An ONIOM and MD Investigation of Possible Monofunctional Activity of Human 8-Oxoguanine–DNA Glycosylase (hOgg1)

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Table S1. List of ONIOM(M06-2X/6-31G(d):PM6) model contents, layer divisions and charges.

Residue	PM6–Freeze	PM6–Move	DFT	Truncations	Charge DFT/PM6
DC21	O3′			Remaining backbone and nucleobase	0/0
DA22	Sugar, phosphate, N9	O3′		Nucleobase truncated to N9.	0/−1
FDG23		P, OP1, OP2	**Sugar, nucleobase**		0/−1
DG24	C1′, C2′, C3′, C4′,O4′, O3′, N9	C5′	**P, OP1, OP2, O5′**	Nucleobase truncated to N9.	−1/−1
DT25	P, OP1, OP2, O5′			Sugar and nucleobase removed.	0/−1
L37	BB, Cβ			R-Group truncated to Cβ	0/0
V38	All				0/0
L39	BB, Cβ			R-Group truncated to Cβ	0/0
P40	All				0/0
S41	All				0/0
G42	N		**Cα, C, O**		0/0
Q43	C, O, R-Group		**N, Cα**		0/0
S44	All				0/0
F45	All				0/0
V130	All				0/0
R131	BB, Cβ			R-Group truncated to Cβ	0/0
L133	All				0/0
R134	BB, Cβ			R-Group truncated to Cβ	0/0
Q135	All				0/0
C140	All				0/0
L141	BB, Cβ			R-Group truncated to Cβ	0/0
F142	BB, Cβ			R-Group truncated to Cβ	0/0
S143	All				0/0
F144	BB	R-Group			0/0
I145	All				0/0
C146	All				0/0
S147	BB		**R-Group**		0/0
S148	All				0/0
C149	All				0/0
N150	All				0/0
N151	All				0/0
I152	All				0/0
A153	All				0/0
R154	BB, Cβ			R-Group truncated to Cβ	0/0
I155	All				0/0
T156	All				0/0
G157	All				0/0

Residue	PM6–Freeze	PM6–Move	DFT	Truncations	Charge DFT/PM6
M158	BB, Cβ			R-Group truncated to Cβ	0/0
V159	All				0/0
T248	All				0/0
K249	BB		**R-Group**		1/1
V250	All				0/0
A251	All				0/0
D252	All				0/−1
C253	BB		**R-Group**		−1/−1
I254	All				0/0
C255	BB, Cβ			R-Group truncated to Cβ	0/0
L256	All				0/0
M257	BB	R-Group			0/0
A264	All				0/0
V265	All				0/0
P266	All				0/0
V267	All				0/0
D268	BB		**R-Group**		−1/−1
V269	All				0/0
H270	BB		**R-Group**		1/1
M271	All				0/0
W272	BB, Cβ			R-Group truncated to Cβ	0/0
H273	BB, Cβ			R-Group truncated to Cβ	0/0
I274	All				0/0
A311	All				0/0
G312	All				0/0
W313	All				0/0
A314	All				0/0
Q315	BB		**R-Group**		0/0
A316	All				0/0
V317	All				0/0
L318	All				0/0
F319	BB		**R-Group**		0/0
S320	All				0/0
A321	All				0/0
D322	All				0/−1
L323	All				0/0
R324	All				0/1
Q325	BB, Cβ			R-Group truncated to Cβ	0/0
Calcium		CA1(C)			0/2
Waters	4(A), 326(A), 328(A), 336(A), 352(A), 364(A), 369(A), 374(A), 389(A)	2 added water molecules to solvate Ca^{2+}	**109(C), 55(C), 1(A)**		0/0

Notes: BB – backbone atoms (N, C, O, Cα).

Table S2. Summary of reaction coordinates and increments used to refine ONIOM(M06-2X/6-31G(d):PM6) transition states.[a]

Mechanism	TS	Coordinates	Increments[b]
All	TS1	Nε–H	0.025, 0.010
K249–Nuc	TS2	C253 Cα–Cβ–S–H	10.0, 5.0, 2.5
K249–Nuc	TS3	C1′–N9, C1′–Nε	0.200, 0.100, 0.050
K249–GB	TS3	C1′–N9, C1′–O$_{Wat}$	0.400, 0.200, 0.050
D268–GB	TS3	C1′–N9, C1′–O$_{Wat}$	0.400, 0.200, 0.050

[a] See Figure 4 for the definitions of the mechanisms and stationary points. [b] Step-sizes used to generated and refine reaction potential energy surface (PES) based on distances (Å) or dihedral angles (degrees).

Table S3. Averages and standard deviations for important dihedral angles (degrees) in the hOgg1 active site from the 3KTU crystal structure and MD simulations [a]

	3KTU	H270^{neu}K249^{+}C253^{-}	H270^{+}K249^{+}C253^{-}	H270^{+}K249^{neu}C253^{neu}
K249 (CγCδCεNζ)	−52.5	−163.9±11.3 (55%) [a]	−165.4±11.8 (23%)	−173.3±11.9 (16%)
		−73.8±12.4 (13%)	−69.9±10.3 (66%)	−60.5±13.2 (33%)
		68.8±8.8 (32%)	68.6±10.0 (10%)	64.7±10.7 (51%)
C253 (CCαCβSγ)	158.2	176.2±9.0	175.9±11.2	168.4±14.0
D268 (CαCβCγOδ)	−51.5	−63.6±12.4	−58.9±9.0	−53.9±9.8
H270 (CαCβCγNδ)	−66.5	71.5±26.3	−72.7±19.6	−78.8±16.0 (20%)
				93.8±11.2 (80%)

[a] The percentage of the simulation that a specific conformation is adopted is shown in brackets. If no number is shown, the noted conformation is adopted over the course of the entire simulation.

Table S4. Hydrogen–bonding occupancies (greater than 10%) in the active site of the hOGG1–DNA complex from MD simulations with various K249, C253 and H270 protonation states.[a]

	H270^{neu}K249$^+$C253$^-$	H270$^+$K249$^+$C253$^-$	H270$^+$K249^{neu}C253^{neu}
$O_{G42}\cdots N1_{OG}$	NB[b]	98.7	99.6
$O_{K249}\cdots H\text{-}N_{C253}$	27.4	80.4	98.0
$O_{K249}\cdots H\text{-}S\gamma_{C253}$	NB	NB	68.9
$S\gamma_{C253}\cdots H1\text{-}N\zeta_{K249}$	22.6	22.7	NB
$S\gamma_{C253}\cdots H2\text{-}N\zeta_{K249}$	25.5	19.1	NB
$S\gamma_{C253}\cdots H3\text{-}N\zeta_{K249}$	51.3	57.0	NB
$O\delta1_{D268}\cdots H\text{-}N_{M271}$	94.8	99.5	99.6
$O\delta1_{D268}\cdots H\text{-}N_{H270}$	NB	NB	18.6
$O\delta2_{D268}\cdots H\text{-}N_{H270}$	95.3	99.1	96.2
$O\delta1_{D268}\cdots N3_{OG}$	95.5	95.9	91.7
$O_{Q315}\cdots H\text{-}N_{F319}$	99.8	99.7	99.7
$O\varepsilon1_{Q315}\cdots H\text{-}N2_{OG}$	100.0	99.3	99.3
$O\varepsilon1_{Q315}\cdots H\text{-}N3_{OG}$	59.6	89.4	91.9
$O\delta2_{D322}\cdots H\text{-}N\varepsilon_{H270}$	95.9	NB	NB
$OP1_{OG}\cdots H\text{-}N\varepsilon_{H270}$	NB	25.6	NB
$OP2_{OG}\cdots H\text{-}N\varepsilon_{H270}$	NB	86.0	17.0
$N4_{OG}\cdots H\text{-}N\zeta_{K249}$	NB	NB	37.8
$O6_{OG}\cdots H\text{-}OG_{S139}$	47.5	26.3	31.9

[a]Data provided for hydrogen bonds within 3.4 Å heavy atom separation and 120° X–H–H angle.
[b]Not observed.

Table S5. Averages and standard deviations for important distances (Å) in the hOgg1 active site from the 3KTU crystal structure and MD simulations.

	3KTU	H270^{neu}K249$^+$C253$^-$	H270$^+$K249$^+$C253$^-$	H270$^+$K249^{neu}C253^{neu}
H270(Nε)-OG(OP2)	3.193	8.565±0.528	2.962±0.470	4.082±0.638
K249(Nζ)-OG(C1')	4.004	4.022±0.211	4.579±0.422	4.061±0.271
D268(Oδ1)-M271(NH)	3.335	3.005±0.188	2.956±0.136	2.960±0.141
D268(Oδ1)-H270(NH)	3.778	3.682±0.257	3.474±0.203	3.471±0.203
D268(Oδ1)-OG(N2)	2.785	2.965±0.233	2.967±0.195	3.042±0.240

Table S6. Hydrogen-bonding occupancies for water molecules in the active site of the hOGG1–DNA complex from MD simulations with different K249 and C253 protontation states, which are occupied for > 20% of the simulation.[a]

	$H270^+K249^+C253^-$	$H270^+K249^{neu}C253^{neu}$
$S\gamma_{C253}$	51.9	NB^b
	46.85	
$O\delta2_{D268}$	80.78	42.9
$H\varepsilon21_{Q315}$	21.6	69.64
	31.7	
$O5'_{OG}$	NB	20.18
$O3'_{OG}$	28.3	99.2
	22.0	
	37.2	
$O4'_{OG}$	NB	25.81
$OP1_{dG}$	36.6	35.5
		34.1
		23.3
$OP2_{dG}$	22.2	21.8
		20.6
$<20\%^c$	24	22

[a] Hydrogen bonds with multiple water molecules are listed as separate lines. Data is provided for hydrogen bonds within 3.4 Å heavy atom separation and 120° X–H–H angle. [b]Not observed. [c]Number of water–active site residue hydrogen bonds occupied for less than 20% of the simulation.

Table S7. Summary of the alternate geometries (°) obtained from an ONIOM(M06-2X/6-31G(d):PM6) conformational search of the hOgg1 active site.

Residue Altered	Count[a]	ΔE[b]	F144 αβ[c]	F144 βγ[d]	K249 αβ[c]	K249 βγ[d]	K249 γδ[e]	K249 δε[f]	C253 αβ[c]	D268 αβ[c]	D268 βγ[d]	H270 αβ[c]	H270 βγ[d]	Q315 αβ[c]	Q315 βγ[d]	Q315 γδ[e]	F319 αβ[c]	F319 βγ[d]
Any	53	0.0	151.1	89.4	55.4	−168.8	165.3	−62.7	173.1	−44.2	128.5	150.0	−80.7	44.6	−83.3	156.9	59.2	88.3
		Std. Dev.[g]	0.01	0.05	0.04	0.02	0.04	0.01	0.01	0.01	0.03	0.02	0.01	0.01	0.03	0.04	0.02	0.02
K249	1	−20.5	150.5	90.2	64.4	−87.6	−170.3	−48.2	177.1	−43.5	126.5	151.5	−81.3	42.5	−84.4	157.2	56.5	85.5
K249	1	−9.7	151.6	91.6	57.7	−76.1	−164.9	−176.4	149.9	−44.7	128.9	149.7	−80.5	44.5	−83.2	156.5	59.7	88.8
Q315	8	−6.0	151.2	91.7	58.0	−167.7	163.4	−62.8	173.5	−44.8	130.8	149.1	−81.5	74.3	−122.4	66.9	57.0	83.6
K249	1	−5.2	150.5	90.0	99.2	−75.1	−55.6	−45.8	176.9	−44.6	128.0	151.0	−80.3	44.3	−84.1	158.3	60.1	89.3
C253	4	0.0	151.1	89.3	55.3	−168.8	165.3	−62.7	−137.2	−44.2	128.5	150.1	−80.7	44.6	−83.3	157.0	59.2	88.3
Q315	2	0.8	149.2	89.6	59.7	−166.5	163.2	−63.5	172.9	−44.4	133.0	150.2	−80.0	−37.0	75.2	47.3	60.0	95.1
K249	1	0.9	150.4	92.2	98.9	−76.9	−55.3	−153.6	176.9	−45.8	128.9	151.2	−80.4	43.7	−82.4	154.5	59.3	88.0
Q315	24	1.6	150.0	88.7	56.2	−169.7	163.9	−64.3	175.1	−45.8	129.3	151.9	−79.7	−23.4	89.4	172.6	61.0	88.8
Q315	13	4.8	149.3	88.7	55.1	−170.7	162.8	−65.4	174.6	−44.8	130.9	151.8	−79.9	54.4	−107.6	−98.7	60.4	97.1
K249	2	5.8	149.6	91.6	71.7	−139.4	55.8	154.4	176.2	−44.9	127.3	152.0	−80.6	43.6	−85.1	159.5	59.8	89.1
Q315	2	6.2	151.2	92.3	58.9	−167.6	162.6	−62.9	173.5	−44.8	131.9	148.7	−81.9	−21.2	94.3	−103.6	55.2	82.0
Q315	4	7.7	149.3	89.7	56.4	−168.8	163.7	−63.8	173.8	−43.8	132.7	149.9	−79.5	39.1	−100.5	−54.8	60.5	91.6
K249	1	8.1	151.1	91.6	45.9	−178.4	176.7	53.4	177.3	−44.7	130.1	149.9	−81.7	43.2	−82.3	153.7	55.2	84.4
K249	1	8.5	151.2	91.5	98.6	−68.9	−75.1	69.2	175.6	−44.6	128.8	150.1	−80.5	44.8	−82.7	156.1	59.8	88.7
K249	2	9.1	150.1	91.1	79.5	−153.4	87.5	90.0	178.0	−43.7	127.4	152.1	−81.0	43.8	−83.9	157.4	59.8	88.6
H270	4	9.5	150.6	87.4	53.2	−170.2	167.2	−64.4	173.4	−44.3	131.5	166.6	106.2	43.7	−86.7	162.6	62.5	90.9
Q315	6	10.4	150.1	86.3	51.5	−171.1	166.7	−64.4	174.2	−45.0	126.9	151.0	−80.0	59.8	−82.9	−9.8	61.1	87.2
K249	1	11.3	148.9	91.6	40.2	−116.3	153.7	58.2	173.4	−45.9	128.5	152.4	−80.5	43.4	−84.3	158.0	59.7	88.9
D268	1	12.2	151.6	91.4	57.9	−166.8	164.5	−62.6	172.3	−29.0	103.3	149.6	−81.8	48.6	−82.4	157.7	58.2	86.6
Q315	35	13.4	149.9	89.8	56.7	−168.5	164.2	−63.3	173.4	−44.4	130.9	149.7	−80.1	154.7	76.2	5.4	60.1	89.5
K249	1	14.5	150.8	89.8	97.2	−103.3	−68.8	−170.4	176.9	−44.4	126.7	151.3	−81.1	44.1	−81.1	158.1	57.8	87.2
Q315	3	14.7	151.5	84.8	50.3	−171.8	169.0	−64.3	174.2	−46.1	120.8	149.7	−81.0	50.1	−179.6	−0.6	61.8	91.6
K249	3	18.8	150.6	93.0	107.9	−123.2	59.7	179.2	176.2	−46.6	132.6	150.9	−81.9	43.8	−81.3	152.4	56.8	85.3
K249	1	26.3	150.7	91.6	−6.8	158.9	−102.2	63.2	177.1	−44.3	128.6	150.5	−80.3	45.0	−83.4	157.6	60.4	89.5
C253	1	26.5	151.0	92.0	54.4	−168.0	167.1	−64.9	24.3	−44.5	128.9	149.9	−80.7	44.2	−83.4	157.0	58.4	87.1
Q315	1	29.2	150.0	88.8	55.0	−168.7	166.2	−63.2	172.9	−44.3	129.0	149.7	−79.5	−11.1	75.0	36.1	62.7	92.3
C253	1	30.0	151.2	90.2	54.6	−167.6	167.4	−64.5	−36.3	−44.4	128.8	149.9	−80.7	44.6	−83.2	157.0	59.2	88.3
Q315	9	31.2	149.8	89.8	56.8	−168.5	164.1	−63.3	173.3	−44.4	131.1	149.7	−80.0	−158.5	−41.5	108.8	60.2	89.5
Q315	2	31.5	150.0	89.1	55.5	−169.1	165.6	−63.5	173.5	−44.2	130.2	150.0	−79.5	0.6	89.1	45.4	62.0	88.7
Q315	1	35.3	149.9	89.5	58.2	−168.2	163.0	−63.7	173.5	−45.2	130.9	150.9	−79.7	−19.0	103.5	90.5	57.7	90.8
Q315	18	36.7	149.9	89.9	56.9	−168.2	164.5	−63.1	173.2	−44.4	130.9	149.4	−80.0	−171.6	−54.2	9.7	60.1	89.4
Q315	5	49.1	149.9	89.9	56.8	−168.3	164.4	−63.2	173.2	−44.4	131.0	149.5	−80.0	153.8	51.7	−78.9	60.1	89.4
Q315	10	62.7	149.9	89.7	57.0	−168.3	164.4	−63.3	173.2	−44.4	131.1	149.9	−79.8	−170.4	−62.8	−92.0	60.2	89.9

