

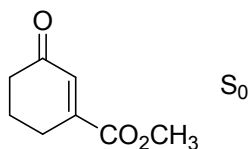
## Supplementary Information

### The chiral photocycloaddition of a cyclohexenone derivative with a chiral alkene. A DFT study

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Italy*

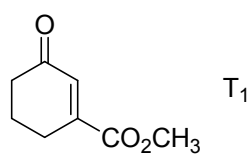
#### Z-matrix and Cartesian coordinates of optimized structures



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5346289		
3	3	C	2	1		1.5346867	111.4010855	
4	4	C	3	2	1	1.5120039	111.8897982	-48.6845679
5	5	C	4	3	2	1.3493757	122.5029850	21.0095127
6	6	C	5	4	3	1.4822391	122.4328824	3.5198268
7	7	O	6	5	4	1.2246937	120.6713075	178.6145444
8	8	C	4	3	2	1.5079783	116.2498479	-151.9239440
9	9	O	8	4	3	1.2118400	120.2802446	50.3458374
10	10	O	8	4	3	1.3516429	120.3425883	-131.0425792
11	11	C	10	8	4	1.4405780	122.7609728	13.7393541
12	12	H	1	6	5	1.1009727	106.8254721	91.1408017
13	13	H	1	6	5	1.0936011	108.1769546	-154.2390490
14	14	H	2	1	6	1.0973064	109.3243522	-66.9146327
15	15	H	2	1	6	1.0950674	110.3328749	175.8577819
16	16	H	3	2	1	1.0941706	111.0390262	-170.0933164
17	17	H	3	2	1	1.1017877	110.1388240	72.3660461
18	18	H	5	4	3	1.0864242	122.1973898	-176.7049334
19	19	H	11	10	8	1.0904273	105.1398516	155.4160140
20	20	H	11	10	8	1.0924512	111.6506665	36.5485808

21 21 H 11 10 8 1.0923394 110.8560454 -86.2331318

Row	Tag	Symbol	X	Y	Z
1	1	C	2.5445470	0.2523450	0.4711900
2	2	C	1.8506430	1.6023290	0.2450790
3	3	C	0.3560160	1.5276610	0.5853410
4	4	C	-0.3093140	0.3315430	-0.0571490
5	5	C	0.3850340	-0.7488830	-0.4711240
6	6	C	1.8460990	-0.8833340	-0.2607800
7	7	O	2.4400700	-1.8896280	-0.6274480
8	8	C	-1.7787820	0.4714590	-0.3655090
9	9	O	-2.1867490	1.4389210	-0.9706010
10	10	O	-2.6492340	-0.4937520	0.0054620
11	11	C	-2.3063250	-1.5357650	0.9392110
12	12	H	2.5323500	-0.0034830	1.5419580
13	13	H	3.5932940	0.2639100	0.1614170
14	14	H	1.9588640	1.8945120	-0.8070610
15	15	H	2.3331560	2.3829660	0.8425400
16	16	H	-0.1665810	2.4322340	0.2599960
17	17	H	0.2180760	1.4652380	1.6766760
18	18	H	-0.0907780	-1.5829310	-0.9793410
19	19	H	-3.2558030	-1.8576620	1.3680530
20	20	H	-1.6508320	-1.1671880	1.7316310
21	21	H	-1.8319510	-2.3760560	0.4272680

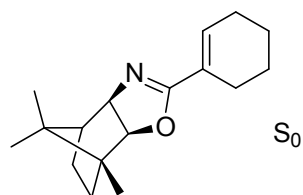


Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
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3	3	C	2	1		1.5335778	112.1612668	
4	4	C	3	2	1	1.5062254	111.0179617	-54.0232886

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6	6	C	5	4	3	1.3914647	121.5087428	-1.4632265
7	7	O	6	5	4	1.2963534	124.7597744	175.2754500
8	8	C	4	3	2	1.4575042	117.9377777	-150.9503456
9	9	O	8	4	3	1.2275727	124.2742516	-0.2180588
10	10	O	8	4	3	1.3652786	113.5233198	-179.8237245
11	11	C	10	8	4	1.4360351	115.6096674	179.6202212
12	12	H	1	2	3	1.0981508	111.6748239	-68.7140738
13	13	H	1	2	3	1.0941355	111.5352138	171.1310462
14	14	H	2	1	6	1.0961381	109.2428734	-71.4915267
15	15	H	2	1	6	1.0967804	108.0892213	172.1564197
16	16	H	3	2	1	1.0936406	111.0452953	-176.1285226
17	17	H	3	2	1	1.1018678	109.5420857	67.2981825
18	18	H	5	4	3	1.0833511	120.2392054	176.9570002
19	19	H	11	10	8	1.0931547	110.6561636	60.1492687
20	20	H	11	10	8	1.0931983	110.6614550	-60.7462311
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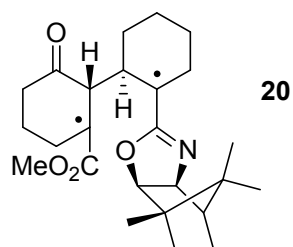
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3	3	C	-0.5940750	1.5998200	-0.2245850
4	4	C	0.1555400	0.3002050	-0.0911940
5	5	C	-0.5437290	-0.9153150	-0.0134210
6	6	C	-1.9345310	-0.9562900	-0.0262590
7	7	O	-2.6418010	-2.0425340	-0.0456330
8	8	C	1.6114340	0.3530190	-0.0475840
9	9	O	2.2680280	1.3879550	-0.1163340
10	10	O	2.1979310	-0.8741980	0.0705060
11	11	C	3.6334460	-0.8749740	0.1091450
12	12	H	-3.0903160	0.4668600	-1.1389240
13	13	H	-3.7054430	0.1707460	0.4904000
14	14	H	-1.8592680	1.4129020	1.5212050
15	15	H	-2.5483490	2.4248430	0.2494340

16	16	H	-0.0027940	2.4093680	0.2125290
17	17	H	-0.7109490	1.8537970	-1.2903940
18	18	H	-0.0037740	-1.8533710	0.0329380
19	19	H	3.9965900	-0.2941180	0.9610370
20	20	H	4.0443120	-0.4511780	-0.8110010
21	21	H	3.9199490	-1.9221550	0.2094280



Row	Tag	Symbol	X	Y	Z
1	1	C	3.5863020	0.1557640	-1.0307300
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3	3	C	1.1751390	0.2148570	-1.2230190
4	4	C	1.0963330	-1.2788850	-0.7779970
5	5	C	3.5305250	-1.3346980	-0.5557580
6	6	C	2.2249760	-1.3773910	0.2844310
7	7	C	2.2558650	0.0207480	0.9883260
8	8	C	3.5056280	0.2150930	1.8813360
9	9	C	1.0674810	0.3532630	1.9137280
10	10	C	2.3587410	2.3336300	-0.3257970
11	11	N	-0.2924550	-1.4746220	-0.3524230
12	12	O	-0.1593850	0.7168060	-0.9502800
13	13	C	-0.9008330	-0.3575770	-0.5144530
14	14	C	-2.3229280	-0.1215310	-0.2361470
15	15	C	-2.8663590	1.0970400	-0.4271750
16	16	C	-4.3068690	1.4248680	-0.1394860
17	17	C	-5.0113190	0.3349590	0.6828970
18	18	C	-4.6381910	-1.0598500	0.1645250
19	19	C	-3.1258430	-1.3033930	0.2704640
20	20	H	4.4984800	0.6582880	-0.6965710
21	21	H	3.5618440	0.2491220	-2.1223230

22	22	H	1.3480370	0.3796160	-2.2913960
23	23	H	1.2957300	-1.9896060	-1.5877170
24	24	H	4.4045010	-1.6007310	0.0441040
25	25	H	3.4957640	-2.0389450	-1.3931580
26	26	H	2.1319020	-2.2451430	0.9432610
27	27	H	3.4679050	-0.4860650	2.7232220
28	28	H	3.5135050	1.2253170	2.3056700
29	29	H	4.4605850	0.0668300	1.3759900
30	30	H	1.0702070	-0.3294720	2.7715350
31	31	H	0.0877140	0.2896980	1.4545020
32	32	H	1.1799820	1.3696580	2.3087210
33	33	H	1.4340870	2.7363980	0.0990140
34	34	H	2.4716320	2.7557540	-1.3317650
35	35	H	3.1998960	2.6923190	0.2779870
36	36	H	-2.2387000	1.8947670	-0.8157260
37	37	H	-4.8310170	1.5758470	-1.0968050
38	38	H	-4.3620620	2.3938060	0.3748720
39	39	H	-6.0968030	0.4853000	0.6556520
40	40	H	-4.7059240	0.4206540	1.7347520
41	41	H	-4.9490690	-1.1492330	-0.8858750
42	42	H	-5.1782160	-1.8355250	0.7196580
43	43	H	-2.8456860	-1.5055680	1.3141370
44	44	H	-2.8341530	-2.2002430	-0.2852490



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5451779		
3	3	C	2	1		1.5551447	112.3226384	
4	4	C	3	2	1	1.5004703	108.1469062	-49.0844361

5	5	C	4	3	2	1.5116068	114.0695847	64.1176768
6	6	C	1	2	3	1.5306854	111.8542744	46.8418580
7	7	C	5	4	3	2.5282444	106.0188537	124.6304859
8	8	C	7	5	4	1.5216050	35.4478190	115.2395476
9	9	O	6	1	2	1.2134044	122.7249980	121.6155742
10	10	C	7	5	4	1.5076868	116.8213650	-142.6665586
11	11	C	10	7	5	1.5378612	112.7539595	-12.7137230
12	12	C	11	10	7	1.5502163	112.5332865	-53.9906024
13	13	C	12	11	10	1.5430154	112.7116847	21.8385485
14	14	C	7	5	4	1.4192378	114.4078073	3.8826344
15	15	C	4	3	2	1.4645053	120.6305404	-93.4355662
16	16	O	15	4	3	1.2224770	125.4762617	144.5524343
17	17	O	15	4	3	1.3637225	112.0949526	-32.9732973
18	18	C	17	15	4	1.4365618	115.1101747	-179.7335978
19	19	O	14	7	5	1.3880530	117.0139068	-144.6341691
20	20	N	14	7	5	1.3053033	126.7150480	36.8895466
21	21	C	19	14	7	1.4460760	107.0533681	175.6334056
22	22	C	21	19	14	1.5508316	116.6455182	118.3967636
23	23	C	22	21	19	1.5626655	102.0893551	174.3283521
24	24	C	23	22	21	1.5649404	104.1422809	72.9882272
25	25	C	20	14	7	1.4593815	107.4259157	-177.2228927
26	26	C	24	23	22	1.5526410	102.7153339	-1.5272600
27	27	C	26	24	23	1.5646638	101.7313735	37.3726983
28	28	C	22	21	19	1.5223836	114.5737317	49.6950082
29	29	C	27	26	24	1.5417673	116.1337866	-179.0119884
30	30	C	27	26	24	1.5478053	112.8721504	60.2303865
31	31	H	1	6	9	1.0994421	107.8553457	-117.9625170
32	32	H	1	6	9	1.0929625	108.1957427	-1.2818948
33	33	H	2	1	6	1.0964259	108.8105602	-73.4603000
34	34	H	2	1	6	1.0963315	109.9199036	169.5484276
35	35	H	3	2	1	1.0914451	110.0138739	-171.2334865
36	36	H	3	2	1	1.0992089	109.0912058	70.3706298
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38	38	H	8	7	5	1.0912890	109.1968727	-117.5337670

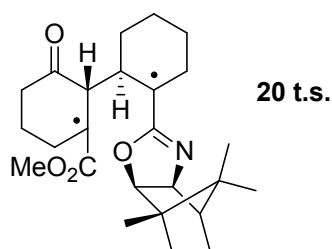
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41	41	H	11	10	7	1.0955783	109.3293838	-177.2652564
42	42	H	11	10	7	1.0975497	108.4192978	67.9455499
43	43	H	12	11	10	1.0963900	110.0215809	-99.4491253
44	44	H	12	11	10	1.0968503	109.5342542	144.8439024
45	45	H	13	12	11	1.0906057	110.4355683	159.9214478
46	46	H	13	12	11	1.0971338	109.0803263	-83.1346241
47	47	H	18	17	15	1.0903576	105.4905263	178.3603521
48	48	H	18	17	15	1.0928522	110.3099415	58.6614655
49	49	H	18	17	15	1.0933170	110.6596675	-62.0060739
50	50	H	21	19	14	1.0953556	106.3286007	-117.5343041
51	51	H	23	22	21	1.0958649	111.2943941	-48.4209769
52	52	H	23	22	21	1.0937211	110.6087392	-166.5762511
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54	54	H	24	23	22	1.0929561	111.7235830	118.1254875
55	55	H	25	20	14	1.0969408	107.4028109	120.3732316
56	56	H	26	24	23	1.0934557	114.8938967	163.5417758
57	57	H	28	22	21	1.0957402	111.2427925	179.4776237
58	58	H	28	22	21	1.0968328	110.8527358	59.9357101
59	59	H	28	22	21	1.0943174	111.2412406	-59.6371173
60	60	H	29	27	26	1.0963031	109.8827519	174.1335697
61	61	H	29	27	26	1.0841883	115.2303213	52.1566550
62	62	H	29	27	26	1.0961783	109.3595148	-68.4633136
63	63	H	30	27	26	1.0962158	109.5641207	64.2236352
64	64	H	30	27	26	1.0905778	114.9411160	-56.8902169
65	65	H	30	27	26	1.0958048	110.1701015	-178.3100211

Row	Tag	Symbol	X	Y	Z
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2	2	C	-4.6758770	1.5700530	-1.3671290
3	3	C	-3.1623430	1.5613750	-1.7243610
4	4	C	-2.4019960	1.0755110	-0.5255200
5	5	C	-2.7095990	-0.3527370	-0.1376500

6	6	C	-4.1781200	-0.2269080	0.3691330
7	7	C	-0.4883330	-1.5596660	-0.1013250
8	8	C	-1.6615210	-1.0966040	0.7498420
9	9	O	-4.5346430	-0.4157740	1.5134980
10	10	C	-0.4794640	-2.9833200	-0.5975610
11	11	C	-1.8935020	-3.5665880	-0.7566590
12	12	C	-2.7356640	-3.4447100	0.5391340
13	13	C	-2.2189210	-2.3394540	1.4837410
14	14	C	0.6350840	-0.7280250	-0.3473810
15	15	C	-1.8547200	2.0248940	0.4460440
16	16	O	-1.7831090	1.8430980	1.6528050
17	17	O	-1.4671130	3.1932790	-0.1407920
18	18	C	-0.9137790	4.1709590	0.7545700
19	19	O	1.6864110	-1.2840430	-1.0630950
20	20	N	0.7972500	0.5033950	0.0540210
21	21	C	2.6561910	-0.2330080	-1.2775430
22	22	C	4.0630080	-0.4484570	-0.6614860
23	23	C	4.8539810	0.7807920	-1.2139640
24	24	C	4.2929280	1.9938020	-0.3997990
25	25	C	2.0670800	0.9761350	-0.4880520
26	26	C	3.2148890	1.3318650	0.5004040
27	27	C	3.8905640	-0.0344870	0.8535590
28	28	C	4.6897210	-1.8007090	-0.9718040
29	29	C	3.0683130	-0.9890760	1.7422150
30	30	C	5.2344460	0.1347630	1.6025830
31	31	H	-5.1715350	-0.5429730	-1.5008950
32	32	H	-6.1345490	0.3331280	-0.2950470
33	33	H	-4.8637010	2.3852930	-0.6584290
34	34	H	-5.2700420	1.7795630	-2.2643560
35	35	H	-2.8436870	2.5611250	-2.0247120
36	36	H	-2.9969350	0.8815570	-2.5721510
37	37	H	-2.8034340	-0.8992690	-1.0855290
38	38	H	-1.3047520	-0.3840090	1.4953860
39	39	H	0.0899210	-3.6051610	0.1158970



40	40	H	0.0785480	-3.0491990	-1.5369870
41	41	H	-1.8206640	-4.6134600	-1.0713740
42	42	H	-2.3940630	-3.0425760	-1.5809560
43	43	H	-2.7300000	-4.3975290	1.0815130
44	44	H	-3.7848030	-3.2589790	0.2785730
45	45	H	-3.0006370	-2.0396990	2.1826600
46	46	H	-1.3939950	-2.7394850	2.0863810
47	47	H	-0.6340670	5.0165580	0.1256000
48	48	H	-0.0394080	3.7632750	1.2679850
49	49	H	-1.6541080	4.4743730	1.4996840
50	50	H	2.7244240	-0.0934970	-2.3618330
51	51	H	4.7059710	0.8967230	-2.2935810
52	52	H	5.9286780	0.6475580	-1.0606640
53	53	H	3.8633890	2.7673400	-1.0447860
54	54	H	5.0719450	2.4760370	0.1961330
55	55	H	1.8509630	1.8488560	-1.1164870
56	56	H	2.8880890	1.9388030	1.3492110
57	57	H	5.6834870	-1.8909820	-0.5191160
58	58	H	4.8067220	-1.9377590	-2.0537330
59	59	H	4.0668490	-2.6207170	-0.6014690
60	60	H	3.5884370	-1.9492870	1.8388910
61	61	H	2.0613170	-1.1912940	1.3950390
62	62	H	2.9821610	-0.5644100	2.7491130
63	63	H	5.0556270	0.6082130	2.5749810
64	64	H	5.9805080	0.7336160	1.0790120
65	65	H	5.6825360	-0.8453790	1.8008890



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
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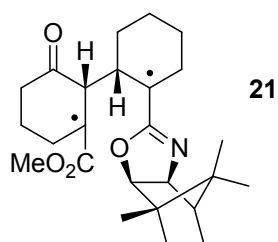
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4	4	C	3	2	1	1.4983822	110.9922044	-57.1693979
5	5	C	4	3	2	1.4744757	118.4842022	36.8547573
6	6	C	5	4	3	1.4478808	121.3332030	-5.3436958
7	7	C	5	4	3	2.9721157	133.9111447	-118.7968688
8	8	C	7	5	4	1.3973964	51.2404171	-11.1436261
9	9	O	6	5	4	1.2433732	121.8164604	172.7407197
10	10	C	7	5	4	1.5046109	119.2271435	98.7235198
11	11	C	10	7	5	1.5344728	113.1360354	-56.7437078
12	12	C	11	10	7	1.5324743	110.6867090	-42.3372532
13	13	C	8	7	5	1.5175771	121.0823603	119.4421180
14	14	C	7	5	4	1.4526204	97.6770016	-132.9024609
15	15	C	4	3	2	1.4482606	122.2374545	-145.5135826
16	16	O	15	4	3	1.2322238	125.0796669	-179.9320197
17	17	O	15	4	3	1.3697465	113.1172845	-0.5913821
18	18	C	17	15	4	1.4349342	115.4122676	-178.9816171
19	19	O	14	7	5	1.3699354	116.3588293	-132.6887054
20	20	N	14	7	5	1.2907652	125.9736299	48.5228574
21	21	C	19	14	7	1.4526556	106.5612450	174.3656762
22	22	C	21	19	14	1.5489529	116.5707553	118.8828327
23	23	C	22	21	19	1.5625270	101.9461946	174.4909173
24	24	C	23	22	21	1.5650287	104.1392946	72.8524856
25	25	C	20	14	7	1.4624868	106.9767499	-176.0704393
26	26	C	24	23	22	1.5529908	102.7845774	-1.3095137
27	27	C	26	24	23	1.5650766	101.7152738	37.1410083
28	28	C	22	21	19	1.5225055	114.7060257	49.8528754
29	29	C	27	26	24	1.5423187	116.1770518	-178.8938122
30	30	C	27	26	24	1.5475338	113.0526770	60.2514565
31	31	H	1	6	5	1.0992653	106.2967421	106.2833471
32	32	H	1	6	5	1.0954876	107.8711619	-140.3946240
33	33	H	2	1	6	1.0975370	110.0679178	-74.4732552
34	34	H	2	1	6	1.0959978	110.1435088	168.4805322

35	35	H	3	2	1	1.0925899	111.6095460	179.1796695
36	36	H	3	2	1	1.1050690	108.4946021	62.6912312
37	37	H	5	4	3	1.0855822	117.1632150	146.5285092
38	38	H	8	7	5	1.0843061	117.4767954	-85.6231974
39	39	H	10	7	5	1.1009438	108.4855052	-179.2203913
40	40	H	10	7	5	1.0967173	108.3946449	66.9082293
41	41	H	11	10	7	1.0956073	109.5349375	-164.9502258
42	42	H	11	10	7	1.0978951	109.5919417	78.4766186
43	43	H	12	11	10	1.0987765	109.1096807	-58.0199655
44	44	H	12	11	10	1.0959809	111.0789955	-175.3348958
45	45	H	13	8	7	1.0953474	110.4739769	-118.6096542
46	46	H	13	8	7	1.0975840	107.5829084	126.9994655
47	47	H	18	17	15	1.0903890	105.4671948	179.6169977
48	48	H	18	17	15	1.0933104	110.6803912	59.9823801
49	49	H	18	17	15	1.0935488	110.7314356	-60.7645026
50	50	H	21	19	14	1.0939929	105.8549399	-116.7998664
51	51	H	23	22	21	1.0957095	111.3080400	-48.5899279
52	52	H	23	22	21	1.0936975	110.5591005	-166.7217187
53	53	H	24	23	22	1.0946839	112.4347875	-121.5779140
54	54	H	24	23	22	1.0928914	111.7395054	118.3627950
55	55	H	25	20	14	1.0959817	107.1293452	119.9423837
56	56	H	26	24	23	1.0932947	114.8791571	163.5162109
57	57	H	28	22	21	1.0956779	111.1162438	179.2187959
58	58	H	28	22	21	1.0964808	110.8361057	59.6474884
59	59	H	28	22	21	1.0944246	111.2657126	-59.9755404
60	60	H	29	27	26	1.0962875	109.9102006	173.3257086
61	61	H	29	27	26	1.0841007	115.1923363	51.3077121
62	62	H	29	27	26	1.0961717	109.3664379	-69.2147749
63	63	H	30	27	26	1.0961123	109.6499137	65.2655976
64	64	H	30	27	26	1.0906394	115.0003195	-55.8422124
65	65	H	30	27	26	1.0958737	110.0805040	-177.2293520

Row	Tag	Symbol	X	Y	Z
1	1	C	-3.5471890	-1.8970730	-1.9611550

2	2	C	-4.7545220	-1.3977020	-1.1610510
3	3	C	-4.8427210	0.1396200	-1.1791080
4	4	C	-3.5857280	0.7557140	-0.6447430
5	5	C	-2.2979690	0.1084590	-0.9558960
6	6	C	-2.2412580	-1.1553760	-1.6600720
7	7	C	-0.1510360	-1.1110670	0.6984640
8	8	C	-1.2388710	-0.3362950	1.1096330
9	9	O	-1.1643490	-1.6441280	-2.0439540
10	10	C	-0.1136030	-2.6056270	0.8680020
11	11	C	-1.4134140	-3.1794140	1.4475420
12	12	C	-1.9345430	-2.2963320	2.5864310
13	13	C	-2.2794590	-0.8911580	2.0648000
14	14	C	0.9801170	-0.4659920	0.0546650
15	15	C	-3.5926780	1.9858450	0.1195790
16	16	O	-2.5927880	2.5380200	0.5818540
17	17	O	-4.8471010	2.5118830	0.2805520
18	18	C	-4.9085840	3.7448120	1.0120860
19	19	O	2.0325040	-1.2763900	-0.2806850
20	20	N	1.0872730	0.7937030	-0.2056440
21	21	C	2.9707670	-0.4512830	-1.0216770
22	22	C	4.3838800	-0.2879360	-0.4087460
23	23	C	5.1292620	0.5139640	-1.5235790
24	24	C	4.5270130	1.9551370	-1.4254400
25	25	C	2.3407350	0.9734280	-0.9373540
26	26	C	3.4785500	1.8127760	-0.2886730
27	27	C	4.2039060	0.8317900	0.6916280
28	28	C	5.0565770	-1.5923830	-0.0038760
29	29	C	3.4211230	0.4348420	1.9598670
30	30	C	5.5466170	1.3885240	1.2226980
31	31	H	-3.7311220	-1.7731970	-3.0378200
32	32	H	-3.3695570	-2.9669290	-1.8064030
33	33	H	-4.6855650	-1.7417750	-0.1211250
34	34	H	-5.6790090	-1.8233370	-1.5677080
35	35	H	-5.7107190	0.4994380	-0.6215570

36	36	H	-4.9918440	0.4699480	-2.2230540
37	37	H	-1.4356730	0.7557570	-1.0821480
38	38	H	-1.1223230	0.7414990	1.0873550
39	39	H	0.7364930	-2.8619120	1.5189490
40	40	H	0.1186360	-3.0584230	-0.1035070
41	41	H	-1.2387710	-4.2036130	1.7952080
42	42	H	-2.1726680	-3.2424420	0.6570140
43	43	H	-1.1631250	-2.2213150	3.3652740
44	44	H	-2.8165370	-2.7429200	3.0595270
45	45	H	-3.2659410	-0.9080090	1.5890320
46	46	H	-2.3734390	-0.1847440	2.8995680
47	47	H	-5.9644060	4.0160870	1.0365410
48	48	H	-4.3237590	4.5207430	0.5108490
49	49	H	-4.5225610	3.6126120	2.0266590
50	50	H	3.0209830	-0.8835690	-2.0253840
51	51	H	4.9755180	0.0617500	-2.5097050
52	52	H	6.2081860	0.5084210	-1.3445080
53	53	H	4.0656140	2.2798730	-2.3635180
54	54	H	5.2901270	2.6966220	-1.1759030
55	55	H	2.0861710	1.4023120	-1.9132800
56	56	H	3.1346080	2.7575320	0.1407840
57	57	H	6.0551890	-1.4101230	0.4085140
58	58	H	5.1714550	-2.2567350	-0.8685780
59	59	H	4.4664090	-2.1270060	0.7468870
60	60	H	3.9684840	-0.3400700	2.5091880
61	61	H	2.4150170	0.0704300	1.7860020
62	62	H	3.3371530	1.3042360	2.6222080
63	63	H	5.3595740	2.2731660	1.8422830
64	64	H	6.2634360	1.6756580	0.4524910
65	65	H	6.0351110	0.6454030	1.8630760



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5429643		
3	3	C	2	1		1.5548820	112.1570062	
4	4	C	3	2	1	1.5023098	109.1253216	-50.4657226
5	5	C	4	3	2	1.5082300	113.1798859	63.3078581
6	6	C	1	2	3	1.5213081	110.8259364	47.7448524
7	7	C	5	4	3	2.5949010	151.1625804	168.6882992
8	8	C	7	5	4	1.5104761	31.8480654	-3.2246620
9	9	O	6	1	2	1.2131239	123.8520336	119.8666030
10	10	C	7	5	4	1.5086038	144.7052289	15.5944054
11	11	C	10	7	5	1.5451738	111.7824704	-36.0247420
12	12	C	11	10	7	1.5358253	109.5676415	-37.8620654
13	13	C	12	11	10	1.5493285	111.2323302	63.2457650
14	14	C	7	5	4	1.4187024	95.5800971	-170.6373833
15	15	C	4	3	2	1.4570473	121.2838200	-101.2486091
16	16	O	15	4	3	1.2279824	126.0750761	167.7690266
17	17	O	15	4	3	1.3677540	112.4280090	-12.5140458
18	18	C	17	15	4	1.4364432	115.4445307	-179.8043362
19	19	O	14	7	5	1.3868018	116.2596654	-172.3348121
20	20	N	14	7	5	1.3086524	127.8097383	9.0504819
21	21	C	19	14	7	1.4440586	107.3073941	175.3065173
22	22	C	21	19	14	1.5500621	116.4679153	118.8936941
23	23	C	22	21	19	1.5624724	102.2007978	174.5601875
24	24	C	23	22	21	1.5648566	104.1445718	73.1145755
25	25	C	20	14	7	1.4609271	107.5666420	-177.3574064
26	26	C	24	23	22	1.5522341	102.7150110	-1.7473824
27	27	C	26	24	23	1.5651100	101.6522108	37.5615033
28	28	C	22	21	19	1.5223564	114.6384251	49.8618786

29	29	C	27	26	24	1.5421166	116.1746430	-179.1409467
30	30	C	27	26	24	1.5481220	113.1016764	59.9684326
31	31	H	1	6	9	1.0974222	107.1421717	-120.0609993
32	32	H	1	6	9	1.0931566	108.6989554	-2.8457376
33	33	H	2	1	6	1.0965792	109.2611923	-72.8848211
34	34	H	2	1	6	1.0960362	109.9568841	169.8325781
35	35	H	3	2	1	1.0903998	109.9329230	-173.2861983
36	36	H	3	2	1	1.0992288	108.6332851	68.5409655
37	37	H	5	4	3	1.0959774	106.8234768	42.6265071
38	38	H	8	7	5	1.0950726	105.9041252	119.2981707
39	39	H	10	7	5	1.0949525	109.3796179	-158.3314319
40	40	H	10	7	5	1.1023464	109.4377344	86.3742178
41	41	H	11	10	7	1.0957611	109.4096955	-159.7036296
42	42	H	11	10	7	1.0966799	110.7979382	83.2042327
43	43	H	12	11	10	1.0983105	108.3583936	-57.7751414
44	44	H	12	11	10	1.0957703	110.7710452	-174.1990937
45	45	H	13	12	11	1.0929683	109.8956959	96.6689525
46	46	H	13	12	11	1.0972203	109.9404276	-145.1706071
47	47	H	18	17	15	1.0901678	105.4087180	-179.7481709
48	48	H	18	17	15	1.0932540	110.6262768	60.6791148
49	49	H	18	17	15	1.0930755	110.6182806	-60.0849067
50	50	H	21	19	14	1.0951233	106.3690381	-116.9560303
51	51	H	23	22	21	1.0957577	111.2426778	-48.2506320
52	52	H	23	22	21	1.0936811	110.6334618	-166.3812128
53	53	H	24	23	22	1.0948371	112.4352806	-122.0582091
54	54	H	24	23	22	1.0928230	111.7161705	117.8527025
55	55	H	25	20	14	1.0970380	107.5200744	120.6524685
56	56	H	26	24	23	1.0938966	114.7518156	163.6649639
57	57	H	28	22	21	1.0956976	111.1451835	-179.9198548
58	58	H	28	22	21	1.0966068	110.8365944	60.5068214
59	59	H	28	22	21	1.0942840	111.2596381	-59.0720131
60	60	H	29	27	26	1.0962236	109.9310273	172.7779372
61	61	H	29	27	26	1.0843614	115.2570680	50.7414441
62	62	H	29	27	26	1.0965899	109.3026499	-69.9435349

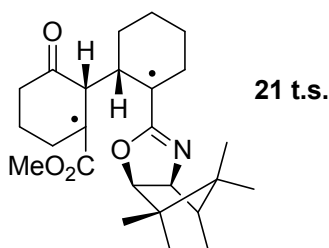
63	63	H	30	27	26	1.0962552	109.7168567	64.3027907
64	64	H	30	27	26	1.0903858	114.9638328	-56.9110787
65	65	H	30	27	26	1.0958133	110.0514097	-178.1890186

Row	Tag	Symbol	X	Y	Z
1	1	C	1.7652750	-2.8065280	-0.8085680
2	2	C	3.0638840	-3.1752690	-0.0613300
3	3	C	3.3653360	-2.1964740	1.1085940
4	4	C	3.2839600	-0.7843730	0.6023250
5	5	C	1.9069310	-0.4060290	0.1171810
6	6	C	1.7333570	-1.3214390	-1.1370210
7	7	C	0.1808450	1.3647570	-0.6691320
8	8	C	1.5660740	1.0674010	-0.1454690
9	9	O	1.6650830	-0.8801220	-2.2649550
10	10	C	0.0065640	2.7783520	-1.1664460
11	11	C	1.0005390	3.7501410	-0.4918670
12	12	C	1.1777050	3.3625100	0.9836350
13	13	C	1.8032370	1.9517770	1.1218020
14	14	C	-0.9334710	0.4867990	-0.6556050
15	15	C	4.4858000	-0.0223440	0.2894920
16	16	O	4.5283380	1.0430550	-0.3196560
17	17	O	5.6212260	-0.6217360	0.7609720
18	18	C	6.8461630	0.0785200	0.4916310
19	19	O	-2.1142810	0.9858850	-1.1846440
20	20	N	-0.9893180	-0.7314040	-0.1807910
21	21	C	-3.0771320	-0.0903050	-1.1769810
22	22	C	-4.3556960	0.1325500	-0.3294350
23	23	C	-5.2021810	-1.1361260	-0.6687770
24	24	C	-4.4757320	-2.2951000	0.0913770
25	25	C	-2.3277790	-1.2497990	-0.4529810
26	26	C	-3.2681960	-1.5709450	0.7448040
27	27	C	-3.9028830	-0.1981290	1.1473540
28	28	C	-5.0635080	1.4560140	-0.5844370
29	29	C	-2.9585640	0.8153370	1.8250370



30	30	C	-5.0884870	-0.3426950	2.1323080
31	31	H	0.8941730	-3.0164980	-0.1749800
32	32	H	1.6657810	-3.3732260	-1.7380540
33	33	H	3.9048320	-3.1527860	-0.7647440
34	34	H	2.9949560	-4.1982170	0.3261300
35	35	H	4.3448660	-2.4163320	1.5342130
36	36	H	2.6098960	-2.3439240	1.8933720
37	37	H	1.1926410	-0.8084300	0.8445230
38	38	H	2.2603700	1.4291040	-0.9111770
39	39	H	-1.0228430	3.1035540	-0.9834420
40	40	H	0.1350970	2.8006260	-2.2610580
41	41	H	0.6270400	4.7760390	-0.5853090
42	42	H	1.9731140	3.7259940	-0.9980500
43	43	H	0.1923120	3.3855040	1.4681440
44	44	H	1.7980990	4.0986550	1.5070040
45	45	H	2.8827560	2.0365340	1.2702040
46	46	H	1.3879350	1.4427320	2.0005960
47	47	H	7.6333610	-0.5363410	0.9283600
48	48	H	6.8323840	1.0698490	0.9523710
49	49	H	6.9967300	0.1905270	-0.5852160
50	50	H	-3.3318180	-0.2840170	-2.2243150
51	51	H	-5.2450620	-1.3072810	-1.7502330
52	52	H	-6.2355950	-1.0108640	-0.3333660
53	53	H	-4.1533040	-3.0975150	-0.5800700
54	54	H	-5.1226420	-2.7531820	0.8436600
55	55	H	-2.2142850	-2.1490720	-1.0709820
56	56	H	-2.7798680	-2.1290740	1.5489400
57	57	H	-5.9557710	1.5544900	0.0438360
58	58	H	-5.3849920	1.5312860	-1.6301550
59	59	H	-4.4033900	2.3047030	-0.3809040
60	60	H	-3.4685250	1.7781490	1.9460530
61	61	H	-2.0251990	0.9979610	1.3041510
62	62	H	-2.7031960	0.4572980	2.8295760
63	63	H	-4.7320170	-0.7597110	3.0814150

64	64	H	-5.9031460	-0.9770920	1.7818730
65	65	H	-5.5146380	0.6421050	2.3544940



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5367771		
3	3	C	2	1		1.5578526	112.3196851	
4	4	C	3	2	1	1.4927028	105.9554239	-59.3906316
5	5	C	4	3	2	1.4739350	115.2891230	59.2082026
6	6	C	5	4	3	1.4403749	119.9580739	-35.6435848
7	7	C	5	4	3	4.5559932	99.1381070	157.1435809
8	8	C	7	5	4	1.3481584	93.4556018	-62.1370655
9	9	O	6	5	4	1.2449829	121.7192493	-178.3528065
10	10	C	7	5	4	1.5162873	114.2583939	66.4237915
11	11	C	10	7	5	1.5354999	112.0009941	-97.3879248
12	12	C	11	10	7	1.5347449	111.4238450	-44.4012077
13	13	C	8	7	5	1.5026628	123.6418049	122.5501930
14	14	C	7	5	4	1.4741791	61.3536051	176.0999378
15	15	C	4	3	2	1.4520966	123.7954131	-103.3407367
16	16	O	15	4	3	1.2291336	124.3063131	168.0006721
17	17	O	15	4	3	1.3657806	112.8503501	-13.0078918
18	18	C	17	15	4	1.4376412	116.1049049	-179.0646649
19	19	O	14	7	5	1.3737325	114.8190001	-132.3839832
20	20	N	14	7	5	1.2815775	127.3775533	49.0049546
21	21	C	19	14	7	1.4548126	106.6549412	178.8345450
22	22	C	21	19	14	1.5537646	116.5785673	116.0067103
23	23	C	22	21	19	1.5599379	102.1557585	173.9826441
24	24	C	23	22	21	1.5646656	104.0841130	71.4307926
25	25	C	20	14	7	1.4706492	107.2489221	-179.6381032

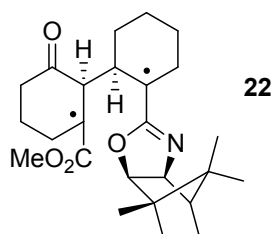
26	26	C	25	20	14	1.5503958	118.5076023	-113.8991024
27	27	C	26	25	20	1.5658979	105.4876973	80.6159383
28	28	C	22	21	19	1.5224943	114.5199514	49.0916498
29	29	C	27	26	25	1.5453231	116.5887877	-69.9224736
30	30	C	27	26	25	1.5472775	112.5624765	169.0417347
31	31	H	1	2	3	1.0981016	110.2660711	-82.5517166
32	32	H	1	2	3	1.0951642	111.2293408	160.2236017
33	33	H	2	1	6	1.0961814	110.3876095	-84.3745135
34	34	H	2	1	6	1.0963770	109.7709168	158.2012917
35	35	H	3	2	1	1.0909847	111.1906288	179.1154680
36	36	H	3	2	1	1.0997262	108.8362219	59.6467165
37	37	H	5	4	3	1.0924440	121.2566577	138.1870407
38	38	H	8	7	5	1.0878728	118.7232516	-57.4677864
39	39	H	10	7	5	1.0990253	109.2050933	140.1960492
40	40	H	10	7	5	1.0957248	109.2629887	24.9959667
41	41	H	11	10	7	1.0964225	109.6316353	-167.0442419
42	42	H	11	10	7	1.0972063	109.1991727	76.2732403
43	43	H	12	11	10	1.0987303	109.3190351	-59.5629488
44	44	H	12	11	10	1.0964995	110.8330971	-176.9620269
45	45	H	13	8	7	1.1029153	108.6613288	-107.5034660
46	46	H	13	8	7	1.0985695	109.3593136	138.2490773
47	47	H	18	17	15	1.0911499	105.2240831	178.3950432
48	48	H	18	17	15	1.0930395	110.6348510	59.0139364
49	49	H	18	17	15	1.0931327	110.6023618	-61.8864946
50	50	H	21	19	14	1.0943679	105.9180820	-120.1493826
51	51	H	23	22	21	1.0958860	111.4851542	-50.1874134
52	52	H	23	22	21	1.0942559	110.2287872	-168.4410163
53	53	H	24	23	22	1.0939721	112.4053081	-119.4793481
54	54	H	24	23	22	1.0930023	111.7558298	120.5220620
55	55	H	25	20	14	1.0935466	107.4714459	121.2644061
56	56	H	26	25	20	1.0937462	113.7095135	-47.5612214
57	57	H	28	22	21	1.0957581	111.1958507	178.3752826
58	58	H	28	22	21	1.0968053	110.8756115	58.8564821
59	59	H	28	22	21	1.0946355	111.2751984	-60.7899847

60	60	H	29	27	26	1.0964132	109.5070464	-166.2534441
61	61	H	29	27	26	1.0851995	115.0103128	73.7250549
62	62	H	29	27	26	1.0958874	110.1263721	-48.5801921
63	63	H	30	27	26	1.0965026	109.3331001	76.0851740
64	64	H	30	27	26	1.0907656	114.9242937	-44.5461496
65	65	H	30	27	26	1.0960672	110.4986854	-166.5278307

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.9409400	-4.0142100	-0.2028460
2	2	C	-3.2535130	-3.7080640	-0.9990270
3	3	C	-3.2737860	-2.2658200	-1.5991680
4	4	C	-3.0183950	-1.2752000	-0.4915870
5	5	C	-1.8761570	-1.6016870	0.3421140
6	6	C	-1.5741660	-2.9225370	0.7972960
7	7	C	-0.2301080	1.9987860	0.1412470
8	8	C	-1.2454360	2.1323810	-0.8313100
9	9	O	-1.0864910	-3.1555360	1.9095310
10	10	C	-0.1090890	3.1204500	1.1307080
11	11	C	-1.0514230	4.3177550	0.8693270
12	12	C	-1.0950050	4.6542560	-0.6299010
13	13	C	-1.6708680	3.4743680	-1.4441620
14	14	C	0.6721320	0.9153890	0.2075300
15	15	C	-3.9233110	-0.2906640	0.1877990
16	16	O	-4.0389270	-0.3506300	1.4268210
17	17	O	-4.6636150	0.6660450	-0.4673450
18	18	C	-5.6758440	1.2435400	0.4000090
19	19	O	1.6469990	0.9046640	1.2016510
20	20	N	0.7093860	-0.0873140	-0.6186250
21	21	C	2.3524950	-0.3403690	1.0697810
22	22	C	3.8643340	-0.2247290	0.7180860
23	23	C	4.3700050	-1.6979650	0.8002440
24	24	C	3.7698910	-2.3559940	-0.4763040
25	25	C	1.7412840	-1.0097400	-0.1795340
26	26	C	2.9720540	-1.1895060	-1.1177090

27	27	C	3.8923660	0.0320420	-0.8267370
28	28	C	4.6441990	0.7460050	1.6040090
29	29	C	3.3466760	1.4028510	-1.3127920
30	30	C	5.3060300	-0.0923950	-1.4677390
31	31	H	-1.1066740	-4.1143480	-0.9196180
32	32	H	-2.0415030	-4.9624160	0.3501780
33	33	H	-4.1199100	-3.8376020	-0.3271260
34	34	H	-3.3573870	-4.4335260	-1.8242270
35	35	H	-4.2271870	-2.0644220	-2.1120290
36	36	H	-2.4680820	-2.1874590	-2.3514060
37	37	H	-1.0386600	-0.9339710	0.5443780
38	38	H	-2.0936870	1.4540370	-0.9155450
39	39	H	0.9399700	3.4620180	1.1483020
40	40	H	-0.3387370	2.7276800	2.1401220
41	41	H	-0.6819560	5.1811880	1.4487830
42	42	H	-2.0833110	4.0776380	1.2499310
43	43	H	-0.0647570	4.8782510	-0.9621750
44	44	H	-1.7038490	5.5560540	-0.8139030
45	45	H	-2.7642170	3.5671600	-1.4917240
46	46	H	-1.3113480	3.5186170	-2.4870820
47	47	H	-6.1942110	1.9813590	-0.2075720
48	48	H	-5.3512740	1.7075780	1.3458310
49	49	H	-6.3389190	0.3895490	0.6146840
50	50	H	2.1923680	-0.9142020	1.9989750
51	51	H	4.0250300	-2.1998330	1.7212230
52	52	H	5.4711890	-1.7461970	0.8047420
53	53	H	3.1242770	-3.2167170	-0.2307130
54	54	H	4.5556190	-2.7269220	-1.1534460
55	55	H	1.2657270	-1.9817420	0.0433870
56	56	H	2.7086300	-1.3488150	-2.1763910
57	57	H	5.7077720	0.7736880	1.3136780
58	58	H	4.5865510	0.4311140	2.6601350
59	59	H	4.2351160	1.7662840	1.5312540
60	60	H	4.1584500	2.1438990	-1.4151570

