

Supplementary Material

Structural, QSAR, machine learning and molecular docking studies of 5-thiophen-2-yl pyrazole derivatives as potent and selective cannabinoid-1 receptor antagonists

Riadh Hanachi, Ridha Ben Said, Hamza Allal, Seyfeddine Rahali, Mohammed A. M. Alkhalifah, Faisal Alresheedi, Bahoueddine Tangour, Majdi Hochlaf

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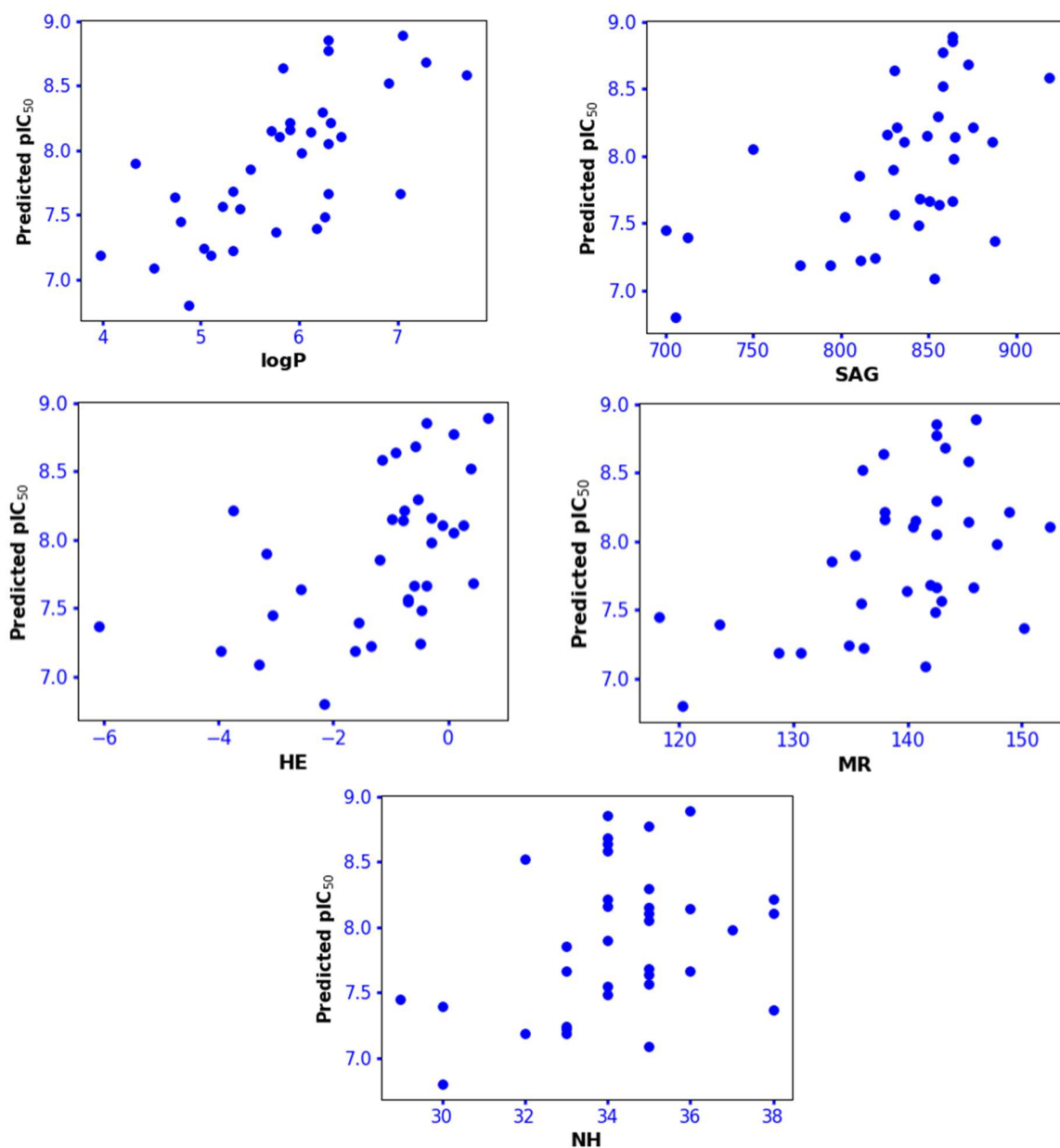


Figure S1: Machine learning derived pIC_{50} evolution along $\log P$, SAG, HE, NH and MR without considering the D3 dispersion correction in the DFT computations. The relation of B3LYP parameters to pIC_{50} is given by: $pIC_{50} = 3.9548 \cdot E_{HOMO} - 13.7532 \cdot E_{LUMO} - 0.0294 \cdot \text{Pol} + 0.0007 \cdot \text{Vol} + 0.0056 \cdot \text{SAG} + 0.3019 \cdot \text{HE} + 0.4842 \cdot \log P - 0.1210 \cdot \text{HBA} + 0.0576 \cdot \text{TPSA} - 0.1551 \cdot N_{\text{atom}} + 0.1106 \cdot N_{\text{brot}} + 0.1877 \cdot \text{NH} + 1.73$

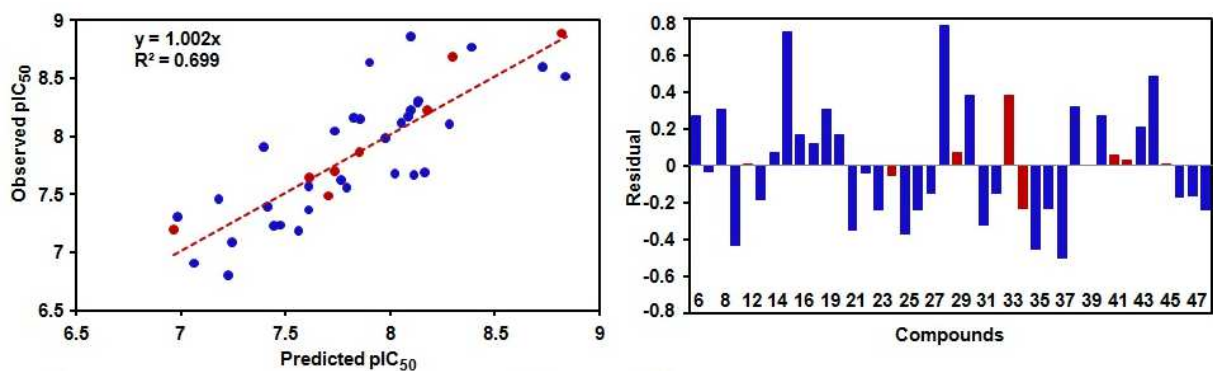


Figure S2: Correlation plots and diagram of residual values of observed (Observed pIC₅₀) vs predicted activity (Predicted pIC₅₀) using B3LYP parameters. The red data are for the external sets for validation. The dotted lines correspond to the linear regression between the predicted and observed pIC₅₀.

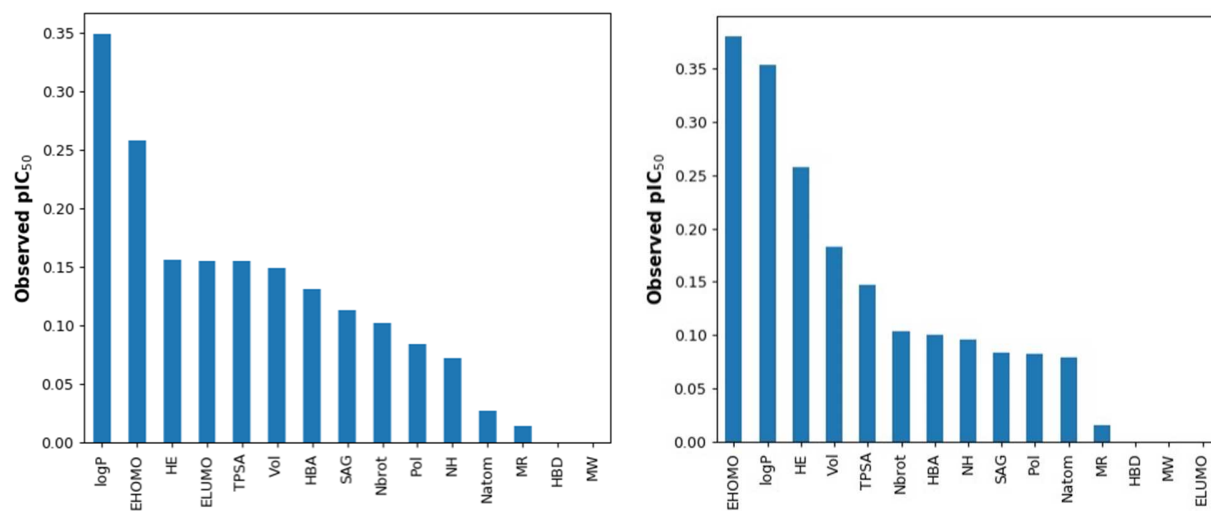
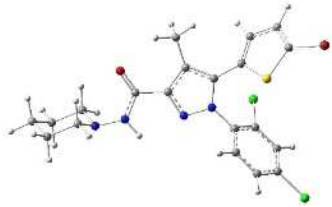
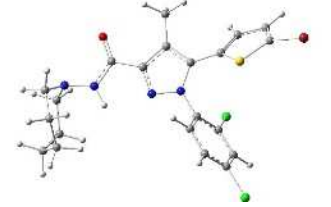
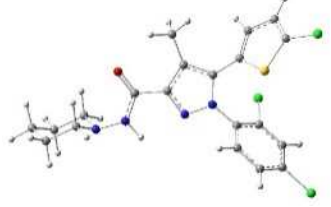
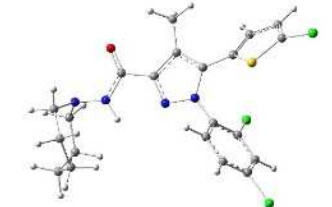
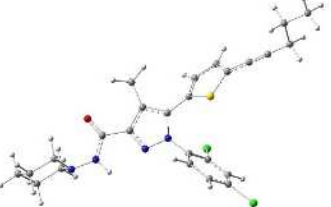
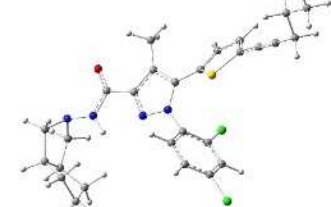
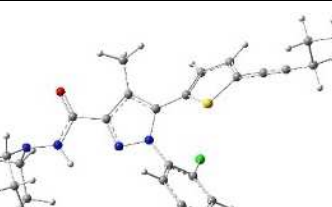
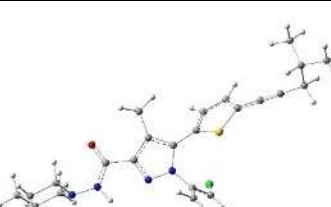
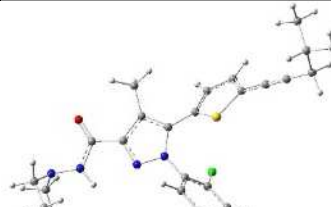



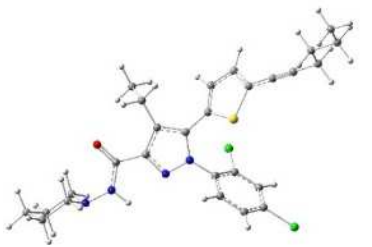
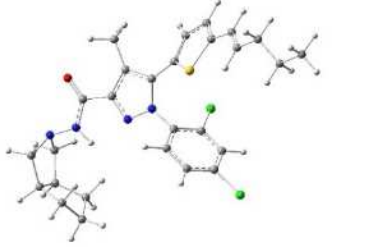
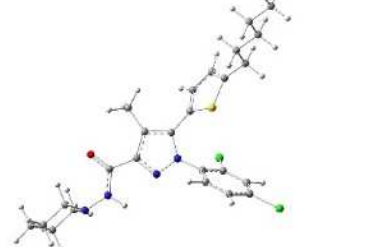
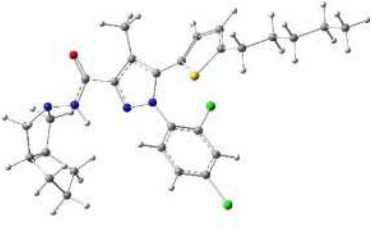
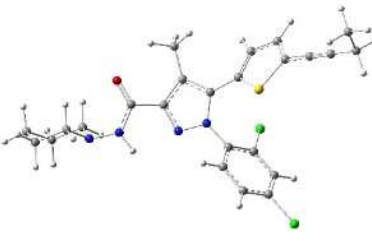
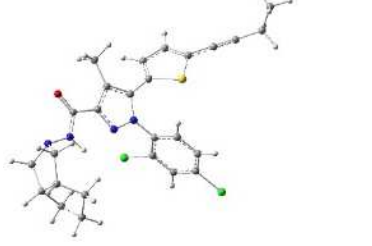
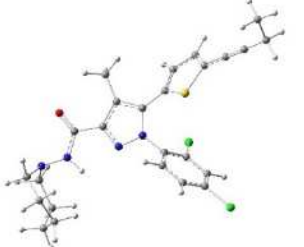
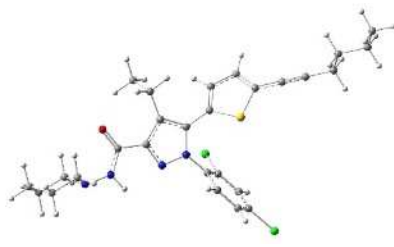
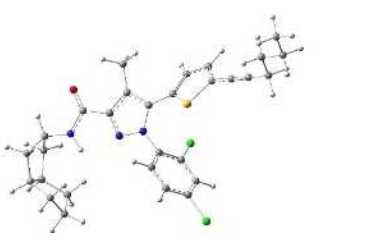
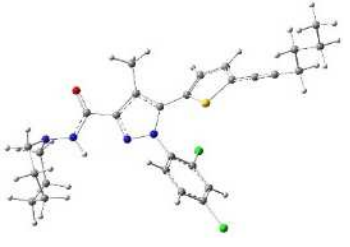
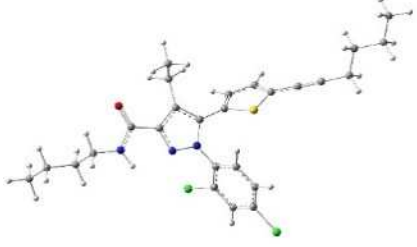
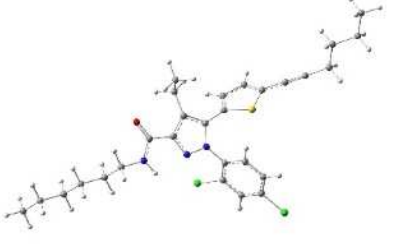
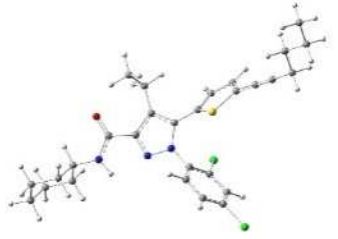
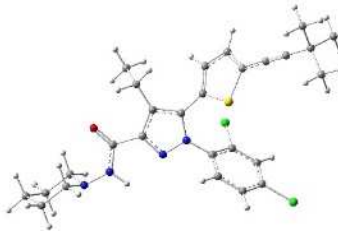
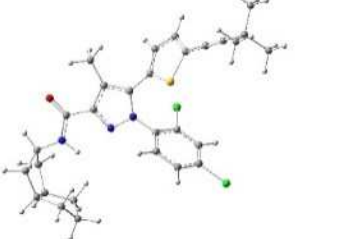
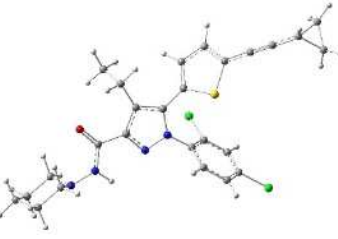
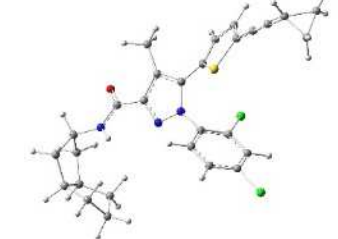
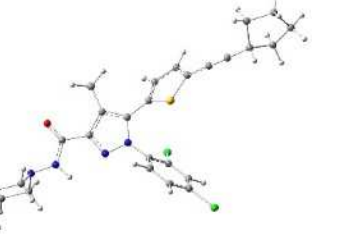
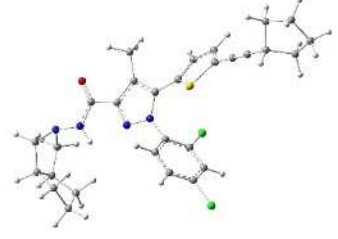
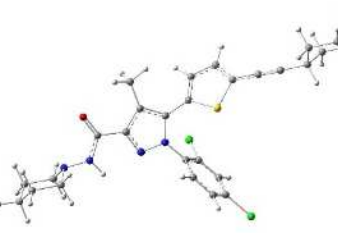
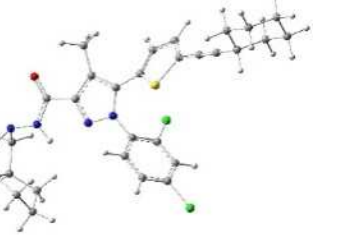
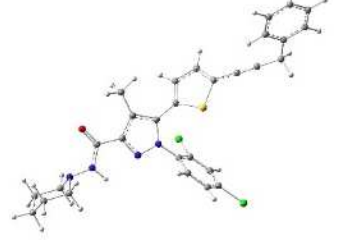
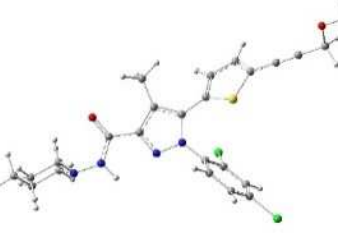
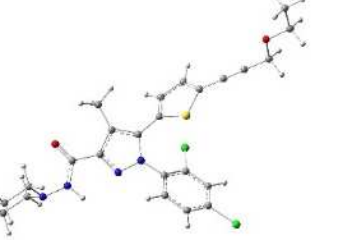


Figure S3: Mutual information diagrams of descriptors obtained using the B3LYP approach.

Table S1: B3LYP+D3/6-311G(d, p) optimized structures of the 5-Thiophen-2-ylpyrazole derivatives under study. We used the numbering used in Ref. [1]. Similar shapes were obtained at the B3LYP/6-311G(d, p). Their Cartesian coordinates are given in Table S7.

N	Structure	N	Structure	N	Structure
6		7		8	
9		12		13	
14		15		16	
18		19		20	

21		22		23	
24		25		26	
27		28		29	
30		31		32	

33		34		35	
36		37		38	
39		40		41	
42		43		44	

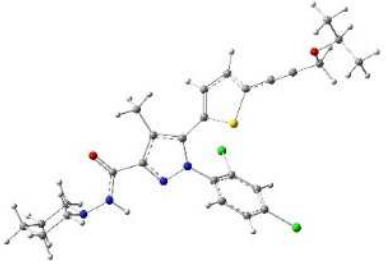
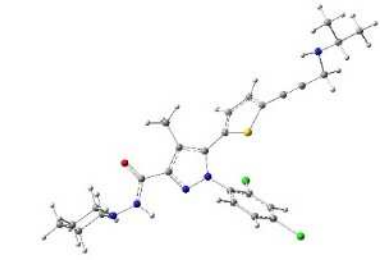
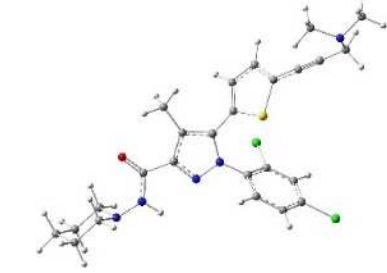
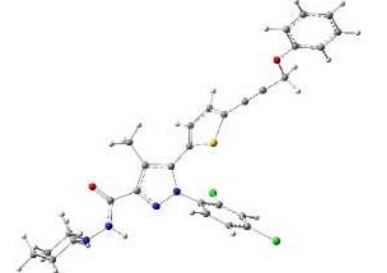
45		46		47	
48					

Table S2: Intramolecular distances between the Cl atom of 2,4-dichlorophenyl and 4-chlorophenyl/thiophenyl (d1, in Å) and between H/S atoms of 4-chlorophenyl/thiophenyl and the 2,4-dichlorophenyl (d2, in Å) as defined in Figure 1. The atoms were described by the 6-311G(d, p) basis set.

Compounds	d1		d2	
	B3LYP	B3LYP+D3	B3LYP	B3LYP+D3
5-(thiophen-2-yl)-1-(2,4-dichlorophenyl) -1H-pyrazole	4.06	3.87	3.88	3.74
5-(5-chlorothiophen-2-yl)-1-(2,4-dichlorophenyl) -1H-pyrazole	4.07	3.87	3.88	3.71
Rimonabant	4.10	3.87	3.42	3.22
6	3.64	3.87	3.87	3.76
7	4.12	3.88	3.90	3.74
8	4.12	3.88	3.91	3.73
9	4.12	3.87	3.90	3.73
12	4.10	3.78	3.88	3.72
13	4.12	3.87	3.87	3.73
14	4.11	3.87	3.87	3.73
15	4.10	3.87	3.87	3.72
16	4.11	3.87	3.87	3.73
18	4.12	3.88	3.89	3.73
19	4.21	3.89	4.02	3.80
20	4.20	3.89	4.03	3.80
21	4.03	3.88	3.89	3.73
22	4.09	3.86	3.87	3.72
23	4.11	3.87	3.91	3.74
24	4.12	3.86	3.91	3.74

25	4.11	3.88	3.88	3.72
26	4.12	3.87	3.88	3.73
27	4.11	3.87	3.87	3.73
28	4.12	3.88	3.89	3.73
29	4.04	3.89	3.92	3.72
30	4.11	3.87	3.88	3.73
31	4.21	3.89	4.02	3.80
32	4.15	3.89	4.04	3.73
33	4.20	3.89	4.02	3.80
34	4.10	3.88	3.89	3.72
35	4.11	3.85	3.87	3.73
36	4.13	3.88	3.89	3.73
37	4.11	3.89	3.89	3.72
38	4.12	3.87	3.97	3.72
39	4.12	3.87	3.87	3.73
40	4.11	3.87	3.87	3.72
41	4.12	3.87	3.87	3.73
42	4.10	3.88	3.88	3.72
43	4.11	3.88	3.87	3.72
44	4.11	3.88	3.87	3.72
45	4.04	3.88	3.84	3.72
46	4.105	3.869	3.88	3.72
47	4.105	3.873	3.87	3.72
48	4.110	3.883	3.87	3.72

Table S3: Volume (Vol, Å³) and volume change (Δ Vol, Å³) and % of changes of the 5-thiophen-2-ylpyrazole derivatives understudy. We used the numbering used in Ref. [1]

Compounds	B3LYP6-311G(d, p)	B3LYP+D3/6-311G(d, p)	Δ Vol	%
6	1202.96	1196.38	6.58	0.549992
7	1253.3	1238.38	14.92	1.2048
8*	1183.98	1176.69	7.29	0.619534
9	1227.01	1218.36	8.65	0.709971
12	1382.04	1376.5	5.54	0.40247
13	1447.29	1434.67	12.62	0.879645
14	1427.54	1417.75	9.79	0.690531
15	1429.17	1420.66	8.51	0.599017
16*	1471.76	1460.29	11.47	0.78546
18	1426.29	1419.35	6.94	0.488956
19	1478.73	1466.11	12.62	0.860781
20	1479.36	1468.72	10.64	0.72444
21	1482.83	1473.91	8.92	0.605193
22	1453.62	1442.35	11.27	0.781364
23	1407.1	1398.13	8.97	0.641571
24	1471.03	1458.37	12.66	0.868092
25	1382.73	1320.98	61.75	4.67456
26	1394.16	1382.42	11.74	0.849235
27*	1374	1365.38	8.62	0.631326
28	1482.83	1473.91	8.92	0.605193
29	1508.8	1491.48	17.32	1.16126
30	1480.63	1471.12	9.51	0.646446

31	1453.88	1445.83	8.05	0.556774
32	1564.05	1556.97	7.08	0.454729
33	1505.29	1494.53	10.76	0.719959
34	1468.01	1461.75	6.26	0.428254
35	1496.48	1469.46	27.02	1.83877
36	1400.69	1392.05	8.64	0.620667
37*	1425.49	1412.76	12.73	0.901073
38	1454.86	1446.25	8.61	0.595333
39	1509.15	1498.01	11.14	0.743653
40	1495.31	1487.32	7.99	0.537208
41	1552.72	1539.03	13.69	0.889521
42	1500.48	1494.19	6.29	0.420964
43	1355.43	1350.92	4.51	0.333847
44	1414.6	1407.82	6.78	0.481596
45	1462.8	1455.33	7.47	0.513286
46	1469.54	1460.57	8.97	0.614144
47*	1412.65	1404.01	8.64	0.61538
48	1523.19	1514.85	8.34	0.55055

Table S4: Measured pIC₅₀, predicted pIC₅₀ and residual values with and without consideration of the dispersion correction.

Compounds	Observed pIC ₅₀	B3LYP/6-311G(d, p)		B3LYP+D3/6-311G(d, p)	
		Predicted pIC ₅₀	Residual	Predicted pIC ₅₀	Residual
6	7.45	7.18	0.27	7.29	0.15
7	7.39	7.42	-0.03	7.14	0.25
8	7.30	6.99	0.31	7.09	0.21
9	6.80	7.23	-0.43	7.12	-0.32
12	7.86	7.85	0.01	7.96	-0.10
13	8.10	8.28	-0.18	8.02	0.08
14	8.16	8.09	0.07	8.12	0.03
15	8.64	7.90	0.73	8.01	0.63
16	8.31	8.14	0.17	8.07	0.24
18	8.22	8.10	0.12	8.14	0.08
19	8.05	7.74	0.31	8.32	-0.27
20	8.29	8.13	0.17	8.25	0.04
21	7.67	8.02	-0.35	8.16	-0.50
22	7.56	7.61	-0.04	7.29	0.27
23	7.24	7.48	-0.24	7.63	-0.39
24	7.69	7.74	-0.05	7.53	0.15
25	7.18	7.56	-0.37	7.76	-0.58
26	7.55	7.79	-0.24	7.75	-0.21
27	7.62	7.77	-0.15	7.86	-0.25
28	8.85	8.10	0.76	8.27	0.58
29	8.89	8.82	0.07	8.68	0.20
30	8.77	8.39	0.38	8.48	0.29
31	8.52	8.84	-0.32	8.94	-0.42
32	8.59	8.73	-0.15	8.50	0.08
33	8.68	8.30	0.38	8.68	0.00
34	7.49	7.71	-0.23	7.74	-0.26
35	7.66	8.11	-0.45	7.98	-0.32
36	7.22	7.45	-0.23	7.52	-0.30
37	7.68	8.17	-0.50	8.07	-0.39
38	8.15	7.83	0.32	8.13	0.01
39	7.98	7.98	0.00	7.94	0.04
40	8.14	7.86	0.27	8.10	0.04
41	8.11	8.05	0.06	8.00	0.11
42	8.22	8.18	0.03	8.35	-0.14
43	7.19	6.97	0.21	7.09	0.09
44	7.90	7.40	0.49	7.58	0.31
45	7.64	7.62	0.01	7.80	-0.17
46	7.08	7.25	-0.17	7.18	-0.10
47	6.91	7.07	-0.16	7.21	-0.30
48	7.37	7.61	-0.24	7.69	-0.33

Table S5: Physicochemical properties of 5-thiophen-2-yl pyrazoles derivatives with and without D3. For each compound, we give the energies of the HOMO (E_{HOMO} , a.u.) and LUMO (E_{LUMO} , a.u.) orbitals, HOMO – LUMO gap (ΔE , eV), Pol, Vol (\AA^3), SAG (in \AA^3) and HE (kcal/mol). The atoms were described using the 6-311G(d, p) basis set.

Compound	B3LYP							B3LYP+D3						
	E_{HOMO}	E_{LUMO}	ΔE	Pol	Vol	SAG	HE	E_{HOMO}	E_{LUMO}	ΔE	Pol	Vol	SAG	HE
6	-0.22308	-0.06218	4.378	47.91	1202.96	700.16	-3.07	-0.22371	-0.06475	4.325	47.91	1196.38	693.22	-3.00
7	-0.22041	-0.06119	4.332	50.23	1253.3	712.58	-1.55	-0.22100	-0.06371	4.280	50.23	1238.38	702.90	-2.07
8	-0.22328	-0.06260	4.372	47.21	1183.98	690.33	-3.07	-0.22388	-0.06503	4.322	47.21	1176.69	684.02	-3.01
9	-0.22051	-0.06153	4.326	49.04	1227.01	705.42	-2.17	-0.22189	-0.06407	4.294	49.04	1218.36	692.98	-2.06
12	-0.21867	-0.06244	4.251	53.35	1382.04	810.77	-1.19	-0.21754	-0.06434	4.168	53.35	1376.50	799.57	-1.15
13	-0.21769	-0.06126	4.256	56.25	1447.29	835.88	0.27	-0.21649	-0.06376	4.156	56.25	1434.67	815.42	-0.16
14	-0.21740	-0.06132	4.247	55.19	1427.54	826.24	-0.29	-0.21636	-0.06340	4.162	55.19	1417.75	814.42	-0.22
15	-0.21886	-0.06277	4.247	55.19	1429.17	830.41	-0.92	-0.21776	-0.06468	4.165	55.19	1420.66	823.11	-0.88
16	-0.21755	-0.06166	4.242	57.02	1471.76	845.91	-0.02	-0.21662	-0.06370	4.161	57.02	1460.29	834.92	-0.06
18	-0.21909	-0.06216	4.270	55.19	1426.29	832.09	-0.76	-0.21761	-0.06401	4.179	55.19	1419.35	821.00	-0.73
19	-0.21839	-0.05864	4.347	57.02	1478.73	749.61	0.09	-0.21789	-0.06104	4.268	57.02	1466.11	839.50	0.17
20	-0.22011	-0.05992	4.359	57.02	1479.36	855.51	-0.53	-0.21905	-0.06227	4.266	57.02	1468.72	849.77	-0.47
21	-0.21881	-0.06196	4.268	57.02	1482.83	863.67	-0.37	-0.21732	-0.06383	4.176	57.02	1473.91	857.74	-0.34
22	-0.21290	-0.06267	4.087	57.16	1453.62	830.87	-0.69	-0.21175	-0.06484	3.997	57.16	1442.35	813.62	-0.57
23	-0.21959	-0.05576	4.458	54.46	1407.10	819.32	-0.49	-0.22012	-0.05773	4.418	54.46	1398.13	814.12	-0.45
24	-0.22323	-0.05490	4.580	57.35	1471.03	844.79	0.44	-0.22128	-0.05725	4.463	57.35	1458.37	823.78	0.54
25	-0.21913	-0.06272	4.256	51.52	1382.73	776.96	-1.63	-0.21800	-0.06469	4.171	51.52	1320.98	772.66	-1.58
26	-0.21823	-0.06155	4.263	54.41	1394.16	802.35	-0.70	-0.21697	-0.06408	4.160	54.41	1382.42	787.00	-0.60
27	-0.21776	-0.06161	4.249	53.35	1374.00	793.67	-0.73	-0.21674	-0.06374	4.163	53.35	1365.38	786.21	-0.66
28	-0.21881	-0.06196	4.268	57.02	1482.83	863.67	-0.37	-0.21732	-0.06383	4.176	57.02	1473.91	857.74	-0.34

29	-0.21736	-0.06118	4.249	58.57	1508.80	863.41	0.69	-0.21624	-0.06370	4.150	58.57	1491.48	849.22	0.67
30	-0.21718	-0.06109	4.247	57.02	1480.63	858.20	0.10	-0.21611	-0.06317	4.161	57.02	1471.12	848.42	0.18
31	-0.22015	-0.05842	4.401	54.61	1453.88	858.47	0.39	-0.21793	-0.06070	4.278	54.61	1445.83	848.70	0.40
32	-0.22012	-0.05837	4.401	58.28	1564.05	919.08	-1.15	-0.21791	-0.06064	4.279	58.28	1556.97	908.44	-1.17
33	-0.21988	-0.05813	4.401	57.51	1505.29	872.99	-0.56	-0.21758	-0.06030	4.279	57.51	1494.53	866.15	0.59
34	-0.21901	-0.06201	4.272	57.02	1468.01	844.29	-0.47	-0.21747	-0.06399	4.176	57.02	1461.75	838.96	-0.44
35	-0.21759	-0.06122	4.255	58.57	1496.48	850.57	-0.59	-0.21681	-0.06423	4.152	58.57	1469.46	819.37	0.56
36	-0.21959	-0.06305	4.259	54.41	1400.69	811.58	-1.34	-0.21823	-0.06484	4.174	54.41	1392.05	802.48	-1.31
37	-0.21832	-0.06246	4.241	55.96	1425.49	814.09	-0.29	-0.21717	-0.06472	4.148	55.96	1412.76	801.23	-0.30
38	-0.21635	-0.06074	4.234	56.25	1454.86	849.00	-0.97	-0.21504	-0.06276	4.143	56.25	1446.25	843.36	-0.93
39	-0.21633	-0.06082	4.231	59.14	1509.15	864.75	-0.28	-0.21513	-0.06334	4.130	59.14	1498.01	849.52	-0.18
40	-0.21663	-0.06052	4.248	58.08	1495.31	865.04	-0.78	-0.21533	-0.06254	4.157	58.08	1487.32	862.44	-0.75
41	-0.21658	-0.06061	4.244	60.98	1552.72	886.83	-0.10	-0.21538	-0.06312	4.197	60.98	1539.03	872.63	0.0
42	-0.22090	-0.06372	4.277	59.34	1500.48	875.62	-3.74	-0.21976	-0.06551	4.197	59.34	1494.19	868.34	-3.70
43	-0.22148	-0.06734	4.194	52.15	1355.43	793.94	-3.97	-0.22193	-0.06891	4.164	52.15	1350.92	787.54	-3.92
44	-0.22137	-0.06699	4.201	53.99	1414.60	829.97	-3.16	-0.22180	-0.06860	4.168	53.99	1407.82	822.27	-3.11
45	-0.22119	-0.06647	4.210	55.82	1462.80	856.03	-2.57	-0.22152	-0.06812	4.174	55.82	1455.33	847.63	-2.52
46	-0.22107	-0.06516	4.242	53.54	1469.54	853.44	-3.29	-0.22084	-0.06703	4.185	53.54	1460.57	850.07	-3.25
47	-0.21966	-0.06551	4.194	54.70	1412.65	818.62	-1.89	-0.21878	-0.06733	4.121	54.70	1404.01	809.65	-1.85
48	-0.22266	-0.07083	4.131	59.98	1523.19	887.61	-6.10	-0.22323	-0.07230	4.107	59.98	1514.85	881.82	-6.05

Table S6: Drug-likeness parameters and lipophilicity indices for the 5-thiophen-2-yl pyrazole derivatives under study. See text for the definition of these parameters and their description. * and # denote the selected compounds for external validation (test sets). * (#) for the model using B3LYP/6-311G(d, p) (B3LYP+D3/6-311G(d, p)) optimized structures.

Comp.	log ₁₀ P	MW	HBA	HBD	TPSA	N _{atom}	MR	N _{brot}	Lipinski Score	Ghose Score	Veber Score	N _H	LE	LLE	ABS %
6	4.79	514.3	5	1	50.16	48	118.27	4	3	3	2	29	0.359	2.656	91.69
7	5.18	528.3	5	1	50.16	52	122.88	4	2	2	2	30	0.345	1.21	91.69
8	4.49	469.8	5	1	50.16	48	115.68	4	4	4	2	29	0.352	2.809	91.69
9	4.88	483.8	5	1	50.16	51	120.28	4	4	3	2	30	0.317	1.919	91.69
12#	5.50	501.5	5	1	50.16	59	133.37	5	2	2	2	33	0.333	2.357	91.69
13	5.80	527.5	5	1	50.16	63	140.51	5	2	1	2	35	0.324	2.302	91.69
14*	5.90	515.5	5	1	50.16	62	137.97	5	2	1	2	34	0.336	2.255	91.69
15	5.83	515.5	5	1	50.16	62	137.91	5	2	1	2	34	0.356	2.808	91.69
16*	6.23	529.5	5	1	50.16	65	142.52	5	2	1	2	35	0.332	2.08	91.69
18	5.90	515.5	5	1	50.16	62	137.97	6	2	1	2	34	0.338	2.315	91.69
19	6.29	529.5	5	1	50.16	65	142.57	6	2	1	2	35	0.322	1.761	91.69
20*	6.23	529.5	5	1	50.16	65	142.52	6	2	1	2	35	0.332	2.062	91.69
21	6.29	529.5	5	1	50.16	65	142.57	7	2	1	2	33	0.325	1.376	91.69
22	5.22	529.5	5	1	50.16	65	142.99	7	2	2	2	35	0.302	2.341	91.69
23	5.03	505.5	5	1	50.16	63	134.89	8	2	2	2	33	0.307	2.207	91.69
24#	5.33	531.5	5	1	50.16	67	142.03	8	2	2	2	35	0.307	2.356	91.69
25	5.10	487.5	5	1	50.16	56	128.76	4	3	3	2	32	0.314	2.084	91.69
26	5.40	513.5	5	1	50.16	60	135.91	4	2	2	2	34	0.311	2.148	91.69
27*	5.50	501.5	5	1	50.16	59	133.37	4	2	2	2	33	0.323	2.116	91.69
28	6.29	529.5	5	1	50.16	65	142.57	6	2	1	2	34	0.365	2.564	91.69

29*#	7.05	540.6	5	1	50.16	67	145.94	6	2	1	2	36	0.346	1.836	91.69
30	6.29	529.5	5	1	50.16	65	142.57	6	2	1	2	35	0.351	2.48	91.69
31	6.91	502.5	4	1	46.92	62	136.10	8	2	1	2	32	0.373	1.613	92.81
32	7.70	530.6	4	1	46.92	68	145.30	10	2	1	1	34	0.354	0.885	92.81
33#	7.29	528.5	4	1	46.92	66	143.24	6	2	1	2	34	0.357	1.388	92.81
34#	6.26	529.5	5	1	50.16	65	142.39	4	2	1	2	34	0.308	1.225	91.69
35	7.02	540.6	5	1	50.16	67	145.76	4	2	1	2	36	0.298	0.644	91.69
36	5.33	513.5	5	1	50.16	60	136.11	4	2	2	2	33	0.306	1.889	91.69
37	6.08	524.5	5	1	50.16	62	139.48	4	2	1	2	35	0.307	1.598	91.69
38	5.72	527.5	5	1	50.16	63	140.71	4	2	1	2	35	0.326	2.429	91.69
39	6.02	553.6	5	1	50.16	67	147.85	4	2	1	2	37	0.302	1.959	91.69
40	6.12	541.5	5	1	50.16	66	145.31	4	2	1	2	36	0.316	2.017	91.69
41*	6.42	567.6	5	1	50.16	70	152.46	4	2	1	2	38	0.299	1.688	91.69
42#	6.32	549.5	5	1	50.16	63	148.86	6	2	1	2	38	0.303	1.895	91.69
43*#	3.98	503.5	6	1	59.40	57	130.69	5	3	2	2	33	0.305	3.205	88.51
44	4.33	517.5	6	1	59.40	60	135.44	6	3	2	2	34	0.325	3.566	88.51
45*#	4.74	531.5	6	1	59.40	63	139.89	6	3	2	2	35	0.305	2.895	88.51
46	4.52	530.5	6	1	62.53	64	141.54	5	3	2	2	35	0.283	2.564	87.43
47#	4.13	516.5	6	1	53.04	61	137.67	6	3	2	2	34	0.284	2.776	90.70
48	5.76	565.5	6	1	59.40	64	150.20	6	2	1	2	38	0.271	1.607	88.51

Table S7: Cartesian coordinates of compounds 6 - 48 (in angstroms) calculated using the B3LYP/6-311 g(d,p) approach with and without considering the dispersion correction (D3).