[a] Number of structures that relax to the this geometry. [b] Energy (kJ mol^{-1}) relative to the geometry closest to the 3KTU crystal structure. [c] Dihedral angle about the Cα–Cβ bond. [d] Dihedral angle about the Cβ–Cγ bond. [e] Dihedral angle about the Cγ–Cδ bond. [f] Dihedral angle about the Cδ–Cε bond. [g] Standard deviation in measured angles for the structures closest to the 3KTU crystal structure.

Table S8. Relaxation of geometries from the ONIOM conformational search of the hOgg1 active site.

Residue	Structures[a]	Residue	Structures[a]
F144	5 / 1	H270	11 / 2
K249	26 / 14	Q315	170 / 17
C253	7 / 3	F319	8 / 1
D268	9 / 2		

[a] Number of structures within 100 kJ mol^{-1} of the minimum after PM6 single-point energy calculation/ Number of unique structures after relaxation with ONIOM.
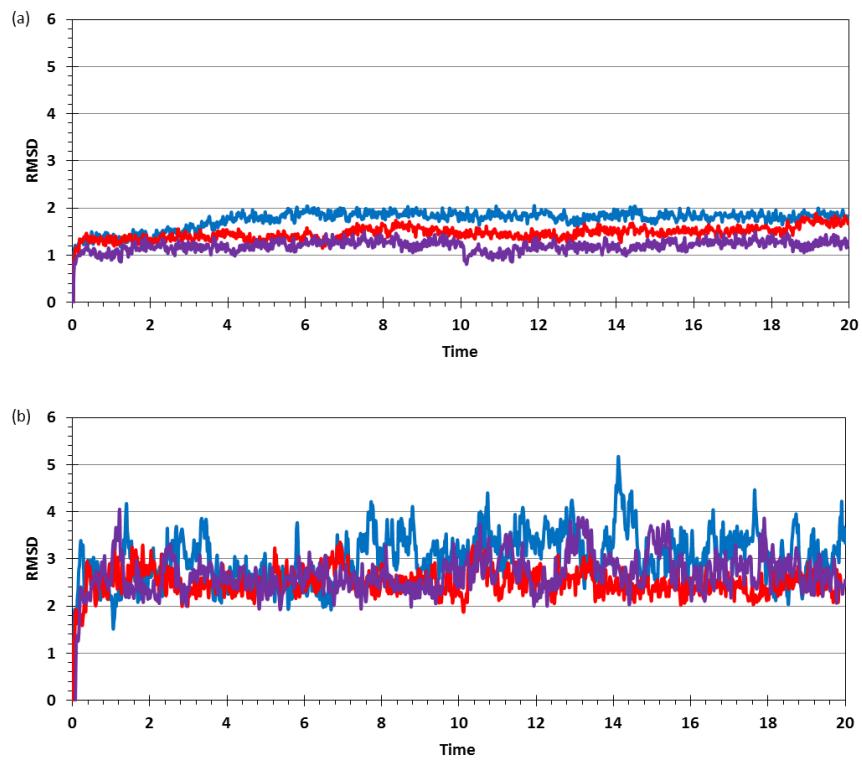
Figure S1. RMSD (Å) of the (a) protein and (b) DNA according to MD simulations on the hOgg1–DNA complex with neutral H270 and K249$^+$–C253$^-$ (purple), cationic H270 and K249$^+$–C253$^-$ (red), and cationic H270 and K249–C253 (blue).
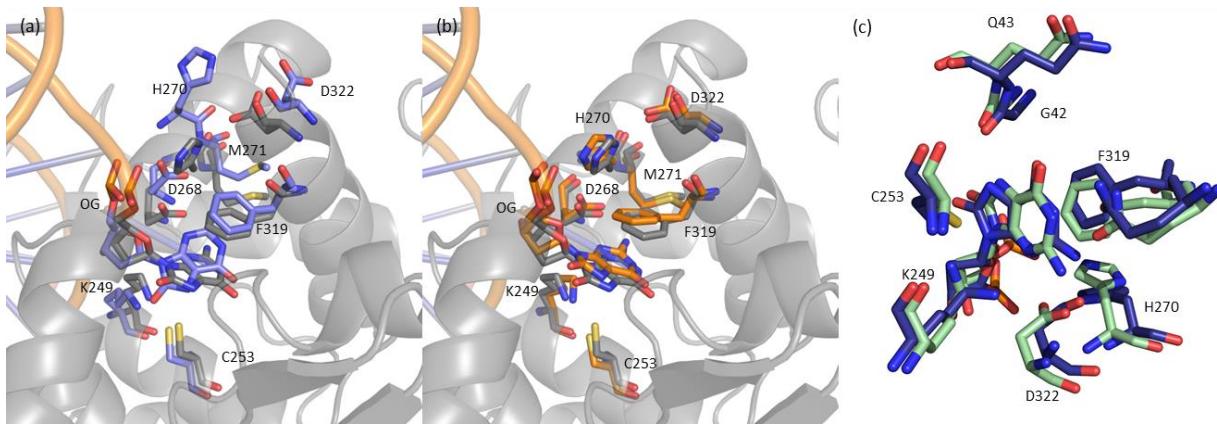
Figure S2. RMSD overlay of (a) the 3KTU crystal structure (grey carbons) and representative structure from the MD simulation with neutral H270 (purple carbons), and (b) the 3KTU crystal structure (grey carbons) and representative structure from the MD simulation with cationic H270 (orange carbons). (c) The optimized ONIOM high-level region (green carbons) and representative structure from the MD simulation with cationic H270 (blue carbons). The charge separated K249$^+$–C253$^-$ was included in both simulations.
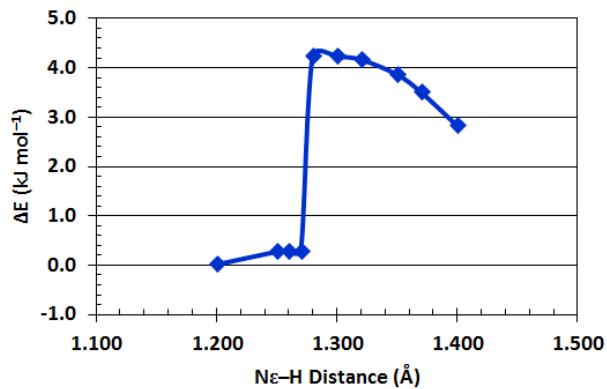
Figure S3. ONIOM(M06-2X/6-31G(d):PM6) reaction potential energy surface for proton transfer from K249 to C253.
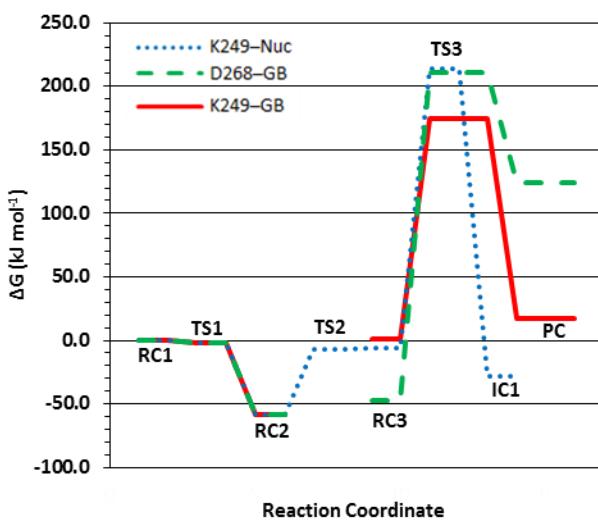
Figure S4. ONIOM(M06-2X/6-311+G(2df,2p):PM6) reaction free energies (ΔG, kJ mol^{-1}) for the three hOgg1 monofunctional mechanisms investigated in the present work. See Figure 4 for the definitions of the mechanisms and stationary points, and Table 1 for the relative free energies.

Full citation for reference 60.
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ONIOM(M06-2X/6-311+G(2df,2p):PM6)//ONIOM(M06-2X/6-31G(d):PM6) energetics and coordinates. (DFT region only, truncation points capped with a hydrogen atom).

Lys Activation: RC1–All   E = −3875.584519 a.u.

```
O          -0.97626300    -6.05723900    -2.30171300
C          -2.10903000    -5.58898800    -1.58949700
C          -1.65570800    -5.34766200    -0.16474900
O          -0.92153400    -4.12698700    -0.10926900
C          -2.79180800    -5.23629400     0.87245300
O          -2.41693500    -6.14540000     1.92775900
C          -2.71874800    -3.79182100     1.33949300
C          -1.24323800    -3.44831500     1.08925400
N          -0.95024300    -2.03864400     0.90257100
C          -1.55567900    -1.23231100    -0.10747200
N          -0.66840900    -0.21986600    -0.35394000
C           0.47350000    -0.37517200     0.43270000
C           1.73196700     0.29062200     0.40987700
O           2.07477300     1.26585600    -0.25447200
N           2.62837000    -0.33830900     1.29347300
C           2.38034800    -1.49174000     1.98512300
N           3.40320900    -1.98857800     2.72884300
N           1.21395800    -2.10747500     1.98137800
C           0.31946600    -1.52133900     1.17091800
O          -2.66687000    -1.38991400    -0.58758700
P          -3.47523500    -6.81683000     2.93338500
O          -2.85506900    -8.17307500     3.34846200
O          -4.84738600    -6.91799600     2.32485800
O          -3.37467900    -5.74293600     4.12257700
C          -1.15179000     1.28469400    -4.32300900
C          -1.03338200     2.37788000    -3.22793000
O          -1.34760600     2.11367200    -2.07566000
N          -0.64681400     3.61390900    -3.62325300
C          -0.76610200     4.77655200    -2.76441800
C          -6.42959700    -1.69237900     0.97647600
O          -6.01894300    -1.60125400     2.31960400
C          -2.05522600    -2.60947800     8.19507500
C          -1.37408900    -2.51213100     6.81603900
C          -2.11060400    -1.62761100     5.80526100
C          -1.64312800    -1.85475900     4.37565100
N          -2.36755100    -0.92695700     3.46562500
C          -2.01731400     2.91079300     4.80925400
S          -0.95636500     1.64062700     4.00894500
C           0.94658800    -5.42506600     4.27565600
C           1.97205800    -5.28782900     3.08459700
O           3.11197400    -4.83443200     3.35295400
O           1.56299400    -5.66484900     1.95592800
C           4.32950100    -6.48979600     0.48253700
C           3.71149500    -6.83934100    -0.84455800
N           4.43090000    -7.24452500    -1.96274500
C           2.39987600    -6.82273200    -1.22062900
C           3.59031800    -7.47427500    -2.96714900
N           2.35212500    -7.22415200    -2.54075400
C           8.21791300     1.42281700     3.55650000
C           7.55799400     0.02299000     3.58209200
C           6.05639800    -0.03579100     3.33615500
O           5.57664700     0.21072700     2.22681300
N           5.30594400    -0.38230400     4.39389800
C           6.33508900    -1.20750200    -0.76247400
C           4.90048600    -1.69112100    -0.94759900
C           4.42201200    -2.81114000    -0.25937400
C           4.02254500    -1.00124800    -1.78899500
```

