

Supporting Information

***N*-Benzyl-Isatin Sulfonamide Analogs as Potent Caspase-3 Inhibitors: Synthesis, In Vitro Activity, and Molecular Modeling Studies**

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Elemental Analysis

Compd	Formula	Calcd			Found		
		C	H	N	C	H	N
10	$C_{19}H_{18}N_2O_5S$	59.06	4.70	7.25	58.99	4.74	7.11
11a	$C_{20}H_{20}N_2O_5S$	59.99	5.03	7.00	59.80	5.03	6.91
2	$C_{26}H_{24}N_2O_5S$	65.53	5.08	5.88	65.27	5.32	5.58
11b	$C_{27}H_{26}N_2O_6S$	64.02	5.17	5.53	64.76	5.24	5.06
11c	$C_{26}H_{23}FN_2O_5S$	63.15	4.69	5.66	63.05	4.69	5.60
11d	$C_{27}H_{26}N_2O_5S_2$	62.05	5.01	5.36	61.81	4.95	5.34
11e	$C_{28}H_{26}N_2O_7S$	62.91	4.90	5.24	62.99	5.02	5.13
11f	$C_{26}H_{24}N_2O_6S \cdot 0.25H_2O$	62.83	4.97	5.64	62.87	4.74	5.69
11g	$C_{25}H_{22}FN_3O_5S$	60.60	4.47	8.48	60.60	4.59	8.33
11h	$C_{25}H_{22}FN_3O_5S$	60.60	4.47	8.48	60.32	4.34	8.35
11i	$C_{25}H_{22}FN_3O_5S \cdot 0.25H_2O$	60.05	4.54	8.40	60.06	4.49	8.24
17	$C_{18}H_{16}N_2O_5S \cdot 0.5H_2O$	56.68	4.49	7.34	56.96	4.39	7.30
18a	$C_{19}H_{18}N_2O_5S$	59.06	4.70	7.25	58.98	4.75	7.19
18b	$C_{25}H_{22}N_2O_5S$	64.92	4.79	6.06	64.82	4.79	5.97
18c	$C_{26}H_{24}N_2O_6S$	63.40	4.91	5.69	63.65	4.93	5.59
18d	$C_{26}H_{24}N_2O_5S_2$	61.40	4.76	5.51	60.99	4.71	5.36
18e	$C_{25}H_{21}FN_2O_5S$	62.49	4.41	5.83	62.27	4.48	5.69
18f	$C_{25}H_{21}FN_2O_5S$	62.49	4.41	5.83	62.25	4.47	5.68
18g	$C_{24}H_{20}FN_3O_5S$	59.87	4.19	8.73	59.81	4.16	8.62
18h	$C_{24}H_{20}FN_3O_5S \cdot 0.5H_2O$	58.87	4.32	8.57	58.69	4.45	8.26
18i	$C_{24}H_{20}FN_3O_5S$	59.87	4.19	8.73	59.59	4.27	8.48
20	$C_{18}H_{17}N_3O_5S \cdot 0.5H_2O$	54.54	4.58	10.60	54.56	4.70	10.04
21a	$C_{19}H_{19}N_3O_5S$	56.85	4.77	10.47	56.48	4.87	10.19
21c	$C_{26}H_{25}N_3O_6S$	61.53	4.96	8.28	61.27	4.95	8.17
23	$C_{18}H_{17}N_3O_5S \cdot 0.75H_2O$	53.92	4.65	10.48	54.14	4.39	10.35

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10 R

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SMALL

USER_CHARGES

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6 H	-99.8880	26.0250	40.9330 H	1	*****	
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7 H	-98.4310	25.0240	40.8600 H	1	*****	
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8 C	-99.9860	24.1790	42.0930 C.3	1	*****	
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9 H	-100.9320	24.5210	42.5320 H	1	*****	
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10 H	-100.2230	23.4200	41.3410 H	1	*****	
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11 C	-99.0540	23.6730	43.1990 C.3	1	*****	
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12 C	-97.9710	22.7230	42.6520 C.3	1	*****	
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33 O	-92.7470	29.4420	48.2510 O.2	1	****	-
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USER_CHARGES

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0.0000
      4 H      -98.0310    26.6710    42.6840 H      1      ****
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      5 C      -99.4610    25.3550    41.7120 C.3      1      ****
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10 H	-100.3140	23.3530	41.5550 H	1	****	
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23 H	-97.4890	26.9920	47.6780 H	1	****	
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30 C	-94.9670	28.3910	48.1210 C.2	1	****	
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32 C	-93.5790	28.7970	47.6950 C.2	1	****	
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33 O	-92.7590	29.5250	48.2460 O.2	1	****	-
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34 N	-93.3960	28.1790	46.4450 N.am	1	****	-
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37 H	-91.7880	27.2890	45.4790 H	1	****	
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38 H	-92.4560	28.7460	44.6830 H	1	****	
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39 C	-94.9880	21.7090	43.3410 C.ar	1	****	-
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42 H	-92.9360	21.2610	42.8590 H	1	****	
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43 C	-94.2200	19.5570	42.5520 C.ar	1	****	-
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44 H	-93.4130	18.9120	42.2160 H	1	****	
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45 C	-95.5250	19.0720	42.6080 C.ar	1	****	-
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46 H	-95.7380	18.0500	42.3040 H	1	****	
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USER_CHARGES

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  5 C      -98.9130    25.4430    41.3440 C.3      1      ****
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  6 H      -99.5690    26.0870    40.7510 H      1      ****
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  7 H      -98.0580    25.1650    40.7170 H      1      ****
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  9 H     -100.5980    24.4870    42.2650 H      1      ****
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 10 H      -99.7810    23.4590    41.0800 H      1      ****
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 11 C      -98.7060    23.7220    42.9940 C.3      1      ****
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22 C	-96.6290	26.9140	46.7480 C.ar	1	****	-
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25 C	-94.3950	27.5570	46.0720 C.ar	1	****	
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26 C	-94.5060	26.8630	44.8800 C.ar	1	****	-
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56 H	-89.6910	32.3490	47.0580 H	1	****	
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SMALL
USER_CHARGES

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6 H	-100.0000	26.1580	41.0940 H	1	****	
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7 H	-98.4940	25.2310	40.9720 H	1	****	
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8 C	-99.9920	24.2710	42.1920 C.3	1	****	
0.0000						
9 H	-100.9480	24.5500	42.6540 H	1	****	
0.0000						
10 H	-100.2030	23.5280	41.4180 H	1	****	
0.0000						
11 C	-99.0230	23.7730	43.2700 C.3	1	****	
0.2700						
12 C	-97.9140	22.8800	42.6820 C.3	1	****	
0.2800						
13 H	-97.3220	23.4030	41.9200 H	1	****	
0.0000						
14 O	-97.1160	22.3130	43.7400 O.3	1	****	-
0.3630						
15 C	-96.0570	21.5370	43.3100 C.ar	1	****	
0.0830						
16 H	-98.3740	22.0240	42.1750 H	1	****	
0.0000						
17 H	-99.5650	23.2300	44.0490 H	1	****	
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18 S	-98.3760	25.3190	45.4720 S.3	1	****	
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19 C	-96.8590	26.1930	45.7240 C.ar	1	****	
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20 O	-99.4530	26.2250	45.8170 O.3	1	****	-
0.2150						
21 O	-98.2640	24.0370	46.1360 O.3	1	****	-
0.2150						
22 C	-96.6800	26.9420	46.8900 C.ar	1	****	-
0.1500						
23 H	-97.4430	26.9970	47.6630 H	1	****	
0.1500						
24 C	-95.4710	27.6160	47.0660 C.ar	1	****	
0.0860						
25 C	-94.4860	27.5670	46.0800 C.ar	1	****	
0.1170						
26 C	-94.6690	26.8620	44.9040 C.ar	1	****	-
0.1500						
27 H	-93.9100	26.8330	44.1310 H	1	****	
0.1500						
28 C	-95.8750	26.1720	44.7220 C.ar	1	****	-
0.1500						
29 H	-96.0330	25.6220	43.7990 H	1	****	
0.1500						
30 C	-94.9610	28.4380	48.1570 C.2	1	****	
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31 O	-95.5250	28.7260	49.1970 O.2	1	****	-
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32 C	-93.5790	28.8800	47.7590 C.2	1	****	
0.6300						
33 O	-92.7740	29.6000	48.3430 O.2	1	****	-
0.5700						
34 N	-93.3690	28.3080	46.4910 N.am	1	****	-
0.4770						
35 C	-92.1540	28.4700	45.7300 C.3	1	****	
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36 H	-91.7800	27.4810	45.4380 H	1	****	
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37 H	-92.3920	28.9880	44.7950 H	1	****	
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38 C	-91.0540	29.1780	46.4900 C.ar	1	****	-
0.1440						
39 C	-96.3410	20.2040	43.0180 C.ar	1	****	-
0.1500						
40 H	-97.3590	19.8360	43.1050 H	1	****	
0.1500						
41 C	-95.3200	19.3470	42.6090 C.ar	1	****	-
0.1500						
42 H	-95.5430	18.3100	42.3740 H	1	****	
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43 C	-94.0110	19.8170	42.5110 C.ar	1	****	-
0.1500						
44 H	-93.2140	19.1480	42.1980 H	1	****	
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45 C	-93.7200	21.1440	42.8300 C.ar	1	****	-
0.1500						
46 H	-92.6970	21.5050	42.7750 H	1	****	
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47 C	-94.7390	22.0050	43.2380 C.ar	1	****	-
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48 H	-94.4940	23.0240	43.5190 H	1	****	
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49 C	-90.2400	28.4750	47.3900 C.ar	1	****	-
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50 H	-90.3770	27.4060	47.5320 H	1	****	
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51 C	-89.2470	29.1310	48.1230 C.ar	1	****	-
0.1500						
52 H	-88.6490	28.5450	48.8100 H	1	****	
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53 C	-89.0550	30.5090	47.9650 C.ar	1	****	
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54 C	-89.8620	31.2150	47.0740 C.ar	1	****	-
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55 H	-89.7230	32.2860	46.9500 H	1	****	
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56 C	-90.8530	30.5590	46.3440 C.ar	1	****	-
0.1500						
57 H	-91.4750	31.1320	45.6600 H	1	****	
0.1500						
58 O	-88.1140	31.2800	48.6340 O.3	1	****	-
0.3630						

59 C	-86.7630	31.1580	48.1850 C.3	1	****
0.2800					
60 H	-86.6710	31.4410	47.1300 H	1	****
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61 H	-86.1530	31.8540	48.7700 H	1	****
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62 H	-86.3780	30.1490	48.3610 H	1	****
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0.2700
      3 H      -99.2590    26.7980    43.2450 H      1      ****
0.0000
      4 H      -97.5930    26.6480    42.6360 H      1      ****
0.0000
      5 C      -99.0730    25.4740    41.5620 C.3      1      ****
0.0000
      6 H      -99.6940    26.1670    40.9870 H      1      ****
0.0000
      7 H      -98.2560    25.1370    40.9150 H      1      ****
0.0000
      8 C      -99.8550    24.2940    42.0960 C.3      1      ****
0.0000
      9 H     -100.8010    24.6430    42.5260 H      1      ****
0.0000
     10 H     -100.0920    23.5610    41.3180 H      1      ****
0.0000
     11 C      -98.9550    23.7370    43.2060 C.3      1      ****
0.2700
     12 C      -97.8940    22.7630    42.6570 C.3      1      ****
0.2800
     13 H      -97.3110    23.2070    41.8400 H      1      ****
0.0000
     14 O      -97.0790    22.2590    43.7330 O.3      1      ****      -
0.3630

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15 C	-96.1300	21.3330	43.3410 C.ar	1	****	
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16 H	-98.3960	21.8860	42.2350 H	1	****	
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17 H	-99.5570	23.2390	43.9690 H	1	****	
0.0000						
18 S	-98.2680	25.2510	45.4170 S.3	1	****	
0.5380						
19 C	-96.7570	26.1290	45.6920 C.ar	1	****	
0.0070						
20 O	-99.3510	26.1590	45.7360 O.3	1	****	-
0.2150						
21 O	-98.1670	23.9730	46.0900 O.3	1	****	-
0.2150						
22 C	-96.6070	26.8960	46.8520 C.ar	1	****	-
0.1500						
23 H	-97.3870	26.9630	47.6050 H	1	****	
0.1500						
24 C	-95.3990	27.5710	47.0470 C.ar	1	****	
0.0860						
25 C	-94.3890	27.5040	46.0880 C.ar	1	****	
0.1170						
26 C	-94.5460	26.7820	44.9180 C.ar	1	****	-
0.1500						
27 H	-93.7670	26.7410	44.1660 H	1	****	
0.1500						
28 C	-95.7470	26.0930	44.7170 C.ar	1	****	-
0.1500						
29 H	-95.8820	25.5280	43.7980 H	1	****	
0.1500						
30 C	-94.9170	28.4100	48.1370 C.2	1	****	
0.4840						
31 O	-95.5100	28.7160	49.1560 O.2	1	****	-
0.5700						
32 C	-93.5240	28.8430	47.7690 C.2	1	****	
0.6300						
33 O	-92.7350	29.5730	48.3600 O.2	1	****	-
0.5700						
34 N	-93.2810	28.2500	46.5170 N.am	1	****	-
0.4770						
35 C	-92.0450	28.3930	45.7880 C.3	1	****	
0.4440						
36 H	-91.6530	27.3960	45.5510 H	1	****	
0.0000						
37 H	-92.2580	28.8690	44.8230 H	1	****	
0.0000						
38 C	-90.9760	29.1440	46.5490 C.ar	1	****	-
0.1440						
39 C	-94.8040	21.7640	43.3330 C.ar	1	****	-
0.1500						
40 H	-94.5580	22.7710	43.6550 H	1	****	
0.1500						
41 C	-93.7940	20.8960	42.9170 C.ar	1	****	-
0.1500						
42 H	-92.7580	21.2270	42.9190 H	1	****	
0.1500						