B3LYP/6-311G(d, p)				B3LYP+D3/6-311G(d, p)			
6							
C	2.21895800	3.10452800	0.94563600	C	2.38690000	2.92390000	0.95360000
C	1.41259400	1.97613800	1.06166400	C	1.52320000	1.83830000	1.05830000
C	0.68792900	1.50468400	-0.03841200	C	0.69140000	1.48940000	-0.01140000
C	0.75275100	2.20552500	-1.24263300	C	0.70830000	2.26640000	-1.16890000
C	1.54043200	3.34125400	-1.37023700	C	1.55190000	3.36240000	-1.28170000
C	2.27565400	3.77337500	-0.27089400	C	2.39360000	3.67230000	-0.21730000
H	2.77937000	3.45996500	1.79859100	H	3.03320000	3.18420000	1.77960000
H	0.17122600	1.84348500	-2.08096400	H	0.04710000	1.99120000	-1.98040000
H	1.58981600	3.87926400	-2.30712600	H	1.56720000	3.96150000	-2.18180000
N	-0.15171600	0.35702200	0.04451100	N	-0.18130000	0.36940000	0.04870000
C	0.19707500	-0.97222600	0.20552500	C	0.14120000	-0.97140000	0.14970000
C	-0.99215200	-1.69191500	0.21615100	C	-1.06270000	-1.66520000	0.14030000
C	-1.99771800	-0.70431500	0.05281500	C	-2.04830000	-0.65150000	0.02570000
C	-3.47550000	-0.91847000	-0.01275100	C	-3.52800000	-0.83860000	-0.03470000
O	-3.97089100	-2.03407500	0.07310400	O	-4.04140000	-1.94880000	0.01480000
N	-4.19050800	0.23196000	-0.17667200	N	-4.22960000	0.32510000	-0.15070000
C	1.56665900	-1.45489500	0.30090900	C	1.49810000	-1.48230000	0.21720000
C	2.05976000	-2.38579000	1.18001200	C	1.94890000	-2.51960000	0.99430000
S	2.81523700	-0.96908300	-0.83756500	S	2.79370000	-0.86250000	-0.79620000
C	3.42786900	-2.71341100	0.97194700	C	3.32380000	-2.82740000	0.80620000
H	1.45946300	-2.81083700	1.97273900	H	1.31180000	-3.03110000	1.70210000
C	3.96412600	-2.02534800	-0.07641800	C	3.90670000	-2.01590000	-0.12310000
H	3.98801000	-3.41290100	1.57578400	H	3.85910000	-3.59920000	1.34000000
Cl	1.30161000	1.19046300	2.61629300	Cl	1.49160000	0.93900000	2.55350000
Cl	3.28798400	5.19717600	-0.41226800	Cl	3.48220000	5.04040000	-0.34550000
H	-3.68833200	1.10718300	-0.22432400	H	-3.72420000	1.19910000	-0.16860000
N	-1.48251100	0.51880900	-0.05752600	N	-1.50880000	0.56530000	-0.03890000
Br	5.74567800	-2.11269900	-0.69867700	Br	5.71630000	-2.03960000	-0.66810000
C	-6.12733600	-0.35231700	-1.46205600	C	-6.17410000	-0.21780000	-1.43240000
C	-6.26434900	-0.09722600	0.98060900	C	-6.28310000	-0.05140000	1.01760000
C	-7.61056700	-0.00613600	-1.61153900	C	-7.66290000	0.11410000	-1.55050000
H	-5.99410200	-1.44187300	-1.40412900	H	-6.02700000	-1.30650000	-1.40780000
H	-5.55987400	0.01154100	-2.32199500	H	-5.62020000	0.17980000	-2.28610000

C	-7.75082800	0.25527300	0.89045600	C	-7.77440000	0.28450000	0.95770000
H	-6.13795300	-1.17370500	1.16339800	H	-6.14070000	-1.13260000	1.15320000
H	-5.79131800	0.44261800	1.80437100	H	-5.80440000	0.46110000	1.85530000
C	-8.39373000	-0.38297900	-0.34747900	C	-8.42100000	-0.32660000	-0.29190000
H	-8.01426200	-0.52587300	-2.48624600	H	-8.07110000	-0.37440000	-2.44080000
H	-7.70789700	1.06948300	-1.79675000	H	-7.77670000	1.19540000	-1.68680000
H	-8.25481300	-0.07755300	1.80335400	H	-8.26260000	-0.08180000	1.86620000
H	-7.85548400	1.34477300	0.83812500	H	-7.89330000	1.37360000	0.93630000
H	-9.43965500	-0.07430800	-0.43842100	H	-9.47530000	-0.04130000	-0.35820000
H	-8.39386200	-1.47424100	-0.23350800	H	-8.38960000	-1.42080000	-0.21620000
N	-5.58702400	0.31388800	-0.26303300	N	-5.62630000	0.41540000	-0.21820000
C	-1.16209400	-3.17481200	0.32863500	C	-1.26070000	-3.14680000	0.19470000
H	-1.43896600	-3.46514700	1.34702200	H	-1.47500000	-3.47750000	1.21600000
H	-1.96853900	-3.51517000	-0.31915600	H	-2.11680000	-3.43560000	-0.41230000
H	-0.23617500	-3.69156900	0.06812400	H	-0.36490000	-3.66810000	-0.14970000
7							
C	1.60805200	3.08965900	1.08206000	C	1.77370000	2.94220000	1.07940000
C	1.05750600	1.81344200	1.15462700	C	1.16930000	1.69130000	1.15380000
C	0.43674200	1.24247200	0.03816800	C	0.41270000	1.20490000	0.08180000
C	0.34134800	1.98728900	-1.13743600	C	0.23750000	2.00580000	-1.04610000
C	0.87176200	3.26724000	-1.22138000	C	0.81950000	3.26280000	-1.12810000
C	1.51082200	3.80167700	-0.10703800	C	1.59410000	3.71310000	-0.06290000
H	2.09028500	3.52173800	1.94733200	H	2.36380000	3.30940000	1.90680000
H	-0.15866300	1.54314800	-1.98877600	H	-0.36310000	1.61990000	-1.85970000
H	0.79842600	3.83892800	-2.13652300	H	0.68670000	3.88060000	-2.00560000
N	-0.14178500	-0.05811500	0.07670500	N	-0.19520000	-0.07870000	0.11100000
C	0.47954700	-1.28974200	0.18331000	C	0.40940000	-1.32130000	0.15690000
C	-0.53190900	-2.24300000	0.16660600	C	-0.61730000	-2.25750000	0.13280000
C	-1.72479300	-1.48406000	0.04554300	C	-1.80060000	-1.47780000	0.06890000
C	-3.12513600	-2.00781200	-0.02393900	C	-3.20900000	-1.97770000	0.01080000
O	-3.36548800	-3.20018400	0.01180700	O	-3.46840000	-3.16510000	-0.05540000
N	-4.06594800	-1.01551200	-0.12799300	N	-4.13380000	-0.96760000	0.03670000
C	1.92078500	-1.47683200	0.25826300	C	1.84540000	-1.52920000	0.19130000
C	2.60635500	-2.31825500	1.09760600	C	2.52320000	-2.47230000	0.92220000
S	3.02974700	-0.69157600	-0.85762300	S	2.95870000	-0.60680000	-0.80860000
C	4.01114700	-2.34049800	0.87734100	C	3.92860000	-2.46840000	0.70900000
H	2.11554100	-2.89312900	1.87093500	H	2.02410000	-3.13550000	1.61470000

C	4.38177500	-1.51168000	-0.14030700	C	4.30610000	-1.51630000	-0.19260000
H	4.71106700	-2.93036900	1.45166000	H	4.62710000	-3.12550000	1.20640000
Cl	1.12991100	0.96275600	2.67700100	Cl	1.36270000	0.75740000	2.61520000
Cl	2.20046800	5.41094000	-0.19374000	Cl	2.35570000	5.28970000	-0.15290000
H	-3.73738000	-0.05532400	-0.13418400	H	-3.78710000	-0.01390000	0.03440000
N	-1.47877700	-0.17661200	-0.01619800	N	-1.53590000	-0.17180000	0.04480000
C	-0.38577700	-3.73175000	0.21821500	C	-0.49250000	-3.74800000	0.13050000
H	-0.59137100	-4.11463900	1.22278000	H	-0.62150000	-4.15500000	1.13860000
H	-1.10638600	-4.20703900	-0.44553500	H	-1.27310000	-4.18960000	-0.48620000
H	0.62682100	-4.03154200	-0.05936400	H	0.49090000	-4.05230000	-0.23480000
C	-6.19198400	-0.96069600	0.98903300	C	-6.29190000	-0.77170000	1.04020000
C	-6.03014400	-0.99280900	-1.49742200	C	-6.01560000	-0.93270000	-1.43200000
C	-6.36870400	0.53207300	1.31124700	C	-6.37250000	0.74480000	1.27800000
H	-7.17703700	-1.42160900	0.85854200	H	-7.30060000	-1.16750000	0.88210000
H	-5.71889700	-1.46712600	1.83469900	H	-5.89350000	-1.26520000	1.93090000
C	-5.88919500	0.44961300	-2.03714400	C	-5.70520000	0.45760000	-2.02800000
H	-7.08888500	-1.24360200	-1.39052200	H	-7.09700000	-1.07700000	-1.36750000
H	-5.62197300	-1.68601500	-2.23985700	H	-5.63830000	-1.70130000	-2.11390000
C	-6.96272700	1.38194300	0.17556400	C	-6.84050000	1.56710000	0.06540000
H	-5.40250000	0.96179500	1.60502600	H	-5.39220000	1.11770000	1.60100000
H	-7.00997300	0.60336000	2.19796800	H	-7.05110000	0.91210000	2.12260000
C	-6.00118000	1.59638200	-1.00798500	C	-5.79500000	1.65990000	-1.06170000
H	-6.65940100	0.57335400	-2.80725300	H	-6.39790000	0.60550000	-2.86410000
H	-4.93180800	0.54873400	-2.55913200	H	-4.70320000	0.44290000	-2.46870000
H	-7.90647500	0.94240400	-0.17249100	H	-7.78360000	1.16170000	-0.32280000
H	-7.22327700	2.36321200	0.58579500	H	-7.06680000	2.58200000	0.40780000
H	-6.29269600	2.50280800	-1.54820000	H	-5.98710000	2.55720000	-1.65820000
H	-5.00843700	1.81730900	-0.59523800	H	-4.81570000	1.83160000	-0.59680000
Br	6.13690900	-1.19429900	-0.76328700	Br	6.06830000	-1.12810000	-0.75510000
N	-5.42106900	-1.30404900	-0.20681800	N	-5.49150000	-1.22240000	-0.09730000
8							
C	2.92512700	2.66189600	0.93921600	C	3.05320000	2.50260000	0.93800000
C	2.02581100	1.60369500	1.03065000	C	2.10770000	1.48550000	1.02210000
C	1.23649700	1.24534300	-0.06759600	C	1.23080000	1.24400000	-0.04120000
C	1.33400400	1.98964800	-1.24324400	C	1.28830000	2.06000000	-1.17020000
C	2.21518700	3.05719900	-1.34544300	C	2.21440000	3.08920000	-1.26170000
C	3.01142600	3.37562900	-0.24977500	C	3.09770000	3.29160000	-0.20520000

H	3.53476700	2.92991500	1.79035700	H	3.73330000	2.67990000	1.75880000
H	0.70314500	1.71620500	-2.07947600	H	0.59210000	1.86860000	-1.97670000
H	2.28937700	3.62917600	-2.26032000	H	2.26070000	3.71870000	-2.13990000
N	0.30160300	0.17223900	-0.00933900	N	0.27210000	0.19580000	-0.00190000
C	0.53600800	-1.18816500	0.08465500	C	0.48750000	-1.16940000	0.04170000
C	-0.71130800	-1.80187900	0.09522900	C	-0.76840000	-1.76400000	0.03540000
C	-1.62975900	-0.72448100	0.00108800	C	-1.67120000	-0.67120000	-0.01810000
C	-3.12185900	-0.80616400	-0.03494300	C	-3.16220000	-0.73690000	-0.05040000
O	-3.71155100	-1.87727800	0.01316600	O	-3.76260000	-1.80340000	-0.03150000
N	-3.73621700	0.40854500	-0.12698400	N	-3.76950000	0.48300000	-0.10460000
C	1.85940900	-1.79163200	0.12493600	C	1.79980000	-1.78920000	0.05860000
C	2.28428100	-2.80737600	0.94330200	C	2.18070000	-2.88970000	0.78400000
S	3.12524300	-1.35294600	-1.01450500	S	3.11940000	-1.23350000	-0.96190000
C	3.61453300	-3.24057600	0.68928000	C	3.52140000	-3.30010000	0.55110000
H	1.66250200	-3.22056600	1.72549100	H	1.51870000	-3.37590000	1.48660000
C	4.18924100	-2.54566700	-0.33241100	C	4.14700000	-2.50130000	-0.35950000
H	4.12457300	-4.01673600	1.24163000	H	4.00580000	-4.13310000	1.03960000
Cl	1.88392800	0.76277700	2.55352500	Cl	2.03210000	0.53560000	2.48410000
Cl	4.14131900	4.71092700	-0.35999600	Cl	4.28910000	4.57340000	-0.30730000
H	-3.16009600	1.23805700	-0.14872100	H	-3.19550000	1.31380000	-0.10130000
N	-1.01185500	0.45311500	-0.06989700	N	-1.03680000	0.50020000	-0.05060000
C	-5.74432000	0.05675900	-1.38745300	C	-5.77660000	0.14950000	-1.36120000
C	-5.80541300	0.20611500	1.06710600	C	-5.82310000	0.22570000	1.09530000
C	-7.19420300	0.53730800	-1.48276700	C	-7.23570000	0.60370000	-1.43220000
H	-5.70637000	-1.04177500	-1.38271400	H	-5.71730000	-0.94770000	-1.38190000
H	-5.16577300	0.41049700	-2.24422500	H	-5.20940000	0.53550000	-2.21150000
C	-7.25668700	0.69034400	1.03126900	C	-7.28330000	0.68180000	1.08250000
H	-5.77032100	-0.88475700	1.19737200	H	-5.76590000	-0.86790000	1.18620000
H	-5.26898200	0.66299100	1.90213700	H	-5.28810000	0.66460000	1.94080000
C	-7.97985400	0.16999700	-0.21747500	C	-8.00180000	0.17470000	-0.17440000
H	-7.66092100	0.09698800	-2.36961400	H	-7.69960000	0.18550000	-2.33100000
H	-7.20043300	1.62492700	-1.61603500	H	-7.26460000	1.69520000	-1.52420000
H	-7.76817900	0.35955400	1.94072600	H	-7.78140000	0.31980000	1.98730000
H	-7.26611000	1.78606500	1.03124900	H	-7.31430000	1.77690000	1.10550000
H	-8.99632200	0.57227200	-0.26726900	H	-9.03070000	0.54560000	-0.20540000
H	-8.07346800	-0.92132700	-0.15341900	H	-8.05710000	-0.92060000	-0.14140000
N	-5.12161900	0.61556000	-0.17357100	N	-5.15540000	0.68760000	-0.13650000

C	-1.00831700	-3.26807100	0.14748000	C	-1.08400000	-3.22610000	0.03950000
H	-1.27945500	-3.58116400	1.16069300	H	-1.30040000	-3.57890000	1.05300000
H	-1.86038600	-3.50577100	-0.48749000	H	-1.97440000	-3.42160000	-0.55520000
H	-0.13973000	-3.85052500	-0.16656000	H	-0.24130000	-3.80320000	-0.34760000
Cl	5.79760600	-2.73278800	-0.94571500	Cl	5.78540000	-2.63380000	-0.90550000
9							
C	2.27317200	2.84748800	1.02619200	C	2.39210000	2.71620000	1.00170000
C	1.64604600	1.60652000	1.08766200	C	1.72050000	1.49910000	1.06060000
C	0.95992300	1.10100000	-0.02208700	C	0.92740000	1.07480000	-0.01130000
C	0.87885000	1.87705500	-1.17841000	C	0.78560000	1.90440000	-1.12310000
C	1.48585600	3.12326300	-1.25057700	C	1.43520000	3.12880000	-1.18920000
C	2.18769800	3.59136600	-0.14418700	C	2.24370000	3.51660000	-0.12460000
H	2.80533800	3.22885300	1.88602100	H	3.00980000	3.03520000	1.82900000
H	0.32859200	1.48442100	-2.02404900	H	0.15670000	1.56690000	-1.93680000
H	1.42309700	3.71930800	-2.15084600	H	1.32790000	3.76890000	-2.05420000
N	0.30227200	-0.16169900	0.00580700	N	0.24900000	-0.17310000	0.00200000
C	0.84804300	-1.43165500	0.06551500	C	0.78310000	-1.44830000	0.01950000
C	-0.22117200	-2.31978700	0.05747100	C	-0.29480000	-2.32480000	-0.01090000
C	-1.36717000	-1.48567300	-0.01061200	C	-1.43280000	-1.47900000	-0.05010000
C	-2.79896200	-1.91977500	-0.05093200	C	-2.86750000	-1.89920000	-0.09980000
O	-3.11230400	-3.09557500	-0.03889300	O	-3.19360000	-3.07120000	-0.13310000
N	-3.67862300	-0.86886600	-0.10020400	N	-3.73290000	-0.83770000	-0.10200000
C	2.27612600	-1.70957200	0.09335200	C	2.20510000	-1.73820000	0.03510000
C	2.93068700	-2.61572400	0.88847900	C	2.83400000	-2.73480000	0.73750000
S	3.39902800	-0.96139700	-1.03481500	S	3.35910000	-0.85820000	-0.95800000
C	4.32426900	-2.71977900	0.62563700	C	4.23500000	-2.80830000	0.50860000
H	2.42626500	-3.18061000	1.66024300	H	2.30370000	-3.38290000	1.42080000
C	4.71576500	-1.88692800	-0.37935700	C	4.65640000	-1.86040000	-0.37580000
H	5.00423300	-3.36738200	1.16036600	H	4.90160000	-3.51470000	0.98180000
Cl	1.70764500	0.71781500	2.58863100	Cl	1.87750000	0.52880000	2.50250000
Cl	2.97397400	5.15632900	-0.21674100	Cl	3.08950000	5.05070000	-0.19480000
H	-3.29099700	0.06903500	-0.09158500	H	-3.33590000	0.09480000	-0.05540000
N	-1.04160300	-0.19485900	-0.05007700	N	-1.09540000	-0.18960000	-0.05290000
C	-0.16724800	-3.81557800	0.07068900	C	-0.25350000	-3.81970000	-0.04010000
H	-0.36567400	-4.20966100	1.07238200	H	-0.38220000	-4.23620000	0.96410000
H	-0.93615300	-4.22865800	-0.58033500	H	-1.07110000	-4.20690000	-0.64530000
H	0.81566400	-4.17069600	-0.24571200	H	0.70320000	-4.17150000	-0.43280000

Cl	6.32065400	-1.67850000	-0.99538000	Cl	6.28180000	-1.58510000	-0.90760000
C	-5.76703500	-0.71918000	1.07838700	C	-5.80770000	-0.68740000	1.07800000
C	-5.67397700	-0.68635900	-1.41165000	C	-5.70300000	-0.52880000	-1.40740000
C	-5.84650000	0.77117800	1.44689800	C	-5.79010000	0.78450000	1.51700000
H	-6.78079700	-1.11780300	0.96347200	H	-6.84380000	-1.01490000	0.94260000
H	-5.30200600	-1.27715800	1.89557200	H	-5.37840000	-1.31480000	1.86390000
C	-5.46021100	0.76036000	-1.91440800	C	-5.36640000	0.91620000	-1.83760000
H	-6.74274700	-0.87623900	-1.28155500	H	-6.78360000	-0.63620000	-1.28360000
H	-5.32878100	-1.38042200	-2.18462400	H	-5.41100000	-1.21140000	-2.21190000
C	-6.41941300	1.68713800	0.35249500	C	-6.29910000	1.78120000	0.46210000
H	-4.84904100	1.13497800	1.72485500	H	-4.77010000	1.06660000	1.80740000
H	-6.45850800	0.85363600	2.35311300	H	-6.39640000	0.86690000	2.42670000
C	-5.47810900	1.88075400	-0.85072800	C	-5.33160000	1.98210000	-0.71930000
H	-6.24039400	0.95202000	-2.66017100	H	-6.10680000	1.20110000	-2.59350000
H	-4.51178000	0.81801100	-2.45850800	H	-4.39910000	0.92140000	-2.35020000
H	-7.39586000	1.31302000	0.01847800	H	-7.28660000	1.47130000	0.09700000
H	-6.61157300	2.66919100	0.79711600	H	-6.44840000	2.74950000	0.95070000
H	-5.73000100	2.81814200	-1.35696200	H	-5.52180000	2.95710000	-1.17870000
H	-4.46376800	2.03164700	-0.45957700	H	-4.31550000	2.05390000	-0.31050000
N	-5.05055900	-1.07162000	-0.14826100	N	-5.10740000	-1.01640000	-0.16470000
12							
C	1.54956900	3.43554300	0.87687000	C	1.76750000	3.23160000	0.93280000
C	0.83300600	2.25672300	1.06108600	C	0.97330000	2.10050000	1.09210000
C	0.23110900	1.61382400	-0.02609100	C	0.26040000	1.57710000	0.00800000
C	0.32379200	2.19377700	-1.29122700	C	0.32210000	2.22590000	-1.22440000
C	1.02159100	3.37719400	-1.48892800	C	1.09600000	3.36500000	-1.39480000
C	1.63773000	3.98126300	-0.39763700	C	1.82210000	3.84940000	-0.31070000
H	2.01626900	3.92322600	1.72081600	H	2.32310000	3.62640000	1.77120000
H	-0.16365500	1.69831900	-2.12118200	H	-0.24780000	1.81580000	-2.04810000
H	1.09335700	3.82080400	-2.47266300	H	1.14660000	3.86450000	-2.35260000
N	-0.51633800	0.41093500	0.12442000	N	-0.53840000	0.40800000	0.12680000
C	-0.07850900	-0.85807800	0.46035900	C	-0.14090000	-0.88600000	0.40950000
C	-1.20704100	-1.67121600	0.47036100	C	-1.29580000	-1.66000000	0.39560000
C	-2.26975200	-0.79758500	0.12466900	C	-2.33030000	-0.73930000	0.09020000
C	-3.71703300	-1.14087200	-0.02127600	C	-3.78600000	-1.03470000	-0.05580000
O	-4.13452200	-2.27779300	0.15419700	O	-4.23600000	-2.16410000	0.08840000
N	-4.50089000	-0.07790100	-0.36498900	N	-4.54430000	0.05720000	-0.36210000

C	1.31192600	-1.21126300	0.70081200	C	1.23530000	-1.28910000	0.63130000
C	1.79358200	-2.03952200	1.68815100	C	1.67840000	-2.21720000	1.54530000
S	2.61456000	-0.69174600	-0.34785000	S	2.57160000	-0.67640000	-0.32000000
C	3.19007600	-2.25366200	1.62428100	C	3.07450000	-2.43720000	1.50250000
H	1.15624300	-2.46171300	2.45279600	H	1.01200000	-2.70310000	2.24400000
C	3.79976000	-1.59199100	0.58153800	C	3.71950000	-1.67860000	0.55080000
H	3.74471200	-2.86299600	2.32440200	H	3.60480000	-3.11820000	2.15340000
Cl	0.67767000	1.62376000	2.68006800	Cl	0.87720000	1.36510000	2.67160000
Cl	2.53682300	5.46942800	-0.62554100	Cl	2.82340000	5.27580000	-0.50810000
H	-4.06314600	0.82582000	-0.47513500	H	-4.09180000	0.95590000	-0.44690000
N	-1.84414800	0.44641000	-0.08798300	N	-1.86480000	0.49810000	-0.07820000
C	-6.27833600	-0.95662200	-1.71125300	C	-6.34290000	-0.76260000	-1.70780000
C	-6.63066200	-0.45295700	0.67017700	C	-6.65950000	-0.32210000	0.68920000
C	-7.76650900	-0.75393400	-2.00533800	C	-7.83420000	-0.54950000	-1.97420000
H	-6.06848300	-2.01861200	-1.52055000	H	-6.13370000	-1.82850000	-1.54130000
H	-5.67231500	-0.64111100	-2.56395300	H	-5.74610000	-0.42960000	-2.56030000
C	-8.12732400	-0.23766200	0.43414000	C	-8.15840000	-0.09810000	0.48010000
H	-6.43890700	-1.48922800	0.98254300	H	-6.46470000	-1.36800000	0.96420000
H	-6.26742700	0.20978800	1.45922300	H	-6.28150000	0.31530000	1.49190000
C	-8.61855300	-1.05684500	-0.76619900	C	-8.66450000	-0.89240000	-0.73080000
H	-8.05816000	-1.39667000	-2.84206200	H	-8.13930000	-1.16450000	-2.82660000
H	-7.92924000	0.28363000	-2.31799800	H	-8.00060000	0.49850000	-2.24800000
H	-8.67694300	-0.51132000	1.34036600	H	-8.69610000	-0.38940000	1.38780000
H	-8.30892300	0.82731800	0.25088500	H	-8.33940000	0.97050000	0.31880000
H	-9.67403200	-0.84841000	-0.96648800	H	-9.72490000	-0.68940000	-0.90820000
H	-8.54571300	-2.12567700	-0.52921300	H	-8.57460000	-1.96570000	-0.52150000
N	-5.88805000	-0.12252700	-0.56009000	N	-5.93380000	0.04290000	-0.54210000
C	-1.27067700	-3.14295800	0.73704200	C	-1.40470000	-3.13670000	0.60850000
H	-1.56501300	-3.34589600	1.77185700	H	-1.65540000	-3.36690000	1.64920000
H	-2.02271800	-3.61078100	0.10381400	H	-2.20490000	-3.54800000	-0.00390000
H	-0.29895300	-3.61018200	0.56440300	H	-0.45990000	-3.63060000	0.37130000
C	5.16222900	-1.56480600	0.22729600	C	5.09140000	-1.62830000	0.24240000
C	6.32985800	-1.53185300	-0.08321000	C	6.26680000	-1.56920000	-0.03040000
C	7.73601100	-1.51681400	-0.46864900	C	7.67960000	-1.52780000	-0.38490000
C	8.11235800	-2.61559500	-1.48596100	C	8.03220000	-2.40030000	-1.60880000
H	8.35487000	-1.62593800	0.43051900	H	8.27600000	-1.85170000	0.47690000
H	7.98118300	-0.53329900	-0.88819200	H	7.97070000	-0.48880000	-0.58350000

C	9.59314900	-2.56967600	-1.86775200	C	9.52150000	-2.33110000	-1.95240000
H	7.86318400	-3.59165100	-1.05901900	H	7.73900000	-3.43390000	-1.40160000
H	7.48933400	-2.49877000	-2.37771900	H	7.43130000	-2.07110000	-2.46180000
H	9.83720900	-3.35479800	-2.58757000	H	9.75490000	-2.95320000	-2.81980000
H	9.85752400	-1.60954500	-2.32159000	H	9.82650000	-1.30610000	-2.18530000
H	10.23446500	-2.71113000	-0.99228800	H	10.13690000	-2.67930000	-1.11690000
13							
C	1.06569900	3.11160400	1.24494100	C	1.24030000	2.90820000	1.29660000
C	0.61134800	1.79772700	1.31156400	C	0.71760000	1.61920000	1.33100000
C	0.13539600	1.15088000	0.16574800	C	0.10970000	1.07040000	0.19640000
C	0.08485000	1.85596800	-1.03677900	C	-0.00290000	1.84580000	-0.95700000
C	0.51965200	3.17174100	-1.11671800	C	0.49750000	3.13930000	-1.00130000
C	1.01643200	3.78324300	0.02987300	C	1.12630000	3.65290000	0.12910000
H	1.43721500	3.60210200	2.13336200	H	1.71680000	3.32340000	2.17300000
H	-0.30221400	1.35121900	-1.91277100	H	-0.48820000	1.41030000	-1.82090000
H	0.48215700	3.71233400	-2.05270700	H	0.41380000	3.73730000	-1.89850000
N	-0.34435900	-0.18908900	0.19721500	N	-0.41550000	-0.24900000	0.18700000
C	0.35275700	-1.36657300	0.40144400	C	0.25090000	-1.45160000	0.33280000
C	-0.58401700	-2.39275700	0.33565100	C	-0.71550000	-2.44730000	0.23740000
C	-1.81302800	-1.72995700	0.08645700	C	-1.92730000	-1.74240000	0.02900000
C	-3.16313300	-2.35685800	-0.08198500	C	-3.29700000	-2.32260000	-0.14490000
O	-3.32283300	-3.56137500	-0.02696100	O	-3.50280000	-3.52010000	-0.08780000
N	-4.15131300	-1.43175300	-0.29709400	N	-4.23980000	-1.35710000	-0.36980000
C	1.79164000	-1.44553000	0.59957500	C	1.68540000	-1.57490000	0.51130000
C	2.45771200	-2.24923600	1.49580700	C	2.33430000	-2.48400000	1.31490000
S	2.93346500	-0.56597000	-0.39515400	S	2.84130000	-0.58860000	-0.35900000
C	3.86640000	-2.16177200	1.40557500	C	3.74410000	-2.39480000	1.25260000
H	1.93987100	-2.86832600	2.21529400	H	1.80080000	-3.17640000	1.95060000
C	4.30115400	-1.28836600	0.43352300	C	4.19360000	-1.41400000	0.39630000
H	4.55156300	-2.70929800	2.03792800	H	4.42020000	-3.01590000	1.82340000
Cl	0.62074300	0.99307200	2.86019200	Cl	0.82380000	0.71620000	2.82030000
Cl	1.58451400	5.44053900	-0.04988300	Cl	1.78400000	5.27860000	0.08970000
H	-3.87996800	-0.45497300	-0.29874200	H	-3.92650000	-0.39440000	-0.34710000
N	-1.65754000	-0.41000000	-0.00222800	N	-1.73620000	-0.42360000	-0.00800000
C	-0.33703700	-3.86468900	0.45208600	C	-0.50830000	-3.92760000	0.29500000
H	-0.56113100	-4.22531900	1.46122200	H	-0.66690000	-4.30780000	1.30940000
H	-0.99126700	-4.41260400	-0.22395300	H	-1.22950000	-4.43370000	-0.34400000

H	0.70606400	-4.10127100	0.23205100	H	0.50860000	-4.18700000	-0.00800000
C	5.61984400	-0.94492200	0.07896600	C	5.51690000	-1.03790000	0.10100000
C	6.74787600	-0.64100300	-0.23096400	C	6.64720000	-0.69910000	-0.15840000
C	8.11162900	-0.29907000	-0.61744700	C	8.01140000	-0.31760000	-0.50020000
C	8.69758000	-1.22229900	-1.70748100	C	8.51210000	-0.94250000	-1.82020000
H	8.75456600	-0.33132900	0.27084000	H	8.68170000	-0.60910000	0.31760000
H	8.13342200	0.73945500	-0.97014900	H	8.07300000	0.77560000	-0.56950000
C	10.12778400	-0.83482900	-2.08828500	C	9.94530000	-0.51890000	-2.14770000
H	8.67009200	-2.25494000	-1.34698900	H	8.44760000	-2.03190000	-1.74170000
H	8.04934300	-1.18372000	-2.58800800	H	7.83630000	-0.64790000	-2.62870000
H	10.52236900	-1.50048000	-2.85987100	H	10.28480000	-0.96870000	-3.08390000
H	10.17314000	0.18726000	-2.47689500	H	10.02260000	0.56780000	-2.25250000
H	10.79878300	-0.89231800	-1.22561300	H	10.63890000	-0.82690000	-1.35910000
C	-6.39726200	-1.28936500	0.56021500	C	-6.42710000	-1.07050000	0.55720000
C	-6.06432700	-1.37872900	-1.75564200	C	-6.17020000	-1.12690000	-1.75800000
H	-5.87492000	-1.21944500	1.51457900	H	-5.89520000	-1.11620000	1.50760000
H	-7.21042400	-2.01318300	0.67591100	H	-7.32940000	-1.68340000	0.64400000
C	-6.72690300	0.00031400	-1.51525300	C	-6.61820000	0.32500000	-1.46130000
H	-6.82130400	-2.11682800	-2.03999800	H	-7.03560000	-1.74740000	-2.01060000
H	-5.29423900	-1.37665900	-2.52743200	H	-5.44360000	-1.21520000	-2.56580000
H	-7.68044600	0.05851700	-2.04594600	H	-7.56510000	0.54210000	-1.96110000
C	-6.95198100	0.05951400	0.03943200	C	-6.79090000	0.36310000	0.10040000
C	-6.21717400	1.33628600	0.51916200	C	-5.85660000	1.49470000	0.59690000
C	-6.15418500	2.23893300	-0.72294100	C	-5.68990000	2.42000000	-0.61840000
H	-5.20066900	1.09237000	0.84827000	H	-4.88170000	1.08970000	0.88920000
H	-6.71602600	1.80779500	1.36944600	H	-6.25610000	2.00660000	1.47550000
C	-5.87073100	1.24472100	-1.85995500	C	-5.59260000	1.43670000	-1.79530000
H	-7.12423200	2.72323900	-0.88313800	H	-6.57980000	3.04950000	-0.73230000
H	-5.40361600	3.02980900	-0.64371500	H	-4.82550000	3.08420000	-0.53850000
H	-6.10048200	1.64532800	-2.85047300	H	-5.78770000	1.90360000	-2.76370000
H	-4.80540800	0.98680000	-1.86505000	H	-4.57980000	1.02210000	-1.84710000
H	-8.01632000	0.14475200	0.27213400	H	-7.82300000	0.59930000	0.36990000
N	-5.48191900	-1.81987200	-0.47162400	N	-5.59670000	-1.67020000	-0.50950000
14							
C	1.08052900	3.19519200	1.19668100	C	1.28850000	2.99970000	1.25060000
C	0.56747500	1.90450400	1.28626000	C	0.70300000	1.73920000	1.31580000
C	0.06500100	1.25872600	0.15124500	C	0.06150000	1.19700000	0.19660000