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C        3.10293900   -3.24341600   -0.40999300
C        2.71497400   -1.44850300   -1.96994700
C        2.24905600   -2.56786800   -1.28277900
O        3.01287700    2.17865800   -2.79101100
O       -4.85114700   -9.14371000    1.11524700
O       -0.01456200   -7.83231700    2.18579500
H       -2.93336900   -6.32717700   -1.57806000
H       -2.49266300   -4.64275100   -2.00203700
H       -1.01691200   -6.18296100    0.14345000
H       -3.78350500   -5.51904100    0.49470700
H       -3.32971100   -3.16146000    0.68556100
H       -3.04688500   -3.68007200    2.37463200
H       -0.59086500   -3.79092800    1.89973600
H       -0.89602300    0.58202000   -0.94249700
H        3.56705300    0.06444900    1.35380600
H        3.27867600   -2.96771500    3.01840500
H        4.32760800   -1.75693900    2.37498000
H       -2.23590700    1.15449000   -4.52956800
H       -0.77452800    0.34137600   -3.87235100
H       -0.45801000    3.77320500   -4.61295100
H       -0.67785800    4.43348000   -1.71526500
H       -5.60699400   -2.19029400    0.44194300
H       -6.55500400   -0.68731400    0.52382200
H       -6.72382600   -1.20217500    2.86703300
H       -1.58489900   -3.44396300    8.75399100
H       -3.11383800   -2.89288600    8.04717500
H       -1.31285100   -3.53173400    6.41783600
H       -0.33834700   -2.16608300    6.92631700
H       -3.19047800   -1.83360700    5.86638900
H       -1.96016500   -0.56094800    6.03712400
H       -1.80894400   -2.88902800    4.06183900
H       -0.57915900   -1.61894500    4.26745900
H       -2.12353400   -1.11633700    2.48742100
H       -3.38454300   -1.01056800    3.55479100
H       -2.77374000    2.45386400    5.48288000
H       -2.58167300    3.47565600    4.04441200
H       -1.98205500    0.17356900    3.70146200
H        0.04006500   -5.94297900    3.94118700
H        0.65214900   -4.38070800    4.52420400
H        3.66309700   -5.80193300    1.01574600
H        5.27410800   -5.95528600    0.24716200
H        5.47847800   -7.32274300   -2.04280300
H        1.52071100   -6.54021700   -0.67494100
H        3.87373900   -7.81410400   -3.95458200
H        1.47733300   -7.29818500   -3.09716000
H        8.62284400    1.65123100    4.55461300
H        7.46667200    2.20476900    3.32978600
H        7.96549500   -0.60669300    2.77583700
H        7.79302300   -0.48730300    4.52326300
H        5.71432700   -0.72858200    5.25291200
H        4.33248100   -0.66280000    4.24980500
H        6.63396500   -1.33705900    0.29569100
H        6.39109000   -0.12287100   -0.95528400
H        5.08758600   -3.34586900    0.41969700
H        4.34663600   -0.09735900   -2.29849500
H        2.71114900   -4.06493700    0.18737500
H        2.04575300   -0.88893300   -2.62426400
H        1.22124500   -2.90760800   -1.39502500
H        2.41183700    1.61815700   -3.31758900
H        2.81259500    1.91370100   -1.87260200
H       -4.93571600   -9.19226100    0.13196000
H       -4.96440800   -8.16592900    1.36727200
H        0.35964000   -6.94514200    1.96874000
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H	-0.95909900	-7.68404100	2.33614000
H	-0.03124790	5.51084550	-3.02074300
H	-1.73535828	5.20554747	-2.91072301
H	-0.63271366	1.52211734	-5.22804486
H	-1.38501646	3.57214130	5.36397758
H	-7.32751717	-2.25249068	0.81863342
H	9.00023939	1.43340718	2.82660051
H	7.02578394	-1.73018305	-1.39068178
H	4.54352288	-7.35895381	1.06876165
H	1.36742228	-5.88566574	5.14493524
H	-3.54975945	-6.15570403	4.97144059
H	-1.20037326	-6.49730855	-3.12494649
H	-1.99158020	-1.72726524	8.79719613

Lys Activation: TS1–All E = -3875.582959 a.u. (348.65i cm^{-1})

O	-0.97444800	-6.06002700	-2.29995900
C	-2.10655100	-5.58977700	-1.58742600
C	-1.65243900	-5.34897400	-0.16296300
O	-0.91410200	-4.13114600	-0.10852200
C	-2.78807000	-5.23311200	0.87421100
O	-2.41454600	-6.14227000	1.93024200
C	-2.71205800	-3.78788100	1.33865500
C	-1.23627600	-3.44761800	1.08784400
N	-0.93988500	-2.04025100	0.89510500
C	-1.54695300	-1.23233000	-0.11054700
N	-0.66199100	-0.21577300	-0.35221000
C	0.47948400	-0.37119600	0.43471500
C	1.73749600	0.29459900	0.41302600
O	2.07995400	1.27240800	-0.24846300
N	2.63466200	-0.33619500	1.29469200
C	2.38725100	-1.49206100	1.98263400
N	3.41031100	-1.99017300	2.72604600
N	1.22196700	-2.10894700	1.97658000
C	0.32632900	-1.52126000	1.16830600
O	-2.65653300	-1.39037300	-0.59439000
P	-3.47340600	-6.81544600	2.93356700
O	-2.85311700	-8.17216200	3.34786700
O	-4.84510800	-6.91759700	2.32372200
O	-3.37479100	-5.74324600	4.12384300
C	-1.15229100	1.28405900	-4.32300900
C	-1.03447300	2.37781600	-3.22854000
O	-1.34923500	2.11431600	-2.07630000
N	-0.64733100	3.61369800	-3.62399400
C	-0.76679500	4.77593400	-2.76487100
C	-6.43002700	-1.69280500	0.97712400
O	-6.02140800	-1.60073000	2.31996500
C	-2.05489400	-2.60894900	8.19284900
C	-1.37168600	-2.50931800	6.81463700
C	-2.10429600	-1.62049200	5.80551700
C	-1.63212200	-1.82661200	4.37397400
N	-2.35447500	-0.88777800	3.48115900
C	-2.01688000	2.90896800	4.81065200
S	-0.94260900	1.65526100	4.00003600
C	0.94770200	-5.42527500	4.27522900
C	1.97418100	-5.28941700	3.08484400
O	3.11378300	-4.83499100	3.35338900

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O          1.56680900   -5.66928600    1.95652400
C          4.33000000   -6.48961900    0.48283200
C          3.70838200   -6.83863200   -0.84264800
N          4.42504400   -7.24551200   -1.96196700
C          2.39609200   -6.81979800   -1.21626700
C          3.58210800   -7.47434400   -2.96471500
N          2.34525000   -7.22182800   -2.53613700
C          8.21836900    1.42388600    3.55738800
C          7.55890900    0.02411700    3.58531100
C          6.05770700   -0.03460000    3.33779500
O          5.57931500    0.21397900    2.22839200
N          5.30609700   -0.38288500    4.39422100
C          6.33486800   -1.20722300   -0.76257400
C          4.90013400   -1.68978300   -0.94917700
C          4.42128500   -2.81144000   -0.26393600
C          4.02247400   -0.99735100   -1.78876800
C          3.10191600   -3.24246700   -0.41522700
C          2.71455700   -1.44335600   -1.97044000
C          2.24808700   -2.56409400   -1.28587700
O          3.01042600    2.18262000   -2.78967300
O         -4.85028300   -9.14187300    1.11594600
O         -0.01477800   -7.83379200    2.18642700
H         -2.93196100   -6.32671900   -1.57599700
H         -2.48850100   -4.64292100   -2.00016200
H         -1.01654700   -6.18639400    0.14560600
H         -3.78033600   -5.51471000    0.49714800
H         -3.32176600   -3.15791400    0.68327800
H         -3.03882400   -3.67055000    2.37347900
H         -0.58532400   -3.78838600    1.90003000
H         -0.89055000    0.58588100   -0.94031500
H          3.57320700    0.06668800    1.35585500
H          3.28453300   -2.96979700    3.01376100
H          4.33450200   -1.75981800    2.37077200
H         -2.23629200    1.15320700   -4.52966200
H         -0.77460600    0.34115900   -3.87185800
H         -0.45834300    3.77300400   -4.61365400
H         -0.67849400    4.43205300   -1.71605800
H         -5.60679700   -2.19105400    0.44382100
H         -6.55563100   -0.68829300    0.52289300
H         -6.72686800   -1.20223900    2.86681900
H         -1.58626900   -3.44448800    8.75159300
H         -3.11363600   -2.89089600    8.04283000
H         -1.31237600   -3.52767700    6.41318100
H         -0.33496700   -2.16658800    6.92763900
H         -3.18390500   -1.82987100    5.85893700
H         -1.96137100   -0.55542900    6.04927800
H         -1.78813800   -2.86111300    4.05293000
H         -0.56662700   -1.58963900    4.27699100
H         -2.12296100   -1.07233700    2.50097500
H         -3.36959000   -0.97356100    3.57750200
H         -2.76224900    2.43581100    5.48445500
H         -2.59001000    3.46986000    4.05029000
H         -1.91396800    0.28686600    3.73525500
H          0.04110300   -5.94281500    3.94052300
H          0.65338400   -4.38074200    4.52312600
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H	3.66608000	−5.80039200	1.01740400
H	5.27522700	−5.95714100	0.24496300
H	5.47195600	−7.32525800	−2.04328500
H	1.51857100	−6.53533500	−0.66889300
H	3.86288100	−7.81504900	−3.95261500
H	1.46912400	−7.29482000	−3.09107600
H	8.62397300	1.65367600	4.55493300
H	7.46661600	2.20525200	3.33028600
H	7.96704400	−0.60701900	2.78049900
H	7.79313900	−0.48457500	4.52753500
H	5.71431100	−0.73070600	5.25272100
H	4.33403400	−0.66709200	4.24745700
H	6.63300900	−1.33785000	0.29569700
H	6.39180900	−0.12245500	−0.95445100
H	5.08675700	−3.34846900	0.41341300
H	4.34704000	−0.09245700	−2.29618000
H	2.70995700	−4.06531200	0.18018800
H	2.04546700	−0.88177200	−2.62317700
H	1.21992100	−2.90279100	−1.39812800
H	2.40901200	1.62256300	−3.31629900
H	2.81205600	1.91582400	−1.87128300
H	−4.93420400	−9.18918200	0.13250600
H	−4.96266500	−8.16380500	1.36902500
H	0.36091700	−6.94706800	1.97008300
H	−0.95904000	−7.68402800	2.33722700
H	−0.03200082	5.51042163	−3.02081129
H	−1.73609095	5.20497019	−2.91079325
H	−1.38513156	3.57145740	5.36463910
H	−7.32765235	−2.25328621	0.81891668
H	−3.54989593	−6.15679203	4.97232278
H	−1.19960292	−6.49860452	−3.12370351
H	1.36788414	−5.88587433	5.14482387
H	−1.99162797	−1.72770376	8.79642521
H	4.54391303	−7.35889391	1.06892273
H	9.00014135	1.43401606	2.82688860
H	7.02563903	−1.72994895	−1.39066075
H	−0.63316772	1.52164471	−5.22797533

Lys Activation:　　　　　RC2–All　　　E = -3875.593005 a.u.

O	−0.97050000	−6.04752700	−2.33144100
C	−2.10135900	−5.58870100	−1.60738200
C	−1.64938000	−5.39272000	−0.17582800
O	−0.88042900	−4.19587700	−0.09154600
C	−2.78941800	−5.26964700	0.85233000
O	−2.42544000	−6.17435100	1.91658600
C	−2.71610300	−3.82333200	1.30905400
C	−1.23526200	−3.48598900	1.08257600
N	−0.93053000	−2.08550600	0.86168300
C	−1.54722800	−1.27362200	−0.12709800
N	−0.67102100	−0.24482300	−0.36105100
C	0.46949700	−0.39519500	0.42712700
C	1.72104400	0.27862900	0.40979600
O	2.05732000	1.26721200	−0.24217100
N	2.62297000	−0.35004100	1.28904700

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C	2.38282500	-1.51415500	1.96618200
N	3.40967800	-2.00650200	2.71272700
N	1.22541200	-2.14193000	1.95162200
C	0.32163300	-1.55561600	1.15054300
O	-2.65459300	-1.43306200	-0.61691200
P	-3.49198400	-6.83221700	2.92143900
O	-2.87677700	-8.18647800	3.35259100
O	-4.85968700	-6.93949800	2.30165500
O	-3.40429700	-5.74886900	4.10100600
N	-0.42683400	1.62065600	-5.57159000
C	-1.14487600	1.29099300	-4.32227700
C	-1.02674300	2.38357700	-3.22646000
O	-1.34159900	2.12019200	-2.07454900
N	-0.63811300	3.62005300	-3.62144600
C	-0.75719900	4.78100800	-2.76172500
C	-6.42664700	-1.69154500	0.98541300
O	-6.02129000	-1.63544800	2.32939200
C	-2.05912500	-2.61962100	8.19726600
C	-1.46933700	-2.50431400	6.77764500
C	-2.35006600	-1.75595700	5.77378700
C	-1.91144900	-1.94235000	4.32548400
N	-2.76439300	-1.13878100	3.44020000
C	-2.05405900	2.93872500	4.83215700
S	-1.02804000	1.58283200	4.14095500
C	0.94581600	-5.42963600	4.26782500
C	1.97667100	-5.30587400	3.08006400
O	3.11488100	-4.84581400	3.34807800
O	1.57823100	-5.70378300	1.95486500
C	4.32880700	-6.49022300	0.48125100
C	3.68883700	-6.83259600	-0.83671800
N	4.39126500	-7.24950800	-1.96128200
C	2.37360400	-6.79864200	-1.19884500
C	3.53677100	-7.46990800	-2.95663200
N	2.30718500	-7.20192000	-2.51790100
C	8.22062900	1.41634500	3.56485500
C	7.55293200	0.02067900	3.59190000
C	6.05245800	-0.02988400	3.33490400
O	5.58079200	0.24056700	2.22824800
N	5.29404100	-0.39650600	4.38096100
C	6.33638200	-1.21090300	-0.76005000
C	4.90206100	-1.69213700	-0.95233100
C	4.42341700	-2.81993900	-0.27727100
C	4.02537600	-0.99431400	-1.78845500
C	3.10478800	-3.25084500	-0.43428000
C	2.71835100	-1.44056200	-1.97630000
C	2.25176000	-2.56712600	-1.30144600
O	3.00877400	2.18870100	-2.77349900
O	-4.86199300	-9.16629900	1.10694900
O	-0.02948200	-7.84880900	2.18062600
H	-2.93384600	-6.31808500	-1.61906200
H	-2.47229900	-4.62739500	-1.99550400
H	-1.03545000	-6.25194100	0.11696100
H	-3.77908300	-5.55322800	0.46959500
H	-3.31582500	-3.19718900	0.64090900
H	-3.05496400	-3.69452800	2.33741400

