SUPPLEMENTARY MATERIAL

Two novel cyclohexanone-monocyclic polycyclic polyprenylated acylphloroglucinols from *Garcinia multiflora* fruits

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ABSTRACT

Two novel cyclohexanone-monocyclic polyprenylated acylphloroglucinol (C-MPAP) derivatives, named norgarmultinones A (**1**) and B (**2**), were isolated from the fruits of *Garcinia multiflora*. Their structures were clarified by NMR, HRESIMS and calculated electronic circular dichroism (ECD) spectra. Compound **2** is the first example of naturally occurring C-MPAPs containing tetrahydropyran moiety by the cyclization of an enolic hydroxyl with an isogeranyl side chain. The reasonable biosynthetic routes of **1** and **2** were also put forward.

Keywords: Garcinia; *Garcinia multiflora*; cyclohexanone-monocyclic polyprenylated acylphloroglucinol (C-MPAP);

Contents

Table S1. ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR Data of **1-2** in $CDCl_3$ (δ in ppm, J in Hz)

No.	**1**		**2**	
	δ_C	δ_H	δ_C	δ_H
1	64.2	4.57, s	132.2	
3	40.6	2.59, dt (17.4, 7.2)	38.9	2.75, m
		2.43, dd (17.4, 7.8)		2.82, m
4	208.2		212.1	
5	66.1		52.7	
6	34.9	1.84, m	34.7	1.50, m
				1.59, m
7	44.4	1.85, m	43.2	1.49, m
8	43.8		37.4	
9	207.3		148.8	
10	197.5		199.4	
11	139.4		139.4	
12	128.1	7.80, d (7.2)	129.6	8.00 d (7.2)
13	128.7	7.45, t (7.8)	128.4	7.45, t (7.8)
14	133.2	7.56, t (7.2)	132.7	7.53, t (7.8)
15	128.7	7.45, t (7.8)	128.4	7.45, t (7.8)
16	128.1	7.80, d (7.2)	129.5	8.00, d (7.2)
17	23.0	2.25, m	22.6	2.33, m
18	123.3	5.08, t (6.6)	123.3	5.16, t (7.2)
19	132.7		133.0	
20	17.8	1.60, s	17.9	1.64, s
21	25.9	1.64, s	25.9	1.72, s
22	36.8	2.21, m	35.2	1.40, m
		2.16, dd (13.8, 7.2)		2.27, m
23	43.3	1.93, m	44.1	1.40, m
24	147.5		82.7	
25	19.3	1.51, s	19.0	0.99, s
26	112.8	4.49, s	28.5	1.01, s
		4.40, s		
27	33.4	2.08, m	30.4	1.60, m
		1.94, m		1.91, dd (14.4, 4.8)
28	122.7	4.92, brs	122.5	5.08, m
29	132.6		133.1	
30	18.1	1.66, s	18.1	1.57, s
31	25.9	1.57, s	25.9	1.72, s
32	27.6	2.31, m	28.2	2.23, m
		1.80, m		1.63, m
33	122.7	5.14, t (7.2)	123.2	5.07, m
34	133.9		133.1	
35	18.2	1.64, s	18.1	1.59, s
36	26.1	1.75, s	26.1	1.72, s

37	17.0	1.21, s	22.3	1.00, s
38	27.8	1.11, s	27.2	1.11, s

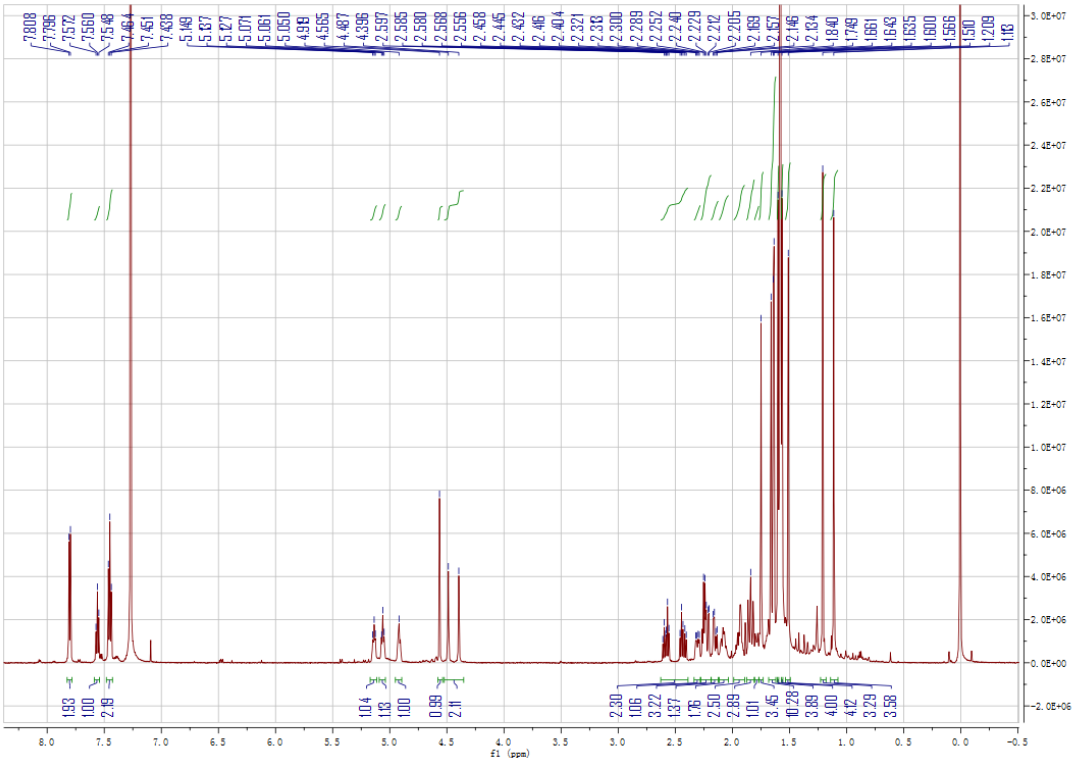


Figure S1. ^{1}H-NMR spectrum of compound **1** ($CDCl_3$, 600 MHz)

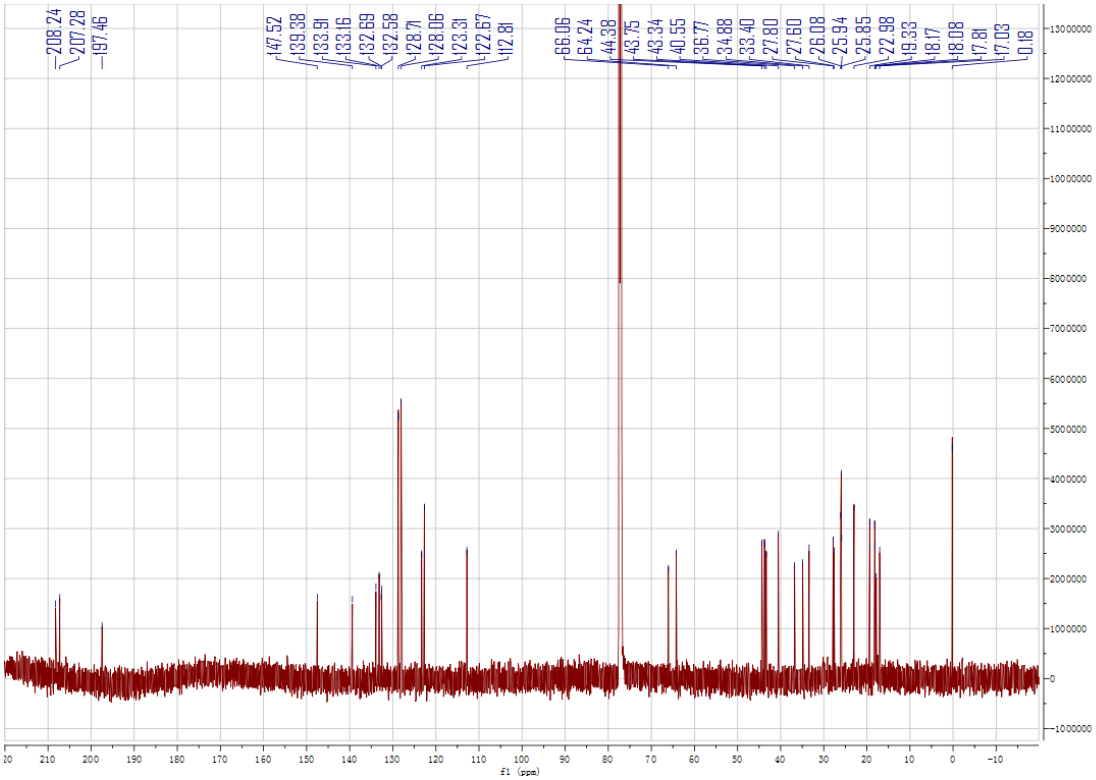


Figure S2. ^{13}C-NMR spectrum of compound **1** ($CDCl_3$, 150 MHz)

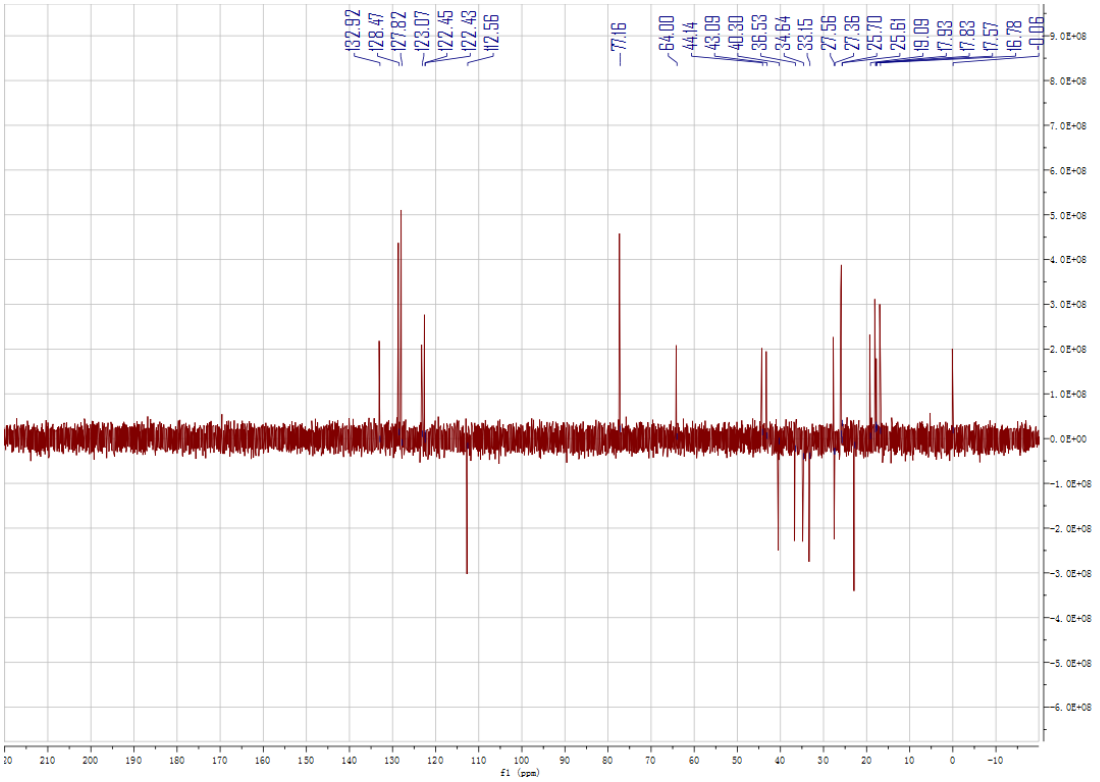


Figure S3. DEPT spectrum of compound **1** ($CDCl_3$, 150 MHz)

