.298077
C	-0.558518	1.263495	4.800381
C	-2.468403	2.103498	7.031414
H	0.367182	-1.136075	6.287271
H	1.965612	1.245472	5.835012
H	0.180966	2.609235	6.280873
H	-1.385652	0.283748	7.404624
H	-0.779411	1.661131	8.258154
H	-1.339599	1.949919	4.499413
H	0.261485	1.378762	4.096987
H	-0.939427	0.256355	4.697867
H	-3.126271	2.039165	7.892814
H	-2.278363	3.156373	6.839105
H	-3.006759	1.703073	6.179312
N	1.624535	0.134949	8.790803
H	0.978993	-0.601056	8.604012
C	2.056048	0.307676	10.161042
H	1.574375	-0.455910	10.758663
H	1.788502	1.281710	10.542231

C	3.565620	0.174490	10.291442
O	4.230222	0.975923	10.888992
N	4.109447	-0.890960	9.658440
H	3.517903	-1.620984	9.320683
C	5.539001	-1.035248	9.619347
H	5.776951	-1.990977	9.166794
H	5.975315	-1.007508	10.607224
C	6.235779	0.058236	8.812790
O	7.365000	0.374501	9.095208
N	5.560517	0.564232	7.781950
C	6.122095	1.732150	7.151180
C	5.506677	3.022334	7.686752
H	5.007124	2.947621	8.651217
O	5.603153	4.057193	7.102411
C	6.018820	1.678819	5.624689
C	6.800787	0.546473	4.991476
C	8.173076	0.399184	5.197993
C	6.161161	-0.364379	4.155921
C	8.885539	-0.612384	4.568227
C	6.871254	-1.373758	3.524991
C	8.237285	-1.497815	3.721170
H	4.638390	0.260910	7.558519
H	7.158684	1.768431	7.450170
H	4.977120	1.590720	5.342930
H	6.367648	2.632409	5.243407
H	8.686791	1.057202	5.877802
H	5.097511	-0.297577	4.028059
H	9.941252	-0.711803	4.753095
H	6.354816	-2.068333	2.886670
H	8.777869	-2.284269	3.227130

N	12.361248	9.925824	-1.111669
H	11.607165	10.236416	-1.695397
C	12.093075	8.575192	-0.609438
C	11.064833	8.708373	0.506884
O	10.076589	8.007466	0.528494
C	13.372990	7.915314	-0.077231
C	14.457403	7.663971	-1.130498
S	13.852162	6.602173	-2.474096
C	15.332976	6.516953	-3.509331
H	13.175987	9.936922	-1.692771
H	11.636210	7.929764	-1.348324
H	13.798365	8.534853	0.706508
H	13.094939	6.969780	0.374010
H	14.829618	8.596577	-1.539453
H	15.298874	7.183920	-0.643812
H	15.095814	5.872993	-4.342489
H	15.603069	7.497037	-3.880799
H	16.166126	6.091458	-2.965280
N	11.273753	9.657624	1.435601
C	10.366455	9.803216	2.556976
C	9.028867	10.442990	2.182404
O	8.044381	10.182399	2.827618
C	11.035541	10.557243	3.712854
C	12.231983	9.773158	4.220211
O	13.357221	10.073305	3.879898
N	11.960963	8.744733	5.033726
H	12.081004	10.237273	1.351557
H	10.096464	8.817616	2.899843
H	11.388413	11.531527	3.398664
H	10.306347	10.688797	4.502252

H	12.722525	8.163167	5.309693
H	11.050654	8.332288	5.065346
N	8.986275	11.257116	1.110692
H	9.824694	11.449963	0.612326
C	7.710276	11.682666	0.574253
H	7.882141	12.446668	-0.173097
H	7.088658	12.098225	1.350430
C	6.920876	10.540892	-0.068393
O	5.719031	10.595894	-0.100007
N	7.623050	9.519392	-0.602366
C	6.960358	8.323386	-1.093860
C	6.455159	7.440744	0.058105
O	5.367844	6.921273	-0.026341
C	7.853574	7.566587	-2.105710
C	8.118482	8.453259	-3.337450
C	7.216500	6.232894	-2.514202
C	9.211617	7.929022	-4.271868
H	8.587225	9.437195	-0.380283
H	6.057923	8.635863	-1.596173
H	8.801229	7.354414	-1.618956
H	7.190092	8.567423	-3.892641
H	8.396868	9.449567	-3.010333
H	7.844015	5.723455	-3.234362
H	7.086215	5.570229	-1.667335
H	6.240564	6.380765	-2.964738
H	9.382972	8.631781	-5.080816
H	10.153718	7.796296	-3.746844
H	8.953630	6.977455	-4.721733
N	7.218120	7.313118	1.162330
C	6.737683	6.556151	2.306925

C	5.372651	7.086484	2.765458
O	4.444387	6.346364	2.983614
C	7.696646	6.645266	3.504442
C	9.131690	6.140408	3.323947
O	10.009432	6.788324	3.887800
O	9.330287	5.097239	2.652589
H	8.170779	7.607712	1.140359
H	6.569782	5.527992	2.026480
H	7.757910	7.664687	3.855564
H	7.259832	6.061540	4.312146
N	5.294712	8.419499	2.941340
H	6.108013	8.982643	2.810320
C	4.087638	9.040679	3.428277
H	4.298045	10.086107	3.616558
H	3.761212	8.596211	4.355205
C	2.922311	8.979805	2.450004
O	1.780343	9.070771	2.838296
N	3.253967	8.852155	1.162305
H	4.213960	8.872983	0.909639
C	2.295757	8.928673	0.103162
H	2.829052	9.148479	-0.812753
H	1.600012	9.738683	0.273361
C	1.420403	7.690813	-0.149664
O	0.380838	7.805684	-0.738045
N	1.912066	6.546181	0.362212
C	1.123506	5.352439	0.553946
C	0.313178	5.409139	1.853539
O	-0.877361	5.209508	1.833230
C	2.012984	4.110251	0.518352
H	2.813662	6.590612	0.787695

H	0.390839	5.297549	-0.233497
H	1.419564	3.220840	0.699178
H	2.479393	4.029755	-0.456658
H	2.795442	4.161629	1.268589
N	0.955799	5.660374	3.011342
C	0.239445	5.450441	4.260131
C	-0.898248	6.451699	4.443906
O	-1.921349	6.116603	5.001188
C	1.170294	5.375023	5.495596
C	1.729503	6.726861	5.965015
C	2.284753	4.345685	5.253594
C	2.583608	6.626235	7.231326
H	1.941700	5.807866	3.023563
H	-0.265507	4.497618	4.190218
H	0.531177	5.000233	6.289362
H	2.314368	7.172563	5.167081
H	0.908238	7.408459	6.161388
H	2.676532	3.981320	6.191941
H	1.909816	3.491205	4.699318
H	3.109279	4.772504	4.692781
H	2.864117	7.618261	7.573014
H	2.032374	6.146875	8.034925
H	3.493833	6.061115	7.073924
N	-0.713871	7.698838	3.986985
H	0.160725	7.965963	3.585406
C	-1.707708	8.711512	4.224758
H	-1.322197	9.656200	3.862518
H	-1.918129	8.817721	5.279115
C	-3.055908	8.418387	3.572063
O	-4.061986	8.598362	4.218495

N	-3.085487	7.934665	2.316397
C	-4.424396	7.823301	1.734004
C	-5.116728	6.512006	2.064702
O	-6.328728	6.465419	2.052662
C	-4.227832	8.114139	0.239506
C	-2.986630	9.013024	0.255735
C	-2.106725	8.338901	1.296390
H	-5.062018	8.581303	2.161601
H	-4.041579	7.202242	-0.312361
H	-5.105584	8.586759	-0.182585
H	-2.486164	9.104999	-0.690577
H	-3.260891	10.009845	0.592859
H	-1.610347	7.471344	0.900543
H	-1.355957	8.996173	1.703517
N	-4.347909	5.461800	2.378965
C	-4.936672	4.237281	2.892134
C	-5.664171	4.491604	4.215738
O	-6.726167	3.954287	4.441223
C	-3.879793	3.126534	3.083612
C	-3.508391	2.339492	1.842038
C	-3.840413	0.993666	1.727777
C	-2.778502	2.895067	0.792263
C	-3.488422	0.236764	0.619653
C	-2.410634	2.155176	-0.311044
C	-2.756568	0.794211	-0.450244
O	-2.435971	0.116882	-1.507373
H	-3.358657	5.587871	2.429389
H	-5.699459	3.898649	2.208395
H	-3.000335	3.572773	3.539111
H	-4.281092	2.432575	3.814075

H	-4.389685	0.516311	2.523769
H	-2.469836	3.919371	0.842249
H	-3.741596	-0.808619	0.575727
H	-1.840033	2.616058	-1.099800
N	-5.067567	5.302063	5.107633
H	-4.145253	5.644315	4.932713
C	-5.693050	5.616465	6.372271
H	-4.926728	5.981968	7.044812
H	-6.143195	4.737061	6.803590
C	-6.790404	6.676691	6.267850
O	-7.850558	6.542823	6.836045
N	-6.502383	7.752530	5.528492
H	-5.606659	7.844328	5.098052
C	-7.450200	8.860410	5.330187
H	-6.985408	9.553054	4.640519
H	-7.641875	9.376803	6.259295
C	-8.807183	8.459359	4.784921
O	-9.801618	9.021967	5.170285
N	-8.848541	7.481791	3.858232
C	-10.122203	7.081631	3.312035
C	-10.996107	6.294821	4.288441
O	-12.127110	6.014457	3.922102
C	-9.957857	6.295381	1.992081
O	-11.202947	6.239333	1.319743
C	-9.383135	4.898576	2.172762
H	-8.000713	7.085166	3.506572
H	-10.697469	7.970397	3.088210
H	-9.295231	6.875273	1.363152
H	-11.886911	6.182756	1.983503
H	-9.240611	4.434163	1.203771

H	-8.424859	4.917573	2.670240
H	-10.059779	4.274645	2.744698
N	-10.493119	5.929455	5.458921
C	-11.290888	5.249506	6.455670
C	-12.227379	6.182969	7.228948
O	-13.145923	5.710381	7.846659
C	-10.417291	4.481507	7.457125
C	-9.518761	3.392849	6.853049
C	-8.677461	2.758808	7.965061
C	-10.308433	2.319055	6.099498
H	-9.557277	6.181496	5.702259
H	-11.953027	4.565534	5.948913
H	-9.795483	5.191083	7.991836
H	-11.093433	4.038694	8.180951
H	-8.833475	3.854093	6.152016
H	-7.992728	2.018660	7.561887
H	-8.089825	3.508385	8.485244
H	-9.307298	2.265549	8.702828
H	-9.636406	1.559004	5.713106
H	-11.032148	1.831378	6.750495
H	-10.850622	2.722898	5.251637
N	-11.934518	7.498613	7.234464
C	-12.824643	8.434965	7.854322
C	-13.986224	8.853713	6.977627
H	-14.699319	9.525147	7.469433
O	-14.140171	8.521188	5.850014
H	-11.256254	7.858362	6.599361
H	-13.222525	8.011962	8.767909
H	-12.274908	9.331477	8.126763
N	-11.802826	10.320195	-2.707646

H	-11.574041	10.515984	-1.753568
C	-12.080551	8.894437	-2.897354
C	-11.661085	8.609736	-4.333310
O	-10.593715	8.108261	-4.591929
C	-13.499574	8.421126	-2.515250
C	-13.765554	8.699174	-1.024442
C	-13.687547	6.936446	-2.853503
C	-15.187413	8.376057	-0.561416
H	-12.598744	10.884176	-2.939163
H	-11.367682	8.347624	-2.295805
H	-14.224940	9.002043	-3.089443
H	-13.052606	8.134577	-0.427428
H	-13.577772	9.748484	-0.819679
H	-14.711016	6.624705	-2.689583
H	-13.451348	6.716628	-3.890397
H	-13.048797	6.318288	-2.230495
H	-15.326440	8.694612	0.465557
H	-15.927280	8.890201	-1.168929
H	-15.400687	7.314264	-0.601578
N	-12.482064	9.026362	-5.328160
H	-13.415170	9.280236	-5.095505
C	-12.231399	8.610726	-6.691936
H	-12.263572	7.534536	-6.795283
H	-13.001719	9.038466	-7.321946
C	-10.872964	9.048477	-7.245658
O	-10.244980	8.339256	-7.978283
N	-10.472282	10.301224	-6.896290
H	-11.035067	10.805894	-6.250380
C	-9.219019	10.889862	-7.340682
H	-9.115474	10.788962	-8.409984

H	-9.227674	11.940526	-7.081967
C	-7.980405	10.233171	-6.713787
O	-7.066038	9.820172	-7.371600
N	-7.951248	10.211886	-5.346525
H	-8.771970	10.475474	-4.849700
C	-6.773204	9.834574	-4.573715
H	-5.890666	10.284242	-5.000350
H	-6.899976	10.209176	-3.565441
C	-6.501152	8.343717	-4.490810
O	-5.355181	7.961999	-4.529533
N	-7.525544	7.484685	-4.328211
C	-7.212550	6.104827	-3.984309
C	-6.697719	5.300123	-5.171359
O	-5.964196	4.357729	-4.977792
C	-8.325959	5.343452	-3.223307
C	-9.530425	4.945661	-4.093763
C	-8.711969	6.118577	-1.958772
C	-10.556737	4.074592	-3.365414
H	-8.470676	7.811758	-4.318455
H	-6.360554	6.132083	-3.321863
H	-7.840997	4.425181	-2.905434
H	-10.018557	5.828581	-4.486623
H	-9.168986	4.382434	-4.950137
H	-9.337015	5.516951	-1.312643
H	-7.830679	6.392646	-1.387496
H	-9.258152	7.024593	-2.195671
H	-11.336698	3.762157	-4.053138
H	-10.099766	3.177811	-2.963036
H	-11.037854	4.604080	-2.551566
N	-7.073816	5.638270	-6.420812

C	-6.450987	4.974479	-7.548094
C	-5.026674	5.464849	-7.812071
O	-4.194572	4.698191	-8.233710
C	-7.341763	5.034464	-8.797238
C	-8.478254	4.005581	-8.715805
C	-7.972126	2.586652	-9.006672
N	-8.874871	1.528173	-8.557812
C	-8.929258	1.019825	-7.329007
N	-8.167173	1.472639	-6.346679
N	-9.763834	0.035226	-7.059737
H	-7.671243	6.424048	-6.562250
H	-6.294403	3.947677	-7.266612
H	-7.750978	6.032684	-8.914300
H	-6.731258	4.842944	-9.674116
H	-8.934965	4.045107	-7.732555
H	-9.258920	4.255105	-9.425698
H	-7.851080	2.449718	-10.072283
H	-6.993488	2.411991	-8.578136
H	-9.394778	1.045896	-9.256042
H	-7.534446	2.227690	-6.471548
H	-8.420750	1.224286	-5.400433
H	-10.408646	-0.319764	-7.729813
H	-9.630508	-0.532613	-6.242181
N	-4.779992	6.748345	-7.543284
H	-5.522997	7.341551	-7.251500
C	-3.485316	7.385726	-7.827284
H	-3.157246	7.158327	-8.829714
H	-3.616712	8.454655	-7.727422
C	-2.411303	6.912320	-6.860550
O	-1.281726	6.704121	-7.226618

N	-2.828457	6.767479	-5.597011
C	-1.933862	6.465321	-4.505927
C	-1.619439	4.984875	-4.401593
O	-0.482104	4.629507	-4.203840
C	-2.524255	7.029328	-3.207201
C	-1.917662	6.322582	-1.996582
C	-2.315398	8.550100	-3.217773
H	-3.754329	7.056494	-5.366174
H	-0.975713	6.928771	-4.692138
H	-3.589324	6.829660	-3.217866
H	-2.138346	6.848850	-1.087086
H	-2.310547	5.315859	-1.902646
H	-0.844625	6.271233	-2.073744
H	-3.050147	9.052153	-2.604354
H	-1.325181	8.804270	-2.854846
H	-2.425205	8.951212	-4.218869
N	-2.622060	4.096465	-4.535400
C	-2.249510	2.701983	-4.666890
C	-1.300735	2.556267	-5.857580
O	-0.352381	1.806056	-5.797896
C	-3.452172	1.756963	-4.766294
C	-4.371062	1.844521	-3.540722
C	-5.377987	0.695911	-3.437060
N	-4.779198	-0.493092	-2.836825
C	-5.420980	-1.630103	-2.679624
N	-6.662734	-1.800277	-3.160596
N	-4.893685	-2.637278	-2.008631
H	-3.547101	4.396667	-4.754613
H	-1.669259	2.409970	-3.805424
H	-4.021020	1.966291	-5.670195

H	-3.053329	0.754143	-4.865686
H	-3.778806	1.873021	-2.639593
H	-4.937775	2.762648	-3.580318
H	-6.218814	1.015974	-2.831531
H	-5.751777	0.452053	-4.427706
H	-3.873939	-0.374788	-2.370380
H	-7.032973	-1.165159	-3.828895
H	-7.042367	-2.728999	-3.173415
H	-4.032180	-2.598623	-1.492245
H	-5.384573	-3.504658	-1.972268
N	-1.566245	3.258454	-6.951797
H	-2.408528	3.780791	-7.050437
C	-0.705504	3.110063	-8.109480
H	-1.081093	3.759599	-8.889565
H	-0.694360	2.092078	-8.471540
C	0.738936	3.490488	-7.797955
O	1.678902	2.890814	-8.255833
N	0.863994	4.538401	-6.969587
H	0.057483	5.074073	-6.741814
C	2.130051	5.040619	-6.542744
H	2.753786	5.334352	-7.377563
H	1.954385	5.918720	-5.934853
C	2.971154	4.092986	-5.704450
O	4.172380	4.256194	-5.621505
N	2.338355	3.115574	-5.046633
C	3.044667	2.277830	-4.112784
C	4.231133	1.506149	-4.702015
O	5.158942	1.213471	-3.974725
C	1.993220	1.369435	-3.474783
C	2.410727	0.551241	-2.258610

C	1.124748	0.122338	-1.560007
N	1.348493	-0.933938	-0.594893
C	0.468646	-1.918857	-0.361199
N	-0.683847	-1.954598	-0.981799
N	0.812819	-2.890773	0.461268
H	1.351437	3.003230	-5.150594
H	3.503519	2.894102	-3.349131
H	1.186624	2.031845	-3.178985
H	1.573820	0.717178	-4.231932
H	2.985510	-0.321632	-2.548607
H	3.035032	1.137878	-1.588586
H	0.645021	0.975608	-1.092811
H	0.436720	-0.255535	-2.299305
H	2.060229	-0.803538	0.088182
H	-1.169330	-1.107744	-1.267857
H	-1.315144	-2.722055	-0.791504
H	1.725740	-2.942064	0.847983
H	0.092020	-3.526417	0.788710
N	4.240680	1.146385	-5.997086
H	3.489390	1.422198	-6.595078
C	5.342997	0.362579	-6.528185
H	5.116615	0.124591	-7.560112
H	5.451333	-0.563932	-5.986890
C	6.697633	1.039094	-6.494589
O	7.719103	0.398703	-6.406783
N	6.689816	2.371358	-6.597599
H	5.821817	2.865356	-6.540036
C	7.908114	3.142744	-6.529888
H	8.618848	2.794830	-7.266098
H	7.672690	4.172779	-6.762091

C	8.658375	3.137022	-5.196083
O	9.787596	3.577964	-5.140840
N	8.033768	2.605874	-4.137287
C	8.626709	2.428875	-2.822709
C	9.916197	1.597634	-2.856545
O	10.736975	1.683746	-1.957497
C	7.546867	1.710575	-1.982732
C	7.753961	1.563742	-0.475517
C	7.378842	2.807633	0.339139
C	7.283515	2.509382	1.831527
N	8.627504	2.502213	2.482073
O	11.015629	1.860772	0.870565
H	10.855107	2.085997	-0.046208
H	11.515347	1.048271	0.801235
H	7.096247	2.278780	-4.252134
H	8.900012	3.385226	-2.396740
H	6.613581	2.230408	-2.152548
H	7.406374	0.727525	-2.417021
H	7.098581	0.758652	-0.157753
H	8.760160	1.235532	-0.250773
H	8.067175	3.632258	0.176046
H	6.401623	3.156858	0.021479
H	6.703350	3.255265	2.352169
H	6.830952	1.546206	2.010013
H	9.347976	2.068717	1.913160
H	8.922083	3.477566	2.653864
H	8.592148	2.006337	3.360750
N	10.048263	0.767818	-3.882324
C	11.120660	-0.183210	-4.140789
C	12.479071	0.423004	-4.495817

O	13.457480	-0.281435	-4.392270
C	10.729413	-1.076474	-5.339706
C	9.621079	-2.111009	-5.097777
C	9.196927	-2.719634	-6.438086
C	10.085480	-3.209472	-4.141253
H	9.306122	0.759165	-4.551083
H	11.298615	-0.784169	-3.261008
H	10.439224	-0.421711	-6.156008
H	11.625048	-1.597996	-5.655393
H	8.753347	-1.612402	-4.677127
H	8.416907	-3.460847	-6.292979
H	8.813745	-1.958866	-7.106148
H	10.034753	-3.214775	-6.922789
H	9.317113	-3.963745	-4.011255
H	10.966963	-3.703454	-4.536675
H	10.334560	-2.826091	-3.156495
N	12.529197	1.674109	-4.960993
C	13.749777	2.301832	-5.429800
C	14.895161	2.499829	-4.418460
O	15.936125	2.918497	-4.849509
C	13.390804	3.634240	-6.091133
O	12.792738	4.515035	-5.183061
H	11.696047	2.222647	-4.940441
H	14.197106	1.663837	-6.182794
H	14.299390	4.086863	-6.456238
H	12.739799	3.441029	-6.937874
H	11.845476	4.479890	-5.240670
N	14.745759	2.156649	-3.119625
C	15.888817	2.094079	-2.230321
C	16.797862	0.886888	-2.488267

O	17.930596	0.893702	-2.081380
C	15.466628	1.980130	-0.760393
C	14.580191	3.100712	-0.221206
C	14.240604	2.810898	1.241228
N	13.194226	3.665261	1.788343
C	13.344071	4.807400	2.439160
N	14.549949	5.311373	2.678313
O	14.869775	7.744209	4.281061
H	14.559394	8.627585	4.064773
H	15.588619	7.856532	4.889987
N	12.278327	5.458053	2.856558
H	13.864843	1.823854	-2.804898
H	16.497298	2.971953	-2.384381
H	14.953772	1.033928	-0.622501
H	16.383573	1.924418	-0.183972
H	15.070472	4.065122	-0.318019
H	13.656352	3.168884	-0.783708
H	13.871479	1.799097	1.326258
H	15.121645	2.862748	1.870126
H	12.261500	3.346651	1.617495
H	15.368948	4.847276	2.365265
H	14.665354	6.158838	3.206931
H	11.329638	5.155213	2.698915
H	12.350647	6.292512	3.393565
N	16.219636	-0.176222	-3.072156
C	16.923677	-1.414983	-3.303777
C	17.713392	-1.343009	-4.607284
H	18.076203	-0.346683	-4.869724
O	17.944470	-2.286793	-5.290166
C	15.953638	-2.601351	-3.303997

C	15.427756	-2.974136	-1.950792
N	14.489769	-2.242001	-1.250289
O	12.538275	-0.116070	-0.541504
H	13.188485	-0.693087	-0.945935
H	12.040395	0.281344	-1.247765
C	15.757560	-4.070970	-1.232846
C	14.282588	-2.895072	-0.153798
N	15.024810	-4.006840	-0.074175
H	15.299861	-0.095232	-3.449370
H	17.657020	-1.530904	-2.513430
H	15.126055	-2.382251	-3.969829
H	16.476123	-3.452464	-3.719471
H	16.434523	-4.872121	-1.438818
H	13.599794	-2.600431	0.617371
H	14.947314	-4.707149	0.630519
O	-14.615809	-2.482410	4.768728
H	-14.852064	-1.958458	4.005649
H	-14.381115	-1.864405	5.453289
O	-13.191662	-0.594781	6.670794
H	-12.500574	-1.061104	7.126518
H	-13.560371	0.016906	7.296437
O	-12.192924	-0.130395	3.899330
H	-12.475726	-0.050048	4.803963
H	-12.977667	-0.344870	3.394555
O	-12.405320	-2.798951	1.211586
H	-11.728545	-2.129098	1.172760
H	-12.301413	-3.242307	2.053422
O	-6.815806	1.307713	0.056255
H	-7.122601	1.524476	0.940636
H	-5.886832	1.122256	0.145264

O	-7.842742	1.787559	2.655195
H	-8.795719	1.803286	2.617068
H	-7.570302	2.464721	3.269371
O	-8.640067	-0.227926	-1.283258
H	-7.940030	0.247482	-0.813982
H	-8.308093	-1.090753	-1.508414
O	-12.290583	-2.121506	-1.641122
H	-12.795314	-2.785666	-1.184193
H	-11.987773	-1.539874	-0.945389
O	-12.763189	1.432073	-1.313844
H	-12.139541	0.861008	-0.866891
H	-12.664237	2.276669	-0.873701
O	-13.848145	3.968839	2.991320
H	-13.378146	4.625144	3.502738
H	-14.765878	4.071430	3.203923
O	-15.159707	0.586181	0.082183
H	-15.883469	0.443557	-0.511663
H	-14.418114	0.868655	-0.452221
O	-12.217179	-0.192514	-3.771701
H	-12.546238	0.566212	-3.293630
H	-12.356182	-0.923388	-3.170533
O	-12.037246	-1.698877	-6.309050
H	-12.302049	-1.130879	-5.586897
H	-12.774237	-2.265124	-6.500076
O	-9.712164	-2.958409	-2.642603
H	-9.649003	-2.605256	-3.529519
H	-10.590330	-2.757793	-2.325358
O	-10.989194	-0.379079	0.185945
H	-10.137952	-0.359434	-0.261297
H	-10.902620	0.223367	0.933169

O	-10.757759	1.531259	2.195718
H	-11.261943	1.136567	2.911674
H	-11.281357	2.236936	1.820157
O	-12.331550	3.511267	0.661366
H	-13.019697	3.628153	1.320285
H	-11.863933	4.342652	0.640087
O	-9.337734	0.612626	-3.890324
H	-10.257950	0.355419	-3.911572
H	-9.049652	0.439643	-2.992154
O	-14.401300	-1.015400	2.311194
H	-14.793411	-0.426865	1.665242
H	-13.901486	-1.656320	1.807755
O	-12.391809	-3.876001	3.886340
H	-13.195693	-3.458100	4.222416
H	-11.684883	-3.529042	4.417399
O	-9.406459	-2.362849	-5.388474
H	-10.279235	-2.531589	-5.736960
H	-8.807301	-2.996491	-5.791534

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(+),Y266(-),E183(0)

POTENTIAL:+35mV

N	15.580942	-6.451471	5.391415
H	14.779104	-6.204513	5.938620
C	15.508191	-5.856005	4.054570
C	14.783016	-6.782958	3.060461
O	14.053577	-6.345859	2.185899
C	16.917677	-5.573721	3.520957
H	16.387759	-6.124395	5.885359
H	14.941991	-4.934023	4.051207

H	16.885963	-5.186741	2.509465
H	17.400751	-4.828476	4.142751
H	17.526242	-6.471247	3.528981
N	15.032385	-8.085607	3.186394
H	15.610982	-8.361763	3.950518
C	14.398655	-9.092381	2.333234
H	14.481873	-8.823219	1.292970
H	14.891987	-10.042050	2.492097
C	12.912988	-9.222114	2.671603
O	12.082257	-9.428517	1.826246
N	12.582805	-9.055890	3.966874
H	13.302554	-8.984003	4.648771
C	11.195103	-9.170806	4.421393
H	11.188255	-9.158111	5.503149
H	10.743824	-10.088262	4.076954
C	10.336955	-8.010603	3.900717
O	9.191198	-8.186526	3.583649
N	10.946779	-6.814294	3.855610
C	10.317527	-5.633912	3.318096
C	10.126103	-5.690555	1.799772
O	9.096116	-5.261786	1.337431
C	11.091289	-4.387807	3.777159
O	12.477603	-4.569759	3.767472
H	11.905030	-6.743480	4.107374
H	9.313636	-5.553631	3.701699
H	10.798291	-3.538963	3.169683
H	10.827436	-4.175602	4.802882
H	12.802544	-4.752241	2.894343
N	11.099667	-6.200188	1.024514
C	10.844275	-6.396400	-0.399882

C	9.694514	-7.386178	-0.602164
O	8.948411	-7.282241	-1.547698
C	12.133011	-6.783990	-1.186532
C	12.336014	-8.289317	-1.401796
C	12.158579	-6.060271	-2.534161
H	11.923084	-6.586725	1.432080
H	10.473896	-5.462260	-0.790979
H	12.964634	-6.412125	-0.598542
H	13.290340	-8.451776	-1.892105
H	12.334419	-8.854739	-0.480691
H	11.569745	-8.698043	-2.053302
H	13.053375	-6.323813	-3.087019
H	11.298193	-6.333473	-3.135146
H	12.157470	-4.984942	-2.402011
N	9.570413	-8.340330	0.328325
H	10.313296	-8.473119	0.975853
C	8.593028	-9.421195	0.241219
H	8.934764	-10.218801	0.888531
H	8.533151	-9.803240	-0.766221
C	7.181546	-9.046150	0.643059
O	6.257862	-9.505041	0.011845
N	7.003139	-8.225180	1.684377
C	5.669236	-7.737017	1.952534
C	5.251026	-6.727546	0.888869
O	4.075011	-6.634436	0.609248
C	5.414749	-7.229137	3.385884
C	5.554761	-8.372063	4.396420
C	6.257705	-6.020635	3.797779
H	7.780632	-7.957153	2.247562
H	4.986299	-8.556668	1.791680

H	4.374383	-6.918810	3.377975
H	5.264683	-8.032966	5.385334
H	4.915597	-9.208967	4.134554
H	6.576433	-8.730676	4.453191
H	5.916925	-5.646780	4.757341
H	7.299661	-6.292262	3.906033
H	6.186856	-5.207074	3.084168
N	6.171317	-6.000952	0.246571
C	5.774690	-5.182491	-0.887395
C	5.343127	-6.067027	-2.065410
O	4.320846	-5.815975	-2.659082
C	6.866981	-4.162911	-1.267457
C	7.064539	-3.145802	-0.129354
C	6.496329	-3.452744	-2.574064
C	8.359106	-2.340455	-0.242737
H	7.132068	-6.054977	0.507757
H	4.876392	-4.646331	-0.620583
H	7.797090	-4.704294	-1.414889
H	6.210170	-2.470840	-0.114628
H	7.072970	-3.658976	0.822973
H	7.201636	-2.662972	-2.793820
H	6.497032	-4.128183	-3.419846
H	5.508375	-3.009311	-2.507758
H	8.460015	-1.666065	0.600945
H	9.220074	-2.998679	-0.241061
H	8.396599	-1.741743	-1.145871
N	6.115468	-7.110232	-2.399910
H	7.009414	-7.232242	-1.972867
C	5.773645	-7.950643	-3.527577
H	6.604258	-8.624483	-3.697228

H	5.618654	-7.364976	-4.421426
C	4.504822	-8.779444	-3.325685
O	3.667639	-8.839480	-4.195014
N	4.393582	-9.432010	-2.161998
H	5.129956	-9.385778	-1.490355
C	3.207574	-10.187543	-1.833506
H	2.968501	-10.900779	-2.608026
H	3.399860	-10.729423	-0.915948
C	1.974222	-9.306874	-1.644766
O	0.887704	-9.697014	-2.006487
N	2.187839	-8.106992	-1.107224
C	1.056881	-7.190771	-1.061929
C	0.613907	-6.716952	-2.448694
O	-0.568610	-6.580259	-2.671111
C	1.259721	-5.955130	-0.190409
O	1.407232	-6.260833	1.156457
H	3.085682	-7.817705	-0.792071
H	0.208261	-7.723964	-0.665600
H	2.093767	-5.367945	-0.558832
H	0.358598	-5.372731	-0.287759
H	2.310452	-6.501650	1.311294
N	1.541502	-6.433051	-3.372548
C	1.144612	-6.026007	-4.707974
C	0.383790	-7.149795	-5.406292
O	-0.599171	-6.894962	-6.070895
C	2.354340	-5.514691	-5.524623
C	2.747885	-4.119911	-5.010065
C	2.064279	-5.491880	-7.030704
C	4.068334	-3.595300	-5.571779
H	2.511686	-6.484301	-3.146650

H	0.420177	-5.228082	-4.628967
H	3.179635	-6.198616	-5.350941
H	1.949819	-3.420754	-5.254002
H	2.821324	-4.147221	-3.930592
H	2.921319	-5.113249	-7.573557
H	1.855346	-6.480629	-7.420792
H	1.214908	-4.856255	-7.260610
H	4.352155	-2.680824	-5.061660
H	4.867104	-4.315145	-5.424277
H	4.008912	-3.373972	-6.631636
N	0.821975	-8.401024	-5.244109
H	1.666597	-8.577992	-4.741098
C	0.045228	-9.507200	-5.750358
H	-0.058497	-9.463811	-6.824338
H	0.556132	-10.424641	-5.487227
C	-1.365283	-9.540071	-5.166931
O	-2.319464	-9.766564	-5.875620
N	-1.472619	-9.318902	-3.858011
C	-2.777211	-9.341795	-3.238828
C	-3.683496	-8.205639	-3.713381
O	-4.881290	-8.411371	-3.773358
C	-2.686235	-9.304950	-1.706232
O	-3.934364	-9.568380	-1.126274
H	-0.656792	-9.234665	-3.288050
H	-3.297513	-10.246270	-3.520891
H	-2.007118	-10.077215	-1.372750
H	-2.297956	-8.346228	-1.379699
H	-4.620589	-9.163800	-1.642351
N	-3.127097	-7.027175	-3.988495
C	-3.875858	-5.902157	-4.525077

C	-4.428434	-6.235589	-5.911243
O	-5.594526	-6.042743	-6.175320
C	-2.949786	-4.666202	-4.544227
C	-3.373636	-3.509459	-5.435319
C	-4.697947	-3.120854	-5.605552
C	-2.390312	-2.795676	-6.113831
C	-5.023269	-2.068499	-6.447795
C	-2.709386	-1.733271	-6.941919
C	-4.034305	-1.370584	-7.119442
H	-2.153793	-6.905736	-3.798098
H	-4.737823	-5.708947	-3.906157
H	-2.836409	-4.330530	-3.517808
H	-1.973752	-4.990062	-4.875339
H	-5.483859	-3.656881	-5.110437
H	-1.358959	-3.079365	-6.000281
H	-6.059029	-1.808492	-6.590088
H	-1.927143	-1.199291	-7.450686
H	-4.288225	-0.560007	-7.780133
N	-3.561181	-6.734650	-6.798636
C	-4.008284	-7.079042	-8.128761
C	-5.137853	-8.106774	-8.097485
O	-6.023010	-8.048974	-8.911236
C	-2.862131	-7.619587	-8.987215
S	-1.637704	-6.375682	-9.506124
H	-2.619240	-6.918672	-6.522129
H	-4.430127	-6.208243	-8.608134
H	-2.362916	-8.439103	-8.487970
H	-3.281972	-7.998857	-9.909110
H	-1.029712	-6.214698	-8.341195
N	-5.078530	-9.066907	-7.155626

H	-4.254666	-9.191008	-6.606637
C	-6.085055	-10.116657	-7.179838
H	-6.256455	-10.458573	-8.188746
H	-5.713640	-10.946041	-6.589259
C	-7.459153	-9.722789	-6.613043
O	-8.482093	-10.083639	-7.127753
N	-7.417997	-9.015713	-5.478473
C	-8.635196	-8.650708	-4.780113
C	-9.497606	-7.639375	-5.527283
O	-10.691395	-7.613337	-5.381408
C	-8.342053	-8.119118	-3.365579
C	-7.452402	-6.868508	-3.254031
C	-8.068524	-5.494773	-3.197106
O	-9.366324	-5.425264	-3.275547
H	-9.662172	-4.515225	-3.141118
O	-7.375167	-4.513003	-3.068626
H	-6.533173	-8.780630	-5.080914
H	-9.261610	-9.526399	-4.683142
H	-9.293825	-7.952404	-2.881705
H	-7.844659	-8.919242	-2.828358
H	-6.864343	-6.931939	-2.346430
H	-6.729514	-6.823488	-4.051081
N	-8.837321	-6.734073	-6.273860
C	-9.562354	-5.706193	-6.995284
C	-10.453969	-6.285518	-8.085558
H	-10.493803	-7.369153	-8.176161
O	-11.080326	-5.574130	-8.814097
C	-8.632453	-4.606929	-7.557429
O	-9.420594	-3.476029	-7.901149
C	-7.779220	-5.029094	-8.745836