H	-0.60396600	-3.80574100	1.91738000
H	-0.90318400	0.55523600	-0.94864300
H	3.55854500	0.05908100	1.35264200
H	3.28303800	-2.98684600	2.99924000
H	4.33121500	-1.78692000	2.34346700
H	-2.22882200	1.16114400	-4.52958800
H	-0.76785500	0.34747800	-3.87197000
H	-0.44965900	3.77988900	-4.61107300
H	-0.67007800	4.43445700	-1.71375200
H	-5.60507400	-2.18090100	0.44128100
H	-6.54814700	-0.67626200	0.55476600
H	-6.70813700	-1.21208300	2.88013300
H	-1.52455700	-3.42970900	8.73436300
H	-3.11252200	-2.94607500	8.11563500
H	-1.31350600	-3.52620300	6.41218600
H	-0.47369500	-2.04238600	6.81504000
H	-3.39027600	-2.10224600	5.87746900
H	-2.35037200	-0.67585500	5.98595600
H	-1.91313900	-3.01478300	4.07994100
H	-0.87862200	-1.58590200	4.20651700
H	-2.47245700	-1.26434100	2.47188600
H	-3.73323100	-1.45876000	3.48265200
H	-2.83791200	2.52765700	5.49982100
H	-2.56174400	3.48463700	4.01934900
H	-2.02136200	0.67690800	3.86640200
H	0.03767600	-5.94456500	3.93307700
H	0.65436400	-4.38342900	4.51122000
H	3.67908800	-5.79407300	1.02411200
H	5.27819500	-5.96956600	0.23211500
H	5.43490800	-7.33918000	-2.04843500
H	1.50533800	-6.50025000	-0.64353500
H	3.80380300	-7.81528500	-3.94679200
H	1.42506600	-7.26717400	-3.06602300
H	8.62728100	1.64273400	4.56280000
H	7.47234500	2.20149300	3.33876800
H	7.96206800	-0.61465300	2.79075200
H	7.77907200	-0.48815100	4.53589600
H	5.69794800	-0.76023300	5.23512100
H	4.32682000	-0.68926300	4.21887400
H	6.63199900	-1.34509200	0.29853400
H	6.39519200	-0.12565700	-0.94871700
H	5.08835900	-3.36245300	0.39620500
H	4.35018100	-0.08529700	-2.28831300
H	2.71283200	-4.07827100	0.15445500
H	2.04971300	-0.87453900	-2.62567900
H	1.22412900	-2.90634500	-1.41733100
H	2.41101900	1.63238600	-3.30826700
H	2.80555000	1.91153100	-1.85878100
H	-4.95135100	-9.22124100	0.12466400
H	-4.97250100	-8.18547800	1.35456500
H	0.35448500	-6.96567500	1.96408900
H	-0.97266100	-7.68907300	2.32743100
H	-0.02166002	5.51550921	-3.01547761
H	-1.72588504	5.21165518	-2.90695022
H	-7.32591020	-2.24623659	0.81646641

H	9.00274037	1.42521356	2.83470217
H	7.02777390	-1.73323675	-1.38777980
H	4.53987315	-7.36149906	1.06539919
H	1.36278404	-5.89024854	5.13895860
H	-1.39240634	3.58089186	5.37505430
H	-1.99594185	-1.73485982	8.79568521
H	-3.56407762	-6.15515615	4.95599191
H	-1.19927438	-6.49317400	-3.15037997

Deglycosylation K249–Nuc: TS2–K$_{Nuc}$ E = −3875.586961 a.u.   (408.60i cm^{-1})

O	-0.97421800	-6.02709400	-2.36237800
C	-2.10577300	-5.57716100	-1.63262200
C	-1.66141000	-5.42440000	-0.19336100
O	-0.87656200	-4.24042000	-0.07262200
C	-2.80742600	-5.31199000	0.82633800
O	-2.44785400	-6.21953000	1.89090600
C	-2.74503300	-3.86942400	1.29133300
C	-1.26348300	-3.52184300	1.08724300
N	-0.96588200	-2.12056100	0.85797900
C	-1.58144500	-1.32215700	-0.14166500
N	-0.71035200	-0.28817700	-0.37879200
C	0.42810800	-0.42745500	0.41364900
C	1.67338000	0.25608200	0.39731300
O	2.00189400	1.24732300	-0.25587500
N	2.57834600	-0.36216400	1.28123200
C	2.34338900	-1.52445400	1.96398400
N	3.37405300	-2.00493500	2.71558800
N	1.18993300	-2.15853400	1.95199300
C	0.28235300	-1.58351600	1.14572000
O	-2.68037600	-1.49610200	-0.64419000
P	-3.51897200	-6.85708100	2.90458000
O	-2.90844200	-8.20748600	3.35333800
O	-4.88507700	-6.96681200	2.28142700
O	-3.43382000	-5.75883200	4.07125900
C	-1.13615900	1.30339800	-4.32155600
C	-1.01509800	2.39191400	-3.22166300
O	-1.32664200	2.12477800	-2.06996700
N	-0.62736300	3.62996000	-3.61490000
C	-0.74545200	4.78996000	-2.75427000
C	-6.42508900	-1.68835100	0.98545900
O	-6.01622500	-1.67828500	2.32734700
C	-2.04500500	-2.65184900	8.22045400
C	-1.51972100	-2.53664300	6.77704000
C	-2.55808100	-2.02466100	5.78074100
C	-2.09386500	-2.05230600	4.32811900
N	-3.06623700	-1.35226900	3.49253000
C	-2.05942000	2.97584000	4.80920400
S	-1.20977200	1.46048200	4.23044200
C	0.93900200	-5.43689500	4.25617900
C	1.97387500	-5.31686200	3.07144900
O	3.10828600	-4.84797100	3.34069800
O	1.58365300	-5.72814100	1.94845000
C	4.32437600	-6.49312400	0.47229800
C	3.67640600	-6.82907700	-0.84320600

N	4.37258100	-7.25065800	-1.96987000
C	2.36041200	-6.78459400	-1.20161300
C	3.51356800	-7.46404900	-2.96305500
N	2.28750600	-7.18679900	-2.52079600
C	8.21977300	1.39979900	3.57120200
C	7.54396800	0.00729800	3.58558000
C	6.04246000	-0.03564100	3.32898200
O	5.56956300	0.24541500	2.22587800
N	5.28386600	-0.40852400	4.37344200
C	6.33824500	-1.21590400	-0.75678200
C	4.90376100	-1.69820800	-0.94635400
C	4.42495700	-2.82304600	-0.26640300
C	4.02699300	-1.00436800	-1.78583600
C	3.10699900	-3.25625600	-0.42409900
C	2.72061800	-1.45258400	-1.97359800
C	2.25463600	-2.57779200	-1.29590000
O	3.02139100	2.17624600	-2.75881100
O	-4.87756300	-9.19407700	1.08685000
O	-0.04381500	-7.85940500	2.16723900
H	-2.94584500	-6.29741700	-1.66879300
H	-2.46383200	-4.60234700	-1.99801700
H	-1.05917900	-6.29797200	0.08046600
H	-3.79266200	-5.59945600	0.43480300
H	-3.34205900	-3.24168400	0.62244400
H	-3.09269300	-3.74917400	2.31653100
H	-0.64439500	-3.82749400	1.93579400
H	-0.94046900	0.50577100	-0.97507100
H	3.51239400	0.05057400	1.34084700
H	3.25319900	-2.98535900	3.00463200
H	4.29285700	-1.78955200	2.33648900
H	-2.22043900	1.17736700	-4.52963900
H	-0.76174300	0.35729900	-3.87456800
H	-0.44123800	3.79118200	-4.60470300
H	-0.65992900	4.44141600	-1.70691800
H	-5.60805600	-2.16414000	0.42220600
H	-6.54461000	-0.66013700	0.58644700
H	-6.67099000	-1.21836700	2.88693900
H	-1.45358200	-3.42289800	8.75611100
H	-3.08375500	-3.02868200	8.19123200
H	-1.18884600	-3.53228700	6.46016100
H	-0.62538700	-1.89887500	6.74438900
H	-3.47803700	-2.62133600	5.87482900
H	-2.84957600	-0.99054800	6.02062900
H	-1.90108900	-3.09739300	4.03549600
H	-1.13108600	-1.52651200	4.24064300
H	-2.71353700	-1.26355700	2.54148200
H	-3.93844700	-1.87592800	3.42266300
H	-2.95094700	2.69595300	5.40139500
H	-2.42698400	3.51085100	3.91774800
H	-1.85620600	0.58620000	5.02335500
H	0.03074800	-5.95033900	3.91926400
H	0.65002000	-4.38989200	4.49841400
H	3.68180800	-5.79414300	1.01954700
H	5.27635500	-5.97862500	0.21949700
H	5.41470500	-7.34630600	-2.05899900

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H	1.49629500	−6.47810700	−0.64385700
H	3.77468700	−7.81087300	−3.95431500
H	1.40321400	−7.24667300	−3.06676100
H	8.62456600	1.61641400	4.57203700
H	7.47648000	2.19072200	3.34859200
H	7.95028900	−0.62377400	2.77957500
H	7.76798100	−0.51031900	4.52525300
H	5.68793700	−0.78280100	5.22301200
H	4.31637100	−0.69896500	4.20871600
H	6.63547500	−1.35032100	0.30128500
H	6.39573200	−0.13055400	−0.94517600
H	5.08937100	−3.36221200	0.41028500
H	4.35183500	−0.09723900	−2.28915300
H	2.71493200	−4.08187700	0.16695800
H	2.05210000	−0.88951400	−2.62560900
H	1.22809500	−2.91980100	−1.41326100
H	2.42005700	1.62932100	−3.29923200
H	2.80920100	1.89567900	−1.84723200
H	−4.97460700	−9.25757700	0.10616400
H	−4.99053500	−8.21260500	1.32903600
H	0.34734500	−6.97990100	1.94903200
H	−0.98772700	−7.69275800	2.30016600
H	−1.71331926	5.22247109	−2.89941521
H	−1.38940683	3.58994511	5.37387848
H	−0.00880885	5.52409986	−3.00585602
H	−0.61554949	1.54339357	−5.22503144
H	−7.32641300	−2.23699232	0.80795481
H	−3.58036607	−6.15676032	4.93252395
H	−1.20319663	−6.47936245	−3.17762155
H	1.35368117	−5.89907713	5.12757379
H	4.53246161	−7.36638892	1.05454258
H	9.00422573	1.41014926	2.84358481
H	7.02942443	−1.73725735	−1.38555993
H	−1.99623779	−1.75309206	8.79903651

Deglycosylation K249–Nuc: RC3–K$_{Nuc}$ E = −3875.582132 a.u.

O	−0.96698400	−5.97852600	−2.52917700
C	−2.08952800	−5.53686800	−1.77738700
C	−1.65427000	−5.51323000	−0.32770400
O	−0.72284900	−4.44472500	−0.14470700
C	−2.80439700	−5.27309200	0.65444600
O	−2.46276200	−5.99824200	1.86651800
C	−2.73005500	−3.77850700	0.88746400
C	−1.22078300	−3.52872200	0.82410400
N	−0.83241600	−2.18175400	0.46580100
C	−1.39608500	−1.37753700	−0.54730200
N	−0.56090900	−0.29065000	−0.65914200
C	0.49731400	−0.40363800	0.24052400
C	1.72872900	0.29680600	0.31809600
O	2.08056900	1.31652400	−0.28006200
N	2.59446800	−0.33344400	1.23062700
C	2.34168000	−1.52057700	1.86183600
N	3.34634100	−2.00371700	2.65443700
N	1.20816600	−2.17691200	1.75963600