C	0.04798600	1.94308700	-1.06407700	C	-0.02020000	1.95200000	-0.97270000
C	0.54163200	3.23627400	-1.16701600	C	0.54330000	3.21780000	-1.04790000
C	1.06364100	3.84581600	-0.03063500	C	1.20410000	3.72370000	0.06770000
H	1.47202100	3.68486100	2.07694200	H	1.79050000	3.40950000	2.11510000
H	-0.36057500	1.44037100	-1.93141700	H	-0.53260000	1.52280000	-1.82400000
H	0.52967000	3.76080400	-2.11276000	H	0.48330000	3.79980000	-1.95730000
N	-0.47469600	-0.05761100	0.20594800	N	-0.52500000	-0.09640000	0.21820000
C	0.16824200	-1.26093700	0.43672400	C	0.08930000	-1.32470000	0.38000000
C	-0.81346000	-2.24496600	0.38690300	C	-0.91940000	-2.27840000	0.30140000
C	-2.01043000	-1.53231500	0.11871700	C	-2.10060000	-1.52370000	0.08740000
C	-3.38535500	-2.10031100	-0.04548800	C	-3.49140000	-2.04750000	-0.08160000
O	-3.60038800	-3.29574500	0.02997300	O	-3.73280000	-3.24000000	-0.11470000
N	-4.33735700	-1.14148000	-0.28218800	N	-4.42450000	-1.05020000	-0.19120000
C	1.60162100	-1.40038600	0.64140000	C	1.51790000	-1.50780000	0.55650000
C	2.22906500	-2.21450800	1.55590000	C	2.12920000	-2.42550000	1.37930000
S	2.78382300	-0.59373800	-0.36783300	S	2.71260000	-0.59540000	-0.34160000
C	3.64045400	-2.19263000	1.46773700	C	3.54130000	-2.40150000	1.30950000
H	1.68246700	-2.79452800	2.28659400	H	1.56820000	-3.07790000	2.03350000
C	4.11595900	-1.36000400	0.47911300	C	4.03020000	-1.46250000	0.42830000
H	4.29902000	-2.75731100	2.11312500	H	4.19160000	-3.03840000	1.89270000
Cl	0.53754200	1.12930500	2.84961700	Cl	0.77460000	0.86400000	2.82360000
Cl	1.70586600	5.47412000	-0.13933300	Cl	1.94170000	5.31330000	-0.01090000
H	-4.03122600	-0.17445800	-0.31477100	H	-4.08950000	-0.09250000	-0.19310000
N	-1.79531500	-0.22282800	0.00456700	N	-1.85230000	-0.21540000	0.02900000
C	-0.63327100	-3.72387300	0.53324900	C	-0.77490000	-3.76540000	0.37920000
H	-0.87917400	-4.05448400	1.54757800	H	-0.96030000	-4.12630000	1.39620000
H	-1.30708800	-4.25536900	-0.13668200	H	-1.50860000	-4.24800000	-0.26340000
H	0.39951900	-4.01087600	0.32494700	H	0.23400000	-4.07010000	0.09190000
C	-6.56280300	-1.08466100	0.62061100	C	-6.66140000	-0.88090000	0.62870000
C	-6.15902500	-1.25169500	-1.83239600	C	-6.17790000	-1.05540000	-1.81000000
C	-6.80592800	0.41822700	0.83550200	C	-6.78240000	0.63570000	0.84570000
H	-7.51924500	-1.58116100	0.42413700	H	-7.64770000	-1.29330000	0.39110000
H	-6.16201900	-1.52787800	1.53621100	H	-6.33110000	-1.36190000	1.55330000
C	-5.99697900	0.16118000	-2.43988400	C	-5.83920000	0.33510000	-2.39010000
H	-7.21759600	-1.52441400	-1.81285300	H	-7.25890000	-1.21510000	-1.83420000
H	-5.66577900	-1.97445700	-2.49020900	H	-5.73440000	-1.82240000	-2.45290000
C	-7.30421400	1.18542800	-0.40074800	C	-7.16260000	1.44180000	-0.40770000

H	-5.88390500	0.89170300	1.19627000	H	-5.83640000	1.02470000	1.24310000
H	-7.53342400	0.52055300	1.64970700	H	-7.52930000	0.79950000	1.63140000
C	-6.23543600	1.36019800	-1.49539400	C	-6.03040000	1.54420000	-1.44690000
H	-6.68966300	0.22015000	-3.28745800	H	-6.45960000	0.46440000	-3.28400000
H	-4.99492300	0.25698900	-2.87062900	H	-4.80300000	0.33300000	-2.74300000
H	-8.19850000	0.70006100	-0.81274900	H	-8.06470000	1.01880000	-0.86790000
H	-7.62660500	2.18035600	-0.07625000	H	-7.43130000	2.45550000	-0.09330000
H	-6.49229500	2.22653800	-2.11344100	H	-6.18980000	2.43220000	-2.06660000
H	-5.29354800	1.63143500	-1.00162500	H	-5.09600000	1.73920000	-0.90530000
C	5.44933500	-1.08343300	0.12101100	C	5.36770000	-1.15320000	0.11960000
C	6.59027200	-0.83664300	-0.19241500	C	6.51080000	-0.87170000	-0.15140000
C	7.96770800	-0.56235800	-0.58427800	C	7.88930000	-0.55950000	-0.50630000
C	8.47939600	-1.46610000	-1.72677100	C	8.35310000	-1.22810000	-1.81820000
H	8.61867500	-0.67851000	0.29099900	H	8.55000000	-0.86870000	0.31300000
H	8.05106900	0.48878900	-0.88700300	H	8.00120000	0.52830000	-0.59370000
C	9.92573700	-1.15016100	-2.11265900	C	9.80270000	-0.87720000	-2.15930000
H	8.39191400	-2.51134700	-1.41557800	H	8.23840000	-2.31200000	-1.72180000
H	7.82285100	-1.34443000	-2.59348700	H	7.68740000	-0.91540000	-2.62830000
H	10.26697300	-1.80063600	-2.92171600	H	10.11580000	-1.35720000	-3.08970000
H	10.02989200	-0.11513700	-2.45267700	H	9.92990000	0.20290000	-2.28200000
H	10.60365800	-1.29122700	-1.26515200	H	10.48550000	-1.20460000	-1.36900000
N	-5.67135700	-1.47247600	-0.47333900	N	-5.76220000	-1.32830000	-0.43450000
15							
C	1.13118500	3.62712600	0.83746200	C	1.36430000	3.44980000	0.86960000
C	0.46948200	2.42002000	1.04250800	C	0.62280000	2.28830000	1.06090000
C	-0.08511900	1.72170100	-0.03559700	C	-0.04880000	1.69190000	-0.01200000
C	-0.00214900	2.27348500	-1.31393300	C	-0.00070000	2.29770000	-1.26660000
C	0.64082300	3.48392100	-1.53282900	C	0.72030000	3.46580000	-1.46950000
C	1.21139900	4.14430900	-0.44942000	C	1.40700000	4.02380000	-0.39510000
H	1.56172400	4.15785000	1.67463400	H	1.88840000	3.90130000	1.69970000
H	-0.45325400	1.73436800	-2.13720100	H	-0.53870000	1.83100000	-2.08160000
H	0.70538700	3.90566700	-2.52662600	H	0.76060000	3.93190000	-2.44440000
N	-0.77607300	0.48823500	0.13606900	N	-0.79270000	0.49090000	0.14000000
C	-0.28272000	-0.74944100	0.50983100	C	-0.33860000	-0.77130000	0.47630000
C	-1.37112900	-1.61548200	0.52658000	C	-1.45490000	-1.60000000	0.47550000
C	-2.46955700	-0.80290800	0.14546200	C	-2.52720000	-0.74200000	0.12170000
C	-3.89683700	-1.21864300	-0.00912300	C	-3.96480000	-1.11200000	-0.03320000

O	-4.26197400	-2.36970700	0.18933200	O	-4.36280000	-2.25590000	0.14520000
N	-4.72588800	-0.20295800	-0.38790600	N	-4.76950000	-0.06920000	-0.38830000
C	1.11953000	-1.02914600	0.77677200	C	1.05170000	-1.09940000	0.73170000
C	1.62618100	-1.80982600	1.79010200	C	1.52410000	-1.97160000	1.68520000
S	2.41055200	-0.47201400	-0.26680600	S	2.37200000	-0.45750000	-0.22280000
C	3.03203400	-1.95795300	1.74966500	C	2.92960000	-2.12570000	1.66980000
H	0.99893100	-2.24414300	2.55629200	H	0.87080000	-2.46340000	2.39200000
C	3.62422100	-1.29236500	0.69925100	C	3.55250000	-1.37140000	0.69990000
H	3.60514300	-2.52297400	2.47173800	H	3.48160000	-2.75640000	2.35250000
Cl	0.32162300	1.82086300	2.67499300	Cl	0.53950000	1.60730000	2.66530000
Cl	2.04113800	5.66803200	-0.70371400	Cl	2.34180000	5.48870000	-0.63280000
H	-4.33027800	0.71782500	-0.51483200	H	-4.35890000	0.84660000	-0.49940000
N	-2.10102400	0.45442700	-0.09360800	N	-2.11850000	0.50940000	-0.08640000
C	-6.44336500	-1.19694500	-1.73197900	C	-6.50650000	-1.02090000	-1.72810000
C	-6.84779900	-0.65467100	0.63268900	C	-6.87990000	-0.51270000	0.64740000
C	-7.93582000	-1.07223700	-2.04701200	C	-8.00220000	-0.88920000	-2.02180000
H	-6.18584500	-2.24298500	-1.51351900	H	-6.24930000	-2.06900000	-1.52100000
H	-5.84273300	-0.87310200	-2.58536800	H	-5.91360000	-0.68940000	-2.58380000
C	-8.35002400	-0.51655700	0.37522800	C	-8.38440000	-0.36860000	0.41040000
H	-6.61094200	-1.67296100	0.97206400	H	-6.63970000	-1.53780000	0.96210000
H	-6.52588700	0.04306300	1.40941900	H	-6.54480000	0.16990000	1.43190000
C	-8.78739800	-1.38621700	-0.81032500	C	-8.83370000	-1.22820000	-0.77810000
H	-8.18669600	-1.74750300	-2.87123800	H	-8.26480000	-1.54760000	-2.85580000
H	-8.14361900	-0.05116800	-2.38613500	H	-8.21420000	0.13930000	-2.33480000
H	-8.89692700	-0.79467800	1.28173600	H	-8.92130000	-0.65340000	1.32060000
H	-8.57966000	0.53394200	0.16437800	H	-8.61370000	0.68380000	0.20860000
H	-9.84907000	-1.23302200	-1.02707700	H	-9.89990000	-1.08290000	-0.97680000
H	-8.66696400	-2.44452400	-0.54695900	H	-8.69590000	-2.28800000	-0.52960000
N	-6.10688500	-0.31837400	-0.59702900	N	-6.15380000	-0.15650000	-0.58640000
C	-1.36813100	-3.08145200	0.83013900	C	-1.49670000	-3.07140000	0.74200000
H	-1.66555000	-3.27227700	1.86639200	H	-1.75070000	-3.27510000	1.78730000
H	-2.08901000	-3.60038400	0.20051700	H	-2.26770000	-3.54270000	0.13540000
H	-0.37318800	-3.50589400	0.68076700	H	-0.52630000	-3.52800000	0.53500000
C	4.98876200	-1.20748100	0.36262700	C	4.92490000	-1.26750000	0.40850000
C	6.15824800	-1.12709800	0.06722000	C	6.10070000	-1.16530000	0.15010000
C	7.56647900	-1.03670400	-0.29983800	C	7.51440000	-1.07170000	-0.18970000
C	8.02355800	-2.07458800	-1.35803600	C	7.93370000	-1.94920000	-1.39750000

H	8.18107700	-1.15232500	0.60257700	H	8.11470000	-1.35860000	0.68360000
H	7.76656100	-0.02714700	-0.67810900	H	7.76060000	-0.02440000	-0.40130000
C	9.46885800	-1.78599900	-1.78088000	C	9.40110000	-1.68110000	-1.75010000
H	7.37598100	-1.94905400	-2.23365400	H	7.31040000	-1.64930000	-2.24820000
H	9.79752700	-2.48906200	-2.55079700	H	9.70690000	-2.27000000	-2.61880000
H	9.57579300	-0.77469500	-2.18415400	H	9.57320000	-0.62590000	-1.98180000
H	10.15294200	-1.88224700	-0.93072000	H	10.05700000	-1.95380000	-0.91610000
C	7.86562700	-3.50989900	-0.84528800	C	7.68960000	-3.43600000	-1.11960000
H	8.50367100	-3.68354500	0.02839600	H	8.29730000	-3.77460000	-0.27310000
H	6.83326400	-3.71797700	-0.55528200	H	6.64120000	-3.62890000	-0.88110000
H	8.15271300	-4.23139300	-1.61507600	H	7.95900000	-4.04300000	-1.98810000
16							
C	0.69111500	3.33171300	1.16926900	C	0.89000000	3.17090000	1.20060000
C	0.22584800	2.02493200	1.28311900	C	0.35690000	1.88940000	1.29820000
C	-0.23371200	1.33317800	0.15704300	C	-0.23690000	1.28230000	0.18620000
C	-0.25723600	1.98678300	-1.07498300	C	-0.32520000	1.99260000	-1.01030000
C	0.18874500	3.29501200	-1.20252700	C	0.18590000	3.27810000	-1.11850000
C	0.66919900	3.95135000	-0.07390600	C	0.80070000	3.84980000	-0.00840000
H	1.04975700	3.85712500	2.04289300	H	1.35570000	3.63120000	2.06020000
H	-0.63266800	1.44801800	-1.93562800	H	-0.80060000	1.51300000	-1.85620000
H	0.17200500	3.79566300	-2.16105400	H	0.12100000	3.82560000	-2.04890000
N	-0.72408300	-0.00110500	0.23626600	N	-0.76830000	-0.03370000	0.24130000
C	-0.04006000	-1.17313800	0.50660800	C	-0.10600000	-1.22810000	0.45790000
C	-0.98307400	-2.19475000	0.46641400	C	-1.07140000	-2.22660000	0.39320000
C	-2.20158500	-1.53492100	0.16247700	C	-2.27890000	-1.53130000	0.12980000
C	-3.55145700	-2.15845400	-0.00838100	C	-3.64240000	-2.12020000	-0.04730000
O	-3.72250900	-3.35913900	0.09214900	O	-3.83290000	-3.32220000	-0.03640000
N	-4.53498800	-1.24223400	-0.28191200	N	-4.61340000	-1.16870000	-0.21730000
C	1.39398400	-1.25296500	0.73687800	C	1.32500000	-1.34330000	0.66830000
C	2.03639300	-2.02100600	1.68047100	C	1.95730000	-2.20610000	1.53370000
S	2.56149000	-0.42521900	-0.27227400	S	2.49850000	-0.41110000	-0.23730000
C	3.44716200	-1.94688400	1.61449800	C	3.36820000	-2.12410000	1.49010000
H	1.50002100	-2.60436300	2.41606300	H	1.41090000	-2.85960000	2.19900000
C	3.90739600	-1.11963600	0.61409400	C	3.83520000	-1.19510000	0.58670000
H	4.11567700	-2.47031200	2.28399900	H	4.03270000	-2.71290000	2.10700000
Cl	0.20047200	1.28712400	2.86453300	Cl	0.43310000	1.07010000	2.83690000
Cl	1.25110100	5.59984500	-0.21327500	Cl	1.47210000	5.46590000	-0.12790000

H	-4.26447800	-0.26553600	-0.33500900	H	-4.32080000	-0.19750000	-0.23930000
N	-2.03407800	-0.22135000	0.01902500	N	-2.08520000	-0.21620000	0.03070000
C	-0.74968000	-3.66174000	0.65230600	C	-0.86580000	-3.70240000	0.52560000
H	-0.99500200	-3.97587900	1.67201300	H	-1.05700000	-4.03610000	1.55080000
H	-1.39527900	-4.23460200	-0.01124300	H	-1.56490000	-4.23780000	-0.11380000
H	0.29548100	-3.91496200	0.46268300	H	0.16090000	-3.97310000	0.26890000
C	-6.77722300	-1.24232400	0.57999700	C	-6.86320000	-1.08920000	0.58270000
C	-6.32268000	-1.46611900	-1.85958300	C	-6.35060000	-1.28100000	-1.84870000
C	-7.07955200	0.25604600	0.74583400	C	-7.05430000	0.42350000	0.77460000
H	-7.71096100	-1.77969800	0.38186100	H	-7.82750000	-1.54960000	0.34330000
H	-6.37725600	-1.64334100	1.51520200	H	-6.52000000	-1.54050000	1.51750000
C	-6.20258300	-0.06661700	-2.50644600	C	-6.07240000	0.11440000	-2.44930000
H	-7.37046400	-1.77822200	-1.85005600	H	-7.42280000	-1.49120000	-1.87860000
H	-5.79079900	-2.18881100	-2.48662800	H	-5.86650000	-2.03660000	-2.47560000
C	-7.58276700	0.96770200	-0.52125400	C	-7.45900000	1.19230000	-0.49450000
H	-6.18253600	0.77406900	1.10844100	H	-6.13020000	0.86070000	1.17350000
H	-7.82533400	0.35467400	1.54378600	H	-7.81470000	0.56570000	1.55140000
C	-6.50116900	1.14968200	-1.60207900	C	-6.32380000	1.32810000	-1.52650000
H	-6.88248400	-0.05835200	-3.36629400	H	-6.69300000	0.20130000	-3.34830000
H	-5.19757000	0.05409400	-2.92384100	H	-5.03520000	0.15420000	-2.79690000
H	-8.45100300	0.43758800	-0.93377700	H	-8.33790000	0.72280000	-0.95480000
H	-7.94720500	1.95907200	-0.23233500	H	-7.77470000	2.19790000	-0.19840000
H	-6.77769000	1.98784000	-2.24979300	H	-6.51670000	2.19860000	-2.16120000
H	-5.57879500	1.46924200	-1.10039500	H	-5.40330000	1.57210000	-0.98100000
C	5.23513600	-0.79953900	0.27176100	C	5.16480000	-0.84160000	0.29210000
C	6.37168300	-0.51710700	-0.02814800	C	6.30160000	-0.52540000	0.03240000
C	7.74097400	-0.18225400	-0.40096400	C	7.67330000	-0.17390000	-0.31050000
C	8.32693800	-1.04984500	-1.54542400	C	8.22520000	-0.91940000	-1.55320000
H	8.38640400	-0.27335600	0.48255000	H	8.32480000	-0.38350000	0.54810000
H	7.77620100	0.87293600	-0.69708900	H	7.73040000	0.90740000	-0.48280000
C	9.70150100	-0.50978200	-1.95762200	C	9.61950000	-0.38670000	-1.90200000
H	7.64823900	-0.95596500	-2.40121700	H	7.54960000	-0.70130000	-2.38860000
H	10.11595600	-1.09025200	-2.78610700	H	10.01320000	-0.88050000	-2.79430000
H	9.64403200	0.53488900	-2.27728000	H	9.60270000	0.69030000	-2.09360000
H	10.41129900	-0.56736000	-1.12522100	H	10.32230000	-0.57180000	-1.08230000
C	8.40114600	-2.52861900	-1.15087000	C	8.24660000	-2.43520000	-1.33160000
H	9.07776300	-2.67114900	-0.30089700	H	8.91350000	-2.69390000	-0.50150000

H	7.41934900	-2.91528700	-0.86851900	H	7.25050000	-2.81650000	-1.09580000
H	8.77735500	-3.13376900	-1.98021700	H	8.60770000	-2.95330000	-2.22400000
N	-5.85216100	-1.62817400	-0.48631700	N	-5.93480000	-1.51180000	-0.46580000
18							
C	1.63667600	3.48455800	1.01736900	C	1.86824500	3.25890600	1.07442400
C	0.90550500	2.30703900	1.14369700	C	1.05459300	2.13410900	1.16665900
C	0.30463100	1.72042000	0.02466600	C	0.34550000	1.67943500	0.04954300
C	0.41304400	2.35540700	-1.21246200	C	0.43083400	2.39022600	-1.14663100
C	1.12541500	3.53837200	-1.35213600	C	1.22446500	3.52379700	-1.24968700
C	1.74040200	4.08575000	-0.23070200	C	1.94620700	3.93933800	-0.13456700
H	2.10244200	3.92861200	1.88556300	H	2.42071400	3.60064200	1.93789800
H	-0.07328300	1.90303600	-2.06730300	H	-0.13581400	2.03238100	-1.99655200
H	1.20945700	4.02465200	-2.31449500	H	1.29351700	4.07130100	-2.17969100
N	-0.45659300	0.51999600	0.11550100	N	-0.47170300	0.51813800	0.09912800
C	-0.03516200	-0.76671700	0.40157500	C	-0.09608100	-0.79474600	0.32107000
C	-1.17220800	-1.56837300	0.36827200	C	-1.26203900	-1.54956900	0.25749500
C	-2.22279000	-0.66779000	0.05029200	C	-2.28008500	-0.59761500	-0.00788600
C	-3.67077400	-0.98643500	-0.13680100	C	-3.73696100	-0.86589200	-0.18137700
O	-4.11195200	-2.11753400	0.02263500	O	-4.20826000	-1.98855300	-0.04550200
N	-4.42749700	0.08898300	-0.50001000	N	-4.47129700	0.23737600	-0.50169400
C	1.35429200	-1.14011100	0.62252700	C	1.27495200	-1.22491400	0.52855800
C	1.84274800	-1.99092000	1.58666400	C	1.70965900	-2.18987100	1.40750800
S	2.64658000	-0.61332800	-0.43568300	S	2.61579800	-0.59554800	-0.40554700
C	3.23602600	-2.21728200	1.49751200	C	3.10261900	-2.42618600	1.35069000
H	1.21349700	-2.42139600	2.35315000	H	1.04074800	-2.69167000	2.09206400
C	3.83669900	-1.54168600	0.45853600	C	3.75398700	-1.64239500	0.42405300
H	3.79485000	-2.84497300	2.17779900	H	3.62634100	-3.13651500	1.97507400
Cl	0.72962700	1.60537100	2.73195900	Cl	0.92874600	1.31980400	2.70480500
Cl	2.65792900	5.57206900	-0.38551200	Cl	2.97196000	5.35757600	-0.24738600
H	-3.97279000	0.98654200	-0.59069900	H	-4.00311600	1.12944300	-0.57121300
N	-1.78179500	0.57897100	-0.10643900	N	-1.79497700	0.63920000	-0.11140500
C	-6.19194600	-0.74987000	-1.88769400	C	-6.27787800	-0.54497800	-1.85804200
C	-6.58522600	-0.25429800	0.48909100	C	-6.59919700	-0.10456200	0.53844200
C	-7.66966200	-0.51814500	-2.21159300	C	-7.76346300	-0.30299200	-2.13189700
H	-6.00547900	-1.81665700	-1.69930500	H	-6.08965200	-1.61500800	-1.69272800
H	-5.56240500	-0.44046000	-2.72542800	H	-5.67026400	-0.22138200	-2.70640700
C	-8.07227800	-0.00946000	0.22300900	C	-8.09221300	0.14910300	0.32183800

H	-6.41989900	-1.29603300	0.79827000	H	-6.42671700	-1.15501100	0.81114400
H	-6.22642600	0.39640200	1.29010400	H	-6.21308400	0.52289300	1.34519200
C	-8.55306200	-0.81233700	-0.99247400	C	-8.60688400	-0.63253300	-0.89363600
H	-7.95530800	-1.15060500	-3.05814200	H	-8.07554500	-0.91041300	-2.98718800
H	-7.80668600	0.52399800	-2.52129700	H	-7.90831700	0.74845900	-2.40437300
H	-8.64585600	-0.27815700	1.11575400	H	-8.64032500	-0.13373700	1.22593900
H	-8.23013200	1.05978300	0.04272500	H	-8.25148700	1.22141500	0.16217000
H	-9.60002900	-0.58314000	-1.21358300	H	-9.66221100	-0.40866100	-1.07632200
H	-8.50504700	-1.88369900	-0.76065100	H	-8.53889200	-1.70783200	-0.68634400
N	-5.81103900	0.06992700	-0.72319800	N	-5.86008600	0.24982700	-0.68808600
C	-1.25054900	-3.05368100	0.57347500	C	-1.40183500	-3.03431100	0.40813200
H	-1.92534100	-3.47154500	-0.17585800	H	-2.10753400	-3.39402400	-0.34251400
H	-0.25893000	-3.48329700	0.40410800	H	-0.43286400	-3.50212000	0.21133000
C	5.19415500	-1.52016200	0.08492300	C	5.12543000	-1.59796500	0.11248100
C	6.35741400	-1.49194400	-0.24195800	C	6.30053100	-1.54366000	-0.16263100
C	7.75796200	-1.48222400	-0.64746000	C	7.71239200	-1.50654200	-0.52136000
C	8.10807000	-2.56049700	-1.69559900	C	8.04556500	-2.31885500	-1.79124900
H	8.38843700	-1.61883700	0.23979900	H	8.30675400	-1.88523200	0.31923600
H	8.00751800	-0.49165800	-1.04738500	H	8.01990200	-0.46341700	-0.66628200
C	9.58363400	-2.52068400	-2.09775100	C	9.53427300	-2.25570400	-2.13821800
H	7.85476000	-3.54375300	-1.28806400	H	7.73619100	-3.35702200	-1.63740400
H	7.47359200	-2.41632500	-2.57519800	H	7.44655000	-1.93534700	-2.62272300
H	9.80906500	-3.29104300	-2.83926900	H	9.75386600	-2.83487400	-3.03846200
H	9.85158900	-1.55285200	-2.53274600	H	9.85521200	-1.22494100	-2.31829400
H	10.23590600	-2.68929700	-1.23528600	H	10.14734200	-2.65751600	-1.32543400
C	-1.76559900	-3.45909400	1.96514200	C	-1.91935700	-3.44653100	1.79629700
H	-1.77577200	-4.54804000	2.06459500	H	-1.97877500	-4.53533600	1.87698900
H	-1.13753400	-3.05148800	2.76272400	H	-1.26582400	-3.07937000	2.59325700
H	-2.78435800	-3.09687500	2.10866700	H	-2.91852500	-3.03770900	1.95261100
19							
C	-0.98776200	3.45454300	-1.03638500	C	1.29353900	3.22868800	1.09522500
C	-0.48780300	2.16430300	-1.18757900	C	0.69843400	1.97934800	1.24156100
C	-0.05976500	1.43271000	-0.07484000	C	0.07671700	1.35892700	0.15291600
C	-0.10333600	2.02964700	1.18466200	C	0.02220200	2.02603200	-1.07012500
C	-0.58476900	3.32094500	1.35096800	C	0.59479100	3.28011500	-1.22724900
C	-1.03268200	4.01722200	0.23297500	C	1.23764900	3.86348400	-0.13936400
H	-1.32090300	4.01157100	-1.90045700	H	1.77977000	3.69952800	1.93753400

H	0.24754900	1.46056500	2.03619400	H	-0.47515400	1.53711300	-1.89786400
H	-0.62026200	3.77782500	2.33060100	H	0.55632800	3.79359600	-2.17821700
N	0.45912400	0.11173400	-0.19385000	N	-0.51047800	0.06955100	0.25491700
C	-0.20671300	-1.05957500	-0.50643100	C	0.10986400	-1.14215300	0.50093600
C	0.74664300	-2.07062200	-0.49172900	C	-0.88547000	-2.10936900	0.44841000
C	1.95591600	-1.40311000	-0.15900400	C	-2.06771300	-1.37856900	0.15950900
C	3.31994600	-2.00381100	-0.02619200	C	-3.44951600	-1.92460400	0.00082200
O	3.50555100	-3.20424400	-0.11092700	O	-3.66705900	-3.12187300	-0.05010300
N	4.30025300	-1.06901800	0.18709900	N	-4.40416700	-0.94511100	-0.07279900
C	-1.64264700	-1.12981100	-0.75567400	C	1.54119300	-1.28097200	0.71967700
C	-2.27649000	-1.67054900	-1.84830200	C	2.16490300	-1.98968600	1.71812700
S	-2.81591200	-0.57868400	0.42039800	S	2.72035100	-0.55948100	-0.35334000
C	-3.68873700	-1.64128200	-1.76237000	C	3.57700700	-1.95929900	1.64074000
H	-1.73334900	-2.05815400	-2.69946000	H	1.61356100	-2.49083100	2.50149700
C	-4.15598100	-1.07463400	-0.59724600	C	4.05155400	-1.22109800	0.57889700
H	-4.35298400	-2.01063800	-2.53143000	H	4.23713100	-2.44705500	2.34433600
Cl	-0.36983000	1.50248700	-2.79866200	Cl	0.72329800	1.22440500	2.81501900
Cl	-1.65841600	5.64479100	0.42033400	Cl	1.98749800	5.43900200	-0.32040400
H	4.01508000	-0.09685400	0.24783000	H	-4.08313600	0.01759900	-0.08935400
N	1.76999900	-0.09620400	0.02135800	N	-1.83059400	-0.07242600	0.03807800
C	0.52284500	-3.54143700	-0.70212900	C	-0.72858700	-3.59748200	0.55780800
H	-0.41715700	-3.68654100	-1.23963000	H	0.20012300	-3.82800200	1.08375400
H	1.32693200	-3.93242200	-1.32855400	H	-1.55655800	-3.99536500	1.14749300
C	6.52503300	-1.03883900	-0.71582700	C	-6.65905800	-0.78864600	0.69500200
C	6.12020400	-1.25840400	1.73304200	C	-6.12230700	-1.00511600	-1.72953400
C	6.80174800	0.46323200	-0.89286500	C	-6.80385400	0.73042300	0.87812100
H	7.47037700	-1.56137900	-0.53369600	H	-7.63491600	-1.21836300	0.44564000
H	6.11319600	-1.44924100	-1.64174400	H	-6.34193800	-1.24592600	1.63611500
C	5.98885300	0.14179400	2.37581300	C	-5.78593500	0.37725800	-2.32943600
H	7.17258200	-1.55340600	1.70506500	H	-7.20056900	-1.17807000	-1.77347100
H	5.61224000	-1.98702000	2.37296500	H	-5.65642000	-1.77994400	-2.34670800
C	7.31792600	1.18748200	0.36181800	C	-7.16697000	1.50623500	-0.39934000
H	5.89049300	0.96642700	-1.24052600	H	-5.87187800	1.14009400	1.28784700
H	7.53091300	0.56959000	-1.70505700	H	-7.56968900	0.90016700	1.64406100
C	6.25387800	1.35862600	1.46165000	C	-6.01389900	1.60274400	-1.41595400
H	6.68242800	0.16410400	3.22439600	H	-6.38603100	0.48079700	-3.24045300
H	4.98904400	0.24885400	2.80908700	H	-4.74153700	0.38077600	-2.65726300

H	8.20120700	0.67170600	0.76033700	H	-8.05359100	1.06243900	-0.86992000
H	7.66260500	2.18272500	0.06218900	H	-7.45518200	2.52237800	-0.11126100
H	6.53043000	2.20308100	2.10108100	H	-6.17169900	2.47554500	-2.05716800
H	5.31805300	1.66337600	0.97596900	H	-5.09403600	1.82171100	-0.85883100
C	-5.48724100	-0.86943200	-0.18589700	C	5.38466700	-0.96491100	0.20777600
C	-6.62590500	-0.68526700	0.17493200	C	6.52370700	-0.73127600	-0.11992200
C	-8.00157400	-0.49009400	0.61726100	C	7.89810800	-0.48433400	-0.53652900
C	-8.55658400	-1.66309000	1.45383500	C	8.39198700	-1.45368800	-1.63193200
H	-8.64115900	-0.33430700	-0.26026900	H	8.55726600	-0.55658900	0.33733100
H	-8.06082100	0.43501700	1.20387800	H	7.98461300	0.54765100	-0.89867300
C	-10.00005100	-1.42442600	1.90113100	C	9.83631900	-1.16423300	-2.04515600
H	-8.49238600	-2.58036700	0.86094700	H	8.30219100	-2.47949600	-1.26203200
H	-7.91153300	-1.81104200	2.32507200	H	7.72763500	-1.37566500	-2.49782500
H	-10.37225500	-2.26579100	2.49078800	H	10.17086400	-1.85794300	-2.82036400
H	-10.08172900	-0.52455800	2.51863300	H	9.93898500	-0.14850600	-2.43971700
H	-10.66732500	-1.29992100	1.04264600	H	10.51816000	-1.26082500	-1.19444900
C	0.48870400	-4.33999500	0.61236000	C	-0.72556600	-4.28201500	-0.81955600
H	1.44584400	-4.25823500	1.12868100	H	-1.67529500	-4.10234400	-1.32463700
H	-0.30382200	-3.97804500	1.27321800	H	0.08880200	-3.90066000	-1.44204000
H	0.30327900	-5.39827000	0.40869500	H	-0.59577700	-5.36222300	-0.71044300
N	5.62660500	-1.43454600	0.36929700	N	-5.73294400	-1.24596300	-0.33986600
20							
C	1.09172500	3.83982800	0.74679200	C	1.43010000	3.61000000	0.78020000
C	0.43416400	2.63490600	0.97743500	C	0.67240000	2.46710000	1.01650000
C	-0.05323700	1.87548400	-0.09127800	C	0.00570000	1.82960000	-0.03500000
C	0.09245100	2.36232700	-1.38977100	C	0.07320000	2.37710000	-1.31520000
C	0.73235600	3.56926700	-1.63597800	C	0.80980000	3.52650000	-1.56350000
C	1.23568600	4.29179400	-0.55895100	C	1.49300000	4.12470000	-0.50880000
H	1.46943300	4.41889200	1.57739400	H	1.94970000	4.09390000	1.59480000
H	-0.30640700	1.77555800	-2.20750900	H	-0.46140000	1.87920000	-2.11390000
H	0.84611200	3.94089500	-2.64523200	H	0.86520000	3.94700000	-2.55830000
N	-0.73291500	0.63950100	0.10894000	N	-0.74690000	0.64030000	0.16110000
C	-0.22297700	-0.57436700	0.53284300	C	-0.29440000	-0.60970000	0.54420000
C	-1.29205300	-1.46191000	0.56229900	C	-1.40500000	-1.44350000	0.54870000
C	-2.40102700	-0.68231400	0.13702800	C	-2.47460000	-0.60020000	0.14690000
C	-3.82463200	-1.11681800	0.00387500	C	-3.91040000	-0.97620000	-0.00180000
O	-4.16945600	-2.27662200	0.19159200	O	-4.29550000	-2.13010000	0.14260000

N	-4.67725400	-0.10715500	-0.33494700	N	-4.73020000	0.07060000	-0.30400000
C	1.18705100	-0.79622800	0.83561900	C	1.10130000	-0.90520000	0.82800000
C	1.72328000	-1.31705700	1.98855400	C	1.60390000	-1.58280000	1.91280000
S	2.44658900	-0.49034200	-0.34039700	S	2.38930000	-0.44890000	-0.26500000
C	3.12995600	-1.46598400	1.94810400	C	3.00960000	-1.73810000	1.88530000
H	1.11659400	-1.56390500	2.84921500	H	0.97360000	-1.92890000	2.72010000
C	3.69089400	-1.05854500	0.75793400	C	3.60100000	-1.17540000	0.77550000
H	3.72533600	-1.84727700	2.76617300	H	3.58420000	-2.23140000	2.65680000
Cl	0.19682100	2.12076700	2.62873900	Cl	0.55350000	1.87050000	2.65250000
Cl	2.06040700	5.81231200	-0.84660700	Cl	2.44820000	5.56600000	-0.80330000
H	-4.29639300	0.81978400	-0.46277800	H	-4.32770000	0.99170000	-0.40080000
N	-2.05253500	0.57434000	-0.13548300	N	-2.06760000	0.64690000	-0.08890000
C	-6.39441000	-1.10875500	-1.67554500	C	-6.45220000	-0.85670000	-1.68150000
C	-6.77942300	-0.60893400	0.70167800	C	-6.83700000	-0.43400000	0.70890000
C	-7.89213500	-1.00167700	-1.97160700	C	-7.94860000	-0.73250000	-1.97450000
H	-6.11919800	-2.15407200	-1.47611400	H	-6.18370000	-1.90830000	-1.50940000
H	-5.80867100	-0.76297700	-2.53068900	H	-5.86120000	-0.48960000	-2.52390000
C	-8.28651500	-0.49021200	0.46376100	C	-8.34260000	-0.30050000	0.47310000
H	-6.52286700	-1.62859400	1.02219800	H	-6.58440000	-1.46620000	0.98880000
H	-6.45899400	0.08155900	1.48542000	H	-6.51180000	0.22540000	1.51700000
C	-8.72444300	-1.34779800	-0.73037400	C	-8.77870000	-1.12410000	-0.74540000
H	-8.14241200	-1.66778100	-2.80342200	H	-8.20140000	-1.36490000	-2.83130000
H	-8.11905300	0.02127400	-2.29224200	H	-8.17210000	0.30360000	-2.25250000
H	-8.81837800	-0.79102900	1.37196200	H	-8.87770000	-0.62310000	1.37160000
H	-8.53465900	0.55979100	0.27235000	H	-8.58440000	0.75530000	0.30720000
H	-9.79073000	-1.20739500	-0.93260300	H	-9.84610000	-0.98490000	-0.94180000
H	-8.58508700	-2.40814400	-0.48518300	H	-8.62850000	-2.19000000	-0.53310000
N	-6.05835600	-0.24240100	-0.53112900	N	-6.11270000	-0.02730000	-0.51020000
C	-1.25504700	-2.92707600	0.89331400	C	-1.44410000	-2.92050000	0.80950000
H	-0.35100500	-3.14015300	1.46843500	H	-0.54940000	-3.21490000	1.36180000
H	-2.11310700	-3.16596300	1.52470600	H	-2.31240000	-3.14410000	1.43200000
C	5.04677200	-1.04901600	0.37719500	C	4.96460000	-1.12750000	0.43110000
C	6.20836800	-1.03435400	0.04298000	C	6.13230000	-1.07490000	0.12570000
C	7.60679400	-1.02473400	-0.36985800	C	7.53530000	-1.04530000	-0.26590000
C	8.02852700	-2.23610500	-1.24195300	C	7.91590000	-2.10360000	-1.33340000
H	8.24435000	-0.98832000	0.52321400	H	8.16080000	-1.19660000	0.62360000
H	7.80357400	-0.09879200	-0.92331700	H	7.77770000	-0.04570000	-0.64560000