61	61	H	2.6116760	1.8554320	-0.6394820
62	62	H	2.8977040	1.3052120	-2.3153560
63	63	H	5.2149500	-0.0947970	-2.5677400
64	64	H	5.8746900	-0.9885040	-1.1897270
65	65	H	5.9259630	0.7759070	-1.1860640



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5386866		
3	3	C	2	1		1.5482757	111.5365568	
4	4	C	3	2	1	1.4966759	110.0029156	-53.3063224
5	5	C	4	3	2	1.5028274	118.1819144	55.0261144
6	6	C	1	2	3	1.5182075	112.3853131	50.7458629
7	7	C	5	4	3	2.5592063	145.1437569	65.5016443
8	8	C	7	5	4	1.5091603	35.3000122	14.5653726
9	9	O	6	1	2	1.2174497	122.6859968	133.0865632
10	10	C	7	5	4	1.5026304	105.3560219	134.4671759
11	11	C	10	7	5	1.5438737	112.2515527	-58.3055797
12	12	C	11	10	7	1.5334102	109.7624039	-34.3100879
13	13	C	12	11	10	1.5424173	111.0526377	65.7362064
14	14	C	7	5	4	1.4177688	123.1714504	-81.1272316
15	15	C	4	3	2	1.4554485	123.1960096	-118.8951297
16	16	O	15	4	3	1.2293188	124.6071793	178.7525348
17	17	O	15	4	3	1.3639487	113.2893224	-1.8768033
18	18	C	17	15	4	1.4370038	115.5380182	-179.5482173
19	19	O	14	7	5	1.3800816	117.6123952	-140.9851028
20	20	N	14	7	5	1.3098636	125.9200328	40.3127627
21	21	C	19	14	7	1.4474738	107.1477517	175.3551741
22	22	C	21	19	14	1.5499740	116.4971445	118.7578556

23	23	C	22	21	19	1.5628857	102.1307581	174.6985403
24	24	C	23	22	21	1.5650173	104.1529792	73.1090990
25	25	C	20	14	7	1.4610862	107.1984749	-177.3492513
26	26	C	24	23	22	1.5521142	102.7210123	-1.6966831
27	27	C	26	24	23	1.5649782	101.7009088	37.4953920
28	28	C	22	21	19	1.5224992	114.6557971	50.0400327
29	29	C	27	26	24	1.5416871	116.1587395	-179.0680390
30	30	C	27	26	24	1.5478453	113.0131672	60.0527765
31	31	H	1	6	9	1.0998579	106.4629629	-106.7296717
32	32	H	1	6	9	1.0934403	108.0769119	9.0438551
33	33	H	2	1	6	1.0970169	109.7968872	-70.3408847
34	34	H	2	1	6	1.0956474	109.7856076	172.2812249
35	35	H	3	2	1	1.0906539	110.6799271	-176.2539548
36	36	H	3	2	1	1.1013607	108.1183651	66.3945287
37	37	H	5	4	3	1.0914602	109.3808265	-165.2684096
38	38	H	8	7	5	1.0915885	107.5189434	-117.2068341
39	39	H	10	7	5	1.0963159	108.7048249	179.5034306
40	40	H	10	7	5	1.1016399	109.4240214	64.8782276
41	41	H	11	10	7	1.0955216	109.3627662	-156.3215329
42	42	H	11	10	7	1.0966793	110.8861884	86.6730295
43	43	H	12	11	10	1.0989524	108.7993541	-55.5298684
44	44	H	12	11	10	1.0958881	110.9702993	-172.5330298
45	45	H	13	12	11	1.0937789	108.5683414	83.5229955
46	46	H	13	12	11	1.0958593	109.4889452	-160.3738764
47	47	H	18	17	15	1.0900765	105.4255732	-179.5180833
48	48	H	18	17	15	1.0931807	110.5846083	60.8874763
49	49	H	18	17	15	1.0930352	110.5753982	-59.8716007
50	50	H	21	19	14	1.0948481	106.2387185	-117.0568238
51	51	H	23	22	21	1.0957862	111.2701326	-48.2701128
52	52	H	23	22	21	1.0937112	110.6101186	-166.3997420
53	53	H	24	23	22	1.0948448	112.4292957	-121.9973044
54	54	H	24	23	22	1.0928527	111.7201654	117.9431538
55	55	H	25	20	14	1.0968302	107.4918014	120.8841691
56	56	H	26	24	23	1.0936423	114.8364216	163.7411735

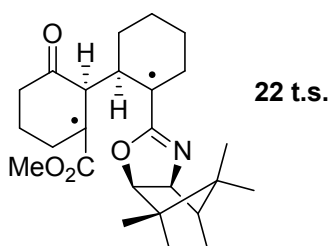
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58	58	H	28	22	21	1.0965877	110.8567956	60.4071650
59	59	H	28	22	21	1.0943148	111.3161288	-59.2166893
60	60	H	29	27	26	1.0961338	109.9195640	173.2468115
61	61	H	29	27	26	1.0842218	115.2190768	51.3360949
62	62	H	29	27	26	1.0964241	109.3334874	-69.3761805
63	63	H	30	27	26	1.0962149	109.6765298	64.0858053
64	64	H	30	27	26	1.0905027	114.9349382	-57.0734657
65	65	H	30	27	26	1.0957464	110.0994266	-178.3856965

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.6541590	-2.4741710	0.8915460
2	2	C	-2.8433860	-2.9922910	0.0639910
3	3	C	-3.3119890	-1.9446760	-0.9752740
4	4	C	-3.5842710	-0.6380360	-0.2980790
5	5	C	-2.4885380	-0.0246030	0.5274870
6	6	C	-1.9147910	-1.0992530	1.4802950
7	7	C	-0.1499580	1.0135830	0.4750430
8	8	C	-1.3335660	0.6010870	-0.3654830
9	9	O	-1.6816160	-0.8273100	2.6438500
10	10	C	-0.2415070	2.2440300	1.3326660
11	11	C	-1.3141710	3.2317510	0.8253740
12	12	C	-1.3773840	3.1869650	-0.7060780
13	13	C	-1.8766340	1.8137400	-1.2000960
14	14	C	1.0398920	0.2436350	0.4362440
15	15	C	-4.8922060	0.0004190	-0.2946960
16	16	O	-5.1499500	1.0610270	0.2709040
17	17	O	-5.8311870	-0.6900750	-1.0031370
18	18	C	-7.1394510	-0.0967340	-1.0401740
19	19	O	2.1132050	0.6868720	1.1820090
20	20	N	1.2272670	-0.8464320	-0.2654590
21	21	C	3.1540050	-0.3125690	1.0678450
22	22	C	4.4889570	0.1489990	0.4296620
23	23	C	5.3895230	-1.1168990	0.6002340



24	24	C	4.8291670	-2.1298860	-0.4529220
25	25	C	2.5680970	-1.3359240	0.0465430
26	26	C	3.6423680	-1.3500900	-1.0794080
27	27	C	4.2092510	0.1079010	-1.1248260
28	28	C	5.0682880	1.4260450	1.0225640
29	29	C	3.2629440	1.1878960	-1.6859970
30	30	C	5.4928120	0.2316910	-1.9809640
31	31	H	-0.7683590	-2.3745430	0.2472480
32	32	H	-1.4004480	-3.1517740	1.7113610
33	33	H	-3.6803130	-3.2375900	0.7294440
34	34	H	-2.5617570	-3.9173830	-0.4511140
35	35	H	-4.1952420	-2.2990310	-1.5080240
36	36	H	-2.5091210	-1.8163650	-1.7181970
37	37	H	-2.9065660	0.7640370	1.1556470
38	38	H	-0.9948980	-0.1794560	-1.0493120
39	39	H	0.7407490	2.7303940	1.3557240
40	40	H	-0.4469520	1.9501170	2.3743080
41	41	H	-1.0753380	4.2406390	1.1793110
42	42	H	-2.2997340	2.9844550	1.2379460
43	43	H	-0.3749610	3.3902090	-1.1079940
44	44	H	-2.0359480	3.9720440	-1.0945560
45	45	H	-2.9700130	1.8095080	-1.1708260
46	46	H	-1.5896000	1.6759640	-2.2486840
47	47	H	-7.7502870	-0.7783180	-1.6322800
48	48	H	-7.1006210	0.8905380	-1.5079670
49	49	H	-7.5438710	0.0049570	-0.0298130
50	50	H	3.3165150	-0.7021390	2.0780520
51	51	H	5.3386090	-1.5060360	1.6233310
52	52	H	6.4387850	-0.8708740	0.4138870
53	53	H	4.5017050	-3.0693190	0.0041550
54	54	H	5.5795380	-2.3888990	-1.2040430
55	55	H	2.4628400	-2.3492040	0.4530170
56	56	H	3.2765890	-1.7541930	-2.0275430
57	57	H	6.0090950	1.6979700	0.5312140

58	58	H	5.2779760	1.3000910	2.0915220
59	59	H	4.3717680	2.2638350	0.9201300
60	60	H	3.7122240	2.1798280	-1.5605870
61	61	H	2.2753100	1.2140160	-1.2394170
62	62	H	3.1271040	1.0278660	-2.7621400
63	63	H	5.2628110	-0.0022430	-3.0269380
64	64	H	6.3144410	-0.4163140	-1.6740250
65	65	H	5.8637380	1.2624580	-1.9566010



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5429689		
3	3	C	2	1		1.5548891	112.1525392	
4	4	C	3	2	1	1.5023680	109.1292320	-50.4649118
5	5	C	4	3	2	1.5081447	113.1730181	63.3228416
6	6	C	1	2	3	1.5213539	110.8045176	47.7613098
7	7	C	5	4	3	2.5948044	151.2174417	168.6692975
8	8	C	7	5	4	1.5107086	31.8597700	-3.2387256
9	9	O	6	1	2	1.2130403	123.8503746	119.7342282
10	10	C	7	5	4	1.5085449	144.7014672	15.6270151
11	11	C	10	7	5	1.5451195	111.7739227	-36.1024119
12	12	C	11	10	7	1.5357890	109.5475836	-37.8230838
13	13	C	12	11	10	1.5492008	111.2119727	63.3912720
14	14	C	7	5	4	1.4186686	95.5263233	-170.9106574
15	15	C	4	3	2	1.4570245	121.2820288	-101.2291856
16	16	O	15	4	3	1.2279553	126.0760909	167.7850514
17	17	O	15	4	3	1.3677894	112.4216318	-12.5010758
18	18	C	17	15	4	1.4364213	115.4496092	-179.7921251
19	19	O	14	7	5	1.3862980	116.3070586	-171.5221582

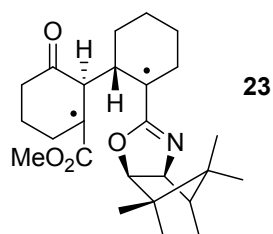
20	20	N	14	7	5	1.3078956	127.7587361	9.4246149
21	21	C	19	14	7	1.4443099	107.3750507	176.2792983
22	22	C	21	19	14	1.5499977	116.0328683	117.6302271
23	23	C	22	21	19	1.5610510	102.5585400	174.9679785
24	24	C	23	22	21	1.5638286	104.2180315	72.9885858
25	25	C	20	14	7	1.4607825	107.6617551	-178.0323193
26	26	C	24	23	22	1.5497417	102.6391718	-1.6396669
27	27	C	26	24	23	1.5651036	102.2162514	37.2713601
28	28	C	22	21	19	1.5224669	114.7144881	50.3980863
29	29	C	27	26	24	1.5564895	115.0254693	-177.3244314
30	30	C	27	26	24	1.5454734	113.1955130	60.2822682
31	31	H	1	6	9	1.0973889	107.1575125	-120.1913745
32	32	H	1	6	9	1.0931517	108.6989405	-2.9630529
33	33	H	2	1	6	1.0965798	109.2638929	-72.8696143
34	34	H	2	1	6	1.0960449	109.9590128	169.8462997
35	35	H	3	2	1	1.0903975	109.9395941	-173.2972277
36	36	H	3	2	1	1.0992470	108.6253208	68.5344330
37	37	H	5	4	3	1.0959565	106.8121044	42.5990917
38	38	H	8	7	5	1.0951344	105.8857143	119.2297630
39	39	H	10	7	5	1.0950993	109.3937183	-158.3793217
40	40	H	10	7	5	1.1023535	109.4796409	86.3479628
41	41	H	11	10	7	1.0957729	109.4292605	-159.6783154
42	42	H	11	10	7	1.0966910	110.7908452	83.2226629
43	43	H	12	11	10	1.0982166	108.3443852	-57.5727134
44	44	H	12	11	10	1.0957748	110.7943709	-174.0387134
45	45	H	13	12	11	1.0929885	109.8962551	96.4110726
46	46	H	13	12	11	1.0972515	109.9286849	-145.4527330
47	47	H	18	17	15	1.0901730	105.4080497	-179.8370427
48	48	H	18	17	15	1.0932491	110.6287842	60.5878014
49	49	H	18	17	15	1.0930816	110.6172155	-60.1783348
50	50	H	21	19	14	1.0951228	106.5134069	-118.0684431
51	51	H	23	22	21	1.0958644	111.2269641	-48.4537220
52	52	H	23	22	21	1.0937749	110.5746181	-166.5304126
53	53	H	24	23	22	1.0949968	112.4575474	-121.9201787

54	54	H	24	23	22	1.0929581	111.7127830	117.9681345
55	55	H	25	20	14	1.0970355	107.8470688	121.3842736
56	56	H	26	24	23	1.0940241	114.8074216	163.5268720
57	57	H	28	22	21	1.0956600	111.0868325	179.1378931
58	58	H	28	22	21	1.0966040	110.7893407	59.6162503
59	59	H	28	22	21	1.0943390	111.5296986	-59.9751155
60	60	H	29	27	26	1.0941578	110.4107559	-122.9081958
61	61	H	29	27	26	1.0924083	112.4009420	117.7353046
62	62	H	29	27	26	1.0911711	112.1100689	-3.5913370
63	63	H	30	27	26	1.0963932	109.6085257	65.9931719
64	64	H	30	27	26	1.0911207	114.8791322	-55.2355744
65	65	H	30	27	26	1.0959733	109.9570779	-176.5657715

Row	Tag	Symbol	X	Y	Z
1	1	C	1.7639360	-2.8072310	-0.8096060
2	2	C	3.0636170	-3.1712920	-0.0619150
3	3	C	3.3614540	-2.1909360	1.1076470
4	4	C	3.2753840	-0.7792680	0.6007990
5	5	C	1.8971080	-0.4059310	0.1155410
6	6	C	1.7277360	-1.3223560	-1.1387770
7	7	C	0.1631600	1.3567180	-0.6715440
8	8	C	1.5498530	1.0660570	-0.1472930
9	9	O	1.6607650	-0.8818020	-2.2670030
10	10	C	-0.0173730	2.7691750	-1.1696210
11	11	C	0.9713950	3.7458050	-0.4943980
12	12	C	1.1492930	3.3585520	0.9810800
13	13	C	1.7846360	1.9523580	1.1188510
14	14	C	-0.9450740	0.4710660	-0.6638970
15	15	C	4.4746820	-0.0134210	0.2876170
16	16	O	4.5136820	1.0521090	-0.3214800
17	17	O	5.6120810	-0.6093050	0.7588850
18	18	C	6.8348060	0.0947900	0.4896270
19	19	O	-2.1231300	0.9563350	-1.2102670
20	20	N	-0.9945610	-0.7457600	-0.1869520

21	21	C	-3.0860650	-0.1198190	-1.1841920
22	22	C	-4.3514880	0.1203680	-0.3219230
23	23	C	-5.2116230	-1.1475740	-0.6208730
24	24	C	-4.4797600	-2.2976260	0.1454930
25	25	C	-2.3316400	-1.2713490	-0.4512650
26	26	C	-3.2585830	-1.5701630	0.7629260
27	27	C	-3.8628900	-0.1795590	1.1509760
28	28	C	-5.0634570	1.4391540	-0.5898950
29	29	C	-2.8474810	0.8346100	1.7535250
30	30	C	-5.0244800	-0.2822650	2.1651990
31	31	H	0.8933750	-3.0197160	-0.1761740
32	32	H	1.6665950	-3.3746730	-1.7388610
33	33	H	3.9046680	-3.1463000	-0.7651190
34	34	H	2.9980500	-4.1942870	0.3260240
35	35	H	4.3415360	-2.4072920	1.5337880
36	36	H	2.6061970	-2.3406320	1.8921990
37	37	H	1.1844240	-0.8110400	0.8429260
38	38	H	2.2424150	1.4300390	-0.9135790
39	39	H	-1.0484350	3.0900250	-0.9873880
40	40	H	0.1111990	2.7922340	-2.2642080
41	41	H	0.5932920	4.7700080	-0.5880170
42	42	H	1.9444060	3.7261120	-0.9999600
43	43	H	0.1628770	3.3732000	1.4636240
44	44	H	1.7633280	4.0987510	1.5062360
45	45	H	2.8639740	2.0444840	1.2643370
46	46	H	1.3752230	1.4416230	1.9994710
47	47	H	7.6237790	-0.5169550	0.9275390
48	48	H	6.8173930	1.0865720	0.9492560
49	49	H	6.9857430	0.2060900	-0.5872470
50	50	H	-3.3514880	-0.3253440	-2.2265950
51	51	H	-5.2774090	-1.3374430	-1.6981570
52	52	H	-6.2372860	-1.0083880	-0.2673390
53	53	H	-4.1740960	-3.1137110	-0.5175250
54	54	H	-5.1162260	-2.7383710	0.9169930

55	55	H	-2.2222430	-2.1796790	-1.0566210
56	56	H	-2.7593570	-2.1150310	1.5696360
57	57	H	-5.9550680	1.5406240	0.0387580
58	58	H	-5.3867590	1.5014030	-1.6359070
59	59	H	-4.4091040	2.2950500	-0.3979520
60	60	H	-3.1789350	1.1643730	2.7427550
61	61	H	-2.7393820	1.7308130	1.1383090
62	62	H	-1.8550870	0.3980400	1.8768750
63	63	H	-4.6444330	-0.6560530	3.1232830
64	64	H	-5.8446110	-0.9337450	1.8594160
65	65	H	-5.4466620	0.7116660	2.3523380



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5405258		
3	3	C	2	1		1.5475442	111.7099442	
4	4	C	3	2	1	1.4961622	110.4863373	-51.9436982
5	5	C	4	3	2	1.5003796	118.5204997	52.9113339
6	6	C	1	2	3	1.5207764	111.4095094	51.9108864
7	7	C	5	4	3	2.5701156	94.9253683	100.6788045
8	8	C	7	5	4	1.5098796	34.7950363	-130.0044628
9	9	O	6	1	2	1.2171484	122.6345531	128.8093019
10	10	C	7	5	4	1.4965867	109.3766986	121.8720272
11	11	C	10	7	5	1.5654712	109.7327351	100.6492350
12	12	C	11	10	7	1.5441546	111.7876890	-24.1136387
13	13	C	12	11	10	1.5348614	111.2331279	-35.1598780
14	14	C	7	5	4	1.4190671	123.3812355	-33.0225251
15	15	C	4	3	2	1.4558630	123.7734509	-121.5502048
16	16	O	15	4	3	1.2291760	124.5873825	-178.8888110

17	17	O	15	4	3	1.3638853	113.3410750	1.2377304
18	18	C	17	15	4	1.4364604	115.4365491	179.9034210
19	19	O	14	7	5	1.3836238	117.4758255	146.8097447
20	20	N	14	7	5	1.3081235	126.1135991	-33.9878490
21	21	C	19	14	7	1.4472177	107.0087870	171.9563280
22	22	C	21	19	14	1.5496665	116.6009378	120.2651984
23	23	C	22	21	19	1.5623417	102.1608035	174.7077877
24	24	C	23	22	21	1.5647644	104.1544936	73.0725088
25	25	C	20	14	7	1.4623341	107.2236769	-174.2961391
26	26	C	24	23	22	1.5525272	102.7265273	-1.7664706
27	27	C	26	24	23	1.5650772	101.6563568	37.4732484
28	28	C	22	21	19	1.5224742	114.6483311	49.9993858
29	29	C	27	26	24	1.5402349	116.0999833	-178.7516523
30	30	C	27	26	24	1.5476478	113.0128438	60.2661197
31	31	H	1	6	9	1.0997376	107.9790596	-111.4471558
32	32	H	1	6	9	1.0930651	108.2749366	5.1153147
33	33	H	2	1	6	1.0969904	109.2581794	-69.2966142
34	34	H	2	1	6	1.0956470	109.7417862	173.6739286
35	35	H	3	2	1	1.0910081	110.4031081	-174.8190766
36	36	H	3	2	1	1.1008615	109.1771772	67.3308417
37	37	H	5	4	3	1.0922464	109.2480003	-165.6036535
38	38	H	8	7	5	1.0938494	107.5988644	119.1422468
39	39	H	10	7	5	1.0978954	108.4186798	-18.3580678
40	40	H	10	7	5	1.0907347	111.5220586	-136.1597326
41	41	H	11	10	7	1.0963315	108.7274847	-145.8213510
42	42	H	11	10	7	1.0953973	109.4858261	97.7113422
43	43	H	12	11	10	1.0959320	110.0854358	-157.4823353
44	44	H	12	11	10	1.0982335	109.7549473	85.6709493
45	45	H	13	12	11	1.0953063	110.7555860	-173.6390104
46	46	H	13	12	11	1.0969261	109.2640741	-57.2945000
47	47	H	18	17	15	1.0901930	105.4552604	-179.6313243
48	48	H	18	17	15	1.0930302	110.5722029	60.7423108
49	49	H	18	17	15	1.0931398	110.5784552	-60.0249198
50	50	H	21	19	14	1.0954222	106.2694200	-115.6674749

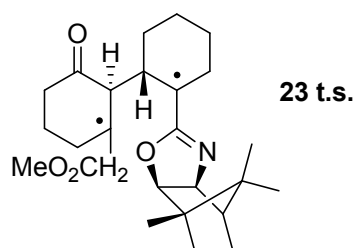
51	51	H	23	22	21	1.0958474	111.2966984	-48.3715071
52	52	H	23	22	21	1.0936696	110.5736780	-166.4869243
53	53	H	24	23	22	1.0947283	112.4624657	-122.1026135
54	54	H	24	23	22	1.0928132	111.7319047	117.8255160
55	55	H	25	20	14	1.0965854	107.1125871	120.6558613
56	56	H	26	24	23	1.0936257	114.7273892	163.6139381
57	57	H	28	22	21	1.0956716	111.1186792	179.8055453
58	58	H	28	22	21	1.0966763	110.8625555	60.3063995
59	59	H	28	22	21	1.0942448	111.3127186	-59.3551688
60	60	H	29	27	26	1.0962137	109.8854245	174.1056544
61	61	H	29	27	26	1.0840191	115.1697610	52.6441751
62	62	H	29	27	26	1.0955634	109.5686852	-68.2512677
63	63	H	30	27	26	1.0962098	109.6623287	64.7716976
64	64	H	30	27	26	1.0906039	115.0134759	-56.4160857
65	65	H	30	27	26	1.0957758	110.0727984	-177.7194329

Row	Tag	Symbol	X	Y	Z
1	1	C	-3.8606460	-0.7432840	2.2222310
2	2	C	-3.0189280	-2.0335030	2.2141410
3	3	C	-1.7177600	-1.8630050	1.3939060
4	4	C	-2.0243360	-1.3273400	0.0309770
5	5	C	-2.8451950	-0.0762550	-0.0790940
6	6	C	-4.0966580	-0.2255830	0.8118960
7	7	C	-0.8353990	1.4703050	-0.4966660
8	8	C	-2.0859680	1.2559150	0.3217780
9	9	O	-5.2043150	0.0546070	0.3923250
10	10	C	-1.0166210	2.1783430	-1.8026570
11	11	C	-1.5314140	3.6345540	-1.5474360
12	12	C	-2.2590780	3.7557030	-0.1908810
13	13	C	-3.0408300	2.4761370	0.1367990
14	14	C	0.4468920	1.2549290	0.0717480
15	15	C	-1.6717670	-2.0105890	-1.2053090
16	16	O	-1.8987820	-1.5754210	-2.3322370
17	17	O	-1.0533190	-3.2092200	-1.0028520



18	18	C	-0.6871740	-3.9235520	-2.1941060
19	19	O	1.5482470	1.6308550	-0.6766580
20	20	N	0.6916340	0.7443130	1.2509680
21	21	C	2.7078080	1.4941230	0.1784220
22	22	C	3.8108850	0.5161800	-0.2994010
23	23	C	4.9291320	0.7335820	0.7697910
24	24	C	4.3719190	0.0342480	2.0538990
25	25	C	2.1341750	0.8370830	1.4720790
26	26	C	2.9766370	-0.4664300	1.5925420
27	27	C	3.2696270	-0.9058940	0.1192820
28	28	C	4.2594310	0.7198410	-1.7399760
29	29	C	2.0673450	-1.4436650	-0.6792440
30	30	C	4.3365140	-2.0228000	0.0218810
31	31	H	-3.3215090	0.0338510	2.7833150
32	32	H	-4.8324500	-0.8895980	2.7007500
33	33	H	-3.6138710	-2.8509740	1.7884980
34	34	H	-2.7704240	-2.3197170	3.2421340
35	35	H	-1.1841460	-2.8121490	1.3254930
36	36	H	-1.0562150	-1.1498310	1.9093060
37	37	H	-3.1921480	0.0373490	-1.1085210
38	38	H	-1.7855670	1.1789240	1.3707480
39	39	H	-1.7643650	1.6321630	-2.3925220
40	40	H	-0.0932810	2.1896610	-2.3831890
41	41	H	-2.2071570	3.9170530	-2.3632230
42	42	H	-0.6867080	4.3312950	-1.5777500
43	43	H	-2.9355310	4.6178790	-0.2023180
44	44	H	-1.5282290	3.9444930	0.6068250
45	45	H	-3.6429050	2.6101630	1.0419170
46	46	H	-3.7533070	2.2703370	-0.6714520
47	47	H	-0.2189130	-4.8451630	-1.8478610
48	48	H	0.0137260	-3.3369500	-2.7935660
49	49	H	-1.5719060	-4.1442540	-2.7970110
50	50	H	3.1127450	2.5034000	0.3100870
51	51	H	5.1284070	1.7997510	0.9261710

52	52	H	5.8707890	0.2877540	0.4371760
53	53	H	4.2968750	0.7195810	2.9042620
54	54	H	5.0090740	-0.7946500	2.3720220
55	55	H	2.2840440	1.4413280	2.3748120
56	56	H	2.5252130	-1.2234810	2.2399270
57	57	H	5.0404670	0.0024780	-2.0154200
58	58	H	4.6708030	1.7264210	-1.8823440
59	59	H	3.4239020	0.6034480	-2.4369090
60	60	H	2.3605830	-1.6210200	-1.7205130
61	61	H	1.1967350	-0.7979420	-0.6925620
62	62	H	1.7503890	-2.4057510	-0.2618850
63	63	H	3.9588110	-2.9360500	0.4962130
64	64	H	5.2951690	-1.7864530	0.4850630
65	65	H	4.5332680	-2.2643680	-1.0286700



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5376807		
3	3	C	2	1		1.5749694	110.3748093	
4	4	C	3	2	1	1.4921298	107.6938155	-52.0566647
5	5	C	4	3	2	1.4814912	117.3912413	58.6208478
6	6	C	5	4	3	1.4429627	108.7577378	-55.9953788
7	7	C	5	4	3	3.8693255	123.1738391	128.5183876
8	8	C	7	5	4	1.4750129	56.2412757	76.6147654
9	9	O	6	5	4	1.1395624	149.4612781	-131.9521158
10	10	C	7	5	4	1.4530367	111.1947145	-169.4439851
11	11	C	10	7	5	1.4627913	119.9645951	-40.5250245
12	12	C	11	10	7	1.5500584	109.5355810	-50.9985893
13	13	C	8	7	5	1.5519161	114.0431650	113.5832347

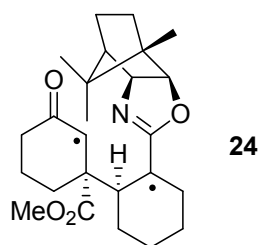
14	14	C	7	5	4	1.4076479	108.4063451	-44.6188841
15	15	C	4	3	2	1.4648872	119.8339818	-104.3222066
16	16	O	15	4	3	1.2159453	126.9164604	159.5977812
17	17	O	15	4	3	1.3744352	111.2000568	-17.6279928
18	18	C	17	15	4	1.4444791	115.6297714	179.8232923
19	19	O	14	7	5	1.4008553	116.4626226	-144.5760602
20	20	N	14	7	5	1.3041059	128.1335223	36.8261672
21	21	C	19	14	7	1.4600555	107.0979700	176.8853452
22	22	C	21	19	14	1.5567070	115.3841545	116.9462543
23	23	C	22	21	19	1.5649768	102.6178306	175.0342533
24	24	C	23	22	21	1.5601165	103.9705936	72.7795748
25	25	C	20	14	7	1.4654288	109.0574869	-178.6067421
26	26	C	24	23	22	1.5549200	103.0672484	-1.1368280
27	27	C	26	24	23	1.5709165	101.7760785	36.9666892
28	28	C	22	21	19	1.5149388	114.2923218	49.8955462
29	29	C	27	26	24	1.5354434	115.6286821	-177.2490540
30	30	C	27	26	24	1.5414860	112.7542250	60.7941842
31	31	H	1	6	5	1.1048830	108.4283572	70.6485245
32	32	H	1	6	5	1.1011785	108.0629178	-173.8501930
33	33	H	2	1	6	1.1028865	110.3714552	-73.8500963
34	34	H	2	1	6	1.1018237	109.9402995	169.3155294
35	35	H	3	2	1	1.1011338	110.4566719	-173.8795993
36	36	H	3	2	1	1.1058939	109.7785943	68.3906982
37	37	H	5	4	3	1.0638180	109.8406801	70.4342311
38	38	H	8	7	5	1.0918333	118.9495069	-104.5310362
39	39	H	10	7	5	1.1075126	108.4404630	-160.0865928
40	40	H	10	7	5	1.1017900	105.6998529	85.8336806
41	41	H	11	10	7	1.0999645	105.2815911	-175.2430075
42	42	H	11	10	7	1.0314651	125.2164184	67.1572493
43	43	H	12	11	10	1.1016104	110.0597278	-77.4056340
44	44	H	12	11	10	1.1011972	107.4801522	166.8726847
45	45	H	13	8	7	1.1006441	107.0417466	-153.1999658
46	46	H	13	8	7	1.1025634	105.8368191	93.8632013
47	47	H	18	17	15	1.0925463	104.0178917	-179.3526863

48	48	H	18	17	15	1.0937188	109.8677933	61.2412561
49	49	H	18	17	15	1.0941257	110.2236735	-59.8928998
50	50	H	21	19	14	1.0970546	105.3491094	-118.6228798
51	51	H	23	22	21	1.0970911	111.7820294	-48.6849944
52	52	H	23	22	21	1.0969483	110.6656468	-166.9829582
53	53	H	24	23	22	1.0970787	112.3333931	-121.9491730
54	54	H	24	23	22	1.0968436	111.7110299	118.4594642
55	55	H	25	20	14	1.1039811	107.9228799	121.5490983
56	56	H	26	24	23	1.0936848	115.0815460	162.6778424
57	57	H	28	22	21	1.0957299	111.5071897	-176.9778098
58	58	H	28	22	21	1.0963383	111.3955915	62.7314497
59	59	H	28	22	21	1.0974310	110.9178769	-56.6787141
60	60	H	29	27	26	1.0958401	111.2041894	-162.3380872
61	61	H	29	27	26	1.0911455	113.6679577	77.2167792
62	62	H	29	27	26	1.0961419	110.5090173	-43.7290519
63	63	H	30	27	26	1.0961598	110.0155286	65.9329976
64	64	H	30	27	26	1.0919912	114.4489090	-54.8280453
65	65	H	30	27	26	1.0959361	110.4349917	-175.7002437

Row	Tag	Symbol	X	Y	Z
1	1	C	5.1515010	0.5948720	-2.0588780
2	2	C	5.4978350	-0.8956860	-1.9080420
3	3	C	4.2065720	-1.7257270	-1.5556210
4	4	C	3.5561670	-1.0755290	-0.3806030
5	5	C	3.1491130	0.3416480	-0.5245910
6	6	C	4.3029650	1.1193120	-0.9066980
7	7	C	-0.4063570	1.6186940	0.3117500
8	8	C	0.6098930	1.2969160	1.3312390
9	9	O	4.9617430	2.0369150	-0.7563030
10	10	C	-0.5970500	2.9827150	-0.1512820
11	11	C	0.4794950	3.9618900	-0.0028720
12	12	C	0.9859790	3.9573310	1.4620970
13	13	C	1.1100090	2.5263120	2.1355480
14	14	C	-1.3414790	0.7173390	-0.2310010

15	15	C	3.6740740	-1.6839070	0.9467510
16	16	O	3.5149740	-1.1334340	2.0192200
17	17	O	4.0611770	-2.9997010	0.8578160
18	18	C	4.2111670	-3.6932760	2.1159800
19	19	O	-2.5284640	1.2722730	-0.7264910
20	20	N	-1.2555650	-0.5815000	-0.3105520
21	21	C	-3.3063890	0.1786190	-1.3013960
22	22	C	-4.6746150	-0.1007000	-0.6134460
23	23	C	-5.2966100	-1.2088420	-1.5268440
24	24	C	-4.4635880	-2.4846430	-1.1916280
25	25	C	-2.4503620	-1.0998140	-0.9823350
26	26	C	-3.4349960	-1.9682310	-0.1461170
27	27	C	-4.2975340	-0.9414320	0.6721070
28	28	C	-5.5383370	1.1290380	-0.4216950
29	29	C	-3.5514280	-0.1781990	1.7759130
30	30	C	-5.5107920	-1.5971750	1.3607180
31	31	H	4.5780260	0.7110790	-2.9961020
32	32	H	6.0417430	1.2369590	-2.1471250
33	33	H	6.2626780	-1.0348660	-1.1257360
34	34	H	5.9413770	-1.2748530	-2.8426640
35	35	H	4.4692560	-2.7731530	-1.3402340
36	36	H	3.5204750	-1.7366850	-2.4228880
37	37	H	2.3217830	0.4139180	-1.1894300
38	38	H	0.5132430	0.3696690	1.8995450
39	39	H	-1.4480650	3.4249520	0.4025990
40	40	H	-0.9137070	2.8989400	-1.2032570
41	41	H	0.0526730	4.9161330	-0.3451660
42	42	H	1.3821970	3.9335290	-0.5011140
43	43	H	0.2811650	4.5055330	2.1072770
44	44	H	1.9344650	4.5162970	1.4859010
45	45	H	2.1307500	2.2953040	2.4763420
46	46	H	0.4850860	2.5666620	3.0430110
47	47	H	4.5284380	-4.6982860	1.8279670
48	48	H	3.2547700	-3.7123470	2.6462270

49	49	H	4.9672460	-3.1984100	2.7328780
50	50	H	-3.4183650	0.4289720	-2.3636170
51	51	H	-5.2399570	-0.9400850	-2.5889970
52	52	H	-6.3611130	-1.3451890	-1.2998230
53	53	H	-3.9737570	-2.9073880	-2.0775930
54	54	H	-5.0914190	-3.2808550	-0.7733690
55	55	H	-2.1222880	-1.6562450	-1.8776150
56	56	H	-2.9432440	-2.7466720	0.4441000
57	57	H	-6.4645840	0.8900310	0.1126890
58	58	H	-5.8154430	1.5770390	-1.3831860
59	59	H	-5.0051400	1.8965040	0.1536760
60	60	H	-4.2511340	0.2697020	2.4905190
61	61	H	-2.9243200	0.6322070	1.4009780
62	62	H	-2.9061430	-0.8581280	2.3440950
63	63	H	-5.1709430	-2.2973570	2.1326080
64	64	H	-6.1671310	-2.1523670	0.6873490
65	65	H	-6.1265150	-0.8376230	1.8557350



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5348667		
3	3	C	2	1		1.5333798	110.2098383	
4	4	C	3	2	1	1.5529493	112.0767801	-64.2348284
5	5	C	4	3	2	1.5053023	110.4915692	43.0505421
6	6	C	5	4	3	1.4391481	125.3450671	-10.0709912
7	7	C	4	3	2	2.6517582	90.2757645	147.2147574
8	8	C	7	4	3	1.5113466	32.7356252	133.5526700
9	9	O	6	5	4	1.2454026	119.9268237	176.8537791
10	10	C	7	4	3	1.5050439	119.4346935	-123.7829509

11	11	C	10	7	4	1.5299502	113.1967187	-23.8859180
12	12	C	11	10	7	1.5414804	112.4968192	-51.2247394
13	13	C	8	7	4	1.5536047	109.0063439	131.0915605
14	14	C	7	4	3	1.4234730	116.7555154	30.0623335
15	15	C	4	3	2	1.5494966	108.9531429	-72.9425623
16	16	O	15	4	3	1.2157100	124.7763820	121.2632272
17	17	O	15	4	3	1.3476832	112.3189747	-58.4730507
18	18	C	17	15	4	1.4422670	116.1193713	179.6995863
19	19	O	14	7	4	1.3828335	116.8767521	-147.6899486
20	20	N	14	7	4	1.3052240	126.5078017	34.6395092
21	21	C	19	14	7	1.4480722	107.0156361	176.5780775
22	22	C	21	19	14	1.5501145	116.6127594	118.3175217
23	23	C	22	21	19	1.5630957	101.9945715	174.4694075
24	24	C	23	22	21	1.5648304	104.1534703	73.2345608
25	25	C	20	14	7	1.4610158	107.2587447	-178.3441642
26	26	C	24	23	22	1.5521891	102.7274217	-1.8169853
27	27	C	26	24	23	1.5648317	101.6728474	37.5801475
28	28	C	22	21	19	1.5222560	114.6479559	49.8392421
29	29	C	27	26	24	1.5421612	116.2253885	-179.1571625
30	30	C	27	26	24	1.5477856	112.9078636	60.0788485
31	31	H	1	6	5	1.0995500	107.4146206	104.7227677
32	32	H	1	6	5	1.0947270	107.5385468	-141.1405444
33	33	H	2	1	6	1.0983375	109.8437437	-72.9759071
34	34	H	2	1	6	1.0957741	110.0296777	170.1715201
35	35	H	3	2	1	1.0915635	112.0810458	172.4529993
36	36	H	3	2	1	1.0951244	108.5959604	55.0883039
37	37	H	5	4	3	1.0839793	119.1883939	176.2487961
38	38	H	8	7	4	1.0927506	105.9957662	-113.2852069
39	39	H	10	7	4	1.1037326	108.3338549	-146.0491292
40	40	H	10	7	4	1.0980568	109.9130324	100.5679643
41	41	H	11	10	7	1.0956994	109.6146701	-173.5780574
42	42	H	11	10	7	1.0947090	108.8150907	71.1094713
43	43	H	12	11	10	1.0965862	108.9147722	-83.8734435
44	44	H	12	11	10	1.0956354	108.9965963	161.3193773

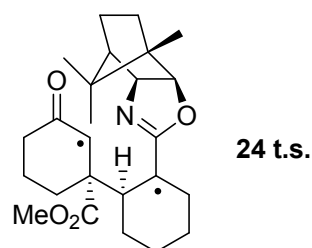
45	45	H	13	8	7	1.0958147	109.7854306	-173.2954310
46	46	H	13	8	7	1.0957028	105.7458913	73.2700235
47	47	H	18	17	15	1.0894701	105.2868266	-179.3732046
48	48	H	18	17	15	1.0924748	110.3485895	61.0278665
49	49	H	18	17	15	1.0923700	110.3457424	-59.7289806
50	50	H	21	19	14	1.0949361	106.2335015	-117.6073544
51	51	H	23	22	21	1.0957737	111.2407953	-48.1238752
52	52	H	23	22	21	1.0936020	110.6572314	-166.2345898
53	53	H	24	23	22	1.0948168	112.5178797	-122.2011461
54	54	H	24	23	22	1.0928855	111.6904572	117.7029399
55	55	H	25	20	14	1.0968007	107.4096375	120.6612040
56	56	H	26	24	23	1.0934670	114.8365758	163.8499548
57	57	H	28	22	21	1.0956720	111.1761222	179.2621999
58	58	H	28	22	21	1.0966941	110.8948649	59.7516272
59	59	H	28	22	21	1.0943839	111.3142125	-59.8806798
60	60	H	29	27	26	1.0960829	109.8673810	173.5996938
61	61	H	29	27	26	1.0843110	115.2445073	51.6653472
62	62	H	29	27	26	1.0963085	109.3330942	-69.0514755
63	63	H	30	27	26	1.0961704	109.6389656	63.4345874
64	64	H	30	27	26	1.0904019	114.9045405	-57.6754046
65	65	H	30	27	26	1.0956514	110.1704881	-179.0193696

Row	Tag	Symbol	X	Y	Z
1	1	C	3.7806100	-0.3881130	2.7545360
2	2	C	3.1602850	0.9811250	2.4443750
3	3	C	2.0481090	0.8342650	1.3990280
4	4	C	2.5937730	0.3397460	0.0317850
5	5	C	3.5943590	-0.7667610	0.2327950
6	6	C	4.1524650	-1.1648100	1.4981890
7	7	C	0.3299480	-0.9674360	-0.4134040
8	8	C	1.3900510	-0.0385900	-0.9589270
9	9	O	4.9309880	-2.1351510	1.5562220
10	10	C	0.3722020	-2.4455240	-0.6938100
11	11	C	1.7176590	-2.9150510	-1.2506200