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C          0.33921000    -1.59869700     0.90940800
O         -2.42373200    -1.58215600    -1.17571500
P         -3.54678800    -6.80553600     2.73579900
O         -2.87695800    -8.12951900     3.18768400
O         -4.84710800    -6.99404900     2.00570300
O         -3.67417600    -5.77174500     3.95559400
C         -1.15510800     1.34298100    -4.30942700
C         -1.03505700     2.43303100    -3.21346100
O         -1.35040000     2.16849800    -2.06095800
N         -0.64319600     3.66991600    -3.59926700
C         -0.75880100     4.81925200    -2.72419900
C         -6.43369000    -1.67554900     0.98371100
O         -6.03593700    -1.62582300     2.32455700
C         -2.15047700    -2.64862500     8.18431800
C         -0.85174700    -3.13914900     7.54490500
C         -1.19391200    -3.89165400     6.26442600
C         -1.31163600    -2.91654400     5.08965900
N         -1.95250200    -3.43706700     3.89520600
C         -2.07434400     2.95460500     4.85653600
S         -1.48142500     1.23434900     4.68331100
C          0.98959100    -5.46780400     4.18499500
C          2.04261400    -5.37305400     3.01549200
O          3.16135800    -4.87385600     3.29533600
O          1.67135800    -5.81420500     1.90005000
C          4.32878900    -6.49073600     0.41018000
C          3.65210500    -6.81937200    -0.89379500
N          4.33078100    -7.24866000    -2.02839500
C          2.33287500    -6.75599800    -1.23956800
C          3.45943300    -7.44927700    -3.01367200
N          2.24205200    -7.15603000    -2.55908400
C          8.21975800     1.39073400     3.56486800
C          7.53326300     0.00372100     3.57478300
C          6.03221800    -0.02476000     3.31153500
O          5.56459800     0.29925000     2.21850100
N          5.26870900    -0.43605200     4.33801300
C          6.32665200    -1.20052500    -0.77804500
C          4.89460300    -1.67503500    -0.99483500
C          4.41185300    -2.81753000    -0.34852900
C          4.02999400    -0.96729200    -1.83503600
C          3.10120900    -3.25649900    -0.54248500
C          2.73131500    -1.42112000    -2.05884100
C          2.26190800    -2.56552100    -1.41688900
O          2.97940100     2.27353100    -2.79593700
O         -4.93120500    -9.31434200     1.01577200
O         -0.08993400    -7.83117300     2.13093800
H         -2.96564900    -6.20922900    -1.87332400
H         -2.38874000    -4.52215500    -2.07864700
H         -1.16049300    -6.45985200    -0.08443500
H         -3.78118400    -5.62261500     0.29751100
H         -3.20950300    -3.26476300     0.04725200
H         -3.16798700    -3.44188800     1.82545200
H         -0.73956900    -3.71896300     1.78218200
H         -0.82163700     0.54118900    -1.18651400
H          3.51919500     0.08842000     1.34603500
H          3.22675600    -2.99062100     2.91827700
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H	4.27455100	-1.79061300	2.29601400
H	-2.23920100	1.21403200	-4.51601100
H	-0.77888100	0.39677500	-3.86350000
H	-0.45197400	3.83913300	-4.58691500
H	-0.66993000	4.45765900	-1.68205500
H	-5.61369700	-2.17126700	0.44203700
H	-6.55116200	-0.66025900	0.54918800
H	-6.72107900	-1.19933300	2.87377300
H	-2.56813600	-3.48329300	8.78818900
H	-2.89715300	-2.45811700	7.39204500
H	-0.29960000	-3.77447000	8.25782100
H	-0.17918500	-2.30427000	7.30358900
H	-0.44417600	-4.65388500	6.05794200
H	-2.15166200	-4.41671900	6.39951600
H	-0.31039900	-2.54437100	4.83003300
H	-1.87983500	-2.02918000	5.40937700
H	-1.58423400	-4.36181700	3.68095200
H	-2.93340200	-3.61932700	4.09647600
H	-3.08005800	2.95218000	5.31823100
H	-2.18824000	3.33153700	3.82632900
H	-1.66626100	0.85592900	5.98281400
H	0.07659800	-5.96996300	3.83852700
H	0.73364900	-4.40735400	4.38845300
H	3.71499100	-5.77227600	0.96267600
H	5.29055700	-6.00477400	0.13484600
H	5.37005700	-7.35133000	-2.12580400
H	1.47842900	-6.42995900	-0.67693800
H	3.70509100	-7.79854400	-4.00827100
H	1.35289000	-7.20506800	-3.09679900
H	8.62953200	1.59826400	4.56570500
H	7.48000300	2.18718500	3.34994000
H	7.93720900	-0.62944200	2.76896900
H	7.75004300	-0.51845500	4.51353200
H	5.66816600	-0.83529700	5.17853000
H	4.30079200	-0.71649300	4.16123000
H	6.61395500	-1.35759600	0.27960400
H	6.39422100	-0.11255300	-0.94698800
H	5.06747900	-3.36792600	0.32749900
H	4.35736800	-0.04567300	-2.30974600
H	2.70523000	-4.09789900	0.02282700
H	2.06872500	-0.84752300	-2.70819800
H	1.24068200	-2.91365700	-1.56255500
H	2.40120700	1.70114100	-3.33571900
H	2.78572600	1.97749800	-1.88428800
H	-5.11463500	-9.50132600	0.06394300
H	-5.00405200	-8.31057300	1.14094600
H	0.33120300	-6.97394300	1.88341800
H	-1.02550100	-7.63430500	2.28420000
H	-0.02215736	5.55530049	-2.97014365
H	-1.72728000	5.25288991	-2.86170021
H	-1.39131950	3.56666405	5.40768140
H	-7.33421864	-2.22674267	0.81012036
H	9.00213513	1.40324891	2.83505337
H	7.01720729	-1.71832733	-1.41043264
H	-0.63548675	1.58833522	-5.21203160

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H          4.52851240   -7.36342480    0.99620460
H          1.36961324   -5.92316939    5.07557091
H         -3.69073006   -6.17956606    4.82450593
H         -1.21004909   -6.46633952   -3.31946640
H         -2.02025666   -1.77675110    8.79076550
```

Deglycosylation K249–Nuc: TS3–K$_{Nuc}$ E = –3875.503694 a.u.   (296.34i cm^{-1})

```
O         -1.23487500   -6.33478200   -1.75806000
C         -1.19766800   -5.01657100   -1.24720500
C         -1.28303500   -5.25549600    0.26433600
O         -0.82829900   -4.10511400    1.03666700
C         -2.69105800   -5.49932300    0.78150600
O         -2.46973200   -6.37883600    1.89576200
C         -3.13824300   -4.10033200    1.21333900
C         -1.82451800   -3.44368700    1.51427200
N         -1.71387600   -1.80212100   -0.16367800
C         -2.53520000   -1.11334400   -1.03202900
N         -1.85594600    0.02732700   -1.47161600
C         -0.65323300    0.11010900   -0.77395200
C          0.44742000    0.97094700   -0.84180800
O          0.62802100    2.01363700   -1.51431900
N          1.46345500    0.56737900    0.05546400
C          1.44255400   -0.58003100    0.79299800
N          2.59007400   -0.84519600    1.53899700
N          0.42822800   -1.39520700    0.83530500
C         -0.60845800   -1.05850500    0.00586600
O         -3.68293000   -1.41696800   -1.36465000
P         -3.62741300   -6.99277500    2.82736400
O         -3.10041000   -8.35644100    3.31568600
O         -4.95171100   -7.01569000    2.12488100
O         -3.53580700   -5.88817900    3.99321400
C         -1.11174100    1.38197600   -4.29468300
C         -1.33970100    2.61546200   -3.40313200
O         -2.18140700    2.58016500   -2.51391200
N         -0.55542200    3.69855000   -3.58749300
C         -0.69380100    4.82191300   -2.68774200
C         -6.42378800   -1.66242000    0.94558100
O         -5.98423100   -1.71928300    2.28007600
C         -2.12252700   -2.75175800    8.15531800
C         -1.23484900   -2.77582200    6.88843400
C         -1.80444300   -2.02829600    5.66442600
C         -2.56630200   -2.85342200    4.61447700
N         -1.71320200   -3.73107600    3.79353000
C         -2.06219200    2.92839800    4.86981900
S         -1.49151600    1.20541100    4.69289300
C          0.94555300   -5.52538200    4.17851400
C          1.97746000   -5.45304300    2.97537700
O          3.08332900   -4.94137000    3.20140400
O          1.56982800   -5.94960400    1.87903600
C          4.32923900   -6.53086200    0.40873100
C          3.70251500   -6.85103400   -0.91743800
N          4.41230900   -7.19597600   -2.05934300
C          2.38377000   -6.87065200   -1.26451800
C          3.55950100   -7.41436500   -3.05679500
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N              2.32329400    -7.22020100    -2.59677900
C              8.27003700     1.32106500     3.67164900
C              7.33778000     0.09002200     3.62982400
C              5.97959200     0.32578200     2.97029300
O              5.86268100     1.02967800     1.97422700
N              4.93172600    -0.30531100     3.54594600
C              6.36643300    -1.27746600    -0.70780500
C              4.92667000    -1.71050100    -0.95165500
C              4.40461700    -2.87347100    -0.37066100
C              4.09017100    -0.92858300    -1.75261100
C              3.08376400    -3.25901400    -0.60175100
C              2.77879800    -1.32625400    -2.01179000
C              2.27444700    -2.49158000    -1.44167900
O              3.08318800     1.95122300    -2.86781400
O             -4.93109300    -9.27438100     0.93605300
O             -0.10204500    -8.00920000     2.11476300
H             -2.02080300    -4.37675100    -1.60187900
H             -0.24560100    -4.50665500    -1.46858100
H             -0.62022100    -6.07778400     0.52525200
H             -3.36045300    -5.96763300     0.04794100
H             -3.55940500    -3.55430500     0.35249800
H             -3.85887600    -4.06920200     2.03148900
H             -1.63356200    -2.47433300     1.93184900
H             -2.32268500     0.83200700    -1.88311700
H              2.32071800     1.10689500    -0.00835100
H              2.57138700    -1.81766700     1.84243500
H              3.44093300    -0.68234500     0.99786300
H             -2.10259700     0.94659100    -4.53480900
H             -0.54926600     0.64979600    -3.66819500
H             -0.03341800     3.80773200    -4.45252500
H             -0.61326800     4.42904400    -1.65318700
H             -5.61481900    -2.07939400     0.32653000
H             -6.56916800    -0.61501700     0.60874600
H             -6.64059100    -1.29496600     2.86433500
H             -1.85002800    -3.62802500     8.77884900
H             -3.17900100    -2.90133300     7.86305200
H             -1.05464900    -3.82504500     6.62159900
H             -0.24385200    -2.37713200     7.14103300
H             -0.99104900    -1.50658300     5.14071100
H             -2.48523400    -1.23751000     6.00936100
H             -3.08697000    -2.14749000     3.95007200
H             -3.34433300    -3.46818000     5.07966100
H             -0.73798600    -3.45604900     3.86937900
H             -1.80171300    -4.70455200     4.06142600
H             -3.07246700     2.93255700     5.32095800
H             -2.15916000     3.31983200     3.84510800
H             -1.64933100     0.84916800     6.00028300
H              0.00900500    -5.99191500     3.84526000
H              0.73280700    -4.46711100     4.43306700
H              3.69022900    -5.82807500     0.95471400
H              5.29383800    -6.03133200     0.17495300
H              5.46104100    -7.26626800    -2.15270600
H              1.50694500    -6.66313000    -0.68298000
H              3.83285800    -7.70599900    -4.06133000
H              1.43427900    -7.27351600    -3.13743300
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H	8.75295800	1.34862400	4.66298000
H	7.65474500	2.23896000	3.57768500
H	7.79586700	-0.73141700	3.05384800
H	7.18477000	-0.30631300	4.64021000
H	5.01148000	-0.91777500	4.35351100
H	4.02001400	-0.24159900	3.10018500
H	6.65102400	-1.50744300	0.33752700
H	6.45790000	-0.18355000	-0.80916700
H	5.03111200	-3.47182800	0.29012600
H	4.44934900	0.00806500	-2.16778100
H	2.66306200	-4.12358300	-0.09106200
H	2.13765900	-0.69723900	-2.62994000
H	1.23868500	-2.77393300	-1.61086100
H	2.85234900	1.27426700	-3.53291300
H	2.22482200	2.09731900	-2.40891700
H	-5.05668400	-9.35936700	-0.03866100
H	-5.04954500	-8.29576900	1.15700800
H	0.41826500	-7.18305900	1.94422200
H	-1.02758100	-7.73048200	2.14520700
H	-1.65962124	5.26364514	-2.81798781
H	0.05013719	5.55657415	-2.91518203
H	-0.57640880	1.61718618	-5.19078322
H	-1.37299978	3.51593815	5.43965288
H	9.03073272	1.31535244	2.91918014
H	7.04660677	-1.77711101	-1.36554242
H	4.51282542	-7.41779681	0.97841747
H	1.33281993	-5.99489706	5.05855941
H	-2.03064150	-1.87874505	8.76712307
H	-3.65433384	-6.27671025	4.86303861
H	-7.32448327	-2.21180570	0.76718993
H	-1.36796147	-6.46923025	-2.69923568

Deglycosylation K249–Nuc: IC1–K$_{Nuc}$ E = –3875.589031 a.u.

O	-1.57285300	-6.19654100	-1.74473800
C	-2.13510100	-4.95349600	-1.36053200
C	-2.13443700	-4.92346700	0.16548200
O	-2.24219700	-3.56599500	0.58069600
C	-3.31065400	-5.67448800	0.81392600
O	-2.73663200	-6.59526700	1.78327000
C	-4.13018500	-4.55533300	1.44854100
C	-3.10376900	-3.45104200	1.70425800
N	-0.87092400	-1.30818100	1.66385200
C	-1.53666600	-0.47211100	0.77144400
N	-0.56446200	0.38529500	0.28365700
C	0.68444000	0.01725600	0.79152100
C	1.99824700	0.50198600	0.59861100
O	2.39941000	1.44786900	-0.09195100
N	2.91664400	-0.26192300	1.35133500
C	2.60626900	-1.37214000	2.08432300
N	3.63785100	-2.04383000	2.67343300
N	1.38054100	-1.79377600	2.28710400
C	0.46465400	-1.05914800	1.63591400
O	-2.72701100	-0.48565600	0.49213200
P	-3.65336800	-7.19717900	2.95977000