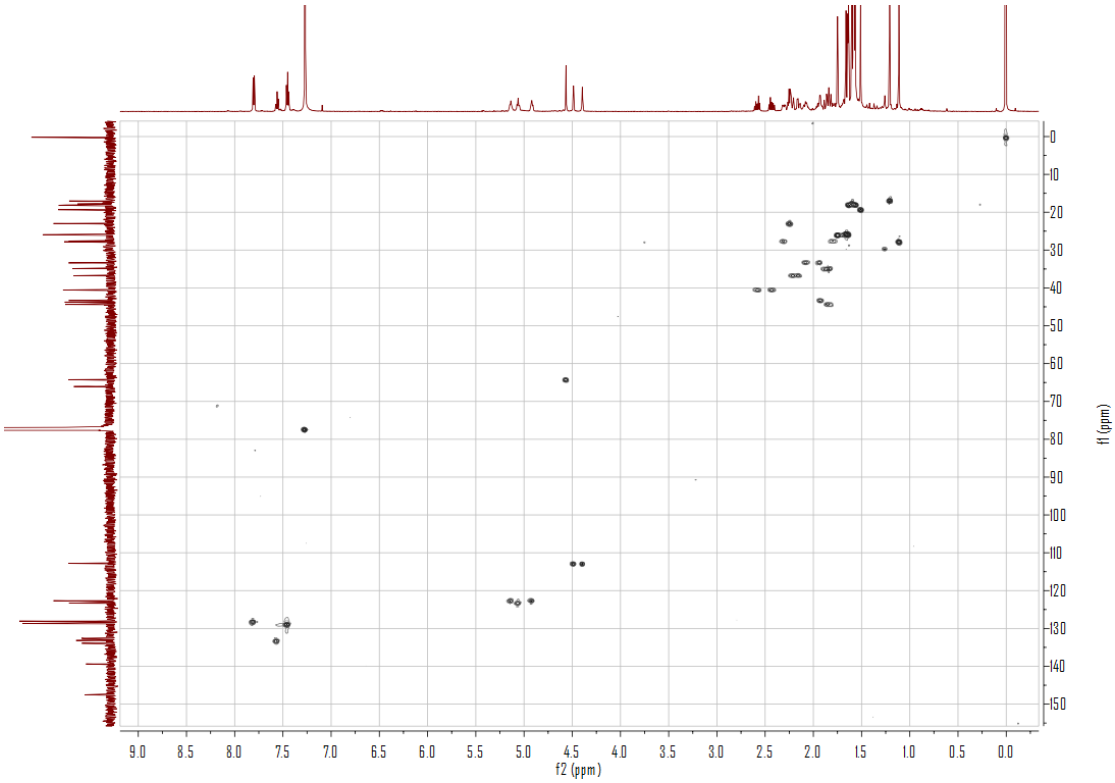


Figure S4. HSQC spectrum of compound **1**

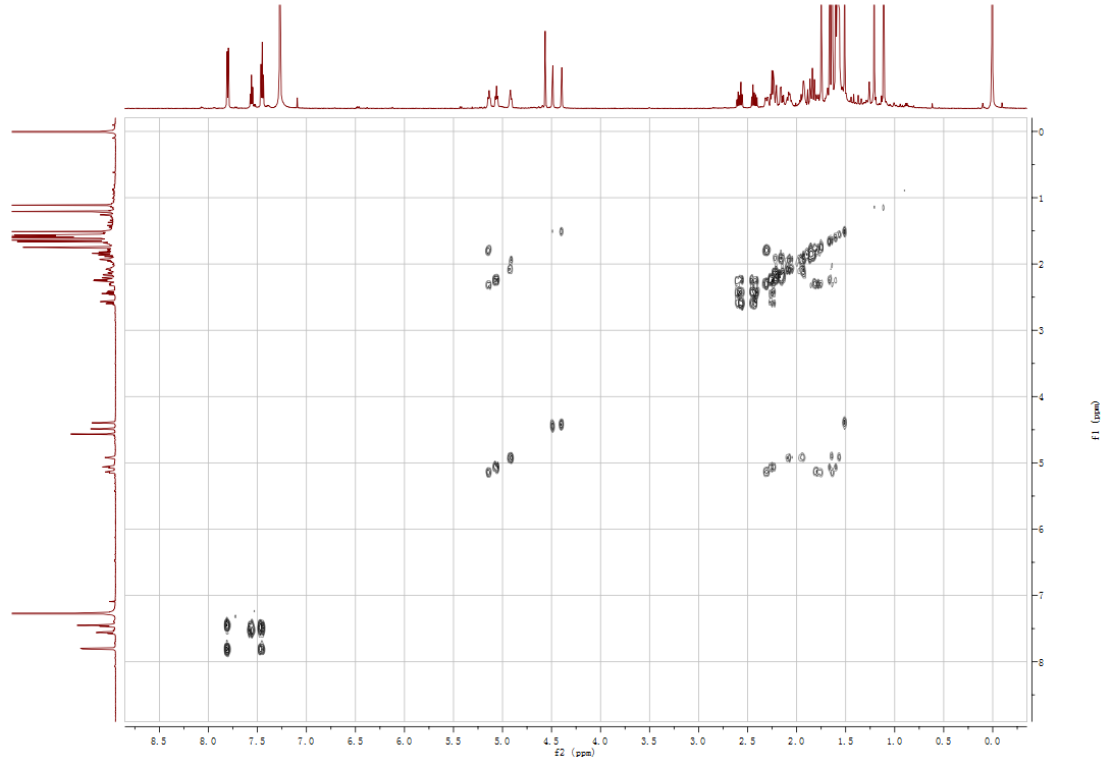


Figure S5. ^{1}H-^{1}H COSY spectrum of compound **1**

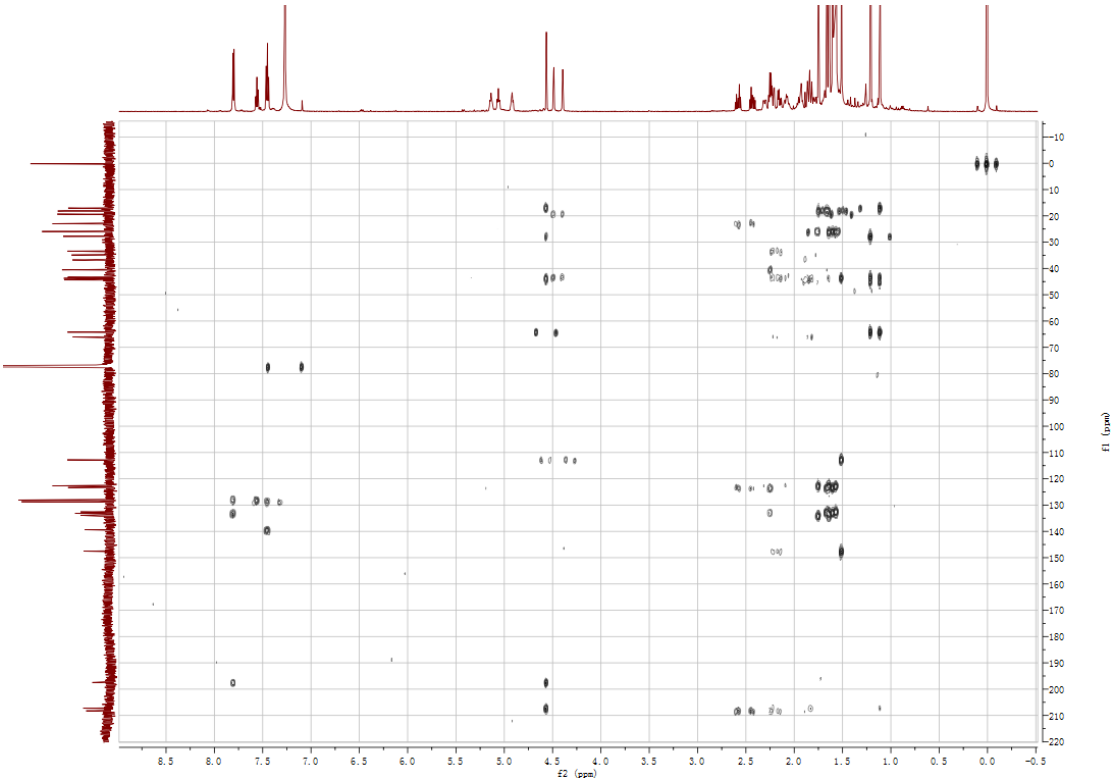


Figure S6. HMBC spectrum of compound **1**

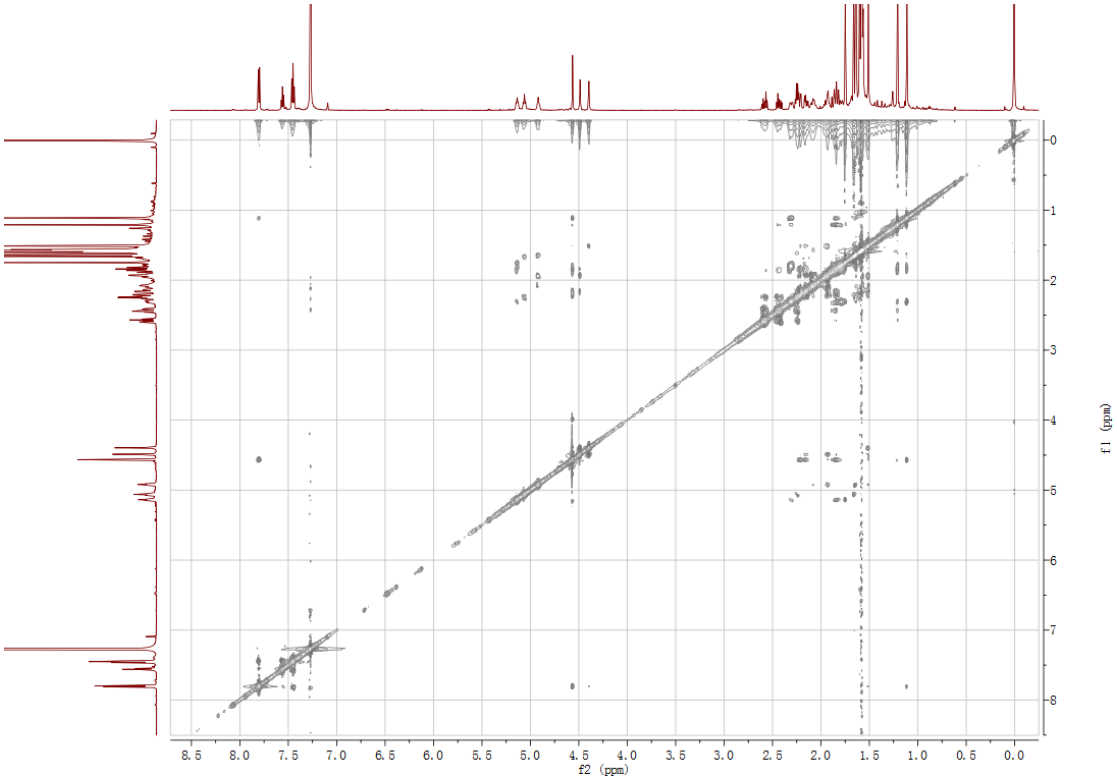


Figure S7. ROESY spectrum of compound **1**

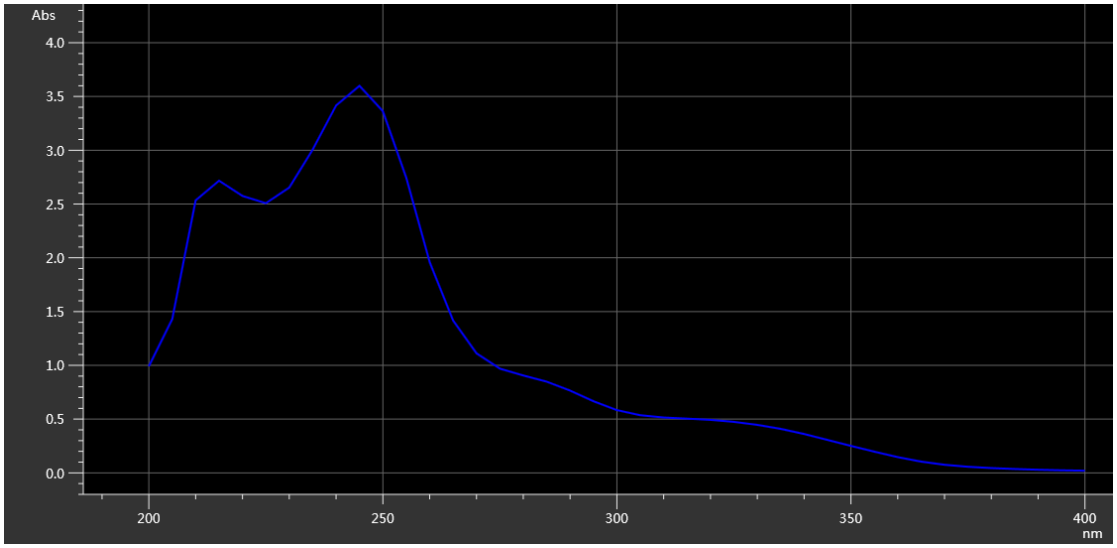


Figure S8. UV spectrum of compound **1**

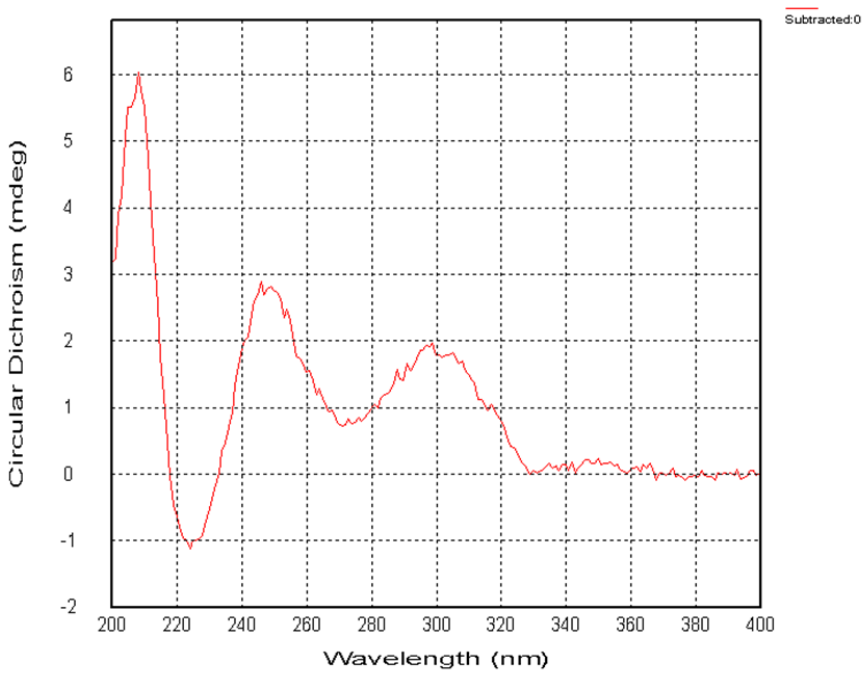