H	-7.863216	-6.859748	-6.448780
H	-10.234601	-5.219725	-6.297852
H	-7.990170	-4.289480	-6.747269
H	-10.129530	-3.784763	-8.459484
H	-7.101539	-4.221406	-9.001021
H	-7.188732	-5.909493	-8.538909
H	-8.399370	-5.232007	-9.612380
N	-12.952337	-9.022034	3.174429
H	-13.221885	-9.548043	2.368927
C	-11.777476	-8.184402	2.899254
C	-10.786110	-8.141422	4.045784
O	-9.651391	-7.750012	3.844839
C	-12.138829	-6.715798	2.593883
O	-12.680666	-6.209730	3.786891
C	-13.123659	-6.564348	1.440448
H	-13.731162	-8.457526	3.453462
H	-11.234242	-8.594444	2.059086
H	-11.219577	-6.198933	2.354009
H	-12.705205	-5.255890	3.753522
H	-13.277809	-5.510731	1.232665
H	-12.760607	-7.035071	0.534081
H	-14.087149	-6.991933	1.690561
N	-11.197283	-8.533693	5.241879
H	-12.125683	-8.893751	5.282445
C	-10.410859	-8.533376	6.450870
H	-10.329987	-7.538596	6.859769
H	-10.935023	-9.139523	7.180325
C	-8.975341	-9.054819	6.376698
O	-8.142020	-8.496097	7.046479
N	-8.658361	-10.127845	5.629560

H	-9.367380	-10.602437	5.117731
C	-7.269006	-10.558267	5.527641
H	-7.250768	-11.535588	5.062448
H	-6.829754	-10.640724	6.508820
C	-6.387520	-9.608326	4.692692
O	-5.220713	-9.464642	4.951299
N	-7.045371	-9.017966	3.701161
C	-6.307965	-7.993244	2.974822
C	-6.272142	-6.694071	3.774969
O	-5.283028	-5.999904	3.736324
C	-6.625165	-7.840081	1.473997
C	-7.801927	-7.000818	1.021176
C	-7.794152	-5.617392	1.177428
C	-8.856280	-7.580120	0.327262
C	-8.823327	-4.839127	0.674747
C	-9.876158	-6.802235	-0.197018
C	-9.868183	-5.429334	-0.017212
H	-8.040034	-9.015732	3.680471
H	-5.283750	-8.321386	2.998909
H	-5.728280	-7.418298	1.033763
H	-6.709424	-8.843478	1.073800
H	-6.967682	-5.138467	1.670053
H	-8.866379	-8.644528	0.166524
H	-8.794761	-3.771443	0.801947
H	-10.663426	-7.264311	-0.764062
H	-10.656637	-4.826606	-0.429629
N	-7.305307	-6.401670	4.567842
C	-7.244328	-5.289935	5.486041
C	-6.123095	-5.500187	6.503005
O	-5.483804	-4.544173	6.886831

C	-8.621845	-5.122928	6.162027
C	-8.871957	-3.782293	6.818762
C	-9.076178	-2.647527	6.038978
C	-8.965864	-3.666117	8.198909
C	-9.355381	-1.424999	6.623682
C	-9.253681	-2.444987	8.791069
C	-9.446161	-1.319898	8.006161
H	-8.166719	-6.890540	4.455286
H	-6.979255	-4.384090	4.959786
H	-9.370832	-5.271045	5.390883
H	-8.751486	-5.915482	6.886766
H	-9.017696	-2.717718	4.966178
H	-8.815944	-4.531878	8.819889
H	-9.498766	-0.559608	6.003100
H	-9.315268	-2.373487	9.862115
H	-9.642429	-0.366151	8.463925
N	-5.874695	-6.736533	6.930564
H	-6.525231	-7.461505	6.724341
C	-4.800131	-7.025983	7.853808
H	-4.840700	-6.391302	8.726234
H	-4.913440	-8.053889	8.174044
C	-3.403101	-6.854342	7.260234
O	-2.530344	-6.355557	7.930301
N	-3.199966	-7.288506	6.011338
C	-1.918226	-7.117567	5.344764
C	-1.662248	-5.648412	4.981286
O	-0.560174	-5.170187	5.147411
C	-1.835701	-8.057293	4.121485
C	-0.667103	-7.706915	3.198450
C	-1.739142	-9.516001	4.582692

H	-3.932129	-7.771843	5.536955
H	-1.129030	-7.365170	6.039841
H	-2.754959	-7.933795	3.553529
H	-0.603814	-8.436220	2.397891
H	-0.772183	-6.733467	2.740400
H	0.276309	-7.720592	3.735539
H	-1.753429	-10.180085	3.724485
H	-0.806460	-9.683338	5.115514
H	-2.557433	-9.800758	5.231252
N	-2.693665	-4.955534	4.488024
C	-2.553130	-3.575509	4.065186
C	-2.426208	-2.654326	5.277356
O	-1.537757	-1.832859	5.330420
C	-3.719576	-3.117929	3.177441
C	-3.943175	-3.893126	1.868659
C	-2.803969	-3.821723	0.864297
O	-1.683336	-4.162278	1.268515
O	-3.070426	-3.447865	-0.292108
H	-3.562126	-5.418546	4.333894
H	-1.634119	-3.470633	3.520465
H	-4.640072	-3.162042	3.751846
H	-3.547007	-2.069801	2.949880
H	-4.110318	-4.937451	2.087417
H	-4.844042	-3.509906	1.402029
N	-3.326633	-2.786991	6.269434
C	-3.116889	-2.037329	7.484968
C	-1.793959	-2.427212	8.154183
O	-1.130467	-1.588153	8.723310
C	-4.246554	-2.025444	8.524777
O	-4.447038	-3.268677	9.129345

C	-5.533431	-1.412348	7.984810
H	-4.004323	-3.515982	6.240661
H	-2.968153	-1.005975	7.204737
H	-3.872128	-1.384804	9.313464
H	-4.896877	-3.842327	8.521013
H	-6.263581	-1.358608	8.782951
H	-5.353504	-0.406617	7.617726
H	-5.954608	-1.999723	7.179927
N	-1.380385	-3.700437	8.043347
H	-2.029686	-4.420959	7.816584
C	-0.188986	-4.105194	8.744524
H	-0.243049	-3.889309	9.802284
H	-0.075393	-5.172767	8.609305
C	1.063269	-3.417761	8.226312
O	1.939020	-3.075595	8.988151
N	1.155018	-3.255737	6.890573
C	2.334927	-2.660226	6.326820
C	2.292759	-1.139308	6.163427
O	3.361594	-0.575856	6.017663
C	2.841729	-3.357628	5.064677
S	1.925438	-3.032480	3.534355
H	0.422091	-3.605818	6.305822
H	3.115321	-2.790801	7.061243
H	3.845673	-3.005743	4.875363
H	2.882985	-4.423240	5.242891
H	0.882413	-3.823131	3.739430
N	1.142366	-0.471603	6.274272
C	1.204810	0.968241	6.492101
C	1.757084	1.271011	7.870353
O	2.373300	2.286503	8.085460

C	-0.097879	1.735804	6.180395
C	-1.202986	1.553051	7.230812
C	-0.549988	1.433407	4.746657
C	-2.471638	2.356726	6.936894
H	0.273967	-0.966412	6.292942
H	1.951090	1.351735	5.814852
H	0.200239	2.777995	6.223840
H	-1.452136	0.506953	7.336813
H	-0.818983	1.869046	8.196355
H	-1.308318	2.135589	4.424419
H	0.284236	1.518660	4.055742
H	-0.955856	0.435440	4.650550
H	-3.145709	2.318657	7.787290
H	-2.246349	3.401972	6.741016
H	-3.007395	1.966692	6.078484
N	1.549778	0.323284	8.791250
H	0.886277	-0.399186	8.614875
C	1.977557	0.513535	10.160150
H	1.469368	-0.221659	10.771273
H	1.736734	1.503327	10.517828
C	3.481545	0.338407	10.305527
O	4.163932	1.129242	10.897436
N	3.999309	-0.752512	9.695188
H	3.389881	-1.465505	9.353007
C	5.424263	-0.937846	9.668203
H	5.637572	-1.908742	9.236097
H	5.854510	-0.903041	10.658459
C	6.156892	0.119125	8.844833
O	7.292547	0.410159	9.129102
N	5.502073	0.621264	7.799016

C	6.105379	1.756770	7.150116
C	5.529225	3.076874	7.656104
H	5.019200	3.037006	8.617190
O	5.664993	4.096776	7.053504
C	6.008315	1.677414	5.624159
C	6.757772	0.509176	5.017373
C	8.124364	0.325373	5.232303
C	6.094020	-0.399426	4.198323
C	8.808452	-0.719816	4.626464
C	6.775845	-1.442301	3.591190
C	8.136909	-1.602992	3.795367
H	4.573923	0.338581	7.573088
H	7.140980	1.765288	7.454008
H	4.965795	1.616528	5.338073
H	6.388812	2.612093	5.226687
H	8.655117	0.982033	5.900270
H	5.033279	-0.303711	4.064790
H	9.860154	-0.846617	4.817437
H	6.241068	-2.134057	2.965019
H	8.655420	-2.415347	3.319818
N	12.613551	9.596234	-1.248798
H	11.870161	9.916292	-1.841104
C	12.304851	8.264736	-0.719492
C	11.274750	8.450359	0.387495
O	10.268003	7.776899	0.418741
C	13.562814	7.581280	-0.165146
C	14.645862	7.276992	-1.205751
S	14.019241	6.202370	-2.529191
C	15.503228	6.052652	-3.552379
H	13.429440	9.571153	-1.827880

H	11.834244	7.616444	-1.447171
H	14.000777	8.205741	0.607669
H	13.255924	6.653893	0.304704
H	15.045770	8.189777	-1.632910
H	15.471079	6.785084	-0.703294
H	15.253026	5.397064	-4.372564
H	15.802981	7.016214	-3.943838
H	16.320884	5.616365	-2.993521
N	11.504585	9.414161	1.296142
C	10.595549	9.609526	2.408512
C	9.278487	10.278160	2.012197
O	8.284015	10.059880	2.657676
C	11.279269	10.369172	3.552065
C	12.449454	9.562313	4.084255
O	13.585196	9.823151	3.746092
N	12.143757	8.559354	4.916978
H	12.327488	9.969979	1.203551
H	10.296014	8.639497	2.770696
H	11.661916	11.325840	3.219140
H	10.549503	10.538802	4.333631
H	12.886454	7.961849	5.209714
H	11.221999	8.173120	4.949741
N	9.264254	11.068704	0.922246
H	10.110289	11.226689	0.424534
C	8.003508	11.517469	0.368849
H	8.200597	12.260284	-0.393480
H	7.389294	11.966561	1.132130
C	7.186379	10.384433	-0.254310
O	5.986874	10.472141	-0.295076
N	7.863138	9.332291	-0.761153

C	7.170537	8.144459	-1.230806
C	6.635013	7.300996	-0.063263
O	5.535074	6.808463	-0.143765
C	8.048175	7.342014	-2.220880
C	8.343851	8.194449	-3.469675
C	7.377236	6.017618	-2.604658
C	9.427595	7.620879	-4.385865
H	8.823223	9.228423	-0.530736
H	6.279762	8.470571	-1.745118
H	8.987067	7.114702	-1.723986
H	7.422047	8.321513	-4.032918
H	8.647254	9.189740	-3.162301
H	7.994568	5.475988	-3.309997
H	7.224312	5.377117	-1.744642
H	6.408172	6.182146	-3.064106
H	9.622354	8.301070	-5.208694
H	10.362841	7.474253	-3.852285
H	9.146447	6.667087	-4.816732
N	7.387521	7.177441	1.048751
C	6.879214	6.459386	2.206267
C	5.526964	7.037691	2.644201
O	4.577394	6.328593	2.872994
C	7.833035	6.547449	3.407935
C	9.254186	5.998826	3.247571
O	10.147089	6.635080	3.801055
O	9.427266	4.935078	2.601900
H	8.347933	7.445473	1.026788
H	6.683997	5.430521	1.946962
H	7.920845	7.572105	3.737535
H	7.375101	5.993760	4.225031

N	5.485400	8.375976	2.789462
H	6.314906	8.913016	2.651009
C	4.293484	9.041756	3.254423
H	4.532220	10.084899	3.420215
H	3.949416	8.627985	4.189136
C	3.132432	8.991223	2.270507
O	1.991571	9.123038	2.649828
N	3.467298	8.824812	0.987996
H	4.428824	8.814090	0.740710
C	2.517177	8.905263	-0.078282
H	3.061156	9.090910	-0.995481
H	1.843277	9.737570	0.070799
C	1.609143	7.687010	-0.310217
O	0.576548	7.817978	-0.906932
N	2.066075	6.540159	0.228970
C	1.242104	5.374512	0.442332
C	0.428577	5.482447	1.736686
O	-0.767067	5.314399	1.714675
C	2.093930	4.105641	0.436329
H	2.965976	6.568616	0.659286
H	0.511204	5.325335	-0.347126
H	1.473322	3.237799	0.630639
H	2.562940	3.992232	-0.534151
H	2.873412	4.148239	1.190229
N	1.071840	5.742054	2.891841
C	0.343362	5.580481	4.141115
C	-0.767537	6.616369	4.295716
O	-1.801826	6.321542	4.854401
C	1.265038	5.506578	5.383483
C	1.859225	6.852475	5.826178

C	2.351500	4.441264	5.171557
C	2.703619	6.756488	7.099342
H	2.061136	5.864514	2.906155
H	-0.187512	4.640745	4.089410
H	0.611135	5.167601	6.181290
H	2.460399	7.263935	5.021996
H	1.056223	7.560748	6.002567
H	2.727585	4.087181	6.120271
H	1.955815	3.585271	4.634418
H	3.190732	4.832107	4.606334
H	3.009861	7.747706	7.420695
H	2.135152	6.310542	7.910127
H	3.598629	6.163010	6.959733
N	-0.547055	7.847522	3.811660
H	0.336411	8.082027	3.409318
C	-1.515086	8.891307	4.019976
H	-1.102635	9.816987	3.638872
H	-1.728707	9.026988	5.070294
C	-2.867019	8.618723	3.365914
O	-3.871382	8.837845	4.002830
N	-2.902654	8.109030	2.120710
C	-4.238565	8.014256	1.531443
C	-4.961964	6.725338	1.881684
O	-6.174628	6.709525	1.859477
C	-4.026558	8.272467	0.032690
C	-2.762923	9.139713	0.039000
C	-1.907400	8.464717	1.098943
H	-4.863158	8.793103	1.940350
H	-3.860806	7.346274	-0.501526
H	-4.889738	8.759425	-0.402883

H	-2.254565	9.199306	-0.905587
H	-3.013536	10.149855	0.354164
H	-1.432418	7.575956	0.724388
H	-1.141521	9.110072	1.496853
N	-4.225552	5.661050	2.224931
C	-4.858214	4.466274	2.755772
C	-5.577685	4.756789	4.076287
O	-6.635886	4.219495	4.318051
C	-3.848725	3.314934	2.960362
C	-3.521157	2.489217	1.732291
C	-4.003564	1.191796	1.596357
C	-2.681720	2.955760	0.723124
C	-3.676542	0.393874	0.510403
C	-2.344660	2.175323	-0.362662
C	-2.828210	0.859856	-0.516628
O	-2.524070	0.142696	-1.553290
H	-3.232572	5.755249	2.273856
H	-5.633555	4.148264	2.076384
H	-2.946482	3.730438	3.399714
H	-4.274050	2.653899	3.707432
H	-4.645736	0.784605	2.361115
H	-2.264199	3.940005	0.792416
H	-4.031251	-0.621635	0.459970
H	-1.690521	2.567564	-1.123518
N	-4.978440	5.593135	4.942756
H	-4.053481	5.921603	4.756816
C	-5.596049	5.948456	6.200554
H	-4.820170	6.300490	6.869449
H	-6.073747	5.090239	6.644421
C	-6.660307	7.040830	6.077578

O	-7.721752	6.950751	6.651545
N	-6.341994	8.091462	5.314146
H	-5.441929	8.148872	4.886995
C	-7.257699	9.220080	5.085083
H	-6.767747	9.891068	4.391851
H	-7.457203	9.753718	6.002575
C	-8.613235	8.823360	4.520535
O	-9.605046	9.420524	4.857066
N	-8.648796	7.802988	3.639425
C	-9.906599	7.387763	3.064012
C	-10.814615	6.618253	4.025119
O	-11.921888	6.301996	3.625580
C	-9.699527	6.576916	1.766145
O	-10.918813	6.514769	1.049618
C	-9.142421	5.179765	1.996862
H	-7.796508	7.388185	3.322476
H	-10.475176	8.272116	2.806595
H	-9.008587	7.137973	1.151109
H	-11.629573	6.499085	1.686700
H	-8.977926	4.690673	1.043133
H	-8.198466	5.203156	2.518144
H	-9.837263	4.575605	2.567492
N	-10.363122	6.325279	5.239884
C	-11.214402	5.721314	6.240613
C	-12.207051	6.706314	6.865822
O	-13.185155	6.280572	7.423061
C	-10.396555	5.060982	7.359045
C	-9.478101	3.911877	6.917843
C	-8.661192	3.427702	8.119731
C	-10.246801	2.746064	6.289385

H	-9.437516	6.588959	5.507287
H	-11.837314	4.985705	5.757037
H	-9.796264	5.822134	7.845268
H	-11.108399	4.696996	8.092892
H	-8.779802	4.285547	6.178014
H	-7.969882	2.641520	7.830025
H	-8.082754	4.239166	8.548896
H	-9.307119	3.032871	8.901334
H	-9.561149	1.949768	6.016503
H	-10.980636	2.338150	6.982615
H	-10.769388	3.037772	5.385163
N	-11.895268	8.017538	6.820323
C	-12.827647	8.999955	7.287868
C	-13.875021	9.388054	6.265499
H	-14.622480	10.098675	6.636203
O	-13.910679	8.993856	5.147651
H	-11.160970	8.329980	6.223270
H	-13.332800	8.632576	8.171896
H	-12.292981	9.901693	7.573044
N	-11.427718	10.616303	-3.022662
H	-11.181784	10.821002	-2.074668
C	-11.805542	9.208255	-3.171993
C	-11.411876	8.859853	-4.600570
O	-10.372408	8.296781	-4.847846
C	-13.251584	8.847022	-2.769678
C	-13.485811	9.183007	-1.285248
C	-13.546072	7.370428	-3.064401
C	-14.920521	8.964482	-0.801260
H	-12.185027	11.226758	-3.265817
H	-11.130048	8.630122	-2.557241

H	-13.938881	9.461455	-3.355672
H	-12.805127	8.589818	-0.678202
H	-13.228457	10.223205	-1.111829
H	-14.588386	7.137580	-2.888916
H	-13.329917	7.104116	-4.094842
H	-12.950770	6.727756	-2.423252
H	-15.028799	9.322482	0.216146
H	-15.632448	9.504830	-1.419559
H	-15.199251	7.917440	-0.803647
N	-12.213403	9.290245	-5.603581
H	-13.132393	9.597055	-5.378919
C	-11.972873	8.843874	-6.959238
H	-12.036120	7.767574	-7.043632
H	-12.729694	9.282233	-7.598216
C	-10.601373	9.232962	-7.517197
O	-9.995633	8.495660	-8.239499
N	-10.162522	10.477376	-7.182169
H	-10.712985	11.009959	-6.548360
C	-8.894347	11.024012	-7.637087
H	-8.789649	10.891462	-8.702767
H	-8.879068	12.081531	-7.407689
C	-7.672369	10.359332	-6.988502
O	-6.753696	9.933719	-7.631003
N	-7.659527	10.350076	-5.619879
H	-8.480817	10.632301	-5.134111
C	-6.495273	9.961231	-4.832324
H	-5.599431	10.376548	-5.265838
H	-6.615523	10.362142	-3.833329
C	-6.266723	8.464845	-4.710641
O	-5.132773	8.048098	-4.719750

N	-7.317132	7.640706	-4.538962
C	-7.031730	6.283162	-4.102747
C	-6.418100	5.430947	-5.206525
O	-5.584341	4.608546	-4.911717
C	-8.199209	5.564407	-3.387622
C	-9.361970	5.169535	-4.313467
C	-8.633670	6.382842	-2.166096
C	-10.484162	4.409860	-3.603906
H	-8.253340	7.991942	-4.551234
H	-6.231077	6.343250	-3.381332
H	-7.753917	4.644906	-3.016860
H	-9.773862	6.044112	-4.799706
H	-8.966171	4.535054	-5.103163
H	-9.310817	5.819887	-1.537922
H	-7.775406	6.646572	-1.556464
H	-9.137245	7.297037	-2.456407
H	-11.217872	4.059045	-4.323485
H	-10.106686	3.542440	-3.073613
H	-11.006150	5.037071	-2.891818
N	-6.820746	5.582730	-6.487696
C	-6.124706	4.841502	-7.520863
C	-4.769596	5.446756	-7.898048
O	-3.906166	4.707721	-8.311091
C	-6.992665	4.548821	-8.753795
C	-8.055759	3.457003	-8.535877
C	-7.451501	2.105427	-8.124890
N	-8.381463	0.972383	-8.170203
C	-9.145668	0.545957	-7.161522
N	-9.387147	1.353847	-6.138685
N	-9.650116	-0.667484	-7.177329

H	-7.464663	6.307747	-6.721633
H	-5.829009	3.908699	-7.075691
H	-7.482563	5.456711	-9.092811
H	-6.328120	4.236451	-9.552056
H	-8.783129	3.791013	-7.801400
H	-8.601200	3.324068	-9.464290
H	-6.640642	1.853746	-8.795998
H	-7.028379	2.146125	-7.130341
H	-8.324676	0.367552	-8.959466
H	-9.187942	2.323896	-6.209231
H	-9.908761	1.064717	-5.327857
H	-9.309925	-1.401990	-7.769560
H	-10.323626	-0.963698	-6.488263
N	-4.571401	6.757467	-7.722150
H	-5.310884	7.354827	-7.430331
C	-3.257802	7.352376	-8.011159
H	-2.929773	7.089171	-9.004152
H	-3.359826	8.427210	-7.941886
C	-2.200638	6.878496	-7.024560
O	-1.071750	6.644367	-7.377119
N	-2.628281	6.767925	-5.761127
C	-1.750491	6.461060	-4.657481
C	-1.472709	4.974917	-4.527491
O	-0.342171	4.593876	-4.332972
C	-2.339329	7.057868	-3.373273
C	-1.752748	6.360792	-2.146915
C	-2.102396	8.574094	-3.408792
H	-3.551036	7.073964	-5.541396
H	-0.780207	6.899126	-4.842254
H	-3.407429	6.876217	-3.388069

H	-1.966145	6.907704	-1.247674
H	-2.166310	5.364057	-2.035887
H	-0.680506	6.286294	-2.218537
H	-2.833593	9.100400	-2.811775
H	-1.110853	8.816640	-3.041412
H	-2.195561	8.958917	-4.417789
N	-2.497811	4.112478	-4.641194
C	-2.166732	2.706235	-4.738411
C	-1.220364	2.507835	-5.924366
O	-0.299613	1.724469	-5.846519
C	-3.394698	1.789820	-4.822878
C	-4.317762	1.918876	-3.603384
C	-5.382998	0.821051	-3.504261
N	-4.858956	-0.390765	-2.879134
C	-5.570174	-1.480609	-2.694283
N	-6.815623	-1.586270	-3.199269
N	-5.121262	-2.493840	-1.979728
H	-3.426274	4.432932	-4.814255
H	-1.595729	2.414244	-3.870318
H	-3.953136	1.996794	-5.734046
H	-3.020653	0.775726	-4.902400
H	-3.729304	1.919009	-2.700063
H	-4.838359	2.862746	-3.645256
H	-6.219089	1.187815	-2.917838
H	-5.752181	0.587600	-4.500392
H	-3.950919	-0.310652	-2.404335
H	-7.065169	-0.991010	-3.953347
H	-7.233590	-2.498455	-3.208162
H	-4.262415	-2.495322	-1.453764
H	-5.653274	-3.337196	-1.951064

N	-1.459796	3.193317	-7.035069
H	-2.275109	3.755058	-7.144634
C	-0.596734	2.996847	-8.183415
H	-0.949731	3.640587	-8.978656
H	-0.612418	1.971696	-8.524569
C	0.856438	3.342222	-7.871335
O	1.782013	2.705251	-8.308357
N	1.006287	4.405059	-7.066829
H	0.213587	4.966413	-6.852763
C	2.282311	4.880660	-6.640289
H	2.920033	5.140173	-7.475915
H	2.126226	5.775339	-6.051617
C	3.092705	3.927578	-5.776448
O	4.297996	4.056843	-5.690801
N	2.428042	2.983351	-5.101928
C	3.098078	2.138002	-4.148361
C	4.271681	1.329667	-4.712376
O	5.187071	1.029301	-3.972538
C	2.012622	1.258937	-3.525104
C	2.383564	0.436981	-2.296646
C	1.071700	0.014275	-1.644960
N	1.261570	-1.019362	-0.648220
C	0.329209	-1.944122	-0.369088
N	-0.822961	-1.947915	-0.990811
N	0.620913	-2.889800	0.501775
H	1.438117	2.903912	-5.207742
H	3.559390	2.748218	-3.381224
H	1.215832	1.941299	-3.249471
H	1.593966	0.613242	-4.288065
H	2.964495	-0.438463	-2.566318

H	2.985475	1.020988	-1.603973
H	0.567986	0.874811	-1.218005
H	0.418636	-0.386703	-2.404574
H	1.961384	-0.877409	0.045179
H	-1.270495	-1.090194	-1.304959
H	-1.492543	-2.673986	-0.771530
H	1.537503	-2.992026	0.869586
H	-0.129527	-3.482597	0.842485
N	4.279931	0.941792	-5.999239
H	3.540628	1.225238	-6.608640
C	5.363429	0.116650	-6.504621
H	5.137543	-0.138155	-7.532654
H	5.442790	-0.800189	-5.942286
C	6.736131	0.756021	-6.476487
O	7.739004	0.089700	-6.367735
N	6.766121	2.085332	-6.608316
H	5.911829	2.604447	-6.567405
C	8.004966	2.823937	-6.549436
H	8.709861	2.441173	-7.273888
H	7.799420	3.854984	-6.804432
C	8.747309	2.825410	-5.211196
O	9.888641	3.234656	-5.158081
N	8.101388	2.335308	-4.145513
C	8.680327	2.169774	-2.823268
C	9.946635	1.302910	-2.830344
O	10.763704	1.385458	-1.927473
C	7.575211	1.499062	-1.976701
C	7.766324	1.380566	-0.464926
C	7.417783	2.651966	0.318509
C	7.302687	2.390078	1.816278

N	8.641120	2.360680	2.477755
O	11.024830	1.615144	0.899022
H	10.877058	1.824607	-0.023627
H	11.500759	0.787047	0.851330
H	7.155314	2.033455	-4.259736
H	8.976984	3.126966	-2.415151
H	6.657446	2.039390	-2.165745
H	7.411936	0.510684	-2.390454
H	7.087260	0.600396	-0.134973
H	8.761622	1.031072	-0.224296
H	8.129169	3.454182	0.142888
H	6.452813	3.019640	-0.015266
H	6.739154	3.162927	2.315438
H	6.822501	1.443850	2.012396
H	9.353189	1.894266	1.924660
H	8.962331	3.330852	2.630295
H	8.585425	1.885879	3.366971
N	10.062473	0.448236	-3.837526
C	11.109423	-0.537452	-4.068766
C	12.486378	0.023107	-4.427190
O	13.444372	-0.705525	-4.301692
C	10.700996	-1.444195	-5.251842
C	9.562735	-2.442398	-4.996623
C	9.130515	-3.066585	-6.327159
C	9.990124	-3.533298	-4.014557
H	9.324421	0.445784	-4.510916
H	11.265041	-1.124702	-3.175583
H	10.434318	-0.798623	-6.083327
H	11.583739	-1.996784	-5.550593
H	8.706536	-1.911341	-4.592493

H	8.329374	-3.782884	-6.172388
H	8.772762	-2.309477	-7.013203
H	9.957405	-3.594522	-6.795802
H	9.200046	-4.262903	-3.874314
H	10.859835	-4.059880	-4.393709
H	10.243703	-3.136659	-3.036216
N	12.574040	1.261815	-4.919241
C	13.814365	1.845027	-5.393453
C	14.959454	2.031091	-4.379514
O	16.015207	2.408283	-4.813084
C	13.496834	3.173240	-6.083867
O	12.919242	4.089092	-5.197601
H	11.755963	1.833054	-4.917152
H	14.247581	1.179477	-6.130689
H	14.419849	3.592385	-6.452815
H	12.845144	2.981116	-6.930316
H	11.971617	4.079044	-5.259625
N	14.792294	1.722323	-3.074273
C	15.927449	1.647073	-2.176062
C	16.804345	0.410268	-2.402952
O	17.934867	0.394781	-1.989920
C	15.492578	1.575149	-0.707132
C	14.633497	2.730365	-0.197460
C	14.275318	2.479761	1.267810
N	13.249920	3.374129	1.789875
C	13.427861	4.525812	2.416443
N	14.646199	5.001311	2.651446
O	15.028483	7.460479	4.200270
H	14.742233	8.347246	3.965182
H	15.744800	7.566168	4.813295

N	12.378597	5.214426	2.813528
H	13.899645	1.424374	-2.757635
H	16.561014	2.504510	-2.343707
H	14.953119	0.646336	-0.553579
H	16.403783	1.506482	-0.123020
H	15.150879	3.678802	-0.309934
H	13.715926	2.812463	-0.768282
H	13.876858	1.480758	1.369856
H	15.153012	2.519180	1.902347
H	12.309593	3.077599	1.620636
H	15.453422	4.508399	2.352244
H	14.782479	5.856907	3.161599
H	11.422466	4.934747	2.656962
H	12.470938	6.058752	3.331732
N	16.200243	-0.648980	-2.967248
C	16.871169	-1.911296	-3.166856
C	17.672697	-1.890181	-4.464988
H	18.056001	-0.908483	-4.752290
O	17.892522	-2.857183	-5.118531
C	15.868545	-3.070246	-3.149067
C	15.323575	-3.399033	-1.792010
N	14.402569	-2.625551	-1.113883
O	12.505261	-0.431587	-0.461793
H	13.140937	-1.034460	-0.851100
H	12.021754	-0.035064	-1.178537
C	15.617382	-4.489055	-1.048507
C	14.169880	-3.248580	-0.005115
N	14.879583	-4.379022	0.103505
H	15.284663	-0.551312	-3.350771
H	17.595216	-2.030652	-2.368481

H	15.051744	-2.842623	-3.825294
H	16.370118	-3.944154	-3.542418
H	16.272300	-5.313503	-1.232667
H	13.490877	-2.918023	0.754754
H	14.777596	-5.061568	0.822398
O	-14.810668	-2.300463	5.221065
H	-15.117954	-1.614369	4.633438
H	-14.385842	-1.854057	5.946330
O	-12.887354	-0.749716	7.017608
H	-12.157408	-1.240044	7.380299
H	-13.143846	-0.123774	7.683721
O	-12.182389	-0.219934	4.191620
H	-12.317790	-0.215653	5.135005
H	-13.062350	-0.213540	3.812117
O	-13.444610	-2.081829	1.043386
H	-12.707094	-1.469625	0.999055
H	-13.253806	-2.667306	1.776452
O	-7.227548	1.027278	-0.132813
H	-7.417762	1.422513	0.721308
H	-6.292804	0.853920	-0.116698
O	-7.800419	2.004921	2.507516
H	-8.737229	1.938269	2.672960
H	-7.464331	2.681235	3.089814
O	-9.391463	-0.255073	-1.399411
H	-8.588874	0.107549	-1.005860
H	-9.193998	-1.131989	-1.714374
O	-12.898664	-2.342439	-1.717073
H	-13.227643	-2.467610	-0.824356
H	-13.559134	-2.657688	-2.325338
O	-13.582322	1.728901	-0.139457

H	-12.969970	1.047323	0.144676
H	-13.096574	2.541090	0.019456
O	-14.214222	4.925261	2.493490
H	-13.815871	5.427744	3.198927
H	-14.742625	4.237703	2.880913
O	-15.511899	2.131104	1.952915
H	-16.374601	2.337125	1.617116
H	-14.938951	2.043800	1.188553
O	-13.352006	0.380953	-2.617827
H	-13.638571	0.979425	-1.926569
H	-13.107532	-0.426616	-2.164391
O	-14.253928	-1.710512	-4.323675
H	-14.310430	-0.848266	-3.916051
H	-15.046048	-1.836794	-4.829677
O	-10.280927	-2.825816	-2.846643
H	-10.563576	-2.516503	-3.706541
H	-11.076214	-2.783319	-2.316075
O	-11.492292	-0.111724	0.552159
H	-10.814978	-0.221725	-0.116904
H	-11.088207	0.400549	1.257364
O	-10.712479	1.650485	2.581335
H	-11.198742	1.216540	3.282895
H	-11.220941	2.398159	2.269761
O	-12.144953	3.759879	1.083310
H	-12.856805	4.177199	1.581844
H	-11.581387	4.476823	0.807283
O	-10.739823	0.825174	-3.610766
H	-11.624638	0.967810	-3.270608
H	-10.209406	0.558524	-2.853536
O	-14.797356	-0.395952	3.050048

H	-15.180792	0.434158	2.765888
H	-14.625983	-0.910082	2.263435
O	-12.786793	-3.291148	3.584722
H	-13.540288	-3.087120	4.150767
H	-12.146449	-2.622532	3.809038
O	-11.464431	-1.464384	-5.064547
H	-12.394426	-1.689741	-5.061388
H	-11.372522	-0.701816	-4.494661

PROTON CONFIGURATION, GIVEN BY NOMINAL CHARGES: R300(+),Y266(-),E183(0)

POTENTIAL:+70mV

N	15.580942	-6.451471	5.391415
H	14.780032	-6.202450	5.939015
C	15.508936	-5.856267	4.054381
C	14.783016	-6.782958	3.060461
O	14.052927	-6.345848	2.186351
C	16.918723	-5.575267	3.520829
H	16.388922	-6.126445	5.884811
H	14.943548	-4.933783	4.050777
H	16.887508	-5.188602	2.509196
H	17.402282	-4.830204	4.142438
H	17.526634	-6.473225	3.529213
N	15.032385	-8.085607	3.186394
H	15.611726	-8.361773	3.949956
C	14.398655	-9.092381	2.333234
H	14.482026	-8.823411	1.292930
H	14.891814	-10.042109	2.492291
C	12.912941	-9.221802	2.671549
O	12.081991	-9.427725	1.826222

N	12.582805	-9.055890	3.966874
H	13.302601	-8.984225	4.648771
C	11.195103	-9.170806	4.421393
H	11.188268	-9.158052	5.503150
H	10.743814	-10.088276	4.076999
C	10.336955	-8.010603	3.900717
O	9.191008	-8.186419	3.583982
N	10.946840	-6.814402	3.855477
C	10.317806	-5.633946	3.317913
C	10.125936	-5.690944	1.799676
O	9.095409	-5.262914	1.337619
C	11.091985	-4.387878	3.776677
O	12.478081	-4.570518	3.768589
H	11.905153	-6.743734	4.107118
H	9.314021	-5.553346	3.701716
H	10.799985	-3.539354	3.168231
H	10.827193	-4.174714	4.801965
H	12.804154	-4.753549	2.895974
N	11.099427	-6.200134	1.024233
C	10.843906	-6.396280	-0.400142
C	9.693932	-7.385891	-0.601949
O	8.946846	-7.281531	-1.546722
C	12.132581	-6.784079	-1.186875
C	12.335091	-8.289392	-1.402676
C	12.158507	-6.059844	-2.534220
H	11.923592	-6.585517	1.431446
H	10.473599	-5.462125	-0.791291
H	12.964299	-6.412703	-0.598709
H	13.289243	-8.451943	-1.893254
H	12.333626	-8.855099	-0.481749