C	9.46367400	-2.04136100	-1.74536000	C	9.37260000	-1.90420000	-1.76660000
H	7.35840300	-2.25801900	-2.10930500	H	7.26800000	-1.93590000	-2.20180000
H	9.76706400	-2.87137900	-2.38887400	H	9.65060000	-2.62350000	-2.54140000
H	9.56601400	-1.11704300	-2.32153400	H	9.54020000	-0.89920000	-2.16530000
H	10.16982500	-1.99536800	-0.90914600	H	10.05290000	-2.04810000	-0.92000000
C	7.87541200	-3.55830100	-0.48281200	C	7.67680000	-3.52700000	-0.81940000
H	8.53567900	-3.58393800	0.39123900	H	8.30910000	-3.73350000	0.05130000
H	6.84996600	-3.70140400	-0.13476700	H	6.63570000	-3.67280000	-0.52270000
H	8.13713800	-4.40595000	-1.12197100	H	7.91830000	-4.26410000	-1.59000000
C	-1.29227700	-3.82847000	-0.35278800	C	-1.53980000	-3.73810000	-0.48970000
H	-2.22071800	-3.67410500	-0.90388000	H	-2.46080000	-3.49040000	-1.01860000
H	-0.44783500	-3.62033000	-1.01555300	H	-0.68700000	-3.53290000	-1.14290000
H	-1.24281200	-4.88125600	-0.06127100	H	-1.55120000	-4.80890000	-0.26850000
21							
C	1.08493300	3.74168900	0.88400500	C	1.34870000	3.52190000	0.96390000
C	0.41985400	2.53360400	1.07198500	C	0.59360000	2.36280000	1.11250000
C	-0.09531600	1.82867700	-0.02122500	C	-0.04330000	1.78600000	0.00830000
C	0.02984100	2.37492900	-1.29847600	C	0.05300000	2.40890000	-1.23520000
C	0.67649400	3.58622800	-1.50091800	C	0.78800000	3.57480000	-1.39590000
C	1.20787400	4.25319200	-0.40172700	C	1.43980000	4.11310000	-0.29020000
H	1.48486400	4.27756800	1.73299100	H	1.84590000	3.95820000	1.81830000
H	-0.39069600	1.83050300	-2.13433500	H	-0.45820000	1.95690000	-2.07530000
H	0.77404200	4.00350100	-2.49391000	H	0.86570000	4.05410000	-2.36220000
N	-0.78747700	0.59329900	0.13197400	N	-0.79850000	0.58740000	0.11680000
C	-0.30378400	-0.63961800	0.53325400	C	-0.36320000	-0.68160000	0.45470000
C	-1.38904200	-1.51061300	0.51783100	C	-1.48340000	-1.50380000	0.40460000
C	-2.47601200	-0.70347200	0.09019700	C	-2.53840000	-0.63370000	0.02650000
C	-3.89324400	-1.12440700	-0.12768800	C	-3.97010000	-0.99620000	-0.18220000
O	-4.27434600	-2.26474800	0.10437300	O	-4.38650000	-2.13010000	0.02260000
N	-4.69463400	-0.12917300	-0.60554300	N	-4.74750000	0.03650000	-0.61620000
C	1.09427800	-0.90830000	0.83654100	C	1.01850000	-1.01680000	0.74820000
C	1.58933400	-1.65298200	1.88169800	C	1.46550000	-1.88660000	1.71580000
S	2.39841500	-0.38268500	-0.20767200	S	2.36320000	-0.38490000	-0.17870000
C	2.99609200	-1.79865500	1.86480600	C	2.87030000	-2.04730000	1.73240000
H	0.95354100	-2.06330400	2.65383200	H	0.79520000	-2.37230000	2.41060000
C	3.60087300	-1.16652000	0.80114400	C	3.51860000	-1.30000000	0.77390000
H	3.56057100	-2.33811900	2.61274400	H	3.40350000	-2.67760000	2.43020000

Cl	0.21608000	1.94293500	2.70154300	Cl	0.44800000	1.66090000	2.70340000
Cl	2.04177000	5.77811800	-0.63458800	Cl	2.39160000	5.57480000	-0.47410000
H	-4.28975100	0.78520800	-0.74898900	H	-4.32470000	0.94560000	-0.73660000
N	-2.10291000	0.55299900	-0.14543600	N	-2.11610000	0.61720000	-0.15390000
C	-6.34624700	-1.17968800	-1.98781800	C	-6.45010000	-0.94630000	-1.97660000
C	-6.86899700	-0.52663200	0.32510700	C	-6.89690000	-0.34500000	0.36430000
C	-7.81964100	-1.06463400	-2.38532900	C	-7.93340000	-0.80970000	-2.32550000
H	-6.10641300	-2.21526300	-1.70782400	H	-6.21240000	-1.98850000	-1.72150000
H	-5.70027900	-0.89814400	-2.82286800	H	-5.82480000	-0.65380000	-2.82340000
C	-8.35508200	-0.39506900	-0.01603400	C	-8.39060000	-0.19280000	0.07100000
H	-6.65646300	-1.52908400	0.72263900	H	-6.68070000	-1.36050000	0.72420000
H	-6.58340100	0.20506000	1.08460900	H	-6.57950000	0.36230000	1.13410000
C	-8.73585700	-1.31736900	-1.18119800	C	-8.81030000	-1.09180000	-1.09890000
H	-8.03159500	-1.77688500	-3.18908300	H	-8.17580000	-1.49650000	-3.14250000
H	-8.00351200	-0.05986100	-2.78203000	H	-8.12210000	0.20840000	-2.68420000
H	-8.94965500	-0.62887200	0.87278800	H	-8.96110000	-0.43700000	0.97250000
H	-8.56718600	0.64534700	-0.28667900	H	-8.59970000	0.85370000	-0.17760000
H	-9.78394600	-1.17052000	-1.45960300	H	-9.86730000	-0.94230000	-1.33910000
H	-8.63565300	-2.36268400	-0.86316800	H	-8.69410000	-2.14290000	-0.80620000
N	-6.06392100	-0.25031200	-0.87889200	N	-6.12570000	-0.04320000	-0.85660000
C	-1.38837600	-2.97845800	0.83375000	C	-1.55020000	-2.97840000	0.66490000
H	-2.00417100	-3.49218000	0.09324200	H	-2.20300000	-3.43310000	-0.08220000
H	-0.36668000	-3.35695500	0.73654100	H	-0.55020000	-3.40440000	0.54280000
C	4.96971700	-1.08888200	0.48027300	C	4.89800000	-1.20170000	0.51430000
C	6.14243000	-1.01351800	0.19763700	C	6.07950000	-1.10220000	0.28270000
C	7.55637200	-0.94724200	-0.15251100	C	7.50230000	-1.01450000	-0.01960000
C	8.01109100	-2.07077600	-1.10824000	C	7.94880000	-1.96560000	-1.14980000
H	8.15403800	-0.98571700	0.76643600	H	8.07640000	-1.23300000	0.88910000
H	7.76532900	0.02754800	-0.61005500	H	7.74800000	0.01860000	-0.29450000
C	9.49908300	-1.97791100	-1.46051600	C	9.44620000	-1.85490000	-1.45030000
H	7.79781700	-3.03946600	-0.64409400	H	7.70020000	-2.99430000	-0.86840000
H	7.40847600	-2.02535700	-2.02151200	H	7.37020000	-1.74210000	-2.05240000
H	9.70321100	-1.00118300	-1.91575700	H	9.68540000	-0.81950000	-1.72180000
H	10.09245500	-2.01469900	-0.53884100	H	10.01550000	-2.07130000	-0.53800000
C	-1.93839100	-3.31038800	2.23149800	C	-2.10420000	-3.31300000	2.05990000
H	-1.88899800	-4.38749400	2.41372500	H	-2.10920000	-4.39420000	2.22270000
H	-1.37029000	-2.80675600	3.01913400	H	-1.50580000	-2.85060000	2.85050000

H	-2.98186100	-3.00205400	2.30730500	H	-3.12940000	-2.95030000	2.14520000
C	9.95917300	-3.08889900	-2.40833700	C	9.89500000	-2.79640000	-2.57100000
H	11.02321500	-2.99703900	-2.64145500	H	10.96600000	-2.70050000	-2.76820000
H	9.79975300	-4.07708500	-1.96629100	H	9.69530000	-3.84040000	-2.31080000
H	9.40783200	-3.05638400	-3.35294900	H	9.36310000	-2.58010000	-3.50250000
22							
C	1.21004500	2.92195900	1.45519900	C	1.38230400	2.69977800	1.47587100
C	0.68980300	1.63097000	1.46659500	C	0.79154500	1.44011600	1.45536900
C	0.20835300	1.04775200	0.28936900	C	0.17415800	0.96565200	0.29281000
C	0.21912600	1.79528200	-0.88834700	C	0.12043800	1.78764000	-0.83222100
C	0.71987300	3.08961400	-0.91341700	C	0.68927000	3.05327600	-0.82198700
C	1.22120800	3.63597900	0.26367300	C	1.32709200	3.49091000	0.33506100
H	1.58503200	3.36291500	2.36781000	H	1.86585400	3.05710900	2.37371000
H	-0.17327600	1.34052300	-1.78897400	H	-0.37348300	1.41018100	-1.71824700
H	0.72904800	3.66317200	-1.83032700	H	0.65104000	3.68714100	-1.69736800
N	-0.33796300	-0.26630800	0.26310300	N	-0.41711400	-0.32353100	0.22578900
C	0.29275500	-1.48445400	0.44549400	C	0.18444500	-1.56394500	0.33556600
C	-0.69323600	-2.45778200	0.31811600	C	-0.83031700	-2.50339400	0.18347200
C	-1.87906300	-1.72458500	0.05785300	C	-1.99992000	-1.72911400	-0.01871000
C	-3.25382700	-2.27436900	-0.16978100	C	-3.39365000	-2.22977400	-0.24145300
O	-3.47741000	-3.46991400	-0.15939400	O	-3.66256800	-3.41609400	-0.23722400
N	-4.18605400	-1.29222600	-0.38265500	N	-4.28077400	-1.20811300	-0.44445500
C	1.71840200	-1.64535200	0.68022400	C	1.60602000	-1.76909700	0.53427400
C	2.31968600	-2.51384000	1.55787100	C	2.19619000	-2.74316400	1.30203900
S	2.93397600	-0.78573000	-0.25256900	S	2.82836700	-0.79972100	-0.27268900
C	3.73479800	-2.48860800	1.50065800	C	3.61140800	-2.71309200	1.26192500
H	1.75490700	-3.13423000	2.24000600	H	1.62128000	-3.43902200	1.89665200
C	4.24131900	-1.60348500	0.57735800	C	4.12651800	-1.71788900	0.46347700
H	4.37232700	-3.09610000	2.13032800	H	4.24413800	-3.39412000	1.81642400
Cl	0.62380500	0.77604500	2.98656100	Cl	0.82665900	0.47959200	2.91145500
Cl	1.87278600	5.26457600	0.25340000	Cl	2.07252000	5.07894100	0.36418200
H	-3.86462500	-0.33155700	-0.34319400	H	-3.91881300	-0.26475800	-0.37689400
N	-1.65442000	-0.41221300	0.01885900	N	-1.74110300	-0.42154100	-0.00056700
C	-0.52473400	-3.94352800	0.39006700	C	-0.69977200	-3.99348000	0.18589100
H	-0.79156500	-4.32516600	1.38096100	H	-0.88791100	-4.40342000	1.18359600
H	-1.18902600	-4.43435800	-0.31919500	H	-1.43869200	-4.43716800	-0.47865900
H	0.51032700	-4.22600800	0.18657700	H	0.30615600	-4.29262900	-0.11761500

C	-6.44586900	-1.05750800	0.41611500	C	-6.47194900	-0.84801200	0.44754700
C	-6.05038600	-1.09549700	-1.89147100	C	-6.16415800	-0.81991400	-1.86171700
H	-5.94849100	-1.04288700	1.38613500	H	-5.96593300	-0.96184700	1.40632200
H	-7.29802200	-1.74116200	0.48720000	H	-7.40630300	-1.41619400	0.48798900
C	-6.65061400	0.30755400	-1.62691100	C	-6.54422400	0.63967900	-1.51187300
H	-6.83426500	-1.78538400	-2.22054800	H	-7.05394600	-1.38334000	-2.15915300
H	-5.25834700	-1.10908900	-2.64058200	H	-5.42441500	-0.91164400	-2.65711300
H	-7.58500200	0.42862200	-2.18055800	H	-7.46694400	0.92666100	-2.02162500
C	-6.91571600	0.33305300	-0.07770200	C	-6.75093400	0.62063800	0.04600000
C	-6.13002200	1.55536900	0.45987100	C	-5.77131400	1.67934400	0.61081100
C	-5.98833700	2.48997900	-0.75166100	C	-5.52876600	2.64548000	-0.55918400
H	-5.13631200	1.24976900	0.80667000	H	-4.82572400	1.21158200	0.90546300
H	-6.62684000	2.02643000	1.31160000	H	-6.16409000	2.17388700	1.50233900
C	-5.72478800	1.51677200	-1.91140800	C	-5.45543500	1.70945800	-1.77568900
H	-6.92820700	3.02767200	-0.92127200	H	-6.38194400	3.32538700	-0.66391900
H	-5.20141500	3.23886800	-0.62899900	H	-4.63313900	3.25909200	-0.43230500
H	-5.90801400	1.95770600	-2.89447200	H	-5.60420300	2.22680600	-2.72658200
H	-4.67399300	1.20527000	-1.89798600	H	-4.46453600	1.24481300	-1.82482100
H	-7.98034200	0.46704300	0.12937000	H	-7.77546700	0.89899800	0.30381000
N	-5.52932700	-1.60405900	-0.60615200	N	-5.64822200	-1.44427000	-0.62607500
C	5.64326000	-1.34758300	0.30339000	C	5.53116000	-1.43019700	0.24300900
C	6.15600500	-0.47734100	-0.57709600	C	6.05289500	-0.44130000	-0.49505200
H	6.32610400	-1.94797600	0.90202700	H	6.20703200	-2.11350000	0.75424200
H	5.48148600	0.12758300	-1.18214900	H	5.38658700	0.24840000	-1.01203000
C	7.62020400	-0.26626500	-0.82028500	C	7.51833100	-0.20594500	-0.69932100
C	8.04824600	-0.58584200	-2.26586600	C	7.94544400	-0.33838600	-2.17370200
H	8.20370000	-0.87580500	-0.12134200	H	8.09941700	-0.90377000	-0.08595000
H	7.87487200	0.78162900	-0.60842600	H	7.77628900	0.80466900	-0.35350100
C	9.53495500	-0.32184200	-2.51770800	C	9.43464300	-0.05278200	-2.38277100
H	7.81353000	-1.63359600	-2.48169800	H	7.70441100	-1.34835900	-2.52213200
H	7.44575500	0.01214500	-2.95948000	H	7.34746400	0.34827600	-2.78420000
H	9.81043700	-0.55811300	-3.54882200	H	9.71600600	-0.15500100	-3.43409300
H	9.78709100	0.72791200	-2.33804100	H	9.68922400	0.96338400	-2.06565600
H	10.16243200	-0.93016900	-1.85898800	H	10.05323900	-0.74510700	-1.80320500
23							
C	1.33656500	3.72481300	0.66794300	C	1.60290000	3.50370000	0.75390000
C	0.66391000	2.54049800	0.95501000	C	0.83940000	2.37020000	1.01570000

C	0.14556400	1.74964700	-0.07613200	C	0.19090000	1.69680000	-0.02520000
C	0.27554400	2.18697800	-1.39420200	C	0.28410000	2.19940000	-1.32230000
C	0.93002800	3.37315200	-1.69628400	C	1.02770000	3.33830000	-1.59700000
C	1.46458700	4.12607300	-0.65580000	C	1.69130000	3.97250000	-0.55100000
H	1.73779300	4.32793400	1.46993600	H	2.10760000	4.01540000	1.56070000
H	-0.14814600	1.57732400	-2.18205300	H	-0.23720000	1.67490000	-2.11260000
H	1.03072300	3.70570200	-2.72048400	H	1.10250000	3.72370000	-2.60460000
N	-0.55383900	0.53591200	0.17855000	N	-0.57310000	0.52060000	0.19910000
C	-0.07450300	-0.66477700	0.67227200	C	-0.14550000	-0.71580000	0.64780000
C	-1.16318100	-1.52819500	0.72219200	C	-1.27010000	-1.53220000	0.66730000
C	-2.24703300	-0.75350900	0.23470200	C	-2.31890000	-0.69580000	0.20710000
C	-3.66732900	-1.18518200	0.06532200	C	-3.75280000	-1.06610000	0.02470000
O	-4.03945100	-2.31625500	0.34829900	O	-4.16890000	-2.19070000	0.27220000
N	-4.48282100	-0.20819900	-0.42830400	N	-4.53320000	-0.04730000	-0.43850000
C	1.31754600	-0.91557300	1.01471700	C	1.23080000	-1.03420000	0.98100000
C	1.79487000	-1.56829100	2.12240800	C	1.66590000	-1.81350000	2.02240000
S	2.64785900	-0.49003600	-0.05002900	S	2.59520000	-0.50150000	0.01200000
C	3.20863300	-1.71729900	2.13051800	C	3.07760000	-1.97690000	2.05700000
H	1.14812800	-1.90904400	2.91952900	H	0.98870000	-2.23140000	2.75430000
C	3.82814800	-1.18627300	1.03260700	C	3.73320000	-1.32880000	1.04680000
H	3.75624000	-2.19189300	2.93516900	H	3.59890000	-2.54610000	2.81610000
Cl	0.45429300	2.08979800	2.62793600	Cl	0.69820000	1.82470000	2.66720000
Cl	2.30918800	5.62115300	-1.01388800	Cl	2.65520000	5.40180000	-0.87760000
H	-4.08295700	0.69954900	-0.61948500	H	-4.10950000	0.85450000	-0.60200000
N	-1.86962900	0.47986400	-0.09728000	N	-1.88930000	0.53230000	-0.08180000
C	-6.15119100	-1.31947100	-1.74179800	C	-6.22460000	-1.08510000	-1.77270000
C	-6.63912600	-0.57819900	0.55174600	C	-6.68690000	-0.39930000	0.54150000
C	-7.63164100	-1.22752900	-2.11873300	C	-7.70620000	-0.96650000	-2.13500000
H	-5.90098400	-2.34200700	-1.42542900	H	-5.98520000	-2.11650000	-1.47830000
H	-5.52082400	-1.06791700	-2.59810900	H	-5.59530000	-0.82200000	-2.62610000
C	-8.13144500	-0.46803600	0.23100500	C	-8.17950000	-0.26400000	0.23450000
H	-6.41367900	-1.56286600	0.98508800	H	-6.46860000	-1.39970000	0.94050000
H	-6.34513800	0.18452000	1.27672100	H	-6.37670000	0.33750000	1.28610000
C	-8.52624600	-1.43747900	-0.89038000	C	-8.58930000	-1.20690000	-0.90400000
H	-7.85291500	-1.97180700	-2.89035300	H	-7.94170000	-1.68350000	-2.92780000
H	-7.82792400	-0.24000000	-2.55123700	H	-7.89630000	0.03720000	-2.53160000
H	-8.70979100	-0.66963900	1.13826300	H	-8.75450000	-0.47710000	1.14120000

H	-8.35419400	0.55976100	-0.07686700	H	-8.39120000	0.77180000	-0.05360000
H	-9.57971900	-1.30729700	-1.15661300	H	-9.64550000	-1.07040000	-1.15550000
H	-8.41441900	-2.46889400	-0.53323800	H	-8.47090000	-2.24600000	-0.57220000
N	-5.85547500	-0.34562700	-0.67540500	N	-5.90940000	-0.14030000	-0.68510000
C	-1.17052600	-2.96263700	1.15013800	C	-1.33710000	-2.97780000	1.04590000
H	-1.53255000	-3.06789400	2.17788600	H	-1.64940000	-3.09790000	2.08830000
H	-1.84587800	-3.54325200	0.52348400	H	-2.07700000	-3.49410000	0.43680000
H	-0.16469300	-3.38476600	1.10091500	H	-0.35930000	-3.45060000	0.92950000
C	5.29360700	-1.16689400	0.70662000	C	5.20550000	-1.29100000	0.76410000
C	5.69934100	-2.10942000	-0.44361200	C	5.61320000	-2.05310000	-0.51040000
H	5.83800200	-1.44851200	1.61407800	H	5.72260000	-1.72270000	1.62740000
H	5.61022400	-0.14593700	0.46309000	H	5.54740000	-0.25210000	0.68660000
C	7.20667800	-2.10025700	-0.71719000	C	7.12430000	-2.03690000	-0.75330000
H	5.37106700	-3.12623800	-0.20060700	H	5.25790000	-3.08680000	-0.43360000
H	5.16004200	-1.82280000	-1.35370000	H	5.09810000	-1.61550000	-1.37320000
C	7.62428900	-3.03057500	-1.86189600	C	7.54120000	-2.78800000	-2.02210000
H	7.52844100	-1.07641300	-0.94833000	H	7.47190000	-0.99750000	-0.81720000
H	7.74374500	-2.38840500	0.19590400	H	7.63700000	-2.47660000	0.11210000
H	7.30147100	-4.05280700	-1.63116600	H	7.19140000	-3.82520000	-1.95730000
H	7.08879500	-2.74179600	-2.77422100	H	7.02880000	-2.34710000	-2.88560000
C	9.13188800	-3.01945400	-2.12981700	C	9.05380000	-2.76960000	-2.25800000
H	9.39599100	-3.69174500	-2.95048700	H	9.32410000	-3.31130000	-3.16830000
H	9.47899900	-2.01659000	-2.39748700	H	9.42390000	-1.74430000	-2.35770000
H	9.69332500	-3.33814000	-1.24602000	H	9.58780000	-3.23360000	-1.42280000
24							
C	0.80456600	3.36402600	1.19600300	C	1.01010000	3.13150000	1.31140000
C	0.41174600	2.03671500	1.34291600	C	0.53950000	1.82520000	1.40470000
C	0.02972200	1.28050700	0.22939600	C	0.01730000	1.17790000	0.27950000
C	0.00894700	1.88937100	-1.02545300	C	-0.06430000	1.87240000	-0.92690000
C	0.38289200	3.21634400	-1.18700900	C	0.38450000	3.18120000	-1.03180000
C	0.78802700	3.93800600	-0.06885400	C	0.93000000	3.79360000	0.09260000
H	1.10246800	3.93969600	2.06075400	H	1.41920000	3.62360000	2.18210000
H	-0.30614700	1.29993500	-1.87705300	H	-0.48430000	1.36120000	-1.78350000
H	0.36857500	3.68187000	-2.16314500	H	0.32480000	3.71610000	-1.96980000
N	-0.38412500	-0.07657300	0.34145100	N	-0.45160000	-0.16120000	0.32970000
C	0.36015300	-1.19598400	0.66901400	C	0.25550000	-1.32120000	0.58690000
C	-0.51819000	-2.27322700	0.63288200	C	-0.66040000	-2.36340000	0.49620000

C	-1.76399600	-1.69903700	0.27158900	C	-1.88620000	-1.72870000	0.17450000
C	-3.06856100	-2.41024000	0.08423500	C	-3.21610000	-2.38120000	-0.04250000
O	-3.17039000	-3.61357300	0.22952600	O	-3.37410000	-3.58140000	0.07730000
N	-4.08814600	-1.56065100	-0.25931200	N	-4.18430000	-1.47610000	-0.38310000
C	1.78839200	-1.17904000	0.94826600	C	1.68060000	-1.36780000	0.85710000
C	2.44502600	-1.83892100	1.95523300	C	2.32060000	-2.18010000	1.75810000
S	2.94664900	-0.35361200	-0.08237900	S	2.85170000	-0.39620000	-0.02030000
C	3.85711300	-1.67863600	1.91526300	C	3.73340000	-2.02270000	1.75970000
H	1.92341200	-2.40341000	2.71617300	H	1.78430000	-2.84920000	2.41650000
C	4.29757100	-0.90072300	0.87994400	C	4.18660000	-1.09430000	0.86360000
H	4.53018500	-2.11517700	2.64259000	H	4.39880000	-2.56980000	2.41530000
Cl	0.37460900	1.35528900	2.94916900	Cl	0.60000000	1.02720000	2.95510000
Cl	1.27926100	5.61239100	-0.25014300	Cl	1.52330000	5.44110000	-0.02110000
H	-3.86557100	-0.57400200	-0.32816600	H	-3.91460000	-0.50010000	-0.40200000
N	-1.67155800	-0.38266400	0.09020800	N	-1.74970000	-0.40710000	0.06660000
C	-0.20229600	-3.71623600	0.87509600	C	-0.39330000	-3.82630000	0.65780000
H	-0.49404100	-4.02139100	1.88504200	H	-0.60770000	-4.15500000	1.67980000
H	-0.76310600	-4.34839800	0.18827200	H	-1.04310000	-4.40300000	0.00200000
H	0.86771800	-3.90157600	0.76062600	H	0.65380000	-4.05190000	0.44290000
C	-6.38387800	-1.45252000	0.45853200	C	-6.43370000	-1.23340000	0.39610000
C	-5.91411200	-1.74819100	-1.81594300	C	-6.03640000	-1.42540000	-1.89160000
H	-5.92139900	-1.26372900	1.42757300	H	-5.95850000	-1.19320000	1.37630000
H	-7.16831500	-2.20257000	0.60243400	H	-7.31240000	-1.88130000	0.47190000
C	-6.65364900	-0.38908400	-1.74952100	C	-6.56410000	0.01980000	-1.71830000
H	-6.61786400	-2.54896800	-2.06533400	H	-6.85730000	-2.10090000	-2.15130000
H	-5.10152000	-1.78026900	-2.54209200	H	-5.25950000	-1.53060000	-2.64890000
H	-7.57719100	-0.43302300	-2.33213300	H	-7.48800000	0.15950000	-2.28450000
C	-6.96935500	-0.19072200	-0.22242800	C	-6.83140000	0.14940000	-0.17490000
C	-6.32269700	1.16287900	0.16496600	C	-5.97850000	1.35300000	0.29760000
C	-6.23162600	1.94262500	-1.15609800	C	-5.77920000	2.20570000	-0.96510000
H	-5.31623200	1.00516400	0.56899200	H	-5.00630000	1.01410000	0.67150000
H	-6.89021300	1.68826200	0.93702600	H	-6.45180000	1.90080000	1.11590000
C	-5.83868300	0.85880100	-2.17225300	C	-5.56940000	1.15500000	-2.06660000
H	-7.21254900	2.35826600	-1.41354300	H	-6.68690000	2.78440000	-1.17100000
H	-5.52425800	2.77525900	-1.11748400	H	-4.95050000	2.91340000	-0.88030000
H	-6.03109500	1.14895300	-3.20821600	H	-5.72640000	1.54950000	-3.07340000
H	-4.76401200	0.65691400	-2.09707500	H	-4.53860000	0.78560000	-2.03310000

H	-8.04801300	-0.13797500	-0.05514900	H	-7.88710000	0.35340000	0.01910000
N	-5.38694500	-2.03218200	-0.46546300	N	-5.51570000	-1.85980000	-0.57910000
C	5.70844200	-0.52540500	0.52952600	C	5.60070000	-0.68050000	0.58450000
C	6.24777800	-1.20582500	-0.74403000	C	6.11710000	-1.12380000	-0.79700000
H	6.34328300	-0.79492700	1.38012700	H	6.23530000	-1.11190000	1.36560000
H	5.79045100	0.56217700	0.41779800	H	5.69880000	0.40800000	0.67250000
C	7.70354700	-0.83612300	-1.04580600	C	7.57570000	-0.72860000	-1.03920000
H	6.15488900	-2.29184500	-0.63160300	H	6.00430000	-2.21020000	-0.88500000
H	5.61593800	-0.93111600	-1.59643400	H	5.48360000	-0.68590000	-1.57690000
C	8.25177600	-1.50286100	-2.31273500	C	8.09960000	-1.15980000	-2.41290000
H	7.78911300	0.25383500	-1.14543500	H	7.68010000	0.35950000	-0.93730000
H	8.33391300	-1.11321800	-0.19077300	H	8.20710000	-1.16940000	-0.25680000
H	8.16524800	-2.59143000	-2.21308400	H	7.99270000	-2.24640000	-2.51370000
H	7.62248100	-1.22531900	-3.16681700	H	7.46860000	-0.71790000	-3.19340000
C	9.70739800	-1.13137100	-2.60929500	C	9.55980000	-0.76320000	-2.64730000
H	10.36697400	-1.42867200	-1.78804700	H	10.21580000	-1.21810000	-1.89840000
H	10.06709200	-1.62215500	-3.51758400	H	9.90840000	-1.08200000	-3.63320000
H	9.81985300	-0.05163700	-2.74864400	H	9.68790000	0.32190000	-2.58300000
25							
C	2.06849600	3.20243400	0.91342200	C	2.25480000	3.00760000	0.94850000
C	1.29293600	2.05669900	1.06438900	C	1.41140000	1.90900000	1.08050000
C	0.62201600	1.50332100	-0.03157700	C	0.63730000	1.47610000	-0.00170000
C	0.70741800	2.14039300	-1.26944200	C	0.68960000	2.18320000	-1.20200000
C	1.46406900	3.29244200	-1.43303400	C	1.51280000	3.29120000	-1.34400000
C	2.14713300	3.80614400	-0.33531300	C	2.29800000	3.68450000	-0.26420000
H	2.58815800	3.62067600	1.76366300	H	2.85710000	3.33230000	1.78470000
H	0.16714800	1.71474600	-2.10541000	H	0.07270000	1.84320000	-2.02380000
H	1.52976100	3.78055900	-2.39589300	H	1.55580000	3.83570000	-2.27730000
N	-0.18679100	0.33698500	0.08586500	N	-0.21360000	0.34190000	0.08810000
C	0.18953600	-0.96957400	0.34318700	C	0.12890000	-0.98240000	0.29210000
C	-0.98207800	-1.71923200	0.35347800	C	-1.06250000	-1.69890000	0.28190000
C	-2.00463200	-0.77224500	0.08947400	C	-2.06010000	-0.71570000	0.06000000
C	-3.47307100	-1.02789000	-0.02084800	C	-3.53270000	-0.93380000	-0.04740000
O	-3.94787400	-2.14788400	0.11266700	O	-4.03270000	-2.04620000	0.05930000
N	-4.20670100	0.09276200	-0.28233200	N	-4.24610000	0.20660000	-0.27440000
C	1.56498100	-1.40990100	0.51715000	C	1.49020000	-1.46120000	0.44350000
C	2.03126500	-2.31047700	1.44684300	C	1.91730000	-2.45630000	1.29240000

S	2.85971200	-0.91162100	-0.55134500	S	2.82250000	-0.86360000	-0.52290000
C	3.41064400	-2.59727600	1.32355200	C	3.29850000	-2.74020000	1.18800000
H	1.39656600	-2.73396500	2.21295700	H	1.25150000	-2.94610000	1.98890000
C	4.02204900	-1.91964400	0.29216900	C	3.94790000	-1.96410000	0.25350000
H	3.95271800	-3.26953900	1.97416300	H	3.81600000	-3.47900000	1.78380000
Cl	1.15323100	1.35194500	2.65488600	Cl	1.33260000	1.09920000	2.62420000
Cl	3.12086500	5.25258400	-0.52113900	Cl	3.36140000	5.06970000	-0.42730000
H	-3.72253400	0.97568900	-0.36284700	H	-3.75310000	1.08590000	-0.33210000
N	-1.51674000	0.45583300	-0.07682200	N	-1.54020000	0.50520000	-0.06390000
C	-6.07537200	-0.61553600	-1.60544800	C	-6.12900000	-0.45950000	-1.58930000
C	-6.31830100	-0.21875900	0.80956900	C	-6.33960000	-0.12210000	0.83590000
C	-7.55854000	-0.31577400	-1.83459200	C	-7.61630000	-0.16230000	-1.78970000
H	-5.92021800	-1.69604300	-1.47624000	H	-5.96750000	-1.54110000	-1.48100000
H	-5.48117700	-0.28984900	-2.46263200	H	-5.54650000	-0.11430000	-2.44680000
C	-7.80740800	0.09066600	0.63947100	C	-7.83190000	0.18320000	0.69360000
H	-6.17530200	-1.27896300	1.06199100	H	-6.18730000	-1.18840000	1.05380000
H	-5.89172200	0.38070800	1.61730300	H	-5.90260000	0.45650000	1.65320000
C	-8.38449000	-0.63588300	-0.58214800	C	-8.41870000	-0.52560000	-0.53370000
H	-7.91428000	-0.89651400	-2.69160000	H	-7.98110000	-0.71960000	-2.65820000
H	-7.67211500	0.74420800	-2.08817300	H	-7.73980000	0.90450000	-2.00730000
H	-8.34096600	-0.19963000	1.55010500	H	-8.35130000	-0.12620000	1.60600000
H	-7.93417000	1.17219700	0.51715500	H	-7.96520000	1.26590000	0.58990000
H	-9.43246700	-0.35918300	-0.73306600	H	-9.47330000	-0.26360000	-0.66180000
H	-8.36489200	-1.71810300	-0.40243600	H	-8.37500000	-1.61100000	-0.37900000
N	-5.59990900	0.13437300	-0.42871100	N	-5.64010000	0.26750000	-0.40300000
C	-1.11983800	-3.19698200	0.54965300	C	-1.23690000	-3.17770000	0.42530000
H	-1.39277000	-3.43589200	1.58264300	H	-1.46280000	-3.44870000	1.46180000
H	-1.91631900	-3.59035200	-0.07987500	H	-2.07700000	-3.51850000	-0.17690000
H	-0.18173000	-3.70710100	0.32143600	H	-0.32640000	-3.70340000	0.12930000
C	5.37162800	-1.94974600	-0.10843000	C	5.30970000	-1.96280000	-0.10080000
C	6.52813600	-1.96642500	-0.45903800	C	6.47660000	-1.94580000	-0.41270000
C	7.92100700	-2.00758700	-0.89144600	C	7.87940000	-1.95060000	-0.81150000
C	8.19628900	-3.06759100	-1.97475300	C	8.14440000	-2.77500000	-2.08610000
H	8.55732300	-2.19751500	-0.01949100	H	8.48210000	-2.34340000	0.01540000
H	8.20526500	-1.01693700	-1.26445500	H	8.20910000	-0.91660000	-0.96500000
H	9.25140500	-3.05265200	-2.25898600	H	9.20640000	-2.74620000	-2.34250000
H	7.95160300	-4.06748000	-1.61081300	H	7.85180000	-3.81700000	-1.94070000

H	7.59645700	-2.87616400	-2.86674400	H	7.57460000	-2.37810000	-2.92880000
26							
C	1.48032400	3.04206700	1.17589600	C	1.62410900	2.86577500	1.19522300
C	1.00334800	1.73610400	1.24004800	C	1.08950600	1.58194600	1.23884500
C	0.46908400	1.11754400	0.10435900	C	0.42796400	1.05155300	0.12574500
C	0.38395400	1.84340300	-1.08376700	C	0.27475800	1.84016900	-1.01389000
C	0.84092000	3.15183700	-1.16040600	C	0.78674800	3.12880000	-1.06649600
C	1.39540000	3.73464500	-0.02537400	C	1.46856400	3.62391200	0.04125500
H	1.89678100	3.51060700	2.05620000	H	2.14192100	3.26683900	2.05465700
H	-0.04793300	1.36077900	-1.95123200	H	-0.25153700	1.41891500	-1.86068400
H	0.77635100	3.70855700	-2.08539800	H	0.67141700	3.73706800	-1.95317400
N	-0.03504200	-0.21350900	0.13398200	N	-0.11161300	-0.26208700	0.12555400
C	0.64669600	-1.40704200	0.29158100	C	0.54719200	-1.47312700	0.23026400
C	-0.31162100	-2.41426800	0.24802700	C	-0.43333600	-2.45754600	0.16678300
C	-1.53659300	-1.72455100	0.05921400	C	-1.64516200	-1.73767900	0.01837400
C	-2.90419400	-2.32342500	-0.06374700	C	-3.02739500	-2.30161500	-0.10122700
O	-3.08466100	-3.52542900	-0.01910600	O	-3.24378200	-3.49729100	-0.04529700
N	-3.88211000	-1.37696200	-0.22635300	N	-3.96825500	-1.32420000	-0.27771300
C	2.09064200	-1.51603100	0.42996200	C	1.98661100	-1.61343500	0.34547200
C	2.77670800	-2.34396400	1.28820200	C	2.65937400	-2.53788000	1.11097900
S	3.20789900	-0.64525400	-0.59965900	S	3.11482900	-0.62985800	-0.56349400
C	4.18202100	-2.28193000	1.14165300	C	4.06605400	-2.46274600	0.98912000
H	2.27642300	-2.96256900	2.02041700	H	2.14620600	-3.23155200	1.76190000
C	4.59372800	-1.40409200	0.16360900	C	4.48909500	-1.47745400	0.12459500
H	4.88153300	-2.85057000	1.73867200	H	4.75918500	-3.09694700	1.52399200
Cl	1.05899500	0.90594900	2.77419400	Cl	1.24937400	0.66206000	2.71289900
Cl	1.99225400	5.38194100	-0.10183100	Cl	2.14147500	5.24302100	-0.00971900
H	-3.59222800	-0.40552100	-0.22612800	H	-3.64345800	-0.36515500	-0.26154700
N	-1.35922600	-0.40649500	-0.01526400	N	-1.44138000	-0.42070600	-0.01356900
C	-0.08879400	-3.89225500	0.33171300	C	-0.24013800	-3.94048000	0.20005300
H	-0.28387200	-4.26553400	1.34224300	H	-0.35809700	-4.32976200	1.21655300
H	-0.77701000	-4.41664500	-0.32911600	H	-0.99427500	-4.43208300	-0.41163100
H	0.94108600	-4.14439000	0.07056300	H	0.75954500	-4.20735900	-0.15030900
C	-6.08932500	-1.20327400	0.72098600	C	-6.11006600	-1.01471500	0.74271000
C	-5.84971900	-1.26905900	-1.60724000	C	-5.95380500	-1.06812000	-1.58139600
H	-5.52836700	-1.15532600	1.65456300	H	-5.53846600	-1.06926400	1.66931800
H	-6.91099200	-1.91320500	0.86023600	H	-7.01508900	-1.61717600	0.86690900