Figure S9. CD spectrum of compound **1**

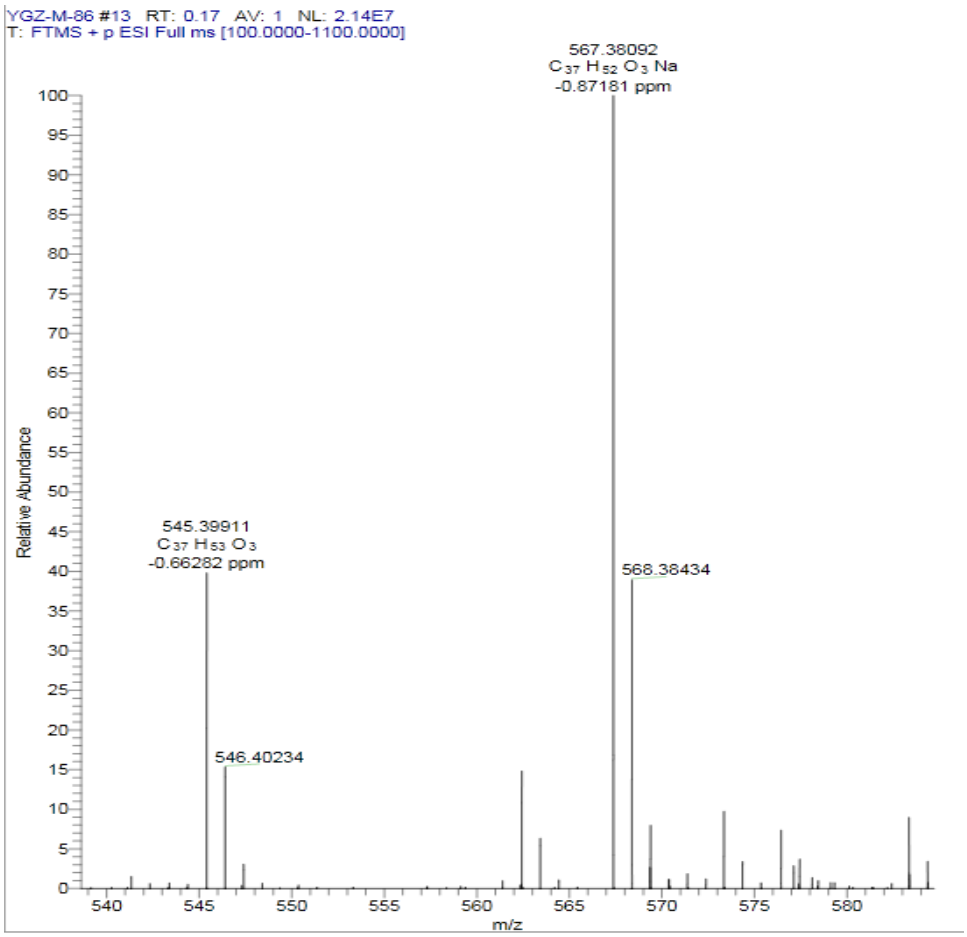


Figure S10. HR-ESI-MS of compound **1**

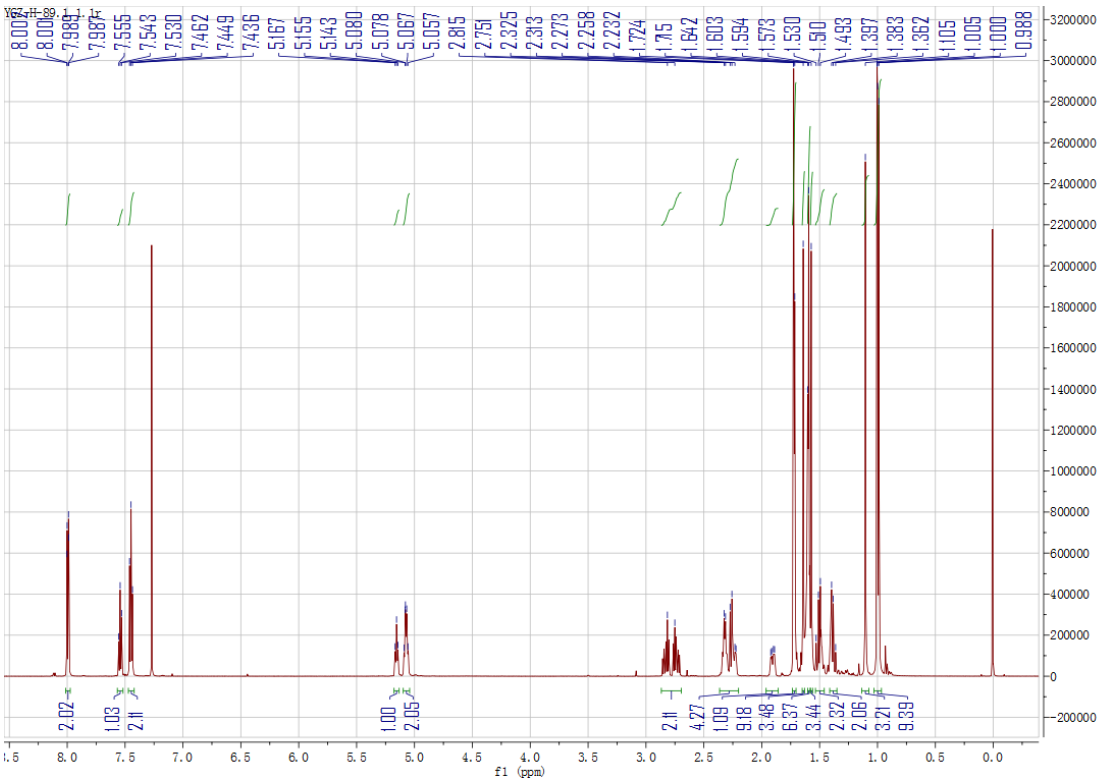


Figure S11. ^{1}H-NMR spectrum of compound **2** ($CDCl_3$, 600 MHz)

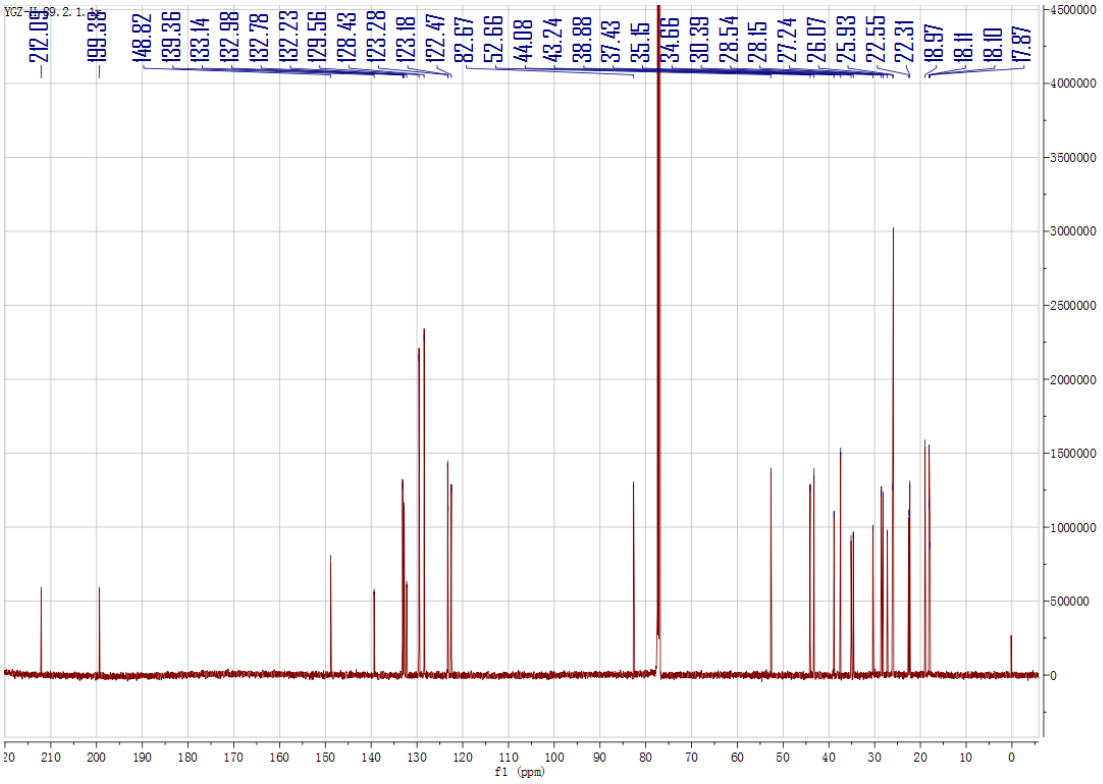


Figure S12. ^{13}C-NMR spectrum of compound **2** ($CDCl_3$, 150 MHz)

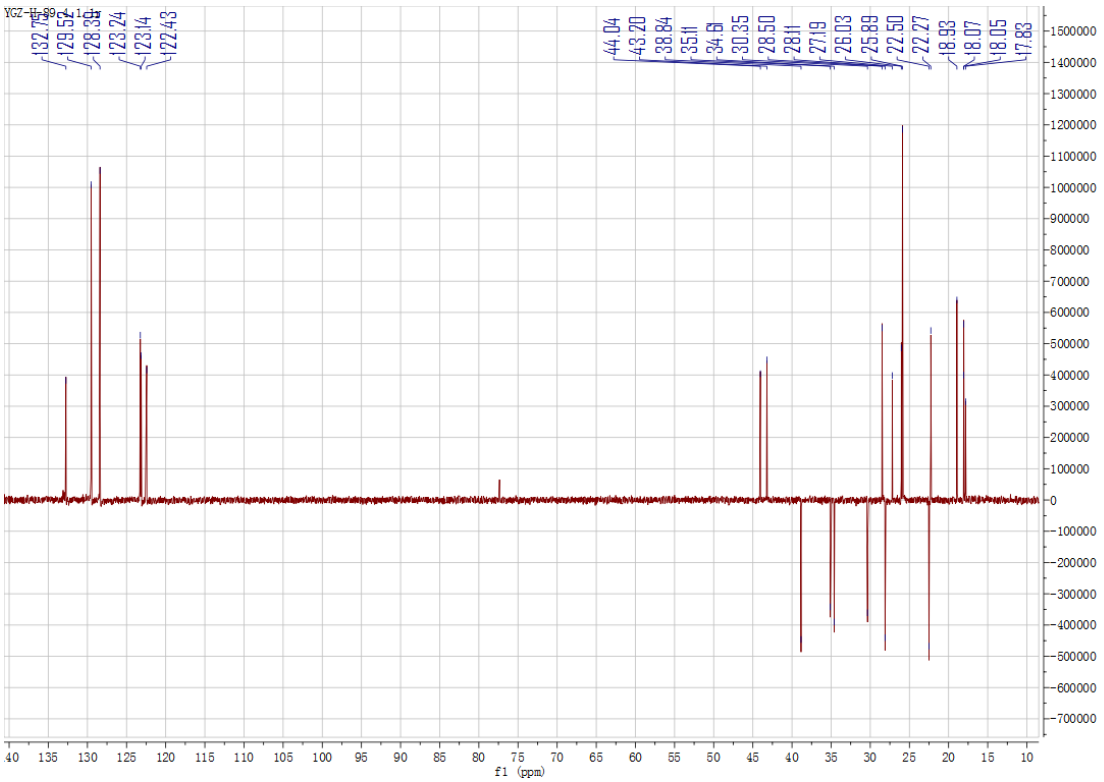


Figure S13. DEPT spectrum of compound **2** ($CDCl_3$, 150 MHz)