H	11.568572	-8.697706	-2.054165
H	13.053324	-6.323369	-3.087025
H	11.298163	-6.332651	-3.135467
H	12.157646	-4.984566	-2.401658
N	9.570413	-8.340330	0.328325
H	10.313985	-8.473695	0.975007
C	8.593028	-9.421195	0.241219
H	8.934730	-10.218716	0.888658
H	8.533182	-9.803389	-0.766172
C	7.181601	-9.046055	0.643019
O	6.257696	-9.504303	0.011540
N	7.003254	-8.225682	1.684795
C	5.669337	-7.737864	1.953248
C	5.250683	-6.728463	0.889688
O	4.074489	-6.635555	0.610319
C	5.415062	-7.230052	3.386666
C	5.555804	-8.372944	4.397153
C	6.257693	-6.021256	3.798335
H	7.780786	-7.958039	2.248181
H	4.986498	-8.557633	1.792534
H	4.374560	-6.920133	3.379027
H	5.265824	-8.033989	5.386151
H	4.916955	-9.210139	4.135403
H	6.577632	-8.731095	4.453691
H	5.917252	-5.647714	4.758148
H	7.299799	-6.292437	3.905981
H	6.186132	-5.207611	3.084889
N	6.170722	-6.001783	0.247305
C	5.774057	-5.183188	-0.886544
C	5.342453	-6.067614	-2.064619

O	4.319611	-5.816967	-2.657693
C	6.866370	-4.163568	-1.266490
C	7.064089	-3.146778	-0.128135
C	6.495640	-3.453091	-2.572901
C	8.358608	-2.341364	-0.241507
H	7.131547	-6.055767	0.508370
H	4.875774	-4.647055	-0.619625
H	7.796413	-4.704961	-1.414136
H	6.209675	-2.471852	-0.113046
H	7.072752	-3.660261	0.824024
H	7.201073	-2.663439	-2.792634
H	6.496123	-4.128372	-3.418814
H	5.507777	-3.009450	-2.506345
H	8.459669	-1.667279	0.602395
H	9.219569	-2.999574	-0.240210
H	8.395924	-1.742331	-1.144429
N	6.115094	-7.110267	-2.399764
H	7.009200	-7.232182	-1.972917
C	5.773166	-7.950654	-3.527407
H	6.603773	-8.624464	-3.697164
H	5.618088	-7.364990	-4.421243
C	4.504391	-8.779437	-3.325286
O	3.666727	-8.839217	-4.194252
N	4.393489	-9.432237	-2.161725
H	5.130116	-9.386274	-1.490282
C	3.207509	-10.187687	-1.833100
H	2.968457	-10.901194	-2.607387
H	3.399729	-10.729245	-0.915337
C	1.974222	-9.306874	-1.644766
O	0.887641	-9.696716	-2.006853

N	2.187839	-8.106992	-1.107224
C	1.057293	-7.190318	-1.062587
C	0.614393	-6.717149	-2.449618
O	-0.568222	-6.580797	-2.672229
C	1.260884	-5.953916	-0.192301
O	1.407207	-6.258096	1.155035
H	3.085630	-7.817890	-0.791642
H	0.208391	-7.722702	-0.665750
H	2.095744	-5.368047	-0.560913
H	0.360409	-5.370723	-0.290954
H	2.310209	-6.499304	1.310800
N	1.541978	-6.433219	-3.373326
C	1.145306	-6.026444	-4.708903
C	0.383926	-7.150161	-5.406686
O	-0.599414	-6.895377	-6.070889
C	2.355364	-5.516309	-5.525830
C	2.750161	-4.121661	-5.011860
C	2.065082	-5.493782	-7.031873
C	4.071113	-3.598567	-5.573819
H	2.512179	-6.484400	-3.147282
H	0.421352	-5.228028	-4.630260
H	3.180097	-6.200860	-5.352025
H	1.952712	-3.421885	-5.256114
H	2.823616	-4.148562	-3.932382
H	2.922287	-5.115928	-7.574977
H	1.855414	-6.482508	-7.421643
H	1.216128	-4.857591	-7.261829
H	4.355835	-2.684147	-5.064138
H	4.869191	-4.319087	-5.425944
H	4.011957	-3.377696	-6.633782

N	0.822029	-8.401361	-5.244419
H	1.666961	-8.578312	-4.741837
C	0.045183	-9.507550	-5.750396
H	-0.058547	-9.464457	-6.824391
H	0.555968	-10.424984	-5.487021
C	-1.365283	-9.540071	-5.166931
O	-2.319660	-9.766341	-5.875532
N	-1.472619	-9.318902	-3.858011
C	-2.777199	-9.341695	-3.238902
C	-3.683450	-8.205506	-3.713465
O	-4.881322	-8.411248	-3.773692
C	-2.686361	-9.304845	-1.706302
O	-3.934868	-9.567478	-1.126550
H	-0.656773	-9.234632	-3.288022
H	-3.297570	-10.246125	-3.521001
H	-2.007741	-10.077477	-1.372691
H	-2.297630	-8.346339	-1.379736
H	-4.620706	-9.163263	-1.643416
N	-3.127111	-7.027015	-3.988257
C	-3.875863	-5.901980	-4.524784
C	-4.428614	-6.235544	-5.910866
O	-5.594890	-6.043062	-6.174788
C	-2.949638	-4.666160	-4.544134
C	-3.373582	-3.509162	-5.434866
C	-4.697943	-3.121138	-5.605936
C	-2.390079	-2.794466	-6.112213
C	-5.023140	-2.068528	-6.447950
C	-2.709037	-1.731822	-6.940011
C	-4.034028	-1.369769	-7.118460
H	-2.153777	-6.905563	-3.797752

H	-4.737744	-5.708640	-3.905770
H	-2.835792	-4.330664	-3.517704
H	-1.973785	-4.990141	-4.875645
H	-5.483973	-3.657794	-5.111689
H	-1.358668	-3.077613	-5.997935
H	-6.058947	-1.809003	-6.590949
H	-1.926647	-1.197125	-7.447783
H	-4.287805	-0.558995	-7.778972
N	-3.561441	-6.734521	-6.798272
C	-4.008508	-7.078851	-8.128429
C	-5.138203	-8.106391	-8.097030
O	-6.023786	-8.048359	-8.910373
C	-2.862308	-7.619503	-8.986796
S	-1.637985	-6.375566	-9.505778
H	-2.619303	-6.918057	-6.521968
H	-4.430210	-6.208006	-8.607851
H	-2.363073	-8.438930	-8.487425
H	-3.282114	-7.998944	-9.908641
H	-1.028311	-6.216387	-8.341476
N	-5.078530	-9.066907	-7.155626
H	-4.254448	-9.191282	-6.606960
C	-6.085060	-10.116602	-7.179909
H	-6.256484	-10.458535	-8.188814
H	-5.713662	-10.945999	-6.589336
C	-7.459153	-9.722789	-6.613043
O	-8.482202	-10.083712	-7.127603
N	-7.417997	-9.015713	-5.478473
C	-8.635228	-8.650794	-4.780214
C	-9.497583	-7.639488	-5.527515
O	-10.691523	-7.613783	-5.382204

C	-8.342204	-8.119479	-3.365555
C	-7.452656	-6.868873	-3.253586
C	-8.068928	-5.495205	-3.197281
O	-9.366890	-5.425967	-3.274947
H	-9.662569	-4.515899	-3.140575
O	-7.375855	-4.513192	-3.069779
H	-6.533145	-8.780549	-5.080936
H	-9.261654	-9.526501	-4.683426
H	-9.293990	-7.952983	-2.881624
H	-7.844713	-8.919716	-2.828593
H	-6.865359	-6.932172	-2.345462
H	-6.729038	-6.824038	-4.049967
N	-8.837321	-6.734073	-6.273860
C	-9.562354	-5.706193	-6.995284
C	-10.454398	-6.285823	-8.085024
H	-10.492575	-7.369440	-8.176611
O	-11.082831	-5.574761	-8.812120
C	-8.632334	-4.607486	-7.558369
O	-9.420395	-3.476450	-7.901913
C	-7.779995	-5.030258	-8.747174
H	-7.862924	-6.858983	-6.447851
H	-10.234191	-5.219167	-6.297860
H	-7.989439	-4.289969	-6.748737
H	-10.129723	-3.785046	-8.459788
H	-7.102240	-4.222849	-9.003008
H	-7.189656	-5.910795	-8.540406
H	-8.400760	-5.233196	-9.613299
N	-12.952337	-9.022034	3.174429
H	-13.221898	-9.547843	2.368800
C	-11.777476	-8.184402	2.899254

C	-10.786206	-8.141049	4.045833
O	-9.651794	-7.748991	3.844940
C	-12.139204	-6.715971	2.593616
O	-12.682500	-6.210242	3.786160
C	-13.123190	-6.564867	1.439408
H	-13.731053	-8.457372	3.453447
H	-11.234128	-8.594502	2.059193
H	-11.220030	-6.198617	2.354573
H	-12.705580	-5.256359	3.753617
H	-13.277812	-5.511284	1.231776
H	-12.759142	-7.035134	0.533219
H	-14.086619	-6.993097	1.688714
N	-11.197283	-8.533693	5.241879
H	-12.125441	-8.894327	5.282310
C	-10.410839	-8.533143	6.450874
H	-10.329810	-7.538243	6.859445
H	-10.935126	-9.138969	7.180508
C	-8.975370	-9.054834	6.377001
O	-8.142317	-8.496461	7.047326
N	-8.658401	-10.127681	5.629597
H	-9.367337	-10.601801	5.117236
C	-7.269036	-10.558230	5.527662
H	-7.250873	-11.535566	5.062507
H	-6.829823	-10.640686	6.508852
C	-6.387520	-9.608326	4.692692
O	-5.220778	-9.464714	4.951348
N	-7.045371	-9.017966	3.701161
C	-6.307770	-7.993249	2.974966
C	-6.271951	-6.694110	3.775155
O	-5.283209	-5.999603	3.736048

C	-6.624645	-7.839933	1.474129
C	-7.801491	-7.000779	1.021382
C	-7.793771	-5.617349	1.177637
C	-8.855869	-7.580140	0.327550
C	-8.823001	-4.839135	0.674989
C	-9.875794	-6.802301	-0.196695
C	-9.867860	-5.429397	-0.016917
H	-8.039999	-9.015706	3.680426
H	-5.283584	-8.321480	2.999193
H	-5.727772	-7.417896	1.034140
H	-6.708627	-8.843258	1.073702
H	-6.967234	-5.138390	1.670106
H	-8.865826	-8.644534	0.166700
H	-8.794372	-3.771435	0.802038
H	-10.662946	-7.264403	-0.763886
H	-10.656231	-4.826671	-0.429504
N	-7.304887	-6.402066	4.568621
C	-7.243633	-5.290399	5.486837
C	-6.122529	-5.500849	6.503923
O	-5.483919	-4.544745	6.888491
C	-8.621133	-5.123009	6.162735
C	-8.870978	-3.782230	6.819262
C	-9.074329	-2.647422	6.039317
C	-8.965227	-3.665869	8.199371
C	-9.352878	-1.424655	6.623845
C	-9.252495	-2.444533	8.791351
C	-9.444026	-1.319377	8.006301
H	-8.166278	-6.890903	4.456207
H	-6.978275	-4.384626	4.960604
H	-9.370110	-5.271048	5.391559

H	-8.750975	-5.915427	6.887595
H	-9.015326	-2.717689	4.966554
H	-8.815744	-4.531611	8.820473
H	-9.495167	-0.559151	6.003164
H	-9.314106	-2.372866	9.862383
H	-9.639479	-0.365401	8.463951
N	-5.873694	-6.737403	6.930639
H	-6.523837	-7.462461	6.723681
C	-4.798918	-7.027219	7.853568
H	-4.839434	-6.392910	8.726262
H	-4.912057	-8.055293	8.173308
C	-3.402041	-6.855021	7.259756
O	-2.529453	-6.356048	7.929815
N	-3.199026	-7.288853	6.010718
C	-1.917440	-7.117395	5.343880
C	-1.661931	-5.648043	4.980942
O	-0.560113	-5.169528	5.147342
C	-1.834981	-8.056581	4.120196
C	-0.666627	-7.705511	3.197092
C	-1.737973	-9.515476	4.580732
H	-3.931066	-7.772440	5.536444
H	-1.128028	-7.365099	6.038671
H	-2.754394	-7.933020	3.552461
H	-0.603247	-8.434485	2.396249
H	-0.772052	-6.731927	2.739407
H	0.276865	-7.719144	3.734016
H	-1.752280	-10.179174	3.722230
H	-0.805135	-9.682838	5.113241
H	-2.556016	-9.800751	5.229403
N	-2.693556	-4.955263	4.487767

C	-2.553158	-3.575182	4.065039
C	-2.426463	-2.653977	5.277199
O	-1.538667	-1.831911	5.330023
C	-3.719679	-3.117509	3.177421
C	-3.943574	-3.892489	1.868582
C	-2.804542	-3.821061	0.863953
O	-1.683850	-4.161187	1.268101
O	-3.071448	-3.447741	-0.292538
H	-3.561739	-5.418545	4.333127
H	-1.634155	-3.470126	3.520324
H	-4.640090	-3.161549	3.752004
H	-3.547026	-2.069386	2.949929
H	-4.110693	-4.936857	2.087166
H	-4.844544	-3.509167	1.402187
N	-3.326750	-2.787077	6.269499
C	-3.116889	-2.037329	7.484968
C	-1.794237	-2.427359	8.154644
O	-1.131337	-1.588396	8.724486
C	-4.246694	-2.024466	8.524552
O	-4.447835	-3.267125	9.130153
C	-5.533301	-1.411439	7.983889
H	-4.003544	-3.516870	6.241112
H	-2.967713	-1.006143	7.204427
H	-3.872217	-1.383373	9.312827
H	-4.896526	-3.841595	8.521772
H	-6.263504	-1.356701	8.781924
H	-5.353002	-0.406131	7.615824
H	-5.954533	-1.999485	7.179516
N	-1.380385	-3.700437	8.043347
H	-2.029276	-4.420959	7.815592

C	-0.188931	-4.105369	8.744389
H	-0.243085	-3.889884	9.802219
H	-0.075224	-5.172869	8.608749
C	1.063302	-3.417566	8.226548
O	1.938496	-3.074993	8.988764
N	1.155534	-3.255591	6.890819
C	2.335628	-2.659989	6.327401
C	2.293225	-1.139129	6.163586
O	3.361827	-0.575540	6.017522
C	2.843026	-3.357441	5.065548
S	1.926576	-3.033088	3.535114
H	0.423034	-3.606058	6.305800
H	3.115762	-2.790277	7.062151
H	3.846755	-3.004983	4.876236
H	2.884937	-4.422992	5.243934
H	0.884375	-3.824861	3.739961
N	1.142633	-0.471584	6.274413
C	1.204810	0.968241	6.492101
C	1.755916	1.271616	7.870712
O	2.370061	2.288207	8.086287
C	-0.097734	1.735605	6.179432
C	-1.203364	1.552573	7.229246
C	-0.548937	1.433114	4.745437
C	-2.472122	2.355834	6.934670
H	0.274371	-0.966553	6.293137
H	1.951539	1.351706	5.815329
H	0.200172	2.777829	6.223077
H	-1.452254	0.506401	7.335103
H	-0.819965	1.868670	8.194982
H	-1.307234	2.135135	4.422711

H	0.285689	1.518562	4.055049
H	-0.954514	0.435057	4.649078
H	-3.146623	2.317607	7.784741
H	-2.247035	3.401138	6.738861
H	-3.007297	1.965581	6.075985
N	1.549778	0.323284	8.791250
H	0.887646	-0.400248	8.614365
C	1.977411	0.513277	10.160240
H	1.469297	-0.222138	10.771158
H	1.736371	1.502965	10.518037
C	3.481464	0.338437	10.305644
O	4.163590	1.129611	10.897343
N	3.999374	-0.752513	9.695502
H	3.390026	-1.465660	9.353573
C	5.424384	-0.937776	9.668387
H	5.637697	-1.908748	9.236466
H	5.854709	-0.902773	10.658595
C	6.156892	0.119125	8.844833
O	7.292422	0.410310	9.129215
N	5.502073	0.621264	7.799016
C	6.105379	1.756770	7.150116
C	5.527844	3.076528	7.655357
H	5.019807	3.036813	8.617533
O	5.660218	4.095982	7.051290
C	6.009871	1.677000	5.624112
C	6.759574	0.508461	5.018261
C	8.125859	0.324149	5.234675
C	6.096367	-0.399896	4.198540
C	8.810160	-0.721369	4.629662
C	6.778403	-1.443104	3.592198

C	8.139152	-1.604335	3.797882
H	4.574258	0.337994	7.572539
H	7.140676	1.765946	7.455081
H	4.967618	1.616394	5.336959
H	6.390954	2.611487	5.226767
H	8.656185	0.980627	5.903151
H	5.035834	-0.303646	4.063675
H	9.861591	-0.848598	4.821775
H	6.244060	-2.134648	2.965419
H	8.657876	-2.416890	3.322938
N	12.613551	9.596234	-1.248798
H	11.871436	9.915304	-1.843204
C	12.304851	8.264736	-0.719492
C	11.274408	8.450403	0.387212
O	10.267132	7.777553	0.417750
C	13.562748	7.581214	-0.165073
C	14.645710	7.276794	-1.205745
S	14.018807	6.202678	-2.529470
C	15.502614	6.053319	-3.553061
H	13.431108	9.571901	-1.825531
H	11.834411	7.616446	-1.447272
H	14.000797	8.205633	0.607734
H	13.255768	6.653868	0.304789
H	15.045970	8.189500	-1.632722
H	15.470760	6.784540	-0.703374
H	15.252313	5.397949	-4.373385
H	15.802203	7.017027	-3.944248
H	16.320373	5.616909	-2.994482
N	11.504217	9.413659	1.296390
C	10.594885	9.608715	2.408553

C	9.277870	10.277202	2.011867
O	8.282950	10.058359	2.656562
C	11.278152	10.368526	3.552276
C	12.449004	9.562346	4.084095
O	13.584327	9.823627	3.745137
N	12.144247	8.559449	4.917297
H	12.327524	9.969043	1.204660
H	10.295446	8.638638	2.770692
H	11.660153	11.325520	3.219551
H	10.548333	10.537494	4.333937
H	12.887462	7.962683	5.210285
H	11.222606	8.173133	4.951167
N	9.264065	11.068466	0.922439
H	10.110333	11.226927	0.425236
C	8.003508	11.517469	0.368849
H	8.200883	12.260155	-0.393534
H	7.389207	11.966707	1.131974
C	7.186379	10.384433	-0.254310
O	5.986762	10.471967	-0.294680
N	7.862975	9.332412	-0.761422
C	7.170216	8.144717	-1.231180
C	6.634121	7.301583	-0.063672
O	5.533542	6.810234	-0.143954
C	8.047953	7.341826	-2.220812
C	8.344214	8.193868	-3.469735
C	7.376724	6.017526	-2.604410
C	9.427799	7.619595	-4.385676
H	8.823171	9.228493	-0.531400
H	6.279689	8.470973	-1.745832
H	8.986622	7.114373	-1.723614

H	7.422527	8.321304	-4.033115
H	8.648074	9.189061	-3.162501
H	7.994074	5.475544	-3.309450
H	7.223435	5.377267	-1.744262
H	6.407815	6.182227	-3.064151
H	9.623064	8.299583	-5.208546
H	10.362875	7.472532	-3.851957
H	9.146213	6.665900	-4.816478
N	7.386803	7.177010	1.048001
C	6.878471	6.458966	2.205533
C	5.526387	7.037544	2.643594
O	4.576348	6.328842	2.872050
C	7.832431	6.546973	3.407115
C	9.253720	5.998440	3.246793
O	10.146174	6.634099	3.801494
O	9.426915	4.935452	2.599915
H	8.347402	7.444505	1.025873
H	6.683101	5.430114	1.946241
H	7.920235	7.571604	3.736778
H	7.374599	5.993215	4.224226
N	5.485186	8.375799	2.789221
H	6.314855	8.912710	2.651013
C	4.293396	9.041619	3.254297
H	4.532121	10.084823	3.419754
H	3.949486	8.628088	4.189184
C	3.132251	8.990779	2.270521
O	1.991221	9.122025	2.649825
N	3.467175	8.824996	0.988015
H	4.428731	8.814459	0.740715
C	2.517177	8.905263	-0.078282

H	3.061296	9.090783	-0.995428
H	1.843247	9.737601	0.070557
C	1.609143	7.687010	-0.310217
O	0.575961	7.817995	-0.906057
N	2.066603	6.540113	0.228298
C	1.243128	5.374178	0.441778
C	0.429102	5.482160	1.735839
O	-0.766627	5.314105	1.713365
C	2.095741	4.105816	0.436590
H	2.966990	6.568467	0.657682
H	0.512481	5.324257	-0.347877
H	1.475672	3.237653	0.631216
H	2.565032	3.992230	-0.533730
H	2.875060	4.149297	1.190578
N	1.071867	5.741877	2.891149
C	0.343102	5.580151	4.140230
C	-0.767934	6.615908	4.294558
O	-1.802740	6.320914	4.852384
C	1.264523	5.506261	5.382840
C	1.858524	6.852144	5.825842
C	2.351129	4.441076	5.171011
C	2.702732	6.755957	7.099120
H	2.061139	5.864756	2.905732
H	-0.187624	4.640344	4.088332
H	0.610483	5.167122	6.180480
H	2.459789	7.263805	5.021839
H	1.055437	7.560337	6.002264
H	2.727135	4.087057	6.119765
H	1.955619	3.585054	4.633775
H	3.190411	4.832017	4.605953

H	3.008906	7.747130	7.420653
H	2.134150	6.309856	7.909746
H	3.597757	6.162523	6.959547
N	-0.547166	7.847269	3.811235
H	0.336647	8.082052	3.409699
C	-1.515070	8.891045	4.019963
H	-1.102613	9.816787	3.639001
H	-1.728571	9.026558	5.070337
C	-2.867019	8.618723	3.365914
O	-3.871542	8.838073	4.002641
N	-2.902654	8.109030	2.120710
C	-4.238446	8.014455	1.531311
C	-4.962235	6.725911	1.882105
O	-6.175023	6.710540	1.860509
C	-4.026033	8.271837	0.032465
C	-2.762245	9.138872	0.038703
C	-1.907041	8.464089	1.099009
H	-4.862895	8.793693	1.939718
H	-3.860235	7.345333	-0.501208
H	-4.889032	8.758703	-0.403610
H	-2.253665	9.198035	-0.905772
H	-3.012754	10.149174	0.353458
H	-1.432187	7.575084	0.724914
H	-1.141107	9.109403	1.496836
N	-4.226116	5.661452	2.225155
C	-4.858905	4.466859	2.756249
C	-5.578253	4.757896	4.076637
O	-6.637196	4.221784	4.318215
C	-3.849571	3.315415	2.961167
C	-3.522554	2.489227	1.733310

C	-4.006256	1.192327	1.597330
C	-2.682196	2.954873	0.724458
C	-3.679641	0.393976	0.511541
C	-2.345570	2.174039	-0.361123
C	-2.830320	0.859002	-0.515103
O	-2.526300	0.141424	-1.551460
H	-3.233060	5.755324	2.273732
H	-5.634268	4.148768	2.076922
H	-2.947150	3.730906	3.400116
H	-4.274834	2.654773	3.708629
H	-4.648977	0.785788	2.361985
H	-2.263497	3.938608	0.793964
H	-4.035128	-0.621264	0.461151
H	-1.690545	2.565435	-1.121639
N	-4.978249	5.593349	4.943342
H	-4.052878	5.920958	4.757670
C	-5.595830	5.948867	6.201061
H	-4.820004	6.301440	6.869721
H	-6.073260	5.090711	6.645348
C	-6.660373	7.040856	6.077506
O	-7.722216	6.950555	6.650877
N	-6.341994	8.091462	5.314146
H	-5.441694	8.149171	4.887399
C	-7.257699	9.220080	5.085083
H	-6.767935	9.890855	4.391520
H	-7.457015	9.753941	6.002489
C	-8.613245	8.822905	4.520945
O	-9.605397	9.419352	4.858020
N	-8.648646	7.802868	3.639474
C	-9.906427	7.387730	3.064070

C	-10.814615	6.618253	4.025119
O	-11.922342	6.303047	3.625709
C	-9.699456	6.577154	1.766027
O	-10.918960	6.515377	1.049630
C	-9.142513	5.179909	1.996305
H	-7.796253	7.388578	3.321987
H	-10.475007	8.272123	2.806771
H	-9.008548	7.138293	1.151057
H	-11.629541	6.500089	1.686895
H	-8.978219	4.691000	1.042450
H	-8.198473	5.203106	2.517425
H	-9.837331	4.575701	2.566939
N	-10.362995	6.324476	5.239523
C	-11.214402	5.721314	6.240613
C	-12.204465	6.707703	6.867696
O	-13.182138	6.283487	7.426952
C	-10.396506	5.058836	7.357807
C	-9.479288	3.909496	6.914686
C	-8.662618	3.422662	8.115655
C	-10.249252	2.745435	6.284559
H	-9.437061	6.587469	5.506673
H	-11.839051	4.987107	5.757154
H	-9.795195	5.818862	7.844521
H	-11.108262	4.694674	8.091654
H	-8.780726	4.283617	6.175345
H	-7.972056	2.636351	7.824574
H	-8.083338	4.232886	8.546012
H	-9.308772	3.027201	8.896768
H	-9.564390	1.949162	6.009681
H	-10.982936	2.336746	6.977519

H	-10.772233	3.039237	5.381240
N	-11.890969	8.018420	6.821510
C	-12.820046	9.002006	7.292926
C	-13.872848	9.389999	6.276136
H	-14.617563	10.101552	6.650702
O	-13.915547	8.994959	5.158858
H	-11.156942	8.330169	6.223743
H	-13.320760	8.636217	8.180174
H	-12.283011	9.903589	7.574076
N	-11.428782	10.616585	-3.022953
H	-11.181466	10.821440	-2.075361
C	-11.805542	9.208255	-3.171993
C	-11.412068	8.859747	-4.600590
O	-10.372868	8.296374	-4.847938
C	-13.251221	8.846068	-2.769246
C	-13.485124	9.181872	-1.284733
C	-13.544905	7.369304	-3.063914
C	-14.919638	8.962969	-0.800354
H	-12.186808	11.226537	-3.265071
H	-11.129483	8.630685	-2.557341
H	-13.939062	9.460100	-3.355054
H	-12.804141	8.588809	-0.677922
H	-13.227943	10.222109	-1.111296
H	-14.586961	7.135733	-2.887775
H	-13.329214	7.103259	-4.094512
H	-12.948756	6.726968	-2.423236
H	-15.027701	9.320778	0.217149
H	-15.631859	9.503270	-1.418386
H	-15.198148	7.915864	-0.802825
N	-12.213547	9.290342	-5.603633

H	-13.132406	9.597526	-5.379013
C	-11.972873	8.843874	-6.959238
H	-12.036058	7.767562	-7.043539
H	-12.729630	9.282181	-7.598332
C	-10.601373	9.232962	-7.517197
O	-9.996079	8.495776	-8.239965
N	-10.162529	10.477325	-7.182123
H	-10.712336	11.009297	-6.547235
C	-8.894347	11.024012	-7.637087
H	-8.789739	10.891343	-8.702753
H	-8.879150	12.081555	-7.407803
C	-7.672369	10.359332	-6.988502
O	-6.753965	9.933366	-7.631082
N	-7.659524	10.350113	-5.619891
H	-8.480443	10.633312	-5.134100
C	-6.495273	9.961231	-4.832324
H	-5.599400	10.376510	-5.265816
H	-6.615483	10.362178	-3.833336
C	-6.266723	8.464845	-4.710641
O	-5.132833	8.048154	-4.719743
N	-7.317133	7.640563	-4.539039
C	-7.031573	6.283107	-4.102678
C	-6.418931	5.430126	-5.206427
O	-5.586728	4.606355	-4.911260
C	-8.198463	5.564610	-3.386362
C	-9.361756	5.169035	-4.311225
C	-8.632279	6.383551	-2.164964
C	-10.482793	4.408545	-3.600702
H	-8.253318	7.991768	-4.551204
H	-6.230345	6.343370	-3.381921

H	-7.752766	4.645382	-3.015459
H	-9.774614	6.043361	-4.797090
H	-8.966287	4.534851	-5.101317
H	-9.309101	5.820863	-1.536192
H	-7.773699	6.647537	-1.555899
H	-9.135988	7.297652	-2.455395
H	-11.216954	4.057318	-4.319632
H	-10.104193	3.541312	-3.070904
H	-11.004489	5.035287	-2.887965
N	-6.820884	5.582674	-6.487785
C	-6.124627	4.841492	-7.520874
C	-4.769750	5.446888	-7.898563
O	-3.906737	4.707881	-8.312407
C	-6.992446	4.547912	-8.753666
C	-8.054183	3.454884	-8.535516
C	-7.448181	2.104001	-8.124832
N	-8.377144	0.970074	-8.169473
C	-9.141568	0.544168	-7.160846
N	-9.383153	1.352333	-6.138252
N	-9.646514	-0.669132	-7.176514
H	-7.463236	6.309046	-6.721803
H	-5.828534	3.909038	-7.075290
H	-7.483445	5.455266	-9.092532
H	-6.327709	4.236324	-9.552057
H	-8.781678	3.788049	-7.800766
H	-8.599796	3.321296	-9.463741
H	-6.637600	1.853063	-8.796527
H	-7.024312	2.145133	-7.130623
H	-8.319372	0.364483	-8.958076
H	-9.181981	2.322015	-6.208071

H	-9.904768	1.063414	-5.327421
H	-9.306774	-1.403720	-7.768900
H	-10.319989	-0.965052	-6.487346
N	-4.571401	6.757467	-7.722150
H	-5.310566	7.354659	-7.429234
C	-3.257802	7.352376	-8.011159
H	-2.929895	7.089195	-9.004186
H	-3.359766	8.427208	-7.941863
C	-2.200566	6.878360	-7.024721
O	-1.071914	6.643833	-7.377519
N	-2.627994	6.768045	-5.761132
C	-1.749940	6.461258	-4.657643
C	-1.472401	4.975118	-4.527434
O	-0.342035	4.593898	-4.332800
C	-2.338366	7.058405	-3.373402
C	-1.752062	6.361076	-2.147056
C	-2.100690	8.574533	-3.409071
H	-3.550440	7.074758	-5.541178
H	-0.779628	6.899122	-4.842729
H	-3.406570	6.877236	-3.388107
H	-1.965353	6.907943	-1.247781
H	-2.165885	5.364428	-2.036170
H	-0.679842	6.286334	-2.218551
H	-2.831816	9.101340	-2.812388
H	-1.109168	8.816643	-3.041388
H	-2.193268	8.959248	-4.418178
N	-2.497671	4.112723	-4.641093
C	-2.166523	2.706506	-4.738287
C	-1.220364	2.507835	-5.924366
O	-0.300102	1.723969	-5.846625

C	-3.394415	1.790021	-4.822486
C	-4.317072	1.918766	-3.602696
C	-5.382627	0.821190	-3.503935
N	-4.858872	-0.390743	-2.878874
C	-5.570099	-1.480473	-2.694072
N	-6.815576	-1.586145	-3.199646
N	-5.121736	-2.493378	-1.978831
H	-3.426010	4.433213	-4.814557
H	-1.595337	2.414685	-3.870258
H	-3.953161	1.997088	-5.733460
H	-3.020314	0.775975	-4.902296
H	-3.728329	1.918131	-2.699561
H	-4.837326	2.862844	-3.643857
H	-6.218791	1.188026	-2.917636
H	-5.751709	0.588009	-4.500175
H	-3.951037	-0.310539	-2.403352
H	-7.063115	-0.992515	-3.955708
H	-7.232775	-2.498664	-3.208983
H	-4.262812	-2.495015	-1.452853
H	-5.653361	-3.336980	-1.950745
N	-1.459796	3.193317	-7.035069
H	-2.274663	3.755702	-7.144273
C	-0.596806	2.996902	-8.183514
H	-0.949862	3.640673	-8.978700
H	-0.612568	1.971759	-8.524674
C	0.856426	3.342190	-7.871520
O	1.781779	2.705154	-8.308745
N	1.006300	4.404904	-7.066843
H	0.213643	4.966346	-6.852996
C	2.282311	4.880660	-6.640289

H	2.920019	5.140127	-7.475932
H	2.126148	5.775415	-6.051758
C	3.092715	3.927752	-5.776302
O	4.297866	4.057240	-5.690502
N	2.428042	2.983351	-5.101928
C	3.098132	2.138091	-4.148255
C	4.271477	1.329244	-4.712126
O	5.186206	1.028106	-3.971893
C	2.012665	1.259397	-3.524524
C	2.383938	0.437214	-2.296295
C	1.072250	0.014581	-1.644206
N	1.262215	-1.019085	-0.647482
C	0.330250	-1.943988	-0.368225
N	-0.822216	-1.947790	-0.989648
N	0.622138	-2.889888	0.502311
H	1.438168	2.903902	-5.207745
H	3.559695	2.748451	-3.381394
H	1.216212	1.942011	-3.248467
H	1.593516	0.613829	-4.287331
H	2.964670	-0.438230	-2.566336
H	2.986166	1.021031	-1.603772
H	0.568823	0.875153	-1.216969
H	0.418899	-0.386302	-2.403636
H	1.963553	-0.878296	0.044610
H	-1.269966	-1.090214	-1.303507
H	-1.491568	-2.673986	-0.770534
H	1.538744	-2.992293	0.870067
H	-0.128173	-3.482747	0.842903
N	4.279927	0.941794	-5.999119
H	3.541075	1.225977	-6.608687

C	5.363429	0.116650	-6.504621
H	5.137453	-0.138134	-7.532634
H	5.442774	-0.800174	-5.942267
C	6.736143	0.756003	-6.476543
O	7.738854	0.089545	-6.367895
N	6.766121	2.085332	-6.608316
H	5.911874	2.604440	-6.567369
C	8.004996	2.823954	-6.549403
H	8.709975	2.440909	-7.273615
H	7.799551	3.854914	-6.804810
C	8.747153	2.825883	-5.211064
O	9.888176	3.235697	-5.157967
N	8.101513	2.335547	-4.145228
C	8.681066	2.170330	-2.823189
C	9.947171	1.303177	-2.830526
O	10.764433	1.385764	-1.927914
C	7.576317	1.500246	-1.975725
C	7.769196	1.380775	-0.464218
C	7.422867	2.651993	0.320468
C	7.309433	2.389262	1.818243
N	8.648470	2.359147	2.478369
O	11.028966	1.615400	0.897874
H	10.880843	1.825153	-0.024643
H	11.505773	0.787783	0.849620
H	7.155623	2.033171	-4.259232
H	8.978157	3.127611	-2.415614
H	6.658798	2.041514	-2.163486
H	7.411794	0.512166	-2.389712
H	7.089851	0.601019	-0.133836
H	8.764499	1.030272	-0.225085

H	8.134690	3.453719	0.144483
H	6.457767	3.020719	-0.011818
H	6.746791	3.162101	2.318405
H	6.829088	1.443113	2.014349
H	9.360186	1.893353	1.924196
H	8.969331	3.329393	2.631134
H	8.593611	1.883776	3.367311
N	10.062473	0.448236	-3.837526
C	11.109385	-0.537499	-4.068892
C	12.486318	0.023018	-4.427498
O	13.444102	-0.705865	-4.302265
C	10.700752	-1.444326	-5.251778
C	9.562247	-2.442193	-4.996372
C	9.129842	-3.066510	-6.326790
C	9.989374	-3.533054	-4.014143
H	9.324430	0.445949	-4.510888
H	11.265082	-1.124645	-3.175660
H	10.434267	-0.798849	-6.083402
H	11.583366	-1.997163	-5.550421
H	8.706186	-1.910840	-4.592279
H	8.328479	-3.782558	-6.171896
H	8.772359	-2.309432	-7.013020
H	9.956567	-3.594776	-6.795320
H	9.199147	-4.262500	-3.873818
H	10.858975	-4.059856	-4.393195
H	10.243041	-3.136330	-3.035863
N	12.574040	1.261815	-4.919241
C	13.814402	1.845124	-5.393451
C	14.959101	2.032366	-4.379294
O	16.014162	2.411657	-4.812553