43 C	-94.1140	19.6070	42.4910 C.ar	1	****	-
0.1500						
44 H	-93.3260	18.9330	42.1630 H	1	****	
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45 C	-95.4430	19.1860	42.4690 C.ar	1	****	-
0.1500						
46 H	-95.6940	18.1910	42.1180 H	1	****	
0.1500						
47 C	-96.4570	20.0510	42.8870 C.ar	1	****	-
0.1500						
48 H	-97.4900	19.7250	42.8340 H	1	****	
0.1500						
49 C	-90.1220	28.4670	47.4360 C.ar	1	****	-
0.1500						
50 H	-90.2010	27.3910	47.5660 H	1	****	
0.1500						
51 C	-89.1620	29.1660	48.1700 C.ar	1	****	-
0.1500						
52 H	-88.5050	28.6470	48.8590 H	1	****	
0.1500						
53 C	-89.0540	30.5420	48.0220 C.ar	1	****	
0.1900						
54 F	-88.1370	31.2120	48.7330 F	1	****	-
0.1900						
55 C	-89.8860	31.2350	47.1530 C.ar	1	****	-
0.1500						
56 H	-89.7890	32.3110	47.0540 H	1	****	
0.1500						
57 C	-90.8460	30.5370	46.4180 C.ar	1	****	-
0.1500						
58 H	-91.5010	31.0860	45.7450 H	1	****	
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      2 C      -98.9290    26.1210    42.9770 C.3      1      ****
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      3 H      -99.7020    26.7460    43.4310 H      1      ****
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      4 H      -98.0640    26.7440    42.7340 H      1      ****
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5 C	-99.4890	25.4370	41.7410 C.3	1	****	
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6 H	-100.1990	26.0690	41.2010 H	1	****	
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7 H	-98.6810	25.1720	41.0500 H	1	****	
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8 C	-100.1300	24.1930	42.3140 C.3	1	****	
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9 H	-101.0800	24.4590	42.7950 H	1	****	
0.0000						
10 H	-100.3430	23.4390	41.5490 H	1	****	
0.0000						
11 C	-99.1250	23.7250	43.3720 C.3	1	****	
0.2700						
12 C	-98.0120	22.8480	42.7660 C.3	1	****	
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13 H	-97.3080	23.4360	42.1630 H	1	****	
0.0000						
14 O	-97.3730	22.0740	43.7990 O.3	1	****	-
0.3630						
15 C	-96.3280	21.2850	43.3530 C.ar	1	****	
0.0830						
16 H	-98.4610	22.1150	42.0870 H	1	****	
0.0000						
17 H	-99.6380	23.1760	44.1660 H	1	****	
0.0000						
18 S	-98.4610	25.3020	45.5470 S.3	1	****	
0.5380						
19 C	-96.9280	26.1550	45.7650 C.ar	1	****	
0.0070						
20 O	-99.5190	26.2280	45.8990 O.3	1	****	-
0.2150						
21 O	-98.3580	24.0240	46.2210 O.3	1	****	-
0.2150						
22 C	-96.7210	26.9170	46.9190 C.ar	1	****	-
0.1500						
23 H	-97.4710	26.9930	47.7020 H	1	****	
0.1500						
24 C	-95.4970	27.5760	47.0690 C.ar	1	****	
0.0860						
25 C	-94.5280	27.4960	46.0690 C.ar	1	****	
0.1170						
26 C	-94.7410	26.7790	44.9050 C.ar	1	****	-
0.1500						
27 H	-93.9930	26.7310	44.1220 H	1	****	
0.1500						
28 C	-95.9580	26.1080	44.7500 C.ar	1	****	-
0.1500						
29 H	-96.1390	25.5500	43.8340 H	1	****	
0.1500						
30 C	-94.9620	28.4070	48.1390 C.2	1	****	
0.4840						
31 O	-95.5100	28.7220	49.1800 O.2	1	****	-
0.5700						
32 C	-93.5790	28.8220	47.7140 C.2	1	****	
0.6300						

33 O	-92.7570	29.5410	48.2750 O.2	1	****	-
0.5700						
34 N	-93.3960	28.2280	46.4540 N.am	1	****	-
0.4770						
35 C	-92.1900	28.3620	45.6710 C.3	1	****	
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36 H	-91.8380	27.3640	45.3850 H	1	****	
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37 H	-92.4350	28.8770	44.7340 H	1	****	
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38 C	-91.0700	29.0600	46.4090 C.ar	1	****	-
0.1440						
39 C	-96.6600	20.0120	42.8920 C.ar	1	****	-
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40 H	-97.6980	19.6970	42.8660 H	1	****	
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41 C	-95.6560	19.1460	42.4560 C.ar	1	****	-
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42 H	-95.9120	18.1570	42.0880 H	1	****	
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43 C	-94.3210	19.5490	42.5000 C.ar	1	****	-
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44 H	-93.5380	18.8730	42.1670 H	1	****	
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45 C	-93.9860	20.8120	42.9900 C.ar	1	****	-
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46 H	-92.9460	21.1160	43.0450 H	1	****	
0.1500						
47 C	-94.9880	21.6810	43.4250 C.ar	1	****	-
0.1500						
48 H	-94.7140	22.6470	43.8360 H	1	****	
0.1500						
49 C	-90.8990	30.4460	46.3020 C.ar	1	****	-
0.1500						
50 H	-91.5860	31.0420	45.7050 H	1	****	
0.1500						
51 C	-89.8460	31.0860	46.9580 C.ar	1	****	-
0.1500						
52 H	-89.7400	32.1630	46.8570 H	1	****	
0.1500						
53 C	-88.9330	30.3560	47.7250 C.ar	1	****	
0.1010						
54 S	-87.6130	31.2330	48.5510 S.3	1	****	-
0.3310						
55 C	-86.5140	31.5840	47.1490 C.3	1	****	
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56 H	-85.6180	32.1150	47.4840 H	1	****	
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57 H	-86.2050	30.6390	46.6940 H	1	****	
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58 H	-87.0280	32.1750	46.3860 H	1	****	
0.0000						
59 C	-89.1060	28.9730	47.8430 C.ar	1	****	-
0.1500						
60 H	-88.4320	28.3770	48.4510 H	1	****	
0.1500						

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        61 C          -90.1560    28.3320    47.1850 C.ar        1      ****    -
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        62 H          -90.2640    27.2530    47.2860 H          1      ****
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USER_CHARGES

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2 C      -99.0770   25.9770   42.9410 C.3      1      ****
0.2700
3 H      -99.9130   26.5200   43.3850 H      1      ****
0.0000
4 H      -98.2950   26.6880   42.6610 H      1      ****
0.0000
5 C      -99.5610   25.1790   41.7430 C.3      1      ****
0.0000
6 H     -100.3560   25.6940   41.1950 H      1      ****
0.0000
7 H      -98.7360   24.9930   41.0450 H      1      ****
0.0000
8 C     -100.0270   23.8850   42.3720 C.3      1      ****
0.0000
9 H     -100.9970   24.0430   42.8610 H      1      ****
0.0000
10 H     -100.1520   23.0820   41.6390 H      1      ****
0.0000
11 C     -98.9540   23.5900   43.4270 C.3      1      ****
0.2700
12 C     -97.7430   22.8490   42.8260 C.3      1      ****
0.2800
13 H     -97.0940   23.5050   42.2330 H      1      ****
0.0000
14 O     -97.0390   22.1160   43.8440 O.3      1      ****      -
0.3630
15 C     -96.0860   21.2100   43.4100 C.ar      1      ****
0.0830
16 H     -98.1090   22.0870   42.1280 H      1      ****
0.0000

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17 H	-99.3770	23.0030	44.2460 H	1	****	
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18 S	-98.5090	25.3250	45.5380 S.3	1	****	
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19 C	-96.9450	26.1170	45.7730 C.ar	1	****	
0.0070						
20 O	-99.5270	26.3190	45.8160 O.3	1	****	-
0.2150						
21 O	-98.4890	24.0720	46.2650 O.3	1	****	-
0.2150						
22 C	-96.7260	26.8970	46.9140 C.ar	1	****	-
0.1500						
23 H	-97.4840	27.0200	47.6820 H	1	****	
0.1500						
24 C	-95.4850	27.5200	47.0630 C.ar	1	****	
0.0860						
25 C	-94.5060	27.3830	46.0820 C.ar	1	****	
0.1170						
26 C	-94.7230	26.6400	44.9340 C.ar	1	****	-
0.1500						
27 H	-93.9690	26.5460	44.1620 H	1	****	
0.1500						
28 C	-95.9620	26.0110	44.7750 C.ar	1	****	-
0.1500						
29 H	-96.1500	25.4430	43.8670 H	1	****	
0.1500						
30 C	-94.9390	28.3730	48.1120 C.2	1	****	
0.4840						
31 O	-95.4850	28.7330	49.1380 O.2	1	****	-
0.5700						
32 C	-93.5430	28.7440	47.6880 C.2	1	****	
0.6300						
33 O	-92.7130	29.4700	48.2270 O.2	1	****	-
0.5700						
34 N	-93.3590	28.0990	46.4530 N.am	1	****	-
0.4770						
35 C	-92.1400	28.1690	45.6810 C.3	1	****	
0.4440						
36 H	-91.8580	27.1610	45.3560 H	1	****	
0.0000						
37 H	-92.3550	28.7380	44.7690 H	1	****	
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38 C	-90.9700	28.7620	46.4330 C.ar	1	****	-
0.1440						
39 C	-94.7750	21.6850	43.3840 C.ar	1	****	-
0.1500						
40 H	-94.5610	22.6970	43.7140 H	1	****	
0.1500						
41 C	-93.7370	20.8650	42.9410 C.ar	1	****	-
0.1500						
42 H	-92.7180	21.2380	42.9300 H	1	****	
0.1500						
43 C	-94.0110	19.5690	42.5070 C.ar	1	****	-
0.1500						
44 H	-93.2070	18.9310	42.1560 H	1	****	
0.1500						

45 C	-95.3240	19.0970	42.5060 C.ar	1	****	-
0.1500						
46 H	-95.5420	18.0950	42.1470 H	1	****	
0.1500						
47 C	-96.3640	19.9160	42.9510 C.ar	1	****	-
0.1500						
48 H	-97.3800	19.5370	42.9050 H	1	****	
0.1500						
49 C	-90.7270	30.1450	46.3830 C.ar	1	****	-
0.1500						
50 H	-91.3900	30.7990	45.8230 H	1	****	
0.1500						
51 C	-89.6400	30.7030	47.0540 C.ar	1	****	-
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52 H	-89.4620	31.7730	47.0040 H	1	****	
0.1500						
53 C	-88.7910	29.8760	47.7900 C.ar	1	****	
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54 C	-88.9880	28.4980	47.8230 C.ar	1	****	-
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55 H	-88.3050	27.8580	48.3700 H	1	****	
0.1500						
56 C	-90.0760	27.9430	47.1470 C.ar	1	****	-
0.1500						
57 H	-90.2260	26.8670	47.1760 H	1	****	
0.1500						
58 O	-87.6720	30.3990	48.4420 O.3	1	****	-
0.2330						
59 C	-86.7510	30.9880	47.5920 C.2	1	****	
0.6590						
60 C	-85.4940	31.2750	48.3600 C.3	1	****	
0.0610						
61 H	-84.6430	31.2830	47.6730 H	1	****	
0.0000						
62 H	-85.5670	32.2570	48.8360 H	1	****	
0.0000						
63 H	-85.3300	30.4950	49.1080 H	1	****	
0.0000						
64 O	-86.8950	31.2500	46.4040 O.2	1	****	-
0.5700						
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SMALL
USER_CHARGES

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0.2700						
3 H	-99.1610	26.8670	43.2130 H	1	*****	
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4 H	-97.5040	26.6630	42.5960 H	1	*****	
0.0000						
5 C	-99.0400	25.6130	41.4730 C.3	1	*****	
0.0000						
6 H	-99.6330	26.3590	40.9340 H	1	*****	
0.0000						
7 H	-98.2400	25.2710	40.8060 H	1	*****	
0.0000						
8 C	-99.8700	24.4420	41.9520 C.3	1	*****	
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9 H	-100.7990	24.8110	42.4030 H	1	*****	
0.0000						
10 H	-100.1410	23.7590	41.1420 H	1	*****	
0.0000						
11 C	-98.9930	23.7960	43.0300 C.3	1	*****	
0.2700						
12 C	-97.9680	22.8130	42.4290 C.3	1	*****	
0.2800						
13 H	-97.2330	23.3180	41.7910 H	1	*****	
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14 O	-97.3710	22.0170	43.4710 O.3	1	*****	-
0.3630						
15 C	-96.2640	21.2890	43.0740 C.ar	1	*****	
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16 H	-98.4930	22.0990	41.7840 H	1	*****	
0.0000						
17 H	-99.6120	23.2810	43.7680 H	1	*****	
0.0000						
18 S	-98.2590	25.1750	45.3140 S.3	1	*****	
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19 C	-96.7660	26.0720	45.6180 C.ar	1	*****	
0.0070						
20 O	-99.3620	26.0410	45.6780 O.3	1	*****	-
0.2150						
21 O	-98.1250	23.8680	45.9230 O.3	1	*****	-
0.2150						
22 C	-96.6510	26.8460	46.7760 C.ar	1	*****	-
0.1500						
23 H	-97.4550	26.9220	47.5030 H	1	*****	
0.1500						
24 C	-95.4540	27.5290	47.0010 C.ar	1	*****	
0.0860						
25 C	-94.4190	27.4620	46.0670 C.ar	1	*****	
0.1170						
26 C	-94.5410	26.7360	44.8950 C.ar	1	*****	-
0.1500						

27 H	-93.7430	26.6990	44.1630 H	1	****	
0.1500						
28 C	-95.7310	26.0370	44.6680 C.ar	1	****	-
0.1500						
29 H	-95.8410	25.4660	43.7490 H	1	****	
0.1500						
30 C	-95.0030	28.3720	48.0990 C.2	1	****	
0.4840						
31 O	-95.6220	28.6900	49.0990 O.2	1	****	-
0.5700						
32 C	-93.5980	28.7950	47.7710 C.2	1	****	
0.6300						
33 O	-92.8110	29.4870	48.4130 O.2	1	****	-
0.5700						
34 N	-93.3230	28.2080	46.5240 N.am	1	****	-
0.4770						
35 C	-92.0720	28.3560	45.8220 C.3	1	****	
0.4440						
36 H	-91.6700	27.3620	45.5940 H	1	****	
0.0000						
37 H	-92.2730	28.8310	44.8540 H	1	****	
0.0000						
38 C	-91.0210	29.1140	46.5990 C.ar	1	****	-
0.1440						
39 C	-96.4990	19.9830	42.6460 C.ar	1	****	-
0.1500						
40 H	-97.5150	19.5990	42.6080 H	1	****	
0.1500						
41 C	-95.4310	19.1720	42.2610 C.ar	1	****	-
0.1500						
42 H	-95.6160	18.1580	41.9190 H	1	****	
0.1500						
43 C	-94.1270	19.6620	42.3220 C.ar	1	****	-
0.1500						
44 H	-93.2950	19.0290	42.0280 H	1	****	
0.1500						
45 C	-93.8870	20.9590	42.7800 C.ar	1	****	-
0.1500						
46 H	-92.8700	21.3320	42.8490 H	1	****	
0.1500						
47 C	-94.9530	21.7730	43.1640 C.ar	1	****	-
0.1500						
48 H	-94.7500	22.7660	43.5500 H	1	****	
0.1500						
49 C	-90.2800	28.4720	47.6060 C.ar	1	****	-
0.1500						
50 H	-90.4320	27.4150	47.8120 H	1	****	
0.1500						
51 C	-89.3410	29.1780	48.3570 C.ar	1	****	-
0.1500						
52 H	-88.7730	28.6780	49.1350 H	1	****	
0.1500						
53 C	-89.1400	30.5300	48.1110 C.ar	1	****	
0.0830						
54 C	-89.8630	31.1940	47.1210 C.ar	1	****	-
0.1500						