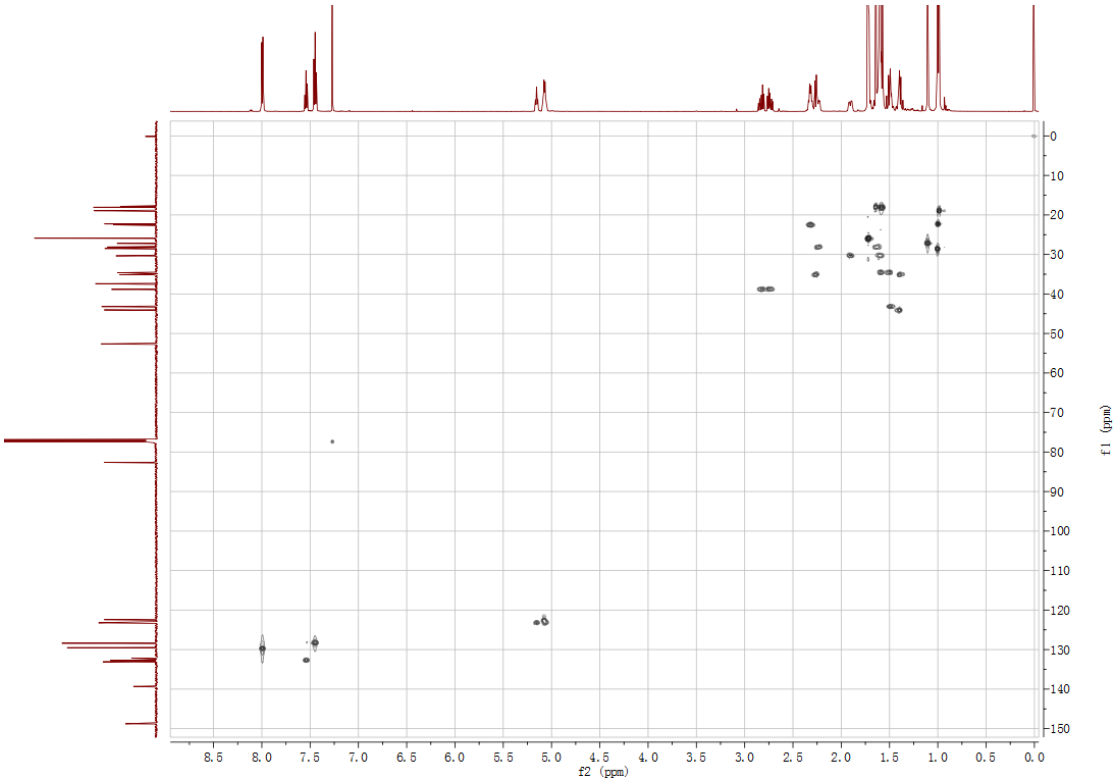


Figure S14. HSQC spectrum of compound **2**

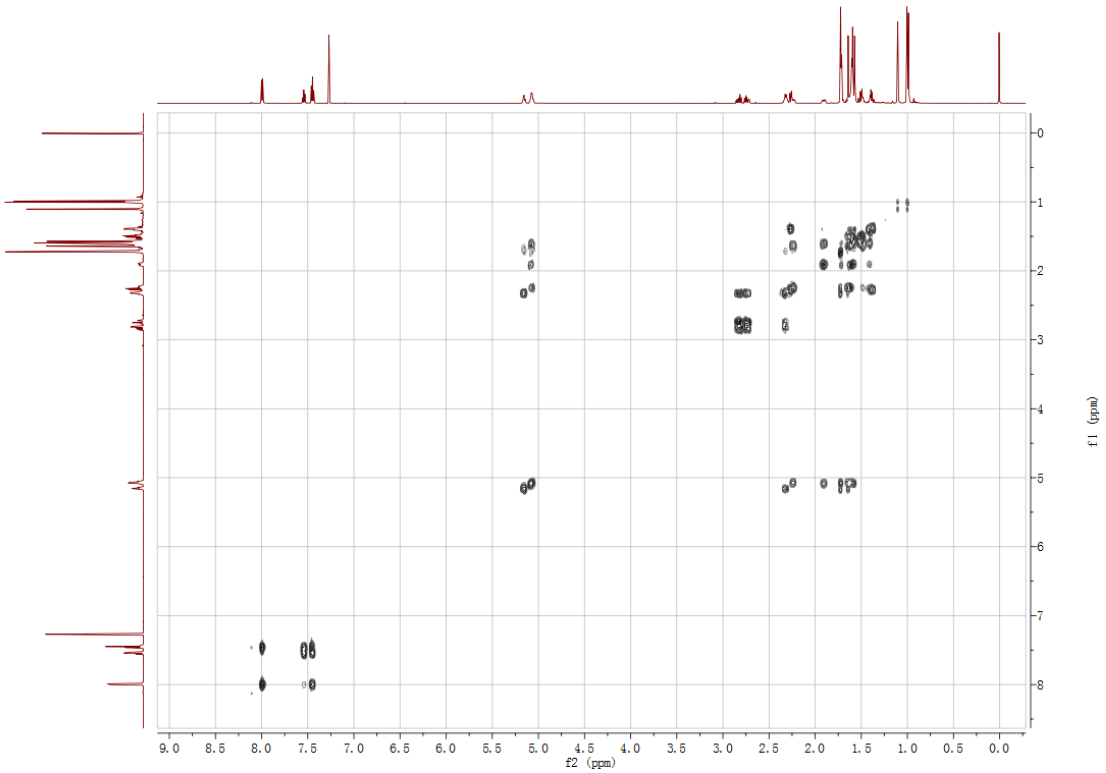


Figure S15. ^{1}H-^{1}H COSY spectrum of compound **2**

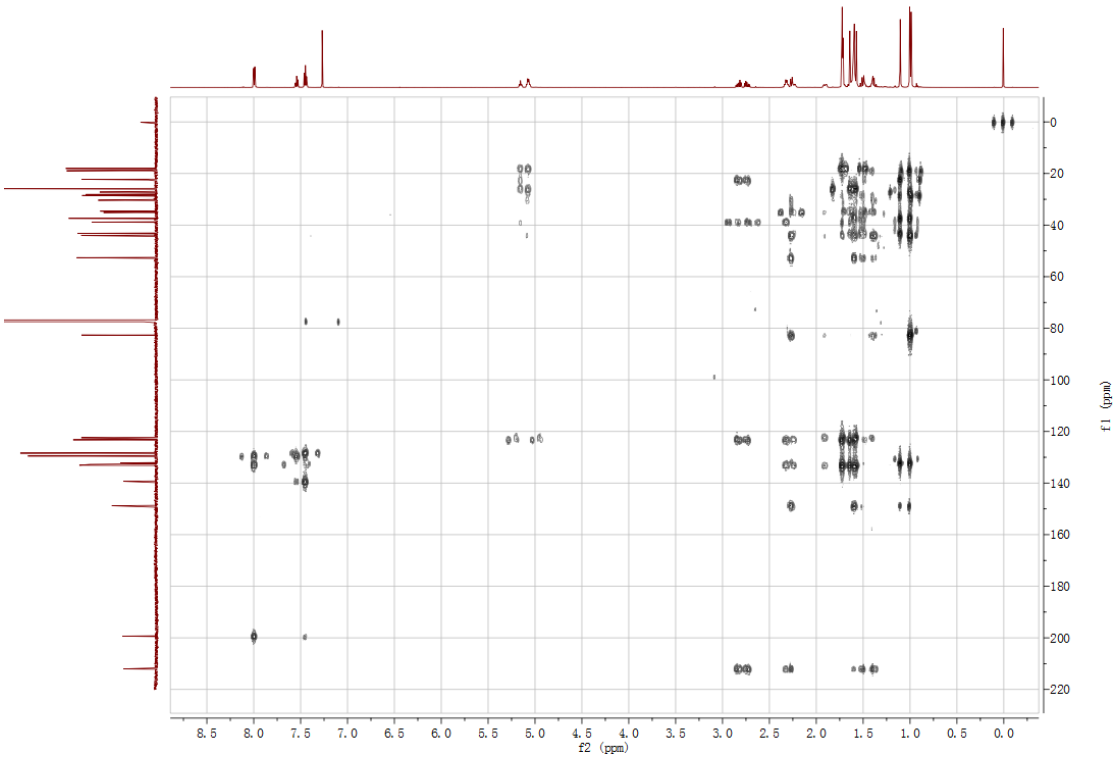


Figure S16. HMBC spectrum of compound **2**

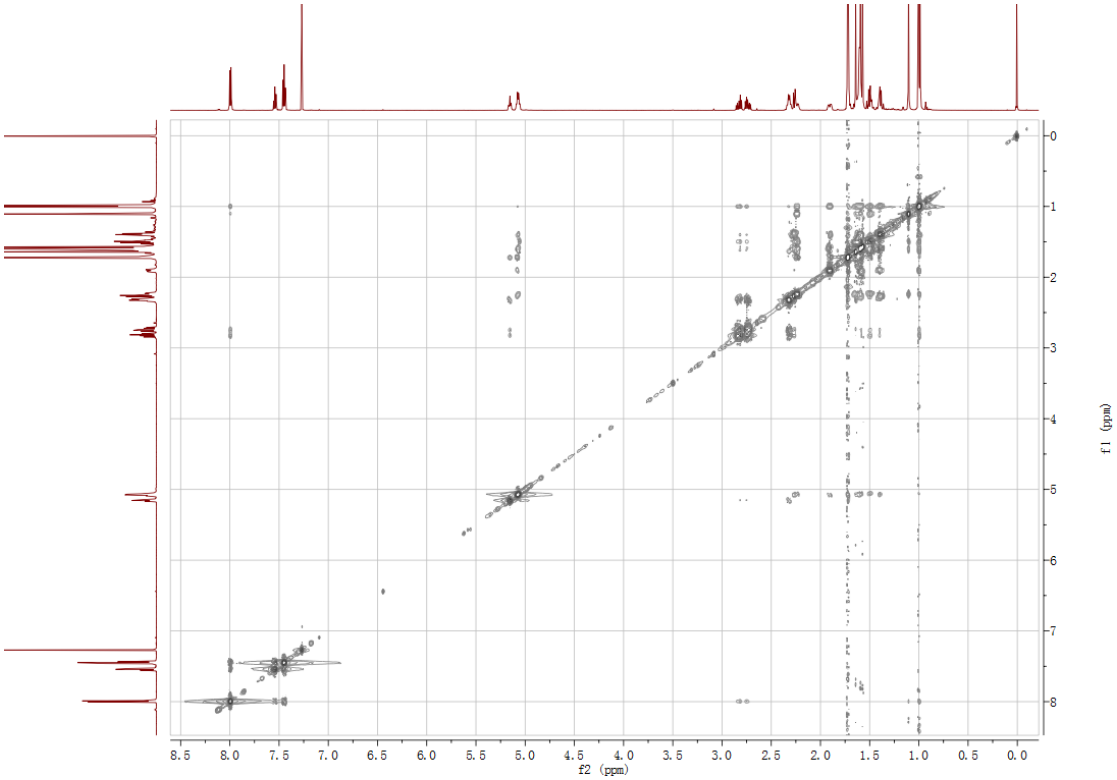


Figure S17. ROESY spectrum of compound **2**

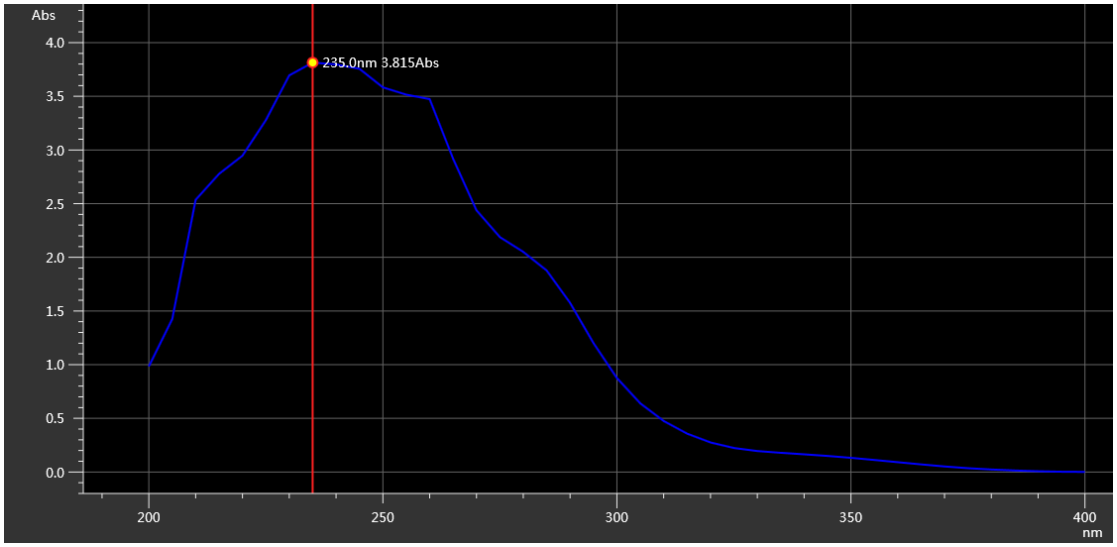