C	13.496699	3.172760	-6.084835
O	12.918485	4.088908	-5.199199
H	11.756268	1.833430	-4.916309
H	14.247968	1.179129	-6.130075
H	14.419688	3.591979	-6.453707
H	12.845327	2.979937	-6.931375
H	11.970943	4.079074	-5.262046
N	14.792294	1.722323	-3.074273
C	15.927719	1.647188	-2.176263
C	16.804389	0.410085	-2.402579
O	17.934553	0.394315	-1.988782
C	15.493418	1.576199	-0.707149
C	14.635029	2.731997	-0.197714
C	14.278053	2.482535	1.268023
N	13.252762	3.377149	1.790066
C	13.430756	4.528612	2.416967
N	14.648942	5.004016	2.652422
O	15.028528	7.461937	4.203427
H	14.743647	8.348737	3.966953
H	15.746372	7.567396	4.814740
N	12.381341	5.217339	2.813920
H	13.900310	1.421993	-2.758069
H	16.561324	2.504420	-2.344669
H	14.953683	0.647645	-0.552865
H	16.404853	1.507479	-0.123427
H	15.152565	3.680213	-0.311232
H	13.717071	2.813876	-0.767959
H	13.879966	1.483506	1.371369
H	15.156187	2.522763	1.901849
H	12.312466	3.080894	1.620435

H	15.456331	4.510925	2.353898
H	14.785053	5.859333	3.163140
H	11.425393	4.937628	2.657052
H	12.473853	6.061264	3.332730
N	16.200243	-0.648980	-2.967248
C	16.870894	-1.911462	-3.167466
C	17.670755	-1.889822	-4.466601
H	18.060349	-0.909366	-4.749612
O	17.882413	-2.854921	-5.125587
C	15.868150	-3.070216	-3.149002
C	15.323809	-3.399061	-1.791707
N	14.402539	-2.626099	-1.113257
O	12.506099	-0.432151	-0.462430
H	13.141962	-1.035492	-0.850861
H	12.023646	-0.035558	-1.179803
C	15.618413	-4.488933	-1.048296
C	14.170588	-3.249263	-0.004407
N	14.880878	-4.379339	0.103926
H	15.285173	-0.550797	-3.351781
H	17.595677	-2.030721	-2.369751
H	15.051075	-2.842552	-3.824865
H	16.369280	-3.944217	-3.542697
H	16.273858	-5.312929	-1.232605
H	13.491731	-2.919058	0.755750
H	14.779630	-5.061789	0.822979
O	-14.807923	-2.300201	5.225778
H	-15.114833	-1.614500	4.637480
H	-14.381301	-1.853417	5.949779
O	-12.881033	-0.751105	7.019263
H	-12.148450	-1.240895	7.377438

H	-13.133124	-0.124765	7.686669
O	-12.181285	-0.220132	4.192191
H	-12.315488	-0.215257	5.135732
H	-13.061658	-0.214532	3.813686
O	-13.444348	-2.081950	1.045259
H	-12.705775	-1.471167	0.998793
H	-13.252860	-2.667409	1.778155
O	-7.228125	1.029560	-0.130575
H	-7.417577	1.424375	0.723910
H	-6.293291	0.856415	-0.115512
O	-7.800955	2.006537	2.509943
H	-8.737809	1.940497	2.675116
H	-7.464497	2.683073	3.091808
O	-9.389751	-0.254834	-1.397153
H	-8.587735	0.109151	-1.003540
H	-9.190521	-1.131292	-1.712271
O	-12.900404	-2.343357	-1.716558
H	-13.229366	-2.469208	-0.823999
H	-13.560377	-2.659081	-2.325070
O	-13.579449	1.728351	-0.139810
H	-12.966518	1.047048	0.143924
H	-13.094119	2.540930	0.018491
O	-14.214072	4.927385	2.494770
H	-13.812294	5.429762	3.198406
H	-14.737755	4.237706	2.884783
O	-15.506305	2.129796	1.954476
H	-16.367951	2.339354	1.618209
H	-14.932993	2.042234	1.190377
O	-13.350841	0.380707	-2.618185
H	-13.636177	0.979357	-1.926566

H	-13.106681	-0.427018	-2.164882
O	-14.252655	-1.708972	-4.324807
H	-14.308315	-0.847013	-3.916393
H	-15.043869	-1.833161	-4.832700
O	-10.281317	-2.826376	-2.845590
H	-10.563412	-2.516751	-3.705510
H	-11.076653	-2.783768	-2.315210
O	-11.491070	-0.112620	0.552589
H	-10.813061	-0.222667	-0.115844
H	-11.087654	0.399932	1.257990
O	-10.714101	1.651582	2.580969
H	-11.200103	1.217835	3.282801
H	-11.222541	2.399231	2.269407
O	-12.145597	3.761965	1.081496
H	-12.857387	4.179540	1.579790
H	-11.581051	4.478575	0.806527
O	-10.736540	0.823996	-3.609666
H	-11.621294	0.967500	-3.269918
H	-10.206422	0.557538	-2.852110
O	-14.797200	-0.398360	3.052640
H	-15.179082	0.432347	2.768201
H	-14.623868	-0.911687	2.265877
O	-12.785738	-3.291256	3.586549
H	-13.538329	-3.087115	4.153694
H	-12.144591	-2.623232	3.810321
O	-11.462580	-1.464169	-5.064183
H	-12.392795	-1.688487	-5.061272
H	-11.369844	-0.701874	-4.494078

Y266F MUTATION, NOMINAL CHARGES R300(O),E183(O),R303(O),E226(O) POTENTIAL:-70mV

N	15.734428	-6.579114	5.125688
H	14.935254	-6.345574	5.679949
C	15.663766	-5.947871	3.801799
C	14.924083	-6.843526	2.790318
O	14.137314	-6.393073	1.979350
C	17.067515	-5.651914	3.264043
H	16.545461	-6.273878	5.624071
H	15.097268	-5.025097	3.826552
H	17.021880	-5.251728	2.257692
H	17.555511	-4.917232	3.895203
H	17.678273	-6.548455	3.251274
N	15.183645	-8.147600	2.874109
H	15.812038	-8.441270	3.588240
C	14.551997	-9.131969	1.993656
H	14.618276	-8.825103	0.962065
H	15.059006	-10.081025	2.111374
C	13.072865	-9.304805	2.341309
O	12.239818	-9.535517	1.503012
N	12.746616	-9.160368	3.638917
H	13.468050	-9.047439	4.311918
C	11.362687	-9.300198	4.098282
H	11.359000	-9.321395	5.180363
H	10.915805	-10.209089	3.725583
C	10.492661	-8.130735	3.619561
O	9.333534	-8.296645	3.346510
N	11.108959	-6.936495	3.561788
C	10.468564	-5.754384	3.042716

C	10.273124	-5.791375	1.524809
O	9.216339	-5.408953	1.081969
C	11.202635	-4.492515	3.520844
O	12.593790	-4.605603	3.503073
H	12.079375	-6.881782	3.761312
H	9.460862	-5.700239	3.421512
H	10.856869	-3.645436	2.933705
H	10.932159	-4.310734	4.552038
H	12.935320	-4.899351	2.669664
N	11.258316	-6.233650	0.721734
C	10.969028	-6.403910	-0.699968
C	9.822409	-7.398711	-0.887994
O	9.063810	-7.295830	-1.824003
C	12.230978	-6.757809	-1.535496
C	12.584381	-8.248178	-1.573730
C	12.078967	-6.232904	-2.964780
H	12.119307	-6.570457	1.096096
H	10.575587	-5.468529	-1.068377
H	13.052102	-6.221241	-1.068483
H	13.537937	-8.374531	-2.075635
H	12.657548	-8.696123	-0.594311
H	11.847694	-8.809194	-2.141886
H	12.965778	-6.467325	-3.543263
H	11.223696	-6.681056	-3.458266
H	11.951431	-5.158936	-2.977010
N	9.705481	-8.354397	0.043515
H	10.468656	-8.511759	0.660989
C	8.735562	-9.439358	-0.071419
H	9.091687	-10.259833	0.539699
H	8.663238	-9.782248	-1.092406

C	7.324929	-9.099481	0.364060
O	6.397058	-9.541147	-0.274745
N	7.148873	-8.330482	1.444373
C	5.812196	-7.871865	1.748015
C	5.361342	-6.831864	0.727546
O	4.173387	-6.711385	0.506318
C	5.576744	-7.412180	3.200591
C	5.752293	-8.581761	4.173994
C	6.409763	-6.202712	3.630146
H	7.929778	-8.072703	2.006497
H	5.136694	-8.695607	1.570160
H	4.532105	-7.115865	3.220218
H	5.475956	-8.275885	5.177783
H	5.119861	-9.419926	3.899113
H	6.779930	-8.926424	4.201189
H	6.081818	-5.862945	4.606955
H	7.457540	-6.461435	3.709960
H	6.309904	-5.370600	2.941199
N	6.270367	-6.114515	0.063468
C	5.865140	-5.265807	-1.044656
C	5.431983	-6.119352	-2.240748
O	4.381978	-5.887230	-2.793874
C	6.961024	-4.250923	-1.415719
C	7.208475	-3.282162	-0.248922
C	6.559048	-3.483558	-2.679999
C	8.543332	-2.550411	-0.352344
H	7.235054	-6.188776	0.299836
H	4.974397	-4.727162	-0.758058
H	7.876945	-4.801518	-1.614063
H	6.389464	-2.568502	-0.218978

H	7.192574	-3.818152	0.690817
H	7.261995	-2.687084	-2.884064
H	6.533210	-4.121872	-3.554164
H	5.576167	-3.039126	-2.564070
H	8.678310	-1.887996	0.495334
H	9.362484	-3.259059	-0.350815
H	8.614436	-1.952255	-1.252682
N	6.232837	-7.115268	-2.641992
H	7.137921	-7.231340	-2.239385
C	5.881109	-7.920762	-3.790628
H	6.710642	-8.587611	-3.992826
H	5.709115	-7.310275	-4.665389
C	4.618612	-8.756614	-3.592763
O	3.770149	-8.800844	-4.452367
N	4.519383	-9.430515	-2.440080
H	5.265057	-9.406598	-1.778221
C	3.335206	-10.192163	-2.125304
H	3.089594	-10.886879	-2.915121
H	3.526940	-10.754672	-1.219543
C	2.103914	-9.316649	-1.911364
O	1.015038	-9.699226	-2.274819
N	2.312311	-8.132395	-1.338198
C	1.175222	-7.233178	-1.240518
C	0.723258	-6.681989	-2.596244
O	-0.460736	-6.490415	-2.772606
C	1.385414	-6.071698	-0.275070
O	1.478788	-6.486420	1.046498
H	3.209933	-7.848270	-1.020684
H	0.329325	-7.798048	-0.881689
H	2.260883	-5.506869	-0.574747

H	0.512575	-5.437934	-0.354416
H	2.374942	-6.730464	1.221180
N	1.639027	-6.412901	-3.530924
C	1.242916	-5.965056	-4.853814
C	0.493000	-7.070430	-5.592398
O	-0.488190	-6.796592	-6.252459
C	2.452484	-5.416064	-5.646619
C	2.825007	-4.033720	-5.085452
C	2.175984	-5.355505	-7.153922
C	4.128312	-3.462694	-5.640915
H	2.608740	-6.505571	-3.320968
H	0.512818	-5.175515	-4.748934
H	3.284222	-6.096537	-5.486151
H	2.011540	-3.341215	-5.294716
H	2.908371	-4.098537	-4.007822
H	3.038291	-4.962351	-7.677695
H	1.973036	-6.334729	-7.571041
H	1.328318	-4.715154	-7.377211
H	4.403741	-2.568254	-5.092377
H	4.941783	-4.174736	-5.539983
H	4.048597	-3.193629	-6.688610
N	0.929810	-8.326151	-5.465463
H	1.777858	-8.518738	-4.976438
C	0.151353	-9.414407	-6.007253
H	0.039898	-9.333713	-7.078762
H	0.662186	-10.341571	-5.778435
C	-1.256369	-9.464904	-5.418388
O	-2.214341	-9.662164	-6.129982
N	-1.356880	-9.285561	-4.102538
C	-2.663912	-9.299065	-3.486583

C	-3.548273	-8.128837	-3.922705
O	-4.748987	-8.309373	-3.981657
C	-2.570434	-9.310726	-1.954853
O	-3.824839	-9.532940	-1.374478
H	-0.538487	-9.239443	-3.533101
H	-3.205141	-10.182020	-3.798706
H	-1.917264	-10.117294	-1.647246
H	-2.140220	-8.375805	-1.607954
H	-4.504799	-9.153250	-1.911169
N	-2.969516	-6.953238	-4.162320
C	-3.694148	-5.792893	-4.655742
C	-4.275556	-6.061957	-6.041239
O	-5.427710	-5.776089	-6.294822
C	-2.731107	-4.581602	-4.665542
C	-3.128597	-3.429235	-5.569550
C	-4.372525	-2.815808	-5.484079
C	-2.228362	-2.966104	-6.521984
C	-4.710883	-1.780043	-6.337740
C	-2.555454	-1.917809	-7.366506
C	-3.802631	-1.324458	-7.279727
H	-1.996474	-6.855031	-3.966955
H	-4.545063	-5.590006	-4.023169
H	-2.617976	-4.243289	-3.640037
H	-1.763723	-4.935587	-4.987697
H	-5.093967	-3.157088	-4.766530
H	-1.265457	-3.436817	-6.614114
H	-5.693520	-1.348276	-6.273287
H	-1.842540	-1.577897	-8.096601
H	-4.066027	-0.522238	-7.947395
N	-3.461900	-6.613021	-6.942978

C	-3.955607	-6.916805	-8.267295
C	-5.112058	-7.914757	-8.211968
O	-6.072898	-7.765640	-8.921549
C	-2.849462	-7.475423	-9.165219
S	-1.581895	-6.268720	-9.668131
H	-2.528391	-6.851580	-6.684717
H	-4.368101	-6.024960	-8.715719
H	-2.374474	-8.330602	-8.702731
H	-3.301576	-7.807825	-10.090659
H	-0.944387	-6.174731	-8.509822
N	-4.985866	-8.958052	-7.368072
H	-4.133959	-9.116239	-6.875719
C	-5.986871	-10.013369	-7.421773
H	-6.170895	-10.316619	-8.442040
H	-5.601492	-10.862824	-6.869374
C	-7.357871	-9.648606	-6.831503
O	-8.377195	-9.998608	-7.358893
N	-7.314770	-8.977255	-5.675499
C	-8.544952	-8.517550	-5.057979
C	-9.297290	-7.451890	-5.851299
O	-10.490730	-7.355628	-5.744975
C	-8.321981	-7.999661	-3.629324
C	-7.380692	-6.799644	-3.458580
C	-7.990028	-5.422695	-3.445239
O	-9.153324	-5.154854	-3.520801
O	-7.050116	-4.505829	-3.295547
H	-7.362665	-3.594269	-3.303819
H	-6.433324	-8.721206	-5.287572
H	-9.233929	-9.348650	-5.005564
H	-9.294970	-7.762051	-3.224590

H	-7.920827	-8.823614	-3.049228
H	-6.860814	-6.882727	-2.510001
H	-6.602939	-6.782339	-4.203912
N	-8.561657	-6.582238	-6.574357
C	-9.221307	-5.523565	-7.301533
C	-10.091055	-6.097012	-8.406984
H	-9.918882	-7.149569	-8.646442
O	-10.909253	-5.451779	-8.980030
C	-8.169818	-4.507747	-7.783909
O	-7.629235	-3.860779	-6.651963
C	-8.720997	-3.428395	-8.703125
H	-7.611955	-6.795459	-6.781359
H	-9.898091	-5.011665	-6.628330
H	-7.378257	-5.040490	-8.302311
H	-6.895251	-4.361819	-6.319946
H	-7.938409	-2.695830	-8.870431
H	-9.037352	-3.832952	-9.653889
H	-9.575473	-2.939798	-8.248607
N	-12.792515	-9.296717	3.007085
H	-13.047198	-9.828823	2.202940
C	-11.617026	-8.454549	2.744241
C	-10.570030	-8.439548	3.891280
O	-9.437123	-8.056103	3.704473
C	-11.972922	-6.984115	2.458914
O	-12.487405	-6.478661	3.661153
C	-12.973491	-6.821367	1.320084
H	-13.573980	-8.737443	3.283884
H	-11.084555	-8.847603	1.888380
H	-11.051906	-6.473796	2.198916
H	-12.629561	-5.541309	3.575768

H	-13.120105	-5.766689	1.117109
H	-12.627061	-7.294204	0.408659
H	-13.937547	-7.240655	1.582952
N	-11.028029	-8.859522	5.078157
H	-11.958160	-9.213996	5.077471
C	-10.257489	-8.909544	6.296271
H	-10.212778	-7.941929	6.774682
H	-10.757934	-9.586680	6.979804
C	-8.803643	-9.366939	6.182595
O	-7.969399	-8.775166	6.823989
N	-8.471588	-10.431366	5.430205
H	-9.178650	-10.931302	4.942703
C	-7.076785	-10.832684	5.312652
H	-7.042082	-11.812933	4.853346
H	-6.622237	-10.899704	6.288791
C	-6.214046	-9.880005	4.465346
O	-5.037717	-9.758043	4.699401
N	-6.882601	-9.263783	3.496980
C	-6.119714	-8.298276	2.706289
C	-6.072070	-6.924243	3.379480
O	-5.082742	-6.231627	3.264179
C	-6.415184	-8.267276	1.196158
C	-7.651627	-7.559282	0.687933
C	-7.717479	-6.167516	0.666841
C	-8.698925	-8.278639	0.130560
C	-8.802986	-5.515353	0.108846
C	-9.783380	-7.628827	-0.438666
C	-9.839008	-6.246624	-0.452647
H	-7.875695	-9.270237	3.467349
H	-5.098788	-8.632853	2.773311

H	-5.545087	-7.806445	0.741501
H	-6.414982	-9.297404	0.859945
H	-6.901575	-5.589324	1.065202
H	-8.653863	-9.354523	0.108769
H	-8.830832	-4.440325	0.079653
H	-10.568643	-8.202782	-0.898060
H	-10.664020	-5.743302	-0.921222
N	-7.114528	-6.576169	4.135348
C	-7.087315	-5.455957	5.043634
C	-6.014429	-5.670767	6.109343
O	-5.334698	-4.734874	6.475045
C	-8.497224	-5.310356	5.653656
C	-8.732960	-4.086806	6.511610
C	-9.035090	-2.862833	5.924300
C	-8.714217	-4.173930	7.898165
C	-9.306388	-1.751171	6.703672
C	-8.989295	-3.064839	8.683046
C	-9.286353	-1.849582	8.087762
H	-7.948348	-7.117645	4.086254
H	-6.805357	-4.547486	4.529391
H	-9.196310	-5.302203	4.824523
H	-8.707211	-6.201031	6.232107
H	-9.074049	-2.776667	4.851831
H	-8.492782	-5.115355	8.371594
H	-9.536390	-0.814241	6.230216
H	-8.968078	-3.150858	9.754933
H	-9.488247	-0.983903	8.694162
N	-5.850491	-6.898095	6.597982
H	-6.529764	-7.598743	6.403526
C	-4.843933	-7.201416	7.589364

H	-4.905526	-6.544745	8.444878
H	-5.014193	-8.216586	7.925902
C	-3.414375	-7.095084	7.070354
O	-2.560718	-6.605043	7.769916
N	-3.155186	-7.566908	5.843120
C	-1.817807	-7.467920	5.286318
C	-1.474804	-6.020372	4.915733
O	-0.365029	-5.594459	5.146867
C	-1.647948	-8.452996	4.108666
C	-0.361328	-8.198032	3.319871
C	-1.668375	-9.897047	4.623804
H	-3.854014	-8.082925	5.353670
H	-1.099876	-7.713552	6.056512
H	-2.491096	-8.310705	3.435290
H	-0.258815	-8.946040	2.540973
H	-0.339217	-7.229877	2.839575
H	0.510119	-8.265064	3.964806
H	-1.617524	-10.589203	3.789566
H	-0.806852	-10.081612	5.260694
H	-2.564563	-10.125845	5.183531
N	-2.427412	-5.271047	4.337174
C	-2.174156	-3.887165	3.977125
C	-2.122583	-2.965714	5.202634
O	-1.227464	-2.154481	5.286751
C	-3.204932	-3.380795	2.960928
C	-3.109078	-4.035004	1.565971
C	-2.185566	-3.336882	0.594486
O	-0.937302	-3.271209	0.993631
H	-0.385782	-2.841943	0.333159
O	-2.547720	-2.892465	-0.457167

H	-3.324677	-5.667636	4.152986
H	-1.187431	-3.811404	3.550638
H	-4.200688	-3.564254	3.347331
H	-3.092226	-2.305401	2.875981
H	-2.784935	-5.065933	1.657024
H	-4.085175	-4.042765	1.102355
N	-3.070267	-3.077549	6.145874
C	-2.905144	-2.335285	7.382761
C	-1.625638	-2.763495	8.101559
O	-0.978373	-1.950203	8.720969
C	-4.096680	-2.334917	8.350219
O	-4.374962	-3.604983	8.858256
C	-5.326409	-1.652390	7.762158
H	-3.770787	-3.781058	6.075021
H	-2.727626	-1.303132	7.123219
H	-3.754947	-1.750331	9.196833
H	-4.828354	-4.109868	8.199437
H	-6.108344	-1.621351	8.510646
H	-5.094945	-0.633840	7.466477
H	-5.707347	-2.182612	6.898580
N	-1.229338	-4.041788	7.968292
H	-1.896363	-4.741797	7.729828
C	-0.082562	-4.478931	8.725203
H	-0.183262	-4.274429	9.782286
H	0.022540	-5.546762	8.580419
C	1.199695	-3.803975	8.271916
O	2.052173	-3.488763	9.069313
N	1.336791	-3.621659	6.942798
C	2.532253	-3.021760	6.424637
C	2.501297	-1.500222	6.258787

O	3.581480	-0.951597	6.201302
C	3.110006	-3.738065	5.206102
S	2.139126	-3.695157	3.674400
H	0.605042	-3.924835	6.336202
H	3.279203	-3.138591	7.195430
H	4.051419	-3.264949	4.963963
H	3.305323	-4.768019	5.473819
H	1.189391	-4.557244	4.007373
N	1.355719	-0.811842	6.286386
C	1.429671	0.628940	6.499796
C	1.897658	0.944470	7.933108
O	2.466151	1.978946	8.181778
C	0.146281	1.401220	6.133311
C	-0.992307	1.201311	7.145028
C	-0.247411	1.115980	4.679396
C	-2.275036	1.958772	6.803399
H	0.480445	-1.288201	6.228225
H	2.218185	1.003872	5.866097
H	0.440810	2.443671	6.200561
H	-1.212455	0.148864	7.256969
H	-0.649730	1.539098	8.118652
H	-0.993771	1.821355	4.334580
H	0.615178	1.209908	4.025252
H	-0.647408	0.118258	4.554798
H	-2.977392	1.900669	7.629482
H	-2.080241	3.011068	6.611791
H	-2.763787	1.544400	5.928648
N	1.675656	-0.021227	8.823607
H	1.041234	-0.757479	8.611033
C	2.099907	0.128901	10.199499

H	1.600441	-0.631549	10.787203
H	1.849915	1.105047	10.587964
C	3.608282	-0.031473	10.341724
O	4.277766	0.752964	10.955584
N	4.142582	-1.100012	9.704939
H	3.542911	-1.818918	9.363522
C	5.570805	-1.264076	9.662300
H	5.794465	-2.230978	9.225399
H	6.010856	-1.226471	10.648884
C	6.284382	-0.191778	8.842048
O	7.419073	0.120280	9.112560
N	5.619219	0.337788	7.816482
C	6.190541	1.508390	7.178754
C	6.228487	2.682421	8.168714
H	5.786670	2.499973	9.149271
O	6.703652	3.732332	7.872241
C	5.439387	1.948294	5.920355
C	5.597046	1.123163	4.656468
C	6.069757	-0.183708	4.627820
C	5.198454	1.703591	3.453500
C	6.105178	-0.900315	3.440237
C	5.226762	0.991122	2.268371
C	5.672036	-0.323335	2.257195
H	4.700987	0.035449	7.582641
H	7.226526	1.303013	6.933021
H	4.383885	2.014198	6.158999
H	5.773437	2.955234	5.702935
H	6.364756	-0.662754	5.541148
H	4.863494	2.726169	3.448406
H	6.457967	-1.917936	3.443550

H	4.915186	1.466886	1.353507
H	5.696949	-0.882430	1.338875
N	12.605097	9.645450	-0.989694
H	11.811783	10.019842	-1.474196
C	12.309724	8.295662	-0.500503
C	11.358265	8.485133	0.678935
O	10.372706	7.800191	0.819562
C	13.587572	7.559801	-0.084249
C	14.603137	7.347577	-1.212949
S	13.871191	6.440892	-2.606847
C	15.302958	6.285570	-3.700731
H	13.344312	9.626370	-1.663160
H	11.767178	7.691727	-1.217401
H	14.075953	8.105162	0.718255
H	13.293052	6.594618	0.306785
H	15.009460	8.292104	-1.558461
H	15.438321	6.780091	-0.817339
H	14.962768	5.735005	-4.565047
H	15.663189	7.258508	-4.009459
H	16.101016	5.731878	-3.223557
N	11.633132	9.508483	1.512139
C	10.803356	9.774034	2.666178
C	9.391406	10.231556	2.272859
O	8.436194	9.887888	2.918276
C	11.428851	10.834619	3.573117
C	12.711544	10.385284	4.254282
O	13.081048	9.235746	4.241846
N	13.391670	11.358819	4.873700
H	12.423569	10.072287	1.295811
H	10.663716	8.862403	3.226757

H	11.616905	11.753676	3.024205
H	10.715465	11.078993	4.355091
H	14.206576	11.123246	5.392662
H	13.056525	12.291776	4.926002
N	9.287052	11.051569	1.205792
H	10.106082	11.286990	0.696468
C	7.991458	11.479987	0.716012
H	8.137413	12.263269	-0.016973
H	7.390674	11.873672	1.521104
C	7.178835	10.360642	0.062912
O	5.979704	10.443531	0.030976
N	7.865769	9.339949	-0.490158
C	7.191788	8.190879	-1.073552
C	6.625966	7.261505	0.008298
O	5.498903	6.840692	-0.095648
C	8.111684	7.466039	-2.082293
C	8.420425	8.393461	-3.272500
C	7.481414	6.149042	-2.549284
C	9.527276	7.891299	-4.201712
H	8.826334	9.237613	-0.264597
H	6.316868	8.553744	-1.592320
H	9.043678	7.230564	-1.570557
H	7.506500	8.541067	-3.844085
H	8.702307	9.373779	-2.900030
H	8.124465	5.657859	-3.267801
H	7.328958	5.461878	-1.725467
H	6.517580	6.315649	-3.019360
H	9.726183	8.623326	-4.977731
H	10.455904	7.722689	-3.663082
H	9.264745	6.963142	-4.695654

N	7.396810	6.977211	1.073194
C	6.870667	6.219922	2.199020
C	5.597065	6.863244	2.756489
O	4.620878	6.194666	3.003143
C	7.954245	6.087259	3.287149
C	8.877118	4.900205	3.014230
O	8.312746	3.792572	3.091685
O	10.070105	5.073631	2.745069
H	8.347648	7.274285	1.101118
H	6.558354	5.235417	1.884578
H	8.512843	7.009524	3.380568
H	7.469175	5.878821	4.234051
N	5.618631	8.193709	2.957647
H	6.466170	8.702491	2.833407
C	4.455927	8.873968	3.476710
H	4.714977	9.913383	3.638085
H	4.141412	8.457332	4.421641
C	3.249080	8.846680	2.543859
O	2.128519	8.961806	2.984634
N	3.519946	8.724741	1.241347
H	4.467098	8.717820	0.947172
C	2.521876	8.841272	0.221535
H	3.021555	9.088019	-0.706909
H	1.840596	9.651214	0.445584
C	1.621509	7.623939	-0.042854
O	0.566567	7.765487	-0.595952
N	2.114075	6.465600	0.435020
C	1.325052	5.275905	0.632023
C	0.521051	5.332272	1.934991
O	-0.665222	5.097145	1.919975

C	2.221393	4.038554	0.605973
H	3.032880	6.490074	0.820726
H	0.586544	5.215106	-0.151268
H	1.642221	3.148854	0.825399
H	2.667555	3.936222	-0.376202
H	3.018817	4.116945	1.337540
N	1.160734	5.612581	3.086106
C	0.445753	5.417564	4.338052
C	-0.688432	6.421301	4.513939
O	-1.715591	6.086282	5.064691
C	1.365414	5.358355	5.583335
C	1.903350	6.719532	6.053495
C	2.490602	4.338333	5.365721
C	2.784614	6.631051	7.301416
H	2.140161	5.794735	3.090161
H	-0.060458	4.464400	4.278000
H	0.719388	4.980710	6.371214
H	2.457740	7.191993	5.248597
H	1.069038	7.377438	6.275109
H	2.862727	3.983365	6.316314
H	2.134669	3.475300	4.812842
H	3.318926	4.770017	4.813867
H	3.036049	7.626730	7.653890
H	2.271645	6.116420	8.108369
H	3.713557	6.104963	7.114495
N	-0.496270	7.670065	4.067139
H	0.383206	7.935521	3.677294
C	-1.482307	8.685751	4.329394
H	-1.098743	9.633836	3.972608
H	-1.680826	8.780515	5.387719

C	-2.837640	8.406102	3.688546
O	-3.836751	8.589636	4.342416
N	-2.877446	7.935275	2.428240
C	-4.220403	7.836635	1.852529
C	-4.943742	6.549192	2.211117
O	-6.153734	6.532863	2.198041
C	-4.022959	8.098999	0.354399
C	-2.778189	8.992138	0.358059
C	-1.898729	8.326332	1.403918
H	-4.843944	8.613510	2.269745
H	-3.838470	7.176028	-0.180426
H	-4.898583	8.567297	-0.076716
H	-2.279065	9.071736	-0.589617
H	-3.047887	9.993701	0.685654
H	-1.403037	7.453915	1.014892
H	-1.146531	8.987927	1.802593
N	-4.206530	5.481044	2.558121
C	-4.850493	4.325074	3.154800
C	-5.508386	4.673999	4.494185
O	-6.601718	4.233176	4.768981
C	-3.863422	3.167891	3.402179
C	-3.562234	2.258476	2.227574
C	-4.265584	1.066274	2.074534
C	-2.532678	2.543873	1.339500
C	-3.919670	0.162834	1.080029
C	-2.184467	1.639896	0.349163
C	-2.859756	0.437984	0.227599
H	-2.543981	-0.291743	-0.496033
H	-3.216320	5.582454	2.618493
H	-5.656491	4.000385	2.514629

H	-2.939961	3.577867	3.796986
H	-4.288460	2.557371	4.189729
H	-5.079725	0.837899	2.740978
H	-1.978071	3.455548	1.437522
H	-4.463735	-0.759548	0.978246
H	-1.367648	1.867138	-0.313212
N	-4.798586	5.430586	5.345921
H	-3.870490	5.714825	5.114979
C	-5.328718	5.798705	6.638834
H	-4.514798	6.194203	7.234486
H	-5.743650	4.940936	7.145710
C	-6.436975	6.846136	6.574470
O	-7.387562	6.793074	7.317466
N	-6.296069	7.791340	5.640483
H	-5.436517	7.847229	5.140913
C	-7.221224	8.920197	5.453612
H	-6.754149	9.597407	4.749698
H	-7.387747	9.444795	6.383351
C	-8.589411	8.538047	4.928208
O	-9.573026	9.111548	5.328641
N	-8.646072	7.566085	4.000131
C	-9.923313	7.209078	3.427515
C	-10.818965	6.437408	4.389075
O	-11.965708	6.220912	4.055364
C	-9.769950	6.442831	2.093494
O	-10.958766	6.545684	1.354121
C	-9.349884	4.987637	2.259810
H	-7.805360	7.150863	3.657528
H	-10.471970	8.115611	3.210235
H	-9.013575	6.967865	1.522689

H	-11.677645	6.275186	1.910390
H	-9.153965	4.551097	1.287678
H	-8.450668	4.897403	2.854885
H	-10.141339	4.411991	2.729064
N	-10.294538	6.001274	5.537719
C	-11.127360	5.378333	6.548334
C	-12.164075	6.334298	7.142836
O	-13.196767	5.888203	7.586332
C	-10.277972	4.818918	7.699419
C	-9.297418	3.696681	7.327125
C	-8.454933	3.339284	8.555516
C	-10.000673	2.453496	6.776122
H	-9.347014	6.207149	5.758566
H	-11.705909	4.592408	6.089703
H	-9.719568	5.636987	8.143712
H	-10.970068	4.455782	8.453996
H	-8.617869	4.061365	6.564274
H	-7.723664	2.572768	8.314265
H	-7.921380	4.208676	8.924371
H	-9.078011	2.960388	9.363199
H	-9.270844	1.678242	6.561906
H	-10.712497	2.055543	7.497675
H	-10.536074	2.652778	5.854776
N	-11.837819	7.634435	7.225023
C	-12.776765	8.587947	7.740207
C	-13.830077	9.025782	6.745453
H	-14.569777	9.723269	7.159464
O	-13.881203	8.680917	5.612976
H	-11.057023	7.981713	6.712469
H	-13.283260	8.176506	8.605351

H	-12.243322	9.475036	8.069918
N	-11.987120	10.578869	-2.764592
H	-11.751692	10.959577	-1.870987
C	-11.843999	9.130699	-2.771738
C	-11.371899	8.816543	-4.181802
O	-10.303173	8.308824	-4.429956
C	-13.097681	8.344887	-2.324940
C	-13.437935	8.683343	-0.862077
C	-12.911609	6.838396	-2.524534
C	-14.763413	8.100056	-0.369997
H	-12.927479	10.865466	-2.954239
H	-11.017331	8.866942	-2.124678
H	-13.934325	8.672613	-2.947305
H	-12.630986	8.332787	-0.222995
H	-13.483546	9.762280	-0.745381
H	-13.831210	6.304279	-2.322028
H	-12.617755	6.591521	-3.540032
H	-12.151435	6.458645	-1.850543
H	-14.977283	8.453926	0.632331
H	-15.589909	8.398488	-1.010071
H	-14.743791	7.017034	-0.331259
N	-12.192657	9.240443	-5.161369
H	-13.089576	9.577737	-4.903483
C	-12.011414	8.884787	-6.567479
H	-12.092493	7.817828	-6.724477
H	-12.784505	9.383186	-7.138846
C	-10.646468	9.301893	-7.121043
O	-10.007899	8.570545	-7.823006
N	-10.257651	10.558634	-6.809092
H	-10.800853	11.059272	-6.144133

C	-8.953652	11.108373	-7.195869
H	-8.831025	11.030151	-8.265539
H	-8.942953	12.154723	-6.917771
C	-7.725399	10.427883	-6.575522
O	-6.814041	10.019586	-7.242355
N	-7.700740	10.405557	-5.227497
H	-8.524363	10.658582	-4.733220
C	-6.528681	9.976762	-4.440793
H	-5.634309	10.408124	-4.860922
H	-6.656793	10.343746	-3.429741
C	-6.295542	8.478017	-4.374212
O	-5.155197	8.078206	-4.433512
N	-7.325650	7.636682	-4.183102
C	-7.006433	6.262528	-3.820324
C	-6.445041	5.466269	-4.990811
O	-5.642453	4.585405	-4.780604
C	-8.129967	5.491217	-3.086373
C	-9.325974	5.105625	-3.972640
C	-8.534021	6.248381	-1.816398
C	-10.308935	4.151738	-3.291972
H	-8.268149	7.968720	-4.160340
H	-6.171691	6.302029	-3.135698
H	-7.647053	4.568492	-2.774381
H	-9.845674	5.996226	-4.304365
H	-8.955628	4.612924	-4.868172
H	-9.177354	5.644811	-1.191102
H	-7.661213	6.506537	-1.224368
H	-9.068568	7.161985	-2.050857
H	-11.105463	3.883409	-3.979581
H	-9.822482	3.232768	-2.990920