12	12	C	2.1825540	-2.0748050	-2.4564480
13	13	C	1.8496720	-0.5566640	-2.3496230
14	14	C	-0.8504990	-0.4194800	0.1632800
15	15	C	3.3690550	1.4959950	-0.6486310
16	16	O	4.5385990	1.4478330	-0.9769570
17	17	O	2.5996460	2.5860520	-0.8384610
18	18	C	3.2428800	3.7165660	-1.4616160
19	19	O	-1.8300120	-1.3148130	0.5520750
20	20	N	-1.1202990	0.8474030	0.3239820
21	21	C	-2.8846670	-0.5440870	1.1770530
22	22	C	-4.2783230	-0.5979250	0.5005330
23	23	C	-5.1603780	0.2069100	1.5092390
24	24	C	-4.7260090	1.6948690	1.2947730
25	25	C	-2.4180630	0.9331800	0.9895780
26	26	C	-3.6105990	1.5742820	0.2221080
27	27	C	-4.1714000	0.4338970	-0.6909760
28	28	C	-4.7811460	-2.0015380	0.1934450
29	29	C	-3.2886780	0.0219280	-1.8865280
30	30	C	-5.5400610	0.7857520	-1.3223280
31	31	H	3.0681620	-1.0032410	3.3229070
32	32	H	4.6810720	-0.3089330	3.3720520
33	33	H	3.9370630	1.6696530	2.0853620
34	34	H	2.7521770	1.4242790	3.3596800
35	35	H	1.4975370	1.7652810	1.2520910
36	36	H	1.3228810	0.0982160	1.7617590
37	37	H	4.0198030	-1.2587370	-0.6343660
38	38	H	0.8972070	0.9248640	-1.1104690
39	39	H	-0.4346670	-2.6867590	-1.4072480
40	40	H	0.1089890	-3.0059020	0.2130660
41	41	H	1.6482210	-3.9696150	-1.5398090
42	42	H	2.4645770	-2.8729300	-0.4514160
43	43	H	1.7087230	-2.4647360	-3.3652600
44	44	H	3.2591320	-2.2202930	-2.5986800
45	45	H	2.7001590	0.0365900	-2.7039270

46	46	H	1.0271400	-0.3313930	-3.0375610
47	47	H	2.4760660	4.4884510	-1.5176070
48	48	H	3.5976870	3.4491910	-2.4596760
49	49	H	4.0889720	4.0525050	-0.8578400
50	50	H	-2.9418670	-0.8887310	2.2147590
51	51	H	-4.9967840	-0.1324320	2.5382210
52	52	H	-6.2228110	0.0558110	1.2985960
53	53	H	-4.3571410	2.1606730	2.2143310
54	54	H	-5.5560900	2.3108220	0.9398560
55	55	H	-2.2677670	1.4708370	1.9336690
56	56	H	-3.3529680	2.5109160	-0.2799010
57	57	H	-5.7733310	-1.9738380	-0.2705580
58	58	H	-4.8630730	-2.5970730	1.1107040
59	59	H	-4.1003490	-2.5291210	-0.4817200
60	60	H	-3.7211700	-0.8533680	-2.3847300
61	61	H	-2.2586030	-0.2121610	-1.6418280
62	62	H	-3.2694630	0.8356840	-2.6209150
63	63	H	-5.4277590	1.6498460	-1.9873990
64	64	H	-6.3280180	1.0238200	-0.6071890
65	65	H	-5.8981750	-0.0477630	-1.9367050



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5351148		
3	3	C	2	1		1.5529990	111.9713976	
4	4	C	3	2	1	1.4906936	108.1660707	-60.5150064
5	5	C	4	3	2	1.4814278	115.3488218	51.4138074
6	6	C	5	4	3	1.4261502	121.9528023	-23.4868623
7	7	C	5	4	3	3.9980209	85.3847815	81.6431808

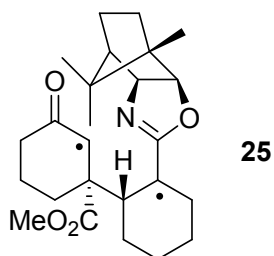
8	8	C	7	5	4	1.3560197	62.3992139	45.1928844
9	9	O	6	5	4	1.2533159	120.5467863	175.0656919
10	10	C	7	5	4	1.5136310	105.9489601	160.0056208
11	11	C	10	7	5	1.5403678	109.9024680	-25.4559039
12	12	C	11	10	7	1.5480886	113.6474592	-53.3584422
13	13	C	8	7	5	1.5027515	121.3010438	96.4764029
14	14	C	7	5	4	1.4698498	101.4318909	-73.2514923
15	15	C	4	3	2	1.4426759	125.8738271	-120.0502323
16	16	O	15	4	3	1.2340576	124.1265762	178.1360384
17	17	O	15	4	3	1.3642022	113.4722611	-4.0142917
18	18	C	17	15	4	1.4363044	115.5798218	-178.1593661
19	19	O	14	7	5	1.3725396	115.2417474	-133.3498737
20	20	N	14	7	5	1.2834724	126.9582973	48.3928755
21	21	C	19	14	7	1.4529135	106.7064857	178.8414776
22	22	C	21	19	14	1.5535572	116.5183462	115.4337036
23	23	C	22	21	19	1.5593066	102.2438896	173.1323211
24	24	C	23	22	21	1.5645872	103.9405083	70.8517143
25	25	C	20	14	7	1.4668236	107.1861839	-178.9332864
26	26	C	25	20	14	1.5493185	118.6175249	-115.1965459
27	27	C	26	25	20	1.5660019	105.1088427	79.5478687
28	28	C	22	21	19	1.5225166	114.4665788	48.2553331
29	29	C	27	26	25	1.5463218	116.3992490	-69.3067233
30	30	C	27	26	25	1.5474017	112.4535240	169.6781980
31	31	H	1	6	5	1.0981198	105.9104817	110.6689457
32	32	H	1	6	5	1.0952286	107.7724265	-135.9452468
33	33	H	2	1	6	1.0967236	110.3835799	-81.0247910
34	34	H	2	1	6	1.0960800	109.5715190	161.5519577
35	35	H	3	2	1	1.0911057	111.5841106	176.7773402
36	36	H	3	2	1	1.1057153	108.8308909	57.5627739
37	37	H	5	4	3	1.0839707	120.2599968	152.8643875
38	38	H	8	7	5	1.0868979	119.6569780	-88.0394263
39	39	H	10	7	5	1.1009865	109.6032728	-146.4967555
40	40	H	10	7	5	1.0925785	110.7349008	96.7233106
41	41	H	11	10	7	1.0956029	109.5476720	-176.6577755

42	42	H	11	10	7	1.0959821	107.4916725	68.0904362
43	43	H	12	11	10	1.0953661	110.2105207	-99.1446394
44	44	H	12	11	10	1.0949758	108.8125914	145.3155685
45	45	H	13	8	7	1.0954064	110.2313873	-159.2866749
46	46	H	13	8	7	1.1014733	106.6782611	86.4548373
47	47	H	18	17	15	1.0900890	105.4224773	-179.8253735
48	48	H	18	17	15	1.0933537	110.6862517	60.6118545
49	49	H	18	17	15	1.0931827	110.6425324	-60.2062317
50	50	H	21	19	14	1.0941662	105.9533109	-120.7114062
51	51	H	23	22	21	1.0957368	111.7317810	-50.9851101
52	52	H	23	22	21	1.0938029	110.1606657	-169.3456912
53	53	H	24	23	22	1.0949204	112.3017497	-118.8787379
54	54	H	24	23	22	1.0925626	111.8539199	121.3145556
55	55	H	25	20	14	1.0961696	107.7112806	119.6352723
56	56	H	26	25	20	1.0936662	113.7676447	-48.2940785
57	57	H	28	22	21	1.0955280	111.1636232	177.9648088
58	58	H	28	22	21	1.0966168	110.8919976	58.4672088
59	59	H	28	22	21	1.0944303	111.3089762	-61.2040529
60	60	H	29	27	26	1.0958602	109.5020659	-160.2386181
61	61	H	29	27	26	1.0857870	115.0298397	79.8263670
62	62	H	29	27	26	1.0955999	110.2329489	-42.4401017
63	63	H	30	27	26	1.0963172	109.3996459	77.3568242
64	64	H	30	27	26	1.0906014	114.9264180	-43.3407850
65	65	H	30	27	26	1.0957167	110.3543276	-165.2136694

Row	Tag	Symbol	X	Y	Z
1	1	C	-2.4508890	-1.9897930	2.6714130
2	2	C	-2.5399880	-2.8701390	1.4169690
3	3	C	-2.2007800	-2.0772790	0.1254130
4	4	C	-3.1829460	-0.9638350	-0.0078530
5	5	C	-3.3393900	-0.1090990	1.1919720
6	6	C	-3.0158430	-0.5773540	2.4996260
7	7	C	-0.0478380	1.7541840	-0.1034170
8	8	C	-1.0144050	1.4804040	-1.0142310

9	9	O	-3.0703590	0.1956790	3.4846380
10	10	C	-0.0411960	3.1069460	0.5756040
11	11	C	-1.4798760	3.5157660	0.9441130
12	12	C	-2.4646220	3.4657680	-0.2493500
13	13	C	-2.0351800	2.5122740	-1.4034930
14	14	C	0.9895720	0.7584930	0.2012770
15	15	C	-4.0917660	-0.7656420	-1.1106130
16	16	O	-4.9158570	0.1508430	-1.1724790
17	17	O	-3.9273820	-1.6692400	-2.1193430
18	18	C	-4.7821170	-1.4883320	-3.2593740
19	19	O	2.1100490	1.2517780	0.8218140
20	20	N	0.9632490	-0.4937760	-0.0787780
21	21	C	2.9893250	0.1195110	1.0580400
22	22	C	4.3479030	0.1272600	0.3045510
23	23	C	5.0769610	-1.1037760	0.9246010
24	24	C	4.2988740	-2.3325360	0.3478320
25	25	C	2.2020820	-1.0807380	0.4430840
26	26	C	3.2247610	-1.6693630	-0.5609260
27	27	C	3.9972310	-0.4315500	-1.1296710
28	28	C	5.1137320	1.4397720	0.3987580
29	29	C	3.1942750	0.5162200	-2.0505970
30	30	C	5.2359150	-0.8395410	-1.9625320
31	31	H	-1.4032000	-1.8602390	2.9737880
32	32	H	-2.9607290	-2.4524680	3.5231880
33	33	H	-3.5452460	-3.2980240	1.3211910
34	34	H	-1.8436510	-3.7116180	1.5087260
35	35	H	-2.2107830	-2.7213740	-0.7552420
36	36	H	-1.1866440	-1.6482980	0.2259600
37	37	H	-3.6526290	0.9235940	1.0898990
38	38	H	-1.0126030	0.5231920	-1.5290990
39	39	H	0.4029690	3.8561410	-0.0978910
40	40	H	0.5890580	3.0887880	1.4678920
41	41	H	-1.4749860	4.5205780	1.3807760
42	42	H	-1.8235350	2.8367050	1.7327520

43	43	H	-2.6082770	4.4695020	-0.6637270
44	44	H	-3.4476060	3.1517540	0.1168600
45	45	H	-2.9159040	2.0282640	-1.8393540
46	46	H	-1.5895220	3.1067650	-2.2166430
47	47	H	-4.5171010	-2.2887460	-3.9503140
48	48	H	-4.6105050	-0.5115360	-3.7196360
49	49	H	-5.8332830	-1.5631080	-2.9686730
50	50	H	3.1437750	0.0793860	2.1405070
51	51	H	5.0665430	-1.0721950	2.0198330
52	52	H	6.1278090	-1.1117650	0.6211880
53	53	H	3.8369060	-2.9382390	1.1343180
54	54	H	4.9541140	-3.0005730	-0.2161540
55	55	H	1.9250290	-1.8457560	1.1776430
56	56	H	2.7790640	-2.3371080	-1.3036080
57	57	H	6.0766160	1.3739570	-0.1196090
58	58	H	5.3197090	1.6981680	1.4444030
59	59	H	4.5435710	2.2651980	-0.0386960
60	60	H	3.8870130	1.1144770	-2.6531850
61	61	H	2.5469740	1.2187870	-1.5345210
62	62	H	2.5763720	-0.0637770	-2.7449590
63	63	H	4.9124640	-1.1813370	-2.9527170
64	64	H	5.8406930	-1.6357630	-1.5270030
65	65	H	5.8904130	0.0248790	-2.1206630



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5338665		
3	3	C	2	1		1.5327388	110.5393135	
4	4	C	3	2	1	1.5719680	113.0893071	-62.0560963

5	5	C	4	3	2	1.5083972	110.2275996	40.8706047
6	6	C	5	4	3	1.4363475	125.5718907	-9.3453153
7	7	C	4	3	2	2.7066777	133.6584743	178.6111818
8	8	C	7	4	3	1.5150032	29.5208640	-29.4606626
9	9	O	6	5	4	1.2467274	119.8824869	176.8532615
10	10	C	7	4	3	1.5110028	141.6638325	-5.7001761
11	11	C	10	7	4	1.5437801	112.3046430	-38.8318126
12	12	C	11	10	7	1.5335865	109.1942280	-36.8890345
13	13	C	12	11	10	1.5477633	111.2230128	63.8911853
14	14	C	7	4	3	1.4164383	98.8154829	163.7390925
15	15	C	4	3	2	1.5430599	104.1513619	-75.4327194
16	16	O	15	4	3	1.2128378	124.6250468	86.9406238
17	17	O	15	4	3	1.3536450	111.9580360	-85.8241918
18	18	C	17	15	4	1.4400575	115.7034519	175.5311580
19	19	O	14	7	4	1.3864756	116.8257191	-170.4595842
20	20	N	14	7	4	1.3039900	126.9667347	10.6995427
21	21	C	19	14	7	1.4484623	106.9989606	175.6625850
22	22	C	21	19	14	1.5505085	116.7083571	118.3693138
23	23	C	22	21	19	1.5625999	102.0748491	174.3599093
24	24	C	23	22	21	1.5648337	104.1480367	73.0893885
25	25	C	20	14	7	1.4591260	107.7500660	-177.3508429
26	26	C	24	23	22	1.5525465	102.7536715	-1.5901070
27	27	C	26	24	23	1.5647096	101.7079064	37.3722024
28	28	C	22	21	19	1.5224642	114.6858182	49.7234782
29	29	C	27	26	24	1.5417788	116.2305883	-178.8357263
30	30	C	27	26	24	1.5474226	113.0636141	60.1494314
31	31	H	1	6	5	1.0999500	107.1581645	103.7945433
32	32	H	1	6	5	1.0945734	107.6894677	-142.1924304
33	33	H	2	1	6	1.0953790	109.7705522	-73.0357860
34	34	H	2	1	6	1.0962555	110.0723890	169.5162813
35	35	H	3	2	1	1.0956025	111.0060657	175.3901190
36	36	H	3	2	1	1.0951693	108.5490358	58.5113549
37	37	H	5	4	3	1.0836657	117.7262350	172.9407163
38	38	H	8	7	4	1.0997551	103.5372330	116.2594900

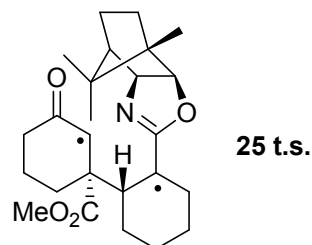
39	39	H	10	7	4	1.0947760	108.9993079	-160.9733109
40	40	H	10	7	4	1.1027901	109.5352808	84.1237269
41	41	H	11	10	7	1.0954811	109.5022121	-158.6755361
42	42	H	11	10	7	1.0976761	111.0143170	84.2829493
43	43	H	12	11	10	1.0976812	108.3512589	-56.8375374
44	44	H	12	11	10	1.0955644	111.1182597	-173.4540199
45	45	H	13	12	11	1.0946812	109.2108218	95.3732059
46	46	H	13	12	11	1.0952105	109.8239982	-147.8591521
47	47	H	18	17	15	1.0899472	105.4526180	179.3569079
48	48	H	18	17	15	1.0924801	110.3140423	59.7620333
49	49	H	18	17	15	1.0927709	110.4823741	-60.9626125
50	50	H	21	19	14	1.0951470	106.1344677	-117.5650149
51	51	H	23	22	21	1.0959429	111.3075606	-48.3844497
52	52	H	23	22	21	1.0935642	110.5355151	-166.4825222
53	53	H	24	23	22	1.0947003	112.4961744	-121.8559362
54	54	H	24	23	22	1.0926327	111.7517492	118.0499577
55	55	H	25	20	14	1.0964077	107.3736457	120.9051524
56	56	H	26	24	23	1.0931111	114.8004465	163.7578126
57	57	H	28	22	21	1.0957014	111.1245438	179.2916683
58	58	H	28	22	21	1.0966830	110.8892908	59.7506326
59	59	H	28	22	21	1.0944475	111.3142480	-59.9403670
60	60	H	29	27	26	1.0962080	109.8986707	173.4542414
61	61	H	29	27	26	1.0842890	115.0785917	51.6452897
62	62	H	29	27	26	1.0961323	109.4388538	-69.0666399
63	63	H	30	27	26	1.0960472	109.6821295	65.0110945
64	64	H	30	27	26	1.0904346	114.8994571	-56.1503385
65	65	H	30	27	26	1.0957267	110.0618449	-177.4560791

Row	Tag	Symbol	X	Y	Z
1	1	C	-4.5098940	-1.9076410	-1.3480270
2	2	C	-4.7949680	-1.3302880	0.0441450
3	3	C	-4.0770100	0.0114690	0.2272100
4	4	C	-2.5122910	-0.1092460	0.1368460
5	5	C	-2.1254170	-1.0560460	-0.9718290



6	6	C	-3.0291860	-1.8977360	-1.7052140
7	7	C	-0.4883390	1.6817990	0.2847650
8	8	C	-1.9217930	1.3382750	-0.0651430
9	9	O	-2.6020070	-2.5990090	-2.6433310
10	10	C	-0.2241170	3.1664610	0.3801330
11	11	C	-1.1996910	3.9920180	-0.4858740
12	12	C	-1.4878850	3.2308340	-1.7856550
13	13	C	-2.2135730	1.8933690	-1.5025730
14	14	C	0.5822770	0.7815940	0.5077220
15	15	C	-2.1039300	-0.7382040	1.4854330
16	16	O	-2.0657410	-1.9301130	1.7064990
17	17	O	-1.9408000	0.1963250	2.4510410
18	18	C	-1.6567290	-0.3101790	3.7688130
19	19	O	1.8066450	1.3371050	0.8463150
20	20	N	0.5474980	-0.5181580	0.4086010
21	21	C	2.7080510	0.2378880	1.1242220
22	22	C	3.9584020	0.1152150	0.2155690
23	23	C	4.7416940	-1.0546090	0.8935690
24	24	C	3.9144720	-2.3315130	0.5276120
25	25	C	1.8602410	-1.0286290	0.7896180
26	26	C	2.7261630	-1.7490450	-0.2842090
27	27	C	3.4226670	-0.6007120	-1.0870350
28	28	C	4.7543530	1.4026980	0.0520250
29	29	C	2.5121440	0.2368280	-2.0071200
30	30	C	4.5529940	-1.1083230	-2.0139700
31	31	H	-5.0332410	-1.3211730	-2.1174770
32	32	H	-4.8693700	-2.9366160	-1.4484180
33	33	H	-4.4690340	-2.0390830	0.8130610
34	34	H	-5.8734950	-1.1870150	0.1784150
35	35	H	-4.3401010	0.4699530	1.1868560
36	36	H	-4.4197200	0.6992890	-0.5530780
37	37	H	-1.0736560	-1.1401750	-1.2189170
38	38	H	-2.5112090	1.9612090	0.6233360
39	39	H	0.8080200	3.3651760	0.0739630

40	40	H	-0.2842680	3.4847540	1.4342760
41	41	H	-0.7622050	4.9745450	-0.6940220
42	42	H	-2.1388120	4.1806500	0.0501880
43	43	H	-0.5330710	3.0353880	-2.2906650
44	44	H	-2.0847670	3.8383370	-2.4748090
45	45	H	-3.2931700	2.0397320	-1.6092270
46	46	H	-1.9207200	1.1467810	-2.2484480
47	47	H	-0.7348650	-0.8963430	3.7592540
49	49	H	-2.4773130	-0.9397310	4.1215940
50	50	H	2.9986710	0.3408610	2.1750710
51	51	H	4.8241120	-0.9040310	1.9759850
52	52	H	5.7641290	-1.1053330	0.5089440
53	53	H	3.5713560	-2.8762780	1.4129770
54	54	H	4.4994470	-3.0357800	-0.0687590
55	55	H	1.7145240	-1.7033550	1.6414520
56	56	H	2.1702870	-2.4827100	-0.8738100
57	57	H	5.6292610	1.2473370	-0.5890370
58	58	H	5.1157590	1.7648910	1.0220330
59	59	H	4.1422150	2.1955300	-0.3890190
60	60	H	3.0770880	1.0777150	-2.4259510
61	61	H	1.6242770	0.6392300	-1.5323070
62	62	H	2.1773720	-0.3803150	-2.8488850
63	63	H	4.1292560	-1.7480040	-2.7966410
64	64	H	5.3359080	-1.6787780	-1.5132960
65	65	H	5.0353990	-0.2624710	-2.5164010



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5354985		

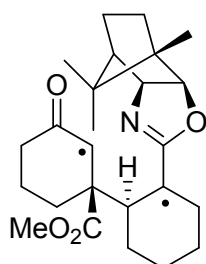
3	3	C	2	1		1.5532582	111.9007821	
4	4	C	3	2	1	1.4905482	107.5816669	-60.4859681
5	5	C	4	3	2	1.4787166	115.9281045	52.4364933
6	6	C	5	4	3	1.4291674	121.4430713	-24.8116818
7	7	C	3	2	1	4.3629495	148.9527251	46.0311194
8	8	C	7	3	2	1.3467447	69.9520236	9.0923082
9	9	O	6	5	4	1.2512559	120.9372195	176.0752171
10	10	C	7	3	2	1.5171151	119.2675640	125.9350908
11	11	C	10	7	3	1.5360112	112.0052407	-68.2064819
12	12	C	11	10	7	1.5341123	111.2005948	-45.6687935
13	13	C	8	7	3	1.5047569	123.9268267	113.4846160
14	14	C	7	3	2	1.4753067	82.5591596	-115.9381526
15	15	C	4	3	2	1.4443150	124.8237930	-117.1837204
16	16	O	15	4	3	1.2335185	124.1068190	176.1703211
17	17	O	15	4	3	1.3651394	113.5060867	-5.2135035
18	18	C	17	15	4	1.4358836	115.5723419	-178.7056056
19	19	O	14	7	3	1.3716339	114.9241235	-137.0602605
20	20	N	14	7	3	1.2826145	127.2507968	45.0924804
21	21	C	19	14	7	1.4559075	106.6252861	178.6618407
22	22	C	21	19	14	1.5491155	116.5543155	117.1053062
23	23	C	22	21	19	1.5630717	101.7819420	174.7674959
24	24	C	23	22	21	1.5652531	104.1605477	73.0753021
25	25	C	20	14	7	1.4683492	107.2667177	179.5816640
26	26	C	24	23	22	1.5529031	102.6788110	-1.6674307
27	27	C	26	24	23	1.5649465	101.7299956	37.4959680
28	28	C	22	21	19	1.5224856	114.7061413	50.2224501
29	29	C	27	26	24	1.5426749	116.4135380	-179.1487623
30	30	C	27	26	24	1.5476620	113.0309170	60.0273703
31	31	H	1	6	5	1.0979651	105.9354429	110.8815120
32	32	H	1	6	5	1.0951714	107.7412455	-135.9232618
33	33	H	2	1	6	1.0965992	110.3034887	-80.5432984
34	34	H	2	1	6	1.0961981	109.8284572	162.0838273
35	35	H	3	2	1	1.0909057	111.5364981	177.3084085
36	36	H	3	2	1	1.1008627	108.6554212	58.3259547

37	37	H	5	4	3	1.0837492	120.3280701	149.8928343
38	38	H	8	7	3	1.0879446	118.2342485	-67.3043138
39	39	H	10	7	3	1.0990247	109.2086026	169.4227982
40	40	H	10	7	3	1.0958172	109.5773270	54.5568860
41	41	H	11	10	7	1.0960051	109.7383193	-168.4192778
42	42	H	11	10	7	1.0990138	109.3221873	74.9210192
43	43	H	12	11	10	1.0985097	109.1476084	-59.7302488
44	44	H	12	11	10	1.0960100	110.8450699	-177.0123511
45	45	H	13	8	7	1.1020218	108.8630119	-108.9770099
46	46	H	13	8	7	1.0980364	109.2105292	136.6856502
47	47	H	18	17	15	1.0901578	105.4499508	-179.6528154
48	48	H	18	17	15	1.0933740	110.6811763	60.8108227
49	49	H	18	17	15	1.0932168	110.6508993	-60.0242828
50	50	H	21	19	14	1.0941664	105.8470292	-118.9430537
51	51	H	23	22	21	1.0958617	111.3032830	-48.2849451
52	52	H	23	22	21	1.0938090	110.5520073	-166.4005411
53	53	H	24	23	22	1.0941262	112.4297985	-121.7985596
54	54	H	24	23	22	1.0928808	111.7045847	118.0115955
55	55	H	25	20	14	1.0946269	107.7223053	121.4933809
56	56	H	26	24	23	1.0935152	114.7425323	163.6356135
57	57	H	28	22	21	1.0956193	111.1148479	179.1978972
58	58	H	28	22	21	1.0967580	110.8884439	59.7020094
59	59	H	28	22	21	1.0945532	111.3259620	-60.0142239
60	60	H	29	27	26	1.0962431	109.8649499	173.1999993
61	61	H	29	27	26	1.0838842	115.4719540	51.1445094
62	62	H	29	27	26	1.0963078	109.3142703	-69.4956976
63	63	H	30	27	26	1.0961626	109.5855495	64.1270698
64	64	H	30	27	26	1.0907127	115.0169365	-56.9797115
65	65	H	30	27	26	1.0958956	110.1405299	-178.3917986

Row	Tag	Symbol	X	Y	Z
1	1	C	-4.6775467	-1.0327222	-1.8130503
2	2	C	-4.9177717	-0.5757681	-0.3669381
3	3	C	-3.6148095	-0.0570660	0.3007810

4	4	C	-2.6343774	-1.1797622	0.3071030
5	5	C	-2.3939184	-1.8355163	-0.9962652
6	6	C	-3.3734315	-1.8080693	-2.0366113
7	7	C	-0.0146360	2.3961934	0.0649900
8	8	C	-0.8157811	2.6496714	-0.9874532
9	9	O	-3.1322775	-2.3026304	-3.1603975
10	10	C	0.2563030	3.4218875	1.1495092
11	11	C	-0.7528101	4.5793067	1.1120692
12	12	C	-0.9625881	5.0863248	-0.3205600
13	13	C	-1.5096032	3.9650096	-1.2172132
14	14	C	0.6539501	1.0849532	0.1658440
15	15	C	-2.0879203	-1.7908773	1.4962072
16	16	O	-1.3292772	-2.7634814	1.4878522
17	17	O	-2.4670344	-1.1695172	2.6511054
18	18	C	-1.9251173	-1.7237203	3.8598016
19	19	O	1.7357933	1.0510192	1.0083662
20	20	N	0.3563371	0.0108690	-0.4688761
21	21	C	2.2305663	-0.3181830	0.9960541
22	22	C	3.6654576	-0.5311651	0.4524691
23	23	C	3.8859106	-2.0549773	0.7218941
24	24	C	2.9923285	-2.7662844	-0.3484191
25	25	C	1.3072892	-1.0241392	-0.0440260
26	26	C	2.3254654	-1.5720962	-1.0837532
27	27	C	3.4911915	-0.5285641	-1.1181152
28	28	C	4.7191027	0.3833181	1.0619892
29	29	C	3.1765445	0.8303811	-1.7769863
30	30	C	4.7409727	-1.0415262	-1.8732143
31	31	H	-4.6322657	-0.1662950	-2.4859404
32	32	H	-5.5023519	-1.6554913	-2.1753423
33	33	H	-5.3151319	-1.4035012	0.2326390
34	34	H	-5.6731878	0.2183720	-0.3485451
35	35	H	-3.8011986	0.3097270	1.3111262
36	36	H	-3.2208705	0.7785581	-0.2979200
37	37	H	-1.4296772	-2.2786133	-1.2163022

38	38	H	-0.9624661	1.8625073	-1.7239853
39	39	H	1.2795622	3.8064716	1.0359702
40	40	H	0.2382710	2.9329814	2.1300503
41	41	H	-0.4090031	5.3913378	1.7629373
42	42	H	-1.7149133	4.2361897	1.5176052
43	43	H	-0.0022890	5.4362619	-0.7231681
44	44	H	-1.6426162	5.9457469	-0.3344621
45	45	H	-2.5895394	3.8336856	-1.0413042
46	46	H	-1.4221312	4.2393896	-2.2768114
47	47	H	-2.3337784	-1.1154502	4.6669247
48	48	H	-0.8331241	-1.6690973	3.8539776
49	49	H	-2.2271043	-2.7681384	3.9743336
50	50	H	2.1441973	-0.6763621	2.0263203
51	51	H	3.6039856	-2.3230124	1.7463883
52	52	H	4.9426878	-2.3152574	0.6128321
53	53	H	2.2478873	-3.4289665	0.1029920
54	54	H	3.5883865	-3.3765635	-1.0315462
55	55	H	0.7307231	-1.8532203	0.3783531
56	56	H	1.8759183	-1.8221583	-2.0487153
57	57	H	5.7112919	0.1736430	0.6472861
58	58	H	4.7789067	0.2416640	2.1479153
59	59	H	4.4858807	1.4369112	0.8786981
60	60	H	4.0195856	1.5167922	-1.6360243
61	61	H	2.2828374	1.3270432	-1.4172372
62	62	H	3.0516805	0.6894611	-2.8570054
63	63	H	4.4917907	-1.2042942	-2.9281964
64	64	H	5.1619108	-1.9718613	-1.4898842
65	65	H	5.5355218	-0.2873250	-1.8438983



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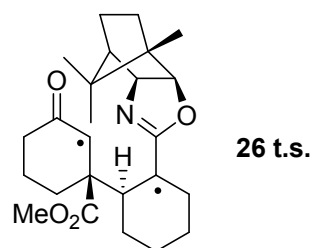
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5325379		
3	3	C	2	1		1.5352539	110.8899151	
4	4	C	3	2	1	1.5518382	114.0115158	-58.8050164
5	5	C	4	3	2	1.5090534	111.9054929	30.5760229
6	6	C	5	4	3	1.4371542	125.7623578	-0.1920229
7	7	C	4	3	2	2.6040324	95.0216795	-66.6820830
8	8	C	7	4	3	1.5138527	34.5102542	-127.6821132
9	9	O	6	5	4	1.2466423	120.0786779	177.8385609
10	10	C	7	4	3	1.5080482	122.7991725	-25.5876629
11	11	C	10	7	4	1.5424733	113.9747777	-58.2243800
12	12	C	11	10	7	1.5314887	110.6074786	-29.2948392
13	13	C	12	11	10	1.5343370	109.5348478	65.1332440
14	14	C	7	4	3	1.4260585	110.2936126	121.5477200
15	15	C	4	3	2	1.5538443	109.0546700	147.3267883
16	16	O	15	4	3	1.2136731	125.3414017	-1.1771735
17	17	O	15	4	3	1.3485153	111.6537507	179.3752614
18	18	C	17	15	4	1.4420681	116.1438704	178.3675890
19	19	O	14	7	4	1.3819283	117.2475945	-139.2360373
20	20	N	14	7	4	1.3038738	126.1324486	43.1119322
21	21	C	19	14	7	1.4511571	106.8787156	175.9215791
22	22	C	21	19	14	1.5504898	116.7882298	118.5203598
23	23	C	22	21	19	1.5626693	101.9692829	174.1837191
24	24	C	23	22	21	1.5649543	104.1494795	72.9201326
25	25	C	20	14	7	1.4602519	107.3849724	-177.3495994
26	26	C	24	23	22	1.5526714	102.7400836	-1.4605020
27	27	C	26	24	23	1.5655249	101.7306759	37.2889541
28	28	C	22	21	19	1.5225612	114.7155251	49.6749794
29	29	C	27	26	24	1.5417226	116.2670652	-178.7873084
30	30	C	27	26	24	1.5474051	112.8949926	60.3150708
31	31	H	1	6	5	1.0997994	107.8718644	96.1388406
32	32	H	1	6	5	1.0943823	108.0170929	-148.8580279
33	33	H	2	1	6	1.0959308	109.1595380	-68.1961600

34	34	H	2	1	6	1.0961720	110.1340361	175.1240669
35	35	H	3	2	1	1.0939828	110.2992886	177.4329563
36	36	H	3	2	1	1.0940064	108.6817201	61.9888337
37	37	H	5	4	3	1.0840530	118.0075442	179.2915348
38	38	H	8	7	4	1.0929441	105.8485410	-113.6958163
39	39	H	10	7	4	1.0971017	107.5688388	-179.9724522
40	40	H	10	7	4	1.1013187	110.5381191	66.8077067
41	41	H	11	10	7	1.0955952	109.2128981	-152.0897838
42	42	H	11	10	7	1.0978716	110.6608817	91.2535827
43	43	H	12	11	10	1.0991332	109.8400322	-56.5280587
44	44	H	12	11	10	1.0962325	110.7207655	-174.1561504
45	45	H	13	12	11	1.0966531	107.4147046	67.1800720
46	46	H	13	12	11	1.0952552	110.2835517	-177.5956321
47	47	H	18	17	15	1.0894380	105.3019349	-179.0722101
48	48	H	18	17	15	1.0925597	110.3770706	61.2911141
49	49	H	18	17	15	1.0923737	110.2736087	-59.5520822
50	50	H	21	19	14	1.0944284	106.0302526	-117.3479092
51	51	H	23	22	21	1.0957088	111.3318385	-48.4885079
52	52	H	23	22	21	1.0935828	110.5187441	-166.6008607
53	53	H	24	23	22	1.0944908	112.4188849	-121.6390824
54	54	H	24	23	22	1.0927317	111.7438238	118.2471887
55	55	H	25	20	14	1.0962633	107.1256751	119.6408434
56	56	H	26	24	23	1.0934860	114.8082234	163.5832063
57	57	H	28	22	21	1.0957024	111.1694390	179.2620037
58	58	H	28	22	21	1.0966442	110.8283078	59.7581326
59	59	H	28	22	21	1.0943941	111.3831682	-59.8969148
60	60	H	29	27	26	1.0962885	109.8468547	175.0652874
61	61	H	29	27	26	1.0844295	115.1641644	53.2469268
62	62	H	29	27	26	1.0963963	109.4415876	-67.5332386
63	63	H	30	27	26	1.0962265	109.5883836	65.1250986
64	64	H	30	27	26	1.0905581	114.9344302	-55.8911391
65	65	H	30	27	26	1.0959070	110.2120059	-177.3630275



Row	Tag	Symbol	X	Y	Z
1	1	C	2.4609110	-2.3538500	-2.2299910
2	2	C	2.5525790	-0.8561260	-2.5415870
3	3	C	3.3337310	-0.1159740	-1.4466070
4	4	C	2.7187190	-0.2548290	-0.0286220
5	5	C	2.0045720	-1.5723160	0.1487600
6	6	C	1.8799920	-2.6009100	-0.8471750
7	7	C	0.5599350	1.0914950	-0.5836430
8	8	C	1.7326140	0.9493530	0.3631250
9	9	O	1.2989910	-3.6692070	-0.5727730
10	10	C	0.5034300	2.1312220	-1.6745070
11	11	C	1.5176200	3.2799990	-1.4985700
12	12	C	1.8149230	3.5140060	-0.0145520
13	13	C	2.5188730	2.2815240	0.5682280
14	14	C	-0.5962760	0.2891260	-0.3533760
15	15	C	3.8623330	-0.2473430	1.0232920
16	16	O	5.0470590	-0.1688580	0.7717630
17	17	O	3.3835470	-0.3520700	2.2795920
18	18	C	4.3672970	-0.3915540	3.3332700
19	19	O	-1.6215820	0.3773970	-1.2757000
20	20	N	-0.7985730	-0.4918590	0.6709410
21	21	C	-2.6275770	-0.5912860	-0.8813850
22	22	C	-4.0295340	-0.0355690	-0.5212270
23	23	C	-4.8531430	-1.3465480	-0.3092420
24	24	C	-4.3315690	-1.9097010	1.0545400
25	25	C	-2.0784640	-1.1630390	0.4618190
26	26	C	-3.2401870	-0.8804970	1.4550560
27	27	C	-3.8776980	0.4645120	0.9698770
28	28	C	-4.6168770	0.9238320	-1.5472730
29	29	C	-3.0336100	1.7365060	1.1854120
30	30	C	-5.2294890	0.7724060	1.6571360
31	31	H	3.4619150	-2.8083220	-2.2616920
32	32	H	1.8466360	-2.8944060	-2.9567220
33	33	H	1.5408850	-0.4477500	-2.6453590

34	34	H	3.0526860	-0.7009970	-3.5046140
35	35	H	3.4325200	0.9434130	-1.7010440
36	36	H	4.3540010	-0.5097030	-1.4169990
37	37	H	1.5470280	-1.7779940	1.1097600
38	38	H	1.3061450	0.6487350	1.3234790
39	39	H	-0.5151320	2.5385050	-1.6913660
40	40	H	0.6236640	1.6609600	-2.6630920
41	41	H	1.1226640	4.1853690	-1.9725360
42	42	H	2.4587460	3.0482270	-2.0142110
43	43	H	0.8795240	3.7166950	0.5258550
44	44	H	2.4537170	4.3948420	0.1188490
45	45	H	3.5078940	2.2159410	0.0989900
46	46	H	2.6991660	2.4185240	1.6398200
47	47	H	3.7966530	-0.4931650	4.2557210
48	48	H	4.9548780	0.5295280	3.3398520
49	49	H	5.0355020	-1.2446630	3.1954750
50	50	H	-2.6920640	-1.3114830	-1.7029270
51	51	H	-4.7037920	-2.0492620	-1.1365660
52	52	H	-5.9238240	-1.1259520	-0.2791920
53	53	H	-3.9194330	-2.9191270	0.9590770
54	54	H	-5.1272320	-1.9621960	1.8016860
55	55	H	-1.8770820	-2.2402470	0.4324680
56	56	H	-2.9365010	-0.9188850	2.5048240
57	57	H	-5.6106930	1.2698300	-1.2420210
58	58	H	-4.7232280	0.4342600	-2.5227920
59	59	H	-3.9763310	1.8001760	-1.6866300
60	60	H	-3.5367780	2.5984000	0.7317500
61	61	H	-2.0261980	1.6945270	0.7862300
62	62	H	-2.9480320	1.9400580	2.2593430
63	63	H	-5.0679670	0.9362030	2.7289540
64	64	H	-5.9845390	-0.0080790	1.5568380
65	65	H	-5.6581350	1.6963280	1.2526080



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5349043		
3	3	C	2	1		1.5342956	111.4441025	
4	4	C	3	2	1	1.5097742	111.8475408	-48.6819735
5	5	C	4	3	2	1.3504486	122.6570294	21.3586112
6	6	C	5	4	3	1.4837011	122.2757410	2.2397885
7	7	C	2	1	6	8.2417404	139.1899720	-101.1665803
8	8	C	7	2	1	1.3467782	94.2657825	-138.8268689
9	9	O	6	5	4	1.2249477	120.5876445	-179.1334189
10	10	C	7	2	1	1.5172359	108.3384695	-12.5146177
11	11	C	10	7	2	1.5361608	112.0679813	-93.0224759
12	12	C	11	10	7	1.5340147	111.2356116	-45.2895103
13	13	C	8	7	2	1.5041590	123.9337456	116.5634006
14	14	C	7	2	1	1.4763545	66.4994580	101.1512331
15	15	C	4	3	2	1.4985773	115.9695623	-159.5794834
16	16	O	15	4	3	1.2179454	123.2003679	-0.8460885
17	17	O	15	4	3	1.3479993	113.4604862	179.4014853
18	18	C	17	15	4	1.4411081	115.8731396	179.8650903
19	19	O	14	7	2	1.3761502	115.1016395	-102.6076210
20	20	N	14	7	2	1.2808474	127.1927376	79.3084770
21	21	C	19	14	7	1.4519311	106.5710223	177.2486936
22	22	C	21	19	14	1.5492993	116.5789686	117.7355185
23	23	C	22	21	19	1.5627276	101.9852893	174.7802725
24	24	C	23	22	21	1.5650063	104.1444171	73.0298217
25	25	C	20	14	7	1.4649401	107.3108089	-179.0241313
26	26	C	24	23	22	1.5526793	102.7426021	-1.7120423
27	27	C	26	24	23	1.5659767	101.6127807	37.5542860
28	28	C	22	21	19	1.5226404	114.6888135	50.2617977

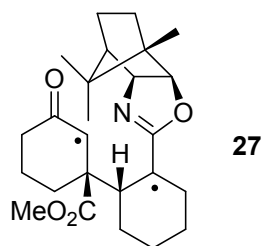
29	29	C	27	26	24	1.5423283	116.4134558	-179.2874378
30	30	C	27	26	24	1.5480042	112.9126979	59.9395814
31	31	H	1	6	5	1.1010429	106.8257318	89.6151791
32	32	H	1	6	5	1.0936201	108.3149471	-155.5629726
33	33	H	2	1	6	1.0982139	109.1982067	-66.7336619
34	34	H	2	1	6	1.0950224	110.2874331	176.2719703
35	35	H	3	2	1	1.0937758	111.2877868	-171.1866522
36	36	H	3	2	1	1.1007222	110.3779399	72.2352109
37	37	H	5	4	3	1.0847287	121.5324530	-179.1088102
38	38	H	8	7	2	1.0875464	118.1386150	-63.5765115
39	39	H	10	7	2	1.0996400	109.2524058	144.6701105
40	40	H	10	7	2	1.0953014	109.5266383	29.7783672
41	41	H	11	10	7	1.0961191	109.7322995	-168.1389701
42	42	H	11	10	7	1.0989629	109.2837904	75.1909505
43	43	H	12	11	10	1.0985793	109.1325940	-59.4822565
44	44	H	12	11	10	1.0961142	110.8725818	-176.8494936
45	45	H	13	8	7	1.1018390	108.7857870	-109.1313453
46	46	H	13	8	7	1.0983064	109.2104285	136.5581090
47	47	H	18	17	15	1.0893499	105.2933282	179.9021925
48	48	H	18	17	15	1.0925200	110.3292743	60.3001840
49	49	H	18	17	15	1.0924934	110.3227888	-60.5022483
50	50	H	21	19	14	1.0944930	105.9812837	-118.2507064
51	51	H	23	22	21	1.0958900	111.2791131	-48.3817882
52	52	H	23	22	21	1.0937315	110.5574523	-166.4543928
53	53	H	24	23	22	1.0947739	112.4131409	-121.9132319
54	54	H	24	23	22	1.0929244	111.6983875	118.0477003
55	55	H	25	20	14	1.0959569	107.7259356	121.1754617
56	56	H	26	24	23	1.0935147	114.7842406	163.6479108
57	57	H	28	22	21	1.0957397	111.1646920	179.1466625
58	58	H	28	22	21	1.0967589	110.8392711	59.6665509
59	59	H	28	22	21	1.0944061	111.3850843	-59.9882210
60	60	H	29	27	26	1.0962202	109.8308151	173.2800544
61	61	H	29	27	26	1.0839577	115.4065181	51.0905644
62	62	H	29	27	26	1.0962800	109.2590135	-69.4522838

63	63	H	30	27	26	1.0962105	109.5710778	64.2131357
64	64	H	30	27	26	1.0904951	114.9702441	-56.8657674
65	65	H	30	27	26	1.0959367	110.1814259	-178.2949105