Figure S18. UV spectrum of compound **2**

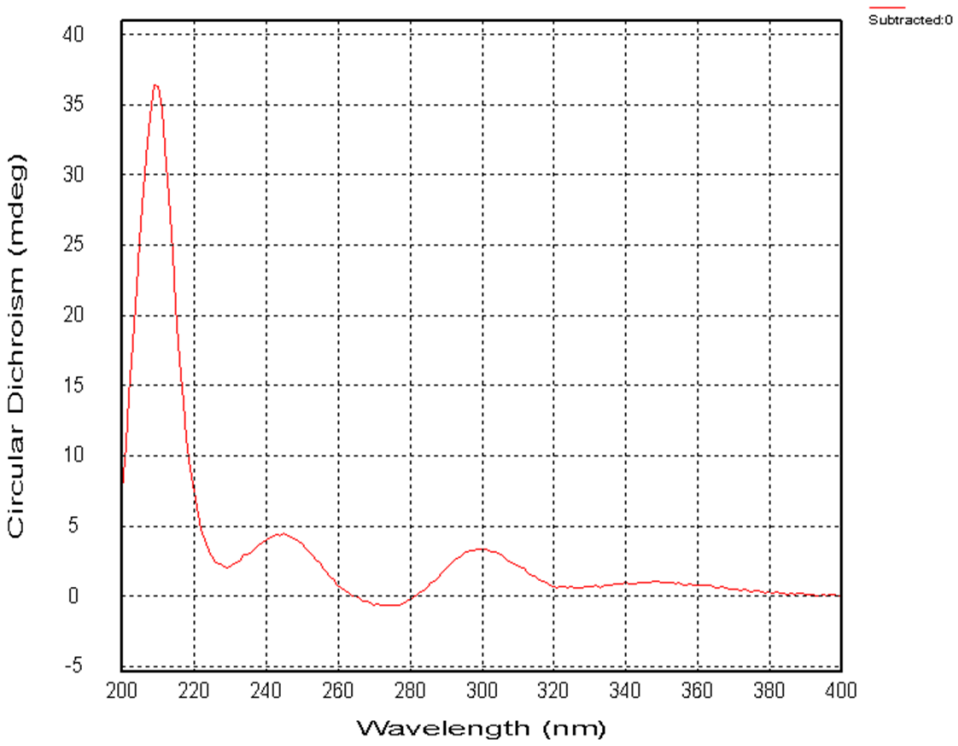


Figure S19. CD spectrum of compound **2**

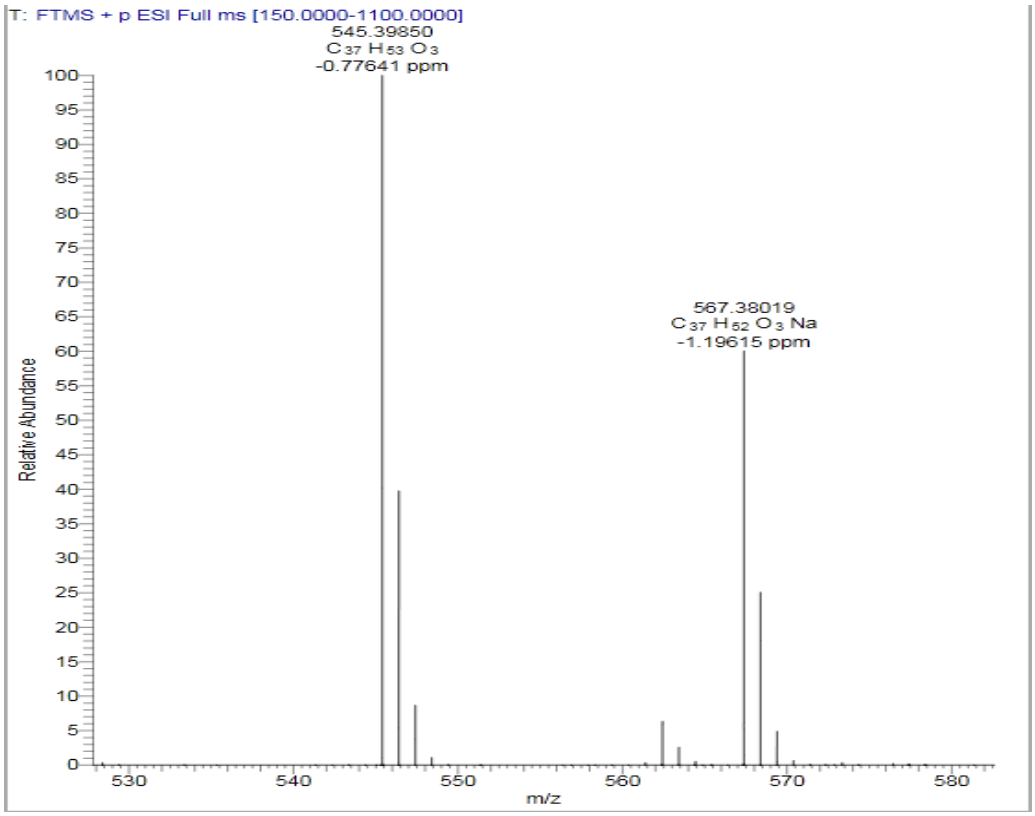


Figure S20. HR-ESI-MS of compound **2**

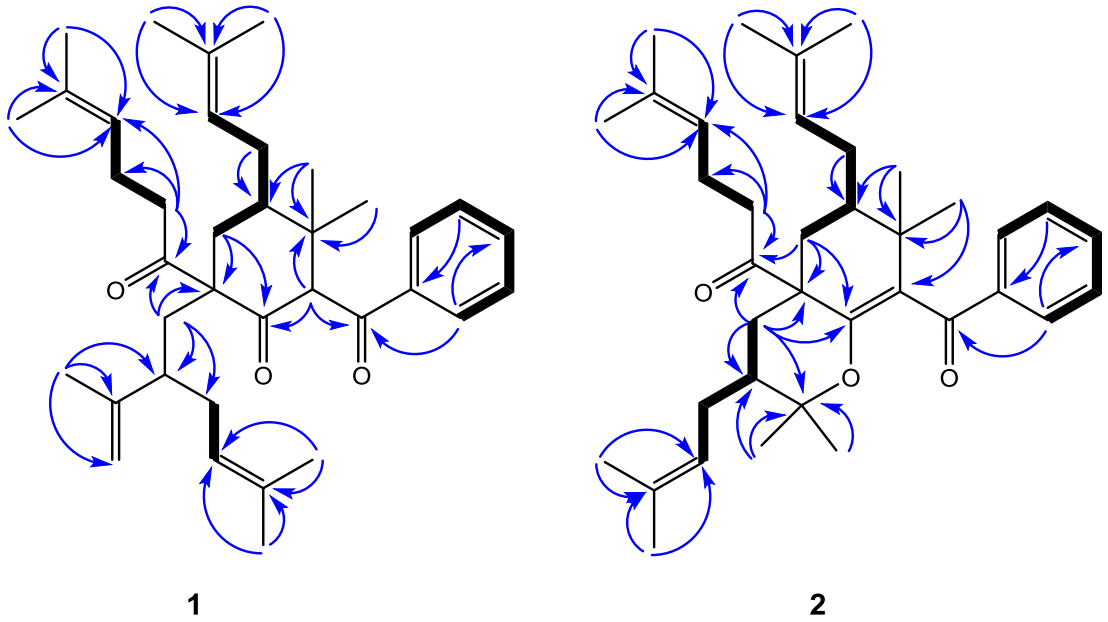


Figure S21. Key HMBC and ^{1}H-^{1}H COSY correlations of compounds **1** and **2**.

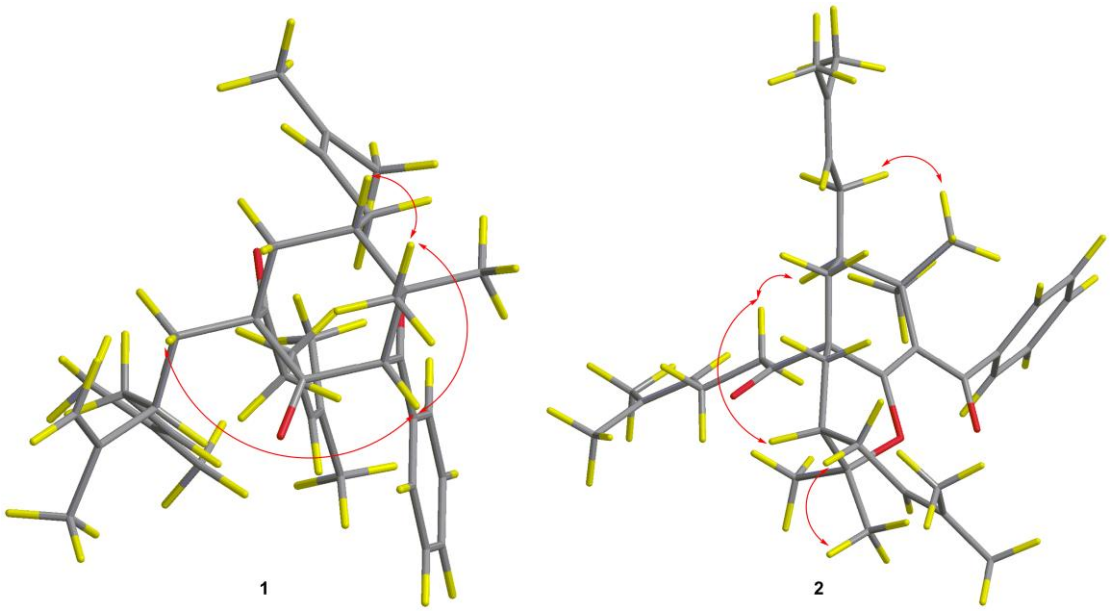


Figure S22. Key ROESY correlations of compounds **1** and **2**.