55 H	-89.7160	32.2500	46.9240 H	1	****	
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56 C	-90.8030	30.4840	46.3720 C.ar	1	****	-
0.1500						
57 H	-91.3690	31.0060	45.6030 H	1	****	
0.1500						
58 O	-88.2100	31.1900	48.8780 O.3	1	****	-
0.5320						
59 H	-87.6040	31.6600	48.2820 H	1	****	
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USER_CHARGES

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      2 C      -98.4700    26.1270    42.8080 C.3      1      ****
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      3 H      -99.2100    26.8160    43.2200 H      1      ****
0.0000
      4 H      -97.5350    26.6660    42.6330 H      1      ****
0.0000
      5 C      -99.0040    25.5060    41.5290 C.3      1      ****
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      6 H      -99.6100    26.2070    40.9480 H      1      ****
0.0000
      7 H      -98.1800    25.1650    40.8920 H      1      ****
0.0000
      8 C      -99.8030    24.3280    42.0420 C.3      1      ****
0.0000
      9 H     -100.7530    24.6830    42.4580 H      1      ****
0.0000
     10 H     -100.0360    23.6030    41.2560 H      1      ****
0.0000
     11 C      -98.9270    23.7570    43.1620 C.3      1      ****
0.2700
     12 C      -97.8670    22.7740    42.6250 C.3      1      ****
0.2800
     13 H      -97.1940    23.2530    41.9020 H      1      ****
0.0000
     14 O      -97.1780    22.1470    43.7230 O.3      1      ****      -
0.3630
     15 C      -96.1840    21.2670    43.3340 C.ar     1      ****
0.0830

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16 H	-98.3690	21.9610	42.0900 H	1	****	
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17 H	-99.5450	23.2620	43.9140 H	1	****	
0.0000						
18 S	-98.2440	25.2490	45.3910 S.3	1	****	
0.5380						
19 C	-96.7340	26.1230	45.6830 C.ar	1	****	
0.0070						
20 O	-99.3280	26.1560	45.7110 O.3	1	****	-
0.2150						
21 O	-98.1490	23.9640	46.0560 O.3	1	****	-
0.2150						
22 C	-96.5920	26.8890	46.8430 C.ar	1	****	-
0.1500						
23 H	-97.3790	26.9560	47.5910 H	1	****	
0.1500						
24 C	-95.3880	27.5660	47.0470 C.ar	1	****	
0.0860						
25 C	-94.3720	27.4970	46.0930 C.ar	1	****	
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26 C	-94.5180	26.7700	44.9250 C.ar	1	****	-
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27 H	-93.7350	26.7220	44.1780 H	1	****	
0.1500						
28 C	-95.7180	26.0840	44.7150 C.ar	1	****	-
0.1500						
29 H	-95.8470	25.5180	43.7960 H	1	****	
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30 C	-94.9140	28.4110	48.1360 C.2	1	****	
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31 O	-95.5130	28.7220	49.1500 O.2	1	****	-
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32 C	-93.5200	28.8450	47.7730 C.2	1	****	
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33 O	-92.7350	29.5820	48.3650 O.2	1	****	-
0.5700						
34 N	-93.2690	28.2480	46.5260 N.am	1	****	-
0.4770						
35 C	-92.0280	28.3920	45.8020 C.3	1	****	
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36 H	-91.6240	27.3950	45.5900 H	1	****	
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37 H	-92.2340	28.8440	44.8250 H	1	****	
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38 C	-90.9800	29.1680	46.5590 C.ar	1	****	-
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39 C	-94.8790	21.7580	43.3280 C.ar	1	****	-
0.1500						
40 H	-94.6800	22.7770	43.6470 H	1	****	
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41 C	-93.8300	20.9360	42.9170 C.ar	1	****	-
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42 H	-92.8110	21.3150	42.9190 H	1	****	
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43 C	-94.0900	19.6320	42.4930 C.ar	1	****	-
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44 H	-93.2730	18.9950	42.1680 H	1	****	
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45 C	-95.4000	19.1510	42.4730 C.ar	1	****	-
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46 H	-95.6020	18.1430	42.1230 H	1	****	
0.1500						
47 C	-96.4510	19.9700	42.8850 C.ar	1	****	-
0.1500						
48 H	-97.4690	19.5970	42.8330 H	1	****	
0.1500						
49 C	-90.1530	28.5460	47.4960 C.ar	1	****	
0.1600						
50 H	-90.2260	27.4800	47.6920 H	1	****	
0.1500						
51 N	-89.2170	29.1840	48.2360 N.ar	1	****	-
0.6200						
52 C	-89.0980	30.5140	48.0350 C.ar	1	****	
0.5000						
53 F	-88.1830	31.1700	48.7650 F	1	****	-
0.1900						
54 C	-89.8590	31.2330	47.1270 C.ar	1	****	-
0.1500						
55 H	-89.7120	32.3010	47.0130 H	1	****	
0.1500						
56 C	-90.8140	30.5490	46.3800 C.ar	1	****	-
0.1500						
57 H	-91.4290	31.0900	45.6650 H	1	****	
0.1500						
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SMALL
USER_CHARGES

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      2 C      -98.3060    26.2310    42.7200 C.3      1      ****
0.2700
      3 H      -99.0610    26.8820    43.1640 H      1      ****
0.0000
      4 H      -97.3650    26.7800    42.6290 H      1      ****
0.0000
      5 C      -98.7930    25.7300    41.3690 C.3      1      ****
0.0000
      6 H      -99.3740    26.4850    40.8310 H      1      ****
0.0000
      7 H      -97.9450    25.4420    40.7370 H      1      ****
0.0000

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8 C	-99.6140	24.5160	41.7440 C.3	1	****	
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9 H	-100.5780	24.8390	42.1540 H	1	****	
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10 H	-99.8170	23.8650	40.8890 H	1	****	
0.0000						
11 C	-98.7820	23.8420	42.8420 C.3	1	****	
0.2700						
12 C	-97.7090	22.9020	42.2620 C.3	1	****	
0.2800						
13 H	-96.9490	23.4740	41.7160 H	1	****	
0.0000						
14 O	-97.0940	22.1750	43.3370 O.3	1	****	-
0.3630						
15 C	-96.0960	21.2750	42.9970 C.ar	1	****	
0.0830						
16 H	-98.1860	22.1840	41.5860 H	1	****	
0.0000						
17 H	-99.4340	23.2920	43.5260 H	1	****	
0.0000						
18 S	-98.1240	25.1150	45.2150 S.3	1	****	
0.5380						
19 C	-96.6490	26.0190	45.5740 C.ar	1	****	
0.0070						
20 O	-99.2440	25.9400	45.6170 O.3	1	****	-
0.2150						
21 O	-97.9690	23.7790	45.7550 O.3	1	****	-
0.2150						
22 C	-96.5820	26.7990	46.7330 C.ar	1	****	-
0.1500						
23 H	-97.4150	26.8720	47.4270 H	1	****	
0.1500						
24 C	-95.4040	27.5000	46.9930 C.ar	1	****	
0.0860						
25 C	-94.3420	27.4440	46.0910 C.ar	1	****	
0.1170						
26 C	-94.4090	26.7000	44.9260 C.ar	1	****	-
0.1500						
27 H	-93.5870	26.6670	44.2200 H	1	****	
0.1500						
28 C	-95.5800	25.9840	44.6630 C.ar	1	****	-
0.1500						
29 H	-95.6510	25.4050	43.7460 H	1	****	
0.1500						
30 C	-95.0030	28.3670	48.0930 C.2	1	****	
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31 O	-95.6560	28.6750	49.0740 O.2	1	****	-
0.5700						
32 C	-93.6040	28.8320	47.7910 C.2	1	****	
0.6300						
33 O	-92.8480	29.5550	48.4350 O.2	1	****	-
0.5700						
34 N	-93.2890	28.2460	46.5530 N.am	1	****	-
0.4770						
35 C	-92.0480	28.4630	45.8490 C.3	1	****	
0.4440						

36 H	-91.6300	27.4980	45.5400 H	1	****	
0.0000						
37 H	-92.2790	29.0190	44.9330 H	1	****	
0.0000						
38 C	-91.0070	29.1860	46.6730 C.ar	1	****	-
0.1440						
39 C	-96.2850	19.9300	42.6530 C.ar	1	****	-
0.1500						
40 H	-97.2690	19.4780	42.6240 H	1	****	
0.1500						
41 C	-95.1830	19.1310	42.3350 C.ar	1	****	-
0.1500						
42 H	-95.3290	18.0890	42.0660 H	1	****	
0.1500						
43 C	-93.8960	19.6670	42.3610 C.ar	1	****	-
0.1500						
44 H	-93.0410	19.0420	42.1150 H	1	****	
0.1500						
45 C	-93.7060	21.0050	42.7050 C.ar	1	****	-
0.1500						
46 H	-92.7050	21.4250	42.7240 H	1	****	
0.1500						
47 C	-94.8040	21.8050	43.0200 C.ar	1	****	-
0.1500						
48 H	-94.6560	22.8490	43.2830 H	1	****	
0.1500						
49 C	-90.7390	30.5400	46.4400 C.ar	1	****	-
0.1500						
50 H	-91.2740	31.1000	45.6800 H	1	****	
0.1500						
51 C	-89.7730	31.1760	47.2120 C.ar	1	****	
0.1600						
52 H	-89.5410	32.2260	47.0610 H	1	****	
0.1500						
53 N	-89.0640	30.5660	48.1840 N.ar	1	****	-
0.6200						
54 C	-89.3250	29.2560	48.3820 C.ar	1	****	
0.5000						
55 F	-88.6180	28.6240	49.3310 F	1	****	-
0.1900						
56 C	-90.2570	28.5280	47.6600 C.ar	1	****	-
0.1500						
57 H	-90.3960	27.4740	47.8790 H	1	****	
0.1500						
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3 H	-99.3320	26.8400	43.1910 H	1	*****	
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4 H	-97.6650	26.7190	42.5820 H	1	*****	
0.0000						
5 C	-99.1380	25.5730	41.4670 C.3	1	*****	
0.0000						
6 H	-99.7730	26.2780	40.9220 H	1	*****	
0.0000						
7 H	-98.3190	25.2760	40.8030 H	1	*****	
0.0000						
8 C	-99.8970	24.3590	41.9540 C.3	1	*****	
0.0000						
9 H	-100.8480	24.6740	42.3980 H	1	*****	
0.0000						
10 H	-100.1230	23.6530	41.1490 H	1	*****	
0.0000						
11 C	-98.9850	23.7760	43.0390 C.3	1	*****	
0.2700						
12 C	-97.8950	22.8580	42.4490 C.3	1	*****	
0.2800						
13 H	-97.1870	23.4390	41.8440 H	1	*****	
0.0000						
14 O	-97.1940	22.2020	43.5160 O.3	1	*****	-
0.3630						
15 C	-96.1700	21.3380	43.1590 C.ar	1	*****	
0.0830						
16 H	-98.3730	22.0950	41.8230 H	1	*****	
0.0000						
17 H	-99.5730	23.2290	43.7790 H	1	*****	
0.0000						
18 S	-98.3440	25.2190	45.3120 S.3	1	*****	
0.5380						
19 C	-96.8360	26.0900	45.6220 C.ar	1	*****	
0.0070						
20 O	-99.4340	26.1100	45.6600 O.3	1	*****	-
0.2150						
21 O	-98.2370	23.9180	45.9400 O.3	1	*****	-
0.2150						
22 C	-96.7050	26.8480	46.7900 C.ar	1	*****	-
0.1500						
23 H	-97.5030	26.9220	47.5240 H	1	*****	
0.1500						
24 C	-95.5050	27.5250	47.0090 C.ar	1	*****	
0.0860						
25 C	-94.4830	27.4640	46.0620 C.ar	1	*****	
0.1170						
26 C	-94.6160	26.7420	44.8880 C.ar	1	*****	-
0.1500						
27 H	-93.8250	26.7110	44.1460 H	1	*****	
0.1500						

28 C	-95.8110	26.0530	44.6640 C.ar	1	****	-
0.1500						
29 H	-95.9310	25.4960	43.7380 H	1	****	
0.1500						
30 C	-95.0420	28.3710	48.1020 C.2	1	****	
0.4840						
31 O	-95.6460	28.6730	49.1150 O.2	1	****	-
0.5700						
32 C	-93.6480	28.8140	47.7460 C.2	1	****	
0.6300						
33 O	-92.8570	29.5210	48.3640 O.2	1	****	-
0.5700						
34 N	-93.3920	28.2290	46.4970 N.am	1	****	-
0.4770						
35 C	-92.1700	28.4120	45.7490 C.3	1	****	
0.4440						
36 H	-91.7580	27.4330	45.4770 H	1	****	
0.0000						
37 H	-92.4030	28.9240	44.8090 H	1	****	
0.0000						
38 C	-91.1250	29.1730	46.5320 C.ar	1	****	
0.1670						
39 C	-96.3160	19.9850	42.8250 C.ar	1	****	-
0.1500						
40 H	-97.2830	19.4970	42.8180 H	1	****	
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41 C	-95.1920	19.2260	42.4880 C.ar	1	****	-
0.1500						
42 H	-95.3060	18.1780	42.2270 H	1	****	
0.1500						
43 C	-93.9260	19.8080	42.4840 C.ar	1	****	-
0.1500						
44 H	-93.0540	19.2140	42.2230 H	1	****	
0.1500						
45 C	-93.7790	21.1540	42.8140 C.ar	1	****	-
0.1500						
46 H	-92.7930	21.6120	42.8100 H	1	****	
0.1500						
47 C	-94.8980	21.9160	43.1490 C.ar	1	****	-
0.1500						
48 H	-94.7830	22.9660	43.4030 H	1	****	
0.1500						
49 C	-90.1780	28.4960	47.3080 C.ar	1	****	-
0.1500						
50 H	-90.1780	27.4100	47.3560 H	1	****	
0.1500						
51 C	-89.2510	29.2350	48.0380 C.ar	1	****	-
0.1500						
52 H	-88.5080	28.7320	48.6490 H	1	****	
0.1500						
53 C	-89.2950	30.6240	47.9830 C.ar	1	****	-
0.1500						
54 H	-88.5950	31.2360	48.5380 H	1	****	
0.1500						
55 C	-90.2700	31.2140	47.1920 C.ar	1	****	
0.5000						

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    56 F      -90.3150   32.5540   47.1340 F      1      ***** -
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    57 N      -91.1750   30.5300   46.4610 N.ar    1      ***** -
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USER_CHARGES