Row	Tag	Symbol	X	Y	Z
1	1	C	-5.6614630	2.8275300	1.2381690
2	2	C	-4.5853570	2.5026180	0.1930090
3	3	C	-5.1313320	1.5828100	-0.9069580
4	4	C	-5.8674940	0.3961990	-0.3329910
5	5	C	-6.3769180	0.3900170	0.9176730
6	6	C	-6.2951740	1.5708290	1.8123070
7	7	C	3.6257700	2.0927300	-0.3863610
8	8	C	3.6693080	2.6696500	-1.6025350
9	9	O	-6.7539910	1.5259610	2.9471950
10	10	C	4.2244020	2.7437970	0.8464230
11	11	C	4.5364290	4.2307800	0.6199040
12	12	C	5.2356270	4.4528340	-0.7273210
13	13	C	4.3366350	3.9881710	-1.8830190
14	14	C	2.9794380	0.7736120	-0.2386950
15	15	C	-6.0239040	-0.7827380	-1.2447900
16	16	O	-5.6056500	-0.8013870	-2.3885150
17	17	O	-6.6765180	-1.8169370	-0.6776660
18	18	C	-6.8587210	-2.9785540	-1.5108770
19	19	O	3.0574770	0.2228960	1.0200390
20	20	N	2.3967490	0.0903130	-1.1520110
21	21	C	2.3146950	-1.0237800	0.9733730
22	22	C	3.1177300	-2.3198650	1.2483760
23	23	C	1.9924640	-3.4042460	1.2518370
24	24	C	1.5946900	-3.5474210	-0.2549880
25	25	C	1.8920390	-1.1339030	-0.5254230
26	26	C	2.5035870	-2.4980320	-0.9503310
27	27	C	3.8290090	-2.6344220	-0.1275690
28	28	C	3.9693580	-2.2847420	2.5100930
29	29	C	4.9893500	-1.7044050	-0.5367800

30	30	C	4.4347430	-4.0575270	-0.1921870
31	31	H	-6.4722960	3.4094840	0.7732230
32	32	H	-5.2750780	3.4270970	2.0671630
33	33	H	-3.7397340	2.0062720	0.6876160
34	34	H	-4.1948470	3.4250920	-0.2492780
35	35	H	-4.3302590	1.2278830	-1.5616750
36	36	H	-5.8196060	2.1369350	-1.5633220
37	37	H	-6.8904010	-0.4781320	1.3167830
38	38	H	3.1959500	2.1514330	-2.4332820
39	39	H	5.1391720	2.2050250	1.1330040
40	40	H	3.5400680	2.6230720	1.6930620
41	41	H	5.1527940	4.6092260	1.4435240
42	42	H	3.5995270	4.8049230	0.6370500
43	43	H	6.1732440	3.8806120	-0.7450090
44	44	H	5.5054040	5.5071360	-0.8582180
45	45	H	3.5599440	4.7428080	-2.0863000
46	46	H	4.9132670	3.9104340	-2.8145390
47	47	H	-7.3944450	-3.6960120	-0.8904440
48	48	H	-5.8906090	-3.3795770	-1.8199720
49	49	H	-7.4418760	-2.7213550	-2.3981880
50	50	H	1.4939040	-0.9124770	1.6887950
51	51	H	1.1483580	-3.0994580	1.8807760
52	52	H	2.3658960	-4.3439050	1.6687760
53	53	H	0.5334800	-3.3414010	-0.4279590
54	54	H	1.7856780	-4.5563610	-0.6292170
55	55	H	0.8066540	-1.1620960	-0.6746410
56	56	H	2.5957940	-2.6173010	-2.0334040
57	57	H	4.4991020	-3.2327010	2.6563480
58	58	H	3.3464180	-2.1151620	3.3966980
59	59	H	4.7100600	-1.4801160	2.4693220
60	60	H	5.8147070	-1.8029730	0.1779010
61	61	H	4.7379970	-0.6526840	-0.6120720
62	62	H	5.3716460	-2.0129360	-1.5168250
63	63	H	4.7312220	-4.2839610	-1.2229660

64	64	H	3.7703680	-4.8561270	0.1395110
65	65	H	5.3412590	-4.1108100	0.4213820



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5342091		
3	3	C	2	1		1.5346884	110.8720011	
4	4	C	3	2	1	1.5521074	114.5321112	-58.6905024
5	5	C	4	3	2	1.5091980	111.2950329	35.0878358
6	6	C	5	4	3	1.4373389	125.7487966	-6.2676596
7	7	C	4	3	2	2.6333641	89.2279375	-108.3229007
8	8	C	7	4	3	1.5186402	33.7140007	144.3215149
9	9	O	6	5	4	1.2466721	119.8309126	-179.5232794
10	10	C	7	4	3	1.4996854	121.0519806	51.4423572
11	11	C	10	7	4	1.5584282	110.5875063	98.5713907
12	12	C	11	10	7	1.5466540	111.5775399	-32.0366142
13	13	C	12	11	10	1.5356775	111.3574987	-26.9021390
14	14	C	7	4	3	1.4185918	111.8791865	-101.5995336
15	15	C	4	3	2	1.5573143	108.4264503	150.6698163
16	16	O	15	4	3	1.2124844	124.9140429	1.4359304
17	17	O	15	4	3	1.3453624	111.3855930	-175.3646025
18	18	C	17	15	4	1.4393829	116.1146829	-177.0461323
19	19	O	14	7	4	1.3839346	117.6173491	147.6679660
20	20	N	14	7	4	1.3062715	125.9273916	-31.8804285
21	21	C	19	14	7	1.4483896	107.0606268	174.7874458
22	22	C	21	19	14	1.5506568	116.6084844	119.0319925
23	23	C	22	21	19	1.5622777	102.1677805	174.7508671
24	24	C	23	22	21	1.5645574	104.1261344	72.8541487
25	25	C	20	14	7	1.4610560	107.3027680	-176.9279331

26	26	C	24	23	22	1.5529397	102.7558979	-1.4584090
27	27	C	26	24	23	1.5660778	101.7500439	37.2238097
28	28	C	22	21	19	1.5224773	114.5233196	50.1663578
29	29	C	27	26	24	1.5409603	116.3467621	-178.7394668
30	30	C	27	26	24	1.5475975	112.7186157	60.4320495
31	31	H	1	6	5	1.0997841	107.2480518	97.7679418
32	32	H	1	6	5	1.0944299	107.9482113	-147.7951762
33	33	H	2	1	6	1.0960588	109.6491586	-72.4913143
34	34	H	2	1	6	1.0960817	109.7876392	171.2274642
35	35	H	3	2	1	1.0932526	110.8620322	176.9118764
36	36	H	3	2	1	1.0941455	108.3866172	61.4887574
37	37	H	5	4	3	1.0859638	118.3701881	173.7403591
38	38	H	8	7	4	1.0946262	107.4386339	116.3877468
39	39	H	10	7	4	1.0991965	108.7949830	-20.0928310
40	40	H	10	7	4	1.0907654	111.2342926	-137.8913123
41	41	H	11	10	7	1.0964603	108.5415582	-153.9302483
42	42	H	11	10	7	1.0952973	109.4166031	89.9140281
43	43	H	12	11	10	1.0955680	110.3455498	-149.6953270
44	44	H	12	11	10	1.0981806	109.8311752	93.3615474
45	45	H	13	12	11	1.0942361	110.3400640	-172.8465229
46	46	H	13	12	11	1.0955863	109.1573228	-56.4528099
47	47	H	18	17	15	1.0897929	105.4005397	-176.8629830
48	48	H	18	17	15	1.0917714	109.3826636	64.0104166
49	49	H	18	17	15	1.0924341	110.4345129	-57.1548076
50	50	H	21	19	14	1.0951550	106.2209742	-116.8894525
51	51	H	23	22	21	1.0960043	111.3789204	-48.6329753
52	52	H	23	22	21	1.0937058	110.4986193	-166.7948833
53	53	H	24	23	22	1.0949838	112.4263584	-121.7694532
54	54	H	24	23	22	1.0927192	111.7542156	118.2450331
55	55	H	25	20	14	1.0965999	107.2231602	121.3004405
56	56	H	26	24	23	1.0931239	114.9159797	163.2427131
57	57	H	28	22	21	1.0956170	111.1727692	179.7302528
58	58	H	28	22	21	1.0968292	110.8439772	60.2379532
59	59	H	28	22	21	1.0943841	111.3155094	-59.4440649

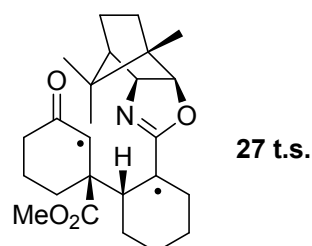


60	60	H	29	27	26	1.0963768	109.5831086	179.4494621
61	61	H	29	27	26	1.0836587	115.1650600	58.2469334
62	62	H	29	27	26	1.0946886	109.8219007	-62.5098681
63	63	H	30	27	26	1.0960352	109.5307618	67.0912263
64	64	H	30	27	26	1.0905709	115.0262496	-54.0757946
65	65	H	30	27	26	1.0956246	110.1079519	-175.5088817

Row	Tag	Symbol	X	Y	Z
1	1	C	4.6948510	-0.6531280	1.9694810
2	2	C	3.4658830	0.2205440	2.2525580
3	3	C	2.2100970	-0.3748300	1.6015590
4	4	C	2.3023460	-0.5469360	0.0617840
5	5	C	3.7012320	-0.9189360	-0.3653140
6	6	C	4.8536980	-0.9759400	0.4917250
7	7	C	0.6049940	1.4456230	-0.2268530
8	8	C	1.8290130	0.7384280	-0.7817590
9	9	O	5.9636000	-1.2894650	0.0184270
10	10	C	0.8321820	2.7606130	0.4574300
11	11	C	1.4749850	3.7856560	-0.5248070
12	12	C	2.3961950	3.0877990	-1.5526720
13	13	C	2.9661000	1.7762170	-0.9929700
14	14	C	-0.7060520	0.9859230	-0.5136230
15	15	C	1.4068390	-1.7514690	-0.3534210
16	16	O	0.7357250	-2.4127930	0.4097140
17	17	O	1.5209070	-2.0176500	-1.6672460
18	18	C	0.6844240	-3.0733710	-2.1747620
19	19	O	-1.7673070	1.7372260	-0.0397490
20	20	N	-1.0104150	-0.0942690	-1.1821240
21	21	C	-2.9783830	1.1389030	-0.5623740
22	22	C	-3.9951910	0.6054660	0.4797790
23	23	C	-5.1965780	0.1764080	-0.4220470
24	24	C	-4.6960680	-1.1254500	-1.1309160
25	25	C	-2.4661360	-0.1370800	-1.2992920
26	26	C	-3.2496660	-1.2778470	-0.5865650

27	27	C	-3.4153100	-0.8026080	0.8964420
28	28	C	-4.3491970	1.5951360	1.5812190
29	29	C	-2.1377200	-0.7920820	1.7579590
30	30	C	-4.4169120	-1.6717180	1.6942510
31	31	H	4.6026720	-1.6097570	2.5041670
32	32	H	5.6247170	-0.1912960	2.3156560
33	33	H	3.6504790	1.2417250	1.8997710
34	34	H	3.3051470	0.2955860	3.3341900
35	35	H	1.3252600	0.2178250	1.8485910
36	36	H	2.0319690	-1.3632940	2.0355680
37	37	H	3.8731140	-1.1688540	-1.4080580
38	38	H	1.5630380	0.3486280	-1.7694430
39	39	H	1.5260530	2.6081470	1.2961970
40	40	H	-0.0954870	3.1541680	0.8749390
41	41	H	2.0413940	4.5204820	0.0595190
42	42	H	0.6841510	4.3371180	-1.0445640
43	43	H	3.2096970	3.7579170	-1.8517130
44	44	H	1.8305560	2.8610290	-2.4662520
45	45	H	3.7110020	1.3617780	-1.6790560
46	46	H	3.4947280	1.9846800	-0.0562710
47	47	H	0.9555600	-3.1778580	-3.2251030
48	48	H	-0.3638630	-2.7860210	-2.0723460
49	49	H	0.8714040	-4.0026190	-1.6316700
50	50	H	-3.4402250	1.8952200	-1.2058420
51	51	H	-5.4634280	0.9656420	-1.1341750
52	52	H	-6.0864870	-0.0063560	0.1869290
53	53	H	-4.7121190	-1.0393320	-2.2223900
54	54	H	-5.3141510	-1.9893470	-0.8746140
55	55	H	-2.7054430	-0.1524820	-2.3693510
56	56	H	-2.8080440	-2.2683680	-0.7235250
57	57	H	-5.0728040	1.1647690	2.2823280
58	58	H	-4.7978880	2.5032680	1.1604970
59	59	H	-3.4613740	1.8964350	2.1457240
60	60	H	-2.3772730	-0.4339370	2.7661200

61	61	H	-1.3309420	-0.1762600	1.3782370
62	62	H	-1.7450260	-1.8095740	1.8520050
63	63	H	-4.0069740	-2.6802710	1.8209980
64	64	H	-5.4031870	-1.7734870	1.2401040
65	65	H	-4.5604750	-1.2558800	2.6976760



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5371372		
3	3	C	2	1		1.5355644	111.6588229	
4	4	C	3	2	1	1.5108136	113.5616269	-50.2925123
5	5	C	4	3	2	1.4789496	117.9108804	22.1961874
6	6	C	5	4	3	1.4252163	123.2510819	2.5764938
7	7	C	4	3	2	3.2063643	89.2213636	-97.4695350
8	8	C	7	4	3	1.3930968	46.7084290	145.1571244
9	9	O	6	5	4	1.2561397	120.6167704	-176.3776302
10	10	C	7	4	3	1.5045188	117.2355193	42.1888643
11	11	C	10	7	4	1.5603165	111.3663910	105.7392921
12	12	C	11	10	7	1.5467103	112.7058317	-32.1110267
13	13	C	8	7	4	1.5157735	116.2959973	-116.0554868
14	14	C	7	4	3	1.4502045	106.3919337	-97.1228174
15	15	C	4	3	2	1.4707465	115.1826593	169.2579081
16	16	O	15	4	3	1.2243025	124.2802490	5.2697278
17	17	O	15	4	3	1.3610616	112.8965602	-174.6958366
18	18	C	17	15	4	1.4378092	115.6141388	-176.9118687
19	19	O	14	7	4	1.3744499	116.6549828	138.9270896
20	20	N	14	7	4	1.2920322	125.9525626	-42.0436856
21	21	C	19	14	7	1.4551121	106.7020676	173.5022600

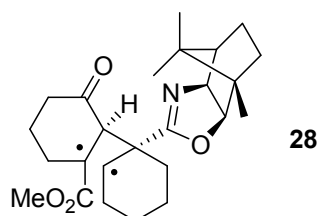
22	22	C	21	19	14	1.5487192	116.6947851	119.5935356
23	23	C	22	21	19	1.5632002	102.0397591	175.6710123
24	24	C	23	22	21	1.5648332	104.1909455	73.2108498
25	25	C	20	14	7	1.4625350	107.1509531	-176.2794635
26	26	C	24	23	22	1.5531038	102.7087815	-1.9548803
27	27	C	26	24	23	1.5671301	101.6489282	37.5691246
28	28	C	22	21	19	1.5225479	114.5951326	51.1722114
29	29	C	27	26	24	1.5406713	116.5252363	-178.9373427
30	30	C	27	26	24	1.5477571	112.6525092	60.2563548
31	31	H	1	6	5	1.1000659	108.0210543	91.0253844
32	32	H	1	6	5	1.0941002	108.0452380	-153.8254881
33	33	H	2	1	6	1.0971726	109.1918621	-68.0621599
34	34	H	2	1	6	1.0957953	110.1141331	175.6314236
35	35	H	3	2	1	1.0956082	111.1682255	-175.1162018
36	36	H	3	2	1	1.1016064	109.2926646	69.7679673
37	37	H	5	4	3	1.0843999	119.4845893	-176.9398757
38	38	H	8	7	4	1.0839807	118.4384633	92.0460175
39	39	H	10	7	4	1.0992912	108.2462243	-13.0226775
40	40	H	10	7	4	1.0903218	111.3233503	-130.1172124
41	41	H	11	10	7	1.0957180	108.1546322	-154.4610801
42	42	H	11	10	7	1.0949771	109.0118817	90.0044440
43	43	H	12	11	10	1.0954986	110.5348601	-143.3985038
44	44	H	12	11	10	1.0963889	110.0112663	99.1085660
45	45	H	13	8	7	1.0924330	110.7661778	-164.6821867
46	46	H	13	8	7	1.0956296	111.6176089	76.9407819
47	47	H	18	17	15	1.0903016	105.4182246	-178.0194245
48	48	H	18	17	15	1.0923000	109.7902133	62.5794660
49	49	H	18	17	15	1.0929932	110.5223023	-58.5164052
50	50	H	21	19	14	1.0947526	105.8741757	-116.2271417
51	51	H	23	22	21	1.0960271	111.3932470	-48.3441123
52	52	H	23	22	21	1.0936485	110.3834104	-166.4334256
53	53	H	24	23	22	1.0948719	112.4435910	-122.3167843
54	54	H	24	23	22	1.0925447	111.7371551	117.6987474
55	55	H	25	20	14	1.0961044	107.0410527	122.3730711

56	56	H	26	24	23	1.0925350	115.1572695	163.7333267
57	57	H	28	22	21	1.0955133	111.1176782	179.4782790
58	58	H	28	22	21	1.0968413	110.9093482	59.9931391
59	59	H	28	22	21	1.0943827	111.3334714	-59.7815639
60	60	H	29	27	26	1.0965535	109.5309922	178.7765963
61	61	H	29	27	26	1.0835006	115.1140726	57.5248346
62	62	H	29	27	26	1.0937184	109.8570676	-62.8211317
63	63	H	30	27	26	1.0958832	109.4684829	66.6224162
64	64	H	30	27	26	1.0905240	115.0477632	-54.5546548
65	65	H	30	27	26	1.0956285	110.1054534	-176.0125769

Row	Tag	Symbol	X	Y	Z
1	1	C	4.7484700	-0.6764830	1.9854710
2	2	C	3.4033580	-0.0244800	2.3437400
3	3	C	2.2223160	-0.7821730	1.7200420
4	4	C	2.3862810	-1.0443860	0.2412190
5	5	C	3.7562030	-1.0339820	-0.3160040
6	6	C	4.9224250	-0.8426890	0.4805980
7	7	C	0.5816080	1.5340710	-0.3715510
8	8	C	1.6784990	0.9617350	-1.0118480
9	9	O	6.0576200	-0.7752270	-0.0529450
10	10	C	0.8310890	2.7626000	0.4603460
11	11	C	1.5870970	3.8573080	-0.3549170
12	12	C	2.5536850	3.2594530	-1.4040070
13	13	C	2.9400330	1.8005650	-1.0615010
14	14	C	-0.7638940	1.0458570	-0.6047130
15	15	C	1.4067350	-1.9736180	-0.3419730
16	16	O	0.4547630	-2.4440110	0.2674500
17	17	O	1.6651270	-2.2657530	-1.6459590
18	18	C	0.7038900	-3.1156380	-2.2948150
19	19	O	-1.7894300	1.7792680	-0.0574500
20	20	N	-1.0826180	-0.0009070	-1.2917700
21	21	C	-3.0289010	1.1962490	-0.5485220
22	22	C	-4.0050030	0.6379640	0.5164070

23	23	C	-5.2321430	0.2162050	-0.3552820
24	24	C	-4.7502240	-1.0745720	-1.0971390
25	25	C	-2.5433140	-0.0600190	-1.3351460
26	26	C	-3.2833120	-1.2218570	-0.6086640
27	27	C	-3.4013950	-0.7716700	0.8877600
28	28	C	-4.3313490	1.6052960	1.6459730
29	29	C	-2.0979600	-0.7649320	1.7091490
30	30	C	-4.3697780	-1.6618790	1.7034280
31	31	H	4.8131420	-1.6726680	2.4476160
32	32	H	5.5968990	-0.0978630	2.3628600
33	33	H	3.4059930	1.0184630	2.0030780
34	34	H	3.2785600	0.0085310	3.4319050
35	35	H	1.2758340	-0.2632870	1.9078890
36	36	H	2.1109860	-1.7575910	2.2197440
37	37	H	3.8997240	-1.1695010	-1.3822870
38	38	H	1.4974110	0.2386040	-1.7988060
39	39	H	1.4599280	2.4772340	1.3156640
40	40	H	-0.0980690	3.1590160	0.8706160
41	41	H	2.1343490	4.4918130	0.3511400
42	42	H	0.8543930	4.5017530	-0.8517170
43	43	H	3.4604950	3.8690880	-1.4824800
44	44	H	2.0837430	3.2671680	-2.3945440
45	45	H	3.6418620	1.4014150	-1.7973850
46	46	H	3.4648930	1.7975280	-0.0997750
47	47	H	1.0868450	-3.2685900	-3.3041260
48	48	H	-0.2696710	-2.6210000	-2.3199430
49	49	H	0.6182870	-4.0693760	-1.7678520
50	50	H	-3.5072810	1.9742860	-1.1520900
51	51	H	-5.5237940	1.0141540	-1.0477360
52	52	H	-6.1015860	0.0226020	0.2792680
53	53	H	-4.8087580	-0.9772960	-2.1861090
54	54	H	-5.3520890	-1.9453210	-0.8265680
55	55	H	-2.8336920	-0.0565870	-2.3920820
56	56	H	-2.8335870	-2.2029730	-0.7783450

57	57	H	-5.0312290	1.1570220	2.3596730
58	58	H	-4.7976200	2.5186200	1.2567540
59	59	H	-3.4290830	1.9006510	2.1903580
60	60	H	-2.3074550	-0.4129400	2.7263230
61	61	H	-1.3042980	-0.1464590	1.3071970
62	62	H	-1.6980400	-1.7804650	1.7796950
63	63	H	-3.9518780	-2.6711500	1.7911300
64	64	H	-5.3724980	-1.7568840	1.2853740
65	65	H	-4.4755340	-1.2694030	2.7208660



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5369790		
3	3	C	2	1		1.5461362	111.4576723	
4	4	C	3	2	1	1.4956224	109.6881176	-54.6359223
5	5	C	4	3	2	1.4978543	119.6521928	53.2921404
6	6	C	1	2	3	1.5231875	113.3968499	50.0514118
7	7	C	5	4	3	1.6494118	115.1662411	86.7297329
8	8	C	7	5	4	1.5045508	109.0247613	43.2789717
9	9	O	6	1	2	1.2189804	121.4975337	138.3651485
10	10	C	7	5	4	1.5596649	108.0839497	163.7665055
11	11	C	10	7	5	1.5356579	113.6677154	-76.5145910
12	12	C	11	10	7	1.5325969	111.5402869	-56.1825758
13	13	C	8	7	5	1.4955975	121.9484791	82.2751145
14	14	C	7	5	4	1.5214472	110.1995896	-76.1983910
15	15	C	4	3	2	1.4576587	122.4404436	-119.2553793
16	16	O	15	4	3	1.2296096	124.8407447	171.9306677
17	17	O	15	4	3	1.3631850	113.2542722	-7.7093789

18	18	C	17	15	4	1.4366540	115.5779029	179.7409923
19	19	O	14	7	5	1.3710097	115.5044431	-89.6910056
20	20	N	14	7	5	1.2780356	126.7703493	91.2283087
21	21	C	19	14	7	1.4546426	106.7562733	176.9404615
22	22	C	21	19	14	1.5483347	116.8855450	117.1611880
23	23	C	22	21	19	1.5643370	101.6424043	174.3688541
24	24	C	23	22	21	1.5652220	104.1479320	73.2499751
25	25	C	20	14	7	1.4698728	107.3976791	-178.2019558
26	26	C	24	23	22	1.5527022	102.7367486	-1.8563845
27	27	C	26	24	23	1.5652323	101.5876464	37.6844445
28	28	C	22	21	19	1.5224219	114.7556557	49.9136290
29	29	C	27	26	24	1.5415872	116.2035684	-179.5019659
30	30	C	27	26	24	1.5480968	113.0743510	59.6631926
31	31	H	1	6	9	1.0978140	106.9878253	-101.1236951
32	32	H	1	6	9	1.0934505	107.4930855	13.7171315
33	33	H	2	1	6	1.0970783	109.6144089	-71.0747792
34	34	H	2	1	6	1.0959145	109.7669382	171.8285720
35	35	H	3	2	1	1.0905492	110.5584707	-177.0398524
36	36	H	3	2	1	1.0996457	109.0871040	64.6810093
37	37	H	5	4	3	1.0912386	108.2223881	-158.5299034
38	38	H	8	7	5	1.0847722	117.2636087	-88.2890406
39	39	H	10	7	5	1.0963419	107.4290067	163.6141809
40	40	H	10	7	5	1.0919023	109.9756250	47.8788772
41	41	H	11	10	7	1.0966802	108.3583145	-177.9852043
42	42	H	11	10	7	1.0976074	110.6363026	66.1177462
43	43	H	12	11	10	1.0988426	109.3139779	-62.5747119
44	44	H	12	11	10	1.0963438	110.6432244	179.8324959
45	45	H	13	8	7	1.1041397	109.5613407	-80.0907569
46	46	H	13	8	7	1.0968334	109.3270788	164.1321211
47	47	H	18	17	15	1.0901035	105.4132966	-179.6919767
48	48	H	18	17	15	1.0931353	110.5888489	60.7519069
49	49	H	18	17	15	1.0931195	110.6012864	-60.0298842
50	50	H	21	19	14	1.0944732	105.7891624	-119.0258318
51	51	H	23	22	21	1.0958064	111.3351494	-48.2409403

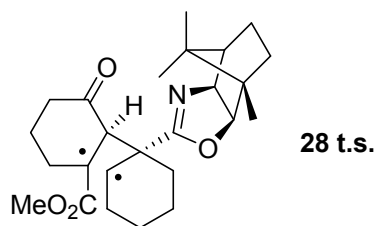


52	52	H	23	22	21	1.0933376	110.5628389	-166.2554151
53	53	H	24	23	22	1.0948611	112.4649764	-122.2795094
54	54	H	24	23	22	1.0927350	111.6647552	117.6312941
55	55	H	25	20	14	1.0958976	107.5111638	120.8767605
56	56	H	26	24	23	1.0934193	114.8066541	163.7995574
57	57	H	28	22	21	1.0955376	111.0882871	179.1463097
58	58	H	28	22	21	1.0964975	110.9183317	59.5778825
59	59	H	28	22	21	1.0941972	111.3357657	-60.0421628
60	60	H	29	27	26	1.0960005	110.0754244	170.4324299
61	61	H	29	27	26	1.0839333	115.2720196	47.8481261
62	62	H	29	27	26	1.0962479	109.2730729	-72.1996124
63	63	H	30	27	26	1.0959957	109.6261573	63.0578643
64	64	H	30	27	26	1.0904890	115.0015331	-58.1407206
65	65	H	30	27	26	1.0956980	110.0268513	-179.4714029

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.0400250	-2.2653380	1.8662490
2	2	C	-1.9022310	-3.0534320	0.8673430
3	3	C	-2.1225180	-2.2582030	-0.4401820
4	4	C	-2.6961940	-0.9141470	-0.1219120
5	5	C	-2.0058500	-0.0299180	0.8706260
6	6	C	-1.5244480	-0.8385790	2.0893930
7	7	C	-0.8168280	0.9288040	0.2480200
8	8	C	-1.2948930	1.5233400	-1.0487660
9	9	O	-1.5468040	-0.3402060	3.2016150
10	10	C	-0.5035050	2.0483430	1.2877390
11	11	C	-1.5542160	3.1676950	1.3238330
12	12	C	-1.7446360	3.8054470	-0.0566980
13	13	C	-2.1631150	2.7404650	-1.0888790
14	14	C	0.4352820	0.1066290	-0.0185330
15	15	C	-3.9956480	-0.4806920	-0.6202140
16	16	O	-4.5720260	0.5494650	-0.2759690
17	17	O	-4.5408490	-1.3437780	-1.5236030
18	18	C	-5.8261930	-0.9674060	-2.0434200

19	19	O	1.3212150	0.0252270	1.0246180
20	20	N	0.7415820	-0.4898940	-1.1065200
21	21	C	2.3969610	-0.8539550	0.5935790
22	22	C	3.8124790	-0.2337920	0.4984640
23	23	C	4.6848440	-1.4882370	0.1630580
24	24	C	4.3396340	-1.8061490	-1.3301540
25	25	C	2.0153690	-1.1879820	-0.8814290
26	26	C	3.2729450	-0.7306780	-1.6713590
27	27	C	3.8207990	0.5129980	-0.8947780
28	28	C	4.2545860	0.5382330	1.7338940
29	29	C	2.9834830	1.8032180	-0.9983420
30	30	C	5.2395760	0.9348410	-1.3483460
31	31	H	-0.0129000	-2.1992970	1.4843480
32	32	H	-0.9903580	-2.7522930	2.8440230
33	33	H	-2.8747350	-3.2822380	1.3206250
34	34	H	-1.4233700	-4.0127600	0.6406040
35	35	H	-2.7781290	-2.8075680	-1.1166950
36	36	H	-1.1557090	-2.1239250	-0.9466110
37	37	H	-2.7325220	0.6910460	1.2487270
38	38	H	-1.1192020	0.9501820	-1.9528420
39	39	H	0.4620290	2.4897350	1.0140920
40	40	H	-0.3781450	1.6110590	2.2803710
41	41	H	-1.2316960	3.9208010	2.0528870
42	42	H	-2.5158140	2.7840160	1.6883350
43	43	H	-0.8024660	4.2736240	-0.3738430
44	44	H	-2.4991610	4.5997420	-0.0147790
45	45	H	-3.2099120	2.4547400	-0.8846690
46	46	H	-2.1558380	3.1582970	-2.1029830
47	47	H	-6.1038660	-1.7637300	-2.7341380
48	48	H	-5.7639180	-0.0093970	-2.5661870
49	49	H	-6.5582940	-0.8842040	-1.2359450
50	50	H	2.3890760	-1.6979420	1.2903540
51	51	H	4.4558020	-2.3240080	0.8337430
52	52	H	5.7464640	-1.2654120	0.2998030

53	53	H	3.9517040	-2.8213420	-1.4628730
54	54	H	5.2171320	-1.7159700	-1.9750840
55	55	H	1.8429610	-2.2550750	-1.0619270
56	56	H	3.0905430	-0.5883140	-2.7400160
57	57	H	5.2671040	0.9371830	1.6080020
58	58	H	4.2620140	-0.1096130	2.6185110
59	59	H	3.5796170	1.3733890	1.9441290
60	60	H	3.3571110	2.5520080	-0.2905760
61	61	H	1.9201460	1.6797090	-0.8281320
62	62	H	3.0935880	2.2263140	-2.0036410
63	63	H	5.2135100	1.2429030	-2.3998330
64	64	H	6.0029210	0.1620080	-1.2524300
65	65	H	5.5770010	1.8008900	-0.7681240



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5351156		
3	3	C	2	1		1.5443264	111.0287228	
4	4	C	3	2	1	1.4943135	110.2864045	-56.0404550
5	5	C	4	3	2	1.5023207	116.9548378	48.3344175
6	6	C	5	4	3	1.4610917	117.8183338	-34.0384539
7	7	C	5	4	3	2.7046250	106.5484064	88.1546083
8	8	C	7	5	4	1.3827474	98.8652264	48.1497161
9	9	O	6	5	4	1.2263141	120.7078129	-155.5070962
10	10	C	7	5	4	1.5310355	98.6990011	169.4216625
11	11	C	10	7	5	1.5339275	112.8849564	-76.1383609
12	12	C	11	10	7	1.5299629	111.5458571	-49.0391946
13	13	C	8	7	5	1.5041546	122.9956063	84.8941374

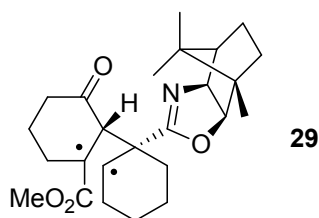
14	14	C	7	5	4	1.5032652	102.1665145	-70.8806537
15	15	C	4	3	2	1.4537591	124.5673059	-125.0687701
16	16	O	15	4	3	1.2132000	123.9245908	177.1420922
17	17	O	15	4	3	1.3419339	113.6582111	-3.1615596
18	18	C	17	15	4	1.4255663	116.5198072	-179.5253042
19	19	O	14	7	5	1.3624975	116.9496584	-90.4913466
20	20	N	14	7	5	1.2658917	125.8642071	91.6302708
21	21	C	19	14	7	1.4441824	107.2366130	179.7368779
22	22	C	21	19	14	1.5486636	117.0254400	115.2029214
23	23	C	22	21	19	1.5570991	102.0491677	174.3274916
24	24	C	23	22	21	1.5598008	103.9809140	72.4987268
25	25	C	20	14	7	1.4581855	108.0858771	179.8548605
26	26	C	25	20	14	1.5456944	118.1964974	-114.2140348
27	27	C	26	25	20	1.5598820	105.2707647	80.1072497
28	28	C	22	21	19	1.5205628	114.5666328	49.7824244
29	29	C	27	26	25	1.5439602	116.2386463	-70.1407874
30	30	C	27	26	25	1.5444435	112.5708019	169.0282053
31	31	H	1	6	5	1.0867677	104.4539196	84.5595890
32	32	H	1	6	5	1.0878493	108.2323371	-161.2198377
33	33	H	2	1	6	1.0921472	109.9105639	-71.6189551
34	34	H	2	1	6	1.0903246	109.9060555	171.2190706
35	35	H	3	2	1	1.0854970	110.9123256	-179.0061117
36	36	H	3	2	1	1.0947135	108.8609521	62.9010800
37	37	H	5	4	3	1.0741879	117.1615043	-177.8694325
38	38	H	8	7	5	1.0802908	118.2611725	-90.7430929
39	39	H	10	7	5	1.0925067	107.3631013	164.0936476
40	40	H	10	7	5	1.0876986	110.6920413	48.5286671
41	41	H	11	10	7	1.0910740	108.4194464	-171.6606748
42	42	H	11	10	7	1.0901131	111.0306916	71.9164202
43	43	H	12	11	10	1.0931232	109.7167272	-61.6714771
44	44	H	12	11	10	1.0909047	110.5399355	-179.3475272
45	45	H	13	8	7	1.0956460	108.9748122	-91.1676068
46	46	H	13	8	7	1.0913592	109.1919119	153.4529115
47	47	H	18	17	15	1.0838755	105.4143364	-178.9195444

48	48	H	18	17	15	1.0862981	110.4756273	61.6670815
49	49	H	18	17	15	1.0861330	110.5473803	-59.3745348
50	50	H	21	19	14	1.0878317	106.0592998	-120.6440711
51	51	H	23	22	21	1.0901740	111.5176079	-48.9635783
52	52	H	23	22	21	1.0878382	110.7031177	-167.1742559
53	53	H	24	23	22	1.0893105	112.3846743	-121.3758122
54	54	H	24	23	22	1.0870059	111.7199423	118.8291040
55	55	H	25	20	14	1.0898679	108.0553875	120.7091308
56	56	H	26	25	20	1.0881167	113.6210136	-47.7955900
57	57	H	28	22	21	1.0898732	111.0984985	179.7553034
58	58	H	28	22	21	1.0911281	110.8978082	60.1572534
59	59	H	28	22	21	1.0887442	111.3305029	-59.5083345
60	60	H	29	27	26	1.0898522	109.9163318	-167.5429070
61	61	H	29	27	26	1.0799318	114.6406844	72.0815953
62	62	H	29	27	26	1.0896158	110.2696821	-49.4740490
63	63	H	30	27	26	1.0909762	109.4092870	66.6177989
64	64	H	30	27	26	1.0843596	114.9991188	-54.3204648
65	65	H	30	27	26	1.0896404	110.2361732	-175.8331059

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.4701890	-2.1928580	2.1909280
2	2	C	-2.1652660	-3.0656710	1.1365820
3	3	C	-2.2579400	-2.3300630	-0.2181270
4	4	C	-2.9559550	-1.0196110	-0.0494160
5	5	C	-2.4929920	-0.1416760	1.0783530
6	6	C	-2.0345740	-0.7912930	2.3041750
7	7	C	-0.4767880	1.3716970	0.0987510
8	8	C	-1.0797280	1.7994010	-1.0698050
9	9	O	-2.0698960	-0.1992760	3.3775410
10	10	C	-0.3385230	2.3554260	1.2637530
11	11	C	-1.4492930	3.4130690	1.2864440
12	12	C	-1.6318550	4.0656640	-0.0852620
13	13	C	-1.9881440	2.9966370	-1.1321550
14	14	C	0.6262550	0.3633420	-0.0634910

15	15	C	-4.1262460	-0.6050510	-0.8057060
16	16	O	-4.7137440	0.4408800	-0.6247950
17	17	O	-4.5040700	-1.4898830	-1.7411780
18	18	C	-5.6407270	-1.1392350	-2.5268600
19	19	O	1.4625170	0.1868390	0.9975990
20	20	N	0.8698700	-0.3076050	-1.1089400
21	21	C	2.4263290	-0.8202050	0.6199860
22	22	C	3.9058350	-0.3744820	0.5162940
23	23	C	4.6338010	-1.7242380	0.2465130
24	24	C	4.2514830	-2.0709680	-1.2254210
25	25	C	2.0213380	-1.1611880	-0.8409430
26	26	C	3.3262430	-0.8948460	-1.6254530
27	27	C	4.0049260	0.3066630	-0.8981310
28	28	C	4.4204970	0.3943920	1.7229700
29	29	C	3.3097770	1.6769760	-1.0492050
30	30	C	5.4543700	0.5460290	-1.3747040
31	31	H	-0.4270390	-2.0445310	1.9246550
32	32	H	-1.4924140	-2.6495110	3.1780400
33	33	H	-3.1644050	-3.3406650	1.4813790
34	34	H	-1.6128400	-3.9960110	1.0020430
35	35	H	-2.7651700	-2.9420160	-0.9574070
36	36	H	-1.2451450	-2.1393400	-0.5872730
37	37	H	-3.0156590	0.7853310	1.2244930
38	38	H	-0.9451490	1.2052860	-1.9619620
39	39	H	0.6236870	2.8605260	1.1515180
40	40	H	-0.2947910	1.8244290	2.2120240
41	41	H	-1.2015170	4.1570110	2.0451270
42	42	H	-2.4009250	2.9745600	1.5871980
43	43	H	-0.7105460	4.5771970	-0.3758510
44	44	H	-2.4168550	4.8222620	-0.0477450
45	45	H	-3.0209600	2.6690170	-0.9696850
46	46	H	-1.9602080	3.4161220	-2.1392880
47	47	H	-5.7952690	-1.9752740	-3.1991260
48	48	H	-5.4484520	-0.2294810	-3.0884840

49	49	H	-6.5109520	-0.9919580	-1.8938490
50	50	H	2.3159700	-1.6276000	1.3406190
51	51	H	4.3211440	-2.4950070	0.9512400
52	52	H	5.7087540	-1.6130210	0.3710070
53	53	H	3.7436770	-3.0312220	-1.3069240
54	54	H	5.1278540	-2.1274930	-1.8660150
55	55	H	1.7143710	-2.1971460	-0.9836820
56	56	H	3.1749550	-0.7788640	-2.6967410
57	57	H	5.4652940	0.6757850	1.5924300
58	58	H	4.3528440	-0.2111550	2.6281200
59	59	H	3.8416120	1.3010020	1.8912390
60	60	H	3.9705470	2.4692250	-0.6977760
61	61	H	2.3841600	1.7750970	-0.5016120
62	62	H	3.0939890	1.8771680	-2.0983100
63	63	H	5.4444900	0.8727810	-2.4155520
64	64	H	6.1059130	-0.3185220	-1.3124220
65	65	H	5.9156950	1.3433110	-0.7926070



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5303048		
3	3	C	2	1		1.5436665	110.3606567	
4	4	C	3	2	1	1.5041490	109.4197555	-58.3557244
5	5	C	4	3	2	1.5179116	113.3518526	65.1948017
6	6	C	1	2	3	1.5275874	115.0695624	46.2516049
7	7	C	5	4	3	1.5717615	122.1336654	170.9303850
8	8	C	7	5	4	1.5200181	110.7293303	-174.4619368
9	9	O	6	1	2	1.2112605	120.3013688	147.7128569

10	10	C	7	5	4	1.5749492	110.3788754	-57.4084939
11	11	C	10	7	5	1.5368438	113.5414028	-69.0301528
12	12	C	11	10	7	1.5330531	112.2281134	-57.4988982
13	13	C	8	7	5	1.4955780	120.2961606	70.1688730
14	14	C	7	5	4	1.5180496	109.7268316	64.4396004
15	15	C	4	3	2	1.4647239	118.9387100	-108.1768972
16	16	O	15	4	3	1.2243200	127.8142715	-165.7634508
17	17	O	15	4	3	1.3699218	111.3301827	12.1232437
18	18	C	17	15	4	1.4355774	115.4524148	-178.5475919
19	19	O	14	7	5	1.3700613	115.1534823	-172.6910743
20	20	N	14	7	5	1.2753155	126.8330079	8.1002376
21	21	C	19	14	7	1.4535416	106.2954997	172.8903139
22	22	C	21	19	14	1.5475619	117.0510151	119.7355060
23	23	C	22	21	19	1.5639710	101.7043304	174.1531888
24	24	C	23	22	21	1.5649715	104.1321982	73.3959696
25	25	C	20	14	7	1.4693393	107.1811362	-174.7150924
26	26	C	24	23	22	1.5522334	102.7391431	-1.9529270
27	27	C	26	24	23	1.5642169	101.5922094	37.8032569
28	28	C	22	21	19	1.5223154	114.8283187	49.7136746
29	29	C	27	26	24	1.5407346	115.4683909	-179.3101558
30	30	C	27	26	24	1.5476066	113.4717296	59.6187386
31	31	H	1	6	9	1.1015750	105.4039362	-91.8542526
32	32	H	1	6	9	1.0932300	107.1223780	21.6745358
33	33	H	2	1	6	1.0957461	110.1919630	-74.2424774
34	34	H	2	1	6	1.0961634	110.0159544	167.7322994
35	35	H	3	2	1	1.0894014	110.4250778	178.7202258
36	36	H	3	2	1	1.1012792	108.4781171	60.7996634
37	37	H	5	4	3	1.1043278	104.3020393	52.4822035
38	38	H	8	7	5	1.0809898	119.6289722	-104.5936661
39	39	H	10	7	5	1.0946111	106.7027480	171.1874660
40	40	H	10	7	5	1.0892405	109.9514488	55.7958896
41	41	H	11	10	7	1.0971022	108.3579676	-179.3130140
42	42	H	11	10	7	1.0999863	110.6516464	65.2572449
43	43	H	12	11	10	1.0979856	109.1512756	-65.4473402