H	-10.770062	4.594278	-2.418601
N	-6.859329	5.742481	-6.243030
C	-6.234516	5.059284	-7.357275
C	-4.828417	5.581984	-7.656692
O	-3.982411	4.820249	-8.062590
C	-7.134704	5.060918	-8.601441
C	-8.262462	4.022738	-8.506346
C	-7.743880	2.597429	-8.724700
N	-8.740287	1.555550	-8.491788
C	-9.000257	0.964199	-7.324725
N	-8.438537	1.378135	-6.203035
N	-9.841373	-0.051720	-7.280511
H	-7.508781	6.481850	-6.397153
H	-6.046038	4.045094	-7.045388
H	-7.557448	6.050080	-8.749381
H	-6.520256	4.852806	-9.472209
H	-8.758643	4.100559	-7.543578
H	-9.017262	4.236462	-9.255855
H	-7.417772	2.482929	-9.750306
H	-6.874296	2.385570	-8.115233
H	-9.160883	1.147081	-9.294192
H	-7.879848	2.196908	-6.192469
H	-8.803682	1.059342	-5.311888
H	-10.200969	-0.427562	-8.127368
H	-9.831710	-0.683540	-6.486956
N	-4.599868	6.879742	-7.441550
H	-5.338150	7.475669	-7.146867
C	-3.292587	7.493378	-7.719943
H	-2.965478	7.263319	-8.722586
H	-3.402807	8.564912	-7.616375

C	-2.225526	6.999452	-6.757111
O	-1.096518	6.788030	-7.123961
N	-2.643483	6.845473	-5.495203
C	-1.750230	6.515475	-4.412904
C	-1.466826	5.028340	-4.317252
O	-0.337836	4.647952	-4.116999
C	-2.320776	7.083777	-3.107291
C	-1.730066	6.349823	-1.904999
C	-2.071008	8.598762	-3.107966
H	-3.566562	7.137295	-5.260576
H	-0.781883	6.957604	-4.602048
H	-3.391560	6.913361	-3.117818
H	-1.938470	6.868730	-0.988943
H	-2.144658	5.349974	-1.824047
H	-0.658230	6.275333	-1.983775
H	-2.797229	9.119510	-2.499711
H	-1.076789	8.824830	-2.736374
H	-2.162209	9.005373	-4.108651
N	-2.488829	4.163540	-4.455760
C	-2.145750	2.764357	-4.598988
C	-1.205798	2.601630	-5.798724
O	-0.272770	1.833217	-5.736683
C	-3.376006	1.849256	-4.673163
C	-4.248226	1.933749	-3.411393
C	-5.382896	0.900075	-3.345627
N	-4.929348	-0.344445	-2.747862
C	-5.747122	-1.420432	-2.548132
N	-6.893250	-1.628524	-3.082175
N	-5.258358	-2.336573	-1.662564
H	-3.407356	4.484360	-4.671915

H	-1.546848	2.466137	-3.750200
H	-3.975485	2.106345	-5.543557
H	-3.020789	0.834990	-4.821411
H	-3.625260	1.835217	-2.526098
H	-4.696058	2.915112	-3.357638
H	-6.209970	1.314217	-2.772438
H	-5.751500	0.697258	-4.345562
H	-4.226947	-0.233303	-2.053460
H	-7.191214	-0.886824	-3.680633
H	-4.276785	-2.394682	-1.497374
H	-5.720509	-3.216774	-1.691743
N	-1.457497	3.319608	-6.885943
H	-2.291982	3.853544	-6.983906
C	-0.598165	3.160353	-8.043207
H	-0.961826	3.818251	-8.822576
H	-0.600798	2.142494	-8.407259
C	0.851686	3.516011	-7.730445
O	1.780674	2.904809	-8.195302
N	0.996656	4.554288	-6.892936
H	0.203311	5.107681	-6.665839
C	2.274462	5.022316	-6.461804
H	2.905535	5.311163	-7.293504
H	2.120529	5.897033	-5.842318
C	3.091684	4.049398	-5.637497
O	4.296290	4.190888	-5.555332
N	2.444256	3.078839	-4.984585
C	3.169500	2.252660	-4.047876
C	4.332543	1.454285	-4.656013
O	5.280287	1.168028	-3.952517
C	2.163836	1.375436	-3.289371

C	2.749656	0.608835	-2.103567
C	1.669330	0.247987	-1.082802
N	2.190891	-0.557952	0.003125
C	2.200503	-1.916450	-0.085782
N	1.352456	-2.526080	-0.816778
N	3.198236	-2.529743	0.643994
H	1.456315	2.973931	-5.077369
H	3.673956	2.893927	-3.334803
H	1.398539	2.059496	-2.932722
H	1.665654	0.699803	-3.976702
H	3.240518	-0.298593	-2.439337
H	3.514344	1.208616	-1.614259
H	1.239877	1.151988	-0.664603
H	0.871836	-0.310411	-1.547965
H	2.922651	-0.147838	0.536419
H	1.544917	-3.504969	-0.838053
H	3.530574	-2.007729	1.425612
H	2.978562	-3.460754	0.924206
N	4.305833	1.076221	-5.946783
H	3.541654	1.348138	-6.527734
C	5.391670	0.279995	-6.494689
H	5.167743	0.077252	-7.535045
H	5.480890	-0.663157	-5.977803
C	6.757888	0.931485	-6.434324
O	7.768019	0.273311	-6.333310
N	6.778946	2.261487	-6.545564
H	5.922709	2.774430	-6.498806
C	8.016502	3.004101	-6.531004
H	8.694264	2.628585	-7.285161
H	7.796154	4.036262	-6.771917

C	8.821096	3.005479	-5.230147
O	9.983291	3.357917	-5.251229
N	8.212780	2.591092	-4.112407
C	8.894197	2.414330	-2.837976
C	10.082265	1.454809	-2.928749
O	10.989464	1.522137	-2.117237
C	7.827250	1.902777	-1.839362
C	8.280908	1.116249	-0.609186
C	8.963161	1.884152	0.522139
C	9.059499	0.960858	1.733999
N	9.654847	1.632783	2.916402
O	12.140230	0.180777	2.408583
H	12.211275	-0.097933	1.499226
H	12.889977	-0.162855	2.866114
H	7.253580	2.316407	-4.165557
H	9.321772	3.351139	-2.506671
H	7.227707	2.755343	-1.536396
H	7.161750	1.251262	-2.390773
H	7.379609	0.663318	-0.207728
H	8.914095	0.292348	-0.913219
H	9.947687	2.221659	0.213277
H	8.381253	2.756424	0.792576
H	8.073196	0.645046	2.030254
H	9.656071	0.085738	1.520292
H	9.465307	1.099347	3.746996
H	10.655773	1.683169	2.829951
H	9.195363	2.597245	3.034014
N	10.045486	0.555561	-3.903113
C	11.054577	-0.458050	-4.167584
C	12.458859	0.070120	-4.457551

O	13.394173	-0.679474	-4.281970
C	10.647497	-1.293354	-5.402092
C	9.518532	-2.315633	-5.203194
C	9.071673	-2.848811	-6.567791
C	9.964305	-3.471556	-4.307153
H	9.262387	0.565409	-4.522440
H	11.170287	-1.089936	-3.297889
H	10.371270	-0.600664	-6.190696
H	11.532247	-1.822960	-5.738476
H	8.665163	-1.819383	-4.750726
H	8.276841	-3.579578	-6.452551
H	8.700873	-2.047111	-7.193313
H	9.895313	-3.337769	-7.082910
H	9.177456	-4.210029	-4.201141
H	10.826255	-3.971259	-4.738764
H	10.233144	-3.142019	-3.307543
N	12.588893	1.304731	-4.952551
C	13.849531	1.853749	-5.423478
C	14.976789	2.048844	-4.390829
O	16.044063	2.430178	-4.788097
C	13.570293	3.172441	-6.147976
O	13.001336	4.121992	-5.292539
H	11.777949	1.881614	-5.004548
H	14.284296	1.163158	-6.138136
H	14.510029	3.560619	-6.511250
H	12.927284	2.975085	-7.000702
H	12.056672	4.113499	-5.344854
N	14.757352	1.720377	-3.100444
C	15.786701	1.762329	-2.093018
C	16.680932	0.520907	-2.138428

O	17.711102	0.515347	-1.515339
C	15.189815	1.836161	-0.677466
C	14.431515	3.118938	-0.306089
C	13.784025	2.925383	1.070417
N	13.059768	4.078874	1.613899
C	13.541495	4.949851	2.495175
N	14.843590	5.014112	2.753055
O	14.894697	7.137387	4.801448
H	14.482511	7.988064	4.692499
H	14.982766	6.988206	5.729444
N	12.723811	5.776198	3.110769
H	13.820841	1.539888	-2.823320
H	16.437986	2.606168	-2.276151
H	14.527330	0.983927	-0.544953
H	16.015596	1.692187	0.009824
H	15.116211	3.963607	-0.294413
H	13.664471	3.354230	-1.034976
H	13.070170	2.118565	1.018358
H	14.526558	2.615696	1.798166
H	12.067240	4.109991	1.502346
H	15.501804	4.509638	2.210846
H	15.168996	5.688788	3.416121
H	11.721887	5.665133	3.034145
H	13.103474	6.420942	3.767874
N	16.216802	-0.533115	-2.833306
C	16.961137	-1.777538	-2.878589
C	17.929767	-1.762363	-4.052072
H	18.394101	-0.791204	-4.248536
O	18.185868	-2.717043	-4.710147
C	16.037036	-2.995273	-2.926916

C	15.157691	-3.107083	-1.721257
C	13.809394	-3.031340	-1.667136
O	12.153260	-0.381310	-0.378832
H	12.852693	-0.785217	-0.869672
H	11.739333	0.252799	-0.958635
N	15.662929	-3.309576	-0.457652
N	13.479516	-3.196227	-0.339149
C	14.640106	-3.352362	0.325705
H	15.371597	-0.457642	-3.355937
H	17.565527	-1.817809	-1.979621
H	15.421091	-2.951937	-3.818950
H	16.657852	-3.877953	-3.014321
H	13.083085	-2.877444	-2.434624
H	12.567873	-3.164785	0.051104
H	14.674147	-3.495071	1.385915
O	-14.991273	-2.648063	4.801082
H	-15.123215	-1.854114	4.296179
H	-14.566571	-2.383588	5.604624
O	-12.965961	-1.514342	6.948920
H	-12.329483	-2.018626	7.433631
H	-13.211906	-0.785417	7.497401
O	-11.972385	-1.083850	4.217796
H	-12.172637	-1.130686	5.144785
H	-12.757303	-0.723459	3.810072
O	-13.204411	-2.028782	0.755849
H	-12.410169	-1.499284	0.776903
H	-13.095257	-2.730149	1.389933
O	-7.138286	1.738246	0.266100
H	-7.393087	1.879711	1.176203
H	-6.206847	1.586701	0.292864

O	-7.703944	1.935504	3.062238
H	-8.619666	1.703470	3.181042
H	-7.509107	2.654848	3.649504
O	-8.853326	-0.035200	-1.102322
H	-8.206100	0.507128	-0.652533
H	-8.443908	-0.855855	-1.346181
O	-12.784135	-2.296437	-2.142829
H	-13.089903	-2.422389	-1.253268
H	-11.851970	-2.508970	-2.144071
O	-13.619059	0.856110	-0.718252
H	-14.008768	-0.005264	-0.756084
H	-12.748168	0.708502	-0.350683
O	-14.182794	4.592813	5.045993
H	-13.687977	5.307461	4.663901
H	-14.211650	4.796021	5.971362
O	-14.856714	2.012773	1.552126
H	-15.584550	2.602099	1.440016
H	-14.524580	1.777574	0.688958
O	-12.457334	0.205109	-3.431325
H	-12.922846	0.860194	-2.931464
H	-12.566874	-0.597990	-2.926209
O	-12.479251	-2.293797	-5.147075
H	-12.684135	-1.386307	-4.971561
H	-12.849305	-2.770288	-4.417400
O	-10.035475	-2.676707	-2.420023
H	-9.779161	-2.116989	-3.141961
H	-9.835892	-3.553714	-2.731861
O	-11.212563	-0.011304	0.514993
H	-10.448995	-0.103824	-0.050706
H	-10.919618	0.426968	1.310908

O	-10.494974	1.114503	3.075921
H	-10.754218	0.342087	3.566999
H	-11.182765	1.754074	3.260670
O	-12.812174	2.564019	3.588412
H	-13.201631	3.171086	4.211108
H	-13.435753	2.495197	2.877570
O	-9.639602	0.761074	-3.731082
H	-10.579565	0.602202	-3.708888
H	-9.323687	0.573992	-2.851963
O	-14.474076	-0.511211	2.917565
H	-14.736609	0.369408	2.674722
H	-14.287208	-0.967790	2.104876
O	-12.899288	-3.661300	3.199433
H	-13.714054	-3.493330	3.672936
H	-12.305584	-3.001790	3.542445
O	-9.670116	-2.113511	-5.368169
H	-10.553945	-2.470830	-5.326220
H	-9.063762	-2.791258	-5.649430

Y266F MUTATION NOMINAL CHARGES R300(+),E183(O),R303(O),E226(-) POTENTIAL: 0mV

N	15.734446	-6.579103	5.125638
H	14.931649	-6.353023	5.677865
C	15.661662	-5.947200	3.802385
C	14.923831	-6.843598	2.790620
O	14.139199	-6.392730	1.978291
C	17.064897	-5.648497	3.264923
H	16.541049	-6.266248	5.626483

H	15.093129	-5.025646	3.827586
H	17.018970	-5.248939	2.258349
H	17.551240	-4.912493	3.895886
H	17.677258	-6.543975	3.252840
N	15.183877	-8.147583	2.873907
H	15.809732	-8.441283	3.590215
C	14.551980	-9.131983	1.993674
H	14.616367	-8.823507	0.962479
H	15.061295	-10.080105	2.109084
C	13.073760	-9.309267	2.342201
O	12.243063	-9.547018	1.503973
N	12.746600	-9.160379	3.638928
H	13.467371	-9.042208	4.311587
C	11.362681	-9.300155	4.098291
H	11.359041	-9.322084	5.180351
H	10.915754	-10.208846	3.725223
C	10.492663	-8.130745	3.619542
O	9.332854	-8.293281	3.351750
N	11.114743	-6.938173	3.549358
C	10.477621	-5.757277	3.023762
C	10.299871	-5.785069	1.502522
O	9.259601	-5.372175	1.049528
C	11.198957	-4.493355	3.512933
O	12.592027	-4.591417	3.490757
H	12.085464	-6.886182	3.746810
H	9.465402	-5.708224	3.390585
H	10.843748	-3.645008	2.933221
H	10.928553	-4.323848	4.546334
H	12.931237	-4.894532	2.659886
N	11.282651	-6.252271	0.709492

C	11.002366	-6.429556	-0.712957
C	9.858589	-7.425679	-0.909835
O	9.135539	-7.345657	-1.875183
C	12.268340	-6.786562	-1.540904
C	12.612627	-8.279226	-1.579060
C	12.128292	-6.259282	-2.970905
H	12.132467	-6.604473	1.094162
H	10.611173	-5.495949	-1.087040
H	13.089141	-6.255237	-1.067370
H	13.570422	-8.411742	-2.071521
H	12.671410	-8.729681	-0.599726
H	11.877329	-8.833117	-2.155821
H	13.020380	-6.492469	-3.541992
H	11.277354	-6.707472	-3.471306
H	12.000227	-5.185110	-2.983531
N	9.705480	-8.354399	0.043523
H	10.451131	-8.499461	0.684311
C	8.735566	-9.439355	-0.071429
H	9.105432	-10.271026	0.516423
H	8.651511	-9.765429	-1.096717
C	7.329417	-9.124903	0.389069
O	6.408579	-9.627280	-0.214489
N	7.148455	-8.314875	1.435518
C	5.809786	-7.827170	1.688613
C	5.391248	-6.855552	0.588773
O	4.222954	-6.782715	0.299499
C	5.547587	-7.275015	3.102243
C	5.675841	-8.385415	4.149556
C	6.393085	-6.058258	3.483788
H	7.928998	-8.011386	1.973223

H	5.131260	-8.655102	1.552664
H	4.508260	-6.961529	3.069932
H	5.387766	-8.012741	5.127323
H	5.029135	-9.224236	3.912821
H	6.694537	-8.751625	4.218395
H	6.040509	-5.648074	4.424433
H	7.431510	-6.334598	3.618221
H	6.339471	-5.270810	2.739893
N	6.325083	-6.142825	-0.064679
C	5.939527	-5.353804	-1.221322
C	5.540616	-6.259635	-2.391410
O	4.553515	-5.999908	-3.040890
C	7.034312	-4.346036	-1.621158
C	7.292386	-3.340260	-0.487167
C	6.631055	-3.613505	-2.905808
C	8.633928	-2.623214	-0.616652
H	7.277710	-6.176012	0.220450
H	5.038561	-4.810167	-0.980284
H	7.951113	-4.899617	-1.806620
H	6.482996	-2.613462	-0.475565
H	7.274762	-3.844448	0.469134
H	7.320010	-2.807123	-3.117837
H	6.623211	-4.269291	-3.766396
H	5.637019	-3.188977	-2.808120
H	8.795071	-1.962583	0.227469
H	9.445061	-3.340806	-0.628396
H	8.696841	-2.026493	-1.519389
N	6.298920	-7.327737	-2.672084
H	7.187265	-7.438561	-2.234407
C	5.956066	-8.199733	-3.773375

H	6.769034	-8.904118	-3.903412
H	5.828574	-7.647476	-4.693116
C	4.662393	-8.983554	-3.554003
O	3.837293	-9.067461	-4.433699
N	4.519394	-9.569109	-2.359664
H	5.244453	-9.496715	-1.679407
C	3.302975	-10.255820	-1.999113
H	3.048342	-11.015891	-2.723239
H	3.459818	-10.730217	-1.037866
C	2.103907	-9.316648	-1.911366
O	1.037264	-9.649217	-2.382579
N	2.312313	-8.132393	-1.338193
C	1.268660	-7.118196	-1.434126
C	0.881652	-6.762026	-2.869876
O	-0.292141	-6.599506	-3.130041
C	1.615422	-5.769003	-0.803964
O	1.415214	-5.759574	0.574055
H	3.168055	-7.897418	-0.886194
H	0.360202	-7.484344	-0.981226
H	2.632605	-5.505962	-1.055397
H	0.962312	-5.039529	-1.263128
H	1.043708	-4.910320	0.784478
N	1.835210	-6.535679	-3.779197
C	1.471669	-6.139287	-5.128694
C	0.630588	-7.229391	-5.778646
O	-0.342505	-6.943901	-6.447000
C	2.713707	-5.764003	-5.972135
C	3.222476	-4.378214	-5.540076
C	2.413898	-5.800102	-7.476570
C	4.575169	-3.997135	-6.141756

H	2.798122	-6.586043	-3.524396
H	0.810876	-5.283546	-5.084106
H	3.483417	-6.501408	-5.762954
H	2.479700	-3.632667	-5.822010
H	3.305911	-4.351096	-4.461110
H	3.292544	-5.516489	-8.042218
H	2.129382	-6.790237	-7.811664
H	1.611625	-5.116186	-7.736233
H	4.943666	-3.080772	-5.692293
H	5.313656	-4.771277	-5.956656
H	4.522444	-3.835778	-7.212755
N	1.000923	-8.494082	-5.569732
H	1.817985	-8.699413	-5.034681
C	0.144747	-9.564730	-6.008547
H	0.029019	-9.569641	-7.082582
H	0.588444	-10.502304	-5.697754
C	-1.256373	-9.464911	-5.418391
O	-2.228049	-9.600033	-6.130526
N	-1.356876	-9.285557	-4.102538
C	-2.656415	-9.224190	-3.479530
C	-3.512677	-8.041625	-3.941161
O	-4.721407	-8.175808	-3.960870
C	-2.525815	-9.184050	-1.951248
O	-3.763628	-9.393055	-1.333248
H	-0.535209	-9.232612	-3.537204
H	-3.232730	-10.099964	-3.748030
H	-1.862556	-9.978212	-1.633795
H	-2.089582	-8.238142	-1.644957
H	-4.456281	-9.013864	-1.853179
N	-2.891715	-6.903402	-4.244263

C	-3.563364	-5.738139	-4.801275
C	-4.210727	-6.106298	-6.132385
O	-5.383739	-5.889025	-6.333913
C	-2.491113	-4.634131	-4.922000
C	-2.702484	-3.385350	-5.773531
C	-3.768780	-3.131581	-6.627341
C	-1.660497	-2.454996	-5.746473
C	-3.767646	-2.010518	-7.452302
C	-1.659993	-1.335991	-6.556235
C	-2.717986	-1.113871	-7.428484
H	-1.906912	-6.851020	-4.087555
H	-4.374819	-5.427063	-4.157910
H	-2.245852	-4.329029	-3.909846
H	-1.601929	-5.107105	-5.317025
H	-4.603403	-3.799488	-6.682900
H	-0.826192	-2.623708	-5.086201
H	-4.591350	-1.860987	-8.129821
H	-0.843248	-0.638905	-6.509749
H	-2.712103	-0.259733	-8.083100
N	-3.405487	-6.641760	-7.056355
C	-3.936979	-6.972395	-8.357133
C	-5.106718	-7.945818	-8.250594
O	-6.070095	-7.815618	-8.960856
C	-2.859536	-7.568445	-9.265958
S	-1.587525	-6.388285	-9.819378
H	-2.462330	-6.871148	-6.824332
H	-4.346981	-6.086459	-8.821320
H	-2.384966	-8.417128	-8.791314
H	-3.335488	-7.916238	-10.173543
H	-0.898692	-6.309710	-8.689150

N	-4.985869	-8.958046	-7.368054
H	-4.128558	-9.114360	-6.882804
C	-5.986846	-10.010389	-7.418493
H	-6.167157	-10.322292	-8.436795
H	-5.609339	-10.857030	-6.856071
C	-7.357892	-9.648668	-6.831488
O	-8.376649	-10.028113	-7.341729
N	-7.314713	-8.977257	-5.675582
C	-8.539003	-8.672110	-4.957869
C	-9.357763	-7.497931	-5.510322
O	-10.486054	-7.331305	-5.116251
C	-8.290639	-8.487059	-3.453379
C	-7.526633	-7.212268	-3.051675
C	-8.342377	-6.000544	-2.687109
O	-9.406299	-6.238191	-1.959825
H	-9.852561	-5.406856	-1.782302
O	-8.002612	-4.878129	-2.959655
H	-6.434865	-8.677541	-5.312341
H	-9.200018	-9.519429	-5.077325
H	-9.248341	-8.512622	-2.953149
H	-7.727301	-9.348214	-3.115591
H	-6.947587	-7.425530	-2.156894
H	-6.816306	-6.900789	-3.800536
N	-8.756093	-6.682539	-6.390137
C	-9.449810	-5.618960	-7.091863
C	-10.091065	-6.097038	-8.407010
H	-9.693586	-7.027185	-8.823577
O	-10.975582	-5.499119	-8.930600
C	-8.483397	-4.429212	-7.306241
O	-8.132258	-3.873691	-6.068871

C	-9.028285	-3.333498	-8.221265
H	-7.811518	-6.870849	-6.645556
H	-10.273472	-5.290761	-6.470283
H	-7.561081	-4.811738	-7.727014
H	-8.913886	-3.627592	-5.589802
H	-8.319071	-2.511368	-8.214035
H	-9.160252	-3.668993	-9.240921
H	-9.986631	-2.969701	-7.861711
N	-12.792520	-9.296693	3.007091
H	-13.053843	-9.901263	2.258280
C	-11.560355	-8.559359	2.703028
C	-10.570027	-8.439517	3.891301
O	-9.457962	-7.997154	3.718391
C	-11.820892	-7.127508	2.203349
O	-12.545608	-6.521881	3.236258
C	-12.567295	-7.078403	0.876280
H	-13.541493	-8.661600	3.197896
H	-11.005970	-9.102244	1.946562
H	-10.857373	-6.641604	2.077330
H	-12.617941	-5.581644	3.112478
H	-12.745930	-6.043597	0.601059
H	-11.988831	-7.537610	0.080273
H	-13.529146	-7.574184	0.943486
N	-11.028025	-8.859560	5.078145
H	-11.943536	-9.252037	5.076584
C	-10.250171	-8.822886	6.294467
H	-10.219736	-7.827204	6.713655
H	-10.729142	-9.472035	7.018694
C	-8.787581	-9.251333	6.171110
O	-7.945875	-8.595872	6.731446

N	-8.466225	-10.364368	5.484504
H	-9.182771	-10.917115	5.074428
C	-7.074892	-10.775374	5.369479
H	-7.049652	-11.778214	4.961470
H	-6.604193	-10.792695	6.340562
C	-6.214055	-9.879991	4.465363
O	-5.029202	-9.781271	4.652703
N	-6.882602	-9.263796	3.496967
C	-6.217934	-8.418763	2.524220
C	-6.045081	-7.003683	3.079642
O	-4.997907	-6.412749	2.961163
C	-6.957957	-8.386859	1.176200
C	-7.235969	-9.754138	0.581079
C	-8.526715	-10.093774	0.196686
C	-6.218362	-10.682542	0.380846
C	-8.805671	-11.333570	-0.360351
C	-6.494106	-11.920125	-0.173474
C	-7.789273	-12.253869	-0.540826
H	-7.870439	-9.344362	3.457341
H	-5.217959	-8.796997	2.383782
H	-7.894027	-7.851871	1.290782
H	-6.340997	-7.801651	0.500442
H	-9.317761	-9.372283	0.305547
H	-5.202372	-10.434136	0.625581
H	-9.810957	-11.572764	-0.660207
H	-5.693086	-12.620741	-0.328306
H	-7.998724	-13.215255	-0.974925
N	-7.104760	-6.499082	3.723628
C	-7.033740	-5.332603	4.566744
C	-6.031202	-5.524384	5.703650

O	-5.439710	-4.556084	6.129842
C	-8.455233	-5.038676	5.088071
C	-8.627053	-3.736335	5.836996
C	-8.536821	-2.517990	5.169872
C	-8.920092	-3.732791	7.193587
C	-8.728280	-1.324189	5.841369
C	-9.117797	-2.537846	7.873045
C	-9.025320	-1.331897	7.197796
H	-7.929949	-7.050286	3.780396
H	-6.664232	-4.486654	4.005673
H	-9.109033	-5.041272	4.221981
H	-8.768728	-5.864689	5.715687
H	-8.313829	-2.495530	4.116702
H	-8.984862	-4.664112	7.729882
H	-8.632950	-0.398373	5.303730
H	-9.319640	-2.552417	8.930318
H	-9.162084	-0.406045	7.726476
N	-5.822899	-6.754803	6.169766
H	-6.485046	-7.467899	5.969514
C	-4.817864	-7.045681	7.168560
H	-4.890140	-6.389778	8.023464
H	-4.974879	-8.062398	7.504068
C	-3.385961	-6.921577	6.656150
O	-2.517866	-6.560198	7.414889
N	-3.153146	-7.224271	5.375235
C	-1.863644	-6.983860	4.755718
C	-1.655728	-5.486102	4.489280
O	-0.590666	-4.976515	4.769117
C	-1.692838	-7.863606	3.499384
C	-0.465533	-7.456785	2.683181

C	-1.604696	-9.340698	3.899387
H	-3.890055	-7.593991	4.821243
H	-1.090600	-7.231286	5.468843
H	-2.572701	-7.722240	2.876241
H	-0.336120	-8.135634	1.847830
H	-0.550127	-6.460379	2.273075
H	0.439815	-7.491125	3.281370
H	-1.538603	-9.961482	3.011074
H	-0.711841	-9.520078	4.493623
H	-2.465331	-9.667028	4.467652
N	-2.674565	-4.780348	3.984062
C	-2.579754	-3.338328	3.793979
C	-2.297768	-2.639184	5.130320
O	-1.428120	-1.802048	5.221675
C	-3.884007	-2.768408	3.212832
C	-4.263978	-3.193978	1.783063
C	-3.597047	-2.366651	0.677111
O	-2.381980	-2.303581	0.662580
O	-4.391192	-1.825138	-0.152484
H	-3.510431	-5.253999	3.718299
H	-1.756396	-3.098210	3.139031
H	-4.693038	-3.035909	3.883987
H	-3.805747	-1.686202	3.251008
H	-4.011198	-4.236358	1.616536
H	-5.339602	-3.104761	1.679518
N	-3.095464	-2.963400	6.160954
C	-2.939464	-2.327720	7.447609
C	-1.754562	-2.850886	8.242134
O	-1.241009	-2.100527	9.045434
C	-4.197170	-2.310161	8.328884

O	-4.620339	-3.597947	8.675449
C	-5.321121	-1.479793	7.724471
H	-3.801935	-3.650884	6.032435
H	-2.679131	-1.297475	7.270561
H	-3.880550	-1.845169	9.253913
H	-5.070986	-3.986002	7.940195
H	-6.152630	-1.447313	8.417708
H	-4.991918	-0.462595	7.536520
H	-5.675170	-1.902275	6.792044
N	-1.229334	-4.041802	7.968335
H	-1.776797	-4.742324	7.521109
C	-0.048500	-4.466073	8.670904
H	-0.108968	-4.261011	9.729127
H	0.068784	-5.532345	8.519936
C	1.194551	-3.764911	8.148284
O	2.074951	-3.407444	8.897363
N	1.264785	-3.600261	6.813297
C	2.442242	-3.008798	6.237847
C	2.461564	-1.482093	6.254595
O	3.549102	-0.950088	6.304727
C	2.796441	-3.561288	4.858146
S	1.856644	-2.927833	3.444988
H	0.516743	-3.920869	6.234324
H	3.266645	-3.264517	6.887056
H	3.820492	-3.279272	4.652281
H	2.740558	-4.641809	4.885742
H	0.711327	-3.553972	3.667683
N	1.323449	-0.776812	6.279895
C	1.425629	0.655966	6.506219
C	1.897655	0.944464	7.933109

O	2.465547	1.978221	8.191566
C	0.159048	1.462605	6.169105
C	-1.005324	1.198233	7.135269
C	-0.200326	1.289570	4.691505
C	-2.267635	2.004817	6.828855
H	0.448196	-1.213816	6.077260
H	2.219718	1.031980	5.878836
H	0.461655	2.493324	6.321192
H	-1.245379	0.144317	7.142360
H	-0.682194	1.443746	8.142196
H	-0.929570	2.028536	4.385489
H	0.676787	1.423126	4.064750
H	-0.604264	0.307850	4.486027
H	-2.984983	1.902927	7.637671
H	-2.048709	3.063745	6.715263
H	-2.751204	1.664480	5.919709
N	1.675654	-0.021225	8.823611
H	1.081328	-0.782670	8.593150
C	2.100401	0.120562	10.198982
H	1.591164	-0.634630	10.785030
H	1.857308	1.098667	10.586244
C	3.606223	-0.053001	10.353721
O	4.268511	0.708011	11.006098
N	4.143030	-1.107136	9.700757
H	3.547921	-1.775669	9.263300
C	5.570377	-1.269428	9.654130
H	5.793819	-2.232706	9.209312
H	6.006571	-1.240482	10.642328
C	6.284386	-0.191779	8.842046
O	7.419465	0.119159	9.118286

N	5.619218	0.337787	7.816479
C	6.241448	1.489915	7.202196
C	6.228486	2.682421	8.168718
H	5.777148	2.503484	9.145550
O	6.691157	3.736387	7.864473
C	5.642712	1.823159	5.839548
C	5.811401	0.738469	4.785865
C	6.701032	-0.324780	4.914108
C	5.021215	0.789274	3.640030
C	6.781269	-1.309513	3.938649
C	5.092867	-0.192543	2.667386
C	5.976243	-1.252944	2.814673
H	4.710941	0.029664	7.550120
H	7.295865	1.276196	7.078122
H	4.585226	2.030496	5.953273
H	6.109289	2.738601	5.490140
H	7.299068	-0.426662	5.800375
H	4.319450	1.596570	3.522113
H	7.458747	-2.135893	4.074043
H	4.445774	-0.137842	1.809074
H	6.038094	-2.024940	2.068497
N	12.605068	9.645440	-0.989737
H	11.813281	10.016706	-1.479100
C	12.309752	8.295709	-0.500458
C	11.349969	8.484824	0.672897
O	10.360067	7.804504	0.804190
C	13.584182	7.561164	-0.070729
C	14.607928	7.340736	-1.190260
S	13.887607	6.422022	-2.582409
C	15.327726	6.262514	-3.664527

H	13.348016	9.626479	-1.659191
H	11.773230	7.689484	-1.219885
H	14.067469	8.110838	0.731909
H	13.285673	6.598935	0.325657
H	15.015158	8.283148	-1.540702
H	15.440854	6.777465	-0.784009
H	14.996658	5.702644	-4.526420
H	15.686405	7.234046	-3.979646
H	16.124669	5.716710	-3.176492
N	11.623863	9.503381	1.512871
C	10.793076	9.760309	2.668178
C	9.384915	10.232748	2.279268
O	8.429509	9.901988	2.930855
C	11.422586	10.805418	3.589993
C	12.699208	10.339467	4.271024
O	13.069918	9.191107	4.233533
N	13.374167	11.298161	4.919474
H	12.420720	10.062194	1.308047
H	10.645917	8.842435	3.216703
H	11.619980	11.729276	3.052357
H	10.707138	11.045996	4.371178
H	14.184737	11.049682	5.439106
H	13.036382	12.228584	4.994210
N	9.285172	11.051262	1.210542
H	10.104064	11.267946	0.692782
C	7.991434	11.480001	0.715991
H	8.140196	12.261200	-0.018629
H	7.389548	11.876449	1.518812
C	7.178859	10.360599	0.062947
O	5.981168	10.454168	0.016108

N	7.863887	9.332233	-0.478635
C	7.182932	8.185716	-1.058783
C	6.598702	7.270955	0.025460
O	5.467799	6.862709	-0.085760
C	8.101138	7.443713	-2.056301
C	8.428034	8.359684	-3.250458
C	7.457238	6.131675	-2.518701
C	9.532497	7.837674	-4.171596
H	8.818953	9.217199	-0.236022
H	6.315492	8.554139	-1.586024
H	9.026987	7.200532	-1.537622
H	7.518860	8.516285	-3.827407
H	8.721115	9.338268	-2.882036
H	8.097622	5.627863	-3.230882
H	7.291596	5.451779	-1.691505
H	6.497885	6.307560	-2.994655
H	9.744433	8.562158	-4.951387
H	10.456465	7.660635	-3.627844
H	9.260662	6.909637	-4.660775
N	7.357108	6.986982	1.098993
C	6.815976	6.238775	2.224872
C	5.549349	6.898414	2.777604
O	4.562334	6.244312	3.014203
C	7.895158	6.091733	3.314277
C	8.805886	4.897444	3.029837
O	8.229648	3.797016	3.101866
O	9.997757	5.066103	2.752565
H	8.312249	7.269571	1.129777
H	6.491197	5.258292	1.910871
H	8.461856	7.008758	3.413910

H	7.406423	5.881754	4.258845
N	5.585351	8.228790	2.983940
H	6.438384	8.729912	2.867563
C	4.422178	8.916159	3.493140
H	4.682273	9.956718	3.645609
H	4.101804	8.509010	4.440327
C	3.220967	8.882064	2.553035
O	2.097607	9.015018	2.981958
N	3.504285	8.737718	1.255799
H	4.453831	8.702315	0.973429
C	2.521915	8.841264	0.221505
H	3.033992	9.074810	-0.703424
H	1.837858	9.653799	0.426236
C	1.621484	7.623962	-0.042825
O	0.586656	7.778614	-0.634227
N	2.071079	6.463016	0.463371
C	1.251511	5.281579	0.615059
C	0.451563	5.305277	1.922259
O	-0.730932	5.065495	1.914218
C	2.105844	4.017403	0.527039
H	2.978515	6.468890	0.876635
H	0.510918	5.275409	-0.167321
H	1.486619	3.138632	0.668164
H	2.573373	3.965514	-0.449346
H	2.887857	4.014286	1.279726
N	1.109127	5.577553	3.070463
C	0.415708	5.379089	4.331647
C	-0.707157	6.392744	4.526066
O	-1.733999	6.072899	5.085785
C	1.361997	5.312196	5.557357