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0.2100
  3 H      -98.0510   27.2180   46.6810 H      1      *****
0.0000
  4 H      -96.7230   26.0250   46.8200 H      1      *****
0.0000
  5 C      -98.6130   25.1510   46.0290 C.3      1      *****
0.0000
  6 H      -98.5350   24.3110   46.7240 H      1      *****
0.0000
  7 H      -99.6580   25.4720   45.9600 H      1      *****
0.0000
  8 C      -97.8990   24.9650   44.6690 C.3      1      *****
0.2100
  9 C      -98.7970   24.7510   43.4620 C.3      1      *****
0.2800
 10 H      -98.2010   24.6590   42.5450 H      1      *****
0.0000
 11 O      -99.5650   23.5590   43.6810 O.3      1      ***** -
0.3630
 12 C     -100.6680   23.3680   42.8620 C.ar     1      *****
0.0830
 13 H      -99.4770   25.6060   43.3700 H      1      *****
0.0000
 14 H      -97.0870   24.2290   44.7320 H      1      *****
0.0000
 15 S      -96.0980   27.1100   43.9990 S.3      1      *****
0.5380
 16 C      -94.7700   26.9000   45.1390 C.ar     1      *****
0.0070
 17 O      -95.7990   26.3360   42.8110 O.3      1      ***** -
0.2150
 18 O      -96.3660   28.5300   43.8980 O.3      1      ***** -
0.2150
 19 C      -94.8020   27.5970   46.3520 C.ar     1      ***** -
0.1500

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20 H	-95.6080	28.2790	46.6070 H	1	****	
0.1500						
21 C	-93.7750	27.3680	47.2660 C.ar	1	****	
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22 C	-92.7420	26.4940	46.9420 C.ar	1	****	
0.1170						
23 C	-92.6750	25.8240	45.7380 C.ar	1	****	-
0.1500						
24 H	-91.8570	25.1490	45.5100 H	1	****	
0.1500						
25 C	-93.7100	26.0340	44.8200 C.ar	1	****	-
0.1500						
26 H	-93.6920	25.5070	43.8700 H	1	****	
0.1500						
27 C	-93.5100	27.8690	48.6100 C.2	1	****	
0.4840						
28 O	-94.1770	28.6520	49.2610 O.2	1	****	-
0.5700						
29 C	-92.2270	27.2210	49.0600 C.2	1	****	
0.6300						
30 O	-91.5740	27.3350	50.0920 O.2	1	****	-
0.5700						
31 N	-91.8390	26.4130	47.9910 N.am	1	****	-
0.5470						
32 H	-91.0070	25.8480	48.0080 H	1	****	
0.3700						
33 C	-100.7370	23.6700	41.4940 C.ar	1	****	-
0.1500						
34 H	-99.8940	24.0870	40.9580 H	1	****	
0.1500						
35 C	-101.9170	23.4300	40.7870 C.ar	1	****	-
0.1500						
36 H	-101.9690	23.6630	39.7270 H	1	****	
0.1500						
37 C	-103.0280	22.8900	41.4340 C.ar	1	****	-
0.1500						
38 H	-103.9440	22.7040	40.8800 H	1	****	
0.1500						
39 C	-102.9600	22.5850	42.7920 C.ar	1	****	-
0.1500						
40 H	-103.8220	22.1610	43.2990 H	1	****	
0.1500						
41 C	-101.7840	22.8240	43.5030 C.ar	1	****	-
0.1500						
42 H	-101.7350	22.5850	44.5610 H	1	****	
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SMALL
USER_CHARGES

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0.2100
      3 H      -98.2330    26.7520    42.6080 H      1      ****
0.0000
      4 H      -99.9300    26.6190    43.1690 H      1      ****
0.0000
      5 C      -99.2700    24.8820    41.9390 C.3      1      ****
0.0000
      6 H     -100.1820    24.9410    41.3380 H      1      ****
0.0000

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7 H	-98.4180	24.6600	41.2860 H	1	****	
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8 C	-99.3600	24.0080	43.2130 C.3	1	****	
0.2100						
9 C	-98.6190	22.6830	43.1730 C.3	1	****	
0.2800						
10 H	-98.9430	22.0810	42.3160 H	1	****	
0.0000						
11 O	-97.2120	22.9590	43.0850 O.3	1	****	-
0.3630						
12 C	-96.3700	21.8690	42.9310 C.ar	1	****	
0.0830						
13 H	-98.8210	22.1350	44.1010 H	1	****	
0.0000						
14 H	-100.3950	23.9100	43.5660 H	1	****	
0.0000						
15 S	-98.5190	25.3630	45.6090 S.3	1	****	
0.5380						
16 C	-96.9970	26.2380	45.7780 C.ar	1	****	
0.0070						
17 O	-99.5970	26.2550	45.9820 O.3	1	****	-
0.2150						
18 O	-98.3620	24.0870	46.2780 O.3	1	****	-
0.2150						
19 C	-96.7720	26.9920	46.9320 C.ar	1	****	-
0.1500						
20 H	-97.5120	27.0720	47.7230 H	1	****	
0.1500						
21 C	-95.5370	27.6220	47.0770 C.ar	1	****	
0.0860						
22 C	-94.5770	27.5240	46.0700 C.ar	1	****	
0.1170						
23 C	-94.8060	26.8110	44.9060 C.ar	1	****	-
0.1500						
24 H	-94.0550	26.7410	44.1260 H	1	****	
0.1500						
25 C	-96.0340	26.1590	44.7590 C.ar	1	****	-
0.1500						
26 H	-96.2240	25.5790	43.8610 H	1	****	
0.1500						
27 C	-94.9680	28.4320	48.1470 C.2	1	****	
0.4840						
28 O	-95.4940	28.7470	49.1990 O.2	1	****	-
0.5700						
29 C	-93.5790	28.8180	47.7090 C.2	1	****	
0.6300						
30 O	-92.7350	29.5130	48.2680 O.2	1	****	-
0.5700						
31 N	-93.4280	28.2290	46.4430 N.am	1	****	-
0.4770						
32 C	-92.2470	28.3280	45.6250 C.3	1	****	
0.3000						
33 H	-91.5440	29.0500	46.0520 H	1	****	
0.0000						
34 H	-91.7600	27.3490	45.5710 H	1	****	
0.0000						

35 H	-92.5280	28.6600	44.6210 H	1	*****	
0.0000						
36 C	-96.7740	20.5280	42.8400 C.ar	1	*****	-
0.1500						
37 H	-97.8170	20.2410	42.8810 H	1	*****	
0.1500						
38 C	-95.8170	19.5220	42.6860 C.ar	1	*****	-
0.1500						
39 H	-96.1320	18.4860	42.6160 H	1	*****	
0.1500						
40 C	-94.4610	19.8450	42.6260 C.ar	1	*****	-
0.1500						
41 H	-93.7200	19.0580	42.5070 H	1	*****	
0.1500						
42 C	-94.0590	21.1760	42.7110 C.ar	1	*****	-
0.1500						
43 H	-93.0040	21.4300	42.6590 H	1	*****	
0.1500						
44 C	-95.0120	22.1840	42.8620 C.ar	1	*****	-
0.1500						
45 H	-94.6940	23.2190	42.9300 H	1	*****	
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18b
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SMALL
USER_CHARGES

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  3 H      -97.3180   26.6470   42.2810 H      1      ****
0.0000
  4 H      -99.0730   26.6680   42.6360 H      1      ****
0.0000
  5 C      -98.4310   24.8840   41.4660 C.3      1      ****
0.0000
  6 H      -99.2600   25.0270   40.7660 H      1      ****
0.0000
  7 H      -97.5330   24.5920   40.9110 H      1      ****
0.0000
  8 C      -98.7440   24.0140   42.7070 C.3      1      ****
0.2100
  9 C      -98.1170   22.6300   42.7290 C.3      1      ****
0.2800
 10 H      -98.4280   22.0480   41.8520 H      1      ****
0.0000
 11 O      -96.6900   22.7820   42.7490 O.3      1      ****      -
0.3630
 12 C      -95.9400   21.6240   42.6050 C.ar     1      ****
0.0830
 13 H      -98.4380   22.1130   43.6420 H      1      ****
0.0000
 14 H      -99.8180   24.0010   42.9340 H      1      ****
0.0000
 15 S      -98.0870   25.2820   45.2080 S.3      1      ****
0.5380
 16 C      -96.6330   26.2250   45.5300 C.ar     1      ****
0.0070

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17 O	-99.2390	26.1220	45.4710 O.3	1	****	-
0.2150						
18 O	-97.9430	24.0050	45.8770 O.3	1	****	-
0.2150						
19 C	-96.5510	26.9640	46.7130 C.ar	1	****	-
0.1500						
20 H	-97.3740	27.0140	47.4200 H	1	****	
0.1500						
21 C	-95.3580	27.6320	46.9920 C.ar	1	****	
0.0860						
22 C	-94.2940	27.5790	46.0900 C.ar	1	****	
0.1170						
23 C	-94.3840	26.8850	44.8960 C.ar	1	****	-
0.1500						
24 H	-93.5610	26.8520	44.1920 H	1	****	
0.1500						
25 C	-95.5700	26.2000	44.6140 C.ar	1	****	-
0.1500						
26 H	-95.6470	25.6310	43.6910 H	1	****	
0.1500						
27 C	-94.9290	28.4250	48.1350 C.2	1	****	
0.4840						
28 O	-95.5770	28.7080	49.1270 O.2	1	****	-
0.5700						
29 C	-93.5080	28.8370	47.8660 C.2	1	****	
0.6300						
30 O	-92.7290	29.4870	48.5590 O.2	1	****	-
0.5700						
31 N	-93.2030	28.2890	46.6070 N.am	1	****	-
0.4770						
32 C	-91.9290	28.4440	45.9480 C.3	1	****	
0.4440						
33 C	-90.9530	29.3070	46.7140 C.ar	1	****	-
0.1440						
34 H	-91.4710	27.4560	45.8150 H	1	****	
0.0000						
35 H	-92.1060	28.8360	44.9400 H	1	****	
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36 C	-96.4500	20.3180	42.5460 C.ar	1	****	-
0.1500						
37 H	-97.5130	20.1150	42.6050 H	1	****	
0.1500						
38 C	-95.5790	19.2360	42.4040 C.ar	1	****	-
0.1500						
39 H	-95.9760	18.2260	42.3560 H	1	****	
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40 C	-94.2030	19.4450	42.3190 C.ar	1	****	-
0.1500						
41 H	-93.5300	18.6010	42.2080 H	1	****	
0.1500						
42 C	-93.6950	20.7420	42.3740 C.ar	1	****	-
0.1500						
43 H	-92.6240	20.9110	42.3040 H	1	****	
0.1500						
44 C	-94.5620	21.8260	42.5160 C.ar	1	****	-
0.1500						

45 H	-94.1610	22.8340	42.5580 H	1	****	
0.1500						
46 C	-90.1840	28.7620	47.7540 C.ar	1	****	-
0.1500						
47 H	-90.2610	27.7070	48.0000 H	1	****	
0.1500						
48 C	-89.3050	29.5640	48.4830 C.ar	1	****	-
0.1500						
49 H	-88.7120	29.1310	49.2830 H	1	****	
0.1500						
50 C	-89.1880	30.9210	48.1870 C.ar	1	****	-
0.1500						
51 H	-88.5040	31.5450	48.7550 H	1	****	
0.1500						
52 C	-89.9510	31.4770	47.1640 C.ar	1	****	-
0.1500						
53 H	-89.8640	32.5350	46.9330 H	1	****	
0.1500						
54 C	-90.8300	30.6770	46.4330 C.ar	1	****	-
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55 H	-91.4170	31.1260	45.6350 H	1	****	
0.1500						

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  2 C      -98.6520   26.1680   42.8140 C.3      1      ****
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  3 H      -97.7660   26.7560   42.5630 H      1      ****
0.0000
  4 H      -99.4730   26.8310   43.1010 H      1      ****
0.0000
  5 C      -99.0340   25.0720   41.8050 C.3      1      ****
0.0000
  6 H      -99.9190   25.2770   41.1980 H      1      ****
0.0000
  7 H      -98.2080   24.7640   41.1540 H      1      ****
0.0000
  8 C      -99.2600   24.1690   43.0410 C.3      1      ****
0.2100
  9 C      -98.7050   22.7570   42.9510 C.3      1      ****
0.2800
 10 H      -98.8500   22.3470   41.9450 H      1      ****
0.0000
 11 O      -97.3070   22.8000   43.2750 O.3      1      ****      -
0.3630

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12 C	-96.5830	21.6360	43.0650 C.ar	1	****	
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13 H	-99.2250	22.1260	43.6810 H	1	****	
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14 H	-100.3050	24.1960	43.3770 H	1	****	
0.0000						
15 S	-98.2960	25.3050	45.5030 S.3	1	****	
0.5380						
16 C	-96.8190	26.2460	45.7090 C.ar	1	****	
0.0070						
17 O	-99.4140	26.1270	45.9210 O.3	1	****	-
0.2150						
18 O	-98.0760	24.0070	46.1070 O.3	1	****	-
0.2150						
19 C	-96.6460	26.9930	46.8760 C.ar	1	****	-
0.1500						
20 H	-97.4100	27.0430	47.6480 H	1	****	
0.1500						
21 C	-95.4310	27.6530	47.0630 C.ar	1	****	
0.0860						
22 C	-94.4360	27.5890	46.0880 C.ar	1	****	
0.1170						
23 C	-94.6170	26.8880	44.9080 C.ar	1	****	-
0.1500						
24 H	-93.8480	26.8410	44.1480 H	1	****	
0.1500						
25 C	-95.8260	26.2090	44.7180 C.ar	1	****	-
0.1500						
26 H	-95.9730	25.6330	43.8080 H	1	****	
0.1500						
27 C	-94.9160	28.4510	48.1680 C.2	1	****	
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28 O	-95.4840	28.7400	49.2050 O.2	1	****	-
0.5700						
29 C	-93.5200	28.8630	47.7890 C.2	1	****	
0.6300						
30 O	-92.7060	29.5590	48.3900 O.2	1	****	-
0.5700						
31 N	-93.3080	28.3000	46.5180 N.am	1	****	-
0.4770						
32 C	-92.0800	28.4370	45.7740 C.3	1	****	
0.4440						
33 C	-90.9890	29.1520	46.5380 C.ar	1	****	-
0.1440						
34 H	-91.7090	27.4390	45.5110 H	1	****	
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35 H	-92.2970	28.9380	44.8240 H	1	****	
0.0000						
36 C	-97.1260	20.3580	42.8640 C.ar	1	****	-
0.1500						
37 H	-98.1970	20.1870	42.8550 H	1	****	
0.1500						
38 C	-96.2800	19.2650	42.6650 C.ar	1	****	-
0.1500						
39 H	-96.7030	18.2760	42.5090 H	1	****	
0.1500						