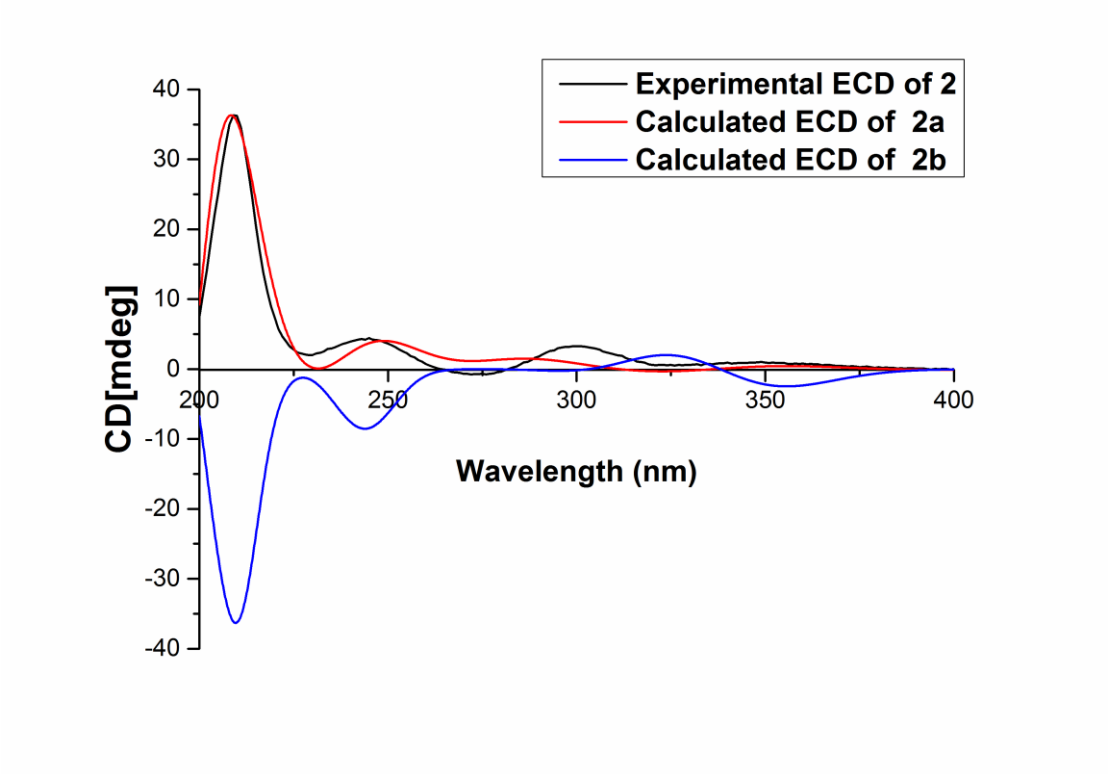
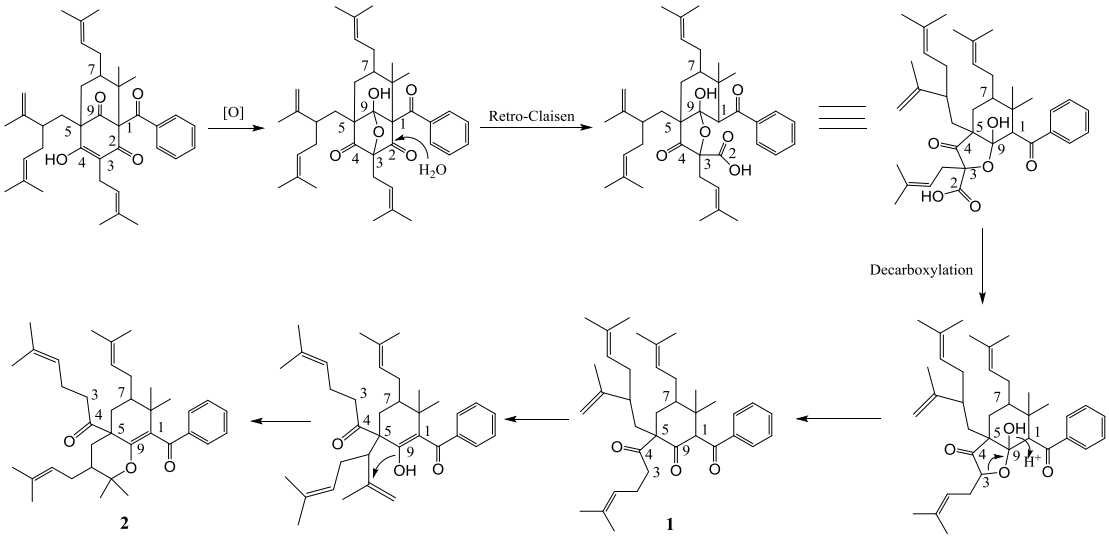


Figure S23. Calculated and experimental ECD spectra of compound **2**.



Scheme S1. Plausible biosynthetic pathway for compounds **1** and **2**.

ECD calculation for Compound 2

Conformational analysis was performed using SYBYL-X 2.1.1 by systematic search at MMFF94s force field, and with an energy cutoff of 8.0 kcal/mol to the global minima. The theoretical calculations were carried out using Gaussian 09. The minimized conformers were further optimized and analysed frequency, using the density functional theory (DFT) at the B3LYP/6-31G(d,p) level in gas phase, and showed no imaginary frequencies. Based on the optimized structures, the ECD were calculated using TD-DFT-B3LYP/6-31G(d,p) level with the IEFPCM model in methanol solution. Rotatory strengths for a total of 60 excited states were calculated. The overall calculated ECD curves of all compounds were generated by Boltzmann weighting of their selected low-energy conformers using SpecDis.

Optimized at the B3LYP/6-31g(d,p) level in gas phase (ECD)

Z-matrix: 2a-1			
C	-1.03212	-0.38287	1.11366
C	-2.47677	-0.6827	0.65933
C	-2.7235	-0.14699	-0.80227
C	-1.47263	-0.33192	-1.68542
C	-0.26037	0.45432	-1.13411
C	-0.04703	0.12184	0.33396
C	-0.71003	-0.54673	2.569
C	0.08161	-1.72894	3.02491
C	0.37327	-2.82219	2.1996
C	0.5225	-1.74765	4.35628
C	1.24699	-2.83421	4.85076
C	1.53353	-3.91523	4.02024
C	1.09688	-3.91044	2.69671
O	-1.11911	0.27092	3.38974
C	-2.72699	-2.19903	0.7661
C	-3.49257	0.0194	1.59602
C	-4.01383	-0.62146	-1.53237
C	-3.9907	-1.98983	-2.16601
C	-4.87393	-2.99672	-2.01177
C	-4.69367	-4.29291	-2.76076
C	-6.09246	-2.96865	-1.12944
C	0.9933	0.05884	-1.93623
C	2.26019	0.67585	-1.32025

C	2.40066	0.23408	0.16087
O	1.17357	0.46457	0.89273
C	-0.56089	1.98438	-1.28148
C	-0.47153	2.59904	-2.67546
O	-0.89471	2.68424	-0.32248
C	-1.17529	3.95258	-2.74755
C	-1.17105	4.49053	-4.15314
C	-0.36561	5.44229	-4.66342
C	-0.52321	5.89829	-6.09054
C	0.74027	6.13131	-3.91177
C	2.80659	-1.22932	0.36685
C	3.44154	1.11301	0.87905
C	3.49997	0.50365	-2.23288
C	3.82268	-0.8902	-2.70179
C	4.97119	-1.57863	-2.54607
C	5.11642	-2.9634	-3.1251
C	6.19409	-1.09313	-1.81636
H	-2.87577	0.938	-0.70248
H	-1.2215	-1.39931	-1.74579
H	-1.69772	-0.01216	-2.70959
H	0.05399	-2.84719	1.16334
H	0.3016	-0.90972	5.01562
H	1.58371	-2.83403	5.88438
H	2.09649	-4.76162	4.40555
H	1.32138	-4.75435	2.04914
H	-2.11697	-2.76432	0.05417
H	-2.50483	-2.57776	1.76975
H	-3.77782	-2.44484	0.59251
H	-3.45815	-0.38565	2.61364
H	-3.29971	1.0969	1.65555
H	-4.52317	-0.11374	1.25224
H	-4.19125	0.08323	-2.35766
H	-4.87182	-0.49347	-0.87015
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H	-6.21105	-2.03749	-0.57278
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H	1.08333	-1.03465	-1.95757
H	2.08998	1.76225	-1.29392

H	0.58636	2.71832	-2.93238
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H	-0.72312	4.65898	-2.04371
H	-1.93449	4.0564	-4.79909
H	-1.33959	5.38034	-6.60487
H	-0.73783	6.97148	-6.12335
H	0.39675	5.70914	-6.65326
H	0.93165	5.6969	-2.92778
H	1.67694	6.06296	-4.47555
H	0.49797	7.18995	-3.77316
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H	3.81999	-1.43123	0.01563
H	2.78795	-1.48246	1.43241
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H	3.18609	2.17489	0.78566
H	3.45658	0.89742	1.95434
H	4.3612	0.98766	-1.76739
H	3.3149	1.09056	-3.14401
H	3.02831	-1.36482	-3.27776
H	4.21488	-3.29122	-3.65326
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H	5.31598	-3.68786	-2.3287
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C	-1.52955	-0.3531	-1.6854
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C	-0.72359	-0.53715	2.56519
C	0.09362	-1.70311	3.01791
C	0.39179	-2.79657	2.19516
C	0.5532	-1.70619	4.34293
C	1.3028	-2.77736	4.83336
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C	1.14116	-3.86925	2.68801
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C	-3.52235	-0.01128	1.61234
C	-4.06175	-0.70123	-1.50636
C	-4.00776	-2.07073	-2.13622
C	-4.85789	-3.10348	-1.96701
C	-4.64506	-4.39762	-2.71107
C	-6.06679	-3.10872	-1.07124
C	0.92746	0.06177	-1.95582
C	2.19297	0.69943	-1.35798
C	2.35275	0.27376	0.12573
O	1.12882	0.49441	0.86601
C	-0.64686	1.97597	-1.29853
C	-0.53569	2.59567	-2.68897

O	-1.02826	2.66294	-0.34771
C	-1.1395	3.99746	-2.74275
C	-1.04634	4.57292	-4.13039
C	-0.12889	5.44541	-4.59133
C	-0.19834	5.96012	-6.00523
C	1.02673	5.98304	-3.79226
C	2.78237	-1.1814	0.34154
C	3.3872	1.17404	0.82685
C	3.42479	0.53207	-2.28189
C	3.75411	-0.86264	-2.7436
C	4.90877	-1.54146	-2.59146
C	5.05986	-2.92944	-3.16084
C	6.13299	-1.04133	-1.87426
H	-2.95199	0.89203	-0.70008
H	-1.26242	-1.41643	-1.74865
H	-1.76842	-0.03463	-2.70723
H	0.05859	-2.8334	1.16371
H	0.3277	-0.86788	5.0003
H	1.65373	-2.76536	5.86212
H	2.1799	-4.69225	4.38705
H	1.37157	-4.71269	2.0421
H	-3.78342	-2.48809	0.63654
H	-2.12443	-2.7902	0.08186
H	-2.49551	-2.59368	1.80017
H	-3.34009	1.06849	1.66406
H	-4.55387	-0.15668	1.27651
H	-3.47632	-0.41	2.63196
H	-4.26726	-0.00436	-2.33173
H	-4.91557	-0.59508	-0.8348
H	-3.19513	-2.20711	-2.84884
H	-5.50905	-4.61608	-3.34717
H	-3.75853	-4.36864	-3.35332
H	-4.5145	-5.22358	-2.00412
H	-6.214	-2.1748	-0.5261
H	-6.97092	-3.28758	-1.66282
H	-5.97851	-3.90799	-0.32763
H	0.82135	0.35624	-3.00668
H	1.03048	-1.03083	-1.96541
H	2.0113	1.78399	-1.33891
H	0.52314	2.64694	-2.96225
H	-1.05115	1.95055	-3.40714
H	-2.19856	3.95935	-2.45697

H	-0.66259	4.65209	-2.00547
H	-1.83623	4.24344	-4.80547
H	-1.05354	5.55264	-6.55452
H	-0.29177	7.05102	-6.00652
H	0.70925	5.68727	-6.55348
H	1.14054	5.50225	-2.81778
H	1.96491	5.82439	-4.33493
H	0.90211	7.05795	-3.62647
H	2.10171	-1.88586	-0.14456
H	3.79547	-1.37137	-0.01706
H	2.77763	-1.42468	1.40953
H	4.39649	1.03904	0.42763
H	3.11238	2.23089	0.73136
H	3.41848	0.96439	1.90301
H	4.28654	1.02711	-1.82901
H	3.22493	1.11058	-3.19532
H	2.95907	-1.34736	-3.31015
H	4.15557	-3.26954	-3.67642
H	5.88317	-2.95529	-3.88219
H	5.27417	-3.64567	-2.36078
H	6.00291	-0.05947	-1.41613
H	6.40716	-1.73557	-1.07259
H	6.97419	-0.97169	-2.57181
Z-matrix:2a-3			
C	-0.95625	-0.58315	1.51541
C	-2.34455	-1.07165	1.05684
C	-2.6055	-0.69487	-0.45177
C	-1.31096	-0.84293	-1.27957
C	-0.20612	0.11627	-0.78291
C	-0.00588	-0.04868	0.71334
C	-0.6617	-0.59545	2.98546
C	0.27182	-1.61921	3.54392
C	0.70229	-2.73922	2.82139
C	0.70641	-1.45694	4.86744
C	1.56205	-2.39113	5.45458
C	1.98606	-3.50037	4.72627
C	1.5563	-3.67561	3.41198
O	-1.20494	0.21174	3.73533
C	-2.43541	-2.59861	1.27326
C	-3.45979	-0.41015	1.90458
C	-3.76326	-1.47647	-1.12315
C	-4.21264	-0.83543	-2.41272