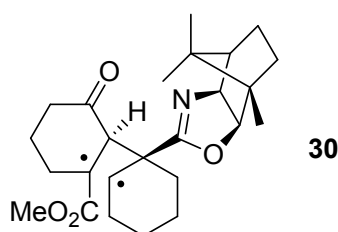


44	44	H	12	11	10	1.0973369	110.8581736	176.8184776
45	45	H	13	8	7	1.1077408	110.8833600	-69.8554204
46	46	H	13	8	7	1.0954718	109.8220955	173.9032590
47	47	H	18	17	15	1.0903245	105.3984301	179.3637399
48	48	H	18	17	15	1.0931671	110.6966108	59.6661630
49	49	H	18	17	15	1.0931410	110.5921007	-61.1406715
50	50	H	21	19	14	1.0941951	105.6925320	-115.9720091
51	51	H	23	22	21	1.0957794	111.2102388	-47.9741099
52	52	H	23	22	21	1.0935627	110.6406231	-166.0304496
53	53	H	24	23	22	1.0949913	112.4309235	-122.3800007
54	54	H	24	23	22	1.0931433	111.6115073	117.5250321
55	55	H	25	20	14	1.0956337	106.9578505	118.6047010
56	56	H	26	24	23	1.0937391	114.7481467	163.7503639
57	57	H	28	22	21	1.0958311	111.1259757	179.5270981
58	58	H	28	22	21	1.0967666	110.8737353	59.9583286
59	59	H	28	22	21	1.0943102	111.2675703	-59.6430648
60	60	H	29	27	26	1.0963347	110.4238236	164.1494281
61	61	H	29	27	26	1.0835689	114.6916065	40.8607708
62	62	H	29	27	26	1.0961398	109.2805469	-78.2560882
63	63	H	30	27	26	1.0961669	109.6357465	61.4260221
64	64	H	30	27	26	1.0909235	115.0817760	-59.8935642
65	65	H	30	27	26	1.0960528	109.9283333	178.7751776

Row	Tag	Symbol	X	Y	Z
1	1	C	2.9332020	-0.2488640	2.8607430
2	2	C	3.5857770	-1.4924380	2.2528760
3	3	C	3.9941780	-1.2233650	0.7887330
4	4	C	2.7789890	-0.8285840	-0.0049470
5	5	C	2.1729200	0.4904300	0.4388300
6	6	C	1.8801910	0.4243890	1.9824370
7	7	C	1.0314270	1.2016640	-0.3745420
8	8	C	0.7132790	2.5628230	0.2225200
9	9	O	0.9316650	0.9845470	2.4860970
10	10	C	1.5001960	1.4752190	-1.8530170

11	11	C	2.5993190	2.5439700	-1.9606680
12	12	C	2.1677280	3.8831050	-1.3518180
13	13	C	1.6935870	3.6861540	0.1047180
14	14	C	-0.2171960	0.3383200	-0.3673010
15	15	C	2.2297720	-1.7754470	-0.9782030
16	16	O	1.4173190	-1.5523020	-1.8665080
17	17	O	2.7781610	-3.0214770	-0.8253490
18	18	C	2.3248170	-4.0137660	-1.7584750
19	19	O	-1.2334510	0.7773780	-1.1744700
20	20	N	-0.4090520	-0.7228000	0.3136140
21	21	C	-2.2481490	-0.2631990	-1.1552210
22	22	C	-3.6488520	0.1293190	-0.6271030
23	23	C	-4.4694230	-1.1725190	-0.9061840
24	24	C	-3.9615240	-2.1834920	0.1750690
25	25	C	-1.7048890	-1.2768740	-0.1020380
26	26	C	-2.8713800	-1.3680890	0.9208120
27	27	C	-3.5095870	0.0597740	0.9467640
28	28	C	-4.2331450	1.3929920	-1.2428760
29	29	C	-2.6589610	1.1535340	1.6205500
30	30	C	-4.8732310	0.1122740	1.6766990
31	31	H	3.7044240	0.5185460	3.0332710
32	32	H	2.4648290	-0.4500620	3.8278510
33	33	H	2.8883970	-2.3371710	2.2802030
34	34	H	4.4661110	-1.7790560	2.8397630
35	35	H	4.4792270	-2.1005310	0.3619980
36	36	H	4.7217030	-0.3967150	0.7755830
37	37	H	3.0199660	1.1988160	0.4232650
38	38	H	-0.1870430	2.6930330	0.8064760
39	39	H	0.6192240	1.8199280	-2.4036870
40	40	H	1.8178430	0.5440940	-2.3205120
41	41	H	2.8513310	2.6749300	-3.0203720
42	42	H	3.5243990	2.1993370	-1.4754620
43	43	H	1.3399100	4.2972010	-1.9424230
44	44	H	2.9872840	4.6118230	-1.3898480

45	45	H	2.5867110	3.4983040	0.7325170
46	46	H	1.2498880	4.6088070	0.4944630
47	47	H	2.8660170	-4.9239950	-1.4988730
48	48	H	2.5495190	-3.7105740	-2.7844370
49	49	H	1.2468430	-4.1677660	-1.6624890
50	50	H	-2.3051640	-0.6399800	-2.1809150
51	51	H	-4.3046860	-1.5336730	-1.9275370
52	52	H	-5.5419230	-0.9789840	-0.8158110
53	53	H	-3.5549470	-3.0989850	-0.2671680
54	54	H	-4.7649830	-2.4872600	0.8511910
55	55	H	-1.5083330	-2.2703110	-0.5202030
56	56	H	-2.5757900	-1.7785530	1.8905600
57	57	H	-5.2261800	1.6093200	-0.8330840
58	58	H	-4.3397760	1.2851540	-2.3291070
59	59	H	-3.5888970	2.2583630	-1.0595940
60	60	H	-3.0338780	2.1485530	1.3534840
61	61	H	-1.6003910	1.1076170	1.3937400
62	62	H	-2.7432850	1.0582730	2.7092820
63	63	H	-4.7420700	-0.1836070	2.7239970
64	64	H	-5.6505680	-0.5236630	1.2507350
65	65	H	-5.2561590	1.1392550	1.6795300



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5336110		
3	3	C	2	1		1.5490564	111.1467848	
4	4	C	3	2	1	1.4936121	107.8308381	-58.8942309
5	5	C	4	3	2	1.5067056	119.6931412	59.1980443
6	6	C	1	2	3	1.5259663	116.0527028	43.1103684

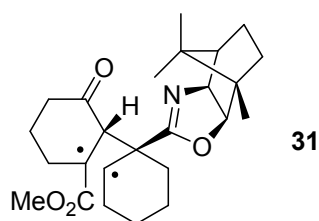
7	7	C	5	4	3	1.6048344	116.2455084	96.2301346
8	8	C	7	5	4	1.5200894	108.9222264	163.9167887
9	9	O	6	1	2	1.2193489	119.6673695	154.7917347
10	10	C	7	5	4	1.5649986	107.9488109	44.8088302
11	11	C	10	7	5	1.5373470	115.6257302	159.6215585
12	12	C	11	10	7	1.5328556	111.2977850	-54.0479012
13	13	C	8	7	5	1.4952521	121.8737417	-154.3427461
14	14	C	7	5	4	1.5249303	112.0529688	-78.1969518
15	15	C	4	3	2	1.4596884	121.5413719	-107.2189047
16	16	O	15	4	3	1.2296034	124.9574971	168.6905728
17	17	O	15	4	3	1.3639270	113.3082021	-11.2989736
18	18	C	17	15	4	1.4366225	115.5243515	-179.9530005
19	19	O	14	7	5	1.3730081	115.2231431	175.8762971
20	20	N	14	7	5	1.2780764	127.4514945	-6.6226137
21	21	C	19	14	7	1.4550686	106.8410585	171.1139045
22	22	C	21	19	14	1.5492312	116.9607327	119.3102135
23	23	C	22	21	19	1.5631847	101.8105411	174.6735148
24	24	C	23	22	21	1.5651174	104.1396362	73.0650188
25	25	C	20	14	7	1.4705712	107.6119676	-172.6616293
26	26	C	24	23	22	1.5528697	102.7391025	-1.7707412
27	27	C	26	24	23	1.5653066	101.5847089	37.5987117
28	28	C	22	21	19	1.5225242	114.8340410	50.1121109
29	29	C	27	26	24	1.5411513	116.3039830	-178.8926215
30	30	C	27	26	24	1.5475214	113.1315860	60.0465384
31	31	H	1	6	9	1.0951414	104.5385738	-84.6558628
32	32	H	1	6	9	1.0943489	106.7769176	29.0930253
33	33	H	2	1	6	1.0973602	110.4235278	-78.0711717
34	34	H	2	1	6	1.0962257	109.7226426	164.4817391
35	35	H	3	2	1	1.0903546	110.6221697	179.4608291
36	36	H	3	2	1	1.0958796	108.1334186	60.0453406
37	37	H	5	4	3	1.0955123	106.8889552	-150.8523196
38	38	H	8	7	5	1.0837548	117.1283992	36.2367739
39	39	H	10	7	5	1.0941600	106.4792996	39.6724858
40	40	H	10	7	5	1.0964399	109.4592427	-75.1357461

41	41	H	11	10	7	1.0973731	108.0546130	-174.9555353
42	42	H	11	10	7	1.0943108	110.6426934	68.1890798
43	43	H	12	11	10	1.0984575	109.4423454	-63.2981825
44	44	H	12	11	10	1.0967082	110.5229706	179.0765160
45	45	H	13	8	7	1.1051493	109.8320593	-78.0841756
46	46	H	13	8	7	1.0965423	109.2321171	166.0110365
47	47	H	18	17	15	1.0901431	105.4228742	-179.7584332
48	48	H	18	17	15	1.0931788	110.5837879	60.6451049
49	49	H	18	17	15	1.0930945	110.6293042	-60.0917428
50	50	H	21	19	14	1.0943066	105.7683926	-116.5359308
51	51	H	23	22	21	1.0956878	111.3375358	-48.3998914
52	52	H	23	22	21	1.0933892	110.5217532	-166.4675392
53	53	H	24	23	22	1.0946636	112.4273386	-122.0497453
54	54	H	24	23	22	1.0927049	111.7092573	117.9098980
55	55	H	25	20	14	1.0954652	107.0979339	119.8527895
56	56	H	26	24	23	1.0938338	114.6114792	163.5298187
57	57	H	28	22	21	1.0956839	111.1504920	178.9879368
58	58	H	28	22	21	1.0965433	110.8563429	59.4831714
59	59	H	28	22	21	1.0944436	111.4102991	-60.2324640
60	60	H	29	27	26	1.0959343	109.9429243	173.2216349
61	61	H	29	27	26	1.0835220	114.9326647	51.5190227
62	62	H	29	27	26	1.0963710	109.5368113	-69.2997099
63	63	H	30	27	26	1.0961642	109.6752695	64.4126453
64	64	H	30	27	26	1.0903605	114.9674126	-56.7770405
65	65	H	30	27	26	1.0956458	110.0496953	-178.0883779

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.8159060	-1.8793240	2.5323130
2	2	C	-2.3151960	-2.7900660	1.4039420
3	3	C	-1.9129750	-2.2320090	0.0160060
4	4	C	-2.5045660	-0.8670210	-0.1170540
5	5	C	-2.1392760	0.2048640	0.8768210
6	6	C	-1.9938120	-0.3799060	2.3117040
7	7	C	-0.9626760	1.2054860	0.4410900

8	8	C	-0.9957020	2.4280310	1.3438440
9	9	O	-2.0684140	0.3668590	3.2727390
10	10	C	-1.2198880	1.6358590	-1.0414220
11	11	C	-0.5203910	2.9295850	-1.4890970
12	12	C	-0.8507100	4.0948770	-0.5496130
13	13	C	-0.4593580	3.7515370	0.9006220
14	14	C	0.4158070	0.5745270	0.6056740
15	15	C	-3.6416770	-0.6099390	-0.9954490
16	16	O	-4.3011420	0.4277760	-1.0087950
17	17	O	-3.9247140	-1.6506040	-1.8304360
18	18	C	-5.0362700	-1.4477350	-2.7176630
19	19	O	1.4666980	1.3422380	0.1681820
20	20	N	0.6958690	-0.5530050	1.1383240
21	21	C	2.6851650	0.6743610	0.6000420
22	22	C	3.6673520	0.2193330	-0.5082790
23	23	C	4.8764320	-0.3061230	0.3317020
24	24	C	4.3665220	-1.6591440	0.9308000
25	25	C	2.1604020	-0.6510540	1.2283750
26	26	C	2.9069350	-1.7373320	0.4064940
27	27	C	3.0575780	-1.1408080	-1.0328290
28	28	C	4.0202970	1.2918490	-1.5296600
29	29	C	1.7659460	-1.0350110	-1.8668800
30	30	C	4.0320870	-1.9458370	-1.9256240
31	31	H	-0.7359900	-2.0127710	2.6560390
32	32	H	-2.2887190	-2.1159220	3.4904720
33	33	H	-3.4071290	-2.8900520	1.4473540
34	34	H	-1.8997940	-3.7966980	1.5298150
35	35	H	-2.2637500	-2.8905790	-0.7790510
36	36	H	-0.8194330	-2.1726150	-0.0238720
37	37	H	-2.9976750	0.8821670	0.9443410
38	38	H	-1.2603960	2.2683130	2.3825700
39	39	H	-2.2995650	1.7842760	-1.1386640
40	40	H	-0.9564760	0.8097730	-1.7125230
41	41	H	-0.8548820	3.1619790	-2.5080850

42	42	H	0.5636930	2.7868130	-1.5326180
43	43	H	-1.9280260	4.3050220	-0.5924870
44	44	H	-0.3326690	5.0065510	-0.8709430
45	45	H	0.6437110	3.7508120	0.9683950
46	46	H	-0.8047620	4.5306460	1.5906150
47	47	H	-5.1167320	-2.3678800	-3.2966890
48	48	H	-4.8524040	-0.5939290	-3.3751190
49	49	H	-5.9533950	-1.2672030	-2.1509660
50	50	H	3.1717850	1.3643840	1.2961570
51	51	H	5.1660720	0.4126160	1.1063340
52	52	H	5.7542170	-0.4448760	-0.3052760
53	53	H	4.4057730	-1.6726770	2.0246760
54	54	H	4.9636000	-2.5056690	0.5830970
55	55	H	2.4112080	-0.7612490	2.2890340
56	56	H	2.4528110	-2.7304390	0.4695990
57	57	H	4.7300270	0.9117540	-2.2728520
58	58	H	4.4849760	2.1572680	-1.0422890
59	59	H	3.1306130	1.6490490	-2.0575590
60	60	H	1.9668930	-0.4975790	-2.8006140
61	61	H	0.9414160	-0.5369280	-1.3708120
62	62	H	1.4224550	-2.0397610	-2.1398650
63	63	H	3.6309630	-2.9515940	-2.0962940
64	64	H	5.0387320	-2.0593060	-1.5222920
65	65	H	4.1256240	-1.4668080	-2.9065530



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5336110		
3	3	C	2	1		1.5490564	111.1467848	

4	4	C	3	2	1	1.4936121	107.8308381	-58.8942309
5	5	C	4	3	2	1.5067056	119.6931412	59.1980443
6	6	C	1	2	3	1.5259663	116.0527028	43.1103684
7	7	C	5	4	3	1.6048344	116.2455084	96.2301346
8	8	C	7	5	4	1.5200894	108.9222264	163.9167887
9	9	O	6	1	2	1.2193489	119.6673695	154.7917347
10	10	C	7	5	4	1.5649986	107.9488109	44.8088302
11	11	C	10	7	5	1.5373470	115.6257302	159.6215585
12	12	C	11	10	7	1.5328556	111.2977850	-54.0479012
13	13	C	8	7	5	1.4952521	121.8737417	-154.3427461
14	14	C	7	5	4	1.5249303	112.0529688	-78.1969518
15	15	C	4	3	2	1.4596884	121.5413719	-107.2189047
16	16	O	15	4	3	1.2296034	124.9574971	168.6905728
17	17	O	15	4	3	1.3639270	113.3082021	-11.2989736
18	18	C	17	15	4	1.4366225	115.5243515	-179.9530005
19	19	O	14	7	5	1.3730081	115.2231431	175.8762971
20	20	N	14	7	5	1.2780764	127.4514945	-6.6226137
21	21	C	19	14	7	1.4550686	106.8410585	171.1139045
22	22	C	21	19	14	1.5492312	116.9607327	119.3102135
23	23	C	22	21	19	1.5631847	101.8105411	174.6735148
24	24	C	23	22	21	1.5651174	104.1396362	73.0650188
25	25	C	20	14	7	1.4705712	107.6119676	-172.6616293
26	26	C	24	23	22	1.5528697	102.7391025	-1.7707412
27	27	C	26	24	23	1.5653066	101.5847089	37.5987117
28	28	C	22	21	19	1.5225242	114.8340410	50.1121109
29	29	C	27	26	24	1.5411513	116.3039830	-178.8926215
30	30	C	27	26	24	1.5475214	113.1315860	60.0465384
31	31	H	1	6	9	1.0951414	104.5385738	-84.6558628
32	32	H	1	6	9	1.0943489	106.7769176	29.0930253
33	33	H	2	1	6	1.0973602	110.4235278	-78.0711717
34	34	H	2	1	6	1.0962257	109.7226426	164.4817391
35	35	H	3	2	1	1.0903546	110.6221697	179.4608291
36	36	H	3	2	1	1.0958796	108.1334186	60.0453406
37	37	H	5	4	3	1.0955123	106.8889552	-150.8523196

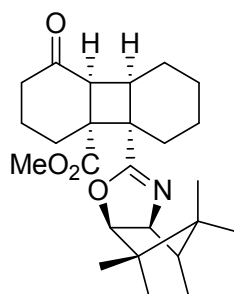


38	38	H	8	7	5	1.0837548	117.1283992	36.2367739
39	39	H	10	7	5	1.0941600	106.4792996	39.6724858
40	40	H	10	7	5	1.0964399	109.4592427	-75.1357461
41	41	H	11	10	7	1.0973731	108.0546130	-174.9555353
42	42	H	11	10	7	1.0943108	110.6426934	68.1890798
43	43	H	12	11	10	1.0984575	109.4423454	-63.2981825
44	44	H	12	11	10	1.0967082	110.5229706	179.0765160
45	45	H	13	8	7	1.1051493	109.8320593	-78.0841756
46	46	H	13	8	7	1.0965423	109.2321171	166.0110365
47	47	H	18	17	15	1.0901431	105.4228742	-179.7584332
48	48	H	18	17	15	1.0931788	110.5837879	60.6451049
49	49	H	18	17	15	1.0930945	110.6293042	-60.0917428
50	50	H	21	19	14	1.0943066	105.7683926	-116.5359308
51	51	H	23	22	21	1.0956878	111.3375358	-48.3998914
52	52	H	23	22	21	1.0933892	110.5217532	-166.4675392
53	53	H	24	23	22	1.0946636	112.4273386	-122.0497453
54	54	H	24	23	22	1.0927049	111.7092573	117.9098980
55	55	H	25	20	14	1.0954652	107.0979339	119.8527895
56	56	H	26	24	23	1.0938338	114.6114792	163.5298187
57	57	H	28	22	21	1.0956839	111.1504920	178.9879368
58	58	H	28	22	21	1.0965433	110.8563429	59.4831714
59	59	H	28	22	21	1.0944436	111.4102991	-60.2324640
60	60	H	29	27	26	1.0959343	109.9429243	173.2216349
61	61	H	29	27	26	1.0835220	114.9326647	51.5190227
62	62	H	29	27	26	1.0963710	109.5368113	-69.2997099
63	63	H	30	27	26	1.0961642	109.6752695	64.4126453
64	64	H	30	27	26	1.0903605	114.9674126	-56.7770405
65	65	H	30	27	26	1.0956458	110.0496953	-178.0883779

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.8159060	-1.8793240	2.5323130
2	2	C	-2.3151960	-2.7900660	1.4039420
3	3	C	-1.9129750	-2.2320090	0.0160060
4	4	C	-2.5045660	-0.8670210	-0.1170540

5	5	C	-2.1392760	0.2048640	0.8768210
6	6	C	-1.9938120	-0.3799060	2.3117040
7	7	C	-0.9626760	1.2054860	0.4410900
8	8	C	-0.9957020	2.4280310	1.3438440
9	9	O	-2.0684140	0.3668590	3.2727390
10	10	C	-1.2198880	1.6358590	-1.0414220
11	11	C	-0.5203910	2.9295850	-1.4890970
12	12	C	-0.8507100	4.0948770	-0.5496130
13	13	C	-0.4593580	3.7515370	0.9006220
14	14	C	0.4158070	0.5745270	0.6056740
15	15	C	-3.6416770	-0.6099390	-0.9954490
16	16	O	-4.3011420	0.4277760	-1.0087950
17	17	O	-3.9247140	-1.6506040	-1.8304360
18	18	C	-5.0362700	-1.4477350	-2.7176630
19	19	O	1.4666980	1.3422380	0.1681820
20	20	N	0.6958690	-0.5530050	1.1383240
21	21	C	2.6851650	0.6743610	0.6000420
22	22	C	3.6673520	0.2193330	-0.5082790
23	23	C	4.8764320	-0.3061230	0.3317020
24	24	C	4.3665220	-1.6591440	0.9308000
25	25	C	2.1604020	-0.6510540	1.2283750
26	26	C	2.9069350	-1.7373320	0.4064940
27	27	C	3.0575780	-1.1408080	-1.0328290
28	28	C	4.0202970	1.2918490	-1.5296600
29	29	C	1.7659460	-1.0350110	-1.8668800
30	30	C	4.0320870	-1.9458370	-1.9256240
31	31	H	-0.7359900	-2.0127710	2.6560390
32	32	H	-2.2887190	-2.1159220	3.4904720
33	33	H	-3.4071290	-2.8900520	1.4473540
34	34	H	-1.8997940	-3.7966980	1.5298150
35	35	H	-2.2637500	-2.8905790	-0.7790510
36	36	H	-0.8194330	-2.1726150	-0.0238720
37	37	H	-2.9976750	0.8821670	0.9443410
38	38	H	-1.2603960	2.2683130	2.3825700

39	39	H	-2.2995650	1.7842760	-1.1386640
40	40	H	-0.9564760	0.8097730	-1.7125230
41	41	H	-0.8548820	3.1619790	-2.5080850
42	42	H	0.5636930	2.7868130	-1.5326180
43	43	H	-1.9280260	4.3050220	-0.5924870
44	44	H	-0.3326690	5.0065510	-0.8709430
45	45	H	0.6437110	3.7508120	0.9683950
46	46	H	-0.8047620	4.5306460	1.5906150
47	47	H	-5.1167320	-2.3678800	-3.2966890
48	48	H	-4.8524040	-0.5939290	-3.3751190
49	49	H	-5.9533950	-1.2672030	-2.1509660
50	50	H	3.1717850	1.3643840	1.2961570
51	51	H	5.1660720	0.4126160	1.1063340
52	52	H	5.7542170	-0.4448760	-0.3052760
53	53	H	4.4057730	-1.6726770	2.0246760
54	54	H	4.9636000	-2.5056690	0.5830970
55	55	H	2.4112080	-0.7612490	2.2890340
56	56	H	2.4528110	-2.7304390	0.4695990
57	57	H	4.7300270	0.9117540	-2.2728520
58	58	H	4.4849760	2.1572680	-1.0422890
59	59	H	3.1306130	1.6490490	-2.0575590
60	60	H	1.9668930	-0.4975790	-2.8006140
61	61	H	0.9414160	-0.5369280	-1.3708120
62	62	H	1.4224550	-2.0397610	-2.1398650
63	63	H	3.6309630	-2.9515940	-2.0962940
64	64	H	5.0387320	-2.0593060	-1.5222920
65	65	H	4.1256240	-1.4668080	-2.9065530

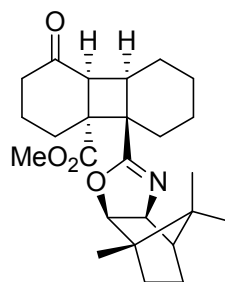


Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5393334		
3	3	C	2	1		1.5418429	112.2190961	
4	4	C	3	2	1	1.5490275	116.7087946	40.2023577
5	5	C	4	3	2	1.5847997	118.2434470	-15.7596527
6	6	C	1	2	3	1.5152212	110.4786174	-60.1624272
7	7	O	6	1	2	1.2209809	122.5618661	-126.9257459
8	8	C	4	3	2	1.6003785	119.3285714	87.9944113
9	9	C	5	4	3	1.5636625	90.2722257	136.9195980
10	10	C	8	4	3	1.5535873	113.1277133	-22.2777570
11	11	C	10	8	4	1.5360586	112.9384661	-144.5163398
12	12	C	11	10	8	1.5341007	109.7326561	62.5819691
13	13	C	9	5	4	1.5360648	124.4265696	-140.8100737
14	14	C	4	3	2	1.5397894	108.0391078	-140.8698936
15	15	O	14	4	3	1.2136070	125.3983960	2.4107799
16	16	O	14	4	3	1.3552669	112.7451250	178.8324508
17	17	C	16	14	4	1.4397944	115.7416533	-179.7250281
18	18	C	8	4	3	1.5089534	115.4795033	104.7067197
19	19	N	18	8	4	1.2762018	125.6820820	-42.9268258
20	20	O	18	8	4	1.3716788	116.1636684	138.1893897
21	21	C	19	18	8	1.4712663	107.1228153	175.3093268
22	22	C	21	19	18	1.5527791	119.9949271	116.4319383
23	23	C	22	21	19	1.5531224	103.8238573	171.6824952
24	24	C	23	22	21	1.5656289	102.7356364	71.8478618
25	25	C	20	18	8	1.4579706	106.2208193	-173.7749984
26	26	C	25	20	18	1.5493130	117.4850098	-119.4055013
27	27	C	22	21	19	1.5644403	105.4338338	-81.9708723
28	28	C	27	22	21	1.5387721	115.8314197	71.0087972
29	29	C	27	22	21	1.5474960	113.1922901	-168.0860648
30	30	C	26	25	20	1.5224634	114.7460824	-49.3217317
31	31	H	1	6	7	1.0932350	108.6472566	-3.4046748
32	32	H	1	6	7	1.1005359	108.0619879	113.7056450
33	33	H	2	1	6	1.0957992	109.3108937	179.3541313

34	34	H	2	1	6	1.0955665	108.6728922	64.4099540
35	35	H	3	2	1	1.0922364	107.8011199	-80.1078666
36	36	H	3	2	1	1.0951108	110.3242414	165.1818303
37	37	H	5	4	3	1.0984610	112.8363807	-108.9860175
38	38	H	9	5	4	1.0901775	106.2150299	93.6603791
39	39	H	10	8	4	1.0947038	109.3528305	90.1218749
40	40	H	10	8	4	1.0913388	109.4580284	-25.8466475
41	41	H	11	10	8	1.0969483	110.8635662	-59.1053718
42	42	H	11	10	8	1.0967755	108.8756022	-176.3889957
43	43	H	12	11	10	1.0966257	110.5195575	177.4072660
44	44	H	12	11	10	1.0970544	109.4457521	60.4497272
45	45	H	13	9	5	1.0944591	109.2890209	-44.7727275
46	46	H	13	9	5	1.0979386	106.5977063	-160.1861375
47	47	H	17	16	14	1.0926078	110.5054451	61.2082594
48	48	H	17	16	14	1.0924814	110.2179640	-59.4463391
49	49	H	17	16	14	1.0900002	105.4145732	-179.1845449
50	50	H	21	19	18	1.0955482	106.9911700	-118.8358690
51	51	H	22	21	19	1.0934696	113.7009676	46.2931823
52	52	H	23	22	21	1.0948241	111.7882169	-48.9797066
53	53	H	23	22	21	1.0927567	111.5014158	-168.4120747
54	54	H	24	23	22	1.0957512	112.5333658	-119.2499461
55	55	H	24	23	22	1.0935663	111.9676283	120.8620765
56	56	H	25	20	18	1.0943835	105.4536949	116.6449829
57	57	H	28	27	22	1.0960824	110.1782959	-173.9264549
58	58	H	28	27	22	1.0962556	109.4729017	68.3832101
59	59	H	28	27	22	1.0824833	114.5555711	-52.0049221
60	60	H	29	27	22	1.0957644	110.0854329	178.1137967
61	61	H	29	27	22	1.0904097	115.0058330	56.7397069
62	62	H	29	27	22	1.0961738	109.6332191	-64.4173568
63	63	H	30	26	25	1.0944247	111.2760416	60.3535402
64	64	H	30	26	25	1.0966592	110.9033381	-59.2463981
65	65	H	30	26	25	1.0956929	111.2354877	-178.8444618

Row	Tag	Symbol	X	Y	Z
1	1	C	5.0094530	-0.0050200	0.8945020
2	2	C	4.0454310	-0.0003620	2.0945800
3	3	C	2.7998610	0.8715660	1.8385010
4	4	C	2.1777700	0.7979520	0.4217900
5	5	C	3.0430840	0.1648960	-0.7452840
6	6	C	4.3187470	-0.5520950	-0.3381900
7	7	O	4.7827510	-1.4674670	-0.9996950
8	8	C	1.0776010	-0.3205520	0.1058970
9	9	C	1.7910400	-0.6185700	-1.2587110
10	10	C	1.1477750	-1.5354520	1.0716750
11	11	C	0.8172970	-2.8678960	0.3825790
12	12	C	1.8515460	-3.1546260	-0.7135870
13	13	C	1.8260260	-2.0592610	-1.7903880
14	14	C	1.7318130	2.2166400	0.0225430
15	15	O	1.8898580	3.2173540	0.6907010
16	16	O	1.1930310	2.2663100	-1.2200330
17	17	C	0.7589380	3.5660540	-1.6618890
18	18	C	-0.3462050	0.1730790	0.0281460
19	19	N	-0.8905420	1.0046100	0.8287360
20	20	O	-1.1116230	-0.3454100	-0.9851690
21	21	C	-2.2401590	1.2824600	0.3130250
22	22	C	-3.4873160	0.8888520	1.1501600
23	23	C	-4.6708360	1.5340260	0.3786550
24	24	C	-4.7760430	0.6400690	-0.9023470
25	25	C	-2.3762620	0.3793450	-0.9520530
26	26	C	-3.6655990	-0.4433320	-0.7047000
27	27	C	-3.7186110	-0.6315110	0.8629800
28	28	C	-2.6855430	-1.5941080	1.4745330
29	29	C	-5.0853690	-1.1471530	1.3736950
30	30	C	-3.8130170	-1.6770350	-1.5845520
31	31	H	5.9057960	-0.6007830	1.0863310
32	32	H	5.3238030	1.0275270	0.6795370
33	33	H	4.5669970	0.3873490	2.9768640

34	34	H	3.7815790	-1.0357800	2.3365670
35	35	H	3.0804730	1.9131660	2.0096930
36	36	H	2.0233600	0.6523920	2.5789580
37	37	H	3.3880710	0.9115260	-1.4733940
38	38	H	1.3355830	0.0056640	-2.0277220
39	39	H	0.5011650	-1.3501300	1.9353460
40	40	H	2.1615540	-1.6293690	1.4646790
41	41	H	-0.1905920	-2.8446950	-0.0497600
42	42	H	0.8228920	-3.6668900	1.1339070
43	43	H	1.6545310	-4.1257190	-1.1834290
44	44	H	2.8501760	-3.2230480	-0.2646050
45	45	H	2.6762610	-2.1732580	-2.4700540
46	46	H	0.9149560	-2.1952990	-2.3878110
47	47	H	1.6023140	4.2597990	-1.6969110
48	48	H	-0.0008130	3.9611610	-0.9835200
49	49	H	0.3470570	3.4104580	-2.6590070
50	50	H	-2.2834420	2.3542810	0.0904220
51	51	H	-3.4174900	1.1739250	2.2035040
52	52	H	-4.4762880	2.5848670	0.1409070
53	53	H	-5.5924860	1.5089150	0.9652110
54	54	H	-4.6186120	1.2089770	-1.8255100
55	55	H	-5.7585760	0.1684960	-0.9925410
56	56	H	-2.4325980	0.9112900	-1.9067970
57	57	H	-2.8716440	-2.6175990	1.1292370
58	58	H	-2.7888060	-1.5957530	2.5659130
59	59	H	-1.6550460	-1.3490650	1.2513740
60	60	H	-5.2080270	-2.2053960	1.1172260
61	61	H	-5.9536850	-0.6154930	0.9833640
62	62	H	-5.1207600	-1.0758550	2.4669750
63	63	H	-2.9859780	-2.3767650	-1.4291500
64	64	H	-3.8171500	-1.4022450	-2.6462180
65	65	H	-4.7514350	-2.2030050	-1.3765370



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5415237		
3	3	C	2	1		1.5369633	112.8732538	
4	4	C	3	2	1	1.5584376	115.9201131	43.8926448
5	5	C	4	3	2	1.5796459	116.3979376	-27.9625045
6	6	C	5	4	3	1.5155128	115.8728821	26.2093112
7	7	O	6	5	4	1.2210107	121.9567766	141.7295864
8	8	C	4	3	2	1.6196645	125.0193139	78.7198989
9	9	C	5	4	3	1.5411227	87.3631637	149.5262392
10	10	C	8	4	3	1.5718850	125.6753997	109.4882278
11	11	C	10	8	4	1.5613991	111.0505355	118.3101848
12	12	C	11	10	8	1.5540429	116.1228500	33.9245997
13	13	C	9	5	4	1.5185205	134.7798182	-154.5558213
14	14	C	4	3	2	1.5274591	103.8888057	-154.1518885
15	15	O	14	4	3	1.2155876	123.8273816	-70.1058236
16	16	O	14	4	3	1.3540965	113.7159218	106.1826137
17	17	C	16	14	4	1.4421626	115.8667469	-175.9956607
18	18	C	8	4	3	1.5191133	113.8050793	-20.7463550
19	19	N	18	8	4	1.2783752	126.1987028	40.2630031
20	20	O	18	8	4	1.3764456	115.7035266	-151.8861213
21	21	C	19	18	8	1.4712232	107.5504448	161.2943705
22	22	C	21	19	18	1.5528348	121.0392414	116.1062832
23	23	C	22	21	19	1.5545092	103.4462281	170.3325732
24	24	C	23	22	21	1.5650507	102.7208205	71.8980232
25	25	C	20	18	8	1.4557256	106.8020671	-159.7756680
26	26	C	25	20	18	1.5492361	117.6986262	-121.8637538
27	27	C	22	21	19	1.5655588	105.5961828	-83.4188107



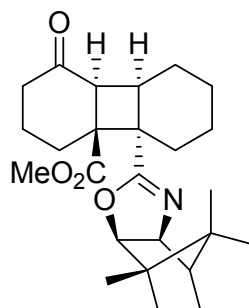
28	28	C	27	22	21	1.5367031	116.2164995	70.4805786
29	29	C	27	22	21	1.5470671	112.9933556	-168.0839337
30	30	C	26	25	20	1.5225550	114.8525169	-49.9484312
31	31	H	1	6	5	1.0933286	108.8673181	-179.7703147
32	32	H	1	6	5	1.1008575	107.8212007	-62.7851294
33	33	H	2	1	6	1.0964872	109.1745312	-178.2687424
34	34	H	2	1	6	1.0904328	109.6303721	65.0388991
35	35	H	3	2	1	1.0990744	107.2943630	-75.0877464
36	36	H	3	2	1	1.0913305	110.2539060	168.6319664
37	37	H	5	4	3	1.0972040	113.7847785	-95.0814233
38	38	H	9	5	4	1.0971017	101.5540969	81.1292697
39	39	H	10	8	4	1.0921948	110.2693424	-3.8146592
40	40	H	10	8	4	1.0942874	109.9355442	-120.2255845
41	41	H	11	10	8	1.0976084	109.1132906	-89.7859742
42	42	H	11	10	8	1.0963869	108.1980172	156.1769460
43	43	H	12	11	10	1.0960603	108.0342833	-176.8812634
44	44	H	12	11	10	1.0918419	108.6090955	67.6647517
45	45	H	13	9	5	1.0912989	112.2799414	51.2895930
46	46	H	13	9	5	1.0963125	109.6410354	-67.7038691
47	47	H	17	16	14	1.0896575	105.3628741	179.3761251
48	48	H	17	16	14	1.0924105	110.3379222	59.6968402
49	49	H	17	16	14	1.0923960	110.3857108	-61.0213700
50	50	H	21	19	18	1.0953747	106.1085421	-119.2506834
51	51	H	22	21	19	1.0937545	113.9958694	45.2682697
52	52	H	23	22	21	1.0946648	111.7756023	-48.8844702
53	53	H	23	22	21	1.0926065	111.5255835	-168.3304377
54	54	H	24	23	22	1.0958636	112.5183266	-119.2465915
55	55	H	24	23	22	1.0936061	111.9481746	120.8633400
56	56	H	25	20	18	1.0952034	105.5631928	114.0492030
57	57	H	28	27	22	1.0952366	110.3541583	-178.1233775
58	58	H	28	27	22	1.0961102	109.9216761	64.1028890
59	59	H	28	27	22	1.0819948	114.6152880	-57.5567784
60	60	H	29	27	22	1.0955703	110.1232043	176.1526767
61	61	H	29	27	22	1.0906227	115.0472945	54.6362763

62	62	H	29	27	22	1.0962994	109.5234181	-66.4584890
63	63	H	30	26	25	1.0943145	111.2928937	60.7440274
64	64	H	30	26	25	1.0967439	110.9642556	-59.1082243
65	65	H	30	26	25	1.0954978	111.0411245	-178.6583903

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.2809190	-3.0318180	1.0475790
2	2	C	-0.9247960	-2.8449410	-0.4405570
3	3	C	-1.8808830	-1.8861500	-1.1677940
4	4	C	-2.2483170	-0.5795930	-0.4018770
5	5	C	-2.2115120	-0.6561970	1.1754810
6	6	C	-1.2810470	-1.6968030	1.7655260
7	7	O	-0.6299040	-1.4828030	2.7760130
8	8	C	-1.3005790	0.7289090	-0.2881750
9	9	C	-1.8272830	0.8362410	1.1679930
10	10	C	-1.5585610	2.1114690	-0.9901690
11	11	C	-1.7387010	3.2501720	0.0628610
12	12	C	-0.8987300	3.1183450	1.3636760
13	13	C	-1.0785540	1.7527680	2.1194590
14	14	C	-3.6103170	-0.1903040	-0.9733150
15	15	O	-3.7767210	0.2219830	-2.1046780
16	16	O	-4.6419810	-0.4205380	-0.1270060
17	17	C	-5.9583020	-0.1538480	-0.6523710
18	18	C	0.1686230	0.4466440	-0.5517600
19	19	N	0.6385730	-0.3298180	-1.4520360
20	20	O	1.0600890	1.2830970	0.0808830
21	21	C	2.0507580	0.0295350	-1.6547590
22	22	C	3.1877280	-0.9766620	-1.3289330
23	23	C	4.4540980	-0.2943970	-1.9182720
24	24	C	4.6992520	0.8918310	-0.9272390
25	25	C	2.3178320	1.1844060	-0.6453950
26	26	C	3.5720310	0.7335880	0.1444660
27	27	C	3.4449500	-0.8375510	0.2090720
28	28	C	2.3435210	-1.3797930	1.1333470

29	29	C	4.7396520	-1.5467830	0.6718390
30	30	C	3.8150840	1.4881950	1.4443380
31	31	H	-0.5839330	-3.7052950	1.5535500
32	32	H	-2.2914660	-3.4601460	1.1325330
33	33	H	-0.9613200	-3.8180470	-0.9445560
34	34	H	0.0996250	-2.4819950	-0.5293010
35	35	H	-2.8223710	-2.4280170	-1.3349620
36	36	H	-1.4814590	-1.6270840	-2.1498060
37	37	H	-3.1869280	-0.8679210	1.6311050
38	38	H	-2.8060790	1.3144910	1.0381180
39	39	H	-2.4420400	2.0521450	-1.6295710
40	40	H	-0.7234030	2.3543280	-1.6542440
41	41	H	-2.8007630	3.3294540	0.3283470
42	42	H	-1.4892450	4.2035380	-0.4176900
43	43	H	-1.1670480	3.9490190	2.0264990
44	44	H	0.1560870	3.2445630	1.1115870
45	45	H	-0.1105140	1.3430660	2.4126760
46	46	H	-1.6633810	1.8888360	3.0367180
47	47	H	-6.6471190	-0.4039810	0.1540520
48	48	H	-6.1486730	-0.7730770	-1.5319590
49	49	H	-6.0517170	0.8989500	-0.9284490
50	50	H	2.1383960	0.3386570	-2.7019500
51	51	H	3.0039320	-1.9900320	-1.6971710
52	52	H	4.2909520	0.0461520	-2.9457450
53	53	H	5.3037090	-0.9808710	-1.9447950
54	54	H	4.6487050	1.8687210	-1.4212510
55	55	H	5.6840160	0.8332710	-0.4552380
56	56	H	2.4766500	2.1710840	-1.0934060
57	57	H	2.6056600	-1.2041420	2.1821430
58	58	H	2.2479760	-2.4640820	1.0043270
59	59	H	1.3673900	-0.9397800	0.9775600
60	60	H	4.9095530	-1.3628830	1.7384170
61	61	H	5.6445470	-1.2482950	0.1412470
62	62	H	4.6283690	-2.6302990	0.5474140

63	63	H	2.9795230	1.3615530	2.1395530
64	64	H	3.9328420	2.5625980	1.2582240
65	65	H	4.7274790	1.1367690	1.9384540



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5526424		
3	3	C	2	1		1.5645041	116.1017494	
4	4	C	3	2	1	1.5507946	108.9214926	-25.5025446
5	5	C	4	3	2	1.5429645	111.2297213	-30.8280550
6	6	C	5	4	3	1.5010710	114.1343910	68.8576522
7	7	O	6	5	4	1.2177944	126.9877540	143.4423526
8	8	C	4	3	2	1.6169936	127.9225737	-133.5137623
9	9	C	5	4	3	1.5482218	92.8072031	-149.1870025
10	10	C	8	4	3	1.5534293	119.6063239	-107.1796756
11	11	C	10	8	4	1.5366366	112.3024599	-120.2142420
12	12	C	11	10	8	1.5325367	110.5974763	57.4687774
13	13	C	12	11	10	1.5456352	112.4931598	-65.3905949
14	14	C	4	3	2	1.5359712	106.0321058	95.4414098
15	15	O	14	4	3	1.2160687	123.5018980	53.4159071
16	16	O	14	4	3	1.3482171	114.1198767	-125.3400882
17	17	C	16	14	4	1.4417530	116.5781001	177.5086160
18	18	C	8	4	3	1.5122252	113.8058241	26.8049711
19	19	N	18	8	4	1.2781492	128.5974646	11.7806679
20	20	O	18	8	4	1.3741232	113.8376508	-172.8040822
21	21	C	19	18	8	1.4698806	107.5418778	171.9785654
22	22	C	21	19	18	1.5523264	119.2163792	114.4738041
23	23	C	22	21	19	1.5534830	103.6841293	171.8209336