40 C	-94.8970	19.4380	42.6640 C.ar	1	****	-
0.1500						
41 H	-94.2430	18.5840	42.5090 H	1	****	
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42 C	-94.3550	20.7060	42.8600 C.ar	1	****	-
0.1500						
43 H	-93.2780	20.8450	42.8540 H	1	****	
0.1500						
44 C	-95.1970	21.8010	43.0570 C.ar	1	****	-
0.1500						
45 H	-94.7700	22.7880	43.2080 H	1	****	
0.1500						
46 C	-90.1610	28.4530	47.4270 C.ar	1	****	-
0.1500						
47 H	-90.2800	27.3800	47.5600 H	1	****	
0.1500						
48 C	-89.1730	29.1160	48.1610 C.ar	1	****	-
0.1500						
49 H	-88.5600	28.5300	48.8360 H	1	****	
0.1500						
50 C	-89.0020	30.4990	48.0170 C.ar	1	****	
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51 C	-89.8230	31.2010	47.1350 C.ar	1	****	-
0.1500						
52 H	-89.6980	32.2740	47.0210 H	1	****	
0.1500						
53 C	-90.8080	30.5370	46.4040 C.ar	1	****	-
0.1500						
54 H	-91.4400	31.1060	45.7270 H	1	****	
0.1500						
55 O	-88.0670	31.2760	48.6870 O.3	1	****	-
0.3630						
56 C	-86.7420	31.2770	48.1530 C.3	1	****	
0.2800						
57 H	-86.3010	30.2740	48.1930 H	1	****	
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58 H	-86.7270	31.6770	47.1340 H	1	****	
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59 H	-86.1310	31.9340	48.7790 H	1	****	
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1 N	-98.5720	25.0790	43.9660 N.3	1	****	-
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2 C	-98.9250	26.1290	42.9640 C.3	1	****	
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3 H	-98.0770	26.7580	42.6820 H	1	****	
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4 H	-99.7640	26.7550	43.2840 H	1	****	
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5 C	-99.2940	25.0190	41.9680 C.3	1	****	
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6 H	-100.2100	25.1850	41.3920 H	1	****	
0.0000						
7 H	-98.4810	24.7470	41.2850 H	1	****	
0.0000						
8 C	-99.4380	24.1070	43.2090 C.3	1	****	
0.2100						
9 C	-98.8280	22.7190	43.0970 C.3	1	****	
0.2800						
10 H	-98.8470	22.3690	42.0580 H	1	****	
0.0000						
11 O	-97.4770	22.7800	43.5790 O.3	1	****	-
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12 C	-96.6610	21.7000	43.2790 C.ar	1	****	
0.0830						
13 H	-99.4050	22.0290	43.7240 H	1	****	
0.0000						
14 H	-100.4700	24.0920	43.5830 H	1	****	
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15 S	-98.4300	25.2820	45.6350 S.3	1	****	
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16 C	-96.9470	26.2240	45.7870 C.ar	1	****	
0.0070						
17 O	-99.5330	26.1060	46.0880 O.3	1	****	-
0.2150						
18 O	-98.1910	23.9850	46.2350 O.3	1	****	-
0.2150						
19 C	-96.7340	26.9730	46.9460 C.ar	1	****	-
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20 H	-97.4670	27.0230	47.7450 H	1	****	
0.1500						
21 C	-95.5130	27.6360	47.0860 C.ar	1	****	
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22 C	-94.5530	27.5670	46.0750 C.ar	1	****	
0.1170						
23 C	-94.7760	26.8640	44.9040 C.ar	1	****	-
0.1500						
24 H	-94.0340	26.8180	44.1160 H	1	****	
0.1500						
25 C	-95.9920	26.1880	44.7590 C.ar	1	****	-
0.1500						
26 H	-96.1740	25.6140	43.8540 H	1	****	
0.1500						
27 C	-94.9630	28.4440	48.1650 C.2	1	****	
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28 O	-95.4980	28.7400	49.2170 O.2	1	****	-
0.5700						

29 C	-93.5810	28.8550	47.7340 C.2	1	****	
0.6300						
30 O	-92.7530	29.5620	48.3040 O.2	1	****	-
0.5700						
31 N	-93.4090	28.2790	46.4640 N.am	1	****	-
0.4770						
32 C	-92.2050	28.4030	45.6800 C.3	1	****	
0.4440						
33 C	-91.0820	29.1110	46.4020 C.ar	1	****	-
0.1440						
34 H	-91.8520	27.4020	45.4070 H	1	****	
0.0000						
35 H	-92.4540	28.9060	44.7380 H	1	****	
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36 C	-97.0930	20.3920	43.0130 C.ar	1	****	-
0.1500						
37 H	-98.1430	20.1260	43.0210 H	1	****	
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38 C	-96.1600	19.3940	42.7260 C.ar	1	****	-
0.1500						
39 H	-96.4990	18.3830	42.5190 H	1	****	
0.1500						
40 C	-94.7990	19.6900	42.7010 C.ar	1	****	-
0.1500						
41 H	-94.0760	18.9090	42.4780 H	1	****	
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42 C	-94.3650	20.9900	42.9600 C.ar	1	****	-
0.1500						
43 H	-93.3050	21.2250	42.9380 H	1	****	
0.1500						
44 C	-95.2940	21.9900	43.2470 C.ar	1	****	-
0.1500						
45 H	-94.9520	23.0010	43.4490 H	1	****	
0.1500						
46 C	-90.9030	30.4930	46.2610 C.ar	1	****	-
0.1500						
47 H	-91.5910	31.0760	45.6560 H	1	****	
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48 C	-89.8460	31.1440	46.9000 C.ar	1	****	-
0.1500						
49 H	-89.7470	32.2180	46.7840 H	1	****	
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50 C	-88.9370	30.4230	47.6820 C.ar	1	****	
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51 C	-89.1150	29.0460	47.8330 C.ar	1	****	-
0.1500						
52 H	-88.4290	28.4640	48.4430 H	1	****	
0.1500						
53 C	-90.1720	28.3950	47.1960 C.ar	1	****	-
0.1500						
54 H	-90.2870	27.3200	47.3220 H	1	****	
0.1500						
55 S	-87.5800	31.2220	48.5210 S.3	1	****	-
0.3310						
56 C	-86.5870	31.7440	47.0940 C.3	1	****	
0.2300						

57 H	-86.2300	30.8750	46.5350 H	1	****
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58 H	-87.1650	32.3920	46.4310 H	1	****
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59 H	-85.7190	32.3070	47.4510 H	1	****
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SMALL
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2 C      -98.2750   26.0490   42.5660 C.3      1      ****
0.2100
3 H      -97.3860   26.6490   42.3520 H      1      ****
0.0000
4 H      -99.1370   26.7040   42.7280 H      1      ****
0.0000
5 C      -98.5310   24.8710   41.6130 C.3      1      ****
0.0000
6 H      -99.3630   25.0020   40.9140 H      1      ****
0.0000
7 H      -97.6410   24.5440   41.0640 H      1      ****
0.0000
8 C      -98.8480   24.0530   42.8890 C.3      1      ****
0.2100
9 C      -98.2520   22.6580   42.9560 C.3      1      ****
0.2800
10 H     -98.2810   22.1750   41.9700 H      1      ****
0.0000
11 O     -96.8980   22.7660   43.4170 O.3      1      ****      -
0.3630
12 C     -96.0510   21.7100   43.1170 C.ar     1      ****
0.0830
13 H     -98.8320   22.0600   43.6700 H      1      ****
0.0000
14 H     -99.9190   24.0730   43.1260 H      1      ****
0.0000
15 S     -98.1430   25.3990   45.3330 S.3      1      ****
0.5380
16 C     -96.6680   26.3240   45.6150 C.ar     1      ****
0.0070
17 O     -99.2730   26.2720   45.5760 O.3      1      ****      -
0.2150

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18 O	-98.0200	24.1460	46.0510 O.3	1	****	-
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19 C	-96.5380	27.0490	46.8020 C.ar	1	****	-
0.1500						
20 H	-97.3290	27.0890	47.5440 H	1	****	
0.1500						
21 C	-95.3250	27.6970	47.0470 C.ar	1	****	
0.0860						
22 C	-94.2930	27.6410	46.1090 C.ar	1	****	
0.1170						
23 C	-94.4350	26.9630	44.9110 C.ar	1	****	-
0.1500						
24 H	-93.6340	26.9230	44.1810 H	1	****	
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25 C	-95.6390	26.2990	44.6610 C.ar	1	****	-
0.1500						
26 H	-95.7560	25.7420	43.7340 H	1	****	
0.1500						
27 C	-94.8490	28.4740	48.1840 C.2	1	****	
0.4840						
28 O	-95.4580	28.7490	49.2010 O.2	1	****	-
0.5700						
29 C	-93.4360	28.8800	47.8680 C.2	1	****	
0.6300						
30 O	-92.6410	29.5620	48.5100 O.2	1	****	-
0.5700						
31 N	-93.1760	28.3330	46.5990 N.am	1	****	-
0.4770						
32 C	-91.9160	28.4630	45.9090 C.3	1	****	
0.4440						
33 C	-90.8850	29.2580	46.6790 C.ar	1	****	-
0.1440						
34 H	-91.5030	27.4620	45.7290 H	1	****	
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35 H	-92.0990	28.8950	44.9200 H	1	****	
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36 C	-96.4490	20.3950	42.8320 C.ar	1	****	-
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37 H	-97.4930	20.1030	42.8210 H	1	****	
0.1500						
38 C	-95.4890	19.4220	42.5480 C.ar	1	****	-
0.1500						
39 H	-95.7990	18.4060	42.3260 H	1	****	
0.1500						
40 C	-94.1340	19.7510	42.5450 C.ar	1	****	-
0.1500						
41 H	-93.3900	18.9900	42.3240 H	1	****	
0.1500						
42 C	-93.7360	21.0570	42.8230 C.ar	1	****	-
0.1500						
43 H	-92.6820	21.3180	42.8180 H	1	****	
0.1500						
44 C	-94.6920	22.0320	43.1080 C.ar	1	****	-
0.1500						
45 H	-94.3780	23.0480	43.3240 H	1	****	
0.1500						

46 C	-90.0550	28.6280	47.6200 C.ar	1	****	-
0.1500						
47 H	-90.1270	27.5570	47.7890 H	1	****	
0.1500						
48 C	-89.1280	29.3670	48.3550 C.ar	1	****	-
0.1500						
49 H	-88.4850	28.8820	49.0830 H	1	****	
0.1500						
50 C	-89.0310	30.7380	48.1560 C.ar	1	****	
0.1900						
51 F	-88.1430	31.4450	48.8680 F	1	****	-
0.1900						
52 C	-89.8400	31.3850	47.2330 C.ar	1	****	-
0.1500						
53 H	-89.7520	32.4580	47.0950 H	1	****	
0.1500						
54 C	-90.7680	30.6470	46.4980 C.ar	1	****	-
0.1500						
55 H	-91.4050	31.1600	45.7800 H	1	****	
0.1500						

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0.2100
  3 H      -97.2480   26.6470   42.1890 H      1      ****
0.0000
  4 H      -99.0110   26.5610   42.4920 H      1      ****
0.0000
  5 C      -98.1920   24.7240   41.5310 C.3      1      ****
0.0000
  6 H      -99.0010   24.7300   40.7970 H      1      ****
0.0000
  7 H      -97.2530   24.4510   41.0360 H      1      ****
0.0000
  8 C      -98.4810   23.9630   42.8470 C.3      1      ****
0.2100
  9 C      -97.7520   22.6430   43.0310 C.3      1      ****
0.2800
 10 H      -97.9070   21.9880   42.1650 H      1      ****
0.0000
 11 O      -96.3540   22.9190   43.2050 O.3      1      ****      -
0.3630
 12 C      -95.4750   21.8860   42.9190 C.ar     1      ****
0.0830

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13 H	-98.1360	22.1500	43.9330 H	1	****	
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14 H	-99.5580	23.8890	43.0450 H	1	****	
0.0000						
15 S	-98.0140	25.5250	45.2200 S.3	1	****	
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16 C	-96.5320	26.4210	45.5520 C.ar	1	****	
0.0070						
17 O	-99.1320	26.4400	45.3330 O.3	1	****	-
0.2150						
18 O	-97.9800	24.3120	46.0110 O.3	1	****	-
0.2150						
19 C	-96.4270	27.1360	46.7470 C.ar	1	****	-
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20 H	-97.2430	27.1840	47.4640 H	1	****	
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21 C	-95.2120	27.7560	47.0410 C.ar	1	****	
0.0860						
22 C	-94.1520	27.6970	46.1370 C.ar	1	****	
0.1170						
23 C	-94.2640	27.0280	44.9300 C.ar	1	****	-
0.1500						
24 H	-93.4410	26.9730	44.2300 H	1	****	
0.1500						
25 C	-95.4710	26.3830	44.6360 C.ar	1	****	-
0.1500						
26 H	-95.5630	25.8290	43.7030 H	1	****	
0.1500						
27 C	-94.7550	28.4910	48.2120 C.2	1	****	
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28 O	-95.3910	28.7530	49.2160 O.2	1	****	-
0.5700						
29 C	-93.3220	28.8700	47.9550 C.2	1	****	
0.6300						
30 O	-92.5250	29.4820	48.6610 O.2	1	****	-
0.5700						
31 N	-93.0420	28.3690	46.6690 N.am	1	****	-
0.4770						
32 C	-91.7670	28.5250	46.0100 C.3	1	****	
0.4440						
33 C	-90.7780	29.3610	46.7810 C.ar	1	****	-
0.1440						
34 H	-91.3220	27.5370	45.8420 H	1	****	
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35 H	-91.9510	28.9440	45.0130 H	1	****	
0.0000						
36 C	-95.7850	20.5190	42.9290 C.ar	1	****	-
0.1500						
37 H	-96.7790	20.1610	43.1660 H	1	****	
0.1500						
38 C	-94.7980	19.5790	42.6230 C.ar	1	****	-
0.1500						
39 H	-95.0410	18.5200	42.6290 H	1	****	
0.1500						
40 C	-93.5050	19.9940	42.3080 C.ar	1	****	-
0.1500						

41 H	-92.7410	19.2590	42.0690 H	1	****	
0.1500						
42 C	-93.1960	21.3530	42.2930 C.ar	1	****	-
0.1500						
43 H	-92.1910	21.6800	42.0440 H	1	****	
0.1500						
44 C	-94.1780	22.2950	42.5980 C.ar	1	****	-
0.1500						
45 H	-93.9340	23.3530	42.5870 H	1	****	
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46 C	-90.6740	30.7420	46.5510 C.ar	1	****	-
0.1500						
47 H	-91.3170	31.2290	45.8210 H	1	****	
0.1500						
48 C	-89.7460	31.5160	47.2520 C.ar	1	****	-
0.1500						
49 H	-89.6800	32.5830	47.0650 H	1	****	
0.1500						
50 C	-88.9020	30.9210	48.1880 C.ar	1	****	-
0.1500						
51 H	-88.1790	31.5230	48.7310 H	1	****	
0.1500						
52 C	-88.9810	29.5510	48.4170 C.ar	1	****	-
0.1500						
53 H	-88.3200	29.0700	49.1320 H	1	****	
0.1500						
54 C	-89.9090	28.7860	47.7160 C.ar	1	****	
0.1900						
55 F	-89.9380	27.4660	47.9430 F	1	****	-
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54 58 1 0 0
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USER_CHARGES