C	-6.47593700	0.11881200	-1.32404600	C	-6.37080100	0.38834400	-1.26268100
H	-6.63118500	-1.98923700	-1.87051500	H	-6.83669200	-1.67757900	-1.79749100
H	-5.11063400	-1.27122200	-2.40877100	H	-5.26395200	-1.16312100	-2.42005500
H	-7.44841400	0.20145600	-1.81569700	H	-7.33542800	0.61844400	-1.72111900
C	-6.63827600	0.16227700	0.23894800	C	-6.47610900	0.42430100	0.30503600
C	-5.86084600	1.41891700	0.70447600	C	-5.50815400	1.54355200	0.76358900
C	-5.82986700	2.33608600	-0.52817400	C	-5.38174800	2.46963900	-0.45602500
H	-4.83691200	1.15209500	0.98998700	H	-4.52668300	1.12643900	1.01375000
H	-6.31664900	1.88866400	1.57954000	H	-5.86399600	2.05826600	1.65918500
C	-5.61054900	1.35145100	-1.68747300	C	-5.34651200	1.48807400	-1.63779500
H	-6.79610900	2.84028200	-0.64380100	H	-6.26782500	3.11027200	-0.53087100
H	-5.06186400	3.11185900	-0.46932500	H	-4.50665100	3.12308900	-0.41156900
H	-5.87160400	1.76889700	-2.66317000	H	-5.57665800	1.95961600	-2.59624900
H	-4.55137800	1.07386100	-1.73805300	H	-4.34217100	1.06093900	-1.73309300
H	-7.69076400	0.26432600	0.51476900	H	-7.49284600	0.67178700	0.61898700
N	-5.22582600	-1.73752000	-0.35273700	N	-5.33343100	-1.62127100	-0.35986300
C	5.90342100	-1.08091600	-0.24021000	C	5.80277400	-1.11183800	-0.22266700
C	7.02341400	-0.79497200	-0.59318900	C	6.92463600	-0.78267100	-0.52687200
C	8.37737300	-0.47122700	-1.02998800	C	8.27923500	-0.41003300	-0.91794200
H	9.05333900	-0.53920200	-0.16988500	H	8.97081900	-0.69336600	-0.11625700
H	8.40378900	0.57531300	-1.35459500	H	8.33824000	0.68146200	-0.99999000
C	8.88957600	-1.37856700	-2.16459900	C	8.72682500	-1.05561400	-2.24359700
H	9.90441800	-1.09075100	-2.45021200	H	9.74489000	-0.74521000	-2.49194400
H	8.90367400	-2.42386300	-1.84953800	H	8.70555800	-2.14486200	-2.16991500
H	8.24830900	-1.29930400	-3.04470400	H	8.06602500	-0.75883600	-3.06070600
27							
C	1.51518700	3.09818200	1.13563100	C	1.69900000	2.92620000	1.16990000
C	0.97256100	1.81891400	1.21410500	C	1.09370000	1.67540000	1.23970000
C	0.40819700	1.21545200	0.08491000	C	0.39140000	1.16570000	0.14200000
C	0.36015400	1.93118700	-1.11137100	C	0.27010000	1.94380000	-1.00860000
C	0.88295600	3.21376300	-1.20234300	C	0.85310000	3.20050000	-1.08730000
C	1.46605900	3.78044700	-0.07350700	C	1.57390000	3.67360000	0.00530000
H	1.95436900	3.55501900	2.01102500	H	2.24790000	3.31090000	2.01750000
H	-0.09608800	1.46152800	-1.97345700	H	-0.28890000	1.53990000	-1.84280000
H	0.84669500	3.76266500	-2.13352300	H	0.76230000	3.80040000	-1.98240000
N	-0.16266500	-0.08810000	0.12877500	N	-0.21770000	-0.11700000	0.16790000
C	0.45799300	-1.31256200	0.30229800	C	0.38000000	-1.35900000	0.27870000

C	-0.54959900	-2.27060800	0.26656300	C	-0.64900000	-2.29280000	0.22920000
C	-1.73772300	-1.52195700	0.06547400	C	-1.82440000	-1.51300000	0.08380000
C	-3.13213100	-2.05185600	-0.05526600	C	-3.23110000	-2.00800000	-0.03100000
O	-3.37420700	-3.24311400	0.00262700	O	-3.49590000	-3.19480000	-0.08470000
N	-4.06854900	-1.06497800	-0.23096800	N	-4.15000000	-0.99230000	-0.06860000
C	1.89415600	-1.49254400	0.44751900	C	1.81140000	-1.57130000	0.38540000
C	2.53459100	-2.34381500	1.31811700	C	2.44230000	-2.51600000	1.16160000
S	3.05756300	-0.69087700	-0.58710100	S	2.98060000	-0.66390000	-0.55050000
C	3.94177400	-2.35406400	1.17694700	C	3.84990000	-2.51650000	1.02650000
H	2.00121500	-2.92779600	2.05539500	H	1.89980000	-3.17050000	1.82910000
C	4.40067400	-1.50928100	0.19083000	C	4.31530000	-1.56990000	0.14080000
H	4.60963000	-2.95001000	1.78350700	H	4.51410000	-3.17660000	1.56670000
Cl	0.98501100	1.00473700	2.75777500	Cl	1.21830000	0.77100000	2.72670000
Cl	2.14585800	5.39430300	-0.16804800	Cl	2.33660000	5.25100000	-0.07900000
H	-3.74145700	-0.10436700	-0.24319200	H	-3.79650000	-0.04120000	-0.07620000
N	-1.49400600	-0.21552000	-0.02330900	N	-1.55440000	-0.20850000	0.03780000
C	-0.40152000	-3.75685700	0.36749100	C	-0.52920000	-3.78330000	0.27280000
H	-0.61795900	-4.10859000	1.38141100	H	-0.67380000	-4.16040000	1.29060000
H	-1.11296800	-4.25370700	-0.29002800	H	-1.30120000	-4.24000000	-0.34350000
C	-6.23923100	-1.00077100	0.79705800	C	-6.35430000	-0.77040000	0.82200000
C	-5.97477500	-1.06960600	-1.67966200	C	-5.95520000	-0.96600000	-1.63040000
C	-6.43359900	0.49584100	1.08940400	C	-6.43650000	0.74960000	1.03430000
H	-7.21664300	-1.46730900	0.63306700	H	-7.35640000	-1.16270000	0.61940000
H	-5.79970800	-1.49301900	1.66879300	H	-6.00370000	-1.25320000	1.73810000
C	-5.81716500	0.36528200	-2.23495200	C	-5.60370000	0.41350000	-2.22820000
H	-7.03613800	-1.32339500	-1.61300100	H	-7.03970000	-1.10120000	-1.61860000
H	-5.53339500	-1.77179900	-2.39415500	H	-5.55040000	-1.74620000	-2.28290000
C	-6.98359900	1.32636800	-0.08221400	C	-6.83920000	1.55780000	-0.21090000
H	-5.48135600	0.93327200	1.41547800	H	-5.47060000	1.12090000	1.39960000
H	-7.11061600	0.57813700	1.94819600	H	-7.15460000	0.93300000	1.84220000
C	-5.97520500	1.52686400	-1.22868400	C	-5.73880000	1.63090000	-1.28610000
H	-6.55566800	0.47429600	-3.03769500	H	-6.24820000	0.55250000	-3.10350000
H	-4.83951800	0.46058100	-2.71866900	H	-4.57910000	0.38640000	-2.61260000
H	-7.91091600	0.87798200	-0.46180900	H	-7.76440000	1.15210000	-0.63980000
H	-7.26389300	2.31268100	0.30216600	H	-7.07610000	2.57840000	0.10650000
H	-6.24751800	2.42392200	-1.79403600	H	-5.89890000	2.51920000	-1.90500000
H	-5.00097500	1.75795600	-0.77913400	H	-4.78360000	1.80810000	-0.77550000

C	5.72650600	-1.25670400	-0.21063700	C	5.64290000	-1.27980000	-0.22440000
C	6.86090100	-1.03127500	-0.56144500	C	6.77740000	-1.01540000	-0.54460000
C	8.23136800	-0.78083500	-0.99491700	C	8.14590000	-0.72220000	-0.95450000
C	8.70809500	-1.73623300	-2.10526700	C	8.55620000	-1.44030000	-2.25470000
H	8.89777300	-0.86091700	-0.12840800	H	8.82770000	-1.00530000	-0.14440000
H	8.30875100	0.25580100	-1.34232600	H	8.25500000	0.36120000	-1.08030000
H	8.67109000	-2.77374800	-1.76716900	H	8.48480000	-2.52350000	-2.13740000
H	8.07719200	-1.64679800	-2.99186100	H	7.90570000	-1.14580000	-3.08090000
H	9.73721300	-1.50258500	-2.38923700	H	9.58630000	-1.18780000	-2.51860000
H	0.61520000	-4.06315400	0.11282500	H	0.45910000	-4.10070000	-0.06710000
N	-5.41852100	-1.35874400	-0.36070000	N	-5.50080000	-1.24190000	-0.26760000
28							
C	1.08493300	3.74168900	0.88400500	C	1.34870000	3.52190000	0.96390000
C	0.41985400	2.53360400	1.07198500	C	0.59360000	2.36280000	1.11250000
C	-0.09531600	1.82867700	-0.02122500	C	-0.04330000	1.78600000	0.00830000
C	0.02984100	2.37492900	-1.29847600	C	0.05300000	2.40890000	-1.23520000
C	0.67649400	3.58622800	-1.50091800	C	0.78800000	3.57480000	-1.39590000
C	1.20787400	4.25319200	-0.40172700	C	1.43980000	4.11310000	-0.29020000
H	1.48486400	4.27756800	1.73299100	H	1.84590000	3.95820000	1.81830000
H	-0.39069600	1.83050300	-2.13433500	H	-0.45820000	1.95690000	-2.07530000
H	0.77404200	4.00350100	-2.49391000	H	0.86570000	4.05410000	-2.36220000
N	-0.78747700	0.59329900	0.13197400	N	-0.79850000	0.58740000	0.11680000
C	-0.30378400	-0.63961800	0.53325400	C	-0.36320000	-0.68160000	0.45470000
C	-1.38904200	-1.51061300	0.51783100	C	-1.48340000	-1.50380000	0.40460000
C	-2.47601200	-0.70347200	0.09019700	C	-2.53840000	-0.63370000	0.02650000
C	-3.89324400	-1.12440700	-0.12768800	C	-3.97010000	-0.99620000	-0.18220000
O	-4.27434600	-2.26474800	0.10437300	O	-4.38650000	-2.13010000	0.02260000
N	-4.69463400	-0.12917300	-0.60554300	N	-4.74750000	0.03650000	-0.61620000
C	1.09427800	-0.90830000	0.83654100	C	1.01850000	-1.01680000	0.74820000
C	1.58933400	-1.65298200	1.88169800	C	1.46550000	-1.88660000	1.71580000
S	2.39841500	-0.38268500	-0.20767200	S	2.36320000	-0.38490000	-0.17870000
C	2.99609200	-1.79865500	1.86480600	C	2.87030000	-2.04730000	1.73240000
H	0.95354100	-2.06330400	2.65383200	H	0.79520000	-2.37230000	2.41060000
C	3.60087300	-1.16652000	0.80114400	C	3.51860000	-1.30000000	0.77390000
H	3.56057100	-2.33811900	2.61274400	H	3.40350000	-2.67760000	2.43020000
Cl	0.21608000	1.94293500	2.70154300	Cl	0.44800000	1.66090000	2.70340000
Cl	2.04177000	5.77811800	-0.63458800	Cl	2.39160000	5.57480000	-0.47410000

H	-4.28975100	0.78520800	-0.74898900	H	-4.32470000	0.94560000	-0.73660000
N	-2.10291000	0.55299900	-0.14543600	N	-2.11610000	0.61720000	-0.15390000
C	-6.34624700	-1.17968800	-1.98781800	C	-6.45010000	-0.94630000	-1.97660000
C	-6.86899700	-0.52663200	0.32510700	C	-6.89690000	-0.34500000	0.36430000
C	-7.81964100	-1.06463400	-2.38532900	C	-7.93340000	-0.80970000	-2.32550000
H	-6.10641300	-2.21526300	-1.70782400	H	-6.21240000	-1.98850000	-1.72150000
H	-5.70027900	-0.89814400	-2.82286800	H	-5.82480000	-0.65380000	-2.82340000
C	-8.35508200	-0.39506900	-0.01603400	C	-8.39060000	-0.19280000	0.07100000
H	-6.65646300	-1.52908400	0.72263900	H	-6.68070000	-1.36050000	0.72420000
H	-6.58340100	0.20506000	1.08460900	H	-6.57950000	0.36230000	1.13410000
C	-8.73585700	-1.31736900	-1.18119800	C	-8.81030000	-1.09180000	-1.09890000
H	-8.03159500	-1.77688500	-3.18908300	H	-8.17580000	-1.49650000	-3.14250000
H	-8.00351200	-0.05986100	-2.78203000	H	-8.12210000	0.20840000	-2.68420000
H	-8.94965500	-0.62887200	0.87278800	H	-8.96110000	-0.43700000	0.97250000
H	-8.56718600	0.64534700	-0.28667900	H	-8.59970000	0.85370000	-0.17760000
H	-9.78394600	-1.17052000	-1.45960300	H	-9.86730000	-0.94230000	-1.33910000
H	-8.63565300	-2.36268400	-0.86316800	H	-8.69410000	-2.14290000	-0.80620000
N	-6.06392100	-0.25031200	-0.87889200	N	-6.12570000	-0.04320000	-0.85660000
C	-1.38837600	-2.97845800	0.83375000	C	-1.55020000	-2.97840000	0.66490000
H	-2.00417100	-3.49218000	0.09324200	H	-2.20300000	-3.43310000	-0.08220000
H	-0.36668000	-3.35695500	0.73654100	H	-0.55020000	-3.40440000	0.54280000
C	4.96971700	-1.08888200	0.48027300	C	4.89800000	-1.20170000	0.51430000
C	6.14243000	-1.01351800	0.19763700	C	6.07950000	-1.10220000	0.28270000
C	7.55637200	-0.94724200	-0.15251100	C	7.50230000	-1.01450000	-0.01960000
C	8.01109100	-2.07077600	-1.10824000	C	7.94880000	-1.96560000	-1.14980000
H	8.15403800	-0.98571700	0.76643600	H	8.07640000	-1.23300000	0.88910000
H	7.76532900	0.02754800	-0.61005500	H	7.74800000	0.01860000	-0.29450000
C	9.49908300	-1.97791100	-1.46051600	C	9.44620000	-1.85490000	-1.45030000
H	7.79781700	-3.03946600	-0.64409400	H	7.70020000	-2.99430000	-0.86840000
H	7.40847600	-2.02535700	-2.02151200	H	7.37020000	-1.74210000	-2.05240000
H	9.70321100	-1.00118300	-1.91575700	H	9.68540000	-0.81950000	-1.72180000
H	10.09245500	-2.01469900	-0.53884100	H	10.01550000	-2.07130000	-0.53800000
C	-1.93839100	-3.31038800	2.23149800	C	-2.10420000	-3.31300000	2.05990000
H	-1.88899800	-4.38749400	2.41372500	H	-2.10920000	-4.39420000	2.22270000
H	-1.37029000	-2.80675600	3.01913400	H	-1.50580000	-2.85060000	2.85050000
H	-2.98186100	-3.00205400	2.30730500	H	-3.12940000	-2.95030000	2.14520000
C	9.95917300	-3.08889900	-2.40833700	C	9.89500000	-2.79640000	-2.57100000

H	11.02321500	-2.99703900	-2.64145500	H	10.96600000	-2.70050000	-2.76820000
H	9.79975300	-4.07708500	-1.96629100	H	9.69530000	-3.84040000	-2.31080000
H	9.40783200	-3.05638400	-3.35294900	H	9.36310000	-2.58010000	-3.50250000
29							
C	0.59915600	3.21825500	1.21551700	C	0.81970000	3.11920000	0.95390000
C	0.18004400	1.89453900	1.31145200	C	0.27600000	1.84030000	1.02140000
C	-0.21469300	1.18923500	0.16930600	C	-0.16800000	1.19700000	-0.13920000
C	-0.22108400	1.84493400	-1.06182200	C	-0.09700000	1.86830000	-1.35890000
C	0.17923300	3.16942300	-1.17207200	C	0.42660000	3.15080000	-1.44010000
C	0.59595500	3.84015000	-0.02671600	C	0.89120000	3.75890000	-0.27750000
H	0.90787000	3.75434200	2.10163300	H	1.16920000	3.60790000	1.85200000
H	-0.54634000	1.29486500	-1.93564600	H	-0.45820000	1.36100000	-2.24420000
H	0.17606600	3.67182100	-2.12982300	H	0.48550000	3.66840000	-2.38780000
N	-0.65668800	-0.16284800	0.22981100	N	-0.70730000	-0.11670000	-0.11110000
C	0.06161900	-1.30911400	0.52128500	C	-0.08540000	-1.30300000	0.23260000
C	-0.84098200	-2.36521700	0.44868600	C	-1.04660000	-2.29940000	0.09910000
C	-2.07194200	-1.75069000	0.10500200	C	-2.20680000	-1.61180000	-0.33560000
C	-3.39491700	-2.41248400	-0.11017500	C	-3.55400000	-2.18570000	-0.62380000
O	-3.53148600	-3.62432800	0.00539600	O	-3.81490000	-3.36620000	-0.42050000
N	-4.39755800	-1.55440400	-0.44019500	N	-4.44760000	-1.28960000	-1.11160000
C	1.48887600	-1.33627800	0.80022200	C	1.30940000	-1.41450000	0.61540000
C	2.12685700	-2.08729100	1.76040800	C	1.82990000	-2.25720000	1.57050000
S	2.65862400	-0.45622500	-0.16112100	S	2.58720000	-0.50540000	-0.16430000
C	3.53517000	-1.95867400	1.74514800	C	3.23620000	-2.17780000	1.69490000
H	1.58787700	-2.69680000	2.47249900	H	1.20530000	-2.89420000	2.18070000
C	3.99811700	-1.10594200	0.76775500	C	3.81210000	-1.27140000	0.83240000
H	4.19939600	-2.46195700	2.43406900	H	3.81930000	-2.75250000	2.40090000
Cl	0.12930500	1.15161300	2.88980900	Cl	0.14790000	1.06950000	2.58150000
Cl	1.11942700	5.50988500	-0.14359100	Cl	1.57540000	5.37200000	-0.35920000
H	-4.15218100	-0.57670600	-0.49004600	H	-4.13140000	-0.33780000	-1.21480000
N	-1.94934000	-0.43177100	-0.03088100	N	-1.99250000	-0.30260000	-0.46480000
C	-0.56006600	-3.82304200	0.64114200	C	-0.87630000	-3.76870000	0.32140000
H	-0.81354000	-4.14482500	1.65649300	H	-1.15060000	-4.04590000	1.34440000
H	-1.17272700	-4.41813500	-0.03395600	H	-1.53420000	-4.32870000	-0.34060000
H	0.49674900	-4.04000700	0.47190700	H	0.16210000	-4.06640000	0.15790000
C	5.32383200	-0.73256300	0.47512100	C	5.16840000	-0.92460000	0.69160000
C	6.45794700	-0.40304700	0.21804800	C	6.32800000	-0.61150000	0.56190000

C	7.83005300	-0.02849100	-0.10333900	C	7.73100000	-0.26290000	0.37890000
C	8.48791500	-0.93639900	-1.16418100	C	8.39380000	-0.99190000	-0.80870000
H	8.42972100	-0.04671500	0.81495500	H	8.28070000	-0.49170000	1.30020000
H	7.84336400	1.01077700	-0.45402900	H	7.81630000	0.82110000	0.23430000
C	9.92770800	-0.52156900	-1.48316800	C	9.86590000	-0.60810000	-0.98310000
H	8.46886100	-1.97133200	-0.80664200	H	8.30590000	-2.07290000	-0.65680000
H	7.88248500	-0.91252600	-2.07640900	H	7.83770000	-0.76070000	-1.72340000
H	9.93633100	0.51858600	-1.83091100	H	9.94280000	0.47680000	-1.12530000
H	10.52246800	-0.53995000	-0.56183300	H	10.41130000	-0.83500000	-0.05900000
C	-5.77072900	-1.99021900	-0.68083000	C	-5.85310000	-1.62650000	-1.33720000
C	-6.77083200	-1.46087600	0.37413500	C	-6.63660000	-1.76840000	-0.01480000
C	-6.34480400	-1.44295300	-2.00744900	C	-6.57380000	-0.46490000	-2.04330000
H	-5.72303200	-3.07841800	-0.67433600	H	-5.87840000	-2.55400000	-1.91270000
H	-6.33405500	-1.43644200	1.37501300	H	-6.06410000	-2.31780000	0.73380000
H	-7.62296600	-2.14727800	0.40881400	H	-7.54670000	-2.34270000	-0.21670000
C	-6.96781400	-0.06563200	-1.67819900	C	-6.99540000	0.51750000	-0.92290000
H	-7.12461000	-2.13079300	-2.34863100	H	-7.45980000	-0.86910000	-2.54010000
H	-5.58778900	-1.39805000	-2.79403300	H	-5.95790000	0.00220000	-2.81730000
H	-7.90704200	0.05956000	-2.22266800	H	-7.99630000	0.90520000	-1.12650000
C	-7.23350700	-0.07378400	-0.12633400	C	-6.99390000	-0.32760000	0.40420000
C	-6.46183000	1.14726300	0.43370200	C	-5.98040000	0.37640000	1.33740000
C	-6.34679100	2.11170400	-0.75690700	C	-5.98590000	1.83870000	0.86920000
H	-5.46090700	0.84946200	0.76551900	H	-4.98190000	-0.04670000	1.19650000
H	-6.95893500	1.59037400	1.30035300	H	-6.23640000	0.25930000	2.39340000
C	-6.07270200	1.17201900	-1.94188100	C	-6.04240000	1.71230000	-0.66170000
H	-7.29769100	2.63572200	-0.90757500	H	-6.88550000	2.34730000	1.23520000
H	-5.57337400	2.87247100	-0.62243400	H	-5.12090000	2.40740000	1.21990000
H	-6.27632900	1.63203700	-2.91228700	H	-6.37650000	2.62680000	-1.15820000
H	-5.01398600	0.88765900	-1.94914400	H	-5.03690000	1.50250000	-1.04320000
H	-8.29889800	0.06288600	0.07573200	H	-7.98150000	-0.29980000	0.87180000
C	10.58841600	-1.41679800	-2.53501900	C	10.52870000	-1.32840000	-2.16040000
H	11.61319900	-1.09731900	-2.74174700	H	11.57770000	-1.03960000	-2.26590000
H	10.62575900	-2.45811500	-2.20096100	H	10.49270000	-2.41400000	-2.02750000
H	10.03558000	-1.39204000	-3.47899200	H	10.02120000	-1.09330000	-3.10090000
30							
C	0.59541700	3.35156700	1.14445800	C	0.83090000	3.13730000	1.24330000
C	0.12734500	2.04792700	1.28068500	C	0.27890000	1.86360000	1.33650000

C	-0.29914500	1.32497200	0.16123000	C	-0.28360000	1.25080000	0.21130000
C	-0.28700300	1.94441500	-1.08847700	C	-0.32150000	1.94830000	-0.99540000
C	0.16215900	3.24910900	-1.23900600	C	0.20910000	3.22620000	-1.10010000
C	0.60945400	3.93673800	-0.11541400	C	0.79210000	3.80310000	0.02430000
H	0.92841500	3.90118900	2.01331900	H	1.27220000	3.60190000	2.11330000
H	-0.63708800	1.38174000	-1.94449000	H	-0.77310000	1.46470000	-1.85190000
H	0.17317900	3.72317100	-2.21103700	H	0.18350000	3.76360000	-2.03820000
N	-0.79121200	-0.00714200	0.26284500	N	-0.83290000	-0.05790000	0.26250000
C	-0.11481500	-1.17052900	0.58483700	C	-0.19300000	-1.25760000	0.51430000
C	-1.05579400	-2.19398400	0.54506800	C	-1.16820000	-2.24500000	0.42850000
C	-2.26522300	-1.54420200	0.18788100	C	-2.35740000	-1.53820000	0.11700000
C	-3.60908600	-2.17403900	-0.00509900	C	-3.72150000	-2.11280000	-0.09770000
O	-3.78259200	-3.37152300	0.12511600	O	-3.92990000	-3.31150000	-0.06350000
N	-4.58456800	-1.26748700	-0.33424700	N	-4.67150000	-1.15300000	-0.32890000
C	1.31189900	-1.24217200	0.85936400	C	1.22860000	-1.38760000	0.77410000
C	1.92637400	-1.98086700	1.84398700	C	1.82090000	-2.24920000	1.66840000
S	2.50855100	-0.44377500	-0.13936400	S	2.44340000	-0.47830000	-0.10020000
C	3.33851900	-1.90703500	1.81752500	C	3.23340000	-2.18420000	1.67190000
H	1.36864800	-2.54257000	2.58057100	H	1.24460000	-2.88970000	2.32090000
C	3.82781000	-1.10954800	0.80689400	C	3.74200000	-1.26990000	0.77600000
H	3.98717400	-2.40968300	2.52157800	H	3.86950000	-2.77470000	2.31650000
Cl	0.05604700	1.35395100	2.88044000	Cl	0.29150000	1.06090000	2.88580000
Cl	1.19473700	5.58143600	-0.28317300	Cl	1.48740000	5.40960000	-0.08970000
H	-4.31407400	-0.29181400	-0.40369800	H	-4.36820000	-0.18510000	-0.34570000
N	-2.09424400	-0.23482100	0.01355300	N	-2.14420000	-0.22680000	0.01000000
C	-0.82718500	-3.65505700	0.77761700	C	-0.98540000	-3.72160000	0.58400000
H	-1.10549400	-3.94231700	1.79676300	H	-1.21280000	-4.04090000	1.60640000
H	-1.45016500	-4.24672800	0.10892800	H	-1.67080000	-4.25610000	-0.07090000
C	-6.84813900	-1.25651700	0.47090800	C	-6.93310000	-1.06050000	0.43850000
C	-6.33132600	-1.52914000	-1.95129200	C	-6.38450000	-1.23880000	-1.98610000
C	-7.15839200	0.24384900	0.59848200	C	-7.11390000	0.45200000	0.63950000
H	-7.77513500	-1.80076200	0.26023500	H	-7.89740000	-1.51090000	0.18060000
H	-6.47096000	-1.63736100	1.42384700	H	-6.60820000	-1.52270000	1.37460000
C	-6.19992300	-0.14276300	-2.62390600	C	-6.08790000	0.15910000	-2.57220000
H	-7.37791000	-1.84523000	-1.96180100	H	-7.45750000	-1.44110000	-2.03380000
H	-5.78118100	-2.26241100	-2.54965300	H	-5.89620000	-1.99290000	-2.61160000
C	-7.63173000	0.92776400	-0.69514200	C	-7.49410000	1.23360000	-0.62940000

H	-6.27197600	0.77192500	0.97245200	H	-6.19160000	0.87790000	1.05450000
H	-7.92408100	0.35655900	1.37544200	H	-7.88390000	0.59510000	1.40670000
C	-6.52410100	1.09087900	-1.75241400	C	-6.34290000	1.36780000	-1.64380000
H	-6.85877200	-0.15461200	-3.49994800	H	-6.69570000	0.25740000	-3.47870000
H	-5.18544700	-0.02702300	-3.01924500	H	-5.04590000	0.19400000	-2.90560000
H	-8.48807700	0.38659200	-1.11803200	H	-8.36980000	0.77460000	-1.10580000
H	-8.00578100	1.92374700	-0.43588600	H	-7.80590000	2.23950000	-0.33030000
H	-6.78664700	1.91469300	-2.42391100	H	-6.51950000	2.24460000	-2.27460000
H	-5.61529300	1.42352600	-1.23472000	H	-5.42850000	1.60030000	-1.08310000
C	5.16503300	-0.79888000	0.49394500	C	5.08470000	-0.93310000	0.52420000
C	6.30922200	-0.52344200	0.21855400	C	6.23230000	-0.62900000	0.30060000
C	7.69243100	-0.21503100	-0.12479100	C	7.61870000	-0.29160000	0.00480000
C	8.30351400	-1.18159100	-1.16152300	C	8.18040000	-1.03120000	-1.22740000
H	8.29898500	-0.22901900	0.78903500	H	8.23820000	-0.51960000	0.88080000
H	7.74459500	0.81141100	-0.50811800	H	7.69960000	0.79110000	-0.15210000
H	8.24617400	-2.20318100	-0.77121200	H	8.09630000	-2.11080000	-1.06360000
H	7.69111700	-1.16187300	-2.06919100	H	7.55600000	-0.79950000	-2.09680000
H	0.22385800	-3.91127000	0.62903400	H	0.04530000	-4.00770000	0.36260000
N	-5.89532900	-1.66092100	-0.56364100	N	-5.99180000	-1.48290000	-0.59900000
C	9.75580200	-0.83562500	-1.50505300	C	9.63720000	-0.66010000	-1.51880000
H	10.35787900	-0.84904900	-0.58839700	H	10.25160000	-0.88760000	-0.63910000
H	9.80301900	0.19185900	-1.88580800	H	9.71120000	0.42340000	-1.67180000
C	10.37013600	-1.78957500	-2.53312100	C	10.19990000	-1.39080000	-2.74080000
H	11.40496600	-1.51853100	-2.75816100	H	11.23960000	-1.11100000	-2.92980000
H	10.36868300	-2.82050900	-2.16637600	H	10.16620000	-2.47550000	-2.60020000
H	9.80997100	-1.77220700	-3.47293100	H	9.62190000	-1.15580000	-3.63980000
31							
C	0.23485900	3.73505500	0.73079800	C	0.71390000	3.55440000	0.77250000
C	-0.31443600	2.46377000	0.87111300	C	0.00400000	2.36470000	0.90300000
C	-0.62028700	1.69317600	-0.25547500	C	-0.50120000	1.71350000	-0.22710000
C	-0.40477800	2.23287100	-1.52309000	C	-0.32290000	2.29290000	-1.48260000
C	0.12818800	3.50486300	-1.68071000	C	0.36690000	3.48810000	-1.62750000
C	0.45232400	4.23998200	-0.54498400	C	0.89020000	4.10080000	-0.49270000
H	0.47269600	4.32247100	1.60616000	H	1.10930000	4.04870000	1.64820000
H	-0.66299600	1.63473100	-2.38776600	H	-0.73300000	1.78260000	-2.34460000
H	0.29721500	3.91725300	-2.66612200	H	0.50900000	3.93320000	-2.60280000
N	-1.18549700	0.39018800	-0.14849500	N	-1.19820000	0.47880000	-0.13690000

C	-0.59602000	-0.78021000	0.29462700	C	-0.71740000	-0.75190000	0.27360000
C	-1.56801300	-1.76934700	0.20336900	C	-1.77010000	-1.64770000	0.13890000
C	-2.70682900	-1.09079600	-0.30695700	C	-2.83680000	-0.85860000	-0.36650000
C	-4.06165300	-1.65476800	-0.58481500	C	-4.22440000	-1.30610000	-0.67830000
O	-4.30811300	-2.84553900	-0.43012700	O	-4.56520000	-2.47870000	-0.56100000
N	-4.97065600	-0.74202300	-1.01839300	N	-5.05920000	-0.32140000	-1.09990000
C	0.79513200	-0.87058700	0.72519800	C	0.65260000	-0.97280000	0.70970000
C	1.27269000	-1.37603300	1.91029500	C	1.06890000	-1.64630000	1.83290000
S	2.12065800	-0.39884200	-0.31595300	S	2.02670000	-0.41560000	-0.21960000
C	2.68490800	-1.38222700	2.00138400	C	2.47540000	-1.71820000	1.96470000
H	0.61722100	-1.71295000	2.70186300	H	0.37290000	-2.04870000	2.55580000
C	3.30927100	-0.87890300	0.88165800	C	3.15410000	-1.09500000	0.94070000
H	3.23765400	-1.73160900	2.86249100	H	2.98730000	-2.19610000	2.78840000
Cl	-0.64985300	1.87672500	2.48057900	Cl	-0.26160000	1.72530000	2.50520000
Cl	1.13997900	5.84385200	-0.71926800	Cl	1.78460000	5.60120000	-0.65410000
H	-4.66483900	0.21894200	-1.07039700	H	-4.70290000	0.62280000	-1.09720000
N	-2.46411400	0.20173800	-0.51743500	N	-2.48130000	0.41470000	-0.53380000
C	-1.41440700	-3.23364700	0.50283900	C	-1.75130000	-3.13000000	0.37010000
H	-0.54386800	-3.37706900	1.14713100	H	-0.89870000	-3.38760000	1.00170000
H	-2.29427400	-3.57262900	1.05323200	H	-2.66210000	-3.41300000	0.90140000
C	4.68666700	-0.72257100	0.63287000	C	4.54260000	-0.95830000	0.75690000
C	5.86623300	-0.58139300	0.41069800	C	5.73170000	-0.82750000	0.58820000
C	7.29191600	-0.43896300	0.13958200	C	7.16690000	-0.70630000	0.36710000
C	7.93676400	-1.70492200	-0.46369000	C	7.74240000	-1.81120000	-0.54350000
H	7.80852300	-0.17458600	1.07044900	H	7.68240000	-0.72620000	1.33510000
H	7.44232700	0.40720900	-0.54196400	H	7.38090000	0.27590000	-0.07200000
C	9.43351400	-1.52960300	-0.73908800	C	9.25060000	-1.66230000	-0.76280000
H	7.78002000	-2.54418500	0.22214600	H	7.52510000	-2.78810000	-0.09870000
H	7.41468800	-1.96140800	-1.39153400	H	7.22160000	-1.78580000	-1.50660000
H	9.57974000	-0.68177700	-1.41933600	H	9.45740000	-0.67780000	-1.19990000
H	9.94478200	-1.26350100	0.19404300	H	9.76100000	-1.67940000	0.20780000
C	-1.26170200	-4.09531000	-0.76240800	C	-1.67700000	-3.92340000	-0.94520000
H	-2.15379400	-4.01420200	-1.38454300	H	-2.55720000	-3.71630000	-1.55500000
H	-0.39126400	-3.78600900	-1.34761500	H	-0.77970000	-3.65710000	-1.51090000
H	-1.13208800	-5.14696200	-0.49206800	H	-1.64760000	-4.99770000	-0.74330000
C	-6.35553800	-1.08337100	-1.30256600	C	-6.46540000	-0.57550000	-1.37530000
C	-7.31763200	-0.73176900	-0.16015100	C	-7.34190000	-0.54310000	-0.11770000

H	-6.38220500	-2.15736000	-1.49433600	H	-6.53630000	-1.56010000	-1.84320000
H	-6.65870700	-0.57095800	-2.22204700	H	-6.80840000	0.16670000	-2.10230000
C	-8.77342500	-1.08261700	-0.48521100	C	-8.81610000	-0.82470000	-0.42050000
H	-6.99809800	-1.26660500	0.74075900	H	-6.95670000	-1.28940000	0.58450000
H	-7.23780700	0.33909000	0.06543400	H	-7.24100000	0.43510000	0.36830000
C	-9.74224200	-0.74010700	0.65009100	C	-9.69400000	-0.80290000	0.83380000
H	-9.07983600	-0.55549100	-1.39729100	H	-9.18850000	-0.08630000	-1.14170000
H	-8.84312200	-2.15265400	-0.71399200	H	-8.90190000	-1.80170000	-0.91080000
H	-10.77091400	-1.00328300	0.38943700	H	-10.74040000	-1.01090000	0.59460000
H	-9.48278300	-1.27962000	1.56596800	H	-9.36050000	-1.55310000	1.55720000
H	-9.72059200	0.32985300	0.87936800	H	-9.65130000	0.17350000	1.32650000
C	10.08157100	-2.78132900	-1.33706000	C	9.82710000	-2.75620000	-1.66550000
H	11.14770100	-2.62682800	-1.52273900	H	10.90350000	-2.63000000	-1.80820000
H	9.98206900	-3.63817900	-0.66383000	H	9.66110000	-3.74860000	-1.23540000
H	9.61419500	-3.05246400	-2.28856300	H	9.35500000	-2.74040000	-2.65260000
32							
C	0.99562900	3.75962100	0.72031000	C	1.47760000	3.56390000	0.78880000
C	0.40924800	2.50287400	0.83993800	C	0.72690000	2.39610000	0.88340000
C	0.11026700	1.74662900	-0.29815700	C	0.23600000	1.77410000	-0.26930000
C	0.37081100	2.28685200	-1.55704500	C	0.47070000	2.36150000	-1.51160000
C	0.94132900	3.54483900	-1.69437800	C	1.20200000	3.53560000	-1.62120000
C	1.25741300	4.26507700	-0.54691100	C	1.70950000	4.11850000	-0.46380000
H	1.22785700	4.33587700	1.60455000	H	1.86150000	4.03550000	1.68200000
H	0.11778900	1.70028700	-2.43113700	H	0.07120000	1.87420000	-2.39170000
H	1.14520100	3.95761500	-2.67301200	H	1.38780000	3.98680000	-2.58630000
N	-0.49185200	0.45871000	-0.21224200	N	-0.50200000	0.56140000	-0.21490000
C	0.05577000	-0.72933800	0.23756300	C	-0.07260000	-0.68860000	0.19430000
C	-0.93987600	-1.69158100	0.11823500	C	-1.14850000	-1.54880000	0.01800000
C	-2.04811900	-0.98009300	-0.41413600	C	-2.17450000	-0.72040000	-0.50860000
C	-3.41083400	-1.50606000	-0.72593900	C	-3.56570000	-1.12000000	-0.86600000
O	-3.69253900	-2.69056200	-0.58351900	O	-3.94640000	-2.28250000	-0.77330000
N	-4.28500600	-0.56723400	-1.17499900	N	-4.35670000	-0.10460000	-1.29900000
C	1.43371400	-0.85902600	0.69947900	C	1.27610000	-0.95780000	0.66800000
C	1.87024700	-1.38264400	1.89248700	C	1.63730000	-1.65600000	1.79510000
S	2.79498200	-0.41779000	-0.30841300	S	2.69420000	-0.43470000	-0.21390000
C	3.27933600	-1.42676300	2.01596300	C	3.03630000	-1.77420000	1.96750000
H	1.18800500	-1.70574100	2.66700800	H	0.90770000	-2.04360000	2.49250000