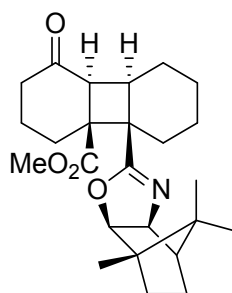
24	24	C	23	22	21	1.5652068	102.7516888	71.9177799
25	25	C	20	18	8	1.4538970	106.8345479	-171.0553161
26	26	C	25	20	18	1.5494708	116.8242653	-118.0789087
27	27	C	22	21	19	1.5658604	105.4172202	-81.7512177
28	28	C	27	22	21	1.5423056	116.2237188	71.2688624
29	29	C	27	22	21	1.5476663	112.9541335	-168.0309973
30	30	C	26	25	20	1.5222285	114.7142480	-49.9975709
31	31	H	1	6	5	1.0983736	106.7260431	104.2829515
32	32	H	1	6	5	1.0951893	107.7558936	-142.2480459
33	33	H	2	1	6	1.0964783	107.9305106	-67.9975482
34	34	H	2	1	6	1.0954037	108.6327302	177.6895643
35	35	H	3	2	1	1.0892539	108.6903641	-145.4491717
36	36	H	3	2	1	1.0921390	111.0488970	95.8132012
37	37	H	5	4	3	1.0993877	104.0493163	-42.4477575
38	38	H	9	5	4	1.0930800	111.0890983	130.3236869
39	39	H	10	8	4	1.0925169	109.8770183	117.1552846
40	40	H	10	8	4	1.0924518	109.8099026	0.9023984
41	41	H	11	10	8	1.0978865	110.0532235	-64.7047422
42	42	H	11	10	8	1.0966496	108.8557369	178.5916045
43	43	H	12	11	10	1.0962179	110.5027953	172.6912045
44	44	H	12	11	10	1.0971613	108.3411404	56.7711697
45	45	H	13	12	11	1.0923289	110.2421494	154.6045868
46	46	H	13	12	11	1.0956664	107.9728666	-89.9039145
47	47	H	17	16	14	1.0893699	105.2725231	-177.3698058
48	48	H	17	16	14	1.0924881	110.3464951	62.9406002
49	49	H	17	16	14	1.0923785	110.2515788	-57.6867631
50	50	H	21	19	18	1.0953760	107.1661135	-120.7125504
51	51	H	22	21	19	1.0935818	113.7677088	46.5673923
52	52	H	23	22	21	1.0947711	111.7209224	-48.7935124
53	53	H	23	22	21	1.0926379	111.5797916	-168.2022717
54	54	H	24	23	22	1.0957293	112.4707595	-119.2321928
55	55	H	24	23	22	1.0935816	112.0034212	120.9211859
56	56	H	25	20	18	1.0944091	105.8093086	117.8609102
57	57	H	28	27	22	1.0961180	109.9992265	-174.3237634

58	58	H	28	27	22	1.0961021	109.3363299	68.3355590
59	59	H	28	27	22	1.0838688	115.3323514	-52.2343700
60	60	H	29	27	22	1.0956932	110.1896796	178.0532016
61	61	H	29	27	22	1.0902719	114.9220119	56.6078941
62	62	H	29	27	22	1.0961076	109.6143991	-64.4606633
63	63	H	30	26	25	1.0943160	111.3344961	60.0315600
64	64	H	30	26	25	1.0966685	110.8997061	-59.6679971
65	65	H	30	26	25	1.0955336	111.1359700	-179.1807489

Row	Tag	Symbol	X	Y	Z
1	1	C	-3.5188560	-2.6617780	-0.2630450
2	2	C	-2.1991250	-3.0664600	0.4477580
3	3	C	-1.4184060	-1.9121750	1.1589380
4	4	C	-1.7760980	-0.5671670	0.4748520
5	5	C	-2.0933690	-0.7684810	-1.0216610
6	6	C	-3.3686650	-1.5156280	-1.2835880
7	7	O	-4.1618140	-1.3174000	-2.1861640
8	8	C	-0.7687860	0.6059010	0.0016690
9	9	C	-1.5677680	0.6376730	-1.4004290
10	10	C	-0.7092760	1.9356940	0.8024510
11	11	C	-1.0723000	3.1534550	-0.0615650
12	12	C	-2.4696510	2.9866570	-0.6684070
13	13	C	-2.5423810	1.8131760	-1.6717220
14	14	C	-2.9071100	0.0473950	1.3129050
15	15	O	-2.8337660	0.2218720	2.5141550
16	16	O	-4.0115580	0.3576260	0.6046390
17	17	C	-5.1274130	0.8868590	1.3485690
18	18	C	0.6242620	0.1182470	-0.3276270
19	19	N	1.0341280	-1.0832550	-0.4761810
20	20	O	1.5215420	1.1283950	-0.5780350
21	21	C	2.4148980	-1.0216750	-0.9764120
22	22	C	3.5687910	-1.5507820	-0.0829390
23	23	C	4.8063020	-1.5148020	-1.0213320
24	24	C	5.0985250	0.0175630	-1.1491430

25	25	C	2.7325440	0.5007170	-1.0813350
26	26	C	4.0195660	0.6890880	-0.2393430
27	27	C	3.8924320	-0.3859020	0.9121640
28	28	C	2.8396300	-0.1110430	2.0052180
29	29	C	5.2103860	-0.6074670	1.6926620
30	30	C	4.3203960	2.1296800	0.1497270
31	31	H	-4.2719400	-2.3375880	0.4678380
32	32	H	-3.9554210	-3.5194120	-0.7858400
33	33	H	-1.5410430	-3.5267510	-0.2987840
34	34	H	-2.4211910	-3.8537110	1.1763400
35	35	H	-0.3503080	-2.1055710	1.0681710
36	36	H	-1.6653700	-1.8683810	2.2218860
37	37	H	-1.3223630	-1.4727120	-1.3655530
38	38	H	-0.8704870	0.5838020	-2.2405010
39	39	H	0.2873370	2.0674120	1.2302430
40	40	H	-1.3974250	1.8888290	1.6496260
41	41	H	-0.3253640	3.2883350	-0.8548170
42	42	H	-1.0370700	4.0542540	0.5629030
43	43	H	-2.7801060	3.9072250	-1.1762120
44	44	H	-3.1849600	2.8326510	0.1491370
45	45	H	-3.5652030	1.4355380	-1.7381080
46	46	H	-2.2971770	2.2027670	-2.6659950
47	47	H	-5.9214200	1.0247930	0.6155930
48	48	H	-4.8572030	1.8378280	1.8135150
49	49	H	-5.4321240	0.1821630	2.1256440
50	50	H	2.4331490	-1.5421370	-1.9400690
51	51	H	3.3653650	-2.5260890	0.3679660
52	52	H	4.5947790	-1.9812820	-1.9888950
53	53	H	5.6532600	-2.0540440	-0.5903590
54	54	H	5.0256430	0.3730020	-2.1830550
55	55	H	6.1042640	0.2730610	-0.8039900
56	56	H	2.8685530	0.8864560	-2.0964400
57	57	H	3.1175050	0.7816720	2.5773370
58	58	H	2.8191030	-0.9512530	2.7088270

59	59	H	1.8257220	0.0276820	1.6481220
60	60	H	5.4101070	0.2476240	2.3480050
61	61	H	6.0936470	-0.7541410	1.0705450
62	62	H	5.1127450	-1.4888300	2.3369580
63	63	H	3.5101110	2.5581110	0.7475670
64	64	H	4.4420380	2.7581560	-0.7407240
65	65	H	5.2475440	2.1969180	0.7294420



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5636656		
3	3	C	2	1		1.5790657	117.2650874	
4	4	C	3	2	1	1.5333418	107.8682999	-4.9935498
5	5	C	4	3	2	1.5617522	105.9502094	-49.3837957
6	6	C	5	4	3	1.5027587	113.1856269	79.6043986
7	7	O	6	5	4	1.2159347	128.6673231	144.6292469
8	8	C	4	3	2	1.6294374	125.0083876	-148.9826702
9	9	C	8	4	3	1.5598222	89.3552535	108.3915709
10	10	C	8	4	3	1.5478367	125.6609853	0.9552142
11	11	C	10	8	4	1.5832696	108.1336617	141.6583009
12	12	C	11	10	8	1.5669254	117.6837917	13.9832049
13	13	C	9	8	4	1.5198314	115.3882830	150.6578524
14	14	C	4	3	2	1.5663036	105.7950252	77.6606268
15	15	O	14	4	3	1.2131745	119.6820423	25.5570089
16	16	O	14	4	3	1.3557394	124.4050838	-156.8757165
17	17	C	16	14	4	1.4423763	130.0896353	14.8497233
18	18	C	8	4	3	1.5182283	109.3710836	-128.5525681
19	19	N	18	8	4	1.2758349	130.8182149	-109.5411287



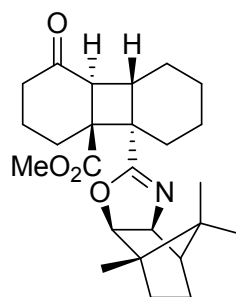
20	20	O	18	8	4	1.3730190	111.4328047	69.9255100
21	21	C	19	18	8	1.4742464	107.0107962	173.2304833
22	22	C	21	19	18	1.5525498	120.1381725	116.0633415
23	23	C	22	21	19	1.5537829	103.6411016	170.7794773
24	24	C	23	22	21	1.5649529	102.7186584	71.5326959
25	25	C	20	18	8	1.4552817	106.6378517	-170.7634203
26	26	C	25	20	18	1.5489922	117.1095119	-120.7649685
27	27	C	22	21	19	1.5653565	105.4296211	-82.9950243
28	28	C	27	22	21	1.5393303	115.9361594	71.1107750
29	29	C	27	22	21	1.5472340	113.0905206	-168.0286080
30	30	C	26	25	20	1.5225629	114.6366745	-50.5889687
31	31	H	1	6	5	1.0981558	106.3448876	104.1221690
32	32	H	1	6	5	1.0947056	107.4562609	-143.2415847
33	33	H	2	1	6	1.0960025	107.8371122	-79.3607905
34	34	H	2	1	6	1.0937970	107.2849356	166.8739713
35	35	H	3	2	1	1.0956288	109.1022271	-123.2153782
36	36	H	3	2	1	1.0893801	111.0552358	117.7890178
37	37	H	5	4	3	1.1016195	104.3611015	-23.1751867
38	38	H	9	8	4	1.0928451	103.6773268	-99.8981046
39	39	H	10	8	4	1.0956076	109.8972655	22.9171382
40	40	H	10	8	4	1.0925908	111.7584865	-95.2341279
41	41	H	11	10	8	1.0962974	108.4435209	-109.8252003
42	42	H	11	10	8	1.0953576	108.6393904	136.1258927
43	43	H	12	11	10	1.0956775	107.2011515	-171.9455117
44	44	H	12	11	10	1.0911140	108.8891458	73.1243101
45	45	H	13	9	8	1.0913921	114.1955821	-72.1382015
46	46	H	13	9	8	1.0959726	110.1038946	165.8561223
47	47	H	17	16	14	1.0902188	105.2597487	-148.8933552
48	48	H	17	16	14	1.0909034	108.7618228	93.4419370
49	49	H	17	16	14	1.0848042	113.6196914	-30.1283495
50	50	H	21	19	18	1.0952057	106.5136771	-119.2324503
51	51	H	22	21	19	1.0937462	113.9329169	45.4630612
52	52	H	23	22	21	1.0946920	111.7555568	-49.2079211
53	53	H	23	22	21	1.0927197	111.5075221	-168.6180739

54	54	H	24	23	22	1.0953751	112.4835424	-118.8086391
55	55	H	24	23	22	1.0934998	111.9769768	121.2924952
56	56	H	25	20	18	1.0933550	105.5237639	114.7483377
57	57	H	28	27	22	1.0961799	110.0452184	-175.2544415
58	58	H	28	27	22	1.0963924	109.5552623	67.1047205
59	59	H	28	27	22	1.0828367	114.6139751	-53.6983168
60	60	H	29	27	22	1.0956349	110.1005703	177.9256993
61	61	H	29	27	22	1.0902732	114.9890169	56.5943217
62	62	H	29	27	22	1.0963439	109.6509711	-64.5662392
63	63	H	30	26	25	1.0944545	111.3762221	60.0900872
64	64	H	30	26	25	1.0963320	110.7580451	-59.3505796
65	65	H	30	26	25	1.0957476	111.2939542	-178.9399048

Row	Tag	Symbol	X	Y	Z
1	1	C	4.6274290	-1.3388640	0.1567560
2	2	C	4.3516090	-1.0725490	1.6726880
3	3	C	2.9268550	-0.5136150	2.0614260
4	4	C	2.1578640	-0.2416300	0.7630370
5	5	C	3.1225570	0.5897270	-0.1410000
6	6	C	4.1539130	-0.2527500	-0.8372910
7	7	O	4.6264830	-0.1108720	-1.9486170
8	8	C	1.0377910	0.9254370	0.5669320
9	9	C	2.0428290	1.7152940	-0.3269750
10	10	C	0.5969820	1.9436030	1.6462020
11	11	C	0.3640540	3.3410790	0.9394150
12	12	C	0.2748360	3.3598280	-0.6248560
13	13	C	1.4133880	2.5921590	-1.3969280
14	14	C	1.6660900	-1.6402790	0.2578180
15	15	O	1.5042620	-2.5430040	1.0519790
16	16	O	1.3521060	-1.9223730	-1.0305400
17	17	C	1.6415620	-1.1899070	-2.2389100
18	18	C	-0.2253430	0.3181620	-0.0167860
19	19	N	-0.7479980	0.4335300	-1.1749210
20	20	O	-0.8630910	-0.4861530	0.8951000

21	21	C	-1.8809910	-0.5079640	-1.2325250
22	22	C	-3.3297440	0.0249960	-1.3982940
23	23	C	-4.1658920	-1.2596340	-1.6528990
24	24	C	-4.1654720	-1.9545490	-0.2506970
25	25	C	-1.9177590	-1.1809400	0.1720570
26	26	C	-3.3704600	-0.9679860	0.6657040
27	27	C	-3.7958480	0.4194920	0.0430460
28	28	C	-3.1332960	1.6713670	0.6458490
29	29	C	-5.3149680	0.6985190	0.1344320
30	30	C	-3.5714720	-1.1847850	2.1592870
31	31	H	4.1460340	-2.2750290	-0.1559740
32	32	H	5.6988950	-1.4906110	-0.0085130
33	33	H	5.1164290	-0.3765810	2.0358690
34	34	H	4.5233390	-2.0128840	2.2043560
35	35	H	3.0480410	0.4285400	2.6073750
36	36	H	2.3952780	-1.2118580	2.7068960
37	37	H	3.8242200	1.0587250	0.5670080
38	38	H	2.4508130	2.4711530	0.3487000
39	39	H	1.3853690	2.0538430	2.3989630
40	40	H	-0.2973760	1.6091720	2.1772710
41	41	H	1.1602240	4.0258830	1.2540970
42	42	H	-0.5637510	3.7778050	1.3244560
43	43	H	0.2602160	4.4102960	-0.9360030
44	44	H	-0.6815050	2.9317280	-0.9292770
45	45	H	0.9774510	2.0380110	-2.2300040
46	46	H	2.1581120	3.2879690	-1.7999050
47	47	H	0.8078290	-1.4008110	-2.9089740
48	48	H	2.5680530	-1.5736180	-2.6683870
49	49	H	1.7058710	-0.1170250	-2.0919790
50	50	H	-1.6604670	-1.2112390	-2.0426170
51	51	H	-3.4333070	0.7972560	-2.1658680
52	52	H	-3.7186850	-1.8874070	-2.4302390
53	53	H	-5.1784850	-1.0191190	-1.9858320
54	54	H	-3.6948030	-2.9433880	-0.2733840

55	55	H	-5.1786590	-2.1016090	0.1334480
56	56	H	-1.6408870	-2.2384010	0.1953650
57	57	H	-3.4646150	1.8100240	1.6815190
58	58	H	-3.4461880	2.5590070	0.0834700
59	59	H	-2.0506180	1.6528310	0.6460460
60	60	H	-5.5932040	0.9331770	1.1678420
61	61	H	-5.9543770	-0.1206180	-0.1955170
62	62	H	-5.5658110	1.5761580	-0.4728550
63	63	H	-2.9554000	-0.4983990	2.7484900
64	64	H	-3.2900880	-2.2051010	2.4451580
65	65	H	-4.6191310	-1.0386430	2.4451470



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5522437		
3	3	C	2	1		1.5717041	116.6663285	
4	4	C	3	2	1	1.5495928	109.8808216	-16.8905261
5	5	C	4	3	2	1.5411370	108.1655227	-38.3382151
6	6	C	5	4	3	1.5053325	114.2353602	72.2719191
7	7	O	6	5	4	1.2187905	126.6332968	142.0071005
8	8	C	4	3	2	1.6249677	123.6731446	-136.0514242
9	9	C	5	4	3	1.5408629	92.3000326	-145.1995385
10	10	C	8	4	3	1.5546512	114.3649710	14.8360434
11	11	C	10	8	4	1.5381905	115.9516095	90.3155010
12	12	C	11	10	8	1.5332934	110.1084070	51.2666210
13	13	C	9	5	4	1.5414390	118.1053387	144.0167106
14	14	C	4	3	2	1.5597936	105.5252977	89.6098610
15	15	O	14	4	3	1.2115048	118.5976491	46.0906717

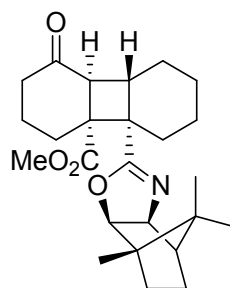
16	16	O	14	4	3	1.3645969	123.4812466	-122.2372699
17	17	C	16	14	4	1.4423765	129.1357527	-56.3278688
18	18	C	8	4	3	1.5136893	118.7620314	-116.3041746
19	19	N	18	8	4	1.2775816	126.4419659	146.7827583
20	20	O	18	8	4	1.3705275	116.0058466	-37.2381355
21	21	C	19	18	8	1.4689808	107.5813840	172.3874034
22	22	C	21	19	18	1.5509732	119.1091250	116.1586269
23	23	C	22	21	19	1.5545614	103.7669853	172.8884012
24	24	C	23	22	21	1.5652868	102.8026088	72.5667479
25	25	C	20	18	8	1.4591025	107.0200337	-172.9468930
26	26	C	25	20	18	1.5506708	117.5947090	-116.0010530
27	27	C	22	21	19	1.5645323	105.3175219	-80.5569257
28	28	C	27	22	21	1.5403787	116.3002571	70.8957903
29	29	C	27	22	21	1.5478832	112.8888477	-168.2979598
30	30	C	26	25	20	1.5226130	114.9328770	-48.6475117
31	31	H	1	6	5	1.0976469	105.9543939	102.9995113
32	32	H	1	6	5	1.0949773	108.1744451	-143.5092927
33	33	H	2	1	6	1.0966356	107.8010840	-73.1128411
34	34	H	2	1	6	1.0945930	108.2070514	173.0644357
35	35	H	3	2	1	1.0927800	107.9159332	-136.6268504
36	36	H	3	2	1	1.0900156	111.2940916	106.0725483
37	37	H	5	4	3	1.0996391	104.7158612	-37.7849856
38	38	H	9	5	4	1.0893927	111.0644565	-87.7443259
39	39	H	10	8	4	1.0938279	109.9351583	-36.5466710
40	40	H	10	8	4	1.0918946	106.6056382	-150.6304629
41	41	H	11	10	8	1.0982655	112.5414173	-72.5294678
42	42	H	11	10	8	1.0965357	107.9896672	171.1563059
43	43	H	12	11	10	1.0958853	110.8343416	172.7097139
44	44	H	12	11	10	1.0978041	107.7895018	56.5617040
45	45	H	13	9	5	1.0956235	109.8388117	146.2910434
46	46	H	13	9	5	1.0973442	107.2375235	31.7228027
47	47	H	17	16	14	1.0910323	104.2561261	-163.0249432
48	48	H	17	16	14	1.0900691	112.4196604	79.2537798
49	49	H	17	16	14	1.0903245	109.9722166	-45.4518770

50	50	H	21	19	18	1.0955663	107.0668410	-119.0673530
51	51	H	22	21	19	1.0934365	113.6236386	47.6073199
52	52	H	23	22	21	1.0950340	111.7107495	-48.2124735
53	53	H	23	22	21	1.0926753	111.5420886	-167.5522529
54	54	H	24	23	22	1.0959753	112.5672128	-120.3706811
55	55	H	24	23	22	1.0933700	111.9542875	119.7479398
56	56	H	25	20	18	1.0941922	105.4224632	119.9150467
57	57	H	28	27	22	1.0945207	110.0552028	-177.5198621
58	58	H	28	27	22	1.0964948	109.3134356	64.4840256
59	59	H	28	27	22	1.0825503	115.3528981	-56.7162876
60	60	H	29	27	22	1.0954320	110.0584691	175.4367704
61	61	H	29	27	22	1.0905470	115.1240114	53.8615262
62	62	H	29	27	22	1.0961869	109.5081565	-67.2049551
63	63	H	30	26	25	1.0939510	111.4838477	60.8095894
64	64	H	30	26	25	1.0972281	110.8507082	-59.4108805
65	65	H	30	26	25	1.0956733	110.8735906	-178.4304029

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.4688810	-2.5142380	1.4731270
2	2	C	-1.6886680	-2.7898350	-0.0485210
3	3	C	-0.9479010	-1.6391460	-0.7168980
4	4	C	-1.8525170	-0.3640400	-0.5203060
5	5	C	-2.3914570	-0.2076680	0.8383670
6	6	C	-2.6189680	-1.5469700	1.6108040
7	7	O	-3.6244750	-1.8380680	2.2137560
8	8	C	-0.9371280	0.7959390	-0.2113040
9	9	C	-1.0370360	0.3285190	1.2346110
10	10	C	-1.7188190	2.0919110	-0.3809980
11	11	C	-1.3388600	3.0637700	0.7283220
12	12	C	-2.1522020	2.5161220	1.6322530
13	13	C	-1.1087060	1.5384980	2.1566510
14	14	C	-2.9666230	-0.5612310	-1.5914100
15	15	O	-3.1767950	-1.5450320	-2.2602310
16	16	O	-3.7462770	0.5257800	-1.5662410

17	17	C	-3.0098410	1.6506430	-1.9635010
18	18	C	0.4625120	0.5982310	-0.7040490
19	19	N	0.7984560	-0.4137860	-1.3753060
20	20	O	1.5659910	1.4735490	-0.5156590
21	21	C	2.2289410	-0.2154690	-1.6494240
22	22	C	3.0683220	-1.2475150	-0.9079130
23	23	C	4.5460980	-0.9714340	-1.1518850
24	24	C	4.8713100	0.5291220	-0.2390270
25	25	C	2.5667960	1.1072010	-0.9741010
26	26	C	3.4306170	0.7170910	0.2179400
27	27	C	2.8579330	-0.9230170	0.5651090
28	28	C	1.3658940	-0.8859620	0.8687340
29	29	C	3.8980450	-1.6576770	1.4004450
30	30	C	3.3711460	1.8169770	1.2696020
31	31	H	-0.5145810	-1.9591960	1.6144690
32	32	H	-1.7029880	-3.4347180	2.0533660
33	33	H	-2.7739320	-2.7178840	-0.2845680
34	34	H	-1.2024130	-3.7523860	-0.3240770
35	35	H	-0.7491440	-1.8958570	-1.7814490
36	36	H	0.0150720	-1.4621470	-0.1877540
37	37	H	-3.3914560	0.2781460	0.7856480
38	38	H	-0.3482770	-0.5313330	1.3933770
39	39	H	-2.8092800	1.8760650	-0.3261460
40	40	H	-1.4754220	2.5441750	-1.3684060
41	41	H	-1.7057590	4.0822450	0.4696520
42	42	H	-0.2813750	2.8882360	1.0277230
43	43	H	-2.9581720	1.9525260	1.1111730
44	44	H	-2.3864970	3.2653800	2.4211580
45	45	H	-0.1153040	2.0392630	2.1875750
46	46	H	-1.3936910	1.2072260	3.1801930
47	47	H	-3.7038360	2.5172350	-1.9234850
48	48	H	-2.7071900	1.4779910	-3.0184200
49	49	H	-2.2099650	1.7925400	-1.2054490
50	50	H	2.3794290	-0.3352980	-2.7456540

51	51	H	2.8160830	-2.2655350	-1.2804900
52	52	H	4.7139560	-0.7881440	-2.2367640
53	53	H	5.1525830	-1.8020750	-0.7264310
54	54	H	5.1431940	1.3422180	-0.9487290
55	55	H	5.5109400	0.2952950	0.6411850
56	56	H	2.8564650	1.8535320	-1.7474050
57	57	H	1.2019810	-0.6493270	1.9437570
58	58	H	0.9064700	-1.8738480	0.6409470
59	59	H	0.8701220	-0.1075990	0.2466290
60	60	H	3.7523020	-1.4265690	2.4793110
61	61	H	4.9215180	-1.3423300	1.0974100
62	62	H	3.8012800	-2.7561120	1.2487980
63	63	H	2.3213740	1.9617530	1.6099880
64	64	H	3.7486980	2.7729270	0.8424640
65	65	H	4.0010310	1.5413300	2.1447780



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5428215		
3	3	C	2	1		1.5385463	110.2167295	
4	4	C	3	2	1	1.5477674	108.9349868	-68.3026391
5	5	C	4	3	2	1.5614558	112.5818293	46.5822279
6	6	C	5	4	3	1.5182645	115.8804607	5.9067971
7	7	O	6	5	4	1.2206912	121.5401237	141.0444161
8	8	C	4	3	2	1.6081708	121.0497282	149.2536627
9	9	C	5	4	3	1.5475863	92.1283869	128.0192611
10	10	C	8	4	3	1.5615424	118.1228053	119.1800517
11	11	C	10	8	4	1.5347473	114.9289674	83.3507664



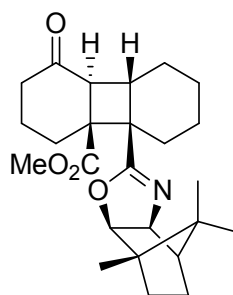
12	12	C	11	10	8	1.5326937	110.3034224	51.0962497
13	13	C	12	11	10	1.5337786	109.9498783	-67.3072767
14	14	C	4	3	2	1.5294368	106.3219161	-81.2268292
15	15	O	14	4	3	1.2152043	123.6382055	-60.1632721
16	16	O	14	4	3	1.3546969	114.1208519	118.4432379
17	17	C	16	14	4	1.4419525	115.7944480	-178.7135354
18	18	C	8	4	3	1.5122132	116.1027541	-5.4059217
19	19	N	18	8	4	1.2752323	128.3907208	41.3514460
20	20	O	18	8	4	1.3777510	113.5457124	-145.1076738
21	21	C	19	18	8	1.4700900	107.2757822	169.1193467
22	22	C	21	19	18	1.5511433	119.4491631	115.2270627
23	23	C	22	21	19	1.5540482	103.6716979	171.6082215
24	24	C	23	22	21	1.5652729	102.7836018	72.3382465
25	25	C	20	18	8	1.4548979	106.5441497	-168.6164829
26	26	C	25	20	18	1.5513784	117.1432402	-118.5041795
27	27	C	22	21	19	1.5662616	105.4758001	-81.9560365
28	28	C	27	22	21	1.5409671	116.5036263	70.5518922
29	29	C	27	22	21	1.5473834	112.8145168	-168.4582759
30	30	C	26	25	20	1.5225266	114.7581742	-49.6333058
31	31	H	1	6	5	1.0959814	106.1941559	141.8974575
32	32	H	1	6	5	1.0983763	107.3874602	-105.1352323
33	33	H	2	1	6	1.0976483	110.4172856	-87.9842499
34	34	H	2	1	6	1.0953546	109.5509526	155.5214193
35	35	H	3	2	1	1.0919856	112.2626066	169.6122791
36	36	H	3	2	1	1.0911090	109.2892426	51.8581567
37	37	H	5	4	3	1.0959778	112.6274639	-115.5982886
38	38	H	9	5	4	1.0908120	111.7025554	-117.6828460
39	39	H	10	8	4	1.0934372	108.6581180	-42.8518147
40	40	H	10	8	4	1.0961653	107.6924346	-157.9594042
41	41	H	11	10	8	1.0982542	111.3617437	-70.3933150
42	42	H	11	10	8	1.0965485	108.3959680	172.8067430
43	43	H	12	11	10	1.0965674	110.7958040	171.7483014
44	44	H	12	11	10	1.0987587	109.3843443	54.2607326
45	45	H	13	12	11	1.0957417	110.4880078	175.8716884

46	46	H	13	12	11	1.0978977	107.4659843	-68.8220242
47	47	H	17	16	14	1.0896736	105.3917382	178.5911646
48	48	H	17	16	14	1.0923146	110.3533763	58.8403412
49	49	H	17	16	14	1.0926061	110.3428408	-61.7892014
50	50	H	21	19	18	1.0952865	106.8988154	-120.0109332
51	51	H	22	21	19	1.0936785	113.7897747	46.4091896
52	52	H	23	22	21	1.0947254	111.6409443	-48.3425296
53	53	H	23	22	21	1.0926767	111.6619711	-167.7069980
54	54	H	24	23	22	1.0958662	112.5279806	-119.7292985
55	55	H	24	23	22	1.0937802	111.9184437	120.3520836
56	56	H	25	20	18	1.0946470	105.7620555	117.4636073
57	57	H	28	27	22	1.0952260	110.1213854	177.6762863
58	58	H	28	27	22	1.0963203	109.7409032	59.9943451
59	59	H	28	27	22	1.0832628	114.9306337	-61.6178564
60	60	H	29	27	22	1.0956373	110.1925902	174.1986322
61	61	H	29	27	22	1.0903760	114.9587720	52.6594413
62	62	H	29	27	22	1.0962804	109.5407573	-68.3325906
63	63	H	30	26	25	1.0942623	111.3424736	60.3048789
64	64	H	30	26	25	1.0967209	110.9152819	-59.4955790
65	65	H	30	26	25	1.0955339	111.0532394	-179.0047116

Row	Tag	Symbol	X	Y	Z
1	1	C	4.1258790	-1.9355960	0.5494750
2	2	C	3.8032590	-1.3118450	1.9337840
3	3	C	2.3940370	-0.6338380	2.0907990
4	4	C	1.7812290	-0.3624250	0.6936450
5	5	C	2.9146400	0.0866070	-0.2491450
6	6	C	3.8579570	-1.0158010	-0.6502380
7	7	O	4.3708560	-1.1717250	-1.7448030
8	8	C	1.0415030	1.0265700	0.2886530
9	9	C	1.9849980	1.0537550	-1.0072010
10	10	C	1.3016650	2.2021950	1.2720970
11	11	C	2.5170450	3.0896470	0.9538040
12	12	C	2.4609880	3.5566840	-0.5055530

13	13	C	2.5757450	2.3870010	-1.5067080
14	14	C	0.9748820	-1.6484030	0.3344500
15	15	O	0.2486350	-2.1312740	1.1753690
16	16	O	1.2067510	-2.3943550	-0.7844410
17	17	C	1.2015080	-1.9862740	-2.1678760
18	18	C	-0.4303520	0.9922420	-0.0630850
19	19	N	-1.2870660	1.9118440	0.1662360
20	20	O	-0.8551260	-0.1059120	-0.7644910
21	21	C	-2.5374280	1.5305590	-0.5039290
22	22	C	-3.7982880	1.2496720	0.3544720
23	23	C	-4.9289160	1.0687890	-0.6970140
24	24	C	-4.5997030	-0.3273020	-1.3236490
25	25	C	-2.2429040	0.1393280	-1.1425250
26	26	C	-3.3252330	-0.8008350	-0.5515620
27	27	C	-3.6196470	-0.2110480	0.8856460
28	28	C	-2.5307100	-0.4200630	1.9548960
29	29	C	-4.9080770	-0.7799770	1.5276820
30	30	C	-3.0182400	-2.2874570	-0.6701400
31	31	H	3.5214760	-2.8360760	0.3801780
32	32	H	5.1715140	-2.2576840	0.5060920
33	33	H	4.5799330	-0.5704120	2.1566390
34	34	H	3.9125340	-2.0916450	2.6941160
35	35	H	2.5325120	0.3096530	2.6244820
36	36	H	1.7240410	-1.2481100	2.6923880
37	37	H	3.5660710	0.7140940	0.3762380
38	38	H	1.4737140	0.5458080	-1.8241190
39	39	H	1.3493590	1.8264250	2.2982460
40	40	H	0.4182940	2.8428060	1.2332760
41	41	H	3.4712520	2.5868410	1.1608360
42	42	H	2.4871520	3.9576520	1.6231800
43	43	H	3.2479030	4.2914410	-0.7101540
44	44	H	1.5048060	4.0747890	-0.6554100
45	45	H	2.1004090	2.6736010	-2.4513280
46	46	H	3.6313590	2.2057790	-1.7454590

47	47	H	1.1240600	-2.9219120	-2.7236950
48	48	H	2.1235700	-1.4811630	-2.4558260
49	49	H	0.3284810	-1.3650340	-2.3695990
50	50	H	-2.7612100	2.3136300	-1.2367230
51	51	H	-3.9938300	2.0158700	1.1096590
52	52	H	-4.9228700	1.8725580	-1.4406660
53	53	H	-5.9167000	1.0801610	-0.2300100
54	54	H	-4.4188510	-0.2716860	-2.4031680
55	55	H	-5.4156960	-1.0412780	-1.1827530
56	56	H	-2.2562780	0.1089980	-2.2362150
57	57	H	-2.4635550	-1.4798530	2.2200580
58	58	H	-2.8024950	0.1325130	2.8621410
59	59	H	-1.5346340	-0.1064840	1.6695610
60	60	H	-4.7565450	-1.8277380	1.8091180
61	61	H	-5.7974710	-0.7359990	0.8981290
62	62	H	-5.1316880	-0.2297690	2.4490370
63	63	H	-2.0978670	-2.5500040	-0.1403180
64	64	H	-2.8971200	-2.5786150	-1.7210760
65	65	H	-3.8361210	-2.8890540	-0.2582520



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5537908		
3	3	C	2	1		1.5697067	116.1640230	
4	4	C	3	2	1	1.5389224	108.9024171	-21.1904695
5	5	C	4	3	2	1.5596830	110.2134194	-35.7731514
6	6	C	5	4	3	1.5030832	112.2665359	72.4519621
7	7	O	6	5	4	1.2171163	126.7055117	139.7612548

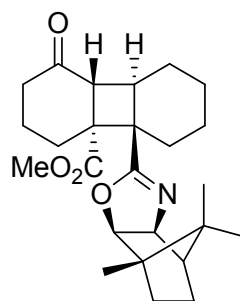
8	8	C	4	3	2	1.6045805	126.4511094	-134.8564165
9	9	C	5	4	3	1.5415151	91.6394707	-149.7644432
10	10	C	8	4	3	1.5602517	112.3249229	20.9900520
11	11	C	10	8	4	1.5373846	114.4449509	139.2002774
12	12	C	11	10	8	1.5343702	110.7860252	-58.0394238
13	13	C	9	5	4	1.5299389	120.9228839	144.3280893
14	14	C	4	3	2	1.5465592	106.7746600	87.6697344
15	15	O	14	4	3	1.2137382	124.0694126	16.0731581
16	16	O	14	4	3	1.3500360	113.6518183	-159.5154039
17	17	C	16	14	4	1.4403375	115.6663618	178.7734360
18	18	C	8	4	3	1.5032482	117.8829620	-106.3502762
19	19	N	18	8	4	1.2750107	127.4948982	12.3649424
20	20	O	18	8	4	1.3757483	114.5657007	-170.0579172
21	21	C	19	18	8	1.4715736	107.2212006	172.8718284
22	22	C	21	19	18	1.5546974	119.9651883	114.3299958
23	23	C	22	21	19	1.5525556	103.7198795	170.5509873
24	24	C	23	22	21	1.5646685	102.6627414	71.0686912
25	25	C	20	18	8	1.4563426	106.3414799	-170.2390941
26	26	C	25	20	18	1.5463249	116.9174006	-120.7110439
27	27	C	22	21	19	1.5659424	105.5227108	-83.2077664
28	28	C	27	22	21	1.5406258	116.1914922	71.3166317
29	29	C	27	22	21	1.5478888	113.2186623	-167.5078155
30	30	C	26	25	20	1.5224877	114.8183648	-51.0204729
31	31	H	1	6	5	1.0981617	106.8014309	104.8103757
32	32	H	1	6	5	1.0951886	107.8733848	-141.7396415
33	33	H	2	1	6	1.0971613	107.8016954	-70.5757786
34	34	H	2	1	6	1.0946702	108.3237748	175.3943240
35	35	H	3	2	1	1.0924266	108.6567320	-142.4701655
36	36	H	3	2	1	1.0901710	110.6385972	99.8132407
37	37	H	5	4	3	1.0999718	105.5814791	-40.2457658
38	38	H	9	5	4	1.0895488	109.5236895	-86.8212274
39	39	H	10	8	4	1.0942294	109.1323854	19.2530852
40	40	H	10	8	4	1.0960438	109.0701770	-95.9139205
41	41	H	11	10	8	1.0970400	108.5072895	-179.2231113

42	42	H	11	10	8	1.0951211	110.2971898	63.7362157
43	43	H	12	11	10	1.0999430	109.4212763	-61.2891353
44	44	H	12	11	10	1.0963678	110.4388276	-177.7186566
45	45	H	13	9	5	1.0979595	107.9312832	173.0044052
46	46	H	13	9	5	1.0973135	108.7659286	57.8610161
47	47	H	17	16	14	1.0893980	105.3695909	-178.5873624
48	48	H	17	16	14	1.0922289	109.9826799	61.6480119
49	49	H	17	16	14	1.0922351	110.3622128	-59.0918115
50	50	H	21	19	18	1.0947577	106.8229750	-120.8783269
51	51	H	22	21	19	1.0934729	113.7703925	45.3085526
52	52	H	23	22	21	1.0946153	111.8454570	-49.7644127
53	53	H	23	22	21	1.0927360	111.4724702	-169.2534870
54	54	H	24	23	22	1.0958530	112.4072160	-118.0357655
55	55	H	24	23	22	1.0935686	112.0475065	122.1872902
56	56	H	25	20	18	1.0948399	105.7668403	115.0773903
57	57	H	28	27	22	1.0958959	110.1203217	-167.9484770
58	58	H	28	27	22	1.0961111	109.1892838	74.8825887
59	59	H	28	27	22	1.0836883	115.1348438	-45.3882556
60	60	H	29	27	22	1.0957902	110.0368698	-179.2179839
61	61	H	29	27	22	1.0905371	115.0204032	59.4774247
62	62	H	29	27	22	1.0962101	109.6647387	-61.7735234
63	63	H	30	26	25	1.0944000	111.3972631	59.7785769
64	64	H	30	26	25	1.0966687	110.8502691	-59.9394013
65	65	H	30	26	25	1.0955383	111.1037483	-179.4043215

Row	Tag	Symbol	X	Y	Z
1	1	C	1.7035720	3.3017840	0.6836760
2	2	C	2.1000350	2.9722420	-0.7704620
3	3	C	1.3916450	1.6885580	-1.2367920
4	4	C	1.9665040	0.4844340	-0.4524410
5	5	C	2.0686350	0.7612570	1.0808830
6	6	C	1.4723980	2.0732840	1.5586000
7	7	O	0.8582100	2.1499960	2.6107290
8	8	C	1.0568810	-0.7993910	-0.1198860

9	9	C	1.3030400	-0.5388890	1.4251330
10	10	C	1.5022980	-2.1841100	-0.6878400
11	11	C	2.5572900	-2.9182590	0.1508890
12	12	C	2.1149290	-2.9913120	1.6165390
13	13	C	2.1086320	-1.5864140	2.2319240
14	14	C	3.2737110	0.1025770	-1.1485530
15	15	O	3.3407310	-0.2449160	-2.3110840
16	16	O	4.3718470	0.2121860	-0.3628770
17	17	C	5.6283030	-0.1115190	-0.9919720
18	18	C	-0.4023240	-0.6983650	-0.5036870
19	19	N	-0.9098100	-0.2061850	-1.5650230
20	20	O	-1.2480570	-1.3404330	0.3741980
21	21	C	-2.3317050	-0.5791050	-1.5826290
22	22	C	-3.4121500	0.5295240	-1.4845170
23	23	C	-4.7416700	-0.2283470	-1.7548390
24	24	C	-4.9422880	-1.0552250	-0.4410260
25	25	C	-2.5530340	-1.3876190	-0.2673130
26	26	C	-3.7204220	-0.6586540	0.4486410
27	27	C	-3.5388630	0.8556690	0.0421620
28	28	C	-2.3507330	1.5939930	0.6885400
29	29	C	-4.7685260	1.7368870	0.3673990
30	30	C	-3.8706230	-0.9934820	1.9262800
31	31	H	0.7737620	3.8809550	0.7181670
32	32	H	2.4626180	3.9207160	1.1808710
33	33	H	3.1887120	2.8602280	-0.8545280
34	34	H	1.8296350	3.8095460	-1.4228480
35	35	H	1.5017860	1.5219390	-2.3103560
36	36	H	0.3207800	1.7789770	-1.0481350
37	37	H	3.1037590	0.7631360	1.4409970
38	38	H	0.3666390	-0.3301780	1.9442320
39	39	H	1.8264970	-2.0495630	-1.7234060
40	40	H	0.6184250	-2.8317530	-0.7179290
41	41	H	3.5337330	-2.4190460	0.0916620
42	42	H	2.6954260	-3.9220660	-0.2682870

43	43	H	2.7868050	-3.6372860	2.1942590
44	44	H	1.1143470	-3.4417190	1.6734580
45	45	H	1.7238850	-1.6186170	3.2573910
46	46	H	3.1527210	-1.2558280	2.3091920
47	47	H	6.3863230	0.0565310	-0.2274110
48	48	H	5.7977880	0.5341990	-1.8565380
49	49	H	5.6320560	-1.1541570	-1.3185910
50	50	H	-2.4953900	-1.1671500	-2.4920590
51	51	H	-3.2306150	1.3821580	-2.1449660
52	52	H	-4.6698300	-0.8658210	-2.6419070
53	53	H	-5.5707330	0.4615010	-1.9300720
54	54	H	-4.9700920	-2.1352200	-0.6247660
55	55	H	-5.8795670	-0.8010860	0.0622400
56	56	H	-2.7808880	-2.4500310	-0.4000360
57	57	H	-2.5658830	1.8047020	1.7415510
58	58	H	-2.1992830	2.5589590	0.1907230
59	59	H	-1.4102540	1.0571190	0.6616340
60	60	H	-4.8745250	1.8528640	1.4517120
61	61	H	-5.7179530	1.3611460	-0.0151280
62	62	H	-4.6213350	2.7400420	-0.0495490
63	63	H	-2.9709180	-0.7258880	2.4887160
64	64	H	-4.0439030	-2.0670060	2.0688180
65	65	H	-4.7209310	-0.4607890	2.3660630