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      2 C      -98.4820    26.0840    42.7030 C.3      1      ****
0.2100
      3 H      -97.5850    26.6590    42.4610 H      1      ****
0.0000
      4 H      -99.3150    26.7610    42.9140 H      1      ****
0.0000
      5 C      -98.8180    24.9370    41.7380 C.3      1      ****
0.0000
      6 H      -99.6830    25.1040    41.0890 H      1      ****
0.0000
      7 H      -97.9680    24.6060    41.1300 H      1      ****
0.0000

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0.2100	8 C	-99.0820	24.0900	43.0060 C.3	1	****	
0.2800	9 C	-98.4940	22.6890	43.0050 C.3	1	****	
0.0000	10 H	-98.6030	22.2210	42.0190 H	1	****	
0.3630	11 O	-97.1080	22.7860	43.3620 O.3	1	****	-
0.0830	12 C	-96.3040	21.6990	43.0540 C.ar	1	****	
0.0000	13 H	-99.0190	22.0840	43.7560 H	1	****	
0.0000	14 H	-100.1390	24.1120	43.2990 H	1	****	
0.5380	15 S	-98.2310	25.3600	45.4470 S.3	1	****	
0.0070	16 C	-96.7330	26.2610	45.6760 C.ar	1	****	
0.2150	17 O	-99.3420	26.2300	45.7740 O.3	1	****	-
0.2150	18 O	-98.0810	24.0840	46.1180 O.3	1	****	-
0.1500	19 C	-96.5730	27.0230	46.8350 C.ar	1	****	-
0.1500	20 H	-97.3540	27.1010	47.5860 H	1	****	
0.0860	21 C	-95.3460	27.6560	47.0460 C.ar	1	****	
0.1170	22 C	-94.3290	27.5650	46.0950 C.ar	1	****	
0.1500	23 C	-94.4980	26.8500	44.9210 C.ar	1	****	-
0.1500	24 H	-93.7110	26.7700	44.1820 H	1	****	
0.1500	25 C	-95.7140	26.1870	44.7130 C.ar	1	****	-
0.1500	26 H	-95.8490	25.5980	43.8090 H	1	****	
0.4840	27 C	-94.8430	28.4440	48.1630 C.2	1	****	
0.5700	28 O	-95.4340	28.7510	49.1820 O.2	1	****	-
0.6300	29 C	-93.4260	28.8160	47.8250 C.2	1	****	
0.5700	30 O	-92.6050	29.4780	48.4560 O.2	1	****	-
0.4770	31 N	-93.1960	28.2550	46.5540 N.am	1	****	-
0.4440	32 C	-91.9420	28.3710	45.8500 C.3	1	****	
0.1440	33 C	-90.9110	29.1800	46.5960 C.ar	1	****	-
0.0000	34 H	-91.5450	27.3600	45.6990 H	1	****	
0.0000	35 H	-92.1040	28.7760	44.8450 H	1	****	

36 C	-96.7460	20.3870	42.8360 C.ar	1	****	-
0.1500						
37 H	-97.7950	20.1210	42.8900 H	1	****	
0.1500						
38 C	-95.8220	19.3840	42.5370 C.ar	1	****	-
0.1500						
39 H	-96.1650	18.3670	42.3650 H	1	****	
0.1500						
40 C	-94.4620	19.6800	42.4540 C.ar	1	****	-
0.1500						
41 H	-93.7460	18.8950	42.2230 H	1	****	
0.1500						
42 C	-94.0210	20.9850	42.6670 C.ar	1	****	-
0.1500						
43 H	-92.9640	21.2230	42.6020 H	1	****	
0.1500						
44 C	-94.9420	21.9900	42.9650 C.ar	1	****	-
0.1500						
45 H	-94.5960	23.0060	43.1310 H	1	****	
0.1500						
46 C	-90.0330	28.5850	47.5070 C.ar	1	****	
0.1600						
47 H	-90.0600	27.5160	47.6970 H	1	****	
0.1500						
48 N	-89.1080	29.2600	48.2310 N.ar	1	****	-
0.6200						
49 C	-89.0400	30.5940	48.0270 C.ar	1	****	
0.5000						
50 F	-88.1350	31.2830	48.7390 F	1	****	-
0.1900						
51 C	-89.8450	31.2830	47.1360 C.ar	1	****	-
0.1500						
52 H	-89.7360	32.3540	47.0140 H	1	****	
0.1500						
53 C	-90.7920	30.5640	46.4120 C.ar	1	****	-
0.1500						
54 H	-91.4370	31.0860	45.7070 H	1	****	
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0.2100
      3 H      -97.6100    26.7490    42.2560 H      1      ****
0.0000

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4 H	-99.3600	26.5810	42.6050 H	1	****	
0.0000						
5 C	-98.5120	24.8490	41.4870 C.3	1	****	
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6 H	-99.3430	24.8800	40.7760 H	1	****	
0.0000						
7 H	-97.5800	24.6410	40.9490 H	1	****	
0.0000						
8 C	-98.7420	23.9870	42.7520 C.3	1	****	
0.2100						
9 C	-97.9760	22.6760	42.8230 C.3	1	****	
0.2800						
10 H	-98.1900	22.0530	41.9450 H	1	****	
0.0000						
11 O	-96.5740	22.9770	42.8930 O.3	1	****	-
0.3630						
12 C	-95.7020	21.9030	42.7950 C.ar	1	****	
0.0830						
13 H	-98.2760	22.1410	43.7310 H	1	****	
0.0000						
14 H	-99.8100	23.8690	42.9730 H	1	****	
0.0000						
15 S	-98.2170	25.3860	45.2150 S.3	1	****	
0.5380						
16 C	-96.7340	26.2790	45.5360 C.ar	1	****	
0.0070						
17 O	-99.3400	26.2720	45.4430 O.3	1	****	-
0.2150						
18 O	-98.1310	24.1180	45.9100 O.3	1	****	-
0.2150						
19 C	-96.6160	26.9940	46.7310 C.ar	1	****	-
0.1500						
20 H	-97.4270	27.0530	47.4510 H	1	****	
0.1500						
21 C	-95.4050	27.6320	46.9980 C.ar	1	****	
0.0860						
22 C	-94.3620	27.5710	46.0750 C.ar	1	****	
0.1170						
23 C	-94.4810	26.8910	44.8760 C.ar	1	****	-
0.1500						
24 H	-93.6710	26.8480	44.1590 H	1	****	
0.1500						
25 C	-95.6860	26.2390	44.6030 C.ar	1	****	-
0.1500						
26 H	-95.7930	25.6870	43.6720 H	1	****	
0.1500						
27 C	-94.9420	28.4130	48.1370 C.2	1	****	
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28 O	-95.5630	28.6920	49.1470 O.2	1	****	-
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29 C	-93.5250	28.8210	47.8360 C.2	1	****	
0.6300						
30 O	-92.7260	29.4610	48.5130 O.2	1	****	-
0.5700						
31 N	-93.2590	28.2850	46.5650 N.am	1	****	-
0.4770						

32 C	-92.0150	28.4640	45.8550 C.3	1	****	
0.4440						
33 C	-90.9790	29.2360	46.6390 C.ar	1	****	-
0.1440						
34 H	-91.5940	27.4840	45.6050 H	1	****	
0.0000						
35 H	-92.2430	28.9660	44.9070 H	1	****	
0.0000						
36 C	-96.0700	20.5520	42.7270 C.ar	1	****	-
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37 H	-97.1080	20.2400	42.7410 H	1	****	
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38 C	-95.0860	19.5650	42.6330 C.ar	1	****	-
0.1500						
39 H	-95.3740	18.5190	42.5780 H	1	****	
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40 C	-93.7380	19.9170	42.6050 C.ar	1	****	-
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41 H	-92.9760	19.1450	42.5320 H	1	****	
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42 C	-93.3690	21.2600	42.6670 C.ar	1	****	-
0.1500						
43 H	-92.3190	21.5380	42.6410 H	1	****	
0.1500						
44 C	-94.3490	22.2480	42.7610 C.ar	1	****	-
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45 H	-94.0570	23.2930	42.8100 H	1	****	
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46 C	-90.1810	28.5830	47.5880 C.ar	1	****	-
0.1500						
47 H	-90.2760	27.5160	47.7670 H	1	****	
0.1500						
48 C	-89.2430	29.3230	48.2990 C.ar	1	****	
0.1600						
49 H	-88.6050	28.8470	49.0380 H	1	****	
0.1500						
50 N	-89.0510	30.6490	48.1420 N.ar	1	****	-
0.6200						
51 C	-89.8370	31.2600	47.2290 C.ar	1	****	
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52 F	-89.6720	32.5810	47.0640 F	1	****	-
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53 C	-90.8070	30.6180	46.4780 C.ar	1	****	-
0.1500						
54 H	-91.4030	31.1930	45.7760 H	1	****	
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26 25 23 ar
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30 29 27 1
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58 54 53 1
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SMALL
USER_CHARGES

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0.2100						
3 H	-97.6830	26.6600	42.3330 H	1	*****	
0.0000						
4 H	-99.4070	26.4760	42.7860 H	1	*****	
0.0000						
5 C	-98.5900	24.7180	41.6860 C.3	1	*****	
0.0000						
6 H	-99.4600	24.7090	41.0230 H	1	*****	
0.0000						
7 H	-97.6870	24.5060	41.1040 H	1	*****	
0.0000						
8 C	-98.7310	23.9000	42.9920 C.3	1	*****	
0.2100						
9 C	-97.9320	22.6080	43.0610 C.3	1	*****	
0.2800						
10 H	-98.3190	21.8750	42.3450 H	1	*****	
0.0000						
11 O	-96.5570	22.9090	42.7740 O.3	1	*****	-
0.3630						
12 C	-95.6990	21.8250	42.6600 C.ar	1	*****	
0.0830						
13 H	-98.0060	22.2010	44.0760 H	1	*****	
0.0000						
14 H	-99.7830	23.7670	43.2760 H	1	*****	
0.0000						
15 S	-98.1460	25.4010	45.3760 S.3	1	*****	
0.5380						
16 C	-96.6680	26.3330	45.6340 C.ar	1	*****	
0.0070						
17 O	-99.2740	26.2810	45.6030 O.3	1	*****	-
0.2150						
18 O	-98.0240	24.1620	46.1150 O.3	1	*****	-
0.2150						
19 C	-96.5210	27.0610	46.8180 C.ar	1	*****	-
0.1500						
20 H	-97.3070	27.1070	47.5670 H	1	*****	
0.1500						
21 C	-95.3000	27.6970	47.0540 C.ar	1	*****	
0.0860						
22 C	-94.2720	27.6280	46.1120 C.ar	1	*****	
0.1170						
23 C	-94.4290	26.9560	44.9110 C.ar	1	*****	-
0.1500						
24 H	-93.6330	26.9120	44.1760 H	1	*****	
0.1500						
25 C	-95.6450	26.3030	44.6720 C.ar	1	*****	-
0.1500						
26 H	-95.7730	25.7470	43.7470 H	1	*****	
0.1500						
27 C	-94.8080	28.4620	48.1900 C.2	1	*****	
0.4840						
28 O	-95.4100	28.7500	49.2090 O.2	1	*****	-
0.5700						

29 C	-93.3890	28.8430	47.8710 C.2	1	****	
0.6300						
30 O	-92.5860	29.5140	48.5150 O.2	1	****	-
0.5700						
31 N	-93.1390	28.2900	46.6030 N.am	1	****	-
0.4770						
32 C	-91.8650	28.3850	45.9250 C.3	1	****	
0.4440						
33 C	-90.7970	29.1710	46.6550 C.ar	1	****	
0.1670						
34 H	-91.4760	27.3700	45.7780 H	1	****	
0.0000						
35 H	-92.0300	28.8010	44.9250 H	1	****	
0.0000						
36 C	-96.0760	20.4740	42.6660 C.ar	1	****	-
0.1500						
37 H	-97.1140	20.1720	42.7580 H	1	****	
0.1500						
38 C	-95.1070	19.4780	42.5450 C.ar	1	****	-
0.1500						
39 H	-95.4020	18.4330	42.5480 H	1	****	
0.1500						
40 C	-93.7600	19.8190	42.4200 C.ar	1	****	-
0.1500						
41 H	-93.0090	19.0390	42.3270 H	1	****	
0.1500						
42 C	-93.3810	21.1600	42.4110 C.ar	1	****	-
0.1500						
43 H	-92.3340	21.4270	42.3090 H	1	****	
0.1500						
44 C	-94.3480	22.1580	42.5300 C.ar	1	****	-
0.1500						
45 H	-94.0480	23.2010	42.5230 H	1	****	
0.1500						
46 C	-90.6910	30.5620	46.5400 C.ar	1	****	-
0.1500						
47 H	-91.3480	31.1240	45.8810 H	1	****	
0.1500						
48 C	-89.7310	31.2360	47.2930 C.ar	1	****	-
0.1500						
49 H	-89.6320	32.3150	47.2160 H	1	****	
0.1500						
50 C	-88.9120	30.5130	48.1510 C.ar	1	****	-
0.1500						
51 H	-88.1570	31.0010	48.7560 H	1	****	
0.1500						
52 C	-89.0910	29.1420	48.2250 C.ar	1	****	
0.5000						
53 F	-88.3120	28.4430	49.0670 F	1	****	-
0.1900						
54 N	-90.0080	28.4570	47.5080 N.ar	1	****	-
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23 23 22 ar
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36 34 32 1
37 35 32 1
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 44 47 1 0 0
 SMALL
 USER_CHARGES

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2 C	-99.2960	25.9150	43.3500 C.3	1	****	
0.2700						
3 H	-100.3510	25.9860	43.6300 H	1	****	
0.0000						
4 H	-98.8340	26.9050	43.4030 H	1	****	
0.0000						
5 C	-99.1710	25.3230	41.9540 C.3	1	****	
0.0000						
6 H	-99.9400	25.6970	41.2720 H	1	****	
0.0000						
7 H	-98.1890	25.5570	41.5250 H	1	****	
0.0000						
8 C	-99.2910	23.8330	42.2160 C.3	1	****	
0.0000						
9 H	-100.3450	23.5770	42.3780 H	1	****	
0.0000						
10 H	-98.9260	23.2300	41.3790 H	1	****	
0.0000						
11 C	-98.5070	23.6250	43.5210 C.3	1	****	
0.2700						
12 C	-97.0380	23.2410	43.2850 C.3	1	****	
0.2800						
13 H	-96.4000	23.7900	43.9850 H	1	****	
0.0000						
14 O	-96.8940	21.8340	43.5070 O.3	1	****	-
0.3630						
15 C	-95.7050	21.2750	43.1400 C.ar	1	****	
0.0830						
16 H	-96.7440	23.4940	42.2580 H	1	****	
0.0000						
17 H	-99.0000	22.8330	44.0930 H	1	****	
0.0000						
18 S	-98.7340	25.0250	45.8720 S.3	1	****	
0.5380						
19 C	-97.2370	25.8430	46.3970 C.ar	1	****	
0.0070						
20 O	-99.8350	25.9150	46.1750 O.3	1	****	-
0.2150						
21 O	-98.6890	23.6780	46.3940 O.3	1	****	-
0.2150						
22 C	-96.8080	25.6970	47.7210 C.ar	1	****	-
0.1500						
23 H	-97.3390	25.0840	48.4430 H	1	****	
0.1500						
24 C	-95.6650	26.3860	48.0750 C.ar	1	****	
0.0860						
25 C	-94.9720	27.2080	47.1870 C.ar	1	****	
0.1170						