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O          −3.05826900    −8.56052700     3.35876500
O          −5.10130600    −7.24765900     2.53825600
O          −3.34359000    −6.05688300     4.04347000
C          −1.11035600     1.38354100    −4.31966200
C          −0.98574300     2.45559800    −3.20307800
O          −1.31103000     2.18068300    −2.05891600
N          −0.57567600     3.69275700    −3.57814100
C          −0.68828600     4.83638200    −2.69716300
C          −6.43426800    −1.64886500     0.94196000
O          −6.01100800    −1.73014700     2.27484800
C          −2.01209600    −2.69799700     8.00791200
C          −2.70654200    −2.45386800     6.62255900
C          −2.13840100    −3.24231800     5.42389900
C          −2.98345100    −3.03078700     4.14986000
N          −2.31428600    −3.53647100     2.94206100
C          −2.04503400     2.90609000     4.85153800
S          −1.45769900     1.18511500     4.66322600
C           0.91609300    −5.52502100     4.13445300
C           1.99167100    −5.36161500     2.99002400
O           3.10929200    −4.88477400     3.30277800
O           1.64803100    −5.75730400     1.84310400
C           4.30657800    −6.53193500     0.36441600
C           3.67345000    −6.83274300    −0.96136200
N           4.37730900    −7.18470600    −2.10475700
C           2.35424800    −6.82443100    −1.30696000
C           3.52172400    −7.38305100    −3.10290000
N           2.28966700    −7.16851200    −2.64045900
C           8.28123400     1.30124600     3.62866800
C           7.64324700    −0.09310200     3.76242200
C           6.16847600    −0.16125300     3.41088000
O           5.77971200     0.11290800     2.27336200
N           5.34659500    −0.51714500     4.40971100
C           6.35480200    −1.24894300    −0.78531100
C           4.90395900    −1.68203700    −0.95905800
C           4.40907900    −2.82033600    −0.31436900
C           4.01990900    −0.90471400    −1.71275000
C           3.05998800    −3.16902600    −0.39294500
C           2.67953800    −1.26672600    −1.82546000
C           2.19225700    −2.38612800    −1.15494100
O           3.03401400     2.25792100    −2.73766300
O          −4.89415000    −9.06484400     0.81428600
O          −0.05780100    −7.81927200     1.94168700
H          −3.16728700    −4.81865200    −1.73400600
H          −1.53507200    −4.09768800    −1.71013800
H          −1.18988300    −5.35872600     0.51691900
H          −3.88235400    −6.27333300     0.09090400
H          −4.83370200    −4.19500200     0.67723000
H          −4.73596600    −4.84875900     2.30126300
H          −0.74637800     1.02986200    −0.47961500
H           3.89376100     0.03394300     1.31528900
H           3.39981600    −3.00312900     2.95696000
H           4.53068500    −1.94594700     2.19949600
H          −2.19455300     1.26836700    −4.53435600
H          −0.74523400     0.42885800    −3.88419400
H          −0.37873400     3.86769800    −4.56338200
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H          -0.60685000    4.46749900   -1.65706800
H          -5.62092600   -2.08061600    0.33817000
H          -6.56248200   -0.59775200    0.61078700
H          -6.65155800   -1.28655700    2.86299600
H          -0.95915700   -2.98902300    7.82818400
H          -2.47008100   -3.57726900    8.50021700
H          -2.63716700   -1.39915200    6.32262400
H          -3.78314600   -2.66504000    6.71946900
H          -1.11489900   -2.89533700    5.22739000
H          -2.07374600   -4.31324500    5.65063700
H          -3.14928200   -1.95235100    4.00116900
H          -3.97539700   -3.48859900    4.29579100
H          -1.27461300   -2.12983200    2.13847800
H          -2.02876000   -4.50086100    3.09791600
H          -3.05374500    2.90410300    5.30638900
H          -2.14809800    3.29622600    3.82493700
H          -1.61582600    0.81459200    5.96790400
H           0.03560600   -6.05433000    3.74996800
H           0.59812400   -4.49081700    4.38720900
H           3.66674000   -5.83299400    0.91446400
H           5.27277600   -6.03406600    0.13415800
H           5.42374100   -7.26988800   -2.19801300
H           1.47726100   -6.60883100   -0.72684100
H           3.79019600   -7.67353600   -4.10904700
H           1.40493600   -7.19887300   -3.18079000
H           8.72169700    1.58769300    4.59760000
H           7.50914100    2.05999500    3.39348200
H           8.10572400   -0.79100100    3.04828000
H           7.81263000   -0.50769800    4.76262500
H           5.70695400   -0.87843800    5.28433100
H           4.41486500   -0.86883700    4.16554300
H           6.65828600   -1.39812500    0.26963200
H           6.43792600   -0.16290600   -0.96147900
H           5.08468200   -3.43092600    0.28652600
H           4.36118000    0.00776500   -2.19401200
H           2.66844200   -4.00863800    0.17981100
H           2.00385800   -0.63635400   -2.40293100
H           1.13651300   -2.64061100   -1.20343800
H           2.43784100    1.68960900   -3.26121400
H           2.85943400    1.98660700   -1.81259200
H          -4.81099200   -8.83416500   -0.14636900
H          -5.14161100   -8.20611300    1.28763900
H           0.43244100   -6.97935000    1.77095200
H          -0.99016500   -7.60380700    1.79057200
H          -3.54268000   -2.44788800    1.67072300
H           0.05542101    5.56820506   -2.93430199
H          -1.65264637    5.27898746   -2.83503788
H          -7.33667816   -2.18922157    0.74556580
H           9.03707751    1.29024009    2.87138374
H           7.03200413   -1.77715030   -1.42350715
H           1.31052720   -6.00147818    5.00755678
H           4.48580280   -7.42572542    0.92469911
H          -3.57663804   -6.35350786    4.92625100
H          -1.36133082    3.50577918    5.41529579
H          -1.99700622   -1.87470252    8.69118244
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H	−1.60454127	−6.37071607	−2.68827332
H	−0.58459447	1.63017015	−5.21835487

Deglycosylation K249–GB: RC3–K$_{GB}$ E = −3875.584189 a.u.

O	−1.00018000	−5.95581800	−2.53428100
C	−2.13402100	−5.56097200	−1.77473900
C	−1.68402900	−5.49852400	−0.33219100
O	−0.81428000	−4.37561500	−0.18132600
C	−2.83019000	−5.31987300	0.67279900
O	−2.46569300	−6.10368900	1.83164100
C	−2.77345400	−3.83998200	0.98562800
C	−1.26620800	−3.56004300	0.89056000
N	−0.91486900	−2.18037700	0.61071700
C	−1.50283700	−1.36184300	−0.38358700
N	−0.64982500	−0.29600000	−0.53601600
C	0.44864000	−0.43490700	0.30921000
C	1.68431500	0.26200600	0.35287500
O	2.02054200	1.27851600	−0.25883900
N	2.56901900	−0.36985100	1.24541200
C	2.32552900	−1.55374100	1.88792500
N	3.34223800	−2.03608300	2.66236300
N	1.18535900	−2.20531200	1.81542300
C	0.29702100	−1.62323500	0.99036100
O	−2.56515600	−1.53977000	−0.95943000
P	−3.53105400	−6.81054400	2.79889800
O	−2.89343600	−8.15022800	3.24642600
O	−4.88093900	−6.95643600	2.14905600
O	−3.52546500	−5.74040400	3.99866600
C	−1.15459200	1.34368100	−4.31040400
C	−1.02969400	2.42883900	−3.20899100
O	−1.33549700	2.15860500	−2.05561000
N	−0.64587800	3.66874100	−3.59591500
C	−0.76161800	4.81947600	−2.72282100
C	−6.43386400	−1.67598800	0.97339100
O	−6.02622500	−1.62398700	2.31236400
C	−2.15595300	−2.66700400	8.19590500
C	−0.85105400	−3.20131200	7.60096400
C	−1.12745200	−3.82753900	6.24096300
C	−1.18368200	−2.73748500	5.17786900
N	−1.64069800	−3.25242200	3.89857000
C	−2.07173700	2.94807900	4.85405500
S	−1.47651500	1.22572200	4.69452900
C	0.99452000	−5.46543500	4.17868900
C	2.03892800	−5.38662600	3.00566500
O	3.16612300	−4.89549400	3.27376800
O	1.66319200	−5.82526700	1.88858500
C	4.33464200	−6.48757700	0.40523800
C	3.66305100	−6.81604500	−0.90086700
N	4.34465500	−7.23759200	−2.03649800
C	2.34358900	−6.76169000	−1.24593200
C	3.47484200	−7.44134600	−3.02232000
N	2.25528700	−7.15788700	−2.56684700
C	8.21710600	1.39012700	3.55860100
C	7.53200900	0.00155700	3.56048400

C	6.03018900	−0.03333800	3.29882200
O	5.55939200	0.27714800	2.20324400
N	5.26863500	−0.43619000	4.33051300
C	6.32710800	−1.19903700	−0.78124700
C	4.89446800	−1.67776500	−0.98913400
C	4.41506600	−2.81903000	−0.33773500
C	4.02345500	−0.97084800	−1.82360100
C	3.10205300	−3.25673000	−0.52049900
C	2.72223500	−1.42296700	−2.03601000
C	2.25608400	−2.56568800	−1.38849400
O	2.98584500	2.24267300	−2.76482500
O	−4.89391100	−9.21658400	1.02552600
O	−0.08016700	−7.85715900	2.11480500
H	−2.97870600	−6.27454700	−1.85270600
H	−2.48707800	−4.56529100	−2.08182500
H	−1.14004600	−6.41603900	−0.08328100
H	−3.80854000	−5.65700500	0.30546800
H	−3.28049700	−3.28607200	0.18896300
H	−3.22820300	−3.58496800	1.94247700
H	−0.74368200	−3.83057800	1.80940700
H	−0.88810100	0.52274700	−1.09367600
H	3.49717300	0.04992800	1.34034600
H	3.22715900	−3.02300500	2.93178100
H	4.26596600	−1.81833700	2.29560800
H	−2.23947100	1.21846800	−4.51550100
H	−0.77900100	0.39543100	−3.86897700
H	−0.46115300	3.83798800	−4.58478800
H	−0.67241400	4.45904400	−1.68030600
H	−5.61370300	−2.16409700	0.42518700
H	−6.55959200	−0.66042600	0.54153500
H	−6.71596300	−1.21339300	2.86822900
H	−2.61306200	−3.47765000	8.80429600
H	−2.87852800	−2.46975300	7.38422500
H	−0.39460100	−3.92945700	8.29154500
H	−0.10383400	−2.40472900	7.48129000
H	−0.36558500	−4.56105800	5.99806200
H	−2.08883700	−4.36136000	6.27383800
H	−0.17333900	−2.32378800	5.04396200
H	−1.80493400	−1.90581000	5.56552300
H	−2.52392000	−3.74747700	4.01461200
H	−1.81556100	−2.46905300	3.26927500
H	−3.07973000	2.94632700	5.31019200
H	−2.17876500	3.31965300	3.82127300
H	−1.66824300	0.85107600	5.99490100
H	0.06169900	−5.93493000	3.84568000
H	0.74653400	−4.40122700	4.37025500
H	3.71700900	−5.77330500	0.95904800
H	5.29574300	−5.99816100	0.13374700
H	5.38477100	−7.33667400	−2.13348100
H	1.48818200	−6.44792700	−0.67856200
H	3.72305500	−7.78613600	−4.01780800
H	1.36738600	−7.20979400	−3.10562000
H	8.62407200	1.59379100	4.56130200
H	7.47767500	2.18724800	3.34517200
H	7.93745200	−0.62646700	2.75145800

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H          7.75091700    -0.52465000    4.49648900
H          5.67003300    -0.82936600    5.17301500
H          4.30220000    -0.72326100    4.15645100
H          6.61893700    -1.35191700    0.27575700
H          6.38913100    -0.11109800   -0.95249800
H          5.07477400    -3.36961100    0.33417100
H          4.34876400    -0.05122000   -2.30350900
H          2.70941800    -4.09749400    0.04821900
H          2.05654200    -0.84990900   -2.68247600
H          1.23331200    -2.91234800   -1.52540900
H          2.39935700     1.68389100   -3.30960800
H          2.78356700     1.94594500   -1.85564000
H         -5.02797400    -9.32181200    0.05312000
H         -4.99802000    -8.22616800    1.23260600
H          0.35148700    -6.99850700    1.88873000
H         -1.00927600    -7.64243100    2.27981200
H         -0.02567953     5.55611723   -2.96910187
H         -1.73026917     5.25264963   -2.86057263
H         -0.63633242     1.59004509   -5.21351625
H         -1.39108231     3.56138586    5.40674287
H         -7.33289750    -2.23118011    0.80486656
H          9.00136158     1.40571071    2.83086456
H          7.01841904    -1.71427360   -1.41490330
H          4.53443055    -7.36167807    0.98913170
H          1.37470724    -5.92417521    5.06746067
H         -3.61524823    -6.15830780    4.85825624
H         -1.22778839    -6.45177713   -3.32410311
H         -2.01983818    -1.78852420    8.79142661
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Deglycosylation K249–GB: TS3–K$_{GB}$ E = –3875.502299 a.u.