C	3.94249300	-0.93484200	0.91361500	C	3.76450000	-1.16200000	0.97120000
H	3.80260100	-1.79472500	2.88768600	H	3.50810000	-2.27680000	2.80030000
Cl	0.01937900	1.91662600	2.43737900	Cl	0.39250000	1.74760000	2.46900000
Cl	1.99190800	5.85069700	-0.69522700	Cl	2.65540000	5.59130000	-0.57990000
H	-3.95286500	0.38556300	-1.21413900	H	-3.97120000	0.82780000	-1.27410000
N	-1.76619100	0.30655100	-0.61147300	N	-1.77420000	0.54270000	-0.64990000
C	-0.83230700	-3.16098700	0.41272300	C	-1.18330000	-3.03340000	0.23170000
H	0.01951800	-3.33102600	1.07530800	H	-0.35810000	-3.32510000	0.88460000
H	-1.73298000	-3.47891600	0.94160600	H	-2.11770000	-3.29330000	0.73290000
C	5.32889100	-0.81342900	0.69745900	C	5.16160000	-1.06760000	0.83010000
C	6.51650700	-0.70168800	0.50316300	C	6.35870000	-0.97300000	0.69850000
C	7.95119100	-0.59429400	0.26544600	C	7.80300000	-0.89500000	0.52160000
C	8.57611000	-1.87031000	-0.33760900	C	8.36790000	-1.99510000	-0.40130000
H	8.45341700	-0.35366500	1.21051300	H	8.28880000	-0.95730000	1.50300000
H	8.13908900	0.25485900	-0.40297000	H	8.06250000	0.09030000	0.11510000
C	10.08270000	-1.73147200	-0.57791700	C	9.88610000	-1.89260000	-0.57270000
H	8.38225300	-2.71240800	0.33514100	H	8.10470000	-2.97510000	0.01060000
H	8.06841300	-2.10308900	-1.27957600	H	7.87730000	-1.92700000	-1.37800000
H	10.26610500	-0.88060300	-1.24523500	H	10.13900000	-0.90470000	-0.97670000
H	10.57972700	-1.48880100	0.36919300	H	10.36650000	-1.95280000	0.41150000
C	-0.67463900	-4.02008900	-0.85365200	C	-1.09550000	-3.81420000	-1.09040000
H	-1.55018900	-3.91187300	-1.49486300	H	-1.95040000	-3.57210000	-1.72290000
H	0.21657800	-3.73140900	-1.41773900	H	-0.17400000	-3.57030000	-1.62650000
H	-0.57929200	-5.07619100	-0.58641200	H	-1.10600000	-4.89100000	-0.90080000
C	-5.67182900	-0.87019500	-1.49176100	C	-5.76170000	-0.31100000	-1.61740000
C	-6.64865100	-0.50656300	-0.36555200	C	-6.67160000	-0.27170000	-0.38390000
H	-5.72172000	-1.94100700	-1.69621200	H	-5.84930000	-1.28560000	-2.10330000
H	-5.94216600	-0.34023400	-2.41146700	H	-6.06140000	0.45270000	-2.34100000
C	-8.10520400	-0.81699400	-0.72599200	C	-8.14370000	-0.50390000	-0.73310000
H	-6.36107000	-1.05943500	0.53505800	H	-6.32820000	-1.04040000	0.31550000
H	-6.54562100	0.55921900	-0.12650700	H	-6.55460000	0.69520000	0.12030000
C	-9.09733400	-0.46568400	0.38834700	C	-9.06530000	-0.47880000	0.49000000
H	-8.37983900	-0.27170400	-1.63863300	H	-8.47580000	0.25730000	-1.45170000
H	-8.19754300	-1.88310200	-0.96907600	H	-8.24600000	-1.47040000	-1.24270000
H	-8.82346500	-1.01065200	1.30072700	H	-8.73160000	-1.23830000	1.20850000
H	-9.00545500	0.60061900	0.63269200	H	-8.96440000	0.48770000	1.00060000
C	10.71119000	-2.99335900	-1.17541300	C	10.45220000	-2.98170000	-1.48780000

H	11.78485100	-2.86491000	-1.33582800	H	11.53610000	-2.88920000	-1.59560000
H	10.57447100	-3.85439500	-0.51415900	H	10.23990000	-3.97870000	-1.08990000
H	10.25827100	-3.24205000	-2.13995100	H	10.01080000	-2.92360000	-2.48740000
C	-10.55559000	-0.77750400	0.03323500	C	-10.53960000	-0.71830000	0.14920000
C	-11.53960300	-0.42423600	1.15211600	C	-11.45060000	-0.69200000	1.37960000
H	-10.64687400	-1.84287800	-0.21038700	H	-10.63850000	-1.68440000	-0.36050000
H	-10.82906800	-0.23313200	-0.87888100	H	-10.87130000	0.04070000	-0.56980000
H	-12.56915500	-0.65846700	0.86793700	H	-12.49590000	-0.86570000	1.10970000
H	-11.31334600	-0.97987700	2.06751700	H	-11.15950000	-1.46280000	2.10020000
H	-11.49660700	0.64224500	1.39470700	H	-11.39390000	0.27470000	1.89010000
33							
C	0.71176200	3.77400900	0.76715200	C	1.14010000	3.56630000	0.78730000
C	0.16330400	2.51985300	1.01987500	C	0.46440000	2.38450000	1.07610000
C	-0.24660800	1.69752000	-0.03481300	C	-0.16330000	1.66020000	0.05720000
C	-0.13598300	2.16901600	-1.34251700	C	-0.14130000	2.15880000	-1.24450000
C	0.39453600	3.42330800	-1.61108100	C	0.51250000	3.34510000	-1.54550000
C	0.82351100	4.21014800	-0.54703500	C	1.15920000	4.03130000	-0.52180000
H	1.03039300	4.40155300	1.58723800	H	1.63030000	4.11730000	1.57700000
H	-0.47417300	1.53159600	-2.14962200	H	-0.64450000	1.59280000	-2.01780000
H	0.48194200	3.78259600	-2.62741900	H	0.53330000	3.72730000	-2.55690000
N	-0.81300800	0.40979000	0.18750800	N	-0.83070000	0.43130000	0.30730000
C	-0.19906200	-0.74438400	0.63987700	C	-0.29140000	-0.76880000	0.73520000
C	-1.18408100	-1.72395000	0.68054500	C	-1.34220000	-1.67570000	0.78050000
C	-2.35567200	-1.05701400	0.23246500	C	-2.46970000	-0.92450000	0.35580000
C	-3.73401900	-1.61779500	0.09654000	C	-3.87790000	-1.39930000	0.22740000
O	-3.96988300	-2.79981000	0.32066200	O	-4.17810000	-2.57590000	0.40270000
N	-4.67149300	-0.71050900	-0.28553600	N	-4.77630000	-0.43050000	-0.08400000
C	1.22252400	-0.83149300	0.95679200	C	1.12260000	-0.95610000	1.02090000
C	1.79373800	-1.28246900	2.12225400	C	1.67510000	-1.55470000	2.12750000
S	2.45973500	-0.43147900	-0.21489100	S	2.37210000	-0.45350000	-0.09650000
C	3.20848900	-1.30328400	2.09479800	C	3.08820000	-1.61200000	2.09770000
H	1.20433000	-1.56956100	2.98242400	H	1.07320000	-1.91280000	2.95110000
C	3.74073600	-0.86599100	0.90214100	C	3.63530000	-1.05230000	0.96400000
H	3.82868400	-1.61575600	2.92354900	H	3.69840000	-2.03380000	2.88420000
Cl	-0.03852800	2.02085300	2.68052800	Cl	0.39780000	1.84810000	2.73560000
Cl	1.51058800	5.79262200	-0.86264700	Cl	2.01080000	5.52190000	-0.88260000
H	-4.35498000	0.23822500	-0.43316400	H	-4.41850000	0.49900000	-0.25460000

N	-2.11961900	0.21968200	-0.06384700	N	-2.15070000	0.33670000	0.06830000
C	-1.01852700	-3.17292800	1.04204400	C	-1.27910000	-3.14070000	1.09830000
H	-0.09962100	-3.29383200	1.62045200	H	-0.36610000	-3.35170000	1.65880000
H	-1.85333200	-3.47256900	1.67864100	H	-2.13020000	-3.39890000	1.73110000
C	5.09358000	-0.73991100	0.53134100	C	4.99110000	-0.92010000	0.61070000
C	6.25155100	-0.62467700	0.20500500	C	6.15060000	-0.79340000	0.29650000
C	7.64963700	-0.51171300	-0.19369600	C	7.54740000	-0.67440000	-0.10170000
C	8.17997100	-1.74877600	-0.94922300	C	7.97490000	-1.71630000	-1.15650000
H	8.26266800	-0.33897700	0.69932000	H	8.18290000	-0.77270000	0.78680000
H	7.77100400	0.37909200	-0.82221900	H	7.72540000	0.33460000	-0.49360000
C	9.64947000	-1.60446100	-1.35737300	C	9.44460000	-1.57040000	-1.56090000
H	8.05442300	-2.63271000	-0.31506200	H	7.79570000	-2.72050000	-0.75800000
H	7.56118700	-1.91432700	-1.83747000	H	7.33400000	-1.61340000	-2.03860000
H	9.76544800	-0.71134400	-1.98333100	H	9.61450000	-0.55880000	-1.94930000
H	10.25865300	-1.43046700	-0.46207200	H	10.07660000	-1.66620000	-0.66960000
C	-0.97632800	-4.10018400	-0.18476200	C	-1.31970000	-4.01220000	-0.16840000
H	-1.91552600	-4.04000100	-0.73584100	H	-2.25690000	-3.84860000	-0.70170000
H	-0.15394900	-3.83232600	-0.85389100	H	-0.48410000	-3.77380000	-0.83240000
H	-0.83370600	-5.13809200	0.12877000	H	-1.25680000	-5.07200000	0.09350000
C	10.18379100	-2.82699300	-2.10855800	C	9.87430000	-2.60130000	-2.60810000
H	11.23282800	-2.69552000	-2.38644900	H	10.92560000	-2.47850000	-2.88150000
H	10.11304600	-3.73024300	-1.49499400	H	9.74350000	-3.62080000	-2.23270000
H	9.61642000	-3.00588000	-3.02692900	H	9.27840000	-2.50600000	-3.52100000
C	-6.07879100	-1.03629000	-0.47861300	C	-6.18790000	-0.71310000	-0.31110000
C	-6.97102800	-0.25179800	0.49881200	C	-7.03920000	0.50200000	0.07560000
C	-6.51083500	-0.79746900	-1.93577100	C	-6.45680000	-1.14370000	-1.76360000
H	-6.16029600	-2.10317500	-0.25487500	H	-6.44150000	-1.55300000	0.34330000
C	-8.45848000	-0.57061000	0.28760900	C	-8.53210000	0.23450000	-0.16290000
H	-6.80293900	0.82359700	0.34920500	H	-6.72520000	1.36390000	-0.53000000
H	-6.66843400	-0.47931000	1.52505400	H	-6.85240000	0.76110000	1.12210000
C	-7.99882300	-1.11589100	-2.14392600	C	-7.94950000	-1.41380000	-1.99630000
H	-6.32221500	0.25341600	-2.19513900	H	-6.11430000	-0.34470000	-2.43400000
H	-5.88882000	-1.40403500	-2.60048000	H	-5.85940000	-2.03210000	-1.98380000
C	-8.88751500	-0.33359400	-1.16698600	C	-8.80320000	-0.19740000	-1.61130000
H	-9.06868300	0.03128000	0.96829700	H	-9.11520000	1.12630000	0.08630000
H	-8.64167500	-1.61984300	0.55174900	H	-8.86580000	-0.55880000	0.51770000
H	-8.28525300	-0.89888700	-3.17780400	H	-8.12320000	-1.68800000	-3.04140000

H	-8.15957400	-2.19133300	-1.99629500	H	-8.25660000	-2.27660000	-1.39160000
H	-9.93686400	-0.61417300	-1.30253600	H	-9.86640000	-0.41940000	-1.74630000
H	-8.81894400	0.73826100	-1.39436800	H	-8.56730000	0.63620000	-2.28560000
34							
C	1.51017700	3.38265000	1.12187200	C	1.72700000	3.16910000	1.13850000
C	0.76251100	2.21148700	1.20251100	C	0.90410000	2.04850000	1.19240000
C	0.12903300	1.69352800	0.06771100	C	0.15720000	1.66390000	0.07370000
C	0.22246200	2.39044600	-1.13684800	C	0.21470000	2.43990000	-1.08300000
C	0.95127700	3.56795500	-1.23021100	C	1.01740000	3.56990000	-1.14670000
C	1.59813800	4.04646600	-0.09529800	C	1.77670000	3.91540000	-0.03260000
H	2.00089400	3.77360000	2.00178400	H	2.30860000	3.45680000	2.00260000
H	-0.28862800	1.99072900	-2.00340900	H	-0.38080000	2.13550000	-1.93400000
H	1.02356800	4.10244900	-2.16762900	H	1.06490000	4.16800000	-2.04640000
N	-0.64969600	0.50178900	0.11258600	N	-0.66970000	0.50840000	0.08270000
C	-0.24298500	-0.80457100	0.32018900	C	-0.30020000	-0.81790000	0.21830000
C	-1.39343400	-1.58600100	0.27136200	C	-1.47480000	-1.55860000	0.14790000
C	-2.43610900	-0.65392100	0.02636700	C	-2.49120000	-0.58500000	-0.03170000
C	-3.89305400	-0.93997500	-0.14306300	C	-3.95520000	-0.83130000	-0.17500000
O	-4.34920400	-2.07099600	-0.03297700	O	-4.43330000	-1.95570000	-0.08540000
N	-4.63988000	0.16466200	-0.43133400	N	-4.68770000	0.29360000	-0.41350000
C	1.14493100	-1.20988800	0.48848200	C	1.07230000	-1.26960000	0.35900000
C	1.64223900	-2.11522000	1.39657500	C	1.52450000	-2.28740000	1.16650000
S	2.42031700	-0.65057100	-0.57390100	S	2.39080000	-0.59550000	-0.57630000
C	3.02925900	-2.35796700	1.26204200	C	2.91340000	-2.52900000	1.05490000
H	1.02449000	-2.57396600	2.15600600	H	0.87180000	-2.82410000	1.84020000
C	3.61596000	-1.64057200	0.24340200	C	3.54380000	-1.69650000	0.15690000
H	3.59365700	-3.02731900	1.89646000	H	3.44930000	-3.27770000	1.62140000
Cl	0.60813100	1.43015200	2.75542600	Cl	0.81570000	1.15010000	2.68560000
Cl	2.53688900	5.52444200	-0.19243400	Cl	2.81480000	5.32760000	-0.09730000
H	-4.17254600	1.05869700	-0.48516500	H	-4.21300000	1.18430000	-0.44820000
N	-1.97843900	0.59260200	-0.07461300	N	-1.99750000	0.65180000	-0.07990000
C	-6.44964400	-0.57220500	-1.81861500	C	-6.54400000	-0.39940000	-1.75110000
C	-6.77974000	-0.19706400	0.58961000	C	-6.78520000	-0.08520000	0.67440000
C	-7.93020000	-0.30027300	-2.09467100	C	-8.03490000	-0.13000000	-1.96410000
H	-6.27710600	-1.65029000	-1.69099600	H	-6.36200000	-1.47830000	-1.64900000
H	-5.83422700	-0.22893800	-2.65364700	H	-5.96000000	-0.03620000	-2.60000000
C	-8.26816100	0.08483600	0.37226600	C	-8.28160000	0.19260000	0.51950000

H	-6.62495900	-1.25617200	0.83957100	H	-6.61510000	-1.15020000	0.88520000
H	-6.39173600	0.40462900	1.41495200	H	-6.36750000	0.49480000	1.50070000
C	-8.79033900	-0.64466700	-0.87206300	C	-8.84240000	-0.51810000	-0.71890000
H	-8.24594500	-0.88231600	-2.96631900	H	-8.38000000	-0.68800000	-2.84020000
H	-8.05642100	0.75888300	-2.34567400	H	-8.17720000	0.93570000	-2.17540000
H	-8.82558800	-0.22179800	1.26301500	H	-8.80390000	-0.13350000	1.42430000
H	-8.41187600	1.16450000	0.25239600	H	-8.43470000	1.27330000	0.42240000
H	-9.83800900	-0.38739400	-1.05580400	H	-9.90050000	-0.27540000	-0.85560000
H	-8.75546700	-1.72746100	-0.69823200	H	-8.77930000	-1.60350000	-0.57160000
N	-6.02830100	0.17877800	-0.62207800	N	-6.08150000	0.32800000	-0.55450000
C	-1.49091500	-3.07886700	0.39886000	C	-1.62440000	-3.04840000	0.21820000
H	-2.18878000	-3.44591900	-0.35594800	H	-2.35680000	-3.35890000	-0.52880000
H	-0.51021800	-3.51319200	0.18395400	H	-0.66670000	-3.51190000	-0.03580000
C	4.96450800	-1.62063600	-0.16212000	C	4.90620000	-1.63980000	-0.19020000
C	6.11908800	-1.59775900	-0.52081500	C	6.07200000	-1.57560000	-0.50170000
C	-1.98105000	-3.55109500	1.77840100	C	-2.10200000	-3.53540000	1.59640000
H	-2.00682000	-4.64355100	1.81933600	H	-2.16970000	-4.62650000	1.61660000
H	-1.32847000	-3.19692300	2.58179700	H	-1.42000000	-3.22000000	2.39170000
H	-2.99022500	-3.18180600	1.96507100	H	-3.09160000	-3.12810000	1.80770000
C	7.52383800	-1.57395000	-0.95056100	C	7.48930000	-1.50030000	-0.87480000
C	7.69444100	-0.51420100	-2.06371500	C	7.67540000	-0.38360000	-1.92740000
C	8.42230400	-1.21219200	0.25547000	C	8.33360000	-1.17910000	0.38010000
C	7.91772600	-2.96787300	-1.49347300	C	7.93580000	-2.85610000	-1.46930000
H	7.06687400	-0.74960100	-2.92621000	H	7.08590000	-0.59080000	-2.82340000
H	7.41981200	0.47931400	-1.70231000	H	7.36380000	0.58420000	-1.52780000
H	8.73703300	-0.48544000	-2.39338200	H	8.72890000	-0.31660000	-2.21410000
H	8.31394700	-1.94669300	1.05670300	H	8.21280000	-1.95510000	1.13940000
H	9.47148100	-1.19171800	-0.05378200	H	9.39230000	-1.12070000	0.11070000
H	8.16107600	-0.23007200	0.65562600	H	8.03410000	-0.22350000	0.81630000
H	8.96307700	-2.96084800	-1.81605800	H	8.99200000	-2.80850000	-1.75060000
H	7.80014000	-3.73381900	-0.72362500	H	7.80830000	-3.66090000	-0.74170000
H	7.29484500	-3.24418600	-2.34704600	H	7.35130000	-3.10250000	-2.35850000
35							
C	0.98539200	2.98206400	1.32584500	C	1.26950000	2.82520000	1.53710000
C	0.50159700	1.67748500	1.35977400	C	0.69190000	1.56030000	1.58720000
C	-0.03926000	1.08964900	0.21098300	C	-0.10170000	1.10180000	0.53030000
C	-0.12424600	1.84460000	-0.95886400	C	-0.34260000	1.94370000	-0.55530000

C	0.33952300	3.15206100	-1.00506100	C	0.21180000	3.21440000	-0.61130000
C	0.90069400	3.70404800	0.14201700	C	1.02500000	3.63700000	0.43630000
H	1.40669700	3.42693100	2.21606200	H	1.88920000	3.17070000	2.35210000
H	-0.56182300	1.38576400	-1.83631100	H	-0.97230000	1.57870000	-1.35650000
H	0.27472100	3.73157800	-1.91592000	H	0.02780000	3.86410000	-1.45600000
N	-0.55069100	-0.23910900	0.20976500	N	-0.69090000	-0.19050000	0.53410000
C	0.12470900	-1.43988100	0.33935700	C	-0.07610000	-1.42950000	0.51510000
C	-0.83978800	-2.44016900	0.27334100	C	-1.09890000	-2.37130000	0.47120000
C	-2.06026300	-1.73884100	0.10096600	C	-2.28730000	-1.59950000	0.46010000
C	-3.43323500	-2.31367800	-0.03796600	C	-3.69910000	-2.07630000	0.36210000
O	-3.62614200	-3.52322700	-0.02201600	O	-3.98050000	-3.24930000	0.14570000
N	-4.41293800	-1.38063000	-0.18014200	N	-4.62200000	-1.09250000	0.50650000
C	1.56801100	-1.56058900	0.47343700	C	1.36040000	-1.63160000	0.49850000
C	2.25020300	-2.41566300	1.30773000	C	2.05380000	-2.62620000	1.14870000
S	2.68971200	-0.66801400	-0.53282500	S	2.44980000	-0.64310000	-0.45190000
C	3.65582200	-2.35741600	1.16179200	C	3.44700000	-2.60070000	0.90760000
H	1.74720700	-3.05132700	2.02329800	H	1.56740000	-3.33650000	1.80240000
C	4.07182000	-1.45533700	0.20795600	C	3.83800000	-1.58440000	0.06440000
H	4.35243800	-2.94605700	1.74259100	H	4.15420000	-3.29250000	1.34360000
Cl	0.55710600	0.81031300	2.87328800	Cl	0.96720000	0.57390000	3.00010000
Cl	1.50634300	5.34948500	0.10375200	Cl	1.75320000	5.23170000	0.37720000
H	-4.11730800	-0.41575100	-0.16604300	H	-4.26890000	-0.15930000	0.65220000
N	-1.87532000	-0.42094600	0.05655000	N	-2.03170000	-0.29160000	0.48660000
C	-0.62625500	-3.92107000	0.32344000	C	-0.96760000	-3.85990000	0.40210000
H	-0.80793100	-4.31379500	1.32916300	H	-1.00000000	-4.30570000	1.40200000
H	-1.32834200	-4.42647800	-0.33757500	H	-1.79810000	-4.28100000	-0.16130000
H	0.39772900	-4.17498200	0.04145100	H	-0.01880000	-4.14290000	-0.05950000
C	5.38303100	-1.12762400	-0.18781100	C	5.13150000	-1.24950000	-0.37660000
C	6.50452100	-0.84106800	-0.53774300	C	6.23410000	-0.94590000	-0.76700000
C	7.86983400	-0.49683200	-0.95729700	C	7.57540000	-0.57970000	-1.23640000
C	-5.82508900	-1.72380900	-0.32552700	C	-6.04380000	-1.29850000	0.23150000
C	-6.72299900	-1.01348200	0.71340900	C	-6.84190000	-0.03450000	0.59530000
C	-6.42503300	-1.26221700	-1.67442900	C	-6.32190000	-1.46020000	-1.27840000
H	-5.86034900	-2.80745300	-0.22090100	H	-6.36320000	-2.17940000	0.79130000
H	-6.23227200	-0.92303200	1.68527200	H	-6.49460000	0.42730000	1.52390000
H	-7.62005000	-1.62317300	0.85960800	H	-7.88410000	-0.32530000	0.75210000
C	-6.90753300	0.19036500	-1.45888200	C	-6.34720000	-0.02470000	-1.84230000

H	-7.27901600	-1.90720700	-1.90470500	H	-7.30250000	-1.93250000	-1.39770000
H	-5.71177700	-1.36431400	-2.49552300	H	-5.58710000	-2.11030000	-1.75550000
H	-7.85243700	0.35445900	-1.98305400	H	-7.09270000	0.06040000	-2.63700000
C	-7.11036500	0.35015700	0.09431100	C	-6.73190000	0.90420000	-0.63220000
C	-6.23683200	1.56216300	0.50690500	C	-5.62920000	1.99260000	-0.56860000
C	-6.07804600	2.38499000	-0.78147200	C	-5.01150000	2.00660000	-1.97630000
H	-5.25250700	1.22820300	0.85474500	H	-4.85670000	1.72800000	0.16180000
H	-6.67849500	2.13110700	1.32893900	H	-6.02240000	2.96500000	-0.26180000
C	-5.91453300	1.30801800	-1.86536300	C	-4.99700000	0.52120000	-2.36620000
H	-6.98742100	2.96794300	-0.96767800	H	-5.65560000	2.56920000	-2.66200000
H	-5.24237700	3.08871000	-0.74243900	H	-4.02140000	2.47010000	-2.00200000
H	-6.10111900	1.68139500	-2.87560300	H	-4.87130000	0.35700000	-3.43940000
H	-4.88631600	0.92882600	-1.85649800	H	-4.16650000	0.02070000	-1.86070000
H	-8.15519700	0.57941800	0.31798800	H	-7.69340000	1.38920000	-0.81540000
C	7.95816300	-0.54649600	-2.50075200	C	7.52310000	-0.29160000	-2.75460000
H	8.97133600	-0.29084500	-2.82468300	H	8.51880000	-0.01630000	-3.11470000
H	7.71807400	-1.54476900	-2.87322700	H	7.18640000	-1.17200000	-3.30650000
H	7.26259100	0.16317200	-2.95437200	H	6.83810000	0.53130000	-2.97120000
C	8.85965700	-1.51544700	-0.34587900	C	8.54680000	-1.75020000	-0.96140000
H	9.88127600	-1.27079000	-0.65079500	H	9.55060000	-1.48780000	-1.30780000
H	8.81262500	-1.49860400	0.74531000	H	8.59710000	-1.97160000	0.10710000
H	8.63314000	-2.52972600	-0.68205000	H	8.22560000	-2.65380000	-1.48450000
C	8.21550000	0.92736500	-0.46197200	C	8.05510000	0.68330000	-0.48380000
H	7.52498700	1.66371000	-0.87923800	H	7.37930000	1.52270000	-0.66240000
H	8.15868100	0.98585900	0.62720900	H	8.09860000	0.50170000	0.59240000
H	9.23100100	1.19340800	-0.77005100	H	9.05470000	0.96430000	-0.82860000
36							
C	1.99166100	3.12087700	1.14889300	C	2.19030000	2.90930000	1.14050000
C	1.18581600	1.98697000	1.19330300	C	1.31480000	1.82830000	1.16560000
C	0.49051300	1.56454400	0.05511500	C	0.51460000	1.53900000	0.05500000
C	0.58336900	2.31980000	-1.11377400	C	0.57420000	2.37060000	-1.06220000
C	1.37057500	3.46154200	-1.17000200	C	1.42990000	3.46250000	-1.09610000
C	2.07680900	3.84416700	-0.03411400	C	2.24010000	3.71240000	0.00760000
H	2.52950700	3.43799500	2.03096400	H	2.81220000	3.12340000	1.99780000
H	0.02522100	1.99425300	-1.98233000	H	-0.06220000	2.14020000	-1.90690000
H	1.44215500	4.04138000	-2.08012400	H	1.47890000	4.10360000	-1.96550000
N	-0.34911100	0.41402700	0.06409300	N	-0.36870000	0.42630000	0.03420000

C	-0.00695600	-0.92093000	0.18989600	C	-0.06260000	-0.92170000	0.09120000
C	-1.19896800	-1.63758400	0.14199200	C	-1.27480000	-1.59960000	0.02560000
C	-2.19720000	-0.64061200	-0.01763000	C	-2.24590000	-0.56950000	-0.07010000
C	-3.67224000	-0.84091800	-0.14978200	C	-3.72440000	-0.73640000	-0.17450000
O	-4.18514100	-1.95049300	-0.07809700	O	-4.25560000	-1.83910000	-0.12410000
N	-4.36698700	0.31429700	-0.35909700	N	-4.40640000	0.43380000	-0.33130000
C	1.36186700	-1.40662700	0.28640200	C	1.28930000	-1.44640000	0.16100000
C	1.83649500	-2.39031800	1.12324300	C	1.71480000	-2.52380000	0.90400000
S	2.63150200	-0.85251300	-0.78389900	S	2.60780000	-0.79410000	-0.78750000
C	3.20269200	-2.69756500	0.92726500	C	3.08480000	-2.82740000	0.73290000
H	1.21805500	-2.86072400	1.87490300	H	1.05780000	-3.05930000	1.57440000
C	3.79735600	-1.95261700	-0.06737100	C	3.72860000	-1.98480000	-0.14690000
H	3.74899400	-3.43339900	1.50105600	H	3.60030000	-3.62830000	1.24440000
Cl	1.03933200	1.13121900	2.70733700	Cl	1.22880000	0.85850000	2.61370000
Cl	3.08920600	5.27510300	-0.08535000	Cl	3.34470000	5.07460000	-0.02080000
H	-3.85397100	1.18417400	-0.38594900	H	-3.88860000	1.30080000	-0.33870000
N	-1.67646300	0.58392700	-0.07043800	N	-1.69210000	0.64250000	-0.07420000
C	-6.25870100	-0.25764300	-1.71446700	C	-6.33730000	-0.09770000	-1.63690000
C	-6.48864900	0.01627700	0.71879700	C	-6.48440000	0.10220000	0.80820000
C	-7.73048200	0.10528600	-1.92499200	C	-7.81870000	0.25470000	-1.78440000
H	-6.14126100	-1.34827300	-1.64361200	H	-6.20680000	-1.18800000	-1.59520000
H	-5.65311000	0.09277200	-2.55369700	H	-5.76320000	0.27990000	-2.48630000
C	-7.96590100	0.38657800	0.56785000	C	-7.96900000	0.46040000	0.71930000
H	-6.38346900	-1.06047600	0.91301400	H	-6.36160000	-0.97930000	0.95940000
H	-6.04167000	0.55560900	1.55731700	H	-6.01150000	0.61760000	1.64750000
C	-8.56758100	-0.25251000	-0.69025600	C	-8.60440000	-0.15720000	-0.53290000
H	-8.10583000	-0.41611300	-2.81127600	H	-8.21960000	-0.23980000	-2.67470000
H	-7.80704400	1.18059700	-2.12145400	H	-7.91380000	1.33570000	-1.93720000
H	-8.50964400	0.06650300	1.46232000	H	-8.47780000	0.11380000	1.62420000
H	-8.05450300	1.47689500	0.50418200	H	-8.07040000	1.55090000	0.68180000
H	-9.60513500	0.06845700	-0.82450200	H	-9.65280000	0.14350000	-0.62060000
H	-8.58606000	-1.34284200	-0.56898900	H	-8.59150000	-1.25060000	-0.44230000
N	-5.75813100	0.41083400	-0.49968700	N	-5.80040000	0.54350000	-0.42210000
C	-1.37327700	-3.12795700	0.19551900	C	-1.49720000	-3.08190000	0.02720000
H	-2.11620200	-3.41642600	-0.55032500	H	-2.26800000	-3.31740000	-0.70850000
H	-0.42606100	-3.60137900	-0.07872200	H	-0.57300000	-3.57820000	-0.28260000
C	5.13035200	-1.98033300	-0.51647900	C	5.07920000	-1.97970000	-0.53710000

C	6.27341400	-1.99460400	-0.91401300	C	6.23720000	-1.95710000	-0.88630000
C	-1.84009800	-3.64718600	1.56624200	C	-1.95450000	-3.61510000	1.39520000
H	-1.92345200	-4.73742500	1.55162100	H	-2.07670000	-4.70120000	1.36320000
H	-1.14196100	-3.37104300	2.36191300	H	-1.23220000	-3.37500000	2.18110000
H	-2.82074400	-3.23626900	1.80937800	H	-2.91490000	-3.17130000	1.66070000
C	7.62668100	-2.02252900	-1.38501500	C	7.61180000	-1.93130000	-1.28890000
C	8.47612300	-0.75865900	-1.34807000	C	8.40970000	-0.63830000	-1.17690000
C	8.78220500	-1.88011800	-0.40314700	C	8.70750000	-1.77160000	-0.24230000
H	7.80429500	-2.68373600	-2.22766000	H	7.85530000	-2.56580000	-2.13580000
H	8.01027700	0.13253900	-0.94791900	H	7.88860000	0.22490000	-0.78270000
H	9.13988700	-0.59014900	-2.18716000	H	9.11090000	-0.42440000	-1.97440000
H	9.65852700	-2.48966200	-0.58639200	H	9.61530000	-2.34350000	-0.39170000
H	8.52475100	-1.75216100	0.64027800	H	8.38900000	-1.68010000	0.78840000
37							
C	1.46195300	2.96183000	0.88936400	C	1.58380000	2.79910000	0.83340000
C	0.87899400	1.69905900	0.94077100	C	0.93200000	1.57050000	0.86780000
C	0.36916400	1.10366000	-0.21824400	C	0.32060000	1.06020000	-0.28270000
C	0.41695800	1.81150100	-1.41919800	C	0.33680000	1.81590000	-1.45400000
C	0.98126700	3.07795400	-1.48438200	C	0.96800000	3.05090000	-1.49980000
C	1.50840800	3.63622200	-0.32429100	C	1.59670000	3.52420000	-0.35190000
H	1.85811300	3.41261100	1.78811900	H	2.06160000	3.18460000	1.72260000
H	0.00237200	1.34858700	-2.30562100	H	-0.15320000	1.41210000	-2.33060000
H	1.01934500	3.62066000	-2.41910600	H	0.98420000	3.63350000	-2.41070000
N	-0.24188000	-0.18227100	-0.20297100	N	-0.33290000	-0.20090000	-0.29020000
C	0.32882000	-1.42327300	0.01870100	C	0.20740000	-1.45890000	-0.09600000
C	-0.70414600	-2.35066100	-0.07284200	C	-0.84990000	-2.35680000	-0.19800000
C	-1.85275300	-1.56838700	-0.35512600	C	-1.97850000	-1.54140000	-0.46090000
C	-3.25442400	-2.04294700	-0.56260200	C	-3.39460000	-1.97510000	-0.64490000
O	-3.55280900	-3.22988500	-0.49555600	O	-3.74050000	-3.14250000	-0.50190000
N	-4.14900300	-1.05609800	-0.82667800	N	-4.24740000	-0.97060000	-0.96600000
C	1.74695800	-1.64588700	0.25295700	C	1.61660000	-1.71740000	0.13200000
C	2.30500500	-2.52097100	1.15687300	C	2.14650000	-2.67260000	0.96970000
S	2.99654200	-0.87522100	-0.70034700	S	2.89090000	-0.86370000	-0.71140000
C	3.71690000	-2.57357600	1.10455600	C	3.55900000	-2.72180000	0.95510000
H	1.70863900	-3.09208500	1.85486600	H	1.52720000	-3.29910000	1.59590000
C	4.26408800	-1.73867700	0.15509800	C	4.13180000	-1.80410000	0.10170000
H	4.32686500	-3.19306300	1.74747000	H	4.15210000	-3.39580000	1.55740000

Cl	0.77242500	0.89578500	2.48652900	Cl	0.88290000	0.69400000	2.37580000
Cl	2.23903500	5.22941500	-0.38484600	Cl	2.41830000	5.07340000	-0.39190000
H	-3.78900000	-0.11574900	-0.89077000	H	-3.85760000	-0.04320000	-1.03450000
N	-1.56409500	-0.27100100	-0.43774100	N	-1.65810000	-0.24890000	-0.52020000
C	-0.61079500	-3.83984100	0.04954200	C	-0.79500000	-3.84820000	-0.09760000
H	-0.87392000	-4.17166500	1.05923500	H	-0.99770000	-4.18090000	0.92560000
H	-1.31575400	-4.31938000	-0.62743300	H	-1.56000000	-4.29670000	-0.72860000
H	0.40300700	-4.18421300	-0.16545600	H	0.19200000	-4.21870000	-0.38400000
C	5.61838900	-1.52438200	-0.15974500	C	5.49350000	-1.56190000	-0.15010000
C	6.77922600	-1.33105400	-0.44255100	C	6.65950000	-1.33710000	-0.38140000
C	-5.56007600	-1.33416900	-1.10099500	C	-5.69340000	-1.17000000	-1.06330000
C	-6.39584200	-1.54158700	0.18263400	C	-6.34760000	-1.36700000	0.32080000
C	-6.24081900	-0.12605100	-1.77378600	C	-6.37400000	0.10550000	-1.58940000
H	-5.58885400	-2.22877400	-1.72606200	H	-5.86160000	-2.03630000	-1.70640000
H	-5.84476700	-2.10681500	0.93602500	H	-5.75390000	-2.02670000	0.95490000
H	-7.27981000	-2.13213300	-0.08029700	H	-7.32160000	-1.84500000	0.17320000
C	-6.75528200	0.78323900	-0.63005000	C	-6.58930000	1.01320000	-0.35330000
H	-7.08448700	-0.49874300	-2.36123900	H	-7.33870000	-0.17850000	-2.01820000
H	-5.57593200	0.39260400	-2.47073900	H	-5.80020000	0.58960000	-2.38510000
H	-7.75100800	1.15896900	-0.87802000	H	-7.56650000	1.49770000	-0.41420000
C	-6.81873700	-0.13200600	0.64847900	C	-6.52910000	0.05390000	0.89240000
C	-5.89627000	0.54928300	1.68790300	C	-5.36640000	0.58610000	1.76350000
C	-5.90553900	2.03345000	1.29260700	C	-5.28790000	2.08040000	1.41960000
H	-4.87906500	0.15435500	1.60335400	H	-4.42960000	0.09840000	1.47950000
H	-6.22653300	0.37389200	2.71503700	H	-5.52260000	0.39450000	2.82800000
C	-5.85343100	1.98385100	-0.24308200	C	-5.51050000	2.09790000	-0.10110000
H	-6.83960400	2.50455700	1.62046100	H	-6.09640000	2.62480000	1.92160000
H	-5.08176500	2.60265800	1.73118100	H	-4.34420000	2.54330000	1.71930000
H	-6.17586900	2.91533600	-0.71559400	H	-5.80870000	3.07770000	-0.48260000
H	-4.81947100	1.81314300	-0.56447600	H	-4.57190000	1.84170000	-0.60510000
H	-7.83719000	-0.15576100	1.04524500	H	-7.45730000	0.11930000	1.46570000
C	8.15554000	-1.11283100	-0.77746000	C	8.04230000	-1.07080000	-0.64420000
C	8.75403200	0.28469200	-0.68238300	C	8.57770000	0.34990000	-0.51750000
C	9.16163200	-0.76064800	0.31030100	C	8.97150000	-0.67970000	0.49820000
H	8.53373500	-1.73199900	-1.58517900	H	8.48640000	-1.67530000	-1.42940000
H	8.09670100	1.07680300	-0.34796300	H	7.87030000	1.11410000	-0.22160000
H	9.45721100	0.56985700	-1.45522700	H	9.31120000	0.66460000	-1.24990000