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5497593		



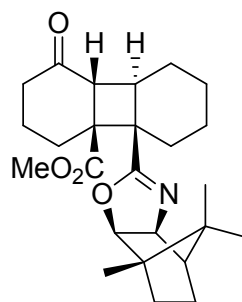
3	3	C	2	1		1.5612081	116.0188587	
4	4	C	3	2	1	1.5524972	109.6874035	29.3657422
5	5	C	4	3	2	1.5613744	111.4425540	26.2549030
6	6	C	5	4	3	1.5050817	114.1601187	-65.8681780
7	7	O	6	5	4	1.2170852	126.2575408	-141.4715880
8	8	C	4	3	2	1.6236518	129.4107861	127.8078458
9	9	C	5	4	3	1.5337455	88.4757448	157.6904730
10	10	C	8	4	3	1.5615334	126.4597836	109.6470707
11	11	C	10	8	4	1.5600751	110.5839046	118.6801390
12	12	C	11	10	8	1.5522371	115.3742849	35.3236431
13	13	C	9	5	4	1.5197490	133.6520403	-154.7435837
14	14	C	4	3	2	1.5334468	106.6246986	-101.0474901
15	15	O	14	4	3	1.2153427	122.8097375	-65.1036305
16	16	O	14	4	3	1.3503621	114.6202926	113.4605267
17	17	C	16	14	4	1.4425536	116.5435262	-178.5473818
18	18	C	8	4	3	1.5203446	111.0765873	-22.2265936
19	19	N	18	8	4	1.2781626	125.7396527	46.8423417
20	20	O	18	8	4	1.3764306	116.7082425	-141.2731528
21	21	C	19	18	8	1.4694718	107.6795661	166.3643860
22	22	C	21	19	18	1.5536332	120.1475833	115.6514051
23	23	C	22	21	19	1.5529570	103.6626203	170.7790832
24	24	C	23	22	21	1.5651716	102.6889573	71.4292522
25	25	C	20	18	8	1.4566574	106.7952067	-164.7496813
26	26	C	25	20	18	1.5490177	117.4224460	-120.4972504
27	27	C	22	21	19	1.5654186	105.5051362	-82.9903288
28	28	C	27	22	21	1.5388497	115.9861925	71.0919180
29	29	C	27	22	21	1.5472711	113.1656112	-167.9234742
30	30	C	26	25	20	1.5227738	114.8230082	-50.4785072
31	31	H	1	6	5	1.0953399	107.9930270	140.6117757
32	32	H	1	6	5	1.0980192	106.3748040	-105.7708044
33	33	H	2	1	6	1.0955962	108.7812363	-177.9826635
34	34	H	2	1	6	1.0970367	108.0365153	67.8152454
35	35	H	3	2	1	1.0934943	110.6944646	-91.8769088
36	36	H	3	2	1	1.0894457	109.9082742	150.5821446

37	37	H	5	4	3	1.1002045	105.5061888	48.0951394
38	38	H	9	5	4	1.0938664	104.7688602	76.2385594
39	39	H	10	8	4	1.0934821	110.4872593	-3.4515325
40	40	H	10	8	4	1.0950425	109.8582710	-119.9525312
41	41	H	11	10	8	1.0974001	109.2759393	-88.0512574
42	42	H	11	10	8	1.0962658	108.4002005	157.4326693
43	43	H	12	11	10	1.0957530	108.3594084	179.7493949
44	44	H	12	11	10	1.0932042	108.5392670	64.1896579
45	45	H	13	9	5	1.0928860	112.5369731	40.2133538
46	46	H	13	9	5	1.0956924	109.3425802	-79.1944081
47	47	H	17	16	14	1.0893509	105.2281554	178.4873470
48	48	H	17	16	14	1.0923778	110.2922785	58.7212041
49	49	H	17	16	14	1.0924289	110.2883620	-61.9419307
50	50	H	21	19	18	1.0952180	106.5807795	-119.7560345
51	51	H	22	21	19	1.0935446	113.8340074	45.4558868
52	52	H	23	22	21	1.0946480	111.8056179	-49.3702064
53	53	H	23	22	21	1.0926010	111.5108894	-168.8450928
54	54	H	24	23	22	1.0956994	112.4804820	-118.6417153
55	55	H	24	23	22	1.0935377	111.9976628	121.5079637
56	56	H	25	20	18	1.0946972	105.6105596	115.3897003
57	57	H	28	27	22	1.0958224	110.1850296	-175.0551272
58	58	H	28	27	22	1.0963382	109.6138346	67.1241123
59	59	H	28	27	22	1.0829493	114.2436629	-53.5807849
60	60	H	29	27	22	1.0956225	110.1153409	178.2995538
61	61	H	29	27	22	1.0903450	114.9669424	56.9098113
62	62	H	29	27	22	1.0962434	109.6159074	-64.2107531
63	63	H	30	26	25	1.0944846	111.4623119	59.9837273
64	64	H	30	26	25	1.0965437	110.8026129	-59.7253928
65	65	H	30	26	25	1.0955952	111.1967567	-179.1809339

Row	Tag	Symbol	X	Y	Z
1	1	C	-4.6706230	-1.2296880	0.0676650
2	2	C	-4.6023120	-0.5985220	-1.3505130
3	3	C	-3.1647780	-0.3118210	-1.9120090

4	4	C	-2.1765010	-0.2324380	-0.7350260
5	5	C	-2.8618110	0.4282630	0.5004640
6	6	C	-3.8670570	-0.4820130	1.1486440
7	7	O	-4.0520980	-0.6286930	2.3426360
8	8	C	-1.0361800	0.8759120	-0.5207670
9	9	C	-1.5206870	1.0109650	0.9884330
10	10	C	-1.3185950	2.1806340	-1.3284350
11	11	C	-1.0049390	3.4797440	-0.5685110
12	12	C	-1.8098290	3.5556180	0.7355930
13	13	C	-1.4585020	2.3826410	1.6632300
14	14	C	-1.6875900	-1.6745620	-0.4646750
15	15	O	-1.8186160	-2.5945290	-1.2454780
16	16	O	-1.1761930	-1.8501100	0.7723590
17	17	C	-0.7325000	-3.1853580	1.0802900
18	18	C	0.3921810	0.4690470	-0.7531480
19	19	N	0.8145950	-0.5966880	-1.3112050
20	20	O	1.3242000	1.3959780	-0.3471640
21	21	C	2.2724060	-0.4620840	-1.4601940
22	22	C	3.2239290	-1.4063920	-0.6728120
23	23	C	4.6212680	-1.1130710	-1.2825950
24	24	C	4.9391460	0.3191110	-0.7385400
25	25	C	2.6078690	0.9383360	-0.8606730
26	26	C	3.7189640	0.6612390	0.1784640
27	27	C	3.3655650	-0.7674320	0.7498070
28	28	C	2.1260370	-0.8540750	1.6606260
29	29	C	4.5102730	-1.3884030	1.5864660
30	30	C	3.9665060	1.7928240	1.1664960
31	31	H	-4.2911160	-2.2599570	0.0457730
32	32	H	-5.7089300	-1.2997150	0.4089170
33	33	H	-5.1712220	0.3393470	-1.3280170
34	34	H	-5.1367900	-1.2543200	-2.0451820
35	35	H	-3.1888610	0.6259820	-2.4717780
36	36	H	-2.8586230	-1.0971400	-2.6033960
37	37	H	-3.4693870	1.2513270	0.0962920

38	38	H	-1.0078540	0.2755120	1.6074870
39	39	H	-2.3787530	2.2135590	-1.5973570
40	40	H	-0.7708290	2.1402930	-2.2769270
41	41	H	-1.2503690	4.3301930	-1.2165830
42	42	H	0.0658770	3.5415110	-0.3475400
43	43	H	-2.8848010	3.5537240	0.5025560
44	44	H	-1.6125970	4.5020320	1.2527220
45	45	H	-0.4358430	2.5307280	2.0343820
46	46	H	-2.1113050	2.3720990	2.5451790
47	47	H	-0.3812780	-3.1425000	2.1106270
48	48	H	0.0732520	-3.4764810	0.4028130
49	49	H	-1.5595130	-3.8923070	0.9841130
50	50	H	2.4903040	-0.5422950	-2.5300450
51	51	H	2.9247800	-2.4577460	-0.7019260
52	52	H	4.6045340	-1.1513730	-2.3764120
53	53	H	5.3632790	-1.8441100	-0.9523320
54	54	H	5.0518370	1.0557020	-1.5420500
55	55	H	5.8698000	0.3430620	-0.1647790
56	56	H	2.9259110	1.6957980	-1.5843960
57	57	H	2.2524300	-0.2020210	2.5323130
58	58	H	2.0276830	-1.8781840	2.0387620
59	59	H	1.1860570	-0.6018150	1.1839890
60	60	H	4.5537260	-0.9143580	2.5734560
61	61	H	5.5030760	-1.3056110	1.1428910
62	62	H	4.3109480	-2.4537100	1.7509870
63	63	H	3.0666310	2.0207780	1.7461280
64	64	H	4.2639200	2.7096680	0.6434050
65	65	H	4.7700790	1.5371260	1.8658480



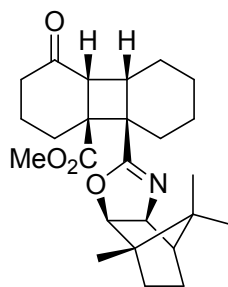
Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5385550		
3	3	C	2	1		1.5352425	110.9292510	
4	4	C	3	2	1	1.5530201	112.0955254	63.1750341
5	5	C	4	3	2	1.5847474	110.9781875	-48.7245960
6	6	C	5	4	3	1.5138509	120.0540968	28.6911675
7	7	O	6	5	4	1.2225524	120.7652535	159.5638891
8	8	C	4	3	2	1.6045302	114.1612979	-145.3978899
9	9	C	8	4	3	1.5524547	85.6135900	87.5863916
10	10	C	8	4	3	1.5414857	125.9552346	-22.3314115
11	11	C	10	8	4	1.5675765	109.5091971	130.5918402
12	12	C	11	10	8	1.5513446	114.7983439	26.1926507
13	13	C	9	8	4	1.5200662	115.5360768	161.4422980
14	14	C	4	3	2	1.5408950	106.1703291	89.4914109
15	15	O	14	4	3	1.2150618	118.3200688	73.9518210
16	16	O	14	4	3	1.3526808	123.8365165	-98.0897268
17	17	C	16	14	4	1.4356681	125.1567504	-22.2152520
18	18	C	8	4	3	1.5299309	106.8774704	-157.2303492
19	19	N	18	8	4	1.2811019	125.6502419	-30.2749129
20	20	O	18	8	4	1.3678321	116.9203042	143.5947811
21	21	C	19	18	8	1.4718679	107.5957117	165.3467838
22	22	C	21	19	18	1.5525891	120.9990104	118.1315614
23	23	C	22	21	19	1.5531791	103.7579336	171.6052834
24	24	C	23	22	21	1.5651067	102.7674846	71.7413201
25	25	C	20	18	8	1.4593429	106.6427628	-164.1450995
26	26	C	25	20	18	1.5484342	117.8343229	-121.4797858
27	27	C	22	21	19	1.5632429	105.3547137	-82.1100038
28	28	C	27	22	21	1.5364929	115.2291414	70.8177357
29	29	C	27	22	21	1.5471043	113.4683366	-168.1318553
30	30	C	26	25	20	1.5224340	114.9618784	-49.1597714
31	31	H	1	6	5	1.0939450	107.8419445	158.9669335
32	32	H	1	6	5	1.1009668	106.9370770	-86.7336313
33	33	H	2	1	6	1.0957317	109.4931810	-175.0194749

34	34	H	2	1	6	1.0975122	110.1659186	68.6591200
35	35	H	3	2	1	1.0953294	107.9420815	-58.0552651
36	36	H	3	2	1	1.0933869	111.2972994	-174.4083185
37	37	H	5	4	3	1.0879359	112.3693247	159.4432378
38	38	H	9	8	4	1.0954051	104.4998812	-82.3083845
39	39	H	10	8	4	1.0939772	109.9847792	10.8051811
40	40	H	10	8	4	1.0898533	110.9503572	-106.9655286
41	41	H	11	10	8	1.0979749	109.4955076	-96.5854211
42	42	H	11	10	8	1.0953419	108.9501490	148.2529214
43	43	H	12	11	10	1.0955379	108.9960396	178.0535433
44	44	H	12	11	10	1.0940592	108.3097183	62.9876315
45	45	H	13	9	8	1.0942521	112.0324632	-81.7355659
46	46	H	13	9	8	1.0962694	110.2442583	159.5615835
47	47	H	17	16	14	1.0906533	104.7484896	-178.0799992
48	48	H	17	16	14	1.0920819	112.2601952	64.0961067
49	49	H	17	16	14	1.0912832	110.3791080	-59.8721155
50	50	H	21	19	18	1.0952512	106.1410944	-116.6758302
51	51	H	22	21	19	1.0937639	113.9486375	46.2108424
52	52	H	23	22	21	1.0945177	111.8524607	-49.0949469
53	53	H	23	22	21	1.0927563	111.3512852	-168.6228772
54	54	H	24	23	22	1.0954008	112.5089633	-119.2534465
55	55	H	24	23	22	1.0934842	112.0025088	120.8385627
56	56	H	25	20	18	1.0934312	105.0797075	114.2745661
57	57	H	28	27	22	1.0960283	110.5035268	-170.5266183
58	58	H	28	27	22	1.0963438	109.5481728	71.5333569
59	59	H	28	27	22	1.0826609	113.8770158	-48.3357695
60	60	H	29	27	22	1.0959301	110.0580618	179.2446036
61	61	H	29	27	22	1.0906426	115.0374142	57.8495900
62	62	H	29	27	22	1.0961047	109.6172239	-63.3078397
63	63	H	30	26	25	1.0945036	111.4189270	60.3807908
64	64	H	30	26	25	1.0964778	110.8832755	-59.3138273
65	65	H	30	26	25	1.0955504	111.0827663	-178.8627851

Row	Tag	Symbol	X	Y	Z
1	1	C	-1.6541590	-2.4741710	0.8915460
2	2	C	-2.8433860	-2.9922910	0.0639910
3	3	C	-3.3119890	-1.9446760	-0.9752740
4	4	C	-3.5842710	-0.6380360	-0.2980790
5	5	C	-2.4885380	-0.0246030	0.5274870
6	6	C	-1.9147910	-1.0992530	1.4802950
7	7	C	-0.1499580	1.0135830	0.4750430
8	8	C	-1.3335660	0.6010870	-0.3654830
9	9	O	-1.6816160	-0.8273100	2.6438500
10	10	C	-0.2415070	2.2440300	1.3326660
11	11	C	-1.3141710	3.2317510	0.8253740
12	12	C	-1.3773840	3.1869650	-0.7060780
13	13	C	-1.8766340	1.8137400	-1.2000960
14	14	C	1.0398920	0.2436350	0.4362440
15	15	C	-4.8922060	0.0004190	-0.2946960
16	16	O	-5.1499500	1.0610270	0.2709040
17	17	O	-5.8311870	-0.6900750	-1.0031370
18	18	C	-7.1394510	-0.0967340	-1.0401740
19	19	O	2.1132050	0.6868720	1.1820090
20	20	N	1.2272670	-0.8464320	-0.2654590
21	21	C	3.1540050	-0.3125690	1.0678450
22	22	C	4.4889570	0.1489990	0.4296620
23	23	C	5.3895230	-1.1168990	0.6002340
24	24	C	4.8291670	-2.1298860	-0.4529220
25	25	C	2.5680970	-1.3359240	0.0465430
26	26	C	3.6423680	-1.3500900	-1.0794080
27	27	C	4.2092510	0.1079010	-1.1248260
28	28	C	5.0682880	1.4260450	1.0225640
29	29	C	3.2629440	1.1878960	-1.6859970
30	30	C	5.4928120	0.2316910	-1.9809640
31	31	H	-0.7683590	-2.3745430	0.2472480
32	32	H	-1.4004480	-3.1517740	1.7113610
33	33	H	-3.6803130	-3.2375900	0.7294440

34	34	H	-2.5617570	-3.9173830	-0.4511140
35	35	H	-4.1952420	-2.2990310	-1.5080240
36	36	H	-2.5091210	-1.8163650	-1.7181970
37	37	H	-2.9065660	0.7640370	1.1556470
38	38	H	-0.9948980	-0.1794560	-1.0493120
39	39	H	0.7407490	2.7303940	1.3557240
40	40	H	-0.4469520	1.9501170	2.3743080
41	41	H	-1.0753380	4.2406390	1.1793110
42	42	H	-2.2997340	2.9844550	1.2379460
43	43	H	-0.3749610	3.3902090	-1.1079940
44	44	H	-2.0359480	3.9720440	-1.0945560
45	45	H	-2.9700130	1.8095080	-1.1708260
46	46	H	-1.5896000	1.6759640	-2.2486840
47	47	H	-7.7502870	-0.7783180	-1.6322800
48	48	H	-7.1006210	0.8905380	-1.5079670
49	49	H	-7.5438710	0.0049570	-0.0298130
50	50	H	3.3165150	-0.7021390	2.0780520
51	51	H	5.3386090	-1.5060360	1.6233310
52	52	H	6.4387850	-0.8708740	0.4138870
53	53	H	4.5017050	-3.0693190	0.0041550
54	54	H	5.5795380	-2.3888990	-1.2040430
55	55	H	2.4628400	-2.3492040	0.4530170
56	56	H	3.2765890	-1.7541930	-2.0275430
57	57	H	6.0090950	1.6979700	0.5312140
58	58	H	5.2779760	1.3000910	2.0915220
59	59	H	4.3717680	2.2638350	0.9201300
60	60	H	3.7122240	2.1798280	-1.5605870
61	61	H	2.2753100	1.2140160	-1.2394170
62	62	H	3.1271040	1.0278660	-2.7621400
63	63	H	5.2628110	-0.0022430	-3.0269380
64	64	H	6.3144410	-0.4163140	-1.6740250
65	65	H	5.8637380	1.2624580	-1.9566010





Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5393907		
3	3	C	2	1		1.5418555	112.3936586	
4	4	C	3	2	1	1.5572193	116.5876169	-39.4155847
5	5	C	4	3	2	1.5721985	118.3158348	17.3547753
6	6	C	5	4	3	1.5164080	116.6674896	-14.1901705
7	7	C	4	3	2	1.6162878	119.2238121	-86.7253747
8	8	C	5	4	3	1.5584258	89.6035988	-140.3838917
9	9	C	7	4	3	1.5469205	112.7694076	27.8242044
10	10	C	9	7	4	1.5387456	112.8598755	144.8511839
11	11	C	10	9	7	1.5345382	110.3426529	-62.2263955
12	12	C	8	5	4	1.5340460	125.2490948	144.0923864
13	13	O	6	5	4	1.2211602	122.4134517	-149.8384509
14	14	C	4	3	2	1.5370179	106.5665929	145.7250326
15	15	O	14	4	3	1.2155535	123.3249407	36.7128195
16	16	O	14	4	3	1.3476533	113.6917471	-140.4822897
17	17	C	16	14	4	1.4396085	116.0357700	-175.4787648
18	18	C	7	4	3	1.5166304	118.3099773	-104.3190289
19	19	O	18	7	4	1.3733987	116.4265282	134.4413391
20	20	N	18	7	4	1.2774487	126.0730727	-47.3933766
21	21	C	19	18	7	1.4531937	106.6372170	171.2831104
22	22	C	21	19	18	1.5366217	116.8930821	120.2966843
23	23	C	22	21	19	1.5567401	102.9735726	174.9529810
24	24	C	23	22	21	1.5649922	103.0215577	73.9882582
25	25	C	20	18	7	1.4703790	107.5313354	-174.7729299
26	26	C	24	23	22	1.5596252	103.8586841	-1.3667990

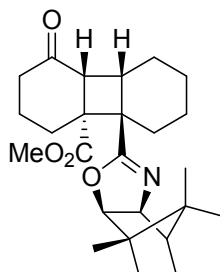
27	27	C	22	21	19	1.5628347	105.2535516	-78.5278178
28	28	C	26	24	23	1.5215100	114.8641720	164.1959303
29	29	C	27	22	21	1.5406608	116.0168694	70.6777899
30	30	C	27	22	21	1.5474678	112.5129020	-168.8462992
31	31	H	1	6	5	1.1006599	107.8912120	62.7330229
32	32	H	1	6	5	1.0931948	108.6690412	179.6371297
33	33	H	2	1	6	1.0945688	108.9474903	-65.6744945
34	34	H	2	1	6	1.0959946	109.2825385	179.2799255
35	35	H	3	2	1	1.0946675	110.2495180	-164.8379315
36	36	H	3	2	1	1.0940357	107.4792343	81.0751210
37	37	H	5	4	3	1.0967593	112.7650130	105.4483086
38	38	H	8	5	4	1.0923942	105.6520812	-89.1820458
39	39	H	9	7	4	1.0908432	109.2375977	26.4073261
40	40	H	9	7	4	1.0933600	110.0197603	-90.4502263
41	41	H	10	9	7	1.0968756	108.8139493	176.7678410
42	42	H	10	9	7	1.0964412	110.2376449	60.1791128
43	43	H	11	10	9	1.0956972	109.5882187	-62.7564190
44	44	H	11	10	9	1.0968126	110.3492421	-179.8514499
45	45	H	12	8	5	1.0996713	106.7259933	163.0882564
46	46	H	12	8	5	1.0951415	109.2591597	48.0767893
47	47	H	17	16	14	1.0899569	105.4052384	-176.1972128
48	48	H	17	16	14	1.0915789	109.4043083	64.6685797
49	49	H	17	16	14	1.0923463	110.5316454	-56.3967033
50	50	H	21	19	18	1.0944163	105.9390391	-114.5966987
51	51	H	22	21	19	1.0940517	114.2310039	50.1623515
52	52	H	23	22	21	1.0953898	111.7672890	-46.9486874
53	53	H	23	22	21	1.0925775	111.1936320	-165.9187485
54	54	H	24	23	22	1.0953818	112.5213198	-122.0488882
55	55	H	24	23	22	1.0936128	111.7053711	118.0429644
56	56	H	25	20	18	1.0956570	106.8862237	122.3176471
57	57	H	28	26	24	1.0936963	111.1311700	-179.4185029
58	58	H	28	26	24	1.0970364	110.7178778	60.6599255
59	59	H	28	26	24	1.0960685	111.1669970	-58.6235689
60	60	H	29	27	22	1.0948952	109.9577332	178.3467528

61	61	H	29	27	22	1.0966614	109.5058621	60.5160615
62	62	H	29	27	22	1.0828851	115.2443359	-61.5914127
63	63	H	30	27	22	1.0953751	110.1038278	173.4351054
64	64	H	30	27	22	1.0906243	115.0956891	51.7792506
65	65	H	30	27	22	1.0963724	109.4866910	-69.2112667

Row	Tag	Symbol	X	Y	Z
1	1	C	-3.9905630	-1.0525560	-2.1359800
2	2	C	-3.3095640	-2.2145750	-1.3917160
3	3	C	-1.9392750	-1.7897280	-0.8486750
4	4	C	-2.0311720	-0.6427240	0.1986690
5	5	C	-2.9621260	0.5082710	-0.3262760
6	6	C	-4.0772520	0.2205130	-1.3087860
7	7	O	-4.9991770	1.0124830	-1.4453780
8	8	C	-0.8401110	0.4111170	0.1615300
9	9	C	-1.6871770	1.2189820	-0.8904830
10	10	C	-0.7293440	1.2039450	1.5037920
11	11	C	-0.4585000	2.7073920	1.3381510
12	12	C	-1.5472130	3.3749200	0.4877760
13	13	C	-1.6135050	2.7457260	-0.9111520
14	14	C	-2.2021480	-1.2818140	1.5896320
15	15	O	-1.2388340	-1.7602000	2.1457870
16	16	O	-3.3931030	-1.3702190	2.2438280
17	17	C	-4.6640200	-0.8841530	1.7907230
18	18	C	0.5214230	-0.0153370	-0.3260660
19	19	N	0.9461050	-1.1887310	-0.5879450
20	20	O	1.3890140	1.0380760	-0.5248150
21	21	C	2.3007540	-1.0531560	-1.1448330
22	22	C	3.5103310	-1.6356680	-0.3619840
23	23	C	4.6985750	-1.4918380	-1.3508900
24	24	C	4.9508200	0.0529970	-1.3640360
25	25	C	2.5868360	0.4789870	-1.1332440
26	26	C	3.9098880	0.6185820	-0.3420400
27	27	C	3.8637940	-0.5573110	0.7140790

28	28	C	2.8569600	-0.4185730	1.8719600
29	29	C	5.2266890	-0.8047820	1.4046230
30	30	C	4.2117810	2.0253530	0.1557090
31	31	H	-4.9984210	-1.2977150	-2.4840020
32	32	H	-3.3988390	-0.8091800	-3.0317880
33	33	H	-3.1782460	-3.0576300	-2.0792050
34	34	H	-3.9576220	-2.5849230	-0.5868670
35	35	H	-1.3248430	-1.4604710	-1.6900460
36	36	H	-1.3993870	-2.6298570	-0.4087370
37	37	H	-3.3809430	1.1206310	0.4729930
38	38	H	-1.4758040	0.8351240	-1.8943600
39	39	H	0.0268450	0.7342140	2.1369760
40	40	H	-1.6727260	1.0998530	2.0529260
41	41	H	0.5215040	2.8654180	0.8761660
42	42	H	-0.4229970	3.1658190	2.3339490
43	43	H	-1.3560340	4.4501930	0.3935340
44	44	H	-2.5185520	3.2803870	0.9937780
45	45	H	-2.4703120	3.1377480	-1.4738200
46	46	H	-0.7117770	3.0314670	-1.4682910
47	47	H	-5.3951330	-1.3582680	2.4468890
48	48	H	-4.8791540	-1.1719110	0.7611720
49	49	H	-4.7364220	0.2005210	1.8996230
50	50	H	2.2792830	-1.4883250	-2.1500990
51	51	H	3.3434290	-2.6496740	0.0111660
52	52	H	4.4538710	-1.8843800	-2.3433230
53	53	H	5.5768830	-2.0404680	-1.0015710
54	54	H	4.8117580	0.4920200	-2.3583900
55	55	H	5.9688640	0.3044930	-1.0542180
56	56	H	2.6672220	0.9512920	-2.1174080
57	57	H	3.0313950	0.5136400	2.4215270
58	58	H	3.0030340	-1.2425180	2.5794760
59	59	H	1.8156320	-0.4562100	1.5744430
60	60	H	5.4074770	-0.0347310	2.1631680
61	61	H	6.0889320	-0.8120770	0.7366200

62	62	H	5.2048780	-1.7685370	1.9260610
63	63	H	3.4329530	2.3850450	0.8352900
64	64	H	4.2716610	2.7315430	-0.6813520
65	65	H	5.1703640	2.0600410	0.6850580



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5525308		
3	3	C	2	1		1.5670786	116.3922294	
4	4	C	3	2	1	1.5487358	109.0635840	22.5757798
5	5	C	4	3	2	1.5437954	110.5235346	33.6778166
6	6	C	5	4	3	1.5038947	113.9406233	-69.9934512
7	7	O	6	5	4	1.2174996	126.7519462	-143.7873330
8	8	C	4	3	2	1.6171774	128.4672132	135.6804751
9	9	C	5	4	3	1.5477526	92.9753527	148.3028571
10	10	C	8	4	3	1.5621462	119.6513805	109.0187787
11	11	C	10	8	4	1.5353413	112.2926887	121.6454743
12	12	C	11	10	8	1.5324096	110.5008075	-57.7635899
13	13	C	12	11	10	1.5452446	112.5549852	64.9711648
14	14	C	4	3	2	1.5357953	106.4243946	-92.4916506
15	15	O	14	4	3	1.2155627	123.4890749	-51.4577942
16	16	O	14	4	3	1.3490583	114.1352044	127.9084358
17	17	C	16	14	4	1.4419886	116.5143737	-178.0133829
18	18	C	8	4	3	1.5104859	115.2175714	-19.8366496
19	19	N	18	8	4	1.2765083	129.8132340	24.8097322
20	20	O	18	8	4	1.3782431	112.6424308	-158.7630211
21	21	C	19	18	8	1.4719904	107.4104087	171.4312023
22	22	C	21	19	18	1.5527238	119.7250388	115.4413119

23	23	C	22	21	19	1.5535677	103.7568542	171.4483246
24	24	C	23	22	21	1.5648693	102.7400105	71.7518761
25	25	C	20	18	8	1.4536730	106.6819159	-170.1433888
26	26	C	25	20	18	1.5492683	117.0400958	-119.3673489
27	27	C	22	21	19	1.5653590	105.4324526	-82.2232477
28	28	C	27	22	21	1.5401763	115.9933987	71.1303599
29	29	C	27	22	21	1.5475591	113.1217334	-168.0476451
30	30	C	26	25	20	1.5224850	114.7392248	-49.9972394
31	31	H	1	6	5	1.0951005	107.8136542	143.0319650
32	32	H	1	6	5	1.0983118	106.6797775	-103.5774766
33	33	H	2	1	6	1.0952354	108.5159850	-176.5538237
34	34	H	2	1	6	1.0969799	107.7236331	69.5616104
35	35	H	3	2	1	1.0921195	111.0300516	-98.8742116
36	36	H	3	2	1	1.0891583	109.6461343	142.7396084
37	37	H	5	4	3	1.1011030	104.5857883	41.0058980
38	38	H	9	5	4	1.0908227	111.1985964	-129.3970763
39	39	H	10	8	4	1.0931691	109.8990749	0.1045893
40	40	H	10	8	4	1.0949937	109.6882808	-115.5144668
41	41	H	11	10	8	1.0968032	108.8430706	-178.8886713
42	42	H	11	10	8	1.0973838	109.9603080	64.2845171
43	43	H	12	11	10	1.0969398	108.3802890	-57.1740800
44	44	H	12	11	10	1.0962299	110.3949401	-173.0749234
45	45	H	13	12	11	1.0956378	107.9886726	90.4475012
46	46	H	13	12	11	1.0921838	110.1435235	-154.1453591
47	47	H	17	16	14	1.0893673	105.2949762	178.0969893
48	48	H	17	16	14	1.0924089	110.2365761	58.4469675
49	49	H	17	16	14	1.0924289	110.3797079	-62.1589851
50	50	H	21	19	18	1.0950743	106.7562960	-119.8207181
51	51	H	22	21	19	1.0935804	113.8160932	46.1482688
52	52	H	23	22	21	1.0946547	111.7738577	-49.0749437
53	53	H	23	22	21	1.0927080	111.4564382	-168.4911630
54	54	H	24	23	22	1.0957125	112.5100607	-119.0917806
55	55	H	24	23	22	1.0935521	111.9629353	121.0559652
56	56	H	25	20	18	1.0945558	105.8194082	116.4955266

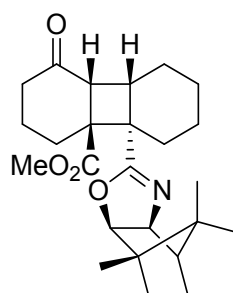
57	57	H	28	27	22	1.0958574	110.1893293	-173.9645921
58	58	H	28	27	22	1.0962433	109.4670975	68.3964300
59	59	H	28	27	22	1.0833306	114.5800476	-52.1679488
60	60	H	29	27	22	1.0956840	110.1306292	178.1761061
61	61	H	29	27	22	1.0903622	114.9438234	56.8051408
62	62	H	29	27	22	1.0961971	109.6464353	-64.3142014
63	63	H	30	26	25	1.0944241	111.3784932	60.1135374
64	64	H	30	26	25	1.0966315	110.8536741	-59.5100183
65	65	H	30	26	25	1.0956583	111.1990980	-179.0213711

Row	Tag	Symbol	X	Y	Z
1	1	C	-2.8802800	-2.8095390	0.6814300
2	2	C	-1.7821200	-2.9959040	-0.3960980
3	3	C	-1.5517770	-1.7860680	-1.3555820
4	4	C	-1.8986380	-0.4628500	-0.6213960
5	5	C	-1.7267060	-0.6055020	0.9239130
6	6	C	-2.6937750	-1.5638710	1.5654560
7	7	O	-3.2384780	-1.4222590	2.6445950
8	8	C	-1.0098130	0.8852320	-0.4513660
9	9	C	-1.5785330	0.9188110	1.0069190
10	10	C	-1.2783400	2.2655570	-1.1303230
11	11	C	-1.5291250	3.3666850	-0.0540060
12	12	C	-0.7008470	3.2223320	1.2508150
13	13	C	-0.9011110	1.8547370	1.9942280
14	14	C	-3.2936380	-0.0464910	-1.1031420
15	15	O	-3.5261780	0.2685450	-2.2536790
16	16	O	-4.2522080	-0.0867360	-0.1528780
17	17	C	-5.5876610	0.2659200	-0.5690030
18	18	C	0.4706880	0.5903850	-0.6320030
19	19	N	0.9841670	-0.1034130	-1.5747030
20	20	O	1.3404470	1.2579540	0.2001220
21	21	C	2.4343960	0.1333810	-1.5641260
22	22	C	3.4128340	-1.0309900	-1.2468320
23	23	C	4.8096950	-0.4350780	-1.5713990

24	24	C	5.0266800	0.5869750	-0.4060290
25	25	C	2.6697910	1.1142670	-0.3778480
26	26	C	3.7535560	0.4251400	0.4881850
27	27	C	3.4672990	-1.1179350	0.3152210
28	28	C	2.2019250	-1.6574400	1.0050190
29	29	C	4.6116460	-2.0202970	0.8350870
30	30	C	3.8941050	0.9817000	1.8986200
31	31	H	-2.9355880	-3.6848750	1.3375530
32	32	H	-3.8700400	-2.7133380	0.2158480
33	33	H	-2.0208150	-3.8828850	-0.9932750
34	34	H	-0.8401650	-3.2289380	0.1156690
35	35	H	-2.1678350	-1.8825180	-2.2538580
36	36	H	-0.5147020	-1.7691240	-1.6888690
37	37	H	-0.7420290	-1.0745750	1.0682450
38	38	H	-2.5959370	1.3044280	0.8940810
39	39	H	-2.1352200	2.1992760	-1.8063900
40	40	H	-0.4237110	2.5452530	-1.7552210
41	41	H	-2.5968260	3.3899610	0.1985010
42	42	H	-1.3122840	4.3437050	-0.5014550
43	43	H	-0.9615930	4.0510410	1.9185930
44	44	H	0.3581000	3.3373040	1.0048310
45	45	H	0.0620250	1.4719720	2.3410130
46	46	H	-1.5422200	1.9801070	2.8738890
47	47	H	-6.2054720	0.1459940	0.3201610
48	48	H	-5.9222470	-0.3968890	-1.3702680
49	49	H	-5.6135790	1.2988890	-0.9235510
50	50	H	2.6886870	0.5591330	-2.5406370
51	51	H	3.1785560	-1.9607600	-1.7726470
52	52	H	4.8290940	0.0428150	-2.5560290
53	53	H	5.5825210	-1.2073730	-1.5801950
54	54	H	5.1325310	1.6164560	-0.7659200
55	55	H	5.9295810	0.3658590	0.1699070
56	56	H	2.9803600	2.1260500	-0.6574980
57	57	H	2.3093260	-1.5957450	2.0938190



58	58	H	2.0668160	-2.7153030	0.7507970
59	59	H	1.2913810	-1.1382100	0.7328260
60	60	H	4.6225100	-2.0214340	1.9306550
61	61	H	5.6097700	-1.7365310	0.5003070
62	62	H	4.4393500	-3.0544230	0.5147010
63	63	H	2.9610320	0.8843820	2.4623580
64	64	H	4.1549670	2.0464530	1.8729270
65	65	H	4.6843190	0.4627680	2.4523350



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5252188		
3	3	C	2	1		1.5272287	111.0378342	
4	4	C	3	2	1	1.5382923	115.1567869	-52.4591277
5	5	C	4	3	2	1.5511764	116.5633476	21.7113358
6	6	C	1	2	3	1.5077965	110.3261790	62.0355059
7	7	C	4	3	2	1.5901960	116.2015245	-82.3227851
8	8	C	5	4	3	1.5630565	90.6593559	-124.0198454
9	9	C	7	4	3	1.5383048	116.6328600	3.3930683
10	10	C	9	7	4	1.5286651	114.2185839	92.4440440
11	11	C	10	9	7	1.5288689	110.4465440	48.8930582
12	12	C	8	5	4	1.5250596	118.9328708	129.3981121
13	13	O	6	1	2	1.2130806	121.2611886	140.7077134
14	14	C	4	3	2	1.5410778	104.7467727	151.1955586
15	15	O	14	4	3	1.2112242	122.4727446	20.2004320
16	16	O	14	4	3	1.3810536	126.6766126	-157.0788940
17	17	C	16	14	4	1.4368107	127.0115869	-6.1944735

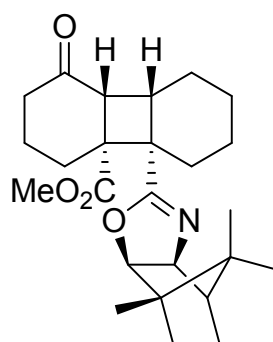
18	18	C	7	4	3	1.5077261	113.1676963	-120.1791614
19	19	O	18	7	4	1.4180178	115.2972289	-105.4036745
20	20	N	18	7	4	1.2968879	129.2886758	76.2601625
21	21	C	19	18	7	1.4685084	106.8580769	178.2315458
22	22	C	21	19	18	1.5467393	114.0213439	115.6370365
23	23	C	22	21	19	1.5567043	103.6727406	174.5316340
24	24	C	23	22	21	1.5533277	103.4668757	72.3714586
25	25	C	20	18	7	1.4778502	109.5269204	-179.9429269
26	26	C	24	23	22	1.5677411	103.9496849	0.3862017
27	27	C	22	21	19	1.5772884	104.7815218	-78.9420941
28	28	C	26	24	23	1.5069364	114.6317106	162.3764697
29	29	C	27	22	21	1.5295339	113.8118789	68.4721189
30	30	C	27	22	21	1.5343162	113.2216332	-168.7761660
31	31	H	1	6	13	1.1106248	109.2762030	-97.0391129
32	32	H	1	6	13	1.1100549	109.8871520	17.8677674
33	33	H	2	1	6	1.1168184	109.4503006	-60.3598750
34	34	H	2	1	6	1.1077536	110.1403091	-176.3149142
35	35	H	3	2	1	1.1144005	110.1237478	-175.5263167
36	36	H	3	2	1	1.1145038	108.4210322	71.0617161
37	37	H	5	4	3	1.1193255	113.0853968	121.8964137
38	38	H	8	5	4	1.1173874	109.5205441	-106.7596291
39	39	H	9	7	4	1.1119149	109.3129564	-32.2191133
40	40	H	9	7	4	1.1149115	109.8452298	-145.9327272
41	41	H	10	9	7	1.1152038	110.1480824	-72.8331961
42	42	H	10	9	7	1.1063458	109.7147161	170.9173385
43	43	H	11	10	9	1.1067670	110.3689453	170.5395936
44	44	H	11	10	9	1.1080576	109.9793637	54.0367590
45	45	H	12	8	5	1.1097868	108.9605907	120.0261004
46	46	H	12	8	5	1.1109746	110.7941895	6.2306004
47	47	H	17	16	14	1.0992338	101.7552621	-174.8151679
48	48	H	17	16	14	1.0980461	110.0444685	67.8446529
49	49	H	17	16	14	1.0987778	111.0765996	-56.8826401
50	50	H	21	19	18	1.0998473	104.1978653	-119.0201462
51	51	H	22	21	19	1.0938071	114.4698636	48.1135160

52	52	H	23	22	21	1.0995772	112.5342494	-48.8933686
53	53	H	23	22	21	1.1009592	110.9221931	-167.6298841
54	54	H	24	23	22	1.0987288	112.2829397	-121.0263440
55	55	H	24	23	22	1.1004516	111.7325094	119.9675512
56	56	H	25	20	18	1.1123506	108.0289707	122.1452715
57	57	H	28	26	24	1.1000301	111.0514938	175.6927179
58	58	H	28	26	24	1.0972099	111.6268065	57.1493197
59	59	H	28	26	24	1.0952897	111.9141548	-63.9236411
60	60	H	29	27	22	1.0976519	111.8390129	-123.2727709
61	61	H	29	27	22	1.0954856	112.4684989	116.9950158
62	62	H	29	27	22	1.0986120	111.8526399	-2.0336126
63	63	H	30	27	22	1.0965969	110.5787198	178.2000693
64	64	H	30	27	22	1.0939006	113.8905943	58.2372275
65	65	H	30	27	22	1.0957582	110.7574005	-62.3751702

Row	Tag	Symbol	X	Y	Z
1	1	C	-4.9056350	0.0663080	0.7798950
2	2	C	-4.7527860	-0.5606300	-0.6167930
3	3	C	-3.5336160	0.0192450	-1.3477780
4	4	C	-2.2034220	-0.3090870	-0.6165780
5	5	C	-2.3072800	0.0274920	0.9285280
6	6	C	-3.6465000	-0.0410340	1.6310510
7	7	O	-3.7099150	-0.1546350	2.8466610
8	8	C	-1.0963770	0.8481000	-0.7160100
9	9	C	-1.7726700	1.4392520	0.5501980
10	10	C	-1.0285530	1.9453410	-1.7965840
11	11	C	-0.8563680	3.3447690	-1.1115660
12	12	C	-0.1768780	3.3075990	0.2825580
13	13	C	-0.9339690	2.4327040	1.3377480
14	14	C	-1.7192970	-1.6548270	-1.1901320
15	15	O	-1.2506350	-1.6684880	-2.3110890
16	16	O	-1.9234460	-2.8479910	-0.5864530
17	17	C	-2.1855100	-3.0322970	0.8130100
18	18	C	0.2622620	0.1841900	-0.4836050

19	19	N	0.4740150	-0.8480950	0.2449350
20	20	O	1.3180060	0.6635690	-1.2092530
21	21	C	1.8157160	-1.3566130	-0.0831550
22	22	C	2.9350800	-1.4109350	0.9913710
23	23	C	4.0785900	-2.1974230	0.2941000
24	24	C	4.6109230	-1.1711800	-0.7608910
25	25	C	2.3772360	-0.3359720	-1.1163480
26	26	C	3.7385570	0.1059880	-0.5254800
27	27	C	3.5332020	0.0325590	1.0393660
28	28	C	2.6188550	1.1000310	1.6600780
29	29	C	4.8551100	0.1255050	1.8377720
30	30	C	4.3116240	1.3854510	-1.1190910
31	31	H	-5.7329750	-0.3675480	1.3490990
32	32	H	-5.1280920	1.1389640	0.6701230
33	33	H	-5.6583570	-0.3709580	-1.2038140
34	34	H	-4.6664160	-1.6516320	-0.5344050
35	35	H	-3.6651430	1.1045790	-1.4148390
36	36	H	-3.4753920	-0.3479490	-2.3760160
37	37	H	-1.5624380	-0.5022030	1.5186450
38	38	H	-2.6305190	2.0015750	0.1657500
39	39	H	-1.9505010	1.9476510	-2.3854750
40	40	H	-0.2127920	1.7556070	-2.4939470
41	41	H	-1.8371410	3.8289530	-1.0156540
42	42	H	-0.2686730	3.9933040	-1.7701940
43	43	H	-0.0734280	4.3322160	0.6562710
44	44	H	0.8405100	2.9247070	0.1589420
45	45	H	-0.2251200	1.9332530	2.0051830
46	46	H	-1.5776930	3.0553930	1.9699540
47	47	H	-2.2605740	-4.1127510	0.9414980
48	48	H	-3.1287020	-2.5759580	1.1208840
49	49	H	-1.3576030	-2.6445860	1.4089540
50	50	H	1.6677180	-2.3569180	-0.5039420
51	51	H	2.6113410	-1.8285930	1.9490110
52	52	H	3.7152520	-3.1208550	-0.1676660