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O         -1.00533500    -6.19027100   -2.12018200
C         -2.12826000    -5.76117900   -1.38193800
C         -1.87462300    -6.09274600    0.08772200
O         -1.18007000    -4.94912300    0.72736700
C         -3.10951300    -6.23229800    0.95582000
O         -2.65246400    -6.94576800    2.11196300
C         -3.39274000    -4.78258700    1.33344000
C         -2.00213800    -4.25073500    1.40024100
N         -2.21222000    -1.64933600    0.53359400
C         -2.78913500    -0.89029900   -0.46747700
N         -1.83631800     0.00229500   -0.96239800
C         -0.67088700    -0.15649500   -0.22490200
C          0.59102300     0.44445800   -0.28495200
O          0.99414300     1.39730900   -0.98342000
N          1.46872300    -0.15417400    0.65579500
C          1.17830900    -1.25154100    1.41937500
N          2.23204900    -1.75840100    2.17324700
N         -0.01250200    -1.78374000    1.49049000
C         -0.94279100    -1.21894700    0.64953800
O         -3.95065500    -0.95859400   -0.88289900
P         -3.68879400    -7.86041800    2.95300200
O         -2.82753000    -8.87178400    3.70860200
O         -4.65157300    -8.56453800    1.98641400
O         -4.51284200    -6.81902900    3.83124700
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C          -1.06518300     1.41556400    -4.31021700
C          -1.19599700     2.59186000    -3.31822900
O          -1.91258100     2.47989700    -2.33474000
N          -0.48663400     3.72118100    -3.55015400
C          -0.64785700     4.85811600    -2.66752500
C          -6.41693200    -1.64966700     0.88545900
O          -6.01170800    -1.71851000     2.23725200
C          -2.06570600    -2.77118600     8.07793200
C          -2.16238000    -2.45399100     6.55933400
C          -3.59336700    -2.53867000     6.00215200
C          -3.91757800    -1.66245400     4.79305800
N          -3.13028000    -1.99342400     3.59303100
C          -2.05296700     2.88445300     4.86226400
S          -1.42009800     1.17545700     4.70156200
C           0.77542800    -5.55390700     4.18671500
C           1.47766200    -5.70400400     2.77549000
O           2.35720800    -4.86640900     2.48745000
O           1.08722800    -6.69658100     2.09645200
C           4.28264500    -6.53374400     0.37985100
C           3.68613100    -6.84735300    -0.96277800
N           4.41094500    -7.19668700    -2.09482400
C           2.37335100    -6.84007500    -1.33159300
C           3.57008600    -7.39548200    -3.10650100
N           2.32939700    -7.18247600    -2.66725300
C           8.26156500     1.29130600     3.71104700
C           7.34693300     0.04852200     3.67588200
C           5.96004200     0.28304900     3.07426400
O           5.78256600     1.08372700     2.16734100
N           4.97222400    -0.48808100     3.58531600
C           6.38119600    -1.24336400    -0.71787300
C           4.92736500    -1.61562400    -0.98202800
C           4.35785300    -2.74347400    -0.38291200
C           4.12483100    -0.82253200    -1.80981800
C           3.02599300    -3.09177100    -0.61917200
C           2.80281700    -1.17883700    -2.07051000
C           2.25039000    -2.31443800    -1.47919100
O           2.98584000     2.27772600    -2.72514300
O          -1.56205000    -9.31703200     1.12600000
O          -2.03101800    -4.40934200     3.69458200
H          -3.06155700    -6.27846200    -1.68320200
H          -2.29358100    -4.67867600    -1.49322600
H          -1.20474600    -6.94380400     0.17500100
H          -3.94179400    -6.75708600     0.47293500
H          -3.88476500    -4.23829300     0.50173400
H          -3.98342200    -4.63392000     2.23463300
H          -1.63923500    -3.30335800     1.75822900
H          -2.06976300     0.81701600    -1.52232600
H           2.42844300     0.17387600     0.60352700
H           2.04504200    -2.71778700     2.48080100
H           3.09831900    -1.77212100     1.63705300
H          -2.09381700     1.08427800    -4.56067300
H          -0.56449200     0.59483600    -3.74537900
H          -0.07583400     3.87255700    -4.46940300
H          -0.58425600     4.49187500    -1.62594700
H          -5.59142500    -2.05928300     0.28728500
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H          -6.53473400    -0.59970000     0.55393700
H          -6.65766400    -1.25337900     2.80195600
H          -1.14174700    -3.34749900     8.27925300
H          -2.89429800    -3.44545700     8.36497600
H          -1.53818000    -3.16716300     6.01454600
H          -1.72820000    -1.46555100     6.34601000
H          -3.81021800    -3.57930400     5.74614500
H          -4.31943100    -2.27578400     6.79033000
H          -3.79784800    -0.60220800     5.06448600
H          -4.97113500    -1.81664700     4.53771000
H          -2.52100100    -3.50572200     3.68584900
H          -3.68751600    -1.82621300     2.75102900
H          -3.06567700     2.86254300     5.30685800
H          -2.15251000     3.26683500     3.83418700
H          -1.61165600     0.80841400     6.00448800
H          -0.24863600    -5.93862800     4.09289000
H           0.72076500    -4.46089000     4.39716000
H           3.60518800    -5.85783100     0.92151200
H           5.22968900    -5.99167500     0.17540000
H           5.45949200    -7.27384200    -2.17689700
H           1.49615000    -6.60787300    -0.75776900
H           3.85430800    -7.68775000    -4.10834100
H           1.45242000    -7.22843900    -3.23033400
H           8.73497500     1.34274300     4.70577700
H           7.63108200     2.19630800     3.59458900
H           7.78881000    -0.75227700     3.05956900
H           7.23792300    -0.37935500     4.67946900
H           5.08645200    -1.08681100     4.39817200
H           4.03224700    -0.42900200     3.20983600
H           6.63497900    -1.48216100     0.33319700
H           6.51570800    -0.15310100    -0.81852300
H           4.96179000    -3.35392400     0.28891400
H           4.51737500     0.09025300    -2.24805000
H           2.58276700    -3.93002700    -0.08508500
H           2.19226600    -0.53302500    -2.70099700
H           1.20847100    -2.57214600    -1.65366700
H           2.44362100     1.82627300    -3.40076300
H           2.51073600     2.01470000    -1.91090700
H          -0.88922700    -9.67665100     0.51319300
H          -1.12275700    -8.60420300     1.62476100
H          -1.12924400    -4.16992500     3.95061800
H          -2.32322600    -1.37391000     3.50073200
H          -1.61193064     5.29997451    -2.80973285
H          -1.37943810     3.48680506     5.43535283
H           0.09832495     5.59056855    -2.89473803
H           9.02759402     1.28549508     2.96400900
H           7.06233539    -1.76305100    -1.35886798
H           4.48768955    -7.42323170     0.93812365
H           1.25379120    -6.02139207     5.02189544
H          -7.32062797    -2.18783798     0.68897596
H          -4.04873056    -6.56976940     4.63378686
H          -1.20891180    -6.44363100    -3.02348992
H          -2.04647601    -1.91196141     8.71531989
H          -0.52675245     1.66241617    -5.20131551
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Deglycosylation K249–GB: PC–K$_{GB}$ E = −3875.577054 a.u.   (107.79i cm^{-1})

O	−1.12719900	−5.94924600	−2.42695800
C	−2.29465300	−5.81070200	−1.62601700
C	−1.96906600	−6.40400900	−0.26387900
O	−0.83558200	−5.74965600	0.28235700
C	−3.02331500	−6.18394400	0.81424100
O	−2.54540200	−6.97321900	1.93898000
C	−2.81032000	−4.71452300	1.13269700
C	−1.30119900	−4.52595700	0.85883800
N	−1.00561900	−1.46119400	1.13736000
C	−1.58913900	−0.62317200	0.18873200
N	−0.57398200	0.21380000	−0.22972700
C	0.59931700	−0.08665600	0.45740500
C	1.90784100	0.45068000	0.40095700
O	2.33888500	1.40112200	−0.26077900
N	2.76249300	−0.25064600	1.27226000
C	2.41104500	−1.34689000	2.00832300
N	3.41356100	−1.93595400	2.72962700
N	1.18684100	−1.81780200	2.08459300
C	0.31690800	−1.14991600	1.29806300
O	−2.75115400	−0.64268000	−0.19127200
P	−3.55516400	−7.72268500	2.94788200
O	−2.69244400	−8.69770600	3.75064100
O	−4.61169100	−8.48505800	2.13192300
O	−4.21669300	−6.52413700	3.78156400
C	−1.15027900	1.37082500	−4.32016600
C	−1.08969100	2.47272000	−3.23240000
O	−1.49332500	2.22934100	−2.10359100
N	−0.63267300	3.69406600	−3.59098800
C	−0.76443800	4.83171600	−2.70320200
C	−6.42611400	−1.71918900	0.94307600
O	−6.05610500	−1.67008700	2.29349400
C	−2.00411900	−2.79782900	8.19144700
C	−1.87390500	−2.66934300	6.66117600
C	−3.19322900	−2.44863100	5.91001500
C	−3.13681700	−2.87001000	4.43805400
N	−2.16185900	−2.14669900	3.62109600
C	−2.09585700	2.89541700	4.85946300
S	−1.48630700	1.17749800	4.71486500
C	0.99032700	−5.48988600	4.15747300
C	2.10060200	−5.31779900	3.04478000
O	3.21145100	−4.84326800	3.39187200
O	1.76921900	−5.69517900	1.89211800
C	4.35619900	−6.47591000	0.37335100
C	3.64874900	−6.77228800	−0.91948600
N	4.30732300	−7.19043200	−2.06937700
C	2.32390600	−6.68720900	−1.24275700
C	3.42003800	−7.36403400	−3.04595500
N	2.21415100	−7.06448100	−2.56840100
C	8.22464400	1.38903400	3.60523100
C	7.57821600	−0.01331800	3.64617700
C	6.08698900	−0.06921800	3.35500700
O	5.64610300	0.21303400	2.23886200
N	5.30458700	−0.43562400	4.38312400

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C            6.35084500    -1.16563400    -0.77907400
C            4.91650200    -1.65286600    -0.94201000
C            4.45290300    -2.77025300    -0.24064400
C            4.02232900    -0.96443100    -1.76724700
C            3.12812000    -3.19635400    -0.35321700
C            2.70906200    -1.40534600    -1.91192900
C            2.25602000    -2.51592000    -1.20251300
O            2.94915500     2.39146800    -2.83083300
O           -1.38016700    -9.42862000     1.27645800
O           -0.63354700    -4.29242200     2.04608900
H           -3.19792800    -6.31247300    -2.03574700
H           -2.53146000    -4.74387400    -1.53883100
H           -1.72316700    -7.46301100    -0.38026700
H           -4.04395800    -6.48189600     0.54450800
H           -3.41010000    -4.07945800     0.46371800
H           -3.06226000    -4.45554200     2.16022100
H           -1.10825800    -3.71918200     0.13138100
H           -0.73719300     0.96628400    -0.89243400
H            3.73259500     0.07103800     1.31670400
H            3.21365400    -2.89260600     3.04304200
H            4.33042100    -1.84009000     2.30095900
H           -2.22501900     1.20077700    -4.54358900
H           -0.74927000     0.44402900    -3.85540300
H           -0.39008300     3.86924300    -4.56607700
H           -0.67848100     4.46047100    -1.66441500
H           -5.59211800    -2.20796600     0.41840100
H           -6.53752300    -0.70425800     0.50918200
H           -6.75360100    -1.24863500     2.83084900
H           -1.16166100    -3.41903600     8.56051800
H           -2.91519000    -3.38103200     8.42320200
H           -1.43284600    -3.60726300     6.30313300
H           -1.14727300    -1.88668000     6.40176500
H           -3.99757600    -3.01039300     6.41352700
H           -3.49346100    -1.39053000     5.96166200
H           -4.11996300    -2.72593500     3.97590900
H           -2.89737000    -3.93613300     4.36778100
H           -1.54720000    -2.04276300     1.79685600
H           -2.30775100    -1.14101500     3.72347900
H           -3.10688100     2.88823000     5.30780800
H           -2.19454400     3.26314200     3.82488900
H           -1.69149400     0.80273100     6.01544300
H            0.11411600    -5.99850300     3.74339800
H            0.65509500    -4.45994000     4.41187700
H            3.75783300    -5.76342600     0.94956900
H            5.31757000    -5.99481700     0.08815400
H            5.34134900    -7.30496600    -2.17738100
H            1.46986300    -6.36916500    -0.66784900
H            3.64558200    -7.69756700    -4.05051900
H            1.31369800    -7.09323200    -3.09901100
H            8.64097300     1.62463500     4.59738800
H            7.46257900     2.16273200     3.38613700
H            8.01028600    -0.65564800     2.86316800
H            7.78779900    -0.50465500     4.60311000
H            5.69431100    -0.81360900     5.23770400
H            4.34762100    -0.74545500     4.18579000
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H            6.66404000   -1.29106200    0.27564700
H            6.39870500   -0.08070100   -0.97346700
H            5.13534300   -3.30905600    0.41830900
H            4.33771600   -0.06280600   -2.28618300
H            2.75711300   -4.02100000    0.25273500
H            2.02511400   -0.84712000   -2.55128300
H            1.22355200   -2.84484100   -1.29413200
H            2.39584600    1.78539300   -3.36063200
H            2.80015800    2.08321700   -1.91427300
H           -0.96932100   -9.66274900    0.41808200
H           -1.23867900   -8.46834600    1.39646700
H            0.31252600   -4.46992800    1.86929200
H           -1.20884500   -2.34995000    3.92421800
H           -0.02897869    5.57215343   -2.93932063
H           -1.73488886    5.26149796   -2.83889504
H           -7.32328438   -2.27117639    0.75520576
H            8.99773959    1.40645132    2.86569071
H            7.03660283   -1.68473536   -1.41560363
H            4.55774799   -7.36075936    0.94020161
H           -3.87347662   -6.46316591    4.67603873
H           -1.28097568   -6.40300025   -3.25885933
H            1.37985599   -5.96753238    5.03212785
H           -1.99001440   -1.89446242    8.76470948
H           -1.41804482    3.50627318    5.41832378
H           -0.62271586    1.62158739   -5.21665658
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Deglycosylation D268–GB: RC3–D$_{GB}$ E = −3875.59852 a.u.