H	10.14777000	-1.20061800	0.22643100	H	9.97820000	-1.07890000	0.47000000
H	8.78179300	-0.67998000	1.32055400	H	8.53210000	-0.61650000	1.48550000
38							
C	0.75484800	3.40044400	0.97936700	C	0.96329500	3.21188800	1.01632900
C	0.15965100	2.15006900	1.11874200	C	0.29764100	1.99421400	1.11619900
C	-0.41245800	1.50799100	0.01504400	C	-0.39384900	1.47225800	0.01745700
C	-0.41445000	2.15796600	-1.21914500	C	-0.44264600	2.20647900	-1.16674400
C	0.16115600	3.41176700	-1.37147200	C	0.20150600	3.43061600	-1.27662100
C	0.75070900	4.01626300	-0.26585300	C	0.90980500	3.91501500	-0.18087500
H	1.19961200	3.88716500	1.83562900	H	1.50338600	3.60577100	1.86530100
H	-0.87726200	1.65987100	-2.06153900	H	-0.99399700	1.79422200	-2.00195200
H	0.16035500	3.90940500	-2.33171100	H	0.16700000	3.99626400	-2.19766600
N	-1.03642600	0.23262500	0.12025800	N	-1.06157300	0.21991100	0.07398500
C	-0.46920200	-1.00400400	0.37298400	C	-0.52316000	-1.04108000	0.25442000
C	-1.51461000	-1.92144800	0.37132500	C	-1.59187300	-1.92951100	0.21977000
C	-2.66729300	-1.13827500	0.10587800	C	-2.72649400	-1.10551400	0.00789300
C	-4.07970300	-1.61907400	-0.01186300	C	-4.14889000	-1.54903900	-0.11028800
O	-4.37323500	-2.79192900	0.12876900	O	-4.47347800	-2.71312100	0.03755600
N	-4.96577700	-0.61203900	-0.29065800	N	-5.00992600	-0.52353000	-0.40093900
C	0.95591400	-1.23290700	0.55313100	C	0.89420000	-1.31038500	0.40909000
C	1.54810300	-2.06185500	1.47769000	C	1.46285200	-2.24727800	1.24081700
S	2.16677600	-0.53429300	-0.50200900	S	2.12641200	-0.49424000	-0.53063300
C	2.95567300	-2.13597600	1.36136100	C	2.87206300	-2.31351400	1.14544600
H	0.98042500	-2.58429100	2.23527800	H	0.87497600	-2.84897200	1.91955600
C	3.46374900	-1.36385300	0.34020100	C	3.40179800	-1.42608500	0.23472400
H	3.58934300	-2.72523700	2.00968000	H	3.49247600	-2.97735700	1.73120700
Cl	0.11691000	1.42286700	2.70472800	Cl	0.33393300	1.14710700	2.64134000
Cl	1.49684200	5.59418700	-0.43716300	Cl	1.74896600	5.45062700	-0.30338900
H	-4.60788900	0.33818300	-0.35052400	H	-4.64597600	0.42652900	-0.37617400
N	-2.36894500	0.15018500	-0.05055800	N	-2.39740700	0.18243600	-0.08657600
C	-1.42909900	-3.40442300	0.55700800	C	-1.54041600	-3.42023600	0.33148200
H	-1.67550800	-3.68987100	1.58479100	H	-1.72665900	-3.74431100	1.36049800
H	-2.14991400	-3.90884200	-0.08439200	H	-2.31752300	-3.87207100	-0.28219400
H	-0.42190600	-3.76481500	0.33767500	H	-0.55977000	-3.79551900	0.03027400
C	4.80398500	-1.18587500	-0.05183700	C	4.74960700	-1.20722300	-0.10302100
C	5.95051500	-1.02658300	-0.40209700	C	5.90173500	-1.00474800	-0.40729600
C	7.33596100	-0.84900600	-0.80979600	C	7.29632000	-0.78404600	-0.75232200

C	8.31358000	-0.51266600	0.34342100	C	8.22305500	-0.50191800	0.45507700
C	7.99237400	-2.09983200	-1.44553200	C	7.99570600	-1.98992500	-1.42534000
H	7.37399200	-0.03134700	-1.54235000	H	7.35018800	0.07289800	-1.43752500
C	9.71190000	-0.76404100	-0.26090800	C	9.64611700	-0.68915300	-0.11340600
H	8.12053600	-1.19726700	1.17467000	H	8.01422300	-1.24319000	1.23232500
H	8.18016400	0.50381900	0.71839000	H	8.05354100	0.48548800	0.88826700
C	9.50377300	-1.78703100	-1.41899000	C	9.49745100	-1.64585900	-1.33630400
H	7.61025300	-2.30633300	-2.44703300	H	7.64693700	-2.15773400	-2.44591700
H	7.76369700	-2.96867000	-0.82125900	H	7.76766500	-2.89005100	-0.84650600
H	10.13139000	0.16757000	-0.64945000	H	10.05637900	0.27232000	-0.43276900
H	10.41050900	-1.13198300	0.49326700	H	10.32723400	-1.08693900	0.64152700
H	9.81826200	-1.35053800	-2.37055200	H	9.82491600	-1.14413300	-2.25061100
H	10.09540400	-2.69402600	-1.27923500	H	10.10794300	-2.54529700	-1.23455900
C	-7.08618300	-0.20297300	0.67167800	C	-7.04136800	-0.25223700	0.78126100
C	-6.81975700	-0.47619300	-1.74621500	C	-6.95947700	-0.14771700	-1.66266500
C	-8.56558600	-0.58446400	0.58712200	C	-8.53081800	-0.59889300	0.75100400
H	-6.98121800	0.89915200	0.62711300	H	-6.91255400	0.84192800	0.89738500
H	-6.65434000	-0.53798400	1.61641300	H	-6.54771800	-0.73831400	1.62466600
C	-8.29150600	-0.86563700	-1.89973900	C	-8.44777900	-0.48891600	-1.76043900
H	-6.70147900	0.61120700	-1.92444100	H	-6.83032500	0.95343500	-1.67621900
H	-6.20245300	-0.99959300	-2.47856200	H	-6.40858000	-0.55558200	-2.51210200
C	-9.14645200	-0.24158100	-0.79007400	C	-9.19934600	-0.02795800	-0.50551200
H	-9.11652900	-0.07035900	1.38075800	H	-9.01044000	-0.21604900	1.65690600
H	-8.65759700	-1.66023200	0.76894600	H	-8.63261800	-1.68898900	0.75952400
H	-8.64636800	-0.55288600	-2.88668400	H	-8.86693900	-0.02537900	-2.65871400
H	-8.36843800	-1.95692900	-1.85504500	H	-8.54838400	-1.57354100	-1.87146200
H	-10.18207200	-0.58621600	-0.86532000	H	-10.24921500	-0.33130100	-0.55397400
H	-9.16688900	0.84873700	-0.91563800	H	-9.18676100	1.06863800	-0.45711000
N	-6.33370100	-0.84423900	-0.41248200	N	-6.38761500	-0.72550700	-0.44479400
39							
C	0.61725400	3.09174500	1.19010400	C	0.77910000	2.92020000	1.17830000
C	0.16161000	1.77827000	1.25593100	C	0.26560000	1.62800000	1.22810000
C	-0.34679100	1.14396600	0.11706400	C	-0.38060000	1.07890000	0.11510000
C	-0.42816400	1.86123300	-1.07654100	C	-0.54030000	1.85680000	-1.03100000
C	0.00757800	3.17677500	-1.15515100	C	-0.04950000	3.15340000	-1.08990000
C	0.53676600	3.77562900	-0.01642100	C	0.61770000	3.66750000	0.01810000
H	1.01387700	3.57249100	2.07298200	H	1.28530000	3.33580000	2.03780000

H	-0.84003000	1.36614100	-1.94671200	H	-1.05450000	1.42090000	-1.87770000
H	-0.05389100	3.72678700	-2.08435900	H	-0.16970000	3.75340000	-1.98150000
N	-0.82878300	-0.19518000	0.14816100	N	-0.89780000	-0.24370000	0.12100000
C	-0.12923400	-1.37613100	0.32189500	C	-0.21890000	-1.44250000	0.23790000
C	-1.07002700	-2.39952400	0.27153500	C	-1.18220000	-2.44390000	0.17650000
C	-2.30370300	-1.73162500	0.06228900	C	-2.40530000	-1.74600000	0.01650000
C	-3.65940000	-2.35390200	-0.07512100	C	-3.77710000	-2.33430000	-0.10560000
O	-3.82081000	-3.55840800	-0.02507200	O	-3.97370000	-3.53290000	-0.03980000
N	-4.65052600	-1.42477700	-0.25708900	N	-4.73340000	-1.37460000	-0.29600000
C	1.31423300	-1.46011000	0.48025100	C	1.22200000	-1.55720000	0.36220000
C	2.00249300	-2.27375200	1.35025600	C	1.90630000	-2.46410000	1.13830000
S	2.43097200	-0.57404500	-0.53734000	S	2.33860000	-0.56040000	-0.54730000
C	3.40842800	-2.18889500	1.22244500	C	3.31210000	-2.36490000	1.02460000
H	1.50282000	-2.89838300	2.07778000	H	1.40140000	-3.16200000	1.79120000
C	3.81902600	-1.30756300	0.24687000	C	3.72340000	-1.37870000	0.15530000
H	4.10906600	-2.74390300	1.83084600	H	4.01310000	-2.98270000	1.56860000
Cl	0.21081000	0.95825800	2.79573200	Cl	0.43220000	0.72140000	2.70960000
Cl	1.10664700	5.43242500	-0.09502400	Cl	1.26410000	5.29720000	-0.04060000
H	-4.37680300	-0.44866100	-0.25818600	H	-4.42510000	-0.41000000	-0.28460000
N	-2.14748800	-0.41119800	-0.01775700	N	-2.22400000	-0.42590000	-0.02390000
C	-0.82356200	-3.87305100	0.36685200	C	-0.96380000	-3.92300000	0.22170000
H	-1.02248700	-4.24334400	1.37775500	H	-1.08030000	-4.30690000	1.24040000
H	-1.49620900	-4.41290000	-0.29752900	H	-1.70620000	-4.43210000	-0.39010000
H	0.21299700	-4.10949700	0.11767000	H	0.04220000	-4.17510000	-0.12160000
C	5.12801100	-0.96371000	-0.14028000	C	5.03220000	-0.99180000	-0.18490000
C	6.24720800	-0.66212300	-0.48528700	C	6.14930000	-0.64560000	-0.49020000
C	-6.87161300	-1.28213100	0.66264300	C	-6.88250000	-1.09860000	0.71940000
C	-6.60284900	-1.35762200	-1.66205800	C	-6.72060000	-1.15780000	-1.60420000
H	-6.32288300	-1.21939900	1.60259700	H	-6.31180000	-1.13970000	1.64730000
H	-7.68309700	-2.00474000	0.79634100	H	-7.77700000	-1.71640000	0.84410000
C	-7.25519300	0.02135900	-1.39485500	C	-7.16390000	0.29230000	-1.29170000
H	-7.36915000	-2.09215900	-1.93022400	H	-7.59220000	-1.78350000	-1.81980000
H	-5.85420700	-1.35233600	-2.45465000	H	-6.02750000	-1.24370000	-2.44110000
H	-8.22287200	0.08507400	-1.89865600	H	-8.13170000	0.50350000	-1.75270000
C	-7.43717500	0.07129000	0.16578300	C	-7.27270000	0.33220000	0.27570000
C	-6.68630300	1.34334800	0.63302600	C	-6.32510000	1.46960000	0.73180000
C	-6.65528800	2.25362500	-0.60472400	C	-6.21290000	2.39350000	-0.49080000

H	-5.66172600	1.09514200	0.93262700	H	-5.33700000	1.07050000	0.98490000
H	-7.16047900	1.81067600	1.49958600	H	-6.69130000	1.98120000	1.62510000
C	-6.40581500	1.26594200	-1.75530700	C	-6.15860000	1.40860000	-1.66910000
H	-7.62815600	2.74122600	-0.73507800	H	-7.10980000	3.01840000	-0.56940000
H	-5.90082400	3.04221800	-0.54130000	H	-5.34930000	3.06230000	-0.44730000
H	-6.66187200	1.67331600	-2.73657300	H	-6.39550000	1.87270000	-2.62950000
H	-5.34170700	1.00554700	-1.79150200	H	-5.14680000	0.99890000	-1.76150000
H	-8.49448000	0.15747300	0.42829700	H	-8.29420000	0.56320000	0.58690000
C	7.60167700	-0.31221000	-0.88551900	C	7.50490000	-0.25040000	-0.83510000
C	8.48915200	0.25436000	0.25049800	C	8.34990000	0.26790000	0.35380000
C	8.45093400	-1.49727700	-1.40863800	C	8.38930000	-1.39330000	-1.39000000
H	7.53816100	0.44254400	-1.68108300	H	7.45030000	0.54350000	-1.59230000
C	9.92411700	0.16803300	-0.31246000	C	9.79710000	0.24990000	-0.18200000
H	8.37778200	-0.38493900	1.13128900	H	8.23580000	-0.42880000	1.18970000
H	8.19778700	1.26558400	0.54066400	H	8.02520000	1.25140000	0.69840000
C	9.89900100	-0.96280600	-1.38560500	C	9.82390000	-0.82920000	-1.30790000
H	8.12957100	-1.83548800	-2.39554000	H	8.09680000	-1.69470000	-2.39740000
H	8.33613200	-2.33920600	-0.71953100	H	8.27660000	-2.26560000	-0.73910000
H	10.21074600	1.11827200	-0.77043000	H	10.06140000	1.22890000	-0.59030000
H	10.65023300	-0.03053000	0.47845500	H	10.51440000	0.03610000	0.61290000
H	10.17156600	-0.56126400	-2.36506800	H	10.10740000	-0.37480000	-2.26080000
H	10.61308700	-1.75825300	-1.16300100	H	10.55130000	-1.61820000	-1.10660000
N	-5.98648700	-1.80826700	-0.39736400	N	-6.09310000	-1.69540000	-0.37950000
40							
C	0.39147800	3.48388900	0.95586400	C	0.61270000	3.29010000	1.00830000
C	-0.18073700	2.22537800	1.11663100	C	-0.03330000	2.06320000	1.12330000
C	-0.71943900	1.54393300	0.01973900	C	-0.69670000	1.50580000	0.02460000
C	-0.71200700	2.16238500	-1.23052300	C	-0.73790000	2.21360000	-1.17590000
C	-0.15923400	3.42360000	-1.40465900	C	-0.11330000	3.44640000	-1.30130000
C	0.39762900	4.06789000	-0.30458500	C	0.56760000	3.96650000	-0.20460000
H	0.81057600	4.00117100	1.80714100	H	1.13120000	3.71150000	1.85750000
H	-1.14917500	1.63373500	-2.06798000	H	-1.26750000	1.77390000	-2.01110000
H	-0.15255700	3.89671400	-2.37719100	H	-0.14180000	3.99160000	-2.23480000
N	-1.31934700	0.25900600	0.14647600	N	-1.34300000	0.24310000	0.09680000
C	-0.73199200	-0.95882400	0.44091900	C	-0.78530000	-1.00370000	0.31370000
C	-1.75835800	-1.89750800	0.44383300	C	-1.83710000	-1.91210000	0.28040000
C	-2.92154100	-1.14538500	0.13754700	C	-2.98250000	-1.11370000	0.03150000

C	-4.32142400	-1.65822700	0.00584200	C	-4.39430000	-1.58590000	-0.10100000
O	-4.59377700	-2.83303800	0.17072300	O	-4.70020000	-2.75230000	0.06710000
N	-5.22216500	-0.67708300	-0.31499800	N	-5.26870000	-0.58310000	-0.42910000
C	0.69395600	-1.15367800	0.65205200	C	0.63390000	-1.24350000	0.49790000
C	1.28593600	-1.94648000	1.60786300	C	1.20500000	-2.15070000	1.36020000
S	1.90929700	-0.45820500	-0.40001200	S	1.86700000	-0.42690000	-0.44030000
C	2.69656600	-1.99559000	1.51726300	C	2.61660000	-2.19370000	1.28920000
H	0.71541200	-2.46068700	2.36894200	H	0.61660000	-2.74720000	2.04300000
C	3.20719800	-1.24006300	0.48518300	C	3.14560000	-1.31790000	0.36700000
H	3.33019700	-2.55551100	2.19112600	H	3.23890000	-2.83270000	1.90000000
Cl	-0.23772500	1.53769500	2.71969900	Cl	-0.00860000	1.24970000	2.66680000
Cl	1.11466200	5.65610300	-0.50295700	Cl	1.38200000	5.51370000	-0.34610000
H	-4.88241800	0.27851300	-0.39246100	H	-4.92270000	0.37390000	-0.41830000
N	-2.64650600	0.14464200	-0.04638100	N	-2.67500000	0.17780000	-0.08540000
C	-1.64620200	-3.37324200	0.66889800	C	-1.76080000	-3.39890000	0.42530000
H	-1.90541000	-3.63767700	1.69914900	H	-1.96110000	-3.70440000	1.45730000
H	-2.34484300	-3.90849500	0.02796500	H	-2.51750000	-3.87810000	-0.19310000
H	-0.62806000	-3.71804600	0.47674600	H	-0.76780000	-3.76220000	0.15090000
C	4.55061300	-1.04621800	0.11074300	C	4.49510000	-1.08290000	0.04580000
C	5.69875700	-0.87034500	-0.22580700	C	5.64740000	-0.86360000	-0.24530000
C	-7.36951400	-0.28896300	0.59494200	C	-7.32420000	-0.32640000	0.71420000
C	-7.04866400	-0.61538100	-1.80965000	C	-7.20360000	-0.26920000	-1.72960000
C	-8.83881500	-0.70320000	0.49068900	C	-8.80620000	-0.70200000	0.66680000
H	-7.28611200	0.81369500	0.52516100	H	-7.21780000	0.77210000	0.81010000
H	-6.95017600	-0.59175100	1.55604200	H	-6.83570000	-0.78610000	1.57520000
C	-8.50876700	-1.03905900	-1.98260700	C	-8.68340000	-0.64060000	-1.84470000
H	-6.94895900	0.46960100	-2.01234500	H	-7.09480000	0.83370000	-1.76330000
H	-6.40612200	-1.14341800	-2.51651500	H	-6.63110000	-0.68340000	-2.56150000
C	-9.39860100	-0.40627400	-0.90578700	C	-9.46440000	-0.16920000	-0.61180000
H	-9.41608600	-0.18147100	1.26027000	H	-9.30800000	-0.31030000	1.55680000
H	-8.91253800	-1.77588700	0.69734700	H	-8.88770000	-1.79340000	0.69580000
H	-8.84983900	-0.75776400	-2.98377900	H	-9.09610000	-0.20300000	-2.75890000
H	-8.56432500	-2.13031800	-1.91261100	H	-8.76180000	-1.72890000	-1.93550000
H	-10.42519200	-0.77433500	-0.99287300	H	-10.50740000	-0.49360000	-0.67120000
H	-9.43887700	0.67998500	-1.05872500	H	-9.47340000	0.92820000	-0.58540000
N	-6.58234000	-0.94067000	-0.45790100	N	-6.64150000	-0.81170000	-0.49120000
C	7.09258600	-0.68345900	-0.61847300	C	7.04900000	-0.63440000	-0.57750000

C	8.02345300	-0.57195700	0.61449300	C	7.93270000	-0.58140000	0.69310000
C	7.57736100	-1.80743300	-1.56854500	C	7.58410000	-1.69900000	-1.56720000
H	7.15587200	0.26638700	-1.16884000	H	7.11860000	0.34490000	-1.07250000
C	9.48690200	-0.37587700	0.19652700	C	9.40480000	-0.33640000	0.33740000
H	7.92544300	-1.48832500	1.20817100	H	7.83260000	-1.53530000	1.22400000
H	7.68966500	0.25292800	1.24983900	H	7.56090000	0.19690000	1.36490000
C	9.04276300	-1.60442100	-1.97603100	C	9.05790000	-1.44750000	-1.91170000
H	7.46294100	-2.76924000	-1.05534600	H	7.47350000	-2.68700000	-1.10550000
H	6.93246600	-1.84226800	-2.45082800	H	6.96880000	-1.70010000	-2.47090000
C	9.96203700	-1.48441100	-0.75282700	C	9.92970000	-1.38770000	-0.65000000
H	10.12206700	-0.33964300	1.08713000	H	10.00970000	-0.33330000	1.24940000
H	9.59369100	0.59704400	-0.30046500	H	9.50660000	0.66120000	-0.10920000
H	9.36526000	-2.43285200	-2.61446300	H	9.41790000	-2.22880000	-2.58800000
H	9.12685200	-0.69382000	-2.58332000	H	9.14430000	-0.49810000	-2.45590000
H	10.99198000	-1.29425700	-1.07068700	H	10.96910000	-1.17260000	-0.91650000
H	9.97267600	-2.44075200	-0.21439500	H	9.92610000	-2.37150000	-0.16350000
41							
C	0.27674100	3.14651800	1.22093000	C	0.43890000	2.96880000	1.23980000
C	-0.16252900	1.82795100	1.29564500	C	-0.05850000	1.67020000	1.28690000
C	-0.63625100	1.17046900	0.15495000	C	-0.66660000	1.10290000	0.16160000
C	-0.70000700	1.86938400	-1.05054600	C	-0.80520000	1.86890000	-0.99520000
C	-0.28035300	3.18955800	-1.13849800	C	-0.33030000	3.17150000	-1.05210000
C	0.21457000	3.81190000	0.00303700	C	0.29940000	3.70400000	0.06910000
H	0.64659600	3.64529100	2.10542700	H	0.91590000	3.39850000	2.10900000
H	-1.08518200	1.35624000	-1.92248100	H	-1.29020000	1.41880000	-1.85170000
H	-0.32798800	3.72530600	-2.07680700	H	-0.43410000	3.76220000	-1.95200000
N	-1.10085800	-0.17458100	0.19471500	N	-1.16610000	-0.22640000	0.16530000
C	-0.38975600	-1.34320500	0.40177800	C	-0.47480000	-1.41490000	0.31090000
C	-1.31543300	-2.37999000	0.34511300	C	-1.42260000	-2.42980000	0.23210000
C	-2.55276800	-1.73212900	0.09793800	C	-2.65010000	-1.74980000	0.03310000
C	-3.89643200	-2.37493100	-0.06120600	C	-4.01010000	-2.35770000	-0.12100000
O	-4.04296000	-3.58060200	0.00434400	O	-4.19210000	-3.55840000	-0.05220000
N	-4.89532600	-1.46254400	-0.28143100	N	-4.97410000	-1.41240000	-0.34290000
C	1.05074800	-1.40528000	0.59376400	C	0.96360000	-1.50900000	0.47540000
C	1.72994300	-2.19804300	1.48976900	C	1.63830000	-2.40080000	1.27690000
S	2.17841500	-0.51787800	-0.41054500	S	2.09140000	-0.50430000	-0.41120000
C	3.13723100	-2.09637000	1.39177500	C	3.04540000	-2.28380000	1.20060000

H	1.22243100	-2.81966400	2.21443700	H	1.12500000	-3.10040000	1.92140000
C	3.55796900	-1.22274400	0.41377800	C	3.46710000	-1.29870000	0.33530000
H	3.83128600	-2.63413900	2.02279100	H	3.73930000	-2.88800000	1.76820000
Cl	-0.13728100	1.03077200	2.84794200	Cl	0.07970000	0.77850000	2.78040000
Cl	0.76364200	5.47512900	-0.08684200	Cl	0.92540000	5.34170000	0.01350000
H	-4.63463500	-0.48291900	-0.29287900	H	-4.67930000	-0.44370000	-0.33070000
N	-2.41238900	-0.41098100	0.00193200	N	-2.48540000	-0.42780000	-0.01390000
C	-1.05156000	-3.84848700	0.46756200	C	-1.18590000	-3.90540000	0.29600000
H	-1.26716400	-4.20668300	1.47940500	H	-1.32550000	-4.28240000	1.31440000
H	-1.70257600	-4.40702300	-0.20287400	H	-1.90420000	-4.42940000	-0.33180000
H	-0.00686200	-4.07443500	0.24396400	H	-0.16750000	-4.14660000	-0.01720000
C	4.87099800	-0.86722300	0.05036900	C	4.77980000	-0.89700000	0.02760000
C	5.99233000	-0.55246700	-0.27516400	C	5.89910000	-0.53410000	-0.24880000
C	-7.14032400	-1.33236200	0.58032000	C	-7.15420000	-1.15970000	0.61030000
C	-6.81310800	-1.45012500	-1.73522800	C	-6.92680000	-1.23270000	-1.70740000
H	-6.61585600	-1.24314600	1.53191800	H	-6.60910000	-1.18620000	1.55400000
H	-7.94490200	-2.06358600	0.70882700	H	-8.04310000	-1.78940000	0.71480000
C	-7.49120200	-0.07578300	-1.51194300	C	-7.39910000	0.21300000	-1.41790000
H	-7.56201500	-2.20091200	-2.00748800	H	-7.78310000	-1.87210000	-1.94270000
H	-6.04505200	-1.44955500	-2.50904100	H	-6.20930000	-1.31430000	-2.52400000
H	-8.44712200	-0.03627100	-2.04008100	H	-8.35640000	0.40720000	-1.90720000
C	-7.71190800	0.00271700	0.04254700	C	-7.55230000	0.26210000	0.14550000
C	-6.99006100	1.29431200	0.50177100	C	-6.63410000	1.41630000	0.61960000
C	-6.94179600	2.18020800	-0.75297800	C	-6.50080000	2.33320000	-0.60620000
H	-5.96965400	1.06665000	0.83045900	H	-5.64780000	1.03310000	0.90310000
H	-7.49123900	1.77189900	1.34728600	H	-7.03240000	1.92860000	1.49850000
C	-6.65081800	1.17352000	-1.87704400	C	-6.39960000	1.34110000	-1.77520000
H	-7.91788300	2.65111900	-0.91637800	H	-7.40400000	2.94450000	-0.71420000
H	-6.20008600	2.98064800	-0.68746200	H	-5.64840000	3.01460000	-0.54350000
H	-6.88862700	1.55757600	-2.87220800	H	-6.61610000	1.79520000	-2.74520000
H	-5.58264100	0.92774200	-1.88237400	H	-5.37980000	0.94540000	-1.83640000
H	-8.77639900	0.07931600	0.27757600	H	-8.58520000	0.48050000	0.42650000
N	-6.22220100	-1.86679200	-0.44693200	N	-6.32630000	-1.75280000	-0.46180000
C	7.35670900	-0.19782400	-0.65541100	C	7.26420000	-0.13260000	-0.56890000
C	8.28420400	-0.09087100	0.58050300	C	8.19160000	-0.24250000	0.66630000
C	7.94080100	-1.19050600	-1.69191600	C	7.83870000	-0.94880000	-1.75350000
H	7.32005300	0.79360100	-1.12962700	H	7.23940000	0.92350000	-0.87360000

C	9.71692600	0.28161300	0.17633300	C	9.62520000	0.18470000	0.32550000
H	8.28311500	-1.05599000	1.10043300	H	8.18630000	-1.28300000	1.01140000
H	7.87677000	0.64463200	1.27946900	H	7.78900000	0.36500000	1.48120000
C	9.37483400	-0.81160500	-2.08518600	C	9.27370000	-0.51680000	-2.08230000
H	7.92717500	-2.19604600	-1.25574800	H	7.82270000	-2.01060000	-1.48190000
H	7.29382400	-1.22029900	-2.57286300	H	7.18930000	-0.83420000	-2.62550000
C	10.28989000	-0.69666300	-0.85833800	C	10.18880000	-0.61900000	-0.85440000
H	10.35411700	0.31097900	1.06574500	H	10.26430000	0.06910000	1.20620000
H	9.72218900	1.29619800	-0.24268300	H	9.63240000	1.25260000	0.07150000
H	9.77138400	-1.55143000	-2.78754600	H	9.66480000	-1.12750000	-2.90190000
H	9.36238300	0.14750700	-2.61905400	H	9.26510000	0.52050000	-2.44130000
H	11.29269900	-0.38073700	-1.16255800	H	11.19700000	-0.27290000	-1.10220000
H	10.40066800	-1.68628900	-0.39683100	H	10.28040000	-1.67260000	-0.56090000
42							
C	-0.05582800	3.86671600	0.66823600	C	0.40870000	3.61780000	0.74260000
C	-0.50924200	2.58366900	0.96030200	C	-0.21520000	2.40740000	1.02760000
C	-0.91207000	1.72139000	-0.06536100	C	-0.71160000	1.60530000	-0.00590000
C	-0.89204600	2.18112000	-1.38219000	C	-0.61000000	2.05200000	-1.32260000
C	-0.45739500	3.46318200	-1.68865200	C	-0.00570000	3.26480000	-1.62170000
C	-0.03293200	4.29117500	-0.65436300	C	0.50880000	4.03140000	-0.58020000
H	0.25873600	4.52468600	1.46575100	H	0.79810000	4.22900000	1.54400000
H	-1.22482000	1.51201400	-2.16544600	H	-1.01180000	1.42520000	-2.10820000
H	-0.44019800	3.81309000	-2.71186700	H	0.07720000	3.60730000	-2.64410000
N	-1.38846400	0.40508500	0.19480600	N	-1.32950000	0.35120000	0.24580000
C	-0.70324600	-0.69896200	0.67050400	C	-0.77370000	-0.79490000	0.78400000
C	-1.62973200	-1.73374900	0.74272100	C	-1.78870000	-1.74430000	0.81310000
C	-2.84041700	-1.15166000	0.28659100	C	-2.91210000	-1.07310000	0.26630000
C	-4.17195100	-1.82227900	0.15355400	C	-4.28250000	-1.63470000	0.06510000
O	-4.33504000	-2.99091200	0.45220400	O	-4.57670000	-2.75720000	0.43370000
N	-5.14466500	-0.98833300	-0.33098900	N	-5.13300000	-0.76610000	-0.56680000
C	0.71918100	-0.71509000	0.97480400	C	0.61550000	-0.91890000	1.18490000
C	1.32524200	-1.31852300	2.05271700	C	1.09300000	-1.60290000	2.27940000
S	1.92215200	-0.02685300	-0.09489500	S	1.93700000	-0.24580000	0.25470000
C	2.73628800	-1.22650400	2.04061600	C	2.50240000	-1.58770000	2.38950000
H	0.76162700	-1.79411600	2.84337200	H	0.43670000	-2.07850000	2.99440000
C	3.23225500	-0.55094200	0.94774600	C	3.12240000	-0.88970000	1.37680000
H	3.37926300	-1.62898400	2.81112600	H	3.05700000	-2.05870000	3.18910000

Cl	-0.59283600	2.09327800	2.63322200	Cl	-0.37540000	1.92460000	2.69690000
Cl	0.53383800	5.91016200	-1.01865200	Cl	1.29480000	5.55830000	-0.93630000
H	-4.89749600	-0.01878600	-0.51395700	H	-4.81630000	0.18990000	-0.71350000
N	-2.68321800	0.12820800	-0.04612700	N	-2.62460000	0.18180000	-0.07830000
C	-1.38693000	-3.15091700	1.15943800	C	-1.69510000	-3.16460000	1.27280000
H	-1.68417700	-3.31395500	2.20036800	H	-2.02510000	-3.26400000	2.31180000
H	-1.98721900	-3.83095700	0.55731200	H	-2.34970000	-3.79820000	0.67720000
H	-0.32969700	-3.40721900	1.06483000	H	-0.66570000	-3.52400000	1.20770000
C	4.57130200	-0.26160100	0.62207600	C	4.49570000	-0.65940000	1.17520000
C	5.71847600	-0.01239500	0.33641400	C	5.66910000	-0.45080000	0.98110000
C	-7.37264300	-0.72141200	0.41308900	C	-7.32510000	-0.39230000	0.24130000
C	-6.87063200	-1.30626600	-1.91018900	C	-6.89090000	-0.82140000	-2.12880000
C	-8.78425200	-1.29901600	0.29031400	C	-8.77820000	-0.84620000	0.09300000
H	-7.39466200	0.36673100	0.20539100	H	-7.26060000	0.70710000	0.12100000
H	-6.98655500	-0.85681700	1.42494600	H	-6.94030000	-0.64340000	1.23130000
C	-8.26789100	-1.90056500	-2.09941200	C	-8.33320000	-1.28460000	-2.34360000
H	-6.86619100	-0.25018200	-2.24607100	H	-6.80750000	0.25640000	-2.37550000
H	-6.13587400	-1.84636800	-2.51000500	H	-6.20500000	-1.36400000	-2.78190000
C	-9.28183200	-1.23776400	-1.15895000	C	-9.27920000	-0.61640000	-1.33810000
H	-9.45748200	-0.75051000	0.95633400	H	-9.40080000	-0.31020000	0.81560000
H	-8.76427000	-2.33969200	0.62999900	H	-8.83420000	-1.91220000	0.33620000
H	-8.57151900	-1.78265200	-3.14424600	H	-8.63550000	-1.06170000	-3.37140000
H	-8.21949700	-2.97455200	-1.89196800	H	-8.37080000	-2.37160000	-2.21730000
H	-10.25946400	-1.72055000	-1.24875600	H	-10.29680000	-1.00020000	-1.45540000
H	-9.41963600	-0.18910700	-1.45271400	H	-9.32050000	0.46180000	-1.53980000
N	-6.46026700	-1.41091100	-0.50615700	N	-6.47980000	-1.07390000	-0.74640000
C	7.10117000	0.30248700	-0.00109000	C	7.08660000	-0.22030000	0.74100000
H	7.58829600	0.74335900	0.87649500	H	7.64150000	-0.48010000	1.65150000
H	7.09850100	1.09154700	-0.76474100	H	7.25080000	0.85360000	0.59010000
C	7.94896600	-0.86472200	-0.50184600	C	7.69070000	-0.98170000	-0.43690000
C	9.34189000	-0.74256900	-0.48714300	C	8.98630000	-0.65550000	-0.85040000
C	7.38139100	-2.03592500	-1.00361000	C	7.00720000	-1.99990000	-1.10020000
C	10.15094700	-1.76747600	-0.96848000	C	9.58820000	-1.33550000	-1.90440000
H	9.79735400	0.16143300	-0.09412900	H	9.52700000	0.13800000	-0.34310000
C	8.19047200	-3.06415700	-1.48538700	C	7.60890000	-2.68200000	-2.15780000
H	6.30321500	-2.14590800	-1.01024800	H	6.00090000	-2.25690000	-0.79100000
C	9.57627600	-2.93399900	-1.47061800	C	8.89930000	-2.35370000	-2.56310000