C	-4.08042	-1.30305	-3.66944
C	-4.62444	-0.5197	-4.83659
C	-3.40548	-2.59046	-4.05397
C	1.10485	-0.22274	-1.51105
C	2.28105	0.59072	-0.94692
C	2.41902	0.34758	0.58089
O	1.15134	0.47319	1.26405
C	-0.65795	1.58269	-1.09455
C	-0.60558	2.05187	-2.54625
O	-1.07442	2.34243	-0.21659
C	-1.39986	3.33782	-2.76122
C	-1.39896	3.73641	-4.21262
C	-0.60958	4.65213	-4.80719
C	-0.7616	4.9639	-6.27302
C	0.47488	5.43312	-4.11669
C	3.0293	-1.00568	0.96023
C	3.29312	1.44728	1.21492
C	3.56399	0.43097	-1.80149
C	3.93182	-0.96678	-2.22803
C	3.76901	-1.53099	-3.44176
C	4.23807	-2.94061	-3.69886
C	3.13121	-0.87228	-4.63442
H	-2.89568	0.36543	-0.47464
H	-0.96403	-1.88395	-1.22507
H	-1.51123	-0.6557	-2.33889
H	0.39236	-2.9013	1.79478
H	0.37834	-0.59542	5.44701
H	1.89291	-2.25131	6.48066
H	2.65072	-4.22856	5.18429
H	1.88805	-4.54184	2.84488
H	-1.72141	-3.13998	0.64386
H	-2.23744	-2.8718	2.31571
H	-3.43613	-2.98293	1.04826
H	-3.37411	0.68267	1.88922
H	-4.45873	-0.6662	1.538
H	-3.42697	-0.73734	2.94975
H	-4.64014	-1.49768	-0.46704
H	-3.47683	-2.52093	-1.27481
H	-4.72213	0.11896	-2.26952
H	-5.11483	0.40805	-4.52334
H	-3.81488	-0.25152	-5.52333
H	-5.36181	-1.11701	-5.38282

H	-2.94019	-3.10779	-3.21264
H	-4.1304	-3.27438	-4.50717
H	-2.61332	-2.39438	-4.78457
H	1.00679	-0.0385	-2.58679
H	1.31181	-1.29605	-1.40927
H	2.00568	1.65006	-1.05434
H	0.4426	2.21788	-2.8164
H	-1.01013	1.26749	-3.19253
H	-2.44123	3.19107	-2.44672
H	-1.01405	4.14129	-2.12478
H	-2.14579	3.22171	-4.81731
H	-1.56337	4.38273	-6.74062
H	-0.99543	6.02449	-6.41213
H	0.16729	4.73852	-6.80712
H	0.2181	6.49718	-4.09646
H	0.65368	5.11003	-3.08847
H	1.42184	5.31694	-4.65487
H	2.47552	-1.83911	0.5185
H	4.07758	-1.08244	0.66002
H	3.00016	-1.1476	2.04603
H	4.32782	1.41706	0.86234
H	2.88209	2.4413	1.00375
H	3.30628	1.35056	2.30749
H	4.42507	0.85802	-1.2757
H	3.45274	1.06709	-2.68732
H	4.42437	-1.56186	-1.46114
H	4.69868	-3.39455	-2.81514
H	3.39421	-3.57264	-3.99456
H	4.98079	-2.9516	-4.50324
H	3.86275	-0.76913	-5.44259
H	2.2984	-1.48332	-4.99899
H	2.72879	0.12043	-4.42275
Z-matrix:2a-4			
C	-1.0535	-0.38984	1.15226
C	-2.49239	-0.65153	0.6604
C	-2.69779	-0.05896	-0.78477
C	-1.4275	-0.22798	-1.6435
C	-0.23115	0.54378	-1.04035
C	-0.04723	0.13353	0.4128
C	-0.75947	-0.6283	2.6035
C	0.04571	-1.81786	3.0126
C	0.33551	-2.88082	2.14805

C	0.49859	-1.87769	4.33855
C	1.23466	-2.97534	4.78934
C	1.51953	-4.02626	3.92049
C	1.07011	-3.98051	2.60196
O	-1.2047	0.13482	3.45753
C	-2.76435	-2.16729	0.70709
C	-3.51924	0.03075	1.5994
C	-3.97515	-0.49036	-1.56221
C	-3.94942	-1.83524	-2.24337
C	-4.84306	-2.8399	-2.14358
C	-4.65175	-4.11272	-2.92914
C	-6.08254	-2.83265	-1.29054
C	1.03485	0.20834	-1.85048
C	2.29303	0.77627	-1.17416
C	2.40698	0.23453	0.27608
O	1.17167	0.41347	1.00799
C	-0.48577	2.08813	-1.11994
C	-1.00736	2.65913	-2.43544
O	-0.26842	2.84314	-0.16951
C	-0.77835	4.16562	-2.53046
C	-1.27087	4.70403	-3.84619
C	-0.53543	5.01878	-4.93015
C	-1.18849	5.59193	-6.16094
C	0.95359	4.842	-5.04439
C	2.80441	-1.24186	0.38604
C	3.43947	1.05686	1.06927
C	3.54736	0.65869	-2.07636
C	3.87083	-0.7017	-2.63537
C	5.012	-1.40777	-2.50628
C	5.15982	-2.75088	-3.17556
C	6.2231	-0.98237	-1.72155
H	-2.83674	1.02361	-0.64401
H	-1.17573	-1.29458	-1.71929
H	-1.6218	0.10765	-2.66911
H	0.00617	-2.87299	1.11468
H	0.27892	-1.06316	5.02689
H	1.58176	-3.00741	5.81901
H	2.09182	-4.8811	4.27196
H	1.29387	-4.80082	1.92469
H	-2.14997	-2.7148	-0.01491
H	-2.56338	-2.58583	1.69948
H	-3.81538	-2.39151	0.50734

H	-3.51949	-0.41679	2.59953
H	-3.30866	1.10103	1.70852
H	-4.54268	-0.06835	1.22409
H	-4.12499	0.2458	-2.3651
H	-4.84745	-0.37757	-0.91611
H	-3.11654	-1.9767	-2.9314
H	-3.74248	-4.09375	-3.53909
H	-4.57722	-4.96876	-2.25047
H	-5.50005	-4.27397	-3.60239
H	-6.04545	-3.65594	-0.5692
H	-6.22035	-1.91076	-0.72298
H	-6.97025	-2.96491	-1.91818
H	0.96071	0.60483	-2.86963
H	1.1247	-0.87998	-1.95633
H	2.12796	1.85996	-1.08271
H	-0.4982	2.16692	-3.26907
H	-2.07807	2.43884	-2.50472
H	-1.32172	4.68026	-1.72774
H	0.27819	4.40235	-2.366
H	-2.34819	4.86781	-3.88362
H	-2.26994	5.71466	-6.0392
H	-0.76636	6.576	-6.38974
H	-1.02342	4.9333	-7.0199
H	1.39212	4.30575	-4.19954
H	1.19558	4.26686	-5.9447
H	1.44405	5.81804	-5.11709
H	2.11698	-1.89251	-0.16218
H	3.81946	-1.42571	0.03026
H	2.77643	-1.56619	1.43191
H	4.45622	0.93165	0.68604
H	3.18735	2.12342	1.04783
H	3.43867	0.76559	2.12675
H	4.40331	1.10434	-1.56505
H	3.38084	1.30792	-2.948
H	3.08457	-1.12937	-3.25719
H	4.2663	-3.03585	-3.74093
H	6.00352	-2.73575	-3.87331
H	5.34036	-3.52919	-2.42673
H	6.09445	-0.03554	-1.19451
H	6.46565	-1.73899	-0.96757
H	7.08399	-0.87423	-2.38954
Z-matrix:2a-5			

C	-1.26561	-0.3396	1.04171
C	-2.63394	-0.80663	0.50295
C	-2.74479	-0.52164	-1.04293
C	-1.39815	-0.76567	-1.75335
C	-0.29877	0.18493	-1.22589
C	-0.23106	0.10485	0.29
C	-1.08583	-0.27269	2.52967
C	-0.21026	-1.27178	3.21313
C	0.22724	-2.45205	2.59884
C	0.15542	-1.02201	4.54361
C	0.95232	-1.93007	5.24366
C	1.38523	-3.09947	4.62231
C	1.02239	-3.36174	3.30242
O	-1.67458	0.57915	3.19057
C	-2.80772	-2.30177	0.83163
C	-3.78419	-0.04201	1.20546
C	-3.92387	-1.18438	-1.81273
C	-3.77626	-2.63605	-2.19286
C	-4.62999	-3.65233	-1.95517
C	-4.31535	-5.04459	-2.44119
C	-5.93862	-3.54697	-1.21975
C	1.05169	-0.24853	-1.81671
C	2.20902	0.56819	-1.22035
C	2.20718	0.42866	0.32732
O	0.89866	0.61334	0.90563
C	-0.63668	1.65276	-1.6567
C	-0.85699	1.93389	-3.14248
O	-0.805	2.55542	-0.8329
C	-0.55571	3.38065	-3.53339
C	0.92137	3.64962	-3.66099
C	1.69534	4.40724	-2.85899
C	3.15913	4.60076	-3.15787
C	1.228	5.12032	-1.61836
C	2.7579	-0.91731	0.82173
C	3.05831	1.54794	0.95603
C	3.55203	0.18293	-1.8821
C	3.62365	0.59522	-3.32968
C	3.62058	-0.19018	-4.42421
C	3.73032	0.41673	-5.79943
C	3.50488	-1.68919	-4.41955
H	-2.95259	0.5555	-1.13442
H	-1.08721	-1.80832	-1.60323

H	-1.52187	-0.63931	-2.83581
H	-0.03455	-2.68334	1.57199
H	-0.18068	-0.11282	5.03956
H	1.23056	-1.72295	6.27391
H	2.00413	-3.80708	5.16845
H	1.35959	-4.2754	2.81935
H	-2.09825	-2.92673	0.27969
H	-2.66486	-2.50199	1.89953
H	-3.82035	-2.6462	0.60642
H	-3.8489	-0.28871	2.27102
H	-3.65311	1.04271	1.11687
H	-4.76039	-0.29307	0.77896
H	-4.03253	-0.63921	-2.76147
H	-4.85617	-0.99638	-1.27763
H	-2.87966	-2.86258	-2.76893
H	-3.35889	-5.09491	-2.97207
H	-4.26151	-5.73764	-1.59513
H	-5.09478	-5.39188	-3.12735
H	-6.16056	-2.54141	-0.85845
H	-6.76258	-3.84777	-1.87547
H	-5.933	-4.21052	-0.34838
H	1.03969	-0.14962	-2.90598
H	1.22198	-1.31647	-1.62389
H	2.01632	1.62368	-1.4549
H	-0.26271	1.25534	-3.75856
H	-1.91312	1.72247	-3.34731
H	-0.99952	3.56967	-4.51948
H	-1.0504	4.0804	-2.8546
H	1.38505	3.17996	-4.52879
H	3.46445	4.10167	-4.08333
H	3.38626	5.66614	-3.26883
H	3.76844	4.19726	-2.34249
H	0.16132	5.00716	-1.42013
H	1.76608	4.7396	-0.7438
H	1.42792	6.1936	-1.70528
H	2.17918	-1.75771	0.42723
H	3.8066	-1.06274	0.5448
H	2.69837	-0.97894	1.91397
H	4.11529	1.47542	0.68497
H	2.68829	2.53387	0.65144
H	2.98763	1.52137	2.05028
H	3.73943	-0.88843	-1.76735

H	4.38135	0.68666	-1.37319
H	3.70777	1.67241	-3.47094
H	3.81868	1.50788	-5.76737
H	4.6134	0.02669	-6.31607
H	2.8429	0.17334	-6.39284
H	3.30853	-2.10764	-3.43025
H	2.67881	-2.00367	-5.06652
H	4.42882	-2.13874	-4.79744
Z-matrix:2a-6			
C	-1.07957	-0.37907	1.34657
C	-2.55105	-0.69166	1.00305
C	-2.89358	-0.25757	-0.47458
C	-1.69705	-0.47414	-1.42208
C	-0.4559	0.3366	-0.98562
C	-0.14581	0.07676	0.4793
C	-0.66397	-0.46732	2.78492
C	0.17422	-1.61473	3.24569
C	0.3974	-2.76053	2.47204
C	0.73169	-1.54415	4.53071
C	1.5029	-2.59571	5.03022
C	1.71889	-3.7307	4.25193
C	1.16666	-3.81424	2.97506
O	-1.03302	0.38321	3.59101
C	-2.80624	-2.19397	1.23334
C	-3.50051	0.08847	1.94872
C	-4.21314	-0.81054	-1.08653
C	-4.14358	-2.16171	-1.75446
C	-4.14658	-2.43573	-3.07467
C	-4.11379	-3.86314	-3.55898
C	-4.17879	-1.41595	-4.17986
C	0.74274	-0.10084	-1.8477
C	2.04704	0.5418	-1.34726
C	2.2855	0.16742	0.13948
O	1.11006	0.44072	0.93874
C	-0.7739	1.85791	-1.18123
C	-0.73552	2.4217	-2.59939
O	-1.09881	2.58524	-0.23917
C	-1.29473	3.84163	-2.66665
C	-1.25884	4.37399	-4.07406
C	-0.33792	5.19898	-4.60968
C	-0.46852	5.68029	-6.0311
C	0.88002	5.71298	-3.89154