26 C	-95.4010	27.3810	45.8870 C.ar	1	****	-
0.1500						
27 H	-94.8780	28.0300	45.1930 H	1	****	
0.1500						
28 C	-96.5550	26.6910	45.4930 C.ar	1	****	-
0.1500						
29 H	-96.9300	26.8230	44.4780 H	1	****	
0.1500						
30 C	-94.9340	26.4670	49.3360 C.2	1	****	
0.4840						
31 O	-95.2090	25.9220	50.3910 O.2	1	****	-
0.5700						
32 C	-93.7480	27.3900	49.1090 C.2	1	****	
0.6300						
33 O	-92.9030	27.7040	49.9160 O.2	1	****	-
0.5700						
34 N	-93.8630	27.7900	47.7920 N.am	1	****	-
0.5470						
35 H	-93.2100	28.4260	47.3570 H	1	****	
0.3700						
36 C	-95.7630	19.9330	42.7690 C.ar	1	****	-
0.1500						
37 H	-96.7110	19.4040	42.7870 H	1	****	
0.1500						
38 C	-94.6040	19.2690	42.3740 C.ar	1	****	-
0.1500						
39 H	-94.6300	18.2250	42.0820 H	1	****	
0.1500						
40 C	-93.4150	19.9780	42.3630 C.ar	1	****	
0.1600						
41 H	-92.4830	19.5060	42.0620 H	1	****	
0.1500						
42 N	-93.3150	21.2760	42.7160 N.ar	1	****	-
0.6200						
43 C	-94.4610	21.8930	43.0990 C.ar	1	****	
0.1600						
44 H	-94.3170	22.9320	43.3780 H	1	****	
0.1500						
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16	16	12	1			
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18	18	1	1			

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19 19 18 1
20 20 18 1
21 21 18 1
22 22 19 ar
23 23 22 1
24 24 22 ar
25 25 24 ar
26 26 25 ar
27 27 26 1
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36 34 32 1
37 35 34 1
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41 39 38 1
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21a R
47 50 1 0 0
SMALL
USER_CHARGES

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0.6550
      2 C      -89.9160    26.9730    47.4200 C.3      1      ****
0.2700
      3 H      -90.2010    26.5320    48.3790 H      1      ****
0.0000
      4 H      -90.6930    26.7700    46.6770 H      1      ****
0.0000
      5 C      -88.5710    26.4220    46.9740 C.3      1      ****
0.0000
      6 H      -88.4720    25.3500    47.1690 H      1      ****
0.0000
      7 H      -88.4250    26.5900    45.9000 H      1      ****
0.0000
      8 C      -87.5880    27.2590    47.7750 C.3      1      ****
0.0000
      9 H      -87.5410    26.8760    48.8020 H      1      ****
0.0000

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10 H	-86.5760	27.2290	47.3610 H	1	****	
0.0000						
11 C	-88.2150	28.6620	47.7810 C.3	1	****	
0.2700						
12 C	-87.6480	29.5750	46.6800 C.3	1	****	
0.2800						
13 H	-88.2100	30.5080	46.5640 H	1	****	
0.0000						
14 O	-86.2520	29.8320	46.8770 O.3	1	****	-
0.3630						
15 C	-85.6720	30.8190	46.1350 C.ar	1	****	
0.0830						
16 H	-87.7340	29.0710	45.7100 H	1	****	
0.0000						
17 H	-88.0350	29.1000	48.7660 H	1	****	
0.0000						
18 S	-90.8070	29.4110	48.2790 S.3	1	****	
0.5380						
19 C	-92.3490	28.5520	48.0200 C.ar	1	****	
0.0070						
20 O	-90.5480	29.4010	49.7030 O.3	1	****	-
0.2150						
21 O	-90.8740	30.6480	47.5340 O.3	1	****	-
0.2150						
22 C	-92.9200	27.8380	49.0780 C.ar	1	****	-
0.1500						
23 H	-92.4710	27.8000	50.0650 H	1	****	
0.1500						
24 C	-94.0960	27.1670	48.8030 C.ar	1	****	
0.0860						
25 C	-94.6970	27.1590	47.5440 C.ar	1	****	
0.1170						
26 C	-94.1210	27.8410	46.4890 C.ar	1	****	-
0.1500						
27 H	-94.5590	27.8400	45.4950 H	1	****	
0.1500						
28 C	-92.9310	28.5400	46.7310 C.ar	1	****	-
0.1500						
29 H	-92.4520	29.0670	45.9050 H	1	****	
0.1500						
30 C	-94.9500	26.3520	49.6590 C.2	1	****	
0.4840						
31 O	-94.7750	26.0930	50.8370 O.2	1	****	-
0.5700						
32 C	-96.1130	25.8640	48.8130 C.2	1	****	
0.6300						
33 O	-97.0240	25.1630	49.1950 O.2	1	****	-
0.5700						
34 N	-95.8730	26.3940	47.5540 N.am	1	****	-
0.4770						
35 C	-96.7160	26.1830	46.4080 C.3	1	****	
0.3000						
36 C	-85.4150	32.0050	46.8200 C.ar	1	****	-
0.1500						
37 H	-85.6620	32.0870	47.8750 H	1	****	
0.1500						

38 C	-84.8480	33.0880	46.1540 C.ar	1	****	-
0.1500						
39 H	-84.6400	34.0170	46.6720 H	1	****	
0.1500						
40 C	-84.5530	32.9450	44.8090 C.ar	1	****	
0.1600						
41 H	-84.1090	33.7610	44.2430 H	1	****	
0.1500						
42 N	-84.7800	31.8140	44.1090 N.ar	1	****	-
0.6200						
43 C	-85.3140	30.7700	44.7920 C.ar	1	****	
0.1600						
44 H	-85.4370	29.8800	44.1860 H	1	****	
0.1500						
45 H	-97.2180	27.1130	46.1250 H	1	****	
0.0000						
46 H	-96.1070	25.8400	45.5680 H	1	****	
0.0000						
47 H	-97.4740	25.4320	46.6490 H	1	****	
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34	33	32	2
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36	34	32	1

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39 37 36 1
40 38 36 ar
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21b
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SMALL
USER_CHARGES

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2 C      -99.3080   25.5760   43.4400 C.3      1      ****
0.2700
3 H     -100.2770   25.7460   43.9230 H      1      ****
0.0000
4 H      -98.8140   26.5370   43.2770 H      1      ****
0.0000
5 C      -99.5090   24.8220   42.1360 C.3      1      ****
0.0000
6 H     -100.3990   25.1550   41.5950 H      1      ****
0.0000
7 H      -98.6410   24.9520   41.4790 H      1      ****
0.0000
8 C      -99.6110   23.3830   42.6040 C.3      1      ****
0.0000
9 H     -100.6050   23.2110   43.0360 H      1      ****
0.0000
10 H     -99.4680   22.6640   41.7930 H      1      ****
0.0000
11 C     -98.5490   23.2900   43.7040 C.3      1      ****
0.2700
12 C     -97.1730   22.8630   43.1580 C.3      1      ****
0.2800
13 H     -96.5980   23.7360   42.8330 H      1      ****
0.0000
14 O     -96.4740   22.0730   44.1310 O.3      1      ****      -
0.3630
15 C     -95.4030   21.4000   43.6230 C.ar     1      ****
0.0830
16 H     -97.2920   22.2370   42.2650 H      1      ****
0.0000

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17 H	-98.8870	22.5640	44.4500 H	1	****	
0.0000						
18 S	-98.7050	24.8490	45.9440 S.3	1	****	
0.5380						
19 C	-97.2700	25.7630	46.4600 C.ar	1	****	
0.0070						
20 O	-99.8540	25.7080	46.1320 O.3	1	****	-
0.2150						
21 O	-98.6430	23.5290	46.5320 O.3	1	****	-
0.2150						
22 C	-96.8020	25.6360	47.7700 C.ar	1	****	-
0.1500						
23 H	-97.2780	24.9920	48.5030 H	1	****	
0.1500						
24 C	-95.6790	26.3730	48.0920 C.ar	1	****	
0.0860						
25 C	-95.0250	27.2140	47.1900 C.ar	1	****	
0.1170						
26 C	-95.5010	27.3540	45.8990 C.ar	1	****	-
0.1500						
27 H	-95.0240	28.0060	45.1760 H	1	****	
0.1500						
28 C	-96.6400	26.6230	45.5340 C.ar	1	****	-
0.1500						
29 H	-97.0400	26.7190	44.5240 H	1	****	
0.1500						
30 C	-94.9340	26.4630	49.3410 C.2	1	****	
0.4840						
31 O	-95.1910	25.9130	50.3980 O.2	1	****	-
0.5700						
32 C	-93.7660	27.4010	49.1050 C.2	1	****	
0.6300						
33 O	-92.9310	27.7040	49.9300 O.2	1	****	-
0.5700						
34 N	-93.9050	27.8140	47.7890 N.am	1	****	-
0.4770						
35 C	-92.9980	28.7340	47.1440 C.3	1	****	
0.4440						
36 C	-95.6220	20.1350	43.0920 C.ar	1	****	-
0.1500						
37 H	-96.6130	19.6940	43.1110 H	1	****	
0.1500						
38 C	-94.5560	19.4330	42.5360 C.ar	1	****	-
0.1500						
39 H	-94.6930	18.4390	42.1250 H	1	****	
0.1500						
40 C	-93.3080	20.0340	42.5200 C.ar	1	****	
0.1600						
41 H	-92.4480	19.5200	42.0990 H	1	****	
0.1500						
42 N	-93.0620	21.2670	43.0210 N.ar	1	****	-
0.6200						
43 C	-94.1240	21.9320	43.5340 C.ar	1	****	
0.1600						
44 H	-93.9050	22.9400	43.8710 H	1	****	
0.1500						

45 H	-92.8880	28.4540	46.0890 H	1	****	
0.0000						
46 H	-93.4450	29.7350	47.1530 H	1	****	
0.0000						
47 C	-89.0750	28.7320	48.9520 C.ar	1	****	-
0.1500						
48 C	-89.7290	29.9410	48.7100 C.ar	1	****	-
0.1500						
49 C	-90.9960	29.9460	48.1230 C.ar	1	****	-
0.1500						
50 C	-91.6250	28.7370	47.7770 C.ar	1	****	-
0.1440						
51 C	-90.9500	27.5270	48.0180 C.ar	1	****	-
0.1500						
52 C	-89.6840	27.5260	48.6040 C.ar	1	****	-
0.1500						
53 H	-88.0870	28.7290	49.4080 H	1	****	
0.1500						
54 H	-89.2490	30.8830	48.9770 H	1	****	
0.1500						
55 H	-91.4850	30.9020	47.9350 H	1	****	
0.1500						
56 H	-91.4070	26.5750	47.7440 H	1	****	
0.1500						
57 H	-89.1710	26.5810	48.7860 H	1	****	
0.1500						

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23	23	22	1
24	24	22	ar
25	25	24	ar
26	26	25	ar
27	27	26	1
28	28	19	ar
29	28	26	ar
30	29	28	1

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33  32 30 1
34  33 32 2
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37  35 34 1
38  36 15 ar
39  37 36 1
40  38 36 ar
41  39 38 1
42  40 38 ar
43  41 40 1
44  42 40 ar
45  43 15 ar
46  43 42 ar
47  44 43 1
48  45 35 1
49  46 35 1
50  48 47 ar
51  49 48 ar
52  50 35 1
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USER_CHARGES

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2 C      -98.4440    25.9820    43.3280 C.3      1      ****
0.2700
3 H      -99.1410    26.6990    43.7780 H      1      ****
0.0000
4 H      -97.4600    26.4490    43.2350 H      1      ****
0.0000
5 C      -98.9800    25.5320    41.9790 C.3      1      ****
0.0000
6 H      -99.4740    26.3440    41.4370 H      1      ****
0.0000
7 H      -98.1700    25.1460    41.3510 H      1      ****
0.0000
8 C      -99.9340    24.4230    42.3680 C.3      1      ****
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9 H	-100.8520	24.8550	42.7870 H	1	****	
0.0000						
10 H	-100.2170	23.7930	41.5200 H	1	****	
0.0000						
11 C	-99.1740	23.6680	43.4630 C.3	1	****	
0.2700						
12 C	-98.2480	22.5920	42.8680 C.3	1	****	
0.2800						
13 H	-97.6640	22.9790	42.0230 H	1	****	
0.0000						
14 O	-97.4470	22.0180	43.9070 O.3	1	****	-
0.3630						
15 C	-96.5240	21.1020	43.4990 C.ar	1	****	
0.0830						
16 H	-98.8590	21.7710	42.4730 H	1	****	
0.0000						
17 H	-99.8810	23.1930	44.1490 H	1	****	
0.0000						
18 S	-98.6740	25.0050	45.8040 S.3	1	****	
0.5380						
19 C	-97.1950	25.7820	46.4060 C.ar	1	****	
0.0070						
20 O	-99.7340	25.9890	45.8850 O.3	1	****	-
0.2150						
21 O	-98.8080	23.7160	46.4490 O.3	1	****	-
0.2150						
22 C	-97.2190	26.4770	47.6180 C.ar	1	****	-
0.1500						
23 H	-98.1050	26.5320	48.2410 H	1	****	
0.1500						
24 C	-96.0430	27.0940	47.9940 C.ar	1	****	
0.0860						
25 C	-94.8820	27.0860	47.2170 C.ar	1	****	
0.1170						
26 C	-94.8620	26.4150	46.0080 C.ar	1	****	-
0.1500						
27 H	-93.9800	26.3790	45.3790 H	1	****	
0.1500						
28 C	-96.0330	25.7590	45.6020 C.ar	1	****	-
0.1500						
29 H	-96.0380	25.2250	44.6510 H	1	****	
0.1500						
30 C	-95.7270	27.8830	49.1790 C.2	1	****	
0.4840						
31 O	-96.4650	28.1380	50.1130 O.2	1	****	-
0.5700						
32 C	-94.2900	28.3500	49.0430 C.2	1	****	
0.6300						
33 O	-93.6920	29.0390	49.8430 O.2	1	****	-
0.5700						
34 N	-93.8640	27.8380	47.8280 N.am	1	****	-
0.4770						
35 C	-92.5580	28.0970	47.2670 C.3	1	****	
0.4440						
36 C	-95.2240	21.5600	43.3270 C.ar	1	****	-
0.1500						