H	11.22951200	-1.65742600	-0.94716900	H	10.59280000	-1.06950000	-2.21380000
H	7.73391500	-3.96933500	-1.87022400	H	7.06420000	-3.47060000	-2.66500000
H	10.20458100	-3.73509700	-1.84308400	H	9.36530000	-2.88360000	-3.38600000
43							
C	1.57788000	3.40663100	0.89583200	C	1.77692900	3.22013200	0.93846900
C	0.85515500	2.23006900	1.06966800	C	0.98345200	2.08735800	1.08924100
C	0.24739800	1.60159800	-0.02266500	C	0.26507900	1.57604600	0.00296300
C	0.34116800	2.19316800	-1.28230200	C	0.32121800	2.23777800	-1.22275500
C	1.04553500	3.37441000	-1.46959300	C	1.09479300	3.37836000	-1.38448900
C	1.66688500	3.96435300	-0.37350500	C	1.82583300	3.85120300	-0.29858900
H	2.04870500	3.88348500	1.74367300	H	2.33629700	3.60604900	1.77857400
H	-0.15041600	1.70871400	-2.11631200	H	-0.25234900	1.83656800	-2.04831500
H	1.11829200	3.82709000	-2.44910500	H	1.14131400	3.88778000	-2.33724700
N	-0.50698600	0.40165500	0.11791400	N	-0.53361000	0.40598200	0.11349100
C	-0.07619500	-0.87352000	0.43885200	C	-0.13534900	-0.89134700	0.37916600
C	-1.20977900	-1.67959600	0.44712200	C	-1.29068300	-1.66456600	0.36680500
C	-2.26850900	-0.79527100	0.11650400	C	-2.32688200	-0.73961000	0.08030000
C	-3.71909200	-1.12756700	-0.02446500	C	-3.78431500	-1.03227400	-0.05590600
O	-4.14260400	-2.26337400	0.14299100	O	-4.23357600	-2.16258900	0.08231900
N	-4.49769700	-0.05640000	-0.35370500	N	-4.54401600	0.06275600	-0.34628000
C	1.31316900	-1.23866500	0.66788900	C	1.24250200	-1.29815500	0.58464000
C	1.79194400	-2.08677700	1.64093900	C	1.69029900	-2.24122900	1.48218000
S	2.61320500	-0.71032000	-0.37661300	S	2.56996800	-0.67332400	-0.36795000
C	3.18592200	-2.30816200	1.56854000	C	3.08483000	-2.46185900	1.42522800
H	1.15413500	-2.51748600	2.40023000	H	1.02818700	-2.73686100	2.17789100
C	3.79512900	-1.63239900	0.53423000	C	3.72247900	-1.68914400	0.47948900
H	3.73986000	-2.93326200	2.25516900	H	3.62003500	-3.15380900	2.06041000
Cl	0.70016900	1.58080000	2.68232800	Cl	0.89545300	1.33375700	2.66079200
Cl	2.57388600	5.44940600	-0.58830500	Cl	2.82613200	5.27945800	-0.48524200
H	-4.05462100	0.84524800	-0.45936300	H	-4.09165200	0.96190400	-0.42692700
N	-1.83555500	0.44792900	-0.08547100	N	-1.86144000	0.49914900	-0.07814900
C	-6.28666500	-0.91135900	-1.70023100	C	-6.35550300	-0.74347900	-1.68299700
C	-6.62520100	-0.42744800	0.68744200	C	-6.65025100	-0.32358700	0.72067600
C	-7.77478900	-0.69642800	-1.98567900	C	-7.84892300	-0.52641900	-1.93413600
H	-6.08281000	-1.97638400	-1.52031600	H	-6.14608700	-1.81104000	-1.52772900
H	-5.68245900	-0.59180800	-2.55271300	H	-5.76602900	-0.40359000	-2.53780300
C	-8.12147300	-0.20047400	0.46007300	C	-8.15066500	-0.09631800	0.52692300

H	-6.43874100	-1.46776100	0.98939800	H	-6.45414200	-1.37210500	0.98480100
H	-6.25424400	0.22569500	1.48088900	H	-6.26438500	0.30645500	1.52551600
C	-8.62323200	-1.00537000	-0.74556300	C	-8.66842800	-0.87938700	-0.68631300
H	-8.07423600	-1.32951400	-2.82697000	H	-8.16224500	-1.13366500	-2.78909900
H	-7.93222700	0.34499100	-2.28803600	H	-8.01652700	0.52404200	-2.19724500
H	-8.66877800	-0.47902700	1.36619500	H	-8.68048800	-0.39496200	1.43683100
H	-8.29705500	0.86729100	0.28751400	H	-8.33189400	0.97388200	0.37664600
H	-9.67820800	-0.78834400	-0.93917900	H	-9.73016400	-0.67365200	-0.85248300
H	-8.55624300	-2.07679200	-0.51879200	H	-8.57793100	-1.95458600	-0.48730500
N	-5.88597100	-0.09044400	-0.54310400	N	-5.93514500	0.05134700	-0.51393500
C	-1.28232900	-3.15356600	0.69862100	C	-1.39963400	-3.14337000	0.56434900
H	-2.04407000	-3.60834200	0.06759900	H	-2.20705000	-3.54644400	-0.04396400
H	-0.31640900	-3.62715400	0.51166800	H	-0.45860900	-3.63669600	0.31123000
C	5.15620300	-1.60827500	0.17883100	C	5.09185800	-1.63665200	0.16503100
C	6.32133300	-1.58291800	-0.13715900	C	6.26375500	-1.58038400	-0.11834400
C	7.73118500	-1.53769700	-0.49584800	C	7.68085000	-1.50379300	-0.43901300
H	8.34241200	-1.67316800	0.41122400	H	8.27091700	-1.73025600	0.46451700
H	7.97228200	-0.54077900	-0.89929300	H	7.93074400	-0.47138800	-0.73493500
H	-1.56884800	-3.36515000	1.73391000	H	-1.63964800	-3.38449600	1.60501100
O	8.03312700	-2.54333300	-1.45044100	O	8.00047700	-2.41171400	-1.48292500
C	9.39798300	-2.52728500	-1.82411500	C	9.37337800	-2.36483900	-1.82721100
H	10.05709300	-2.71186400	-0.96331400	H	10.01654300	-2.63590500	-0.97657900
H	9.53567400	-3.32495100	-2.55356400	H	9.52321400	-3.08799300	-2.62873800
H	9.68222000	-1.56933300	-2.28344300	H	9.67006700	-1.36769400	-2.18547800
44							
C	1.04952400	3.64758200	0.76828700	C	1.27755300	3.46698400	0.82505000
C	0.38841800	2.44543600	1.00198100	C	0.53915700	2.30662900	1.03454700
C	-0.13743200	1.70516900	-0.06244300	C	-0.11153700	1.67871700	-0.03311100
C	-0.02595000	2.20939500	-1.35808600	C	-0.04543300	2.25125900	-1.30249100
C	0.61723400	3.41409200	-1.60624800	C	0.67301000	3.41753800	-1.52408300
C	1.15855200	4.11715600	-0.53471900	C	1.33851600	4.00767400	-0.45356300
H	1.45744300	4.21122100	1.59521900	H	1.78508300	3.94331300	1.65156500
H	-0.45460800	1.63787500	-2.17144200	H	-0.56709400	1.76014200	-2.11377000
H	0.70422800	3.79893000	-2.61321500	H	0.72749600	3.85777200	-2.51031500
N	-0.82754500	0.47556400	0.13897400	N	-0.85190500	0.47808700	0.13855100
C	-0.33809700	-0.74579000	0.56723600	C	-0.39735900	-0.77242600	0.51522800
C	-1.42388500	-1.61482500	0.59550600	C	-1.50958600	-1.60658700	0.52088600

C	-2.51732300	-0.82038700	0.16481200	C	-2.58052600	-0.76339900	0.12914400
C	-3.94054200	-1.24650000	-0.00063200	C	-4.01436900	-1.14445500	-0.03583600
O	-4.30567100	-2.39067900	0.23391200	O	-4.40916400	-2.28505800	0.16845500
N	-4.76520500	-0.24854800	-0.43196400	N	-4.81846000	-0.11586300	-0.43080100
C	1.05970900	-1.01078900	0.87038800	C	0.99071900	-1.08707900	0.79856500
C	1.54732000	-1.76010900	1.91732700	C	1.45174300	-1.93571400	1.77967900
S	2.36788500	-0.47881100	-0.16216400	S	2.32001100	-0.46247600	-0.15180200
C	2.95345900	-1.90256700	1.91013400	C	2.85704400	-2.08352100	1.78806500
H	0.90564900	-2.17497500	2.68217200	H	0.78973600	-2.41408500	2.48746200
C	3.56359600	-1.26447800	0.85271700	C	3.48999700	-1.34893700	0.80939000
H	3.51452500	-2.44486500	2.65858300	H	3.40238900	-2.69647400	2.49203800
Cl	0.20519500	1.90480200	2.65131800	Cl	0.43323500	1.66676500	2.65466700
Cl	1.98760900	5.63451200	-0.82536000	Cl	2.26931100	5.47093300	-0.71418800
H	-4.36990500	0.66806100	-0.58693700	H	-4.41069500	0.79859700	-0.56151100
N	-2.14780400	0.42872700	-0.11264700	N	-2.17432000	0.48397700	-0.10601100
C	-6.45357300	-1.29780400	-1.77110800	C	-6.53180800	-1.11223300	-1.76877500
C	-6.90488100	-0.67027800	0.56395600	C	-6.94155800	-0.54149600	0.58655000
C	-7.94009500	-1.19020400	-2.11877800	C	-8.02369700	-0.99600100	-2.08701800
H	-6.19716900	-2.33415500	-1.50941500	H	-6.27278400	-2.15309500	-1.52968100
H	-5.83768200	-1.00334000	-2.62426300	H	-5.92827300	-0.80109100	-2.62472000
C	-8.40230300	-0.54735400	0.27305800	C	-8.44311600	-0.41137600	0.32435100
H	-6.67153500	-1.67450800	0.94505400	H	-6.70126800	-1.55650800	0.93238400
H	-6.59997100	0.05677800	1.32038700	H	-6.62078200	0.16375100	1.35683500
C	-8.81420900	-1.46166200	-0.88776400	C	-8.87137300	-1.30521100	-0.84645800
H	-8.17313600	-1.89621600	-2.92219400	H	-8.27126900	-1.67802400	-2.90642500
H	-8.14437900	-0.18306600	-2.49916200	H	-8.23583800	0.02260700	-2.43084600
H	-8.96554600	-0.79407800	1.17864100	H	-8.99157200	-0.67401000	1.23432500
H	-8.63112300	0.49382000	0.01942200	H	-8.67429700	0.63396400	0.09073100
H	-9.87198400	-1.32052600	-1.13017400	H	-9.93519700	-1.17066000	-1.06417100
H	-8.69561400	-2.50910300	-0.58334900	H	-8.73223000	-2.35713000	-0.56723400
N	-6.14158700	-0.37678400	-0.66305500	N	-6.19947600	-0.21543700	-0.64604100
C	-1.42279800	-3.06887800	0.95171700	C	-1.54893800	-3.07058900	0.82574000
H	-2.13511700	-3.61097900	0.33208200	H	-2.31047900	-3.56085700	0.22233100
H	-0.42585700	-3.49740900	0.83026100	H	-0.57453100	-3.52896500	0.64294100
C	4.93406100	-1.18308100	0.54488400	C	4.86604600	-1.24462400	0.53996900
C	6.10722700	-1.11078700	0.26818000	C	6.04355500	-1.14685000	0.29347100
C	7.52554300	-1.00268600	-0.04162700	C	7.46653500	-1.01525400	0.01873600

H	8.10670600	-1.04563900	0.89355100	H	8.03115400	-1.14252100	0.95695600
H	7.72415500	-0.01953100	-0.49785800	H	7.67315800	0.00504100	-0.34403200
H	-1.73337300	-3.22259600	1.99029500	H	-1.81549700	-3.24728300	1.87287700
O	7.92211000	-2.04461300	-0.91936900	O	7.87332200	-1.97752000	-0.94230400
C	9.30311800	-1.97841100	-1.25319200	C	9.25965100	-1.89122200	-1.25013100
H	9.91410100	-2.04097200	-0.33916300	H	9.85983600	-2.03966400	-0.33828500
H	9.52781700	-1.01314200	-1.73318500	H	9.49883600	-0.88967500	-1.64175900
C	9.61963500	-3.12930200	-2.18944800	C	9.57483300	-2.95965600	-2.28001500
H	10.67590200	-3.11388000	-2.47071100	H	10.63385800	-2.93312600	-2.54974000
H	9.40177800	-4.08418700	-1.70650300	H	9.33903600	-3.94885000	-1.88202500
H	9.01649800	-3.05889800	-3.09706900	H	8.97927300	-2.80218400	-3.18168600
45							
C	0.66705200	3.71771000	0.80575500	C	0.90290000	3.53920000	0.86120000
C	0.02988300	2.50163500	1.03383600	C	0.18750000	2.36340000	1.06400000
C	-0.46190000	1.74558500	-0.03576200	C	-0.43410000	1.71820000	-0.01070000
C	-0.34135300	2.24747000	-1.33150500	C	-0.36290000	2.28860000	-1.28080000
C	0.27801100	3.46565100	-1.57435100	C	0.33260000	3.46990000	-1.49590000
C	0.78606500	4.18482800	-0.49724600	C	0.96970000	4.07760000	-0.41810000
H	1.04881200	4.29356700	1.63674800	H	1.38820000	4.02890000	1.69330000
H	-0.74380000	1.66324200	-2.14920900	H	-0.86210000	1.78370000	-2.09780000
H	0.37222200	3.84865800	-2.58136600	H	0.39110000	3.90850000	-2.48270000
N	-1.12665200	0.50115400	0.15963200	N	-1.15020000	0.50200000	0.15440000
C	-0.61604500	-0.70689500	0.60072400	C	-0.67350000	-0.73710000	0.54100000
C	-1.68180800	-1.60068800	0.61529000	C	-1.76720000	-1.59540000	0.53410000
C	-2.78621100	-0.83348500	0.16371700	C	-2.85090000	-0.77710000	0.12530000
C	-4.19628600	-1.29314400	-0.02277700	C	-4.27380000	-1.18970000	-0.05750000
O	-4.53931200	-2.44373900	0.21379600	O	-4.64680000	-2.33760000	0.14660000
N	-5.03587700	-0.31743600	-0.47576800	N	-5.09430000	-0.18040000	-0.46820000
C	0.78251900	-0.93829800	0.92707100	C	0.71710000	-1.02040000	0.84420000
C	1.27074000	-1.67089400	1.98543200	C	1.18300000	-1.85670000	1.83350000
S	2.09432000	-0.38167800	-0.08788300	S	2.04560000	-0.36850000	-0.08890000
C	2.67976900	-1.78106100	2.00086900	C	2.59100000	-1.97310000	1.86210000
H	0.62683300	-2.09652500	2.74246500	H	0.52190000	-2.34820000	2.53310000
C	3.29175200	-1.13446700	0.94972100	C	3.22140000	-1.22670000	0.89080000
H	3.24132600	-2.30657400	2.76083100	H	3.13990000	-2.57230000	2.57520000
Cl	-0.16725900	1.96312000	2.68226000	Cl	0.07330000	1.72560000	2.68440000
Cl	1.58490000	5.71966700	-0.78089400	Cl	1.87150000	5.56050000	-0.67020000

H	-4.65932700	0.60729800	-0.62915000	H	-4.70470000	0.74220000	-0.59700000
N	-2.44124500	0.42277800	-0.11310000	N	-2.46900000	0.47830000	-0.10810000
C	-6.67861500	-1.41428700	-1.83310800	C	-6.76850000	-1.21920000	-1.82330000
C	-7.18113100	-0.78011900	0.48963800	C	-7.22070000	-0.64700000	0.52390000
C	-8.16141100	-1.34295600	-2.20511700	C	-8.25840000	-1.13650000	-2.16110000
H	-6.40319900	-2.44261000	-1.55935600	H	-6.49040000	-2.25320000	-1.57600000
H	-6.05586300	-1.11227000	-2.67859800	H	-6.16080000	-0.89900000	-2.67290000
C	-8.67613600	-0.69346300	0.17420600	C	-8.72120000	-0.55040000	0.24190000
H	-6.93111500	-1.77590000	0.88215700	H	-6.96310000	-1.65500000	0.87760000
H	-6.90494600	-0.04071600	1.24514400	H	-6.92520000	0.06840000	1.29490000
C	-9.04872500	-1.62523800	-0.98602900	C	-9.11510000	-1.45840000	-0.93010000
H	-8.36557400	-2.05993700	-3.00667800	H	-8.48070000	-1.82730000	-2.98040000
H	-8.38229600	-0.34353100	-2.59642100	H	-8.48790000	-0.12420000	-2.51240000
H	-9.24801800	-0.94640300	1.07263300	H	-9.27560000	-0.82090000	1.14600000
H	-8.92438600	0.34038500	-0.09086300	H	-8.97180000	0.48860000	0.00050000
H	-10.10542100	-1.50989200	-1.24615300	H	-10.17870000	-1.34780000	-1.16200000
H	-8.91137600	-2.66749400	-0.67185500	H	-8.95700000	-2.50590000	-0.64420000
N	-6.40521600	-0.47833000	-0.72740800	N	-6.47000000	-0.31050000	-0.70070000
C	-1.65269200	-3.05297300	0.97766500	C	-1.77870000	-3.05920000	0.84250000
H	-2.34275400	-3.61380500	0.34955600	H	-2.52210000	-3.56730000	0.23130000
H	-0.64433900	-3.45870000	0.87308700	H	-0.79240000	-3.49680000	0.67280000
C	4.66464400	-1.02348500	0.66238200	C	4.59840000	-1.09250000	0.64010000
C	5.84047900	-0.92806700	0.40445900	C	5.77720000	-0.97120000	0.41090000
C	7.26042900	-0.78659300	0.11243500	C	7.20020000	-0.80550000	0.15200000
H	7.82562400	-0.76960100	1.05814200	H	7.75090000	-0.85390000	1.10570000
H	7.42589000	0.18296300	-0.37910500	H	7.36910000	0.19730000	-0.26670000
H	-1.97536200	-3.20975900	2.01207800	H	-2.05400000	-3.23910000	1.88680000
O	7.69943300	-1.86357400	-0.70239700	O	7.65170000	-1.82180000	-0.73200000
C	9.11666000	-1.90613000	-0.92064000	C	9.07320000	-1.86730000	-0.91440000
H	9.62228200	-1.71707700	0.03971900	H	9.55720000	-1.80410000	0.07390000
C	9.56464600	-0.85564300	-1.93913200	C	9.56870000	-0.71620000	-1.79180000
H	10.64215200	-0.92591600	-2.11211800	H	10.64530000	-0.80220000	-1.96250000
H	9.04958200	-1.01395400	-2.89040300	H	9.05870000	-0.74320000	-2.75840000
H	9.35287600	0.16122300	-1.59961900	H	9.38450000	0.25790000	-1.33240000
C	9.42688700	-3.32557100	-1.37673000	C	9.36520000	-3.22900000	-1.52890000
H	9.09607100	-4.04565500	-0.62612700	H	8.99180000	-4.02300000	-0.87990000
H	8.90384000	-3.54211000	-2.31184200	H	8.86510000	-3.31440000	-2.49710000

H	10.49987800	-3.45462500	-1.54026400	H	10.43940000	-3.36590000	-1.67640000
46							
C	0.59502500	3.76163500	0.74388500	C	0.83430000	3.58940000	0.79610000
C	-0.01562600	2.53410200	0.98312000	C	0.14400000	2.40090000	1.01190000
C	-0.52050500	1.77317500	-0.07690700	C	-0.48990000	1.74710000	-0.05040000
C	-0.44089900	2.28168500	-1.37325800	C	-0.45720000	2.32160000	-1.32020000
C	0.15114700	3.51121400	-1.62670100	C	0.21250000	3.51540000	-1.54780000
C	0.67369800	4.23522400	-0.55980100	C	0.86310000	4.13170000	-0.48290000
H	0.98741900	4.34107400	1.56740000	H	1.32950000	4.08570000	1.61830000
H	-0.85391100	1.69358600	-2.18288100	H	-0.96610000	1.81010000	-2.12700000
H	0.21331300	3.89949200	-2.63419300	H	0.24080000	3.95740000	-2.53430000
N	-1.15853600	0.51668000	0.12967900	N	-1.18060000	0.51810000	0.12710000
C	-0.61689300	-0.68305900	0.55635400	C	-0.67410000	-0.71300000	0.50170000
C	-1.66580400	-1.59591600	0.59096000	C	-1.75210000	-1.59090000	0.51390000
C	-2.79323700	-0.84782700	0.16490100	C	-2.85810000	-0.79170000	0.12750000
C	-4.19831600	-1.33266600	0.00719300	C	-4.27640000	-1.22990000	-0.02900000
O	-4.51483600	-2.49043200	0.24579000	O	-4.62390000	-2.38550000	0.17690000
N	-5.06549700	-0.37066700	-0.42265400	N	-5.12360000	-0.23420000	-0.41840000
C	0.79224000	-0.88991800	0.85251400	C	0.72680000	-0.97180000	0.77800000
C	1.31712500	-1.60769300	1.90281300	C	1.22740000	-1.79600000	1.75990000
S	2.07217100	-0.31521900	-0.19397600	S	2.02590000	-0.29700000	-0.18130000
C	2.72845000	-1.69193800	1.88850600	C	2.63820000	-1.88510000	1.76320000
H	0.69793000	-2.04031000	2.67640800	H	0.58910000	-2.29770000	2.47340000
C	3.30575000	-1.04041500	0.82126100	C	3.23620000	-1.12970000	0.77890000
H	3.31597500	-2.20227100	2.63909900	H	3.21160000	-2.47100000	2.46790000
Cl	-0.16384500	1.98781800	2.63400500	Cl	0.07650000	1.75870000	2.63300000
Cl	1.43905100	5.78444500	-0.85735400	Cl	1.73310000	5.63060000	-0.75140000
H	-4.70941200	0.56153600	-0.57967800	H	-4.75380000	0.69610000	-0.55020000
N	-2.47702700	0.41509800	-0.11584400	N	-2.50360000	0.47080000	-0.11070000
C	-6.71777300	-1.49190500	-1.74818700	C	-6.80540000	-1.29820000	-1.74420000
C	-7.18007400	-0.87634700	0.58786200	C	-7.22050000	-0.74440000	0.61420000
C	-8.20953000	-1.44611700	-2.08698000	C	-8.30300000	-1.24180000	-2.05150000
H	-6.41773900	-2.51613100	-1.48514900	H	-6.50310000	-2.32780000	-1.50740000
H	-6.11954300	-1.17518000	-2.60592400	H	-6.22100000	-0.96300000	-2.60450000
C	-8.68301200	-0.81555700	0.30593000	C	-8.72790000	-0.67470000	0.36300000
H	-6.90347300	-1.86900700	0.97033700	H	-6.93700000	-1.74890000	0.95810000
H	-6.90058200	-0.13512300	1.34035400	H	-6.92270000	-0.02680000	1.38230000

C	-9.06432900	-1.74934000	-0.84983100	C	-9.12840000	-1.58500000	-0.80490000
H	-8.41843500	-2.16348000	-2.88698400	H	-8.52910000	-1.93310000	-2.86940000
H	-8.45710900	-0.44931200	-2.46887800	H	-8.55840000	-0.23250000	-2.39330000
H	-9.23020100	-1.08235800	1.21565200	H	-9.25870000	-0.95930000	1.27690000
H	-8.95568000	0.21465100	0.05087600	H	-9.00260000	0.36050000	0.13150000
H	-10.12844400	-1.65218800	-1.08604500	H	-10.19840000	-1.49340000	-1.01480000
H	-8.90123100	-2.79016600	-0.54331800	H	-8.94500000	-2.63050000	-0.52710000
N	-6.43690700	-0.55558500	-0.64469900	N	-6.50100000	-0.38880000	-0.62370000
C	-1.60257200	-3.04807500	0.94936400	C	-1.73100000	-3.05490000	0.82030000
H	-2.29084700	-3.62141700	0.33057500	H	-2.47410000	-3.57650000	0.22010000
H	-0.58799800	-3.43331200	0.82868600	H	-0.73930000	-3.47340000	0.63470000
C	4.67053900	-0.90819900	0.50248300	C	4.60620000	-0.97170000	0.50100000
C	5.84127500	-0.79508500	0.22665400	C	5.78050000	-0.83020000	0.25810000
C	7.25126100	-0.65299400	-0.12133900	C	7.19470000	-0.66440000	-0.05670000
H	7.80730700	-0.36916900	0.77838200	H	7.73840000	-0.45330000	0.87010000
H	7.35235600	0.19438600	-0.82558800	H	7.30710000	0.23460000	-0.69210000
H	-1.90627500	-3.21336000	1.98815300	H	-1.98640000	-3.24130000	1.86850000
C	9.15644700	-1.76564600	-1.23068400	C	9.10280000	-1.68910000	-1.24090000
H	9.20587000	-0.89109000	-1.90725100	H	9.14370000	-0.78440000	-1.87760000
C	9.45978800	-3.02021400	-2.05122500	C	9.42880000	-2.90290000	-2.11250000
H	10.45701600	-2.96356900	-2.49393900	H	10.42750000	-2.81200000	-2.54630000
H	9.41060000	-3.90901100	-1.41629800	H	9.38950000	-3.81690000	-1.51370000
H	8.73941100	-3.14334300	-2.86623000	H	8.71420000	-3.00280000	-2.93570000
C	10.19885300	-1.56632400	-0.12559900	C	10.13670000	-1.52630000	-0.12200000
H	10.02777200	-0.64703800	0.43998400	H	9.95970000	-0.62750000	0.47360000
H	10.16832200	-2.40637500	0.57365100	H	10.10030000	-2.39140000	0.54580000
H	11.20254100	-1.50265400	-0.55439000	H	11.14310000	-1.44720000	-0.54140000
N	7.81000400	-1.90142700	-0.65494900	N	7.75700000	-1.87060000	-0.67740000
H	7.17808600	-2.24989400	-1.36903800	H	7.12610000	-2.17020000	-1.41410000
47							
C	1.20785700	3.63891900	0.82009400	C	1.47040000	3.43560000	0.87500000
C	0.54320900	2.43518800	1.03505600	C	0.71610000	2.28340000	1.07270000
C	-0.01451400	1.73022000	-0.03710100	C	0.04230000	1.68560000	0.00210000
C	0.06847000	2.27192800	-1.31973500	C	0.10140000	2.28070000	-1.25720000
C	0.71446100	3.47892000	-1.54851400	C	0.83530000	3.43960000	-1.46650000
C	1.28803500	4.14610000	-0.47081500	C	1.52380000	3.99900000	-0.39410000
H	1.64069100	4.17491300	1.65271900	H	1.99610000	3.88830000	1.70350000

H	-0.38512500	1.72788500	-2.13838900	H	-0.43860000	1.81320000	-2.07050000
H	0.77896500	3.89295100	-2.54555200	H	0.88390000	3.89750000	-2.44500000
N	-0.70871000	0.49993900	0.14485700	N	-0.71440000	0.49340000	0.16080000
C	-0.21864000	-0.73602000	0.52825600	C	-0.27440000	-0.77060000	0.50890000
C	-1.30939400	-1.59881500	0.55418900	C	-1.39910000	-1.58810000	0.51090000
C	-2.40606100	-0.78610800	0.16817900	C	-2.46130000	-0.72200000	0.14660000
C	-3.83485900	-1.19919600	0.01945300	C	-3.90230000	-1.07880000	-0.01020000
O	-4.20219600	-2.34784400	0.22742300	O	-4.31170000	-2.21750000	0.17510000
N	-4.66195700	-0.18434500	-0.36535000	N	-4.69530000	-0.03070000	-0.37530000
C	1.18331400	-1.01801800	0.79470900	C	1.11150000	-1.11100000	0.77130000
C	1.68890700	-1.79242700	1.81380800	C	1.57110000	-1.98280000	1.73200000
S	2.47341400	-0.47249400	-0.25489000	S	2.44110000	-0.48810000	-0.18160000
C	3.09394700	-1.94450600	1.77241000	C	2.97450000	-2.15170000	1.72230000
H	1.06143500	-2.21871400	2.58423600	H	0.91010000	-2.46350000	2.43930000
C	3.68614800	-1.28846500	0.71587400	C	3.60850000	-1.40930000	0.75030000
H	3.66688000	-2.50543200	2.49781100	H	3.51780000	-2.78440000	2.41030000
Cl	0.39570100	1.84870500	2.67222200	Cl	0.62010000	1.61580000	2.68210000
Cl	2.12143400	5.66543600	-0.73761100	Cl	2.47470000	5.45190000	-0.63990000
H	-4.26431400	0.73443500	-0.50020700	H	-4.27550000	0.88020000	-0.49180000
N	-2.03408600	0.46806400	-0.08173800	N	-2.03910000	0.52340000	-0.06980000
C	-6.38420800	-1.18390600	-1.69923300	C	-6.43700000	-0.97480000	-1.71470000
C	-6.78336500	-0.62296800	0.66207300	C	-6.81380000	-0.44610000	0.65590000
C	-7.87684700	-1.05760400	-2.01273000	C	-7.93020000	-0.83040000	-2.01470000
H	-6.12907400	-2.22897600	-1.47344500	H	-6.19090000	-2.02390000	-1.49930000
H	-5.78416000	-0.86794700	-2.55598400	H	-5.83780000	-0.65510000	-2.57060000
C	-8.28563400	-0.48283200	0.40598500	C	-8.31590000	-0.28880000	0.41240000
H	-6.54864900	-1.63932900	1.00864000	H	-6.58490000	-1.47130000	0.97860000
H	-6.45836900	0.07970300	1.43304500	H	-6.47470000	0.23870000	1.43670000
C	-8.72720400	-1.36013400	-0.77235800	C	-8.76950000	-1.15230000	-0.77160000
H	-8.13082600	-1.73831600	-2.83149700	H	-8.19630000	-1.49200000	-2.84490000
H	-8.08250900	-0.03855200	-2.35912100	H	-8.13080000	0.19790000	-2.33570000
H	-8.83175600	-0.75278300	1.31541800	H	-8.85880000	-0.56180000	1.32260000
H	-8.51287500	0.56666900	0.18773300	H	-8.53400000	0.76430000	0.20230000
H	-9.78880600	-1.20574000	-0.98853400	H	-9.83340000	-0.99790000	-0.97520000
H	-8.60914500	-2.41676800	-0.50132100	H	-8.64300000	-2.21160000	-0.51510000
N	-6.04360400	-0.29781800	-0.57135000	N	-6.07980000	-0.10590000	-0.57770000
C	-1.31049400	-3.06220500	0.87003300	C	-1.45710000	-3.05670000	0.78900000

H	-2.03390700	-3.58400500	0.24574100	H	-2.23150000	-3.52460000	0.18410000
H	-0.31721200	-3.49127400	0.72288100	H	-0.49120000	-3.52550000	0.58830000
C	5.05055000	-1.21010000	0.37784500	C	4.98260000	-1.32110000	0.46340000
C	6.22110200	-1.12997800	0.08395400	C	6.16100000	-1.22610000	0.21120000
C	7.64431400	-1.07290000	-0.29492700	C	7.58390000	-1.18040000	-0.16520000
H	8.25285600	-1.10135300	0.61551100	H	8.19040000	-1.46450000	0.70150000
H	7.84294500	-0.10643400	-0.77084300	H	7.85500000	-0.14760000	-0.40950000
H	-1.60725700	-3.24323300	1.90821100	H	-1.71620000	-3.24930000	1.83520000
N	8.11636000	-2.12833900	-1.19172000	N	7.96450000	-2.03400000	-1.29310000
C	8.05150800	-3.45560000	-0.59196900	C	7.78070000	-3.45360000	-1.01040000
H	8.59160900	-3.45620800	0.35856200	H	8.32190000	-3.72050000	-0.09880000
H	7.02191700	-3.80461000	-0.40426200	H	6.72300000	-3.73970000	-0.88080000
H	8.53928200	-4.17323700	-1.25615600	H	8.19650000	-4.04040000	-1.83310000
C	7.48644300	-2.08261200	-2.50574300	C	7.31920000	-1.63680000	-2.54000000
H	7.61694200	-1.08853300	-2.94158300	H	7.52410000	-0.58200000	-2.74110000
H	7.97631400	-2.80491500	-3.16330000	H	7.73510000	-2.22370000	-3.36260000
H	6.40749500	-2.31171800	-2.48549100	H	6.22530000	-1.78080000	-2.53080000
48							
C	-0.17877400	3.87165700	0.64690600	C	0.08949200	3.69343300	0.72300800
C	-0.76965700	2.64478400	0.93389400	C	-0.59021800	2.50704500	0.97969100
C	-1.18642800	1.79802800	-0.09899000	C	-1.13998800	1.76421000	-0.07077200
C	-1.03868000	2.21853000	-1.42062900	C	-1.03390500	2.24629900	-1.37450800
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C	-0.03062500	4.25713100	-0.67969300	C	0.19292300	4.14306300	-0.58783900
H	0.14480900	4.51828400	1.45008000	H	0.51908000	4.25937400	1.53712800
H	-1.38350000	1.56380000	-2.21080400	H	-1.47779900	1.66610500	-2.17317200
H	-0.34918100	3.76555400	-2.74966800	H	-0.28742100	3.80665300	-2.65716200
N	-1.80254400	0.53940100	0.15660000	N	-1.81718200	0.53486500	0.15197800
C	-1.25610500	-0.61188700	0.69559300	C	-1.31156500	-0.65450400	0.64376100
C	-2.28084100	-1.55166800	0.73422600	C	-2.37193800	-1.55355100	0.65829000
C	-3.40053200	-0.86804500	0.19447500	C	-3.46783400	-0.80868100	0.15265300
C	-4.78101800	-1.40487000	-0.00816500	C	-4.86654600	-1.28891300	-0.05192200
O	-5.07973600	-2.55250100	0.29358700	O	-5.20464800	-2.43292200	0.22266000
N	-5.64626300	-0.50162000	-0.55321800	N	-5.70624900	-0.34526400	-0.56627000
C	0.13820500	-0.75601900	1.08451400	C	0.07535600	-0.86110500	1.01761500
C	0.61846000	-1.39431900	2.20607100	C	0.53205900	-1.61009100	2.07902000
S	1.45992800	-0.20641600	0.07957000	S	1.41388500	-0.22070200	0.09181600

C	2.02908200	-1.43758300	2.27674400	C	1.94084300	-1.66850700	2.16749600
H	-0.03362700	-1.79871800	2.96761500	H	-0.13761800	-2.07941900	2.78553900
C	2.64946000	-0.83308700	1.20551100	C	2.58014500	-0.96397700	1.17087700
H	2.58485100	-1.88540100	3.08893700	H	2.48286400	-2.19621100	2.93980400
Cl	-1.00528300	2.20679100	2.60693400	Cl	-0.75139400	1.97918200	2.63530400
Cl	0.70988700	5.80524100	-1.03777700	Cl	1.04966100	5.63899500	-0.90808400
H	-5.30614900	0.42769900	-0.75606600	H	-5.34606600	0.58035500	-0.74821700
N	-3.10123300	0.38193700	-0.15425400	N	-3.12277600	0.44117900	-0.15550400
C	-7.18667800	-1.76068700	-1.88987900	C	-7.28732900	-1.54463200	-1.90051500
C	-7.80318900	-1.00107700	0.36694500	C	-7.85168300	-0.82073200	0.37965500
C	-8.65621400	-1.78331100	-2.31650500	C	-8.76469500	-1.54475800	-2.29780600
H	-6.87628300	-2.75502500	-1.53890100	H	-6.98215800	-2.54625200	-1.56695700
H	-6.54693000	-1.48541100	-2.73180000	H	-6.65857000	-1.26388100	-2.74876600
C	-9.28776800	-1.00567900	-0.00473400	C	-9.34248500	-0.80376600	0.03667600
H	-7.52369800	-1.95629000	0.83344900	H	-7.57167900	-1.78934800	0.81664800
H	-7.58886300	-0.20179700	1.08038600	H	-7.61288700	-0.03979900	1.10542900
C	-9.57487500	-2.02730400	-1.11246200	C	-9.65688500	-1.80932300	-1.07830700
H	-8.79807000	-2.55955500	-3.07514200	H	-8.92946300	-2.30158100	-3.07106000
H	-8.90664300	-0.82285000	-2.78075800	H	-9.01667300	-0.57052200	-2.73155000
H	-9.88084000	-1.22638000	0.88842200	H	-9.92166600	-1.02912500	0.93755000
H	-9.57196900	-0.00406200	-0.34635400	H	-9.62095600	0.20441900	-0.29005500
H	-10.62521400	-1.97880200	-1.41571500	H	-10.71383500	-1.75737500	-1.35640300
H	-9.40299500	-3.03938900	-0.72517300	H	-9.47232600	-2.82621800	-0.70991700
N	-6.99671100	-0.74303700	-0.84024700	N	-7.06618200	-0.54554500	-0.83836300
C	-2.20171700	-2.97391100	1.19478800	C	-2.34254000	-2.99134100	1.07020100
H	-2.83806000	-3.60719700	0.57895300	H	-3.04399600	-3.56913800	0.47149500
H	-1.17269500	-3.33731300	1.15841200	H	-1.33578800	-3.40209900	0.96662300
C	4.02582800	-0.67760300	0.95959000	C	3.95994700	-0.79154700	0.96405900
C	5.20438900	-0.54541400	0.73375200	C	5.14054300	-0.63728800	0.76761300
C	6.62455000	-0.35213200	0.49236200	C	6.56280500	-0.42531200	0.56175200
H	7.15846200	-0.29464500	1.45023400	H	7.08723500	-0.47095500	1.52603800
H	6.78384000	0.59678500	-0.03687400	H	6.72929900	0.57410500	0.13694100
H	-2.56190800	-3.07747700	2.22345000	H	-2.65035700	-3.10754800	2.11446200
O	7.12473900	-1.44091600	-0.28646800	O	7.06477000	-1.42941900	-0.32331000
C	8.45179300	-1.43513400	-0.62002900	C	8.39340000	-1.39450800	-0.64706500
C	9.36267300	-0.44042600	-0.25568400	C	9.30775400	-0.44869800	-0.17558000
C	8.88189200	-2.52750400	-1.38343300	C	8.82126200	-2.40290200	-1.51926400

C	10.69594000	-0.54906500	-0.65923500	C	10.64235900	-0.52226500	-0.58274500
H	9.05725600	0.41378300	0.33342800	H	9.00459400	0.34043400	0.49899800
C	10.20880500	-2.62040200	-1.77599400	C	10.14959800	-2.46204900	-1.91385800
H	8.15542600	-3.28454200	-1.65233900	H	8.09071400	-3.12212100	-1.86855100
C	11.12724800	-1.63072800	-1.41652500	C	11.07161300	-1.52087700	-1.44807200
H	11.39642600	0.22731000	-0.37218700	H	11.34571700	0.21531300	-0.21254500
H	10.53000300	-3.47091600	-2.36689200	H	10.46906400	-3.24746200	-2.58963500
H	12.16315000	-1.70616600	-1.72471700	H	12.10858500	-1.56945200	-1.75800000

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