C	1.925978	6.667971	6.011986
C	2.473662	4.280871	5.315631
C	2.828038	6.571785	7.244499
H	2.090427	5.746642	3.063712
H	-0.099334	4.430756	4.278367
H	0.731278	4.942840	6.361221
H	2.474118	7.127350	5.195421
H	1.105070	7.338854	6.245244
H	2.860202	3.919252	6.258487
H	2.095894	3.424283	4.768474
H	3.296118	4.703643	4.748276
H	3.099764	7.565200	7.588960
H	2.322599	6.066935	8.062302
H	3.745880	6.031953	7.043023
N	-0.506922	7.641164	4.076779
H	0.371603	7.899590	3.680796
C	-1.483815	8.662817	4.341826
H	-1.089445	9.610803	3.995981
H	-1.689393	8.750272	5.399407
C	-2.837595	8.406077	3.688540
O	-3.840913	8.610537	4.331020
N	-2.877489	7.935289	2.428242
C	-4.217339	7.889276	1.842381
C	-4.972031	6.625367	2.206688
O	-6.184175	6.618353	2.162603
C	-3.995910	8.135921	0.345216
C	-2.726562	8.993938	0.360502
C	-1.877307	8.302582	1.414507
H	-4.816047	8.690752	2.250191
H	-3.827093	7.204981	-0.182070

H	-4.853231	8.624982	-0.100236
H	-2.214433	9.060076	-0.581439
H	-2.971845	10.002564	0.685970
H	-1.402809	7.416646	1.029578
H	-1.111457	8.942579	1.821539
N	-4.245826	5.567959	2.582585
C	-4.881610	4.372656	3.097316
C	-5.515294	4.625903	4.471481
O	-6.575699	4.116845	4.750087
C	-3.893615	3.209489	3.203628
C	-3.364350	2.621443	1.907506
C	-2.656125	1.425261	1.993822
C	-3.505375	3.212799	0.662206
C	-2.062839	0.856829	0.885432
C	-2.910216	2.646449	-0.456530
C	-2.177527	1.481074	-0.347383
H	-1.714579	1.040843	-1.212230
H	-3.250906	5.643276	2.602052
H	-5.705185	4.103909	2.451687
H	-3.049544	3.529628	3.808715
H	-4.389473	2.421932	3.761846
H	-2.566238	0.930907	2.944315
H	-4.058972	4.124440	0.548929
H	-1.558202	-0.085400	0.971031
H	-3.024736	3.128425	-1.411784
N	-4.828447	5.408443	5.322804
H	-3.910601	5.718047	5.084171
C	-5.352588	5.769196	6.619635
H	-4.530968	6.132360	7.225434
H	-5.790440	4.914144	7.111073

C	-6.436971	6.846135	6.574466
O	-7.383478	6.805059	7.324530
N	-6.296072	7.791340	5.640484
H	-5.437689	7.845459	5.138067
C	-7.221222	8.920186	5.453602
H	-6.753342	9.600000	4.752853
H	-7.394675	9.441931	6.383607
C	-8.586084	8.529464	4.920432
O	-9.576464	9.101216	5.306484
N	-8.632744	7.543786	4.004680
C	-9.900814	7.173284	3.419814
C	-10.818979	6.437427	4.389095
O	-11.966881	6.229851	4.052049
C	-9.716080	6.341626	2.129525
O	-10.890552	6.401399	1.360717
C	-9.302375	4.894493	2.373394
H	-7.785100	7.150718	3.652281
H	-10.441889	8.070021	3.148137
H	-8.948466	6.838128	1.549510
H	-11.621970	6.175429	1.920630
H	-9.084141	4.418316	1.424093
H	-8.422336	4.821232	2.999236
H	-10.109587	4.340743	2.842202
N	-10.294540	6.001277	5.537721
C	-11.131185	5.393282	6.554142
C	-12.169270	6.356053	7.134058
O	-13.210485	5.916253	7.563802
C	-10.282718	4.839370	7.707426
C	-9.289711	3.732198	7.325051
C	-8.476636	3.335915	8.560948

C	-9.975299	2.509395	6.712118
H	-9.346560	6.206947	5.756711
H	-11.710438	4.603654	6.103268
H	-9.734684	5.659674	8.160453
H	-10.974572	4.462483	8.455547
H	-8.592127	4.120989	6.591416
H	-7.733358	2.584081	8.310923
H	-7.957680	4.194433	8.973752
H	-9.116854	2.925100	9.339115
H	-9.237375	1.747953	6.484081
H	-10.703365	2.081032	7.399252
H	-10.488533	2.741816	5.785849
N	-11.837511	7.654650	7.216421
C	-12.776032	8.614181	7.720921
C	-13.819828	9.054470	6.717451
H	-14.558364	9.757156	7.124778
O	-13.866038	8.706826	5.585445
H	-11.048320	7.996576	6.713104
H	-13.291339	8.208116	8.583451
H	-12.241010	9.499657	8.052314
N	-11.987120	10.578869	-2.764592
H	-11.139682	11.102772	-2.676643
C	-11.737367	9.147430	-2.773520
C	-11.361431	8.791069	-4.206373
O	-10.359481	8.165733	-4.477956
C	-12.975329	8.367330	-2.266495
C	-13.129235	8.550420	-0.742548
C	-12.898791	6.881089	-2.631403
C	-14.480890	8.096924	-0.188093
H	-12.574648	10.851296	-2.004626

H	-10.882923	8.861425	-2.166123
H	-13.846959	8.798736	-2.758167
H	-12.330786	8.012691	-0.239519
H	-13.000741	9.596235	-0.476320
H	-13.783720	6.359803	-2.289763
H	-12.831628	6.724392	-3.703062
H	-12.038266	6.414534	-2.164161
H	-14.539261	8.311762	0.873026
H	-15.302950	8.612982	-0.676992
H	-14.636770	7.030777	-0.309175
N	-12.192658	9.240443	-5.161369
H	-12.937053	9.837603	-4.884379
C	-12.011414	8.884787	-6.567478
H	-12.085161	7.816396	-6.710172
H	-12.792692	9.368464	-7.140618
C	-10.649820	9.302759	-7.126326
O	-10.006084	8.572941	-7.824409
N	-10.257651	10.558633	-6.809092
H	-10.833141	11.091346	-6.200194
C	-8.953654	11.108373	-7.195869
H	-8.829082	11.038793	-8.266124
H	-8.936298	12.151967	-6.907837
C	-7.736646	10.405276	-6.576984
O	-6.847009	9.949786	-7.240820
N	-7.700741	10.405557	-5.227497
H	-8.491737	10.745233	-4.734724
C	-6.528678	9.976769	-4.440791
H	-5.631644	10.397924	-4.866069
H	-6.650898	10.354226	-3.432867
C	-6.298977	8.478461	-4.356947

O	-5.160100	8.079944	-4.429601
N	-7.321731	7.634119	-4.128670
C	-6.973982	6.274899	-3.734636
C	-6.414448	5.452652	-4.888680
O	-5.629780	4.563804	-4.654157
C	-8.059456	5.493070	-2.955784
C	-9.261839	5.034157	-3.798194
C	-8.469207	6.271075	-1.700925
C	-10.110615	3.962412	-3.108893
H	-8.270205	7.950115	-4.120408
H	-6.129581	6.350490	-3.065266
H	-7.533480	4.599086	-2.630608
H	-9.881408	5.882869	-4.059661
H	-8.899814	4.623037	-4.738209
H	-9.115743	5.680862	-1.065616
H	-7.600095	6.543018	-1.110208
H	-9.005529	7.178328	-1.954826
H	-10.923071	3.648057	-3.757542
H	-9.521107	3.082391	-2.866881
H	-10.554718	4.320020	-2.188119
N	-6.822678	5.718329	-6.146765
C	-6.203981	5.029879	-7.261290
C	-4.813200	5.571762	-7.606212
O	-3.964984	4.810359	-8.007131
C	-7.119648	5.009309	-8.492052
C	-8.344139	4.097115	-8.336593
C	-7.978738	2.611117	-8.268580
N	-9.148160	1.732216	-8.268408
C	-9.728394	1.155628	-7.219459
N	-9.398739	1.477169	-5.984088

N	-10.665539	0.247291	-7.435587
H	-7.445531	6.479320	-6.305991
H	-5.993971	4.022517	-6.940476
H	-7.456961	6.017337	-8.715548
H	-6.530497	4.682666	-9.343524
H	-8.919322	4.380364	-7.460042
H	-8.995436	4.250949	-9.191741
H	-7.384030	2.334928	-9.130720
H	-7.378081	2.374407	-7.401333
H	-9.556507	1.538081	-9.154444
H	-8.800778	2.247705	-5.804070
H	-9.709367	0.939426	-5.188834
H	-10.769877	-0.153603	-8.338713
H	-11.234283	-0.139405	-6.704079
N	-4.599878	6.879766	-7.441561
H	-5.334680	7.474332	-7.135570
C	-3.292582	7.493362	-7.719931
H	-2.967402	7.266071	-8.723802
H	-3.402951	8.564609	-7.614227
C	-2.224332	6.995185	-6.760772
O	-1.100230	6.772264	-7.134219
N	-2.637167	6.848483	-5.496649
C	-1.742436	6.511690	-4.416874
C	-1.466378	5.021090	-4.331742
O	-0.336995	4.630764	-4.159685
C	-2.305604	7.082488	-3.110315
C	-1.694144	6.358794	-1.914519
C	-2.064747	8.598925	-3.116508
H	-3.553638	7.155104	-5.256772
H	-0.772057	6.948699	-4.607607

H	-3.375847	6.904101	-3.110124
H	-1.905998	6.870274	-0.995136
H	-2.083374	5.351210	-1.830057
H	-0.621861	6.308243	-2.001031
H	-2.781763	9.114687	-2.493088
H	-1.065662	8.829011	-2.761351
H	-2.175193	9.006998	-4.114860
N	-2.493846	4.160668	-4.464856
C	-2.165514	2.758006	-4.617042
C	-1.205775	2.601595	-5.798724
O	-0.280099	1.822621	-5.736851
C	-3.427376	1.870774	-4.769353
C	-3.455939	0.691703	-3.786939
C	-4.653004	-0.215545	-4.051698
N	-4.765857	-1.267278	-3.049887
C	-5.617151	-2.282415	-3.146375
N	-6.315761	-2.494605	-4.262325
N	-5.794567	-3.080984	-2.117814
H	-3.424001	4.482421	-4.617107
H	-1.594930	2.439507	-3.756879
H	-4.306640	2.483108	-4.611594
H	-3.488302	1.495246	-5.786434
H	-2.545853	0.108077	-3.873219
H	-3.510632	1.069389	-2.773408
H	-5.566885	0.376698	-4.064610
H	-4.528521	-0.660949	-5.029704
H	-4.347477	-1.151486	-2.140414
H	-6.004641	-2.102166	-5.117485
H	-6.832339	-3.345272	-4.363246
H	-5.354188	-2.832263	-1.240879

H	-6.470670	-3.809268	-2.191192
N	-1.457551	3.319595	-6.885953
H	-2.281871	3.870894	-6.972275
C	-0.599719	3.167663	-8.045740
H	-0.963171	3.833200	-8.818581
H	-0.605689	2.153522	-8.420370
C	0.851838	3.516468	-7.732641
O	1.776862	2.899237	-8.196469
N	0.998040	4.554871	-6.896949
H	0.205008	5.107891	-6.668979
C	2.274483	5.022348	-6.461770
H	2.906919	5.313785	-7.291461
H	2.118574	5.895484	-5.840594
C	3.092094	4.048117	-5.639735
O	4.297124	4.182955	-5.566668
N	2.444250	3.078801	-4.984622
C	3.172094	2.245621	-4.056294
C	4.354513	1.495130	-4.680445
O	5.323292	1.242551	-3.993584
C	2.202121	1.280820	-3.353116
C	2.870995	0.495152	-2.228958
C	1.939159	-0.457640	-1.488107
N	2.753905	-1.242905	-0.578572
C	2.306191	-2.430662	-0.037338
N	1.121486	-2.843526	0.073690
N	3.375944	-3.216324	0.388331
H	1.452622	2.996693	-5.052042
H	3.646414	2.872067	-3.310030
H	1.390225	1.882654	-2.956186
H	1.761786	0.611286	-4.085447

H	3.689207	-0.086693	-2.639310
H	3.314534	1.181407	-1.512411
H	1.186493	0.090634	-0.931326
H	1.418221	-1.099918	-2.197625
H	3.694272	-1.334332	-0.892237
H	0.416185	-2.236068	-0.292920
H	3.984840	-2.706656	0.993501
H	3.052967	-4.036440	0.858793
N	4.307489	1.085164	-5.959499
H	3.536205	1.340891	-6.538162
C	5.391673	0.280012	-6.494636
H	5.170432	0.061584	-7.532282
H	5.477397	-0.656325	-5.962956
C	6.758118	0.931300	-6.437819
O	7.766735	0.271236	-6.340521
N	6.778946	2.261504	-6.545618
H	5.924112	2.775814	-6.499020
C	8.018536	3.002914	-6.530038
H	8.695485	2.626639	-7.284514
H	7.799375	4.035359	-6.770782
C	8.823915	3.002762	-5.228361
O	9.986383	3.354173	-5.249894
N	8.210480	2.586977	-4.115147
C	8.872139	2.397050	-2.830976
C	10.060106	1.434922	-2.909824
O	10.949801	1.489322	-2.078824
C	7.775150	1.887658	-1.863268
C	8.166759	1.084199	-0.624239
C	8.826805	1.818252	0.543318
C	8.676790	0.942788	1.783083

N	9.353110	1.508769	2.974516
O	11.850475	0.120031	2.393514
H	11.961694	-0.156113	1.486953
H	12.556414	-0.258241	2.891386
H	7.249749	2.319689	-4.177599
H	9.297559	3.329103	-2.483504
H	7.175055	2.744626	-1.574551
H	7.121009	1.248385	-2.439815
H	7.235918	0.653338	-0.263543
H	8.786395	0.243510	-0.909851
H	9.872036	2.014397	0.325216
H	8.343458	2.770184	0.727011
H	7.634747	0.847952	2.040484
H	9.081880	-0.045824	1.619120
H	9.048310	1.015018	3.796349
H	10.352221	1.396664	2.901554
H	9.042821	2.521920	3.078578
N	10.045455	0.555560	-3.903137
C	11.055414	-0.456381	-4.175724
C	12.460763	0.073762	-4.448352
O	13.397061	-0.672095	-4.263016
C	10.666097	-1.263271	-5.436647
C	9.572250	-2.327485	-5.271047
C	9.134402	-2.823666	-6.652443
C	10.060894	-3.501054	-4.421047
H	9.266776	0.570106	-4.527586
H	11.161147	-1.106401	-3.318498
H	10.366937	-0.553119	-6.200761
H	11.564289	-1.755168	-5.794046
H	8.707150	-1.874614	-4.796037

H	8.365137	-3.584271	-6.560718
H	8.734140	-2.011901	-7.246188
H	9.970774	-3.265635	-7.189151
H	9.297819	-4.266431	-4.335734
H	10.934822	-3.958519	-4.875817
H	10.327783	-3.199195	-3.412883
N	12.588928	1.304758	-4.952501
C	13.850354	1.856476	-5.420953
C	14.978463	2.052987	-4.388079
O	16.044296	2.440013	-4.784073
C	13.569668	3.175792	-6.143669
O	13.004361	4.125775	-5.286644
H	11.776208	1.879199	-5.007782
H	14.286201	1.167378	-6.136519
H	14.508655	3.563587	-6.509255
H	12.924090	2.979451	-6.994809
H	12.059273	4.112757	-5.330134
N	14.757274	1.720286	-3.100410
C	15.774445	1.754063	-2.081167
C	16.679174	0.521349	-2.138103
O	17.713561	0.520832	-1.522010
C	15.154506	1.792404	-0.673159
C	14.371939	3.056995	-0.290247
C	13.704646	2.837052	1.073677
N	12.979244	3.985428	1.624910
C	13.470017	4.863015	2.493686
N	14.774724	4.924626	2.741787
O	14.848226	7.058436	4.784771
H	14.445677	7.913525	4.674631
H	14.920431	6.903404	5.713152

N	12.661501	5.699637	3.107158
H	13.821356	1.526529	-2.831286
H	16.419723	2.607809	-2.237975
H	14.502693	0.927958	-0.567732
H	15.970942	1.646163	0.024936
H	15.044541	3.910725	-0.255502
H	13.612502	3.294593	-1.026231
H	12.986517	2.035371	0.997628
H	14.436527	2.510935	1.805612
H	11.984659	4.007982	1.529886
H	15.426419	4.398990	2.212346
H	15.107795	5.601431	3.398440
H	11.657478	5.600070	3.032458
H	13.049848	6.343563	3.759743
N	16.216815	-0.533118	-2.833292
C	16.969897	-1.771894	-2.888631
C	17.940836	-1.738371	-4.059716
H	18.396046	-0.761191	-4.247669
O	18.208513	-2.685268	-4.724605
C	16.053653	-2.994764	-2.949957
C	15.172515	-3.121165	-1.747224
C	13.824406	-3.045846	-1.694092
O	12.076126	-0.451516	-0.368918
H	12.809847	-0.826571	-0.831080
H	11.674414	0.185693	-0.953917
N	15.676509	-3.337053	-0.485314
N	13.493045	-3.223613	-0.368373
C	14.652594	-3.388805	0.296157
H	15.367553	-0.461618	-3.349901
H	17.572765	-1.817104	-1.988814

H	15.439536	-2.947447	-3.843095
H	16.679945	-3.872944	-3.043338
H	13.099127	-2.882465	-2.460459
H	12.579478	-3.210483	0.018739
H	14.685009	-3.544388	1.354404
O	-14.785306	-2.853004	5.042749
H	-15.042258	-2.023152	4.661043
H	-14.255184	-2.645040	5.799988
O	-12.545104	-1.840413	6.941536
H	-11.772675	-2.304524	7.232415
H	-12.696860	-1.154137	7.572938
O	-11.981242	-1.151500	4.149820
H	-11.991757	-1.254641	5.093654
H	-12.824778	-0.768318	3.925013
O	-13.461874	-2.005687	0.887427
H	-12.667188	-1.472041	0.876074
H	-13.334323	-2.678622	1.555932
O	-7.007523	-0.750818	0.541836
H	-7.007741	-0.116551	1.247866
H	-6.103202	-1.016015	0.380226
O	-7.662875	1.233100	2.940078
H	-8.611301	1.283941	2.915736
H	-7.369096	1.976154	3.447035
O	-9.236623	-1.030641	-1.128112
H	-8.431234	-0.932376	-0.611337
H	-9.422161	-1.960310	-1.201142
O	-13.386941	-2.981249	-1.707811
H	-13.511753	-2.742852	-0.788205
H	-14.029476	-3.637309	-1.927577
O	-13.934675	0.647455	-0.617564

H	-14.332668	-0.152190	-0.302717
H	-13.034733	0.601961	-0.293346
O	-14.165092	4.583169	5.025512
H	-13.656100	5.293940	4.653903
H	-14.209403	4.787666	5.950333
O	-15.068736	1.968808	1.715866
H	-15.724696	2.647249	1.702588
H	-14.804343	1.791693	0.820338
O	-12.988103	-0.498343	-3.105002
H	-13.428207	0.098742	-2.508674
H	-13.083601	-1.361671	-2.710440
O	-12.678692	-1.100021	-5.803588
H	-12.964079	-0.788839	-4.946636
H	-13.443852	-1.407167	-6.263975
O	-10.547578	-3.663152	-1.872988
H	-10.366108	-3.544033	-2.800161
H	-11.483896	-3.533861	-1.778936
O	-11.439731	-0.082422	0.460583
H	-10.685585	-0.346610	-0.062402
H	-11.102243	0.358908	1.241279
O	-10.597966	1.022779	2.907114
H	-10.826694	0.259383	3.428410
H	-11.233572	1.687581	3.168448
O	-12.866486	2.483491	3.621170
H	-13.209788	3.123077	4.239438
H	-13.520481	2.421865	2.938981
O	-10.164796	-0.023702	-3.615688
H	-11.077711	-0.044086	-3.343141
H	-9.657647	-0.222090	-2.827999
O	-14.656102	-0.532202	3.236760

H	-14.903039	0.361756	3.034546
H	-14.550338	-0.967883	2.401822
O	-12.930023	-3.670491	3.101963
H	-13.664187	-3.585565	3.712393
H	-12.297689	-3.041474	3.436580
O	-10.438575	-2.724507	-4.653410
H	-11.258910	-2.593408	-5.108073
H	-10.158823	-1.854756	-4.391222

R303cit MUTATION: NOMINAL CHARGES, Y266(0), E183(0) POTENTIAL: -70mV

N	15.580944	-6.451469	5.391416
H	14.778721	-6.221506	5.942956
C	15.496182	-5.852360	4.058535
C	14.783013	-6.782961	3.060453
O	14.059772	-6.346221	2.181659
C	16.898622	-5.543534	3.522670
H	16.387053	-6.123736	5.883073
H	14.912587	-4.940419	4.059364
H	16.856096	-5.149452	2.514323
H	17.371781	-4.795364	4.148834
H	17.520987	-6.432039	3.521605
N	15.032379	-8.085604	3.186404
H	15.604488	-8.359632	3.954624
C	14.398661	-9.092386	2.333235
H	14.473079	-8.817195	1.293410
H	14.898004	-10.040740	2.484013
C	12.915566	-9.237106	2.674696

O	12.091047	-9.472910	1.831600
N	12.582804	-9.055884	3.966877
H	13.300401	-8.952342	4.644778
C	11.195108	-9.170814	4.421376
H	11.186121	-9.158618	5.503549
H	10.743031	-10.087116	4.073834
C	10.336944	-8.010595	3.900734
O	9.189623	-8.187785	3.593898
N	10.947888	-6.814647	3.844867
C	10.307915	-5.635464	3.316218
C	10.122054	-5.677140	1.796732
O	9.101972	-5.229344	1.334258
C	11.066256	-4.386316	3.786757
O	12.455638	-4.545396	3.745752
H	11.906296	-6.741332	4.089670
H	9.301194	-5.569087	3.696350
H	10.744266	-3.531790	3.201132
H	10.816125	-4.198601	4.821679
H	12.762907	-4.720594	2.869165
N	11.093922	-6.194189	1.021791
C	10.834858	-6.389726	-0.401802
C	9.692850	-7.388519	-0.606448
O	8.955961	-7.295761	-1.558787
C	12.123852	-6.767009	-1.190596
C	12.355672	-8.272145	-1.373227
C	12.126409	-6.071633	-2.552874
H	11.907714	-6.594654	1.431659
H	10.454906	-5.457753	-0.790548
H	12.951582	-6.365225	-0.615949
H	13.314463	-8.427505	-1.857860

H	12.359749	-8.818307	-0.440328
H	11.598129	-8.708184	-2.017473
H	13.018871	-6.336159	-3.109741
H	11.262212	-6.366445	-3.138180
H	12.114070	-4.994064	-2.441309
N	9.570431	-8.340344	0.328319
H	10.307980	-8.465745	0.980619
C	8.593019	-9.421180	0.241223
H	8.936112	-10.222208	0.884479
H	8.528603	-9.797854	-0.768425
C	7.182085	-9.050582	0.647345
O	6.260842	-9.524975	0.024190
N	7.005575	-8.223203	1.682776
C	5.668735	-7.741118	1.951776
C	5.235307	-6.754245	0.873617
O	4.064959	-6.719838	0.570307
C	5.415152	-7.215973	3.378629
C	5.562643	-8.344244	4.404104
C	6.247746	-5.995348	3.773988
H	7.784102	-7.941227	2.234165
H	4.992284	-8.569225	1.804641
H	4.372370	-6.912641	3.368443
H	5.273821	-7.992184	5.389018
H	4.924983	-9.186424	4.155111
H	6.586332	-8.698508	4.461968
H	5.901885	-5.610026	4.727236
H	7.291890	-6.258982	3.887928
H	6.169958	-5.193840	3.048309
N	6.132684	-5.989047	0.244728
C	5.696855	-5.158945	-0.870091

C	5.296702	-6.033333	-2.065134
O	4.302267	-5.776276	-2.699429
C	6.770930	-4.116630	-1.241972
C	6.976245	-3.122041	-0.086118
C	6.376579	-3.383046	-2.528637
C	8.267475	-2.311858	-0.201250
H	7.089896	-6.000462	0.517461
H	4.785693	-4.650049	-0.585442
H	7.707106	-4.644429	-1.413025
H	6.115579	-2.457998	-0.041052
H	7.000815	-3.654869	0.855292
H	7.060830	-2.569160	-2.731544
H	6.390446	-4.037683	-3.390735
H	5.376000	-2.973446	-2.445487
H	8.371653	-1.641675	0.645580
H	9.129858	-2.969217	-0.207601
H	8.299973	-1.708681	-1.102124
N	6.077711	-7.079449	-2.385043
H	6.959866	-7.205789	-1.940342
C	5.752414	-7.908953	-3.523653
H	6.591369	-8.571842	-3.700329
H	5.587881	-7.314560	-4.410563
C	4.495136	-8.757486	-3.333983
O	3.664721	-8.828911	-4.209262
N	4.393710	-9.421895	-2.176055
H	5.115840	-9.348134	-1.493595
C	3.210276	-10.180583	-1.848728
H	2.968650	-10.885962	-2.630339
H	3.406768	-10.731622	-0.936782
C	1.974185	-9.306852	-1.644812

O	0.890526	-9.709539	-2.006858
N	2.187876	-8.107002	-1.107175
C	1.012886	-7.252376	-0.965832
C	0.545710	-6.702050	-2.313977
O	-0.642021	-6.600070	-2.533184
C	1.163378	-6.146269	0.075942
O	1.421534	-6.707870	1.327333
H	3.065164	-7.832942	-0.730040
H	0.197103	-7.876550	-0.638504
H	1.933350	-5.442946	-0.200343
H	0.220235	-5.622796	0.131930
H	2.356605	-6.752795	1.430579
N	1.458863	-6.375799	-3.241601
C	1.040325	-5.948927	-4.561843
C	0.321333	-7.075681	-5.302065
O	-0.658091	-6.824655	-5.976063
C	2.227309	-5.367300	-5.366608
C	2.554205	-3.967123	-4.821865
C	1.946409	-5.329650	-6.873968
C	3.829406	-3.354337	-5.397458
H	2.429656	-6.387940	-3.016204
H	0.283541	-5.183419	-4.460645
H	3.083019	-6.015458	-5.200400
H	1.713446	-3.307480	-5.032170
H	2.651703	-4.016589	-3.745072
H	2.794532	-4.913266	-7.403438
H	1.774907	-6.318716	-7.281928
H	1.077492	-4.719480	-7.100870
H	4.072811	-2.440208	-4.866028
H	4.670031	-4.032369	-5.289350

H	3.730978	-3.105296	-6.448950
N	0.787067	-8.321965	-5.181476
H	1.629515	-8.498347	-4.676282
C	0.045256	-9.425831	-5.745357
H	-0.060609	-9.330635	-6.816446
H	0.586385	-10.338900	-5.529478
C	-1.365274	-9.540101	-5.166933
O	-2.306887	-9.811308	-5.877044
N	-1.472642	-9.318870	-3.858023
C	-2.775758	-9.368202	-3.235321
C	-3.698644	-8.231569	-3.681698
O	-4.892287	-8.459293	-3.766303
C	-2.685085	-9.371581	-1.702540
O	-3.930809	-9.672021	-1.134250
H	-0.658585	-9.198186	-3.293558
H	-3.288101	-10.270066	-3.541002
H	-1.991739	-10.141827	-1.391851
H	-2.310860	-8.416028	-1.349806
H	-4.619006	-9.252255	-1.627732
N	-3.166169	-7.033680	-3.913437
C	-3.942967	-5.920828	-4.435541
C	-4.476161	-6.248018	-5.830667
O	-5.641613	-6.070728	-6.108422
C	-3.061297	-4.651732	-4.438918
C	-3.544043	-3.522635	-5.333580
C	-4.871491	-3.106840	-5.366701
C	-2.631681	-2.871704	-6.155345
C	-5.268512	-2.084391	-6.211351
C	-3.022446	-1.837478	-6.990360
C	-4.348248	-1.444785	-7.025850

H	-2.203200	-6.886787	-3.691052
H	-4.815495	-5.760781	-3.821248
H	-2.965740	-4.309135	-3.412733
H	-2.072591	-4.936163	-4.769910
H	-5.604410	-3.595238	-4.752880
H	-1.601039	-3.180188	-6.149539
H	-6.305927	-1.795034	-6.236729
H	-2.293378	-1.349711	-7.612756
H	-4.658954	-0.652154	-7.685253
N	-3.592131	-6.727714	-6.713717
C	-4.015210	-7.045249	-8.057310
C	-5.138068	-8.080755	-8.068498
O	-6.012741	-8.009181	-8.893646
C	-2.854374	-7.568232	-8.906784
S	-1.618410	-6.317742	-9.381269
H	-2.645681	-6.876065	-6.434715
H	-4.434719	-6.167874	-8.528775
H	-2.364209	-8.397281	-8.413644
H	-3.259501	-7.928939	-9.843102
H	-1.023930	-6.185661	-8.204100
N	-5.078558	-9.066914	-7.155618
H	-4.269966	-9.185399	-6.585169
C	-6.089593	-10.108532	-7.194207
H	-6.270510	-10.427377	-8.209590
H	-5.720335	-10.953218	-6.623276
C	-7.459140	-9.722569	-6.613184
O	-8.482033	-10.093281	-7.124002
N	-7.417942	-9.016208	-5.478355
C	-8.648379	-8.662987	-4.796849
C	-9.505958	-7.661910	-5.564683

O	-10.706016	-7.670725	-5.474841
C	-8.384496	-8.139675	-3.375761
C	-7.525130	-6.872785	-3.235898
C	-8.183013	-5.515585	-3.207105
O	-9.481231	-5.502387	-3.330568
H	-9.835700	-4.614888	-3.215774
O	-7.531239	-4.513280	-3.057680
H	-6.537742	-8.775970	-5.075678
H	-9.269992	-9.544580	-4.717237
H	-9.346082	-7.994797	-2.905184
H	-7.880184	-8.936557	-2.839395
H	-6.974302	-6.920610	-2.303748
H	-6.773404	-6.815661	-4.005850
N	-8.837305	-6.733964	-6.273853
C	-9.555190	-5.702612	-7.000840
C	-10.380280	-6.277583	-8.142491
H	-10.392379	-7.361959	-8.250254
O	-10.986939	-5.567424	-8.889810
C	-8.627868	-4.567856	-7.490331
O	-9.428216	-3.446960	-7.840235
C	-7.714316	-4.938660	-8.650180
H	-7.850313	-6.816355	-6.387291
H	-10.271827	-5.251866	-6.322526
H	-8.028611	-4.260170	-6.643559
H	-10.101156	-3.752726	-8.436041
H	-7.033710	-4.116418	-8.843519
H	-7.125703	-5.820183	-8.442640
H	-8.291137	-5.118858	-9.551435
N	-12.952117	-9.022533	3.174166
H	-13.212203	-9.555727	2.372042

C	-11.773529	-8.180033	2.898782
C	-10.792793	-8.116127	4.050703
O	-9.669187	-7.695095	3.859858
C	-12.153157	-6.724244	2.562295
O	-12.723325	-6.208781	3.737452
C	-13.124624	-6.608058	1.393589
H	-13.729904	-8.455274	3.445915
H	-11.219375	-8.597694	2.069698
H	-11.238230	-6.195980	2.323962
H	-12.860811	-5.272517	3.643058
H	-13.297627	-5.559704	1.174797
H	-12.738583	-7.078720	0.497661
H	-14.082253	-7.054128	1.635469
N	-11.197265	-8.533586	5.241923
H	-12.114878	-8.917725	5.275612
C	-10.414054	-8.496029	6.449928
H	-10.332269	-7.489763	6.832138
H	-10.934868	-9.083468	7.197584
C	-8.979364	-9.016494	6.388596
O	-8.152341	-8.455039	7.063068
N	-8.662777	-10.094113	5.648233
H	-9.369412	-10.557222	5.125428
C	-7.274548	-10.528739	5.553415
H	-7.256904	-11.519385	5.115981
H	-6.833488	-10.582569	6.536179
C	-6.387408	-9.608374	4.692653
O	-5.216063	-9.491131	4.937578
N	-7.045394	-9.018027	3.701138
C	-6.281229	-8.044831	2.926661
C	-6.253481	-6.681700	3.616578

O	-5.277898	-5.980226	3.501055
C	-6.554224	-7.997241	1.413761
C	-7.770313	-7.255633	0.907918
C	-7.800398	-5.863374	0.911688
C	-8.834615	-7.940773	0.338571
C	-8.876105	-5.176643	0.376460
C	-9.904410	-7.255451	-0.213846
C	-9.931750	-5.871913	-0.190922
H	-8.038231	-9.006758	3.677930
H	-5.259464	-8.373646	3.004627
H	-5.671805	-7.543731	0.976290
H	-6.569828	-9.023644	1.066034
H	-6.965550	-5.311779	1.307104
H	-8.812053	-9.016725	0.293425
H	-8.873356	-4.101167	0.370812
H	-10.700827	-7.800970	-0.688164
H	-10.750407	-5.341772	-0.641330
N	-7.286215	-6.346127	4.398547
C	-7.231011	-5.196327	5.266954
C	-6.174944	-5.392765	6.353500
O	-5.552435	-4.433941	6.752902
C	-8.635410	-4.967568	5.860679
C	-8.832236	-3.673185	6.620149
C	-8.878552	-2.455145	5.947342
C	-9.022153	-3.678344	7.995597
C	-9.097850	-1.273200	6.631889
C	-9.249177	-2.495711	8.687335
C	-9.287765	-1.290147	8.006929
H	-8.139320	-6.853184	4.328992
H	-6.909320	-4.322168	4.718249

H	-9.335619	-5.002465	5.032151
H	-8.869900	-5.802679	6.508530
H	-8.744451	-2.427953	4.879607
H	-8.985396	-4.608427	8.536438
H	-9.121671	-0.343685	6.092499
H	-9.377058	-2.519061	9.755470
H	-9.447539	-0.370421	8.541589
N	-5.968943	-6.622483	6.822068
H	-6.616773	-7.342709	6.602262
C	-4.936727	-6.909935	7.791769
H	-4.985848	-6.246334	8.642485
H	-5.087668	-7.924222	8.140212
C	-3.520611	-6.791823	7.233634
O	-2.647363	-6.327873	7.927344
N	-3.313612	-7.225201	5.986939
C	-2.023899	-7.080235	5.331026
C	-1.727440	-5.611796	4.999885
O	-0.642418	-5.158598	5.283452
C	-1.947857	-8.008121	4.101670
C	-0.782326	-7.644813	3.183260
C	-1.845430	-9.470236	4.550164
H	-4.047453	-7.693078	5.505117
H	-1.246428	-7.350840	6.031699
H	-2.869370	-7.879982	3.537413
H	-0.717256	-8.358455	2.370046
H	-0.883956	-6.662057	2.743314
H	0.162211	-7.668069	3.716065
H	-1.881878	-10.128440	3.687663
H	-0.898477	-9.641550	5.056619
H	-2.647551	-9.757208	5.217736