37 H	-94.9700	22.5910	43.5520 H	1	****	
0.1500						
38 C	-94.2430	20.6830	42.8750 C.ar	1	****	-
0.1500						
39 H	-93.2180	21.0090	42.7460 H	1	****	
0.1500						
40 C	-94.6090	19.3790	42.5840 C.ar	1	****	
0.1600						
41 H	-93.8760	18.6610	42.2270 H	1	****	
0.1500						
42 N	-95.8690	18.9070	42.7100 N.ar	1	****	-
0.6200						
43 C	-96.8000	19.7830	43.1600 C.ar	1	****	
0.1600						
44 H	-97.8050	19.3770	43.2130 H	1	****	
0.1500						
45 H	-92.6720	28.6300	46.3160 H	1	****	
0.0000						
46 H	-92.0190	28.7830	47.9340 H	1	****	
0.0000						
47 C	-90.1150	24.5490	46.8380 C.ar	1	****	
0.0830						
48 C	-90.0250	25.5890	45.9090 C.ar	1	****	-
0.1500						
49 C	-90.8210	26.7310	46.0360 C.ar	1	****	-
0.1500						
50 C	-91.7200	26.8530	47.1010 C.ar	1	****	-
0.1440						
51 C	-91.8060	25.8060	48.0300 C.ar	1	****	-
0.1500						
52 C	-91.0090	24.6630	47.9000 C.ar	1	****	-
0.1500						
53 H	-89.3280	25.5090	45.0790 H	1	****	
0.1500						
54 H	-90.7190	27.5230	45.2970 H	1	****	
0.1500						
55 H	-92.4900	25.8780	48.8750 H	1	****	
0.1500						
56 H	-91.1150	23.8840	48.6480 H	1	****	
0.1500						
57 O	-89.2930	23.4860	46.5850 O.3	1	****	-
0.3630						
58 C	-89.8470	22.1890	46.7740 C.3	1	****	
0.2800						
59 H	-89.1600	21.4650	46.3260 H	1	****	
0.0000						
60 H	-89.9400	21.9480	47.8380 H	1	****	
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61 H	-90.8100	22.0950	46.2620 H	1	****	
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USER_CHARGES

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      2 C      -99.2320   25.9870   43.4450 C.3      1      ****
0.2700
      3 H     -100.2460   25.9750   43.8620 H      1      ****
0.0000
      4 H      -98.7960   26.9830   43.5640 H      1      ****
0.0000
      5 C      -99.2550   25.5640   41.9880 C.3      1      ****
0.0000
      6 H     -100.0800   26.0170   41.4330 H      1      ****
0.0000
      7 H      -98.3130   25.8340   41.4940 H      1      ****
0.0000
      8 C      -99.3770   24.0580   42.0990 C.3      1      ****
0.0000
      9 H     -100.4140   23.7980   42.3500 H      1      ****
0.0000
     10 H      -99.1290   23.5440   41.1670 H      1      ****
0.0000
     11 C      -98.4630   23.6890   43.2770 C.3      1      ****
0.2700
     12 C      -97.0480   23.2820   42.8160 C.3      1      ****
0.2800
     13 H      -96.4280   24.1760   42.6820 H      1      ****
0.0000
     14 O      -96.4970   22.4190   43.8210 O.3      1      ****      -
0.3630
     15 C      -95.8490   21.2970   43.4000 C.ar     1      ****
0.0830
     16 H      -97.0870   22.7180   41.8780 H      1      ****
0.0000
     17 H      -98.9260   22.8750   43.8440 H      1      ****
0.0000
     18 S      -98.5730   24.8430   45.7800 S.3      1      ****
0.5380
     19 C      -97.1890   25.7770   46.3810 C.ar     1      ****
0.0070
     20 O      -99.7610   25.5830   46.1460 O.3      1      ****      -
0.2150
     21 O      -98.4030   23.4570   46.1550 O.3      1      ****      -
0.2150
     22 C      -96.8030   25.6820   47.7180 C.ar     1      ****      -
0.1500

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23 H	-97.3250	25.0550	48.4340 H	1	****	
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24 C	-95.6740	26.3920	48.0770 C.ar	1	****	
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25 C	-94.9430	27.1810	47.1840 C.ar	1	****	
0.1170						
26 C	-95.3520	27.3100	45.8690 C.ar	1	****	-
0.1500						
27 H	-94.8130	27.9170	45.1530 H	1	****	
0.1500						
28 C	-96.4900	26.5990	45.4670 C.ar	1	****	-
0.1500						
29 H	-96.8290	26.6680	44.4340 H	1	****	
0.1500						
30 C	-94.9600	26.4600	49.3460 C.2	1	****	
0.4840						
31 O	-95.2720	25.9240	50.3950 O.2	1	****	-
0.5700						
32 C	-93.7330	27.3270	49.1310 C.2	1	****	
0.6300						
33 O	-92.8920	27.5830	49.9680 O.2	1	****	-
0.5700						
34 N	-93.8080	27.7260	47.8080 N.am	1	****	-
0.4770						
35 C	-92.8170	28.5580	47.1650 C.3	1	****	
0.4440						
36 C	-94.4770	21.4340	43.2060 C.ar	1	****	-
0.1500						
37 H	-93.9820	22.3750	43.4360 H	1	****	
0.1500						
38 C	-93.7330	20.3650	42.7150 C.ar	1	****	-
0.1500						
39 H	-92.6630	20.4540	42.5580 H	1	****	
0.1500						
40 C	-94.3960	19.1850	42.4280 C.ar	1	****	
0.1600						
41 H	-93.8610	18.3210	42.0440 H	1	****	
0.1500						
42 N	-95.7270	19.0160	42.5930 N.ar	1	****	-
0.6200						
43 C	-96.4220	20.0740	43.0810 C.ar	1	****	
0.1600						
44 H	-97.4840	19.8840	43.1790 H	1	****	
0.1500						
45 H	-92.9070	28.4530	46.0770 H	1	****	
0.0000						
46 H	-93.0400	29.6080	47.3940 H	1	****	
0.0000						
47 C	-88.7740	27.5210	48.3020 C.ar	1	****	
0.1010						
48 C	-89.5440	26.6300	47.5510 C.ar	1	****	-
0.1500						
49 C	-90.8520	26.9630	47.1860 C.ar	1	****	-
0.1500						
50 C	-91.4040	28.1960	47.5580 C.ar	1	****	-
0.1440						

51 C	-90.6250	29.0830	48.3170 C.ar	1	****	-
0.1500						
52 C	-89.3170	28.7500	48.6800 C.ar	1	****	-
0.1500						
53 H	-89.1320	25.6720	47.2440 H	1	****	
0.1500						
54 H	-91.4330	26.2470	46.6070 H	1	****	
0.1500						
55 H	-91.0310	30.0420	48.6330 H	1	****	
0.1500						
56 H	-88.7300	29.4570	49.2600 H	1	****	
0.1500						
57 S	-87.1050	27.0990	48.7620 S.3	1	****	-
0.3310						
58 C	-86.2380	28.4260	47.8860 C.3	1	****	
0.2300						
59 H	-85.1630	28.2370	47.9230 H	1	****	
0.0000						
60 H	-86.5500	28.4610	46.8380 H	1	****	
0.0000						
61 H	-86.4390	29.3920	48.3560 H	1	****	
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21e
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SMALL
USER_CHARGES

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0.2700
3 H     -100.0760   25.4550   43.6240 H      1      ****
0.0000
4 H      -98.5370   26.2560   43.1820 H      1      ****
0.0000
5 C      -99.0000   24.4790   42.0270 C.3      1      ****
0.0000
6 H      -99.7410   24.8180   41.2960 H      1      ****
0.0000
7 H      -98.0070   24.5250   41.5660 H      1      ****
0.0000
8 C      -99.2800   23.0820   42.5410 C.3      1      ****
0.0000

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9 H	-100.3520	22.9850	42.7590 H	1	****	
0.0000						
10 H	-99.0260	22.3050	41.8150 H	1	****	
0.0000						
11 C	-98.4870	22.9950	43.8540 C.3	1	****	
0.2700						
12 C	-97.1030	22.3350	43.6660 C.3	1	****	
0.2800						
13 H	-96.6170	22.1660	44.6360 H	1	****	
0.0000						
14 O	-97.3150	21.0830	42.9940 O.3	1	****	-
0.3630						
15 C	-96.2090	20.4040	42.5860 C.ar	1	****	
0.0830						
16 H	-96.4610	22.9610	43.0330 H	1	****	
0.0000						
17 H	-99.0800	22.4210	44.5790 H	1	****	
0.0000						
18 S	-98.6950	24.8160	45.9190 S.3	1	****	
0.5380						
19 C	-97.2690	25.7380	46.4480 C.ar	1	****	
0.0070						
20 O	-99.8100	25.7400	45.9080 O.3	1	****	-
0.2150						
21 O	-98.7570	23.5810	46.6720 O.3	1	****	-
0.2150						
22 C	-96.8400	25.6630	47.7810 C.ar	1	****	-
0.1500						
23 H	-97.3250	25.0280	48.5190 H	1	****	
0.1500						
24 C	-95.7050	26.3850	48.0950 C.ar	1	****	
0.0860						
25 C	-95.0220	27.1930	47.1720 C.ar	1	****	
0.1170						
26 C	-95.4770	27.3050	45.8650 C.ar	1	****	-
0.1500						
27 H	-94.9770	27.9200	45.1200 H	1	****	
0.1500						
28 C	-96.6110	26.5640	45.5020 C.ar	1	****	-
0.1500						
29 H	-96.9830	26.6250	44.4740 H	1	****	
0.1500						
30 C	-94.9370	26.4510	49.3300 C.2	1	****	
0.4840						
31 O	-95.1800	25.8840	50.3810 O.2	1	****	-
0.5700						
32 C	-93.7500	27.3610	49.0810 C.2	1	****	
0.6300						
33 O	-92.8910	27.6350	49.8930 O.2	1	****	-
0.5700						
34 N	-93.8890	27.7820	47.7610 N.am	1	****	-
0.4770						
35 C	-93.0170	28.7620	47.1280 C.3	1	****	
0.4440						
36 C	-96.4170	19.4530	41.5910 C.ar	1	****	-
0.1500						

37 H	-97.4040	19.3210	41.1540 H	1	****	
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38 C	-95.3580	18.6680	41.1450 C.ar	1	****	-
0.1500						
39 H	-95.5060	17.9220	40.3720 H	1	****	
0.1500						
40 C	-94.1150	18.8680	41.7170 C.ar	1	****	
0.1600						
41 H	-93.2560	18.2830	41.4020 H	1	****	
0.1500						
42 N	-93.8750	19.7760	42.6870 N.ar	1	****	-
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43 C	-94.9290	20.5240	43.1000 C.ar	1	****	
0.1600						
44 H	-94.6880	21.2180	43.8960 H	1	****	
0.1500						
45 H	-92.9730	28.5520	46.0490 H	1	****	
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46 H	-93.4330	29.7730	47.2240 H	1	****	
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47 C	-88.9500	28.6420	48.5780 C.ar	1	****	
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48 C	-89.5950	27.4580	48.2570 C.ar	1	****	-
0.1500						
49 C	-90.9260	27.4830	47.8190 C.ar	1	****	-
0.1500						
50 C	-91.6080	28.6920	47.7050 C.ar	1	****	-
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51 C	-90.9380	29.8740	48.0540 C.ar	1	****	-
0.1500						
52 C	-89.6080	29.8470	48.4880 C.ar	1	****	-
0.1500						
53 F	-87.6680	28.6130	48.9740 F	1	****	-
0.1900						
54 H	-89.0560	26.5280	48.3350 H	1	****	
0.1500						
55 H	-91.4100	26.5470	47.5650 H	1	****	
0.1500						
56 H	-91.4440	30.8290	47.9730 H	1	****	
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57 H	-89.0910	30.7670	48.7350 H	1	****	
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SMALL
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2 C	-98.7600	26.1330	42.9170 C.3	1	****	
0.2700						
3 H	-99.4680	26.8330	43.3660 H	1	****	
0.0000						
4 H	-97.8320	26.6650	42.6840 H	1	****	
0.0000						
5 C	-99.3760	25.5150	41.6730 C.3	1	****	
0.0000						
6 H	-100.0250	26.2130	41.1380 H	1	****	
0.0000						
7 H	-98.5920	25.1840	40.9790 H	1	****	
0.0000						
8 C	-100.1280	24.3270	42.2310 C.3	1	****	
0.0000						
9 H	-101.0520	24.6720	42.7130 H	1	****	
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10 H	-100.4050	23.6020	41.4590 H	1	****	
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11 C	-99.1720	23.7600	43.2870 C.3	1	****	
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12 C	-98.1320	22.8040	42.6670 C.3	1	****	
0.2800						
13 H	-97.4650	23.2970	41.9510 H	1	****	
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14 O	-97.4260	22.0720	43.6870 O.3	1	****	-
0.3630						
15 C	-96.4000	21.2330	43.2820 C.ar	1	****	
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16 H	-98.6640	22.0390	42.0910 H	1	****	
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17 H	-99.7330	23.2390	44.0680 H	1	****	
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18 S	-98.4380	25.2590	45.4910 S.3	1	****	
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19 C	-96.9110	26.1150	45.7410 C.ar	1	****	
0.0070						
20 O	-99.5050	26.1760	45.8380 O.3	1	****	-
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21 O	-98.3370	23.9740	46.1540 O.3	1	****	-
0.2150						
22 C	-96.7330	26.8810	46.8990 C.ar	1	****	-
0.1500						
23 H	-97.4980	26.9570	47.6680 H	1	****	
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24 C	-95.5210	27.5510	47.0680 C.ar	1	****	
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25 C	-94.5460	27.4730	46.0780 C.ar	1	****	
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26 C	-94.7130	26.7530	44.9150 C.ar	1	****	-
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27 H	-93.9390	26.7190	44.1560 H	1	****	
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28 C	-95.9200	26.0670	44.7410 C.ar	1	****	-
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29 H	-96.0800	25.5020	43.8270 H	1	****	
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30 C	-94.9930	28.4050	48.1270 C.2	1	****	
0.4840						
31 O	-95.5380	28.7320	49.1660 O.2	1	****	-
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32 C	-93.6150	28.8250	47.6870 C.2	1	****	
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33 O	-92.7810	29.5590	48.2080 O.2	1	****	-
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34 N	-93.4350	28.2210	46.4440 N.am	1	****	-
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35 H	-92.5950	28.3270	45.9010 H	1	****	
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36 C	-95.1470	21.8370	43.2010 C.ar	1	****	-
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37 H	-95.0130	22.8810	43.4560 H	1	****	
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38 C	-94.0700	21.0640	42.7860 C.ar	1	****	
0.1600						
39 H	-93.0760	21.4900	42.7140 H	1	****	
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40 N	-94.1660	19.7600	42.4460 N.ar	1	****	-
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41 C	-95.3980	19.2100	42.5080 C.ar	1	****	
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42 H	-95.4570	18.1680	42.2060 H	1	****	
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43 C	-96.5370	19.8920	42.9150 C.ar	1	****	-
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