53	53	H	4.8565590	-2.4833450	1.0062300
54	54	H	4.5132710	-1.5374820	-1.7886020
55	55	H	5.6699460	-0.9429490	-0.6122690
56	56	H	2.4966080	-0.7193330	-2.1333910
57	57	H	3.0369260	2.1011750	1.5044970
58	58	H	2.5513750	0.9407320	2.7426860
59	59	H	1.6076310	1.0894530	1.2734660
60	60	H	5.2308110	1.1549360	1.8242350
61	61	H	5.6581720	-0.5185640	1.4775390
62	62	H	4.6707700	-0.1349830	2.8863950
63	63	H	3.6399080	2.2350770	-0.9613840
64	64	H	4.4631490	1.2811590	-2.2000290
65	65	H	5.2816470	1.6277030	-0.6712070



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5406826		
3	3	C	2	1		1.5517850	116.6051097	
4	4	C	3	2	1	1.5265358	109.4635347	15.2030788
5	5	C	4	3	2	1.5575680	108.2058296	41.2628146
6	6	C	5	4	3	1.4980913	111.3952235	-75.0886974
7	7	C	4	3	2	1.5847661	127.0872098	142.1144150
8	8	C	5	4	3	1.5459597	90.5325956	147.6858786
9	9	C	7	4	3	1.5289309	118.9416912	109.1005587
10	10	C	9	7	4	1.5322531	115.0609384	79.7140267
11	11	C	10	9	7	1.5321059	111.9785558	44.5658412
12	12	C	8	5	4	1.5216512	115.9862824	98.9634007

13	13	O	6	5	4	1.2059468	126.9445320	-142.4068540
14	14	C	4	3	2	1.5266769	106.0828211	-87.9154121
15	15	O	14	4	3	1.2093500	126.7978024	-60.4016110
16	16	O	14	4	3	1.3771693	112.3542542	117.7764274
17	17	C	16	14	4	1.4529358	117.2319952	-179.6887978
18	18	C	7	4	3	1.5065593	109.8050216	-17.0042730
19	19	O	18	7	4	1.4178244	114.3127511	-79.0046198
20	20	N	18	7	4	1.2981144	130.3938574	99.5862188
21	21	C	19	18	7	1.4641405	107.1125040	177.4572582
22	22	C	21	19	18	1.5474813	114.1541978	114.2833730
23	23	C	22	21	19	1.5567211	103.6056706	174.0872240
24	24	C	23	22	21	1.5534096	103.4319924	72.2776161
25	25	C	20	18	7	1.4791439	109.4570339	-178.2956308
26	26	C	24	23	22	1.5679193	103.9560076	0.6157352
27	27	C	22	21	19	1.5772342	104.9272120	-79.4080774
28	28	C	26	24	23	1.5070747	114.6115312	162.2104711
29	29	C	27	22	21	1.5292684	114.1800315	68.4942803
30	30	C	27	22	21	1.5346126	113.1668780	-168.6061192
31	31	H	1	6	5	1.1079722	109.0332593	141.4231034
32	32	H	1	6	5	1.1123867	106.9341192	-105.5648332
33	33	H	2	1	6	1.1079463	108.2720005	-171.5641051
34	34	H	2	1	6	1.1083222	108.4955385	74.1682993
35	35	H	3	2	1	1.1091481	110.7868753	-107.9547284
36	36	H	3	2	1	1.1071678	109.7543491	136.8814300
37	37	H	5	4	3	1.1314433	110.0314145	40.1797927
38	38	H	8	5	4	1.1081905	112.8799308	-132.4222032
39	39	H	9	7	4	1.1136310	109.1154411	-44.3343006
40	40	H	9	7	4	1.1121026	109.1971440	-158.3227927
41	41	H	10	9	7	1.1079375	110.3984550	-78.1329983
42	42	H	10	9	7	1.1075976	108.9760519	166.5903495
43	43	H	11	10	9	1.1062515	110.0902040	175.3733861
44	44	H	11	10	9	1.1067648	110.2211695	58.7388277
45	45	H	12	8	5	1.1072297	109.5545782	95.9589926
46	46	H	12	8	5	1.1134896	110.2083714	-18.9094427

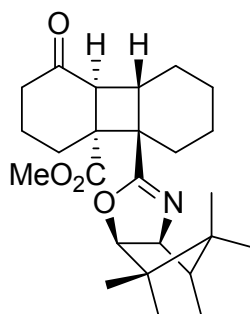
47	47	H	17	16	14	1.0940866	108.6671802	-75.3050670
48	48	H	17	16	14	1.0949513	110.3726570	46.3397736
49	49	H	17	16	14	1.0957422	102.5399535	166.1185431
50	50	H	21	19	18	1.0998009	104.1191112	-120.5533419
51	51	H	22	21	19	1.0939356	114.3933531	47.7078663
52	52	H	23	22	21	1.0994041	112.5403711	-49.0387222
53	53	H	23	22	21	1.1010374	110.9204725	-167.7453247
54	54	H	24	23	22	1.0982979	112.2981676	-120.8750902
55	55	H	24	23	22	1.1005413	111.6948108	120.1153317
56	56	H	25	20	18	1.1107339	108.1874208	122.7172494
57	57	H	28	26	24	1.1004516	110.9713250	175.2398180
58	58	H	28	26	24	1.0966296	111.7262380	56.5671613
59	59	H	28	26	24	1.0954220	111.8751742	-64.5584807
60	60	H	29	27	22	1.0963893	111.6121663	-125.1890552
61	61	H	29	27	22	1.0958687	112.4513364	115.2552757
62	62	H	29	27	22	1.0971566	112.2176860	-3.7062053
63	63	H	30	27	22	1.0966331	110.5768696	178.4231842
64	64	H	30	27	22	1.0937214	113.9422149	58.3982404
65	65	H	30	27	22	1.0958737	110.7117997	-62.2348443

Row	Tag	Symbol	X	Y	Z
1	1	C	-4.6498130	0.9783400	1.2414610
2	2	C	-3.5739390	0.7509930	2.3187410
3	3	C	-2.1711840	1.1855500	1.8488930
4	4	C	-1.8014490	0.8662410	0.3702890
5	5	C	-2.9638120	0.5268050	-0.6324590
6	6	C	-4.3166330	0.2110080	-0.0244780
7	7	C	-1.1666530	-0.5756820	0.0093480
8	8	C	-2.0700840	-0.5741500	-1.2788640
9	9	C	-1.6088310	-1.6870070	0.9903670
10	10	C	-1.7896630	-3.0525400	0.3045410
11	11	C	-2.8975090	-2.9750830	-0.7544610
12	12	C	-2.5738040	-1.9177070	-1.8214670
13	13	O	-5.1114890	-0.5490440	-0.5552860

14	14	C	-0.9097870	2.0193290	-0.1173080
15	15	O	-0.0911020	2.5749940	0.5887810
16	16	O	-1.1610000	2.3990290	-1.3857280
17	17	C	-0.2877270	3.4066850	-1.9284030
18	18	C	0.3209830	-0.6558870	-0.2746840
19	19	O	1.0045470	-1.6814020	0.3313550
20	20	N	0.9822630	0.1182960	-1.0461920
21	21	C	2.3402370	-1.6865790	-0.2410760
22	22	C	3.5135270	-1.4840940	0.7303130
23	23	C	4.7599790	-1.6770220	-0.1821430
24	24	C	4.7920170	-0.3552500	-1.0194560
25	25	C	2.3564590	-0.3993700	-1.1211690
26	26	C	3.5419660	0.4330650	-0.5210960
27	27	C	3.5522760	0.0523520	1.0136580
28	28	C	3.5290990	1.9098120	-0.8872180
29	29	C	2.4002630	0.6107280	1.8708150
30	30	C	4.8387880	0.4856000	1.7565170
31	31	H	-4.6878500	2.0487290	0.9879400
32	32	H	-5.6433240	0.6758280	1.5827780
33	33	H	-3.5934980	-0.2998590	2.6243690
34	34	H	-3.8325390	1.3256500	3.2154570
35	35	H	-1.4045620	0.7720380	2.5119130
36	36	H	-2.1036420	2.2701540	1.9753300
37	37	H	-3.1797930	1.3487540	-1.3257360
38	38	H	-1.5102960	-0.0717850	-2.0710710
39	39	H	-2.5759150	-1.4228990	1.4204070
40	40	H	-0.9023790	-1.7549170	1.8220820
41	41	H	-2.0453470	-3.7996490	1.0658490
42	42	H	-0.8456150	-3.3772560	-0.1487980
43	43	H	-3.8514430	-2.7360170	-0.2713360
44	44	H	-3.0283030	-3.9490630	-1.2415480
45	45	H	-1.7788710	-2.3156810	-2.4687500
46	46	H	-3.4445920	-1.7447200	-2.4626680
47	47	H	-0.6831660	3.6293480	-2.9193900



48	48	H	0.7264930	3.0089340	-1.9969340
49	49	H	-0.2940980	4.2989200	-1.2982470
50	50	H	2.4283970	-2.6293770	-0.7898080
51	51	H	3.4878550	-2.1371070	1.6077320
52	52	H	4.6683400	-2.5686260	-0.8118440
53	53	H	5.6679010	-1.8067100	0.4116450
54	54	H	4.7451820	-0.5406000	-2.0980260
55	55	H	5.7072990	0.2155440	-0.8393390
56	56	H	2.5664170	-0.5927850	-2.1789840
57	57	H	2.6335410	2.4041820	-0.5002480
58	58	H	3.5423390	2.0397380	-1.9764530
59	59	H	4.4090570	2.4249420	-0.4851220
60	60	H	2.5405510	1.6846430	2.0315050
61	61	H	2.4086190	0.1272980	2.8551380
62	62	H	1.4106480	0.4939490	1.4469460
63	63	H	4.8807210	1.5776130	1.8313220
64	64	H	5.7712880	0.1523190	1.2995390
65	65	H	4.8188550	0.0949590	2.7807410



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5619452		
3	3	C	2	1		1.5230065	103.0487441	
4	4	C	3	2	1	1.5757138	106.1058974	-74.7501854
5	5	C	4	3	2	1.4700003	114.3227537	45.1132821
6	6	C	1	2	3	1.5090601	95.4360914	84.3815175
7	7	O	6	1	2	1.2080288	121.6975931	109.0763215
8	8	C	4	3	2	1.5096260	107.4108077	140.0370281

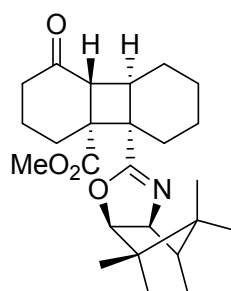
9	9	C	5	4	3	1.5096231	87.2171589	78.9201685
10	10	C	8	4	3	1.5229512	108.6525469	165.1048820
11	11	C	10	8	4	1.5229805	109.5001733	139.9764825
12	12	C	11	10	8	1.3336172	94.5599730	-81.5256019
13	13	C	9	5	4	1.5229391	113.5083374	138.0053053
14	14	C	4	3	2	1.5580052	102.8462733	-77.4582482
15	15	O	14	4	3	1.2080390	127.4523830	9.4830269
16	16	O	14	4	3	1.3379412	107.5139125	-175.9351866
17	17	C	16	14	4	1.4019523	109.9037190	64.5853147
18	18	C	8	4	3	1.4969563	113.4587574	23.3155082
19	19	N	18	8	4	1.2600090	122.0544884	3.7722249
20	20	O	18	8	4	1.4210342	126.9457573	-176.8376694
21	21	C	19	18	8	1.4699516	104.5039754	179.9981461
22	22	C	21	19	18	1.5229964	110.7397604	112.2719162
23	23	C	22	21	19	1.5230118	109.5079147	-177.0186231
24	24	C	23	22	21	1.7862645	104.3041818	70.6520577
25	25	C	20	18	8	1.1601683	115.0224536	179.0861382
26	26	C	25	20	18	1.5229361	105.1226783	-108.3980465
27	27	C	22	21	19	1.5229433	104.5007130	-65.5512807
28	28	C	27	22	21	1.5230698	109.4711209	53.5109274
29	29	C	27	22	21	1.5229394	109.4745661	-166.3228220
30	30	C	26	25	20	1.5229179	109.4731383	-46.9251280
31	31	H	1	6	7	1.1129859	108.7974300	-138.2759676
32	32	H	1	6	7	1.1129990	108.7982006	-3.5713547
33	33	H	2	1	6	1.1129659	109.4157857	-31.9413520
34	34	H	2	1	6	1.1130496	109.4081513	-159.3066590
35	35	H	3	2	1	1.1129572	109.4119256	161.7053284
36	36	H	3	2	1	1.1129416	109.4115718	41.5103108
37	37	H	5	4	3	1.1130106	109.3933866	-147.6768849
38	38	H	9	5	4	1.1130773	108.5561943	-80.1641880
39	39	H	10	8	4	1.1129705	109.4126178	20.0717377
40	40	H	10	8	4	1.1129957	109.4140372	-100.1149633
41	41	H	11	10	8	1.1130213	109.4146986	166.0472802
42	42	H	11	10	8	1.1129814	109.4110653	30.9084326

43	43	H	12	11	10	1.1129926	109.4054161	-22.0835627
44	44	H	12	11	10	1.1129478	109.4138775	-157.2426565
45	45	H	13	9	5	1.1129103	109.4090693	-164.9965034
46	46	H	13	9	5	1.1129222	109.4127322	74.8079424
47	47	H	17	16	14	1.1109510	106.7097378	-179.9958100
48	48	H	17	16	14	1.1109727	106.7068175	63.5780507
49	49	H	10	8	4	1.0052695	95.0908807	-40.1521066
50	50	H	21	19	18	1.1129806	107.5014719	-128.2745877
51	51	H	22	21	19	1.1130152	109.3855427	63.1050169
52	52	H	23	22	21	1.1129843	109.4106472	-46.3152999
53	53	H	23	22	21	1.1130138	109.4024578	-172.3816921
54	54	H	24	23	22	1.1129793	109.4090898	-115.2256752
55	55	H	24	23	22	1.1129127	109.4101304	109.8795561
56	56	H	25	20	18	1.1130666	106.6962431	117.5531594
57	57	H	28	27	22	1.1128962	110.0002315	-179.9985379
58	58	H	28	27	22	1.1130481	109.9964377	59.9226404
59	59	H	28	27	22	1.1129481	109.9967352	-59.9181409
60	60	H	29	27	22	1.1129258	110.0051975	179.9976044
61	61	H	29	27	22	1.1130009	109.9993626	59.9206840
62	62	H	29	27	22	1.1130677	109.9958062	-59.9205843
63	63	H	30	26	25	1.1130337	109.9962162	60.0050312
64	64	H	30	26	25	1.1130287	110.0013001	-60.0715916
65	65	H	30	26	25	1.1129553	110.0016448	-179.9220658

Row	Tag	Symbol	X	Y	Z
1	1	C	-3.1356120	-2.7834330	0.4321210
2	2	C	-2.0838980	-3.0571090	-0.6766400
3	3	C	-1.5943990	-1.8133690	-1.4947090
4	4	C	-1.8357230	-0.5316730	-0.6594840
5	5	C	-1.6529400	-0.8238790	0.8453450
6	6	C	-2.7348730	-1.6857830	1.4354650
7	7	O	-3.2110370	-1.5945340	2.5522670
8	8	C	-0.8393320	0.7209580	-0.4284360
9	9	C	-1.1324650	0.6032980	1.1416720

10	10	C	-1.1587200	2.0961060	-1.0972110
11	11	C	-1.2991140	3.2260200	-0.0672320
12	12	C	-2.3960260	2.8922160	0.9494480
13	13	C	-2.0471830	1.6604180	1.8147590
14	14	C	-3.2179740	-0.0011930	-1.0677000
15	15	O	-3.5507850	0.1852790	-2.2218480
16	16	O	-4.0480380	0.2314670	-0.0300000
17	17	C	-5.3756810	0.6889810	-0.3576830
18	18	C	0.6196230	0.4418430	-0.7025030
19	19	N	1.1558700	-0.4350670	-1.4594320
20	20	O	1.4583930	1.3348670	-0.0712130
21	21	C	2.5968730	-0.1411700	-1.5218070
22	22	C	3.6159970	-1.1588000	-0.9414910
23	23	C	4.9935260	-0.6011730	-1.3943030
24	24	C	5.1651880	0.6672490	-0.4940510
25	25	C	2.7913650	1.1025450	-0.6026050
26	26	C	3.8866360	0.6735560	0.4056520
27	27	C	3.6550910	-0.8773850	0.5978680
28	28	C	2.4030110	-1.2938620	1.3922140
29	29	C	4.8263600	-1.5894120	1.3162590
30	30	C	3.9867720	1.5479910	1.6479470
31	31	H	-3.3463000	-3.6957370	1.0000620
32	32	H	-4.0934840	-2.4742800	-0.0074180
33	33	H	-2.4916900	-3.8040190	-1.3661120
34	34	H	-1.2166470	-3.5342860	-0.2038370
35	35	H	-2.1181980	-1.7419920	-2.4503580
36	36	H	-0.5324110	-1.9144130	-1.7143390
37	37	H	-0.7722090	-1.4828840	0.8948730
38	38	H	-0.1987110	0.5736130	1.7048030
39	39	H	-2.0841630	2.0230930	-1.6744830
40	40	H	-0.3779360	2.3429900	-1.8241470
41	41	H	-1.5416330	4.1571430	-0.5937030
42	42	H	-0.3416820	3.3880190	0.4439740
43	43	H	-3.3320160	2.7193410	0.4041830

44	44	H	-2.5799700	3.7489880	1.6081030
45	45	H	-1.5187490	2.0127550	2.7075290
46	46	H	-2.9610180	1.1818510	2.1735690
47	47	H	-5.8910410	0.7832580	0.5974280
48	48	H	-5.8776150	-0.0373700	-1.0009820
49	49	H	-5.3301400	1.6513700	-0.8725950
50	50	H	2.8348070	0.0502760	-2.5734360
51	51	H	3.4231680	-2.1939990	-1.2366150
52	52	H	5.0031760	-0.3609130	-2.4622220
53	53	H	5.7931150	-1.3268660	-1.2268580
54	54	H	5.2449000	1.5897710	-1.0798710
55	55	H	6.0670680	0.6125630	0.1219670
56	56	H	3.0733360	2.0272810	-1.1158380
57	57	H	2.4862520	-0.9589680	2.4323200
58	58	H	2.3280190	-2.3874080	1.4090270
59	59	H	1.4699160	-0.9130450	0.9948260
60	60	H	4.8264790	-1.3338290	2.3817170
61	61	H	5.8167030	-1.3540170	0.9254910
62	62	H	4.6956170	-2.6755680	1.2468370
63	63	H	3.0496640	1.5467680	2.2132710
64	64	H	4.2065850	2.5876100	1.3768840
65	65	H	4.7884290	1.2041130	2.3109410



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
1	1	C						
2	2	C	1			1.5619457		
3	3	C	2	1		1.5230068	103.0486956	
4	4	C	3	2	1	1.5229700	109.4960018	-78.3933863

5	5	C	4	3	2	1.7525959	109.4729668	46.2278976
6	6	C	5	4	3	1.5089892	109.8981586	-29.3913707
7	7	O	6	5	4	1.2080290	121.7012305	-134.6274026
8	8	C	4	3	2	1.5230481	109.4698802	134.3038190
9	9	C	8	4	3	1.5228701	90.0029804	-79.2357325
10	10	C	8	4	3	1.5229509	109.4698578	170.0601292
11	11	C	10	8	4	1.5229811	109.5001728	145.5352042
12	12	C	11	10	8	1.3336170	94.5599357	-81.5256685
13	13	C	9	8	4	1.5229391	109.5159100	-143.8405065
14	14	C	4	3	2	1.5089995	107.8042315	-70.7752639
15	15	O	14	4	3	1.2080392	125.2956744	0.6597355
16	16	O	14	4	3	1.3379407	109.9034295	-179.9996809
17	17	C	16	14	4	1.4019525	109.9037322	60.0032963
18	18	C	8	4	3	1.4969557	109.4661902	31.4695187
19	19	N	18	8	4	1.2600087	122.0545254	-0.0017497
20	20	O	18	8	4	1.4210347	126.9457608	179.3883398
21	21	C	19	18	8	1.4699513	104.5040082	179.9981193
22	22	C	21	19	18	1.5229969	110.7397750	112.2718768
23	23	C	22	21	19	1.5230117	109.5079272	-177.0186049
24	24	C	23	22	21	1.7862645	104.3041710	70.6520955
25	25	C	20	18	8	1.1601675	115.0224959	179.0861675
26	26	C	25	20	18	1.5229361	105.1226882	-108.3980333
27	27	C	22	21	19	1.5229434	104.5007092	-65.5512297
28	28	C	27	22	21	1.5230692	109.4711511	53.5109242
29	29	C	27	22	21	1.5229399	109.4745227	-166.3228338
30	30	C	26	25	20	1.5229183	109.4730943	-46.9251682
31	31	H	1	6	5	1.1129855	108.7974469	41.1201626
32	32	H	1	6	5	1.1129993	108.7981921	175.8248156
33	33	H	2	1	6	1.1129653	109.4158067	-31.9412969
34	34	H	2	1	6	1.1130495	109.4081898	-159.3066670
35	35	H	3	2	1	1.1129575	109.4119046	161.7053831
36	36	H	3	2	1	1.1129411	109.4116004	41.5103033
37	37	H	5	4	3	1.1130099	109.3933638	-147.6769258
38	38	H	9	8	4	1.1130774	109.3865814	77.5128928

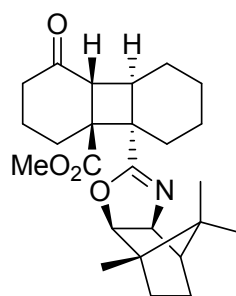
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40	40	H	10	8	4	1.1129957	109.4139850	-94.5562986
41	41	H	11	10	8	1.1130208	109.4146592	166.0472448
42	42	H	11	10	8	1.1129806	109.4110459	30.9084065
43	43	H	12	11	10	1.1129922	109.4054515	-22.0835371
44	44	H	12	11	10	1.1129474	109.4138869	-157.2426812
45	45	H	13	9	8	1.1129110	109.4090431	-71.5529353
46	46	H	13	9	8	1.1129220	109.4127923	168.2515491
47	47	H	17	16	14	1.1109510	106.7097636	-179.9957646
48	48	H	17	16	14	1.1109730	106.7068223	63.5780437
49	49	H	10	8	4	1.0052695	95.0909071	-34.5934267
50	50	H	21	19	18	1.1129798	107.5015298	-128.2745692
51	51	H	22	21	19	1.1130160	109.3854929	63.1050463
52	52	H	23	22	21	1.1129844	109.4106449	-46.3152877
53	53	H	23	22	21	1.1130137	109.4024328	-172.3816354
54	54	H	24	23	22	1.1129799	109.4090632	-115.2256928
55	55	H	24	23	22	1.1129131	109.4101187	109.8795813
56	56	H	25	20	18	1.1130663	106.6962708	117.5531122
57	57	H	28	27	22	1.1128962	110.0002477	-179.9985448
58	58	H	28	27	22	1.1130478	109.9964540	59.9225736
59	59	H	28	27	22	1.1129490	109.9967135	-59.9181495
60	60	H	29	27	22	1.1129254	110.0051713	179.9976423
61	61	H	29	27	22	1.1130007	109.9993848	59.9206378
62	62	H	29	27	22	1.1130684	109.9958238	-59.9206158
63	63	H	30	26	25	1.1130340	109.9962150	60.0050782
64	64	H	30	26	25	1.1130279	110.0013210	-60.0715910
65	65	H	30	26	25	1.1129555	110.0016021	-179.9220943

Row	Tag	Symbol	X	Y	Z
1	1	C	5.0057890	-0.0092610	0.4919720
2	2	C	4.1227170	0.3041710	1.6953990
3	3	C	2.9431030	-0.6624600	1.7764110
4	4	C	2.1086470	-0.7851260	0.4899510
5	5	C	2.8064640	-0.3699550	-0.8317270

6	6	C	4.2252230	0.1554160	-0.7875000
7	7	C	1.0083750	0.3390640	0.2568810
8	8	C	1.6649660	0.6541890	-1.1338150
9	9	C	0.9484510	1.4713660	1.2964400
10	10	C	1.7916830	2.6954910	0.9396560
11	11	C	1.5163880	3.1326920	-0.4992700
12	12	C	2.0368910	2.0894900	-1.4907320
13	13	O	4.7311930	0.6459280	-1.7748990
14	14	C	1.5374420	-2.2159340	0.5278220
15	15	O	1.4567570	-2.8570290	1.5522980
16	16	O	1.1062010	-2.9608350	-0.5522070
17	17	C	0.9838860	-2.5191850	-1.9139740
18	18	C	-0.3912430	-0.2125160	0.1565470
19	19	O	-0.9394100	-0.2400370	-1.1509430
20	20	N	-1.1756270	-0.6381320	1.0975630
21	21	C	-2.2735850	-0.8436530	-1.0407540
22	22	C	-3.4306030	0.1147830	-1.4083300
23	23	C	-4.6934820	-0.7935450	-1.3499750
24	24	C	-4.8960770	-1.0341060	0.1711800
25	25	C	-2.4552280	-1.0859040	0.5092070
26	26	C	-3.7296620	-0.2278660	0.8399590
27	27	C	-3.6220720	1.0223420	-0.1325890
28	28	C	-3.9225370	0.0551590	2.3074580
29	29	C	-2.4574080	1.9799140	0.1244860
30	30	C	-4.9022600	1.8668670	-0.1775590
31	31	H	5.4019670	-1.0452520	0.5490070
32	32	H	5.9030280	0.6440760	0.4736740
33	33	H	3.7625060	1.3591310	1.6276430
34	34	H	4.7160160	0.2468060	2.6291140
35	35	H	2.2651290	-0.3708900	2.6114120
36	36	H	3.3288420	-1.6646140	2.0747590
37	37	H	2.8367450	-1.1932520	-1.5894570
38	38	H	1.0206210	0.2626070	-1.9584590
39	39	H	1.2374140	1.0714280	2.2928860



40	40	H	-0.1066060	1.8053020	1.4319730
41	41	H	2.8754470	2.4660900	1.0681480
42	42	H	1.5699190	3.5195330	1.6437700
43	43	H	1.9932110	4.1105430	-0.7026920
44	44	H	0.4292050	3.2883230	-0.6462520
45	45	H	1.6454180	2.3224190	-2.5027200
46	46	H	3.1374870	2.1967680	-1.5977110
47	47	H	0.5229540	-3.3947220	-2.3928180
48	48	H	1.9782240	-2.3250200	-2.3374090
49	49	H	0.3250980	-1.6428840	-1.9875110
50	50	H	-2.2145410	-1.7449960	-1.6682560
51	51	H	-3.2884290	0.6574720	-2.3473130
52	52	H	-4.5621470	-1.7339620	-1.9044450
53	53	H	-5.5613280	-0.2898440	-1.8030090
54	54	H	-4.8644880	-2.1009360	0.4321030
55	55	H	-5.8742660	-0.6656590	0.5152540
56	56	H	-2.6085950	-2.1515110	0.7890000
57	57	H	-3.0394550	0.5542910	2.7330160
58	58	H	-4.0630620	-0.8687120	2.8824230
59	59	H	-4.7890680	0.7000140	2.4889670
60	60	H	-2.0270550	1.8402290	1.1245480
61	61	H	-2.7578960	3.0314130	0.0601000
62	62	H	-1.6521960	1.8513980	-0.6117650
63	63	H	-5.0082870	2.4553640	0.7416550
64	64	H	-5.8184000	1.2776360	-0.2781220
65	65	H	-4.8771620	2.5655290	-1.0213170



Row	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral
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1	1	C						
2	2	C	1			1.5388232		
3	3	C	2	1		1.5339754	110.9406667	
4	4	C	3	2	1	1.5559539	112.9356375	62.5479270
5	5	C	4	3	2	1.5706789	110.5019158	-47.6316549
6	6	C	5	4	3	1.5138152	120.9458039	27.3398017
7	7	O	6	5	4	1.2230370	120.3093598	160.7710075
8	8	C	4	3	2	1.5907817	115.3670662	-144.4557671
9	9	C	5	4	3	1.5649072	88.3047159	-93.3278507
10	10	C	8	4	3	1.5628541	111.6589597	-160.1255079
11	11	C	10	8	4	1.5366022	114.5986818	-138.1048146
12	12	C	11	10	8	1.5342840	111.1222947	57.5089444
13	13	C	9	5	4	1.5286602	119.8496004	-146.4544567
14	14	C	4	3	2	1.5402749	107.9723757	89.0433067
15	15	O	14	4	3	1.2108408	119.3672131	77.4322184
16	16	O	14	4	3	1.3616760	123.9097472	-101.3268084
17	17	C	16	14	4	1.4341528	126.9617814	-1.0841179
18	18	C	8	4	3	1.5077757	119.7546224	-28.0781138
19	19	N	18	8	4	1.2750643	128.8633547	-9.4181041
20	20	O	18	8	4	1.3790918	113.4936402	169.3863102
21	21	C	19	18	8	1.4709109	107.4383146	174.9383820
22	22	C	21	19	18	1.5541072	119.4413209	115.1733860
23	23	C	22	21	19	1.5525933	103.8921831	171.6878770
24	24	C	23	22	21	1.5653484	102.7149665	71.4300640
25	25	C	20	18	8	1.4551783	106.5364402	-173.6167732
26	26	C	25	20	18	1.5478880	117.0785664	-118.2024683
27	27	C	22	21	19	1.5638739	105.3111280	-81.8833656
28	28	C	27	22	21	1.5406659	115.5634311	71.3840779
29	29	C	27	22	21	1.5477647	113.3133596	-167.7264527
30	30	C	26	25	20	1.5224645	114.8304477	-49.9792242
31	31	H	1	6	5	1.0940749	107.9454155	158.7916999
32	32	H	1	6	5	1.1008366	106.7507851	-86.9242056
33	33	H	2	1	6	1.0957314	109.3038723	-173.5940991
34	34	H	2	1	6	1.0976879	110.3730438	70.5176149

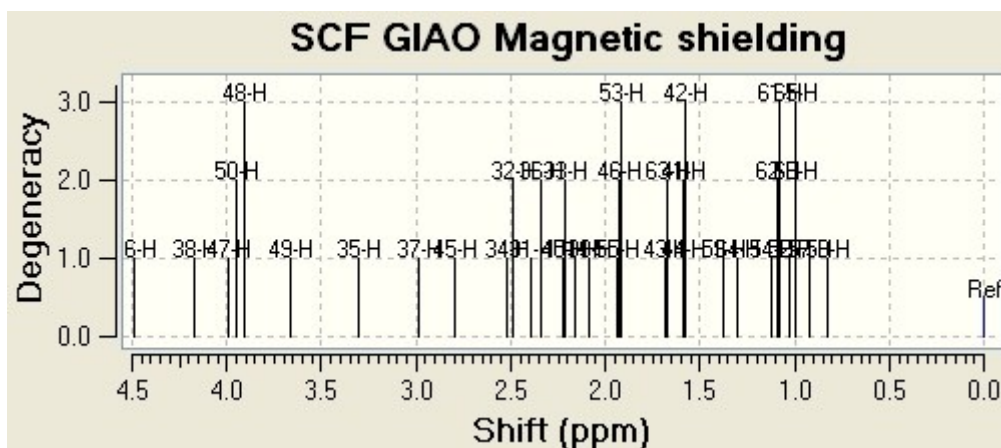
35	35	H	3	2	1	1.0926308	108.2518090	-58.5281421
36	36	H	3	2	1	1.0912567	111.8046237	-174.0970386
37	37	H	5	4	3	1.0905152	113.2140968	156.9198524
38	38	H	9	5	4	1.0953513	109.1771428	86.6505830
39	39	H	10	8	4	1.0924244	109.1918176	96.4474088
40	40	H	10	8	4	1.0965185	108.7220647	-17.9853480
41	41	H	11	10	8	1.0949019	110.1490603	-64.3784361
42	42	H	11	10	8	1.0968270	108.4681136	178.7195253
43	43	H	12	11	10	1.0961948	110.5280838	178.8074519
44	44	H	12	11	10	1.0993061	109.5396433	62.1979497
45	45	H	13	9	5	1.0974492	109.0304322	-56.6062811
46	46	H	13	9	5	1.0978002	107.8428308	-172.1494115
47	47	H	17	16	14	1.0908094	104.8683707	165.9397399
48	48	H	17	16	14	1.0904415	112.5626545	47.9069932
49	49	H	17	16	14	1.0925287	111.3288752	-76.2187596
50	50	H	21	19	18	1.0956244	107.0208438	-120.2606311
51	51	H	22	21	19	1.0933002	113.6248265	46.1965171
52	52	H	23	22	21	1.0949395	111.9042838	-49.4356854
53	53	H	23	22	21	1.0929060	111.4055888	-168.9457553
54	54	H	24	23	22	1.0958190	112.4920662	-118.7681654
55	55	H	24	23	22	1.0934583	112.0018289	121.3781887
56	56	H	25	20	18	1.0945833	105.7001997	117.6552824
57	57	H	28	27	22	1.0961170	110.4502653	-165.0439091
58	58	H	28	27	22	1.0958111	109.2940373	77.3363192
59	59	H	28	27	22	1.0836498	114.7410569	-41.8130408
60	60	H	29	27	22	1.0959258	109.9817342	-178.5724566
61	61	H	29	27	22	1.0907540	115.0820157	60.0613399
62	62	H	29	27	22	1.0959913	109.5932729	-61.2460342
63	63	H	30	26	25	1.0944321	111.4432984	60.5951229
64	64	H	30	26	25	1.0967958	110.8701029	-59.1404886
65	65	H	30	26	25	1.0955798	111.1442842	-178.6375131

Row	Tag	Symbol	X	Y	Z
1	1	C	-3.6055560	-2.4696820	0.2903510

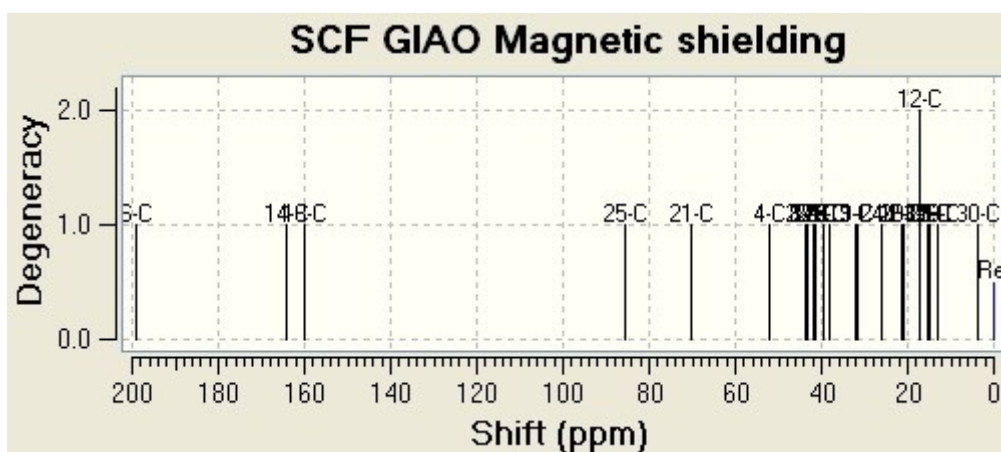
2	2	C	-2.5102160	-2.9195550	-0.6953200
3	3	C	-1.6441460	-1.7994420	-1.3303840
4	4	C	-1.8309960	-0.5044460	-0.5440100
5	5	C	-1.8528800	-0.8553670	0.9733540
6	6	C	-3.1532740	-1.4845480	1.3700710
7	7	C	-0.7221820	0.5755100	-0.2038480
8	8	C	-1.1954970	0.5023650	1.3115890
9	9	C	-0.7710450	1.9326530	-0.9062760
10	10	C	-1.7802510	2.9283590	-0.3250080
11	11	C	-1.7347640	2.9630730	1.2060290
12	12	C	-2.1384540	1.6020280	1.7774170
13	13	O	-3.7549400	-1.3164350	2.4015960
14	14	C	-3.0345800	0.1986110	-1.1667770
15	15	O	-3.1423140	0.5730690	-2.3116360
16	16	O	-4.0722890	0.3501950	-0.2741530
17	17	C	-5.2767860	1.0019590	-0.7593470
18	18	C	0.6476760	-0.0207770	-0.3978890
19	19	O	1.0796760	-0.8500320	0.6679150
20	20	N	1.4781820	0.0845810	-1.3899880
21	21	C	2.3879100	-1.3889980	0.2914220
22	22	C	3.5542710	-0.9016000	1.1840270
23	23	C	4.7729090	-1.7271420	0.6772900
24	24	C	5.0869940	-1.0946470	-0.7063220
25	25	C	2.6817920	-0.7295290	-1.1135560
26	26	C	4.0224920	0.0474750	-0.8504180
27	27	C	3.8964920	0.5433040	0.6522330
28	28	C	4.3520230	1.0847180	-1.8929200
29	29	C	2.8105740	1.5848320	0.9254790
30	30	C	5.2093850	1.1000300	1.2191580
31	31	H	-4.0563750	-3.3571600	0.7769180
32	32	H	-4.4433630	-1.9862030	-0.2589500
33	33	H	-2.9907920	-3.5004210	-1.5072230
34	34	H	-1.8389830	-3.6310880	-0.1742200
35	35	H	-1.9009690	-1.6623390	-2.4006430

36	36	H	-0.5800890	-2.1053750	-1.3332570
37	37	H	-1.0769790	-1.6472780	1.1992270
38	38	H	-0.3426560	0.4054150	2.0125520
39	39	H	-0.9745720	1.7753650	-1.9897940
40	40	H	0.2380900	2.3987410	-0.8719130
41	41	H	-2.8055420	2.6818590	-0.6649220
42	42	H	-1.5692750	3.9355650	-0.7346390
43	43	H	-2.4134960	3.7483860	1.5886500
44	44	H	-0.7207110	3.2398840	1.5524400
45	45	H	-2.1562970	1.6307210	2.8841310
46	46	H	-3.1847740	1.3625030	1.4812730
47	47	H	-5.0871440	2.0768330	-0.8348940
48	48	H	-5.5681110	0.5899210	-1.7310840
49	49	H	-6.0054770	0.7698120	0.0253620
50	50	H	2.2408550	-2.4789070	0.2973620
51	51	H	3.3588180	-0.9669590	2.2583740
52	52	H	4.5522990	-2.8015830	0.6024760
53	53	H	5.6239520	-1.6374760	1.3700880
54	54	H	5.0233740	-1.8262020	-1.5230460
55	55	H	6.1075150	-0.6843810	-0.7438690
56	56	H	2.8051470	-1.4585100	-1.9424710
57	57	H	3.5295450	1.8074700	-2.0031620
58	58	H	4.5041060	0.6333970	-2.8807340
59	59	H	5.2560240	1.6478900	-1.6368560
60	60	H	2.4916530	2.0868850	0.0044460
61	61	H	3.1488710	2.3731310	1.6074380
62	62	H	1.9234480	1.1450510	1.3980810
63	63	H	5.4197800	2.0918470	0.8012620
64	64	H	6.0839250	0.4790610	1.0051400
65	65	H	5.1485140	1.2026070	2.3085210

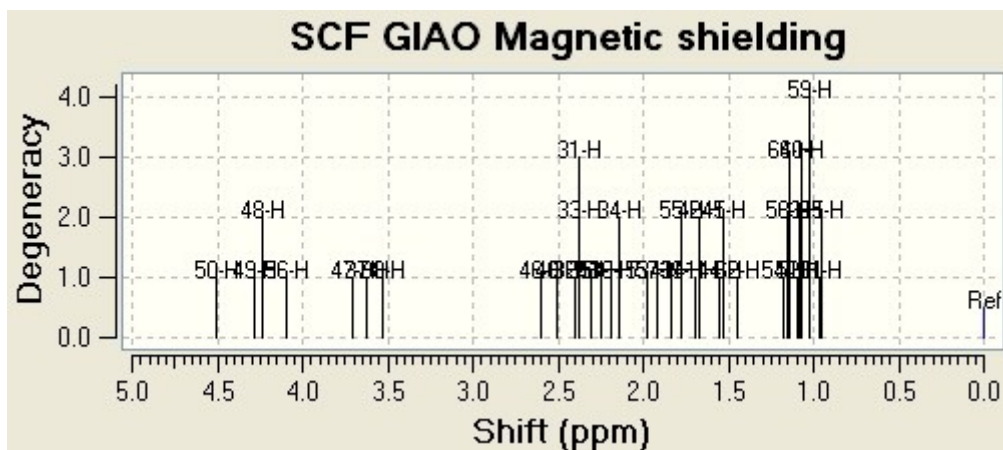
### Simulated NMR Spectra



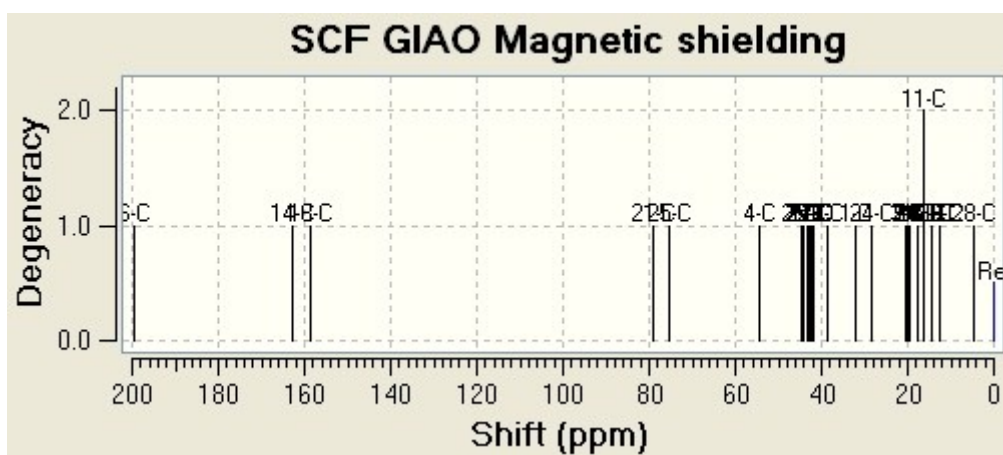
### <sup>1</sup>H NMR Spectrum of 13



### <sup>13</sup>C NMR spectrum of 13



<sup>1</sup>H NMR spectrum of 17



<sup>13</sup>C NMR Spectrum of 17

**Table S1.** Imaginary frequencies of the transition states.

<b>Transition state</b>	<b>Frequency</b>
20 s.t.	210i
21 s.t.	545i
22 s.t.	37i
23 s.t.	40i
24 s.t.	809i
25 s.t.	202i
27 s.t.	53i