N	-2.697994	-4.887143	4.428764
C	-2.466689	-3.509800	4.021656
C	-2.398438	-2.589531	5.241026
O	-1.569728	-1.709008	5.303561
C	-3.556754	-3.001271	3.064987
C	-3.679714	-3.710336	1.704639
C	-2.464778	-3.543636	0.783731
O	-1.410756	-4.044011	1.206315
O	-2.625470	-2.943721	-0.289097
H	-3.541901	-5.335782	4.150844
H	-1.505798	-3.439917	3.541250
H	-4.519089	-3.059012	3.569678
H	-3.356747	-1.946732	2.897048
H	-3.833950	-4.771418	1.857844
H	-4.561270	-3.316238	1.208713
N	-3.291291	-2.769819	6.236592
C	-3.094021	-2.024920	7.456986
C	-1.786791	-2.428838	8.150580
O	-1.130556	-1.592446	8.734475
C	-4.242891	-1.992992	8.472703
O	-4.510070	-3.238765	9.045472
C	-5.493579	-1.325861	7.914669
H	-3.938971	-3.522276	6.199064
H	-2.922578	-0.996869	7.179416
H	-3.863446	-1.380191	9.282717
H	-4.949560	-3.782419	8.408517
H	-6.244984	-1.270510	8.693232
H	-5.272676	-0.317350	7.578128
H	-5.905376	-1.881915	7.083152
N	-1.380380	-3.700423	8.043288

H	-2.005425	-4.420007	7.762130
C	-0.131383	-4.094491	8.640062
H	-0.100608	-3.880771	9.699635
H	-0.018107	-5.160627	8.490034
C	1.071994	-3.389833	8.026149
O	1.978890	-2.997871	8.730124
N	1.088060	-3.259934	6.690709
C	2.236638	-2.668978	6.053454
C	2.270063	-1.144384	6.153809
O	3.355672	-0.594733	6.163659
C	2.440696	-3.150150	4.612360
S	1.368543	-2.312481	3.402094
H	0.367655	-3.683296	6.139395
H	3.112261	-2.971438	6.609986
H	3.474707	-2.967510	4.352720
H	2.256195	-4.215830	4.580498
H	1.799554	-2.978468	2.339088
N	1.126092	-0.463369	6.261850
C	1.204069	0.968501	6.491363
C	1.761855	1.265767	7.869776
O	2.372713	2.286572	8.087135
C	-0.093933	1.751377	6.198872
C	-1.193707	1.550710	7.251800
C	-0.553896	1.488869	4.759637
C	-2.470932	2.344346	6.971336
H	0.249518	-0.931163	6.150316
H	1.952272	1.357753	5.816338
H	0.212971	2.790517	6.266463
H	-1.431127	0.501322	7.351322
H	-0.807476	1.861995	8.218303

H	-1.300533	2.213126	4.457739
H	0.279673	1.573372	4.068374
H	-0.978650	0.501693	4.639085
H	-3.142173	2.289393	7.823588
H	-2.256835	3.394750	6.787147
H	-3.004586	1.957990	6.109793
N	1.549785	0.323276	8.791268
H	0.924729	-0.426893	8.596421
C	1.986100	0.500666	10.156042
H	1.462325	-0.222220	10.769782
H	1.768585	1.496342	10.513755
C	3.484960	0.295346	10.316365
O	4.161388	1.050551	10.963138
N	4.001659	-0.777718	9.680608
H	3.398860	-1.426421	9.220989
C	5.426736	-0.958277	9.643657
H	5.641165	-1.918858	9.188737
H	5.856108	-0.943200	10.634972
C	6.156884	0.119116	8.844831
O	7.283485	0.430639	9.147134
N	5.502075	0.621284	7.799030
C	6.098618	1.759274	7.146316
C	5.535843	3.077053	7.670198
H	5.003130	3.023929	8.619908
O	5.700657	4.107370	7.091428
C	5.964102	1.686659	5.622494
C	6.677912	0.506854	4.995244
C	8.044724	0.295989	5.182068
C	5.977747	-0.387754	4.191070
C	8.693856	-0.763895	4.563679

C	6.625182	-1.445010	3.571495
C	7.986595	-1.634263	3.749286
H	4.595003	0.300639	7.538209
H	7.141665	1.764832	7.428581
H	4.913698	1.641632	5.362190
H	6.348743	2.618160	5.219726
H	8.602098	0.941641	5.840004
H	4.915916	-0.274367	4.077565
H	9.747028	-0.912451	4.733408
H	6.060426	-2.123407	2.957097
H	8.477856	-2.459462	3.265491
N	12.613550	9.596234	-1.248802
H	11.875371	9.913983	-1.846612
C	12.304853	8.264740	-0.719488
C	11.274242	8.447550	0.387609
O	10.270539	7.770142	0.419851
C	13.561105	7.577803	-0.166669
C	14.640145	7.267853	-1.209184
S	14.005701	6.195739	-2.530673
C	15.483639	6.038081	-3.560022
H	13.436386	9.575614	-1.815741
H	11.832859	7.616957	-1.447424
H	14.003238	8.201298	0.605228
H	13.250621	6.651952	0.304501
H	15.043433	8.178707	-1.638947
H	15.464443	6.771810	-0.708456
H	15.222801	5.383944	-4.378108
H	15.786540	7.000480	-3.952794
H	16.301059	5.595840	-3.005150
N	11.501599	9.413469	1.295150

C	10.592248	9.606047	2.407507
C	9.279666	10.287585	2.017629
O	8.289452	10.086012	2.674527
C	11.279972	10.350479	3.558211
C	12.451052	9.538400	4.079766
O	13.587794	9.816673	3.756854
N	12.148272	8.513112	4.883471
H	12.320437	9.972402	1.198453
H	10.284423	8.634277	2.760936
H	11.664064	11.310587	3.235747
H	10.551426	10.510527	4.343261
H	12.896017	7.923884	5.174477
H	11.228061	8.125410	4.909339
N	9.265352	11.070902	0.921775
H	10.107337	11.207311	0.413431
C	8.003503	11.517468	0.368862
H	8.196834	12.261331	-0.393975
H	7.387903	11.963042	1.133693
C	7.186383	10.384438	-0.254326
O	5.988474	10.483090	-0.309205
N	7.860524	9.323653	-0.745051
C	7.162093	8.138573	-1.212865
C	6.623560	7.303803	-0.041159
O	5.517599	6.824139	-0.115549
C	8.033450	7.325747	-2.199734
C	8.345605	8.174069	-3.447106
C	7.346039	6.010593	-2.585652
C	9.423005	7.585403	-4.360416
H	8.817926	9.215641	-0.510349
H	6.271104	8.467798	-1.726386

H	8.968023	7.086894	-1.698317
H	7.426845	8.314760	-4.012990
H	8.662508	9.165172	-3.138097
H	7.961327	5.456951	-3.283239
H	7.173736	5.375467	-1.725469
H	6.384126	6.188718	-3.055437
H	9.626960	8.261504	-5.184671
H	10.355911	7.428425	-3.825425
H	9.130994	6.633998	-4.789345
N	7.378441	7.176113	1.068804
C	6.865001	6.461093	2.226701
C	5.515601	7.045285	2.664267
O	4.566882	6.338845	2.900772
C	7.818996	6.544802	3.427786
C	9.234998	5.988958	3.259695
O	10.139158	6.633744	3.787157
O	9.396311	4.913683	2.632075
H	8.341397	7.429992	1.040426
H	6.663211	5.432694	1.968582
H	7.913693	7.569808	3.756351
H	7.360165	5.991522	4.244777
N	5.475394	8.385157	2.800808
H	6.304186	8.919766	2.658608
C	4.282462	9.052707	3.260188
H	4.522217	10.094631	3.434622
H	3.928259	8.633895	4.189280
C	3.125895	9.015483	2.270588
O	1.987567	9.179845	2.644986
N	3.462275	8.827414	0.992053
H	4.422548	8.780775	0.750309

C	2.517195	8.905257	-0.078303
H	3.063976	9.089531	-0.994780
H	1.841813	9.737275	0.068108
C	1.609130	7.687023	-0.310195
O	0.568239	7.818812	-0.891663
N	2.082674	6.540758	0.214374
C	1.265121	5.376763	0.458801
C	0.458403	5.531164	1.751648
O	-0.745011	5.431769	1.724406
C	2.121409	4.111815	0.480560
H	2.984319	6.576380	0.637504
H	0.527066	5.306962	-0.323636
H	1.510397	3.244212	0.703312
H	2.581753	3.973798	-0.490833
H	2.908039	4.178233	1.225514
N	1.103380	5.766666	2.910707
C	0.359919	5.601859	4.152269
C	-0.753277	6.635729	4.301341
O	-1.787484	6.338089	4.859958
C	1.268752	5.522648	5.403488
C	1.867566	6.865444	5.848299
C	2.349872	4.449223	5.205032
C	2.698719	6.767947	7.129597
H	2.097415	5.824520	2.934193
H	-0.173209	4.662680	4.094578
H	0.603494	5.188930	6.194680
H	2.480416	7.267876	5.047847
H	1.068097	7.581322	6.013013
H	2.705719	4.086686	6.158550
H	1.956054	3.598741	4.658550

H	3.201779	4.836539	4.655611
H	3.011170	7.758047	7.449572
H	2.118517	6.330220	7.936793
H	3.589461	6.165249	7.001109
N	-0.537734	7.868344	3.819129
H	0.340631	8.105230	3.410001
C	-1.517047	8.902494	4.019313
H	-1.113762	9.831023	3.633584
H	-1.735897	9.041250	5.068751
C	-2.866969	8.618760	3.365891
O	-3.873013	8.835243	4.002903
N	-2.902694	8.108965	2.120754
C	-4.240747	8.006926	1.538818
C	-4.985005	6.744200	1.937892
O	-6.197583	6.757516	1.931133
C	-4.025738	8.210828	0.034049
C	-2.777443	9.099328	0.019839
C	-1.911386	8.462277	1.093741
H	-4.857319	8.807367	1.920528
H	-3.837180	7.267635	-0.462653
H	-4.894798	8.664946	-0.425313
H	-2.268609	9.143979	-0.924756
H	-3.046329	10.112660	0.310987
H	-1.419707	7.575449	0.736816
H	-1.158349	9.130327	1.480642
N	-4.272419	5.671195	2.306342
C	-4.944660	4.508958	2.862948
C	-5.649229	4.863615	4.175098
O	-6.762293	4.446846	4.412822
C	-3.984662	3.328790	3.119143

C	-3.566245	2.524101	1.904560
C	-4.156942	1.297363	1.616047
C	-2.530891	2.947897	1.083945
C	-3.733907	0.521921	0.547046
C	-2.103023	2.189271	0.011706
C	-2.696939	0.968417	-0.267370
O	-2.242895	0.273562	-1.321877
H	-2.952690	-0.231068	-1.719485
H	-3.278257	5.741763	2.345946
H	-5.728252	4.202213	2.187212
H	-3.108952	3.707165	3.637974
H	-4.489221	2.664240	3.811690
H	-4.954290	0.931394	2.240961
H	-2.039409	3.876870	1.278128
H	-4.172302	-0.439677	0.359116
H	-1.304354	2.533385	-0.621596
N	-4.975134	5.619849	5.057657
H	-4.033333	5.895763	4.874980
C	-5.590535	6.005783	6.305803
H	-4.816268	6.383175	6.963109
H	-6.068038	5.161270	6.777593
C	-6.653547	7.089065	6.140512
O	-7.707896	7.042151	6.734549
N	-6.342148	8.091247	5.313908
H	-5.447310	8.133900	4.875928
C	-7.257687	9.220268	5.085303
H	-6.780977	9.874221	4.365771
H	-7.425267	9.773907	5.998204
C	-8.631028	8.841954	4.565103
O	-9.609634	9.436787	4.949337

N	-8.689665	7.852504	3.658311
C	-9.953936	7.451761	3.088773
C	-10.769603	6.546741	3.997573
O	-11.817458	6.083081	3.565386
C	-9.759684	6.810649	1.692333
O	-10.952324	6.896525	0.954858
C	-9.237764	5.377501	1.739069
H	-7.846122	7.423083	3.337882
H	-10.571911	8.331416	2.960916
H	-9.040690	7.431820	1.172827
H	-11.637837	6.496969	1.472067
H	-8.969437	5.050165	0.742518
H	-8.358262	5.288511	2.361358
H	-9.998394	4.702991	2.115269
N	-10.353337	6.327942	5.240899
C	-11.263937	5.755933	6.221480
C	-12.430178	6.704185	6.510430
O	-13.521427	6.260257	6.782760
C	-10.540844	5.423961	7.534519
C	-9.544386	4.255508	7.460538
C	-8.723890	4.208798	8.752885
C	-10.237545	2.911150	7.217389
H	-9.456611	6.643768	5.544060
H	-11.721310	4.869439	5.813842
H	-10.022944	6.313219	7.877814
H	-11.305429	5.193593	8.272050
H	-8.857468	4.436276	6.639877
H	-8.000651	3.398671	8.724251
H	-8.183136	5.136740	8.900808
H	-9.364036	4.048091	9.618118

H	-9.500781	2.113113	7.199477
H	-10.947203	2.691551	8.013377
H	-10.770374	2.881265	6.274128
N	-12.161548	8.022371	6.508919
C	-13.213370	8.981115	6.674726
C	-13.981245	9.276037	5.404614
H	-14.806318	9.987713	5.534383
O	-13.739401	8.809974	4.340737
H	-11.296639	8.348955	6.135131
H	-13.917311	8.632615	7.421011
H	-12.797121	9.917795	7.034850
N	-11.441241	10.613163	-3.010180
H	-11.171665	10.805432	-2.067594
C	-11.816457	9.206991	-3.172692
C	-11.416593	8.871301	-4.602200
O	-10.367825	8.327599	-4.850535
C	-13.263658	8.844362	-2.777744
C	-13.505983	9.186420	-1.295966
C	-13.551523	7.366187	-3.069339
C	-14.938026	8.950945	-0.813600
H	-12.199822	11.226667	-3.235231
H	-11.144625	8.621479	-2.559970
H	-13.950309	9.455497	-3.370072
H	-12.816999	8.610086	-0.682292
H	-13.265469	10.232331	-1.130718
H	-14.596292	7.132332	-2.908960
H	-13.318975	7.095146	-4.095053
H	-12.964200	6.728604	-2.415942
H	-15.050112	9.306023	0.204720
H	-15.657067	9.483055	-1.431648

H	-15.205308	7.900551	-0.818003
N	-12.221605	9.293884	-5.606697
H	-13.144303	9.585644	-5.383198
C	-11.972872	8.843880	-6.959258
H	-12.030826	7.766437	-7.041610
H	-12.727332	9.277620	-7.605113
C	-10.601635	9.233244	-7.517693
O	-10.001429	8.500085	-8.247884
N	-10.163627	10.478873	-7.182432
H	-10.705002	11.000804	-6.533973
C	-8.894341	11.023967	-7.637100
H	-8.788447	10.888364	-8.702796
H	-8.876005	12.081928	-7.407754
C	-7.672564	10.359017	-6.988311
O	-6.750720	9.944631	-7.632766
N	-7.659883	10.351601	-5.619712
H	-8.489577	10.606490	-5.135691
C	-6.495254	9.961264	-4.832349
H	-5.598896	10.375427	-5.266935
H	-6.614392	10.359253	-3.831602
C	-6.268291	8.463911	-4.714277
O	-5.133276	8.049574	-4.714449
N	-7.319505	7.640709	-4.554014
C	-7.041022	6.286202	-4.100339
C	-6.399273	5.427597	-5.182974
O	-5.555778	4.625980	-4.865138
C	-8.230441	5.578173	-3.412387
C	-9.372729	5.197623	-4.369143
C	-8.686920	6.403628	-2.204162
C	-10.520284	4.447573	-3.692671

H	-8.252791	7.995231	-4.566114
H	-6.257136	6.350501	-3.359957
H	-7.804402	4.654646	-3.027832
H	-9.763026	6.078375	-4.863312
H	-8.964088	4.563062	-5.151621
H	-9.402396	5.859321	-1.603640
H	-7.843656	6.639114	-1.562733
H	-9.152445	7.333392	-2.508425
H	-11.234943	4.101822	-4.434147
H	-10.161814	3.579350	-3.151526
H	-11.057496	5.078299	-2.995191
N	-6.791003	5.554791	-6.471692
C	-6.079039	4.805068	-7.486926
C	-4.754681	5.444973	-7.908168
O	-3.894153	4.728963	-8.364366
C	-6.944630	4.429443	-8.697814
C	-7.972902	3.318009	-8.426847
C	-7.335488	1.999228	-7.961437
N	-8.248833	0.854884	-7.954140
C	-9.058522	0.500921	-6.954248
N	-9.287055	1.345625	-5.960773
N	-9.639824	-0.678275	-6.960157
H	-7.450829	6.258333	-6.720152
H	-5.738748	3.902187	-7.010489
H	-7.463536	5.306941	-9.073984
H	-6.271884	4.102933	-9.483573
H	-8.709286	3.661953	-7.705928
H	-8.516934	3.129205	-9.347103
H	-6.525225	1.733545	-8.628448
H	-6.900295	2.090101	-6.974335

H	-8.192204	0.217291	-8.715211
H	-8.928770	2.268224	-5.991742
H	-9.780791	1.079953	-5.126944
H	-9.336528	-1.443270	-7.533272
H	-10.356064	-0.895104	-6.288737
N	-4.571382	6.757518	-7.721942
H	-5.298999	7.337833	-7.376967
C	-3.257813	7.352386	-8.011369
H	-2.929746	7.080324	-9.002182
H	-3.360944	8.428528	-7.952678
C	-2.193219	6.896491	-7.027526
O	-1.061215	6.684714	-7.383873
N	-2.614922	6.781484	-5.763570
C	-1.730110	6.466737	-4.669021
C	-1.453232	4.979585	-4.555254
O	-0.320391	4.598179	-4.370159
C	-2.311053	7.055944	-3.378256
C	-1.724824	6.346597	-2.158742
C	-2.067587	8.571886	-3.408271
H	-3.541599	7.067290	-5.539318
H	-0.760260	6.905461	-4.858082
H	-3.380917	6.879752	-3.391464
H	-1.936497	6.883760	-1.253143
H	-2.138679	5.348614	-2.058455
H	-0.652297	6.271921	-2.232441
H	-2.806351	9.102365	-2.824136
H	-1.080458	8.810160	-3.025697
H	-2.143649	8.955910	-4.419238
N	-2.480494	4.124610	-4.674163
C	-2.164161	2.717524	-4.734154

C	-1.272670	2.436910	-5.935556
O	-0.408422	1.595377	-5.885649
C	-3.392490	1.790010	-4.722420
C	-4.258321	1.918120	-3.461106
C	-5.303866	0.801541	-3.300541
N	-4.771050	-0.372108	-2.635142
C	-5.548932	-1.357423	-2.405906
N	-6.887078	-1.413741	-2.801361
N	-5.164690	-2.418476	-1.664709
H	-3.415252	4.445085	-4.798683
H	-1.555259	2.458807	-3.879215
H	-4.000706	1.972948	-5.607935
H	-3.015117	0.776604	-4.803676
H	-3.623573	1.924969	-2.587144
H	-4.777778	2.866653	-3.485464
H	-6.144568	1.211814	-2.738029
H	-5.696595	0.561343	-4.295261
H	-7.071232	-0.913658	-3.641916
H	-7.273165	-2.337867	-2.840603
H	-4.229898	-2.489266	-1.295686
H	-5.683003	-3.262984	-1.740791
N	-1.459779	3.193346	-7.035076
H	-2.264018	3.767364	-7.143528
C	-0.596738	2.980726	-8.177683
H	-0.945588	3.613755	-8.984380
H	-0.605399	1.950878	-8.505996
C	0.856772	3.335685	-7.872241
O	1.784264	2.709096	-8.321503
N	1.007506	4.397742	-7.065992
H	0.209314	4.934998	-6.822421

C	2.282349	4.880604	-6.640357
H	2.921372	5.136843	-7.476466
H	2.123623	5.776550	-6.053644
C	3.090814	3.928324	-5.777631
O	4.297674	4.051600	-5.702333
N	2.428078	2.983428	-5.101794
C	3.113691	2.135740	-4.164098
C	4.318215	1.403883	-4.753426
O	5.285285	1.187363	-4.050692
C	2.103548	1.144773	-3.576669
C	2.725784	0.179901	-2.582098
C	1.699092	-0.716628	-1.914718
N	2.418546	-1.721620	-1.171285
C	1.868896	-2.613520	-0.294751
N	0.545579	-2.727780	-0.299407
O	2.621483	-3.260498	0.423983
H	1.432989	2.943196	-5.156082
H	3.544148	2.732272	-3.367565
H	1.325049	1.728995	-3.095183
H	1.622291	0.603034	-4.383402
H	3.452177	-0.452627	-3.080198
H	3.270475	0.731223	-1.817586
H	1.040213	-0.131031	-1.277087
H	1.076015	-1.189557	-2.668227
H	3.371363	-1.540542	-0.959886
H	-0.050824	-2.153350	-0.847864
H	0.049119	-3.332430	0.338568
N	4.284556	0.951822	-6.016429
H	3.508524	1.169822	-6.604581
C	5.363401	0.116580	-6.504631

H	5.141461	-0.157579	-7.529028
H	5.444896	-0.791660	-5.926553
C	6.735556	0.755735	-6.484745
O	7.739593	0.088468	-6.387531
N	6.766097	2.085339	-6.608338
H	5.914177	2.605595	-6.566033
C	8.008019	2.818112	-6.552164
H	8.713131	2.428925	-7.273911
H	7.808806	3.850147	-6.810441
C	8.752414	2.822116	-5.214784
O	9.896112	3.229690	-5.165797
N	8.104621	2.336859	-4.150538
C	8.678169	2.169284	-2.826204
C	9.942813	1.301192	-2.829377
O	10.756994	1.383099	-1.923027
C	7.567816	1.496961	-1.986522
C	7.740156	1.380299	-0.472963
C	7.361160	2.645127	0.306255
C	7.227282	2.380697	1.801701
N	8.556181	2.360637	2.481696
O	10.975135	1.600057	0.910496
H	10.836546	1.807037	-0.009990
H	11.440399	0.771211	0.877074
H	7.154458	2.045838	-4.264762
H	8.976417	3.124846	-2.412874
H	6.650361	2.032676	-2.188140
H	7.412051	0.507304	-2.401124
H	7.067158	0.590988	-0.153072
H	8.736734	1.043884	-0.217908
H	8.063206	3.458725	0.140984

H	6.394783	2.996917	-0.041234
H	6.648879	3.148266	2.293578
H	6.750010	1.430569	1.989859
H	9.271622	1.890043	1.940201
H	8.876580	3.331280	2.632790
H	8.485699	1.887566	3.369657
N	10.062459	0.448217	-3.837523
C	11.108353	-0.538444	-4.063358
C	12.484382	0.019845	-4.433381
O	13.443189	-0.709995	-4.317075
C	10.690947	-1.458251	-5.232494
C	9.531307	-2.429423	-4.966306
C	9.094242	-3.067810	-6.288311
C	9.926922	-3.509712	-3.960361
H	9.324155	0.443221	-4.509301
H	11.270825	-1.117051	-3.164859
H	10.438866	-0.821597	-6.076204
H	11.566371	-2.031151	-5.516049
H	8.682480	-1.874320	-4.578335
H	8.279027	-3.765900	-6.124898
H	8.753571	-2.314937	-6.987849
H	9.913735	-3.619496	-6.743547
H	9.117215	-4.214699	-3.808339
H	10.784145	-4.065934	-4.325834
H	10.185820	-3.099001	-2.989098
N	12.574048	1.261825	-4.919242
C	13.814758	1.840629	-5.394045
C	14.958271	2.031677	-4.379289
O	16.013181	2.413631	-4.812566
C	13.501679	3.164654	-6.094152

O	12.926293	4.090133	-5.218451
H	11.755408	1.831045	-4.920136
H	14.251680	1.170192	-6.125856
H	14.428563	3.575930	-6.465265
H	12.851126	2.965494	-6.940836
H	11.981521	4.069876	-5.263840
N	14.792298	1.722328	-3.074282
C	15.930482	1.649333	-2.180230
C	16.805629	0.411917	-2.408434
O	17.938979	0.397411	-2.001491
C	15.502896	1.578241	-0.709013
C	14.629921	2.722246	-0.198775
C	14.253766	2.452893	1.258476
N	13.218520	3.336161	1.778853
C	13.386550	4.493213	2.396111
N	14.602013	4.980632	2.623990
O	15.039639	7.450799	4.160770
H	14.748831	8.335504	3.942971
H	15.759562	7.540610	4.764607
N	12.332054	5.174672	2.789703
H	13.902607	1.418488	-2.757875
H	16.565136	2.505622	-2.354128
H	14.974155	0.643993	-0.551634
H	16.418127	1.522193	-0.129001
H	15.141677	3.676153	-0.296016
H	13.718456	2.803224	-0.779860
H	13.856413	1.451108	1.338634
H	15.123908	2.485351	1.905478
H	12.281509	3.028699	1.615279
H	15.407527	4.489738	2.322747

H	14.732423	5.837673	3.129132
H	11.380330	4.880723	2.640349
H	12.414666	6.024369	3.297594
N	16.200237	-0.648976	-2.967239
C	16.873232	-1.911333	-3.155405
C	17.690170	-1.897370	-4.443379
H	18.039344	-0.909140	-4.756666
O	17.957088	-2.875825	-5.061927
C	15.871409	-3.071161	-3.142299
C	15.317297	-3.394693	-1.788203
N	14.402693	-2.609434	-1.116482
O	12.562337	-0.372519	-0.476237
H	13.157748	-1.001902	-0.875328
H	12.043072	0.012939	-1.168529
C	15.595997	-4.485851	-1.040674
C	14.157981	-3.226642	-0.006971
N	14.854271	-4.364863	0.107724
H	15.281178	-0.557338	-3.341499
H	17.591357	-2.028102	-2.350123
H	15.058108	-2.844791	-3.824032
H	16.377719	-3.945471	-3.529396
H	16.241966	-5.318000	-1.222201
H	13.478569	-2.885218	0.748276
H	14.742258	-5.043928	0.827194
O	-14.960527	-2.469725	5.344596
H	-15.102336	-1.594511	5.005496
H	-14.426088	-2.371683	6.120447
O	-12.680208	-1.808938	7.362317
H	-11.956090	-2.343237	7.656457
H	-12.783232	-1.130069	8.011127

O	-11.943052	-0.969095	4.626111
H	-11.999187	-1.156846	5.554799
H	-12.763460	-0.538730	4.398975
O	-13.427561	-1.434041	1.204091
H	-12.556946	-1.039012	1.184793
H	-13.381570	-2.183735	1.792252
O	-7.254553	2.154569	0.018657
H	-7.410356	2.204124	0.961019
H	-6.339914	1.929911	-0.071088
O	-7.592412	2.119624	2.821497
H	-8.353679	1.648725	3.136834
H	-7.455797	2.865375	3.393781
O	-8.959903	0.258077	-1.133245
H	-8.391808	0.940214	-0.767266
H	-8.374413	-0.427159	-1.440636
O	-13.031259	-1.860031	-1.615205
H	-13.333741	-1.922675	-0.714345
H	-13.753684	-2.059220	-2.194057
O	-13.671463	1.576011	0.463493
H	-14.093183	0.744781	0.629069
H	-12.750601	1.404956	0.645641
O	-14.672397	5.278923	4.160493
H	-13.982154	5.830178	3.817334
H	-14.612989	5.395416	5.099982
O	-14.717613	2.679824	3.054362
H	-14.899455	3.558542	3.385524
H	-14.552860	2.728958	2.122264
O	-13.172071	0.927910	-2.304205
H	-13.457425	1.424996	-1.545266
H	-12.968144	0.059200	-1.967183

O	-14.434016	-0.889227	-4.096995
H	-14.305837	-0.064049	-3.641581
H	-15.232280	-0.825088	-4.595505
O	-10.644895	-3.038237	-2.964691
H	-10.923718	-2.629968	-3.774432
H	-11.313554	-2.811417	-2.332035
O	-11.141332	0.223138	0.862571
H	-10.463164	0.115265	0.201670
H	-10.703109	0.478736	1.673257
O	-10.187929	0.963592	3.413774
H	-10.599986	0.280385	3.932086
H	-10.696201	1.758444	3.566935
O	-11.945023	3.112422	3.762167
H	-11.899126	4.055844	3.675573
H	-12.857440	2.879980	3.640466
O	-10.521877	0.898844	-3.359850
H	-11.345589	1.219059	-3.006754
H	-9.958729	0.697615	-2.609779
O	-14.503463	-0.058467	3.756269
H	-14.716174	0.866892	3.663925
H	-14.425442	-0.410955	2.879894
O	-13.121954	-3.336938	3.387866
H	-13.869905	-3.201636	3.969829
H	-12.449569	-2.774306	3.757953
O	-11.636768	-1.169560	-4.915529
H	-12.586803	-1.181519	-4.885835
H	-11.346665	-0.549056	-4.253497

R303cit MUTATION: NOMINAL CHARGES, Y266(0), E183(0) POTENTIAL: 0mV

N	15.811987	-6.063897	5.314056
H	15.005750	-5.858786	5.869538
C	15.703106	-5.466092	3.982355
C	15.011770	-6.415695	2.986877
O	14.271932	-5.998632	2.112517
C	17.093375	-5.116519	3.439914
H	16.610099	-5.712546	5.802433
H	15.093416	-4.571364	3.987180
H	17.034516	-4.722581	2.432342
H	17.548103	-4.355873	4.064725
H	17.740892	-5.986851	3.434534
N	15.298586	-7.710857	3.110135
H	15.882089	-7.969294	3.875166
C	14.689227	-8.734397	2.259151
H	14.750118	-8.455942	1.219324
H	15.216488	-9.668167	2.405900
C	13.212818	-8.922313	2.608213
O	12.391403	-9.181811	1.769230
N	12.881523	-8.750874	3.902113
H	13.599293	-8.627004	4.576374
C	11.499986	-8.905480	4.363628
H	11.496386	-8.894461	5.445847
H	11.072283	-9.833972	4.017562
C	10.606664	-7.769565	3.848581
O	9.463166	-7.976763	3.547347
N	11.184934	-6.556843	3.789943
C	10.508735	-5.396226	3.266180

C	10.321283	-5.436208	1.746623
O	9.292961	-5.003164	1.288125
C	11.229132	-4.126011	3.738713
O	12.622781	-4.239507	3.685649
H	12.142285	-6.457206	4.029248
H	9.501137	-5.362203	3.648581
H	10.874504	-3.279167	3.160749
H	10.981460	-3.952756	4.776768
H	12.927445	-4.406230	2.806495
N	11.300464	-5.933899	0.968546
C	11.043277	-6.135289	-0.454640
C	9.933729	-7.169723	-0.661122
O	9.205593	-7.106529	-1.622420
C	12.340873	-6.469959	-1.248270
C	12.619208	-7.966964	-1.432681
C	12.316198	-5.773844	-2.609987
H	12.122861	-6.318009	1.376748
H	10.633314	-5.214763	-0.839894
H	13.157265	-6.042539	-0.675981
H	13.582257	-8.092405	-1.917656
H	12.639765	-8.513595	-0.500230
H	11.875062	-8.425228	-2.077011
H	13.214629	-6.009306	-3.170381
H	11.459597	-6.095648	-3.192097
H	12.269939	-4.697235	-2.497540
N	9.831339	-8.117556	0.279877
H	10.566330	-8.215520	0.939380
C	8.884542	-9.225591	0.196546
H	9.259721	-10.021441	0.828458
H	8.822932	-9.596883	-0.815136

C	7.466191	-8.909913	0.617296
O	6.563459	-9.436300	0.007963
N	7.261555	-8.077627	1.641684
C	5.910133	-7.614860	1.879577
C	5.480697	-6.671643	0.761453
O	4.339514	-6.713459	0.384756
C	5.622610	-7.056094	3.285621
C	5.776985	-8.153007	4.343732
C	6.424100	-5.809441	3.663982
H	8.032151	-7.747256	2.176536
H	5.252883	-8.459763	1.747362
H	4.573773	-6.776682	3.243801
H	5.464977	-7.782337	5.314863
H	5.162350	-9.015544	4.106806
H	6.807162	-8.483538	4.427004
H	6.064210	-5.414870	4.608470
H	7.474050	-6.045622	3.789505
H	6.332613	-5.023641	2.923243
N	6.369416	-5.852603	0.173178
C	5.919052	-5.051594	-0.953623
C	5.531874	-5.952799	-2.134618
O	4.547277	-5.705407	-2.790549
C	6.967731	-3.988483	-1.338923
C	7.144766	-2.973407	-0.195125
C	6.560021	-3.278846	-2.634533
C	8.415624	-2.132018	-0.313537
H	7.307901	-5.787383	0.496889
H	4.997401	-4.555940	-0.679072
H	7.916713	-4.494995	-1.501945
H	6.268339	-2.329489	-0.161717

H	7.177014	-3.491583	0.753832
H	7.224715	-2.450918	-2.844092
H	6.589098	-3.941761	-3.489474
H	5.549948	-2.890577	-2.558139
H	8.501088	-1.454358	0.529601
H	9.294621	-2.767008	-0.313706
H	8.435069	-1.533196	-1.217869
N	6.314468	-7.007042	-2.418208
H	7.192921	-7.113820	-1.961461
C	6.006173	-7.872766	-3.533949
H	6.859015	-8.522264	-3.693131
H	5.831682	-7.304976	-4.436126
C	4.766767	-8.745168	-3.327817
O	3.940451	-8.850797	-4.204678
N	4.677913	-9.391187	-2.159729
H	5.389309	-9.275280	-1.471742
C	3.506322	-10.158937	-1.810717
H	3.282337	-10.898499	-2.565688
H	3.708120	-10.669311	-0.876606
C	2.255477	-9.297031	-1.655394
O	1.186606	-9.701469	-2.061393
N	2.437859	-8.092144	-1.117479
C	1.301238	-7.181561	-1.081027
C	0.832358	-6.784518	-2.480004
O	-0.354425	-6.727332	-2.718646
C	1.557608	-5.871176	-0.351131
O	1.666550	-6.083433	1.018962
H	3.284514	-7.822316	-0.667940
H	0.455967	-7.674223	-0.624156
H	2.446603	-5.402590	-0.745406

H	0.708121	-5.233380	-0.567453
H	2.005366	-5.278480	1.384316
N	1.747642	-6.457087	-3.402413
C	1.327376	-6.056997	-4.731587
C	0.592123	-7.199011	-5.424613
O	-0.399409	-6.972511	-6.089652
C	2.516615	-5.514008	-5.558564
C	2.860130	-4.099929	-5.061671
C	2.228138	-5.522078	-7.064903
C	4.156170	-3.532316	-5.636859
H	2.715822	-6.429553	-3.163695
H	0.581157	-5.278417	-4.647505
H	3.365679	-6.166074	-5.374684
H	2.034152	-3.434055	-5.307937
H	2.942457	-4.114730	-3.982560
H	3.076034	-5.128000	-7.611616
H	2.047386	-6.522462	-7.440017
H	1.362178	-4.913258	-7.306361
H	4.407045	-2.602864	-5.136454
H	4.981894	-4.219974	-5.485276
H	4.082574	-3.322892	-6.698895
N	1.066470	-8.436456	-5.262601
H	1.903959	-8.589886	-4.741458
C	0.311296	-9.562967	-5.751662
H	0.197138	-9.532664	-6.825669
H	0.842280	-10.467377	-5.481525
C	-1.094210	-9.621495	-5.160577
O	-2.047506	-9.869825	-5.866798
N	-1.200902	-9.404752	-3.850754
C	-2.505780	-9.442079	-3.231062

C	-3.436521	-8.315636	-3.688828
O	-4.631692	-8.543545	-3.747522
C	-2.409783	-9.417849	-1.698523
O	-3.652703	-9.703242	-1.116714
H	-0.387201	-9.276761	-3.286551
H	-3.016955	-10.350401	-3.519953
H	-1.715743	-10.183252	-1.377196
H	-2.030884	-8.456667	-1.366552
H	-4.344397	-9.308365	-1.625819
N	-2.907718	-7.121938	-3.947207
C	-3.687861	-6.001300	-4.445128
C	-4.253921	-6.312512	-5.829036
O	-5.420071	-6.089996	-6.093073
C	-2.787662	-4.740829	-4.456753
C	-3.214561	-3.632982	-5.402415
C	-4.501208	-3.105953	-5.397751
C	-2.296328	-3.118017	-6.309044
C	-4.859339	-2.106654	-6.285188
C	-2.644778	-2.104178	-7.186759
C	-3.932271	-1.599037	-7.181051
H	-1.937117	-6.982029	-3.755264
H	-4.548470	-5.838659	-3.813345
H	-2.725777	-4.368925	-3.438637
H	-1.792292	-5.051450	-4.739275
H	-5.233482	-3.489987	-4.712426
H	-1.297894	-3.517595	-6.335629
H	-5.868782	-1.734593	-6.282756
H	-1.913743	-1.719649	-7.875569
H	-4.210348	-0.821084	-7.871226
N	-3.409280	-6.833648	-6.719482