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O           -0.96326000   -6.10003500   -2.23704400
C           -2.10865800   -5.71109900   -1.48860800
C           -1.67154900   -5.73125200   -0.03685800
O           -0.71027300   -4.68568200    0.16567500
C           -2.79219900   -5.48211100    0.97434400
O           -2.42039700   -6.14481500    2.21722000
C           -2.72090700   -3.98482200    1.18457500
C           -1.21472400   -3.70575900    1.05372300
N           -0.87445500   -2.36715200    0.58863200
C           -1.54224100   -1.58721400   -0.38817300
N           -0.73942200   -0.48665100   -0.59144500
C            0.39875600   -0.56738900    0.20669300
C            1.59527500    0.19882000    0.22298900
O            1.85977700    1.23096400   -0.39380900
N            2.53395100   -0.37659100    1.10304400
C            2.37230500   -1.56430400    1.76060900
N            3.40699500   -1.97966800    2.54002100
N            1.26853400   -2.28008400    1.70188300
C            0.32477700   -1.75199200    0.90279200
O           -2.61736000   -1.81760200   -0.91685800
P           -3.30735400   -7.33011100    2.84723300
O           -2.31889900   -8.30524700    3.51665200
O           -4.17165200   -8.07700400    1.83043100
O           -4.27337700   -6.59667300    3.89026500
C           -1.18345400    1.32760100   -4.31242300
C           -1.06854000    2.40441600   -3.20033500
O           -1.36442400    2.11429600   -2.04969600
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N            -0.70502600     3.65373300    -3.58433200
C            -0.83450200     4.80915700    -2.71886000
C            -6.42383800    -1.75751900     0.97263600
O            -6.01691100    -1.70288700     2.31226500
C            -2.04667400    -2.75304300     8.25053000
C            -1.34113400    -2.76521200     6.89018600
C            -2.21611200    -2.26761700     5.74303600
C            -1.57953500    -2.51251600     4.37685400
N            -0.19283100    -2.05056200     4.36556300
C            -2.12873400     2.93987700     4.84594200
S            -1.53067000     1.22353500     4.69447000
C             1.00636000    -5.42339300     4.22369100
C             2.04127800    -5.28715900     3.04048600
O             3.16237800    -4.79245300     3.31129500
O             1.66953700    -5.71426900     1.91532900
C             4.38784800    -6.42750300     0.41571900
C             3.70831900    -6.75829800    -0.88519500
N             4.38590600    -7.17637400    -2.02396600
C             2.38656400    -6.70364000    -1.22411200
C             3.51087100    -7.37723000    -3.00690600
N             2.29433400    -7.09553800    -2.54523000
C             8.18562500     1.49243600     3.55758700
C             7.51480600     0.09601300     3.55692000
C             6.01605200     0.03869400     3.27955000
O             5.55063900     0.33266400     2.17650000
N             5.24953200    -0.37141900     4.30479800
C             6.32703900    -1.11667200    -0.78924500
C             4.90681100    -1.61299300    -1.03221400
C             4.43860200    -2.77350100    -0.40900100
C             4.04382700    -0.91585300    -1.88300300
C             3.14220400    -3.23858400    -0.63245900
C             2.76053300    -1.39593100    -2.13835800
C             2.30519200    -2.55702000    -1.51617600
O             2.95234600     2.29031200    -2.79139200
O            -1.30035400    -9.49216700     0.71413100
O             0.11123700    -7.78009000     2.12798700
H            -2.96218800    -6.40437900    -1.61894900
H            -2.43231900    -4.69358900    -1.76126900
H            -1.19574300    -6.69258500     0.16792200
H            -3.76876900    -5.85320900     0.64244800
H            -3.24850400    -3.47829100     0.36927800
H            -3.14348800    -3.66040000     2.13673600
H            -0.69664200    -3.81715800     2.01109300
H            -1.02688900     0.31938200    -1.14473500
H             3.43616700     0.09682500     1.17956300
H             3.33826200    -2.96287200     2.83790100
H             4.32358800    -1.68294500     2.21341500
H            -2.26730100     1.19374900    -4.51885000
H            -0.79864800     0.37947300    -3.87847300
H            -0.52857500     3.82421700    -4.57441700
H            -0.74206300     4.45612900    -1.67396300
H            -5.59734000    -2.23271000     0.42260100
H            -6.56355300    -0.74262400     0.54337200
H            -6.71163000    -1.30037300     2.86795900
H            -1.59967500    -3.55014100     8.88209100
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H               -3.10803900    -3.03282100     8.11262100
H               -1.03460800    -3.79598300     6.67294800
H               -0.40628400    -2.19588600     6.91820800
H               -3.19671400    -2.76208700     5.77658400
H               -2.42566500    -1.19528700     5.87109900
H               -2.20796900    -2.05164000     3.59552200
H               -1.56899700    -3.59149900     4.18650400
H                0.29226700    -2.38899300     3.53741000
H               -0.16962300    -1.03182300     4.30529200
H               -3.13891600     2.93368200     5.29708200
H               -2.22977500     3.31475800     3.81328000
H               -1.68405200     0.87043100     6.00504600
H                0.08790100    -5.91956200     3.88925100
H                0.73299600    -4.37813600     4.50040300
H                3.76162800    -5.72664400     0.97924200
H                5.33594700    -5.91633400     0.13928500
H                5.42386800    -7.27254200    -2.12506900
H                1.52858200    -6.38135900    -0.66372100
H                3.75411800    -7.71810500    -4.00485200
H                1.39581700    -7.14426200    -3.08046800
H                8.58991600     1.69754400     4.56097200
H                7.43827100     2.28280700     3.34650500
H                7.93695400    -0.52957500     2.75458200
H                7.72961900    -0.42425700     4.49700800
H                5.64226300    -0.75049300     5.15810900
H                4.28564700    -0.65944700     4.12635500
H                6.60341800    -1.27557000     0.27064800
H                6.38267100    -0.02716600    -0.95223600
H                5.09319700    -3.31605100     0.27372500
H                4.36162100     0.01547600    -2.34476400
H                2.75469700    -4.09048100    -0.07785800
H                2.10033900    -0.83050900    -2.79762800
H                1.29488900    -2.92511100    -1.68538100
H                2.36366300     1.74467700    -3.34754600
H                2.74338500     1.97549600    -1.89091100
H               -0.97085100   -10.01768700    -0.05012600
H               -0.55556500    -8.91811800     1.02250000
H                0.49440400    -6.87896300     1.91681200
H               -0.74562900    -7.64717500     2.57305100
H               -1.80789383     5.23078152    -2.85900677
H               -0.10862995     5.55505803    -2.96713691
H                8.97043783     1.51893761     2.83076756
H                7.02773375    -1.62447476    -1.41858054
H                4.61065011    -7.30211988     0.99044026
H               -3.85699645    -6.46716731     4.74551672
H               -7.31563383    -2.32404314     0.80337115
H               -1.17339396    -6.47384586    -3.09594397
H               -1.44947400     3.54881205     5.40514139
H               -0.66779682     1.58290691    -5.21454082
H               -1.98269069    -1.83926599     8.80353788
H                1.42581773    -5.90013363     5.08489573
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Deglycosylation D268–GB: TS3–D$_{GB}$ E = −3875.500019 a.u.   (334.58i cm^{-1})

O	−1.45704000	−5.56075500	−2.61388000
C	−2.61756600	−5.39470600	−1.82006800
C	−2.33019800	−6.03183100	−0.46161600
O	−1.04612900	−5.44436800	−0.06231100
C	−3.29153500	−5.78180500	0.72307100
O	−3.45717100	−7.03902600	1.41555300
C	−2.54320700	−4.74932400	1.54543100
C	−1.13304900	−4.99397700	1.13608000
N	−0.99916500	−2.36672800	0.52812700
C	−1.73569000	−1.57743500	−0.33225300
N	−0.98592800	−0.43685700	−0.64906500
C	0.20844100	−0.49334800	0.06102100
C	1.36338200	0.30102700	0.06825000
O	1.60402800	1.37915600	−0.50796000
N	2.35322800	−0.27314400	0.90986500
C	2.23900100	−1.47369600	1.54575000
N	3.32429200	−1.86048900	2.31478300
N	1.17008900	−2.22299100	1.50979400
C	0.15171300	−1.71865600	0.74312300
O	−2.87510500	−1.80875800	−0.75847000
P	−3.72067900	−7.53204400	2.91774500
O	−2.43242900	−8.22408900	3.42819900
O	−4.82852600	−8.58730100	2.83013600
O	−4.05181300	−6.20157100	3.74726900
C	−1.15329300	1.35793100	−4.30547000
C	−1.09989500	2.45785500	−3.21436600
O	−1.51325300	2.20922700	−2.09347800
N	−0.62950500	3.68048700	−3.57322800
C	−0.76232000	4.83008600	−2.70336300
C	−6.43001800	−1.68902300	0.97277600
O	−6.04842900	−1.65521400	2.32028000
C	−2.07626000	−2.74345800	8.22862100
C	−1.34666400	−2.75626600	6.87546300
C	−2.21308800	−2.29600000	5.70341600
C	−1.59508500	−2.61147300	4.34303800
N	−0.20204100	−2.17174600	4.28344400
C	−2.08954700	2.94748900	4.85516700
S	−1.50761900	1.22451100	4.70413300
C	0.94544600	−5.40123000	4.24138300
C	1.95115800	−5.42572300	3.04160500
O	3.04194600	−4.85778200	3.15664900
O	1.59159800	−6.13305700	2.02944500
C	4.34545800	−6.47581400	0.39977700
C	3.74708200	−6.80065100	−0.94178600
N	4.48362600	−7.16307000	−2.06213100
C	2.43961300	−6.78306500	−1.33294900
C	3.65888200	−7.36278200	−3.08490900
N	2.41298700	−7.13637700	−2.66602900
C	8.22805200	1.41920900	3.60796100
C	7.49780100	0.05927900	3.66873500
C	6.03621500	0.04996100	3.22717100
O	5.70070700	0.43910200	2.10994800
N	5.15900200	−0.42527000	4.13057000

C	6.33255200	-1.16925400	-0.77923600
C	4.89512100	-1.54807700	-1.10975700
C	4.35014300	-2.74212000	-0.63007100
C	4.09732900	-0.71934200	-1.90412400
C	3.04151500	-3.10856700	-0.93887400
C	2.79738500	-1.09547800	-2.23581900
C	2.26169600	-2.28720000	-1.75351000
O	2.93718200	2.35575000	-2.76093100
O	-1.57168700	-9.34627100	0.98024700
O	-0.75112000	-6.78954800	1.92984100
H	-3.53425000	-5.85480200	-2.24271800
H	-2.78968400	-4.32058700	-1.68803100
H	-2.15407100	-7.10686900	-0.56152200
H	-4.28698400	-5.44427300	0.39002900
H	-2.75081900	-3.73738800	1.15704300
H	-2.74488000	-4.76935900	2.61051500
H	-0.25259900	-4.49920800	1.53329600
H	-1.33483000	0.36315000	-1.16639900
H	3.23216600	0.23493300	0.97523500
H	3.24538500	-2.83675200	2.60849500
H	4.21766600	-1.65429600	1.86874400
H	-2.22693200	1.17925900	-4.52867900
H	-0.74346800	0.43435300	-3.84022500
H	-0.39765500	3.84860400	-4.55176800
H	-0.68243000	4.47190600	-1.66054600
H	-5.59963100	-2.16744900	0.43061200
H	-6.54998300	-0.66909100	0.55137800
H	-6.73121800	-1.21392700	2.86093000
H	-1.65363400	-3.55445600	8.85897700
H	-3.13876800	-3.00548400	8.06840400
H	-1.01574900	-3.78410600	6.67829200
H	-0.42226000	-2.16923900	6.91335600
H	-3.20046400	-2.77478200	5.76258500
H	-2.40888200	-1.21667500	5.78296400
H	-2.22808700	-2.19349500	3.54438100
H	-1.59282600	-3.70146200	4.21614200
H	0.17929200	-2.36001300	3.35460600
H	-0.16954500	-1.15488700	4.38143000
H	-3.10163700	2.95085200	5.30231400
H	-2.18610200	3.32184200	3.82366700
H	-1.67208400	0.87718000	6.01482100
H	-0.03129300	-5.81291400	3.96040100
H	0.77970100	-4.33101500	4.50781000
H	3.69111800	-5.77722200	0.93072100
H	5.30360000	-5.95851000	0.18053700
H	5.53799900	-7.23519400	-2.13773400
H	1.54887700	-6.51946700	-0.79507000
H	3.95927800	-7.66538500	-4.07908000
H	1.54853100	-7.17689100	-3.23689900
H	8.66902600	1.62567100	4.59673200
H	7.50239200	2.23195200	3.40471700
H	7.97281300	-0.65616300	2.97918300
H	7.58315500	-0.37661800	4.67012300
H	5.44983200	-0.85011200	5.00476100
H	4.22596500	-0.69437500	3.81281600

H	6.55379100	-1.40027900	0.28006100
H	6.47218700	-0.07950200	-0.87777700
H	4.95913700	-3.39122100	0.00067200
H	4.47509600	0.23323500	-2.26314600
H	2.61238300	-4.01182000	-0.51159700
H	2.18410800	-0.42556000	-2.83861100
H	1.23392600	-2.56215000	-1.97788400
H	2.34511800	1.86613700	-3.36311600
H	2.63990600	2.03470700	-1.88208700
H	-1.30350700	-9.67602100	0.09547400
H	-1.24082900	-8.42575300	1.06258800
H	0.28240500	-6.60107200	2.05250700
H	-1.20904200	-7.18461700	2.70861800
H	-0.02728793	5.56886058	-2.94593254
H	-1.73071038	5.26356954	-2.84197066
H	-1.40742166	3.54988453	5.41794995
H	-0.63079672	1.60990381	-5.20458475
H	8.99864687	1.41772819	2.86561246
H	7.02309235	-1.69362246	-1.40620629
H	4.54052041	-7.35478903	0.97792365
H	1.35797373	-5.91635307	5.08362352
H	-3.83284986	-6.31682210	4.67483157
H	-7.32985519	-2.23880190	0.79129268
H	-1.49062637	-6.20747194	-3.32256128
H	-2.00844511	-1.83785745	8.79447327

Deglycosylation D268–GB: PC–D$_{GB}$ E = –3875.53412 a.u.

O	-1.40178600	-5.79074200	-2.23776200
C	-2.65996600	-5.38290300	-1.71005200
C	-2.88348200	-6.13190400	-0.39402700
O	-1.68381700	-6.05354800	0.37714300
C	-3.94638400	-5.54050100	0.52969800
O	-4.43374300	-6.57696800	1.44350900
C	-3.18807600	-4.40815900	1.19387100
C	-1.72163400	-4.85410200	1.14267600
N	-1.41784800	-1.82392200	0.42194900
C	-2.25540000	-1.25584700	-0.52138200
N	-1.63139600	-0.12841000	-1.06954900
C	-0.41926800	0.05090200	-0.41345400
C	0.65229400	0.91850100	-0.61271800
O	0.78191700	1.89851100	-1.39030000
N	1.71853100	0.61469300	0.27182200
C	1.76362200	-0.49525700	1.06668500
N	2.95267300	-0.70928900	1.75908100
N	0.77343600	-1.32138100	1.23302600
C	-0.33047100	-1.05145200	0.46612100
O	-3.37710000	-1.65247200	-0.86106800
P	-3.93190000	-7.15248700	2.82833900
O	-2.44549500	-7.59422800	2.81421300
O	-4.77654800	-8.40358400	3.11554900
O	-4.13258700	-5.91505000	3.82223400
C	-1.10761300	1.29657900	-4.30582600
C	-1.28115800	2.50166600	-3.35965000
O	-2.03446400	2.40691300	-2.40224300

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N           -0.55855000     3.62112400    -3.60628600
C           -0.70188400     4.77576300    -2.74798900
C           -6.41676900    -1.66649400     0.99588000
O           -6.02055400    -1.67474300     2.34066100
C           -2.07351300    -2.66404000     8.26225700
C           -1.48277700    -2.67285700     6.83893700
C           -2.44276600    -2.17916200     5.75273500
C           -2.09354700    -2.64489500     4.33728800
N           -0.67778600    -2.43292900     4.01186000
C           -2.04948600     2.98017300     4.83033800
S           -1.44014900     1.26577300     4.67989200
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C            4.30935000    -6.53292300     0.49170900
C            3.73612000    -6.87189900    -0.85898500
N            4.49668500    -7.25314400    -1.95723300
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C            3.69497600    -7.46626800    -2.99517500
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C            7.41681000     0.09949900     3.67292200
C            6.01817500     0.24538900     3.08264000
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C            4.92163400    -1.68473700    -0.94080000
C            4.39975900    -2.84115100    -0.34842500
C            4.07708100    -0.90002400    -1.72789700
C            3.07123200    -3.20895100    -0.54790700
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C            2.24256800    -2.43193500    -1.36107000
O            3.10570400     1.95111900    -2.88631500
O           -1.43041500    -8.90074700     0.78328200
O           -1.16088200    -5.18870300     2.39304600
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