C	-3.877422	-7.177754	-8.042300
C	-4.992113	-8.220776	-7.981720
O	-5.954482	-8.119815	-8.699683
C	-2.740821	-7.705605	-8.921105
S	-1.530090	-6.452642	-9.449271
H	-2.465870	-7.023500	-6.453047
H	-4.322751	-6.311337	-8.509184
H	-2.227295	-8.523199	-8.432740
H	-3.171697	-8.084203	-9.839009
H	-0.884940	-6.322265	-8.298675
N	-4.829289	-9.251610	-7.129472
H	-3.980523	-9.372875	-6.619846
C	-5.811687	-10.322426	-7.162249
H	-5.990778	-10.648701	-8.176289
H	-5.413752	-11.155295	-6.593528
C	-7.189253	-9.976452	-6.575336
O	-8.202787	-10.379393	-7.077825
N	-7.159766	-9.266859	-5.440989
C	-8.389918	-8.950158	-4.743239
C	-9.281417	-7.964883	-5.492732
O	-10.476759	-7.986715	-5.365030
C	-8.109551	-8.426473	-3.325710
C	-7.328256	-7.108834	-3.202788
C	-8.083707	-5.804871	-3.212528
O	-9.382894	-5.905354	-3.273801
H	-9.797889	-5.046105	-3.177912
O	-7.517431	-4.744590	-3.133842
H	-6.282254	-9.009661	-5.042295
H	-8.986906	-9.848088	-4.657777
H	-9.059484	-8.343522	-2.818405

H	-7.537715	-9.195093	-2.816432
H	-6.797636	-7.101987	-2.256985
H	-6.564296	-7.020411	-3.957704
N	-8.647837	-7.027884	-6.226384
C	-9.403915	-6.017282	-6.945316
C	-10.395649	-6.668173	-7.903164
H	-10.166205	-7.692806	-8.204030
O	-11.349074	-6.088089	-8.315033
C	-8.401504	-5.085310	-7.657832
O	-7.707016	-4.339748	-6.682817
C	-9.046356	-4.093491	-8.615290
H	-7.680911	-7.149608	-6.429986
H	-9.989947	-5.431685	-6.247059
H	-7.693940	-5.696475	-8.210664
H	-6.940634	-4.809013	-6.372559
H	-8.279586	-3.408383	-8.959829
H	-9.485234	-4.588514	-9.470478
H	-9.829694	-3.529784	-8.120065
N	-12.647666	-9.440103	3.241040
H	-12.898347	-9.972873	2.435603
C	-11.501621	-8.556151	2.963498
C	-10.512041	-8.480381	4.105006
O	-9.397927	-8.033106	3.908978
C	-11.930212	-7.101151	2.677307
O	-12.490136	-6.641577	3.880507
C	-12.926191	-6.971009	1.531694
H	-13.442415	-8.903620	3.525970
H	-10.947995	-8.936515	2.116694
H	-11.034277	-6.540372	2.439664
H	-12.532916	-5.691736	3.877981

H	-13.128211	-5.921188	1.347006
H	-12.547187	-7.404494	0.613942
H	-13.868502	-7.446589	1.776741
N	-10.896810	-8.903383	5.300230
H	-11.809741	-9.295757	5.353085
C	-10.101206	-8.807718	6.497020
H	-10.047376	-7.788763	6.851158
H	-10.588786	-9.394465	7.267177
C	-8.650595	-9.277564	6.416904
O	-7.823871	-8.663640	7.044143
N	-8.315248	-10.371080	5.707132
H	-9.017894	-10.878963	5.221841
C	-6.917801	-10.769106	5.606705
H	-6.876480	-11.765410	5.183885
H	-6.464933	-10.796766	6.585472
C	-6.061356	-9.841470	4.724496
O	-4.887190	-9.700855	4.950271
N	-6.741060	-9.268556	3.737273
C	-6.005690	-8.317886	2.913195
C	-5.987681	-6.944049	3.572170
O	-5.019466	-6.232993	3.444479
C	-6.331144	-8.310133	1.408023
C	-7.540760	-7.542144	0.923625
C	-7.541335	-6.149372	0.923395
C	-8.632682	-8.204595	0.380481
C	-8.619201	-5.440556	0.422036
C	-9.703166	-7.497413	-0.142519
C	-9.705833	-6.113611	-0.112789
H	-7.734119	-9.291786	3.715097
H	-4.978522	-8.634627	2.971353

H	-5.450405	-7.903028	0.924040
H	-6.393890	-9.345799	1.094746
H	-6.684969	-5.613442	1.292739
H	-8.633818	-9.280784	0.334884
H	-8.594671	-4.365222	0.418132
H	-10.521641	-8.025995	-0.597627
H	-10.528382	-5.565783	-0.533868
N	-7.027445	-6.607658	4.340758
C	-6.989933	-5.440679	5.182317
C	-5.951015	-5.605925	6.291840
O	-5.406780	-4.618758	6.737722
C	-8.405674	-5.178018	5.737984
C	-8.653892	-3.772714	6.242775
C	-8.610355	-2.689775	5.365788
C	-8.970415	-3.538527	7.573006
C	-8.852478	-1.402212	5.811715
C	-9.225034	-2.252004	8.024141
C	-9.159031	-1.180672	7.149193
H	-7.866336	-7.141076	4.296945
H	-6.652454	-4.586028	4.614222
H	-9.100321	-5.387394	4.931164
H	-8.615106	-5.893646	6.524150
H	-8.365527	-2.848542	4.328962
H	-9.009290	-4.360511	8.266398
H	-8.775936	-0.578427	5.123902
H	-9.451863	-2.087457	9.062924
H	-9.312184	-0.179073	7.508953
N	-5.665572	-6.835936	6.713391
H	-6.283055	-7.576812	6.477611
C	-4.629301	-7.109633	7.683142

H	-4.689737	-6.449326	8.535214
H	-4.765074	-8.127200	8.027754
C	-3.214993	-6.964580	7.124584
O	-2.362465	-6.438607	7.800172
N	-2.978486	-7.435541	5.895767
C	-1.702198	-7.208287	5.235206
C	-1.503304	-5.719783	4.933584
O	-0.434088	-5.201017	5.162215
C	-1.584272	-8.089231	3.972900
C	-0.421501	-7.656935	3.075148
C	-1.440956	-9.563224	4.368458
H	-3.687449	-7.949656	5.422200
H	-0.902276	-7.453219	5.920307
H	-2.504420	-7.968883	3.404427
H	-0.326909	-8.348182	2.244844
H	-0.554881	-6.668752	2.655582
H	0.519034	-7.662658	3.617241
H	-1.433675	-10.187913	3.480848
H	-0.502044	-9.723371	4.892898
H	-2.248959	-9.902830	5.004003
N	-2.546547	-5.047006	4.432279
C	-2.412220	-3.659895	4.030916
C	-2.312557	-2.744475	5.250489
O	-1.473099	-1.867330	5.280469
C	-3.567913	-3.210495	3.126760
C	-3.633715	-3.875210	1.739154
C	-2.448864	-3.528633	0.833428
O	-1.348443	-3.933164	1.205225
O	-2.695607	-2.865465	-0.198973
H	-3.370288	-5.543114	4.174300

H	-1.487647	-3.543575	3.493605
H	-4.508981	-3.382612	3.641977
H	-3.472734	-2.135938	3.004823
H	-3.666500	-4.950928	1.850853
H	-4.554946	-3.560770	1.260069
N	-3.170251	-2.925742	6.267478
C	-2.974287	-2.171410	7.485231
C	-1.646980	-2.536353	8.159257
O	-1.006610	-1.676658	8.725501
C	-4.115598	-2.192800	8.511501
O	-4.341385	-3.462658	9.047428
C	-5.389764	-1.545075	7.982436
H	-3.828186	-3.670672	6.237470
H	-2.840601	-1.136870	7.208056
H	-3.746104	-1.592162	9.335004
H	-4.800474	-3.990394	8.410614
H	-6.136481	-1.537002	8.767951
H	-5.201028	-0.519707	7.679601
H	-5.793443	-2.083929	7.135389
N	-1.206549	-3.796924	8.055904
H	-1.817723	-4.537873	7.796708
C	0.062188	-4.144138	8.643552
H	0.099596	-3.914717	9.699595
H	0.208001	-5.208421	8.507489
C	1.231615	-3.408852	7.999780
O	2.149485	-2.994528	8.673355
N	1.195881	-3.276215	6.665068
C	2.299613	-2.658816	5.971783
C	2.327646	-1.141441	6.129368
O	3.403889	-0.577093	6.129324

C	2.355580	-3.079035	4.492778
S	1.432122	-2.063482	3.302752
H	0.478485	-3.740366	6.146609
H	3.217282	-2.985866	6.441584
H	3.381601	-3.009826	4.157443
H	2.047747	-4.112708	4.413307
H	0.249061	-2.079107	3.898112
N	1.174584	-0.481707	6.279328
C	1.228527	0.949825	6.498120
C	1.800391	1.255515	7.870039
O	2.395847	2.285750	8.083778
C	-0.091113	1.707767	6.235951
C	-1.159109	1.503768	7.321489
C	-0.592220	1.425527	4.814999
C	-2.454798	2.276063	7.065919
H	0.305811	-0.967311	6.210681
H	1.956049	1.350919	5.807870
H	0.200749	2.751891	6.284079
H	-1.379458	0.452035	7.442640
H	-0.752017	1.833238	8.273063
H	-1.342760	2.148921	4.523085
H	0.220326	1.490467	4.097766
H	-1.029982	0.440460	4.725231
H	-3.102102	2.222166	7.936414
H	-2.260750	3.326698	6.863207
H	-3.006270	1.872691	6.223449
N	1.612303	0.307477	8.793116
H	1.005984	-0.457617	8.600248
C	2.051429	0.495691	10.155553
H	1.548493	-0.239040	10.772753

H	1.811237	1.485779	10.514377
C	3.555334	0.327731	10.310887
O	4.211958	1.094060	10.964528
N	4.099120	-0.725840	9.665137
H	3.514583	-1.380496	9.191176
C	5.528692	-0.865960	9.622083
H	5.768664	-1.818866	9.163905
H	5.960450	-0.840893	10.612006
C	6.223546	0.233873	8.822826
O	7.341890	0.577654	9.119791
N	5.549411	0.718265	7.780935
C	6.111205	1.873315	7.127100
C	5.522793	3.174903	7.663004
H	5.005725	3.105642	8.620349
O	5.652608	4.210582	7.085251
C	5.960156	1.802705	5.604558
C	6.694008	0.644067	4.960117
C	8.065147	0.455529	5.138927
C	6.008233	-0.250563	4.143552
C	8.731421	-0.581788	4.500667
C	6.672692	-1.285127	3.503641
C	8.038127	-1.451727	3.673651
H	4.647519	0.377507	7.529041
H	7.156838	1.902658	7.397750
H	4.907873	1.733522	5.357041
H	6.316005	2.745140	5.200827
H	8.613397	1.100674	5.804907
H	4.944291	-0.154215	4.034227
H	9.787813	-0.713210	4.664437
H	6.118562	-1.963078	2.878846

H	8.543439	-2.259629	3.175069
N	12.357062	9.899479	-1.293582
H	11.607207	10.196712	-1.887394
C	12.088942	8.559269	-0.764141
C	11.059086	8.711851	0.348237
O	10.074730	8.006776	0.384374
C	13.366957	7.907687	-0.218484
C	14.448915	7.629383	-1.266891
S	13.838112	6.541308	-2.586471
C	15.314815	6.425848	-3.623170
H	13.177333	9.902767	-1.864587
H	11.631813	7.899043	-1.490385
H	13.795251	8.542722	0.551806
H	13.085242	6.972969	0.253247
H	14.824240	8.551708	-1.697521
H	15.289382	7.156142	-0.770996
H	15.068447	5.765136	-4.440452
H	15.588667	7.396632	-4.016637
H	16.147002	6.006346	-3.072613
N	11.263823	9.682568	1.256036
C	10.354863	9.848184	2.373039
C	9.021522	10.492385	1.990254
O	8.040516	10.261618	2.651403
C	11.026786	10.610903	3.521095
C	12.223068	9.832010	4.036032
O	13.349817	10.142999	3.708052
N	11.953547	8.797517	4.839799
H	12.066207	10.264347	1.156185
H	10.076559	8.867743	2.726993
H	11.381799	11.581837	3.197735

H	10.297897	10.749469	4.309906
H	12.719213	8.229685	5.126712
H	11.044851	8.383851	4.869871
N	8.979602	11.276431	0.895672
H	9.814963	11.438031	0.383786
C	7.702859	11.687848	0.349739
H	7.871252	12.437565	-0.413280
H	7.078839	12.115166	1.118155
C	6.914954	10.532689	-0.270426
O	5.714316	10.596800	-0.317902
N	7.616172	9.492344	-0.766803
C	6.948911	8.288608	-1.232522
C	6.439666	7.437884	-0.059161
O	5.347318	6.927296	-0.128766
C	7.837817	7.501380	-2.224482
C	8.120747	8.359475	-3.472146
C	7.185017	6.168296	-2.608988
C	9.209022	7.801308	-4.391693
H	8.577622	9.411286	-0.537806
H	6.046566	8.593243	-1.741381
H	8.780919	7.287723	-1.727691
H	7.195699	8.476142	-4.033243
H	8.412367	9.358347	-3.163284
H	7.812053	5.632504	-3.310034
H	7.034004	5.527673	-1.748892
H	6.216500	6.320636	-3.074291
H	9.390821	8.483976	-5.215713
H	10.148388	7.668414	-3.861522
H	8.940410	6.843166	-4.820928
N	7.203398	7.330444	1.046884

C	6.716303	6.600319	2.206722
C	5.353578	7.146568	2.652028
O	4.425488	6.414257	2.892053
C	7.674095	6.709649	3.402766
C	9.104395	6.193990	3.226964
O	9.992370	6.862756	3.752067
O	9.292833	5.124963	2.596386
H	8.158666	7.611408	1.013922
H	6.541785	5.566946	1.948613
H	7.741694	7.736583	3.731974
H	7.235388	6.142974	4.221632
N	5.277230	8.484587	2.791054
H	6.090069	9.042301	2.645414
C	4.068208	9.117886	3.256706
H	4.278351	10.166900	3.426882
H	3.732133	8.691443	4.189078
C	2.907686	9.043868	2.273864
O	1.766416	9.169049	2.654824
N	3.243034	8.870134	0.993151
H	4.203026	8.855292	0.746156
C	2.290477	8.921686	-0.072058
H	2.826773	9.122092	-0.991279
H	1.591938	9.733605	0.078476
C	1.416146	7.678398	-0.300637
O	0.370924	7.783061	-0.880569
N	1.916743	6.544070	0.223913
C	1.128936	5.356414	0.454411
C	0.320164	5.469890	1.750471
O	-0.877636	5.311962	1.731128
C	2.017953	4.113775	0.461532

H	2.820270	6.597875	0.641250
H	0.393349	5.276716	-0.329298
H	1.430600	3.227883	0.675280
H	2.481063	3.998832	-0.511471
H	2.803071	4.192480	1.206870
N	0.964323	5.731963	2.904258
C	0.241257	5.544979	4.153640
C	-0.896347	6.549330	4.317259
O	-1.917255	6.224071	4.884868
C	1.166726	5.488477	5.393997
C	1.735929	6.845831	5.833538
C	2.272888	4.443656	5.181227
C	2.581023	6.769172	7.107110
H	1.954546	5.837634	2.917427
H	-0.266853	4.591985	4.099810
H	0.519604	5.137637	6.192821
H	2.331136	7.263379	5.027691
H	0.920372	7.541352	6.006076
H	2.651501	4.091706	6.130101
H	1.894626	3.582821	4.639752
H	3.106505	4.853063	4.620106
H	2.870810	7.766867	7.424666
H	2.019585	6.316766	7.919492
H	3.485835	6.189742	6.970471
N	-0.716685	7.787511	3.835132
H	0.152658	8.048162	3.421109
C	-1.720054	8.796192	4.046304
H	-1.342853	9.736264	3.662289
H	-1.935887	8.924681	5.097625
C	-3.065581	8.479544	3.399396

O	-4.073417	8.668598	4.041715
N	-3.093200	7.970199	2.153867
C	-4.428845	7.829750	1.574117
C	-5.119888	6.531579	1.954580
O	-6.331916	6.496599	1.963569
C	-4.228965	8.065691	0.071098
C	-3.000308	8.981249	0.060560
C	-2.115385	8.352627	1.124114
H	-5.072997	8.599181	1.972961
H	-4.025101	7.135806	-0.444113
H	-5.111277	8.508861	-0.373429
H	-2.497549	9.046621	-0.886543
H	-3.289238	9.985412	0.363674
H	-1.607693	7.479019	0.756282
H	-1.373518	9.032202	1.512033
N	-4.359732	5.481725	2.293074
C	-4.968660	4.290482	2.860305
C	-5.695395	4.615970	4.168757
O	-6.774949	4.123481	4.413715
C	-3.932482	3.184798	3.151335
C	-3.496027	2.295837	2.002336
C	-3.988137	0.999691	1.889907
C	-2.508084	2.680869	1.103534
C	-3.492204	0.107074	0.953795
C	-1.989938	1.797109	0.176041
C	-2.445702	0.485742	0.116018
O	-1.849363	-0.353492	-0.732860
H	-3.368518	5.592084	2.319685
H	-5.729044	3.921346	2.187998
H	-3.065831	3.649815	3.611252

H	-4.368754	2.545903	3.911372
H	-4.762663	0.664525	2.561021
H	-2.103055	3.670692	1.145898
H	-3.880490	-0.889505	0.883567
H	-1.204707	2.103109	-0.492680
H	-2.176898	-1.255360	-0.634712
N	-5.068854	5.423468	5.041382
H	-4.141332	5.742582	4.856208
C	-5.686618	5.770323	6.300796
H	-4.918552	6.163048	6.956485
H	-6.129316	4.902435	6.763777
C	-6.788528	6.820077	6.167600
O	-7.836106	6.718951	6.765161
N	-6.514331	7.852000	5.364461
H	-5.623702	7.926344	4.922486
C	-7.462506	8.954972	5.142173
H	-7.002497	9.628543	4.429907
H	-7.649073	9.497015	6.058385
C	-8.819936	8.541166	4.615540
O	-9.813855	9.115377	4.986428
N	-8.852379	7.540652	3.717576
C	-10.112923	7.117423	3.163297
C	-10.956051	6.267129	4.105949
O	-12.050357	5.897268	3.714210
C	-9.913370	6.383780	1.818754
O	-11.149346	6.316142	1.133997
C	-9.298352	4.999363	1.970431
H	-7.999608	7.135850	3.391528
H	-10.719956	7.994171	2.974885
H	-9.258635	7.001762	1.216652

H	-11.830240	6.204142	1.788127
H	-9.128021	4.561865	0.993415
H	-8.347178	5.036425	2.479380
H	-9.961743	4.344429	2.521080
N	-10.474378	5.976392	5.310489
C	-11.318450	5.358173	6.316616
C	-12.342330	6.320807	6.925022
O	-13.306537	5.870352	7.487333
C	-10.482005	4.742649	7.446114
C	-9.459980	3.686226	7.004058
C	-8.698714	3.171522	8.229059
C	-10.096671	2.529348	6.233115
H	-9.563170	6.281028	5.577938
H	-11.915105	4.596306	5.840341
H	-9.956035	5.538145	7.964604
H	-11.183572	4.307975	8.151692
H	-8.738158	4.156288	6.347875
H	-7.930307	2.460054	7.939807
H	-8.214492	3.987102	8.756684
H	-9.367011	2.675056	8.930446
H	-9.338052	1.807621	5.949355
H	-10.848628	2.019476	6.832613
H	-10.572528	2.860979	5.317619
N	-12.070920	7.640112	6.858893
C	-13.023350	8.608950	7.310968
C	-13.928471	9.134993	6.219267
H	-14.684838	9.848831	6.571524
O	-13.853372	8.842805	5.072412
H	-11.329212	7.966051	6.279992
H	-13.640194	8.171312	8.085705

H	-12.510341	9.462456	7.748699
N	-11.803319	10.245201	-2.923053
H	-11.555021	10.454220	-1.978245
C	-12.081744	8.817744	-3.090505
C	-11.659906	8.509079	-4.520736
O	-10.586906	8.014797	-4.768819
C	-13.502304	8.355143	-2.702014
C	-13.767855	8.659113	-1.216178
C	-13.696579	6.866364	-3.016239
C	-15.188580	8.343963	-0.745757
H	-12.599529	10.806940	-3.153309
H	-11.371313	8.276768	-2.479770
H	-14.225833	8.930594	-3.285990
H	-13.053850	8.105173	-0.609878
H	-13.579361	9.712197	-1.030206
H	-14.722396	6.562690	-2.851981
H	-13.456228	6.627238	-4.047920
H	-13.064529	6.255522	-2.379467
H	-15.324903	8.678460	0.276578
H	-15.929526	8.848974	-1.360356
H	-15.402746	7.281845	-0.768103
N	-12.483337	8.899582	-5.524731
H	-13.418222	9.146350	-5.296968
C	-12.227292	8.456234	-6.878662
H	-12.256120	7.377532	-6.961182
H	-12.995244	8.869968	-7.521675
C	-10.868344	8.883357	-7.439409
O	-10.242872	8.163305	-8.162683
N	-10.469649	10.144592	-7.114873
H	-11.026873	10.654117	-6.469800

C	-9.215260	10.723366	-7.569981
H	-9.108942	10.597982	-8.636948
H	-9.221439	11.779500	-7.332374
C	-7.977128	10.080286	-6.928057
O	-7.055078	9.673747	-7.578108
N	-7.952448	10.083289	-5.560306
H	-8.784216	10.322256	-5.071871
C	-6.773002	9.726201	-4.778822
H	-5.891433	10.166685	-5.217771
H	-6.899798	10.121366	-3.777930
C	-6.499696	8.237642	-4.664834
O	-5.353052	7.857152	-4.702496
N	-7.520102	7.383617	-4.468411
C	-7.193719	6.020597	-4.070931
C	-6.607821	5.203961	-5.215411
O	-5.793724	4.344706	-4.977393
C	-8.330608	5.263700	-3.343414
C	-9.503545	4.859533	-4.253385
C	-8.760118	6.052051	-2.101336
C	-10.585309	4.039525	-3.548048
H	-8.464859	7.707284	-4.462119
H	-6.371742	6.080033	-3.372434
H	-7.856604	4.348836	-2.997457
H	-9.952508	5.739093	-4.699410
H	-9.114570	4.259714	-5.071975
H	-9.409067	5.458198	-1.472546
H	-7.898088	6.329086	-1.502572
H	-9.295376	6.957053	-2.366296
H	-11.337793	3.721796	-4.263100
H	-10.175665	3.144314	-3.095498

H	-11.090765	4.609942	-2.777743
N	-7.018956	5.442207	-6.479222
C	-6.375230	4.738827	-7.568791
C	-4.984277	5.280357	-7.895096
O	-4.139657	4.532989	-8.327171
C	-7.270416	4.676722	-8.814215
C	-8.352936	3.596343	-8.697094
C	-7.763189	2.191292	-8.845627
N	-8.724080	1.117248	-8.613085
C	-9.051315	0.591755	-7.434458
N	-8.560123	1.049910	-6.301582
N	-9.911964	-0.415168	-7.387958
H	-7.674880	6.169605	-6.658059
H	-6.161660	3.742131	-7.220149
H	-7.732397	5.644394	-8.985578
H	-6.645587	4.472954	-9.678338
H	-8.869705	3.689209	-7.746735
H	-9.100904	3.742865	-9.469663
H	-7.394494	2.054531	-9.853825
H	-6.908313	2.038464	-8.199403
H	-9.078991	0.649826	-9.414654
H	-7.907183	1.796195	-6.284347
H	-8.972179	0.764234	-5.419823
H	-10.240826	-0.810670	-8.238036
H	-9.855844	-1.045558	-6.600293
N	-4.773232	6.580669	-7.681188
H	-5.511241	7.160217	-7.356719
C	-3.479244	7.213377	-7.976907
H	-3.148364	6.956564	-8.971586
H	-3.613098	8.285337	-7.910482

C	-2.396876	6.780364	-7.001585
O	-1.260917	6.604381	-7.364954
N	-2.810535	6.641800	-5.737302
C	-1.911758	6.357890	-4.645441
C	-1.587278	4.880549	-4.526083
O	-0.443484	4.536072	-4.336778
C	-2.507278	6.930903	-3.353422
C	-1.895038	6.244968	-2.133528
C	-2.313976	8.453548	-3.384154
H	-3.744900	6.899987	-5.510563
H	-0.957172	6.827155	-4.838964
H	-3.571250	6.720637	-3.363244
H	-2.125525	6.776768	-1.229151
H	-2.272396	5.232875	-2.030859
H	-0.820723	6.209180	-2.208350
H	-3.059981	8.957718	-2.785981
H	-1.329149	8.722952	-3.016457
H	-2.419273	8.837067	-4.392592
N	-2.587924	3.993530	-4.636211
C	-2.233138	2.594004	-4.706746
C	-1.337556	2.351590	-5.914538
O	-0.434867	1.551922	-5.868306
C	-3.450208	1.654090	-4.690641
C	-4.290911	1.760634	-3.410594
C	-5.398685	0.697148	-3.305987
N	-4.926102	-0.476639	-2.609323
C	-5.666337	-1.493477	-2.480364
N	-6.957043	-1.636130	-3.006573
N	-5.305663	-2.545214	-1.692861
H	-3.525271	4.286172	-4.803538

H	-1.612208	2.349389	-3.856661
H	-4.075892	1.855003	-5.559699
H	-3.073719	0.642243	-4.794689
H	-3.651130	1.652647	-2.542979
H	-4.743259	2.743582	-3.366194
H	-6.246342	1.139946	-2.779740
H	-5.758231	0.470252	-4.316799
H	-7.125956	-1.111620	-3.835887
H	-7.254382	-2.585590	-3.115539
H	-4.379607	-2.552533	-1.309577
H	-5.710337	-3.432777	-1.886834
N	-1.558189	3.105534	-7.012690
H	-2.397025	3.627955	-7.124192
C	-0.696793	2.918943	-8.161218
H	-1.068304	3.543008	-8.964881
H	-0.677086	1.889770	-8.491552
C	0.747189	3.315896	-7.863486
O	1.689898	2.717834	-8.319990
N	0.871729	4.380384	-7.056137
H	0.059674	4.894286	-6.807924
C	2.135358	4.897749	-6.637158
H	2.761409	5.174181	-7.476623
H	1.955303	5.787526	-6.047131
C	2.972650	3.968185	-5.782665
O	4.175886	4.127039	-5.712864
N	2.343282	3.004398	-5.101701
C	3.082909	2.200275	-4.161229
C	4.293212	1.491719	-4.766737
O	5.275628	1.300658	-4.077229
C	2.144710	1.184385	-3.498270

C	2.824884	0.382876	-2.393708
C	1.879878	-0.603570	-1.732623
N	2.611518	-1.353011	-0.732828
C	2.094158	-2.437907	-0.069997
N	0.766031	-2.554933	-0.097491
O	2.852250	-3.226536	0.472494
H	1.350306	2.921762	-5.148931
H	3.517737	2.837630	-3.399778
H	1.308128	1.740634	-3.086792
H	1.729974	0.527065	-4.255623
H	3.671877	-0.163099	-2.795768
H	3.222933	1.055759	-1.637632
H	1.058703	-0.069951	-1.267061
H	1.446201	-1.260658	-2.484840
H	3.588309	-1.456850	-0.883422
H	0.189227	-1.819627	-0.432040
H	0.284064	-3.216017	0.483347
N	4.253844	1.030071	-6.025822
H	3.466315	1.226168	-6.606404
C	5.351309	0.223258	-6.522314
H	5.129754	-0.056814	-7.545123
H	5.461963	-0.681811	-5.944437
C	6.705026	0.900869	-6.509706
O	7.727769	0.261864	-6.419081
N	6.697146	2.230905	-6.631135
H	5.831462	2.727313	-6.585484
C	7.918740	2.998098	-6.582245
H	8.629585	2.629347	-7.309062
H	7.688987	4.024319	-6.838349
C	8.672153	3.022380	-5.249869

O	9.804905	3.460380	-5.209453
N	8.044646	2.521019	-4.181151
C	8.630117	2.368503	-2.860015
C	9.918372	1.536097	-2.871021
O	10.737055	1.641839	-1.971384
C	7.544155	1.663412	-2.015304
C	7.728359	1.549798	-0.503042
C	7.315745	2.802351	0.278853
C	7.196209	2.532985	1.774340
N	8.528656	2.547721	2.447902
O	10.961441	1.858936	0.863104
H	10.813017	2.064500	-0.056144
H	11.450561	1.044050	0.824787
H	7.102208	2.203794	-4.289780
H	8.903340	3.331647	-2.446992
H	6.610547	2.172672	-2.210748
H	7.414946	0.670244	-2.430555
H	7.081011	0.740390	-0.180292
H	8.736087	1.243538	-0.254023
H	7.992663	3.636475	0.110961
H	6.337646	3.125224	-0.063817
H	6.600120	3.284433	2.269946
H	6.745277	1.570408	1.963264
H	9.253932	2.097692	1.902043
H	8.822837	3.526477	2.599058
H	8.475148	2.071358	3.335197
N	10.052776	0.685290	-3.879050
C	11.124839	-0.270655	-4.116735
C	12.483579	0.328506	-4.482879
O	13.463853	-0.372010	-4.365049

C	10.734981	-1.185970	-5.299525
C	9.620503	-2.210654	-5.043630
C	9.198672	-2.840509	-6.374658
C	10.072201	-3.293028	-4.063743
H	9.309109	0.659564	-4.544358
H	11.303920	-0.855778	-3.225656
H	10.450050	-0.544946	-6.129229
H	11.630774	-1.717040	-5.600421
H	8.752900	-1.699643	-4.637167
H	8.415320	-3.575774	-6.218644
H	8.820263	-2.089050	-7.056071
H	10.036642	-3.347816	-6.847538
H	9.296025	-4.036312	-3.919957
H	10.950276	-3.803244	-4.447042
H	10.321211	-2.891240	-3.086368
N	12.534695	1.570690	-4.972734
C	13.756147	2.185168	-5.452963
C	14.898598	2.408413	-4.443794
O	15.939404	2.822324	-4.881903
C	13.402134	3.500041	-6.150830
O	12.806333	4.409277	-5.271881
H	11.699158	2.114820	-4.973814
H	14.208600	1.527940	-6.187400
H	14.315082	3.936966	-6.527076
H	12.752572	3.282950	-6.993898
H	11.862275	4.360574	-5.309807
N	14.748508	2.092146	-3.138682
C	15.893161	2.050653	-2.250858
C	16.801777	0.838735	-2.484974
O	17.937397	0.856235	-2.084437

C	15.475829	1.966498	-0.777396
C	14.573729	3.085121	-0.261597
C	14.213816	2.804857	1.197686
N	13.156301	3.657748	1.724047
C	13.293983	4.818355	2.342015
N	14.495975	5.340167	2.565072
O	14.870543	7.819484	4.103502
H	14.553875	8.695778	3.887774
H	15.590698	7.929147	4.703776
N	12.222161	5.468921	2.741322
H	13.870526	1.759596	-2.818606
H	16.502268	2.924731	-2.427484
H	14.974516	1.017600	-0.617883
H	16.395437	1.935887	-0.202419
H	15.057633	4.053208	-0.361309
H	13.657060	3.140262	-0.837484
H	13.846134	1.791968	1.279957
H	15.086267	2.862480	1.839783
H	12.227744	3.323750	1.564312
H	15.313839	4.872904	2.259548
H	14.604139	6.199890	3.070917
H	11.278627	5.148035	2.595864
H	12.282795	6.319877	3.250195
N	16.223616	-0.238416	-3.041419
C	16.931013	-1.481233	-3.233577
C	17.739114	-1.444028	-4.526610
H	18.060199	-0.446438	-4.840326
O	18.027721	-2.414057	-5.148701
C	15.962807	-2.669110	-3.214066
C	15.426494	-3.008018	-1.856578

N	14.495168	-2.248224	-1.178604
O	12.592125	-0.068118	-0.532443
H	13.205196	-0.679567	-0.932809
H	12.059910	0.301046	-1.223705
C	15.739323	-4.091624	-1.111593
C	14.274117	-2.872577	-0.068106
N	15.001824	-3.991424	0.041482
H	15.299838	-0.172983	-3.409508
H	17.657207	-1.577252	-2.432792
H	15.139155	-2.466239	-3.890761
H	16.491342	-3.528771	-3.604260
H	16.406300	-4.905966	-1.297824
H	13.590197	-2.550369	0.691500
H	14.911300	-4.674518	0.760216
O	-14.263520	-2.279454	5.036254
H	-14.661796	-1.757324	4.347938
H	-13.925328	-1.662476	5.670572
O	-12.705352	-0.285101	6.665424
H	-11.840735	-0.641906	6.811742
H	-12.996088	0.076252	7.488570
O	-12.882577	1.207988	4.065773
H	-12.801768	0.926833	4.967629
H	-13.437193	0.561187	3.627719
O	-12.791843	-2.334923	1.314238
H	-12.061805	-1.770307	1.069737
H	-12.507682	-2.900907	2.022523
O	-7.031903	1.655996	0.279357
H	-7.231878	1.642531	1.212548
H	-6.125816	1.396592	0.196984
O	-7.829237	1.683990	3.051748

H	-8.768624	1.743037	2.920923
H	-7.562676	2.461487	3.528575
O	-8.717730	0.008436	-1.252479
H	-8.166693	0.610558	-0.749631
H	-8.132409	-0.646518	-1.622549
O	-13.069448	-2.747541	-1.520904
H	-13.250723	-2.687834	-0.590830
H	-12.212512	-3.143257	-1.593245
O	-13.028741	1.284014	-0.893261
H	-12.437088	0.660145	-0.482262
H	-12.662909	2.136839	-0.686430
O	-13.791133	3.644190	2.810443
H	-13.560248	4.442493	3.269336
H	-13.553427	2.923543	3.385485
O	-15.289890	1.547186	1.053870
H	-15.101177	2.364711	1.492816
H	-14.674900	1.472088	0.332642
O	-12.596678	-0.496353	-3.164347
H	-12.917570	0.291831	-2.741701
H	-12.776503	-1.196593	-2.536956
O	-12.283320	-2.581802	-5.057630
H	-12.581425	-1.770628	-4.655023
H	-13.047893	-3.101007	-5.252479
O	-10.616172	-3.451517	-2.867206
H	-9.929234	-2.811838	-2.992993
H	-11.255400	-3.271743	-3.550003
O	-10.985858	-0.391705	0.416285
H	-10.238419	-0.411343	-0.177086
H	-10.755351	0.212503	1.117153
O	-10.662813	1.652359	2.347127

H	-11.343623	1.510024	3.000148
H	-10.986283	2.327191	1.758999
O	-12.064326	3.543173	0.577354
H	-12.727825	3.627324	1.260141
H	-11.668434	4.400600	0.486943
O	-9.864109	0.509767	-3.824055
H	-10.735226	0.149809	-3.698077
H	-9.446130	0.475274	-2.968160
O	-14.559623	-0.593415	2.740235
H	-15.027353	0.034846	2.192865
H	-14.068455	-1.163529	2.154433
O	-12.254859	-3.757407	3.830499
H	-12.977498	-3.311268	4.281571
H	-11.462978	-3.491924	4.272535
O	-9.400406	-2.417981	-5.450020
H	-10.257943	-2.819795	-5.430550
H	-8.776261	-3.075039	-5.752754

SUPPORTINGINF_06_07_19.docx (272.06 KiB)

[view on ChemRxiv](#) • [download file](#)