C	2.69966	-1.2876	0.38569
C	3.37519	1.07119	0.74566
C	3.22231	0.32608	-2.33274
C	3.5158	-1.08882	-2.75519
C	4.67613	-1.76724	-2.65131
C	4.7838	-3.18021	-3.16696
C	5.9481	-1.24343	-2.04231
H	-3.0655	0.82813	-0.43329
H	-1.4469	-1.54322	-1.45404
H	-1.98287	-0.19292	-2.442
H	-0.01124	-2.85375	1.47172
H	0.56615	-0.6633	5.14906
H	1.93054	-2.52653	6.02714
H	2.31745	-4.55013	4.64179
H	1.33693	-4.70006	2.36816
H	-2.23181	-2.81319	0.53663
H	-2.53775	-2.50066	2.25042
H	-3.86626	-2.44482	1.12426
H	-3.41938	-0.25576	2.98581
H	-3.28309	1.1629	1.93201
H	-4.5507	-0.03881	1.66723
H	-4.58014	-0.06674	-1.80319
H	-4.99864	-0.85328	-0.32397
H	-4.13013	-3.00678	-1.06828
H	-4.09184	-4.58315	-2.73411
H	-5.0009	-4.07814	-4.16375
H	-3.22328	-4.03483	-4.17257
H	-4.12406	-0.38461	-3.82564
H	-3.32843	-1.56685	-4.85366
H	-5.1011	-1.52007	-4.76067
H	0.5805	0.15353	-2.90183
H	0.83233	-1.19438	-1.8201
H	1.87843	1.62861	-1.35791
H	0.30369	2.42675	-2.94323
H	-1.31914	1.76922	-3.25624
H	-2.33718	3.84873	-2.32317
H	-0.75725	4.50143	-1.9772
H	-2.0973	4.05708	-4.69433
H	-1.37143	5.29763	-6.51843
H	-0.51515	6.77395	-6.05746
H	0.39288	5.35382	-6.62287
H	1.02939	5.25636	-2.91029

H	1.77973	5.5015	-4.47949
H	0.80604	6.79638	-3.75242
H	1.97475	-1.99548	-0.02588
H	3.68341	-1.51414	-0.02931
H	2.75951	-1.48868	1.46083
H	4.35768	0.8976	0.29728
H	3.1173	2.12945	0.62247
H	3.4623	0.90361	1.82618
H	4.11162	0.83118	-1.94962
H	2.97415	0.869	-3.25608
H	2.68263	-1.59304	-3.24484
H	3.84625	-3.53634	-3.6067
H	5.55797	-3.24406	-3.9386
H	5.04711	-3.86159	-2.35128
H	5.85609	-0.23716	-1.63041
H	6.26892	-1.89756	-1.22446
H	6.74252	-1.21974	-2.79571
Z-matrix:2a-7			
C	-0.99231	-0.53709	1.41663
C	-2.43714	-0.93034	1.0497
C	-2.7713	-0.53012	-0.43834
C	-1.545	-0.75306	-1.34944
C	-0.35477	0.13547	-0.92449
C	-0.06463	-0.05814	0.55507
C	-0.60423	-0.5776	2.86426
C	0.27456	-1.67711	3.36497
C	0.58053	-2.81761	2.61196
C	0.78654	-1.56565	4.66591
C	1.59536	-2.57069	5.20057
C	1.89579	-3.69946	4.44162
C	1.38884	-3.82406	3.14942
O	-1.03057	0.2697	3.64496
C	-2.61737	-2.44866	1.27077
C	-3.44735	-0.19938	1.96901
C	-4.01685	-1.23369	-1.03446
C	-4.50694	-0.55727	-2.29069
C	-4.48216	-1.02278	-3.55489
C	-5.04923	-0.19961	-4.68308
C	-3.91177	-2.34568	-3.98546
C	0.8826	-0.26563	-1.7475
C	2.13716	0.46717	-1.24413
C	2.36561	0.1554	0.25886

O	1.16102	0.3804	1.02863
C	-0.74222	1.62953	-1.19164
C	-0.76892	2.1112	-2.63965
O	-1.04602	2.40314	-0.28045
C	-1.52662	3.42802	-2.79086
C	-1.62739	3.82955	-4.23798
C	-0.84924	4.70996	-4.89711
C	-1.10722	5.03138	-6.34596
C	0.32228	5.44007	-4.29943
C	2.8594	-1.26392	0.56013
C	3.38685	1.14127	0.85579
C	3.3435	0.28746	-2.19855
C	3.726	-1.12121	-2.56666
C	4.91898	-1.72954	-2.4117
C	5.11867	-3.14902	-2.87936
C	6.14281	-1.11645	-1.78733
H	-2.99599	0.54622	-0.44037
H	-1.25895	-1.81339	-1.31814
H	-1.8022	-0.5494	-2.39328
H	0.20904	-2.94208	1.60084
H	0.55611	-0.68904	5.26926
H	1.98716	-2.46988	6.20953
H	2.52514	-4.48193	4.85811
H	1.62523	-4.70473	2.55751
H	-1.98345	-3.03388	0.59649
H	-2.37321	-2.73976	2.29841
H	-3.65419	-2.76313	1.10975
H	-3.36507	-0.52908	3.01066
H	-3.29241	0.88563	1.94452
H	-4.48308	-0.39001	1.67095
H	-4.84885	-1.20471	-0.3225
H	-3.80658	-2.29291	-1.20698
H	-4.94814	0.42479	-2.11208
H	-5.45414	0.75755	-4.33793
H	-4.27105	0.01711	-5.42229
H	-5.8596	-0.74417	-5.17857
H	-3.42508	-2.89516	-3.17719
H	-4.70415	-2.98222	-4.39244
H	-3.15767	-2.19259	-4.76502
H	0.73026	-0.05368	-2.8124
H	1.0306	-1.35096	-1.68062
H	1.90678	1.54157	-1.29609

H	0.26504	2.23992	-2.97713
H	-1.24486	1.3494	-3.26386
H	-2.54423	3.32222	-2.39318
H	-1.05877	4.21385	-2.18826
H	-2.44379	3.35014	-4.77837
H	-1.97116	4.4893	-6.74467
H	-1.30203	6.10199	-6.46719
H	-0.23726	4.7642	-6.95478
H	0.56878	5.10888	-3.2879
H	1.21618	5.28103	-4.91221
H	0.11688	6.51474	-4.26203
H	2.19071	-2.02608	0.15026
H	3.86648	-1.44183	0.17893
H	2.8998	-1.43056	1.64203
H	4.38695	1.01326	0.43182
H	3.0689	2.17767	0.69363
H	3.46127	1.01274	1.9425
H	4.19426	0.85523	-1.81577
H	3.08492	0.78472	-3.14449
H	2.93553	-1.68605	-3.06072
H	4.21345	-3.57147	-3.32805
H	5.91341	-3.19189	-3.63127
H	5.40042	-3.78906	-2.0368
H	5.98105	-0.10867	-1.40128
H	6.48269	-1.73119	-0.94694
H	6.95202	-1.06228	-2.52305
Z-matrix:2a-8			
C	-0.82138	-1.30609	0.89097
C	-2.19618	-1.92626	0.60892
C	-2.93209	-1.09232	-0.50965
C	-1.98799	-0.76996	-1.68933
C	-0.72431	0.01178	-1.26344
C	-0.16108	-0.4763	0.0575
C	-0.11668	-1.68149	2.15722
C	0.06356	-0.66183	3.23565
C	-0.56754	0.58846	3.21675
C	0.88649	-0.99289	4.32207
C	1.08238	-0.08642	5.36632
C	0.45481	1.15716	5.33506
C	-0.36866	1.49443	4.26231
O	0.29018	-2.83074	2.31226
C	-2.00251	-3.40058	0.20252

C	-3.0575	-1.89581	1.89632
C	-4.29617	-1.64138	-1.01921
C	-4.25585	-2.66546	-2.12589
C	-4.54861	-2.49011	-3.43048
C	-4.48676	-3.65162	-4.38986
C	-4.94768	-1.18942	-4.0713
C	0.36252	-0.19762	-2.34152
C	1.722	0.39306	-1.91667
C	2.14773	-0.17491	-0.53338
O	1.07469	0.04138	0.41455
C	-1.15064	1.50053	-1.06248
C	-1.20612	2.42772	-2.27223
O	-1.57501	1.90505	0.02763
C	-1.0507	3.90017	-1.89009
C	0.31984	4.19821	-1.34065
C	1.41163	4.59027	-2.02538
C	2.71199	4.8505	-1.3107
C	1.46948	4.78806	-3.51438
C	2.53054	-1.66297	-0.5034
C	3.32844	0.62974	0.03715
C	2.768	0.33976	-3.05476
C	3.0632	-1.01164	-3.64589
C	4.24883	-1.64804	-3.7254
C	4.34448	-3.00322	-4.38011
C	5.55994	-1.13325	-3.1979
H	-3.19062	-0.13055	-0.04143
H	-1.69459	-1.70718	-2.17842
H	-2.53424	-0.19097	-2.44478
H	-1.21475	0.88447	2.39605
H	1.38154	-1.96147	4.35674
H	1.72474	-0.35286	6.2016
H	0.60774	1.86442	6.14612
H	-0.85739	2.46523	4.23369
H	-1.4398	-3.96383	0.95422
H	-2.9616	-3.91798	0.10849
H	-1.46171	-3.49762	-0.74439
H	-2.58581	-2.44645	2.71819
H	-3.22782	-0.86867	2.23822
H	-4.03627	-2.36081	1.74521
H	-4.89502	-0.78105	-1.33969
H	-4.87221	-2.06864	-0.19231
H	-3.99061	-3.67089	-1.80397

H	-4.19593	-4.58516	-3.89688
H	-5.46561	-3.81191	-4.8536
H	-3.75517	-3.45183	-5.17969
H	-5.96674	-1.26153	-4.46517
H	-4.91447	-0.33708	-3.38983
H	-4.27272	-0.95911	-4.90272
H	0.0501	0.21535	-3.3069
H	0.4823	-1.27414	-2.52129
H	1.54297	1.46499	-1.7562
H	-0.4287	2.18107	-2.99571
H	-2.17531	2.27103	-2.75811
H	-1.25919	4.52645	-2.7645
H	-1.79721	4.18748	-1.13956
H	0.39893	4.06905	-0.25926
H	2.62975	4.69912	-0.22915
H	3.48946	4.17456	-1.68203
H	3.0367	5.88256	-1.47866
H	0.53991	4.51919	-4.02187
H	1.68681	5.83547	-3.74729
H	2.26187	4.16627	-3.9448
H	1.76534	-2.29748	-0.96042
H	3.48155	-1.85437	-1.00473
H	2.63324	-2.01	0.53204
H	4.2449	0.49173	-0.54346
H	3.09316	1.69987	0.06901
H	3.53557	0.33294	1.07244
H	3.67722	0.85104	-2.73035
H	2.38575	0.95698	-3.88026
H	2.19922	-1.50392	-4.09251
H	3.37732	-3.35501	-4.75433
H	5.03518	-2.9661	-5.22887
H	4.71191	-3.7448	-3.66312
H	5.48559	-0.16051	-2.70925
H	5.969	-1.83447	-2.46267
H	6.28045	-1.03378	-4.01656
Z-matrix:2a-9			
C	-0.92495	0.06584	0.35666
C	-2.40398	-0.24971	0.04823
C	-2.65239	-0.27764	-1.50703
C	-1.43502	-0.85692	-2.25788
C	-0.17005	0.01617	-2.03985
C	0.07098	0.16937	-0.55378

C	-0.56226	0.41602	1.7673
C	0.10862	-0.59343	2.63966
C	0.2842	-1.93216	2.26879
C	0.56106	-0.17323	3.89903
C	1.18158	-1.07304	4.76819
C	1.35189	-2.4024	4.38835
C	0.90337	-2.83236	3.14107
O	-0.83073	1.53367	2.20221
C	-2.77746	-1.58701	0.71558
C	-3.32674	0.83776	0.65359
C	-3.98628	-0.90124	-2.0105
C	-4.06143	-2.40561	-2.08499
C	-5.0026	-3.22309	-1.57142
C	-4.91287	-4.714	-1.77692
C	-6.20466	-2.78927	-0.77772
C	1.01467	-0.68187	-2.73544
C	2.35706	-0.05803	-2.32622
C	2.50176	-0.07494	-0.78115
O	1.34619	0.53113	-0.14992
C	-0.41007	1.37756	-2.76844
C	0.10148	2.68408	-2.18318
O	-0.95853	1.39535	-3.87924
C	-0.9973	3.74253	-2.20433
C	-0.50586	5.05512	-1.65821
C	-0.5579	5.46978	-0.37735
C	-0.04278	6.82831	0.01688
C	-1.0937	4.65306	0.76752
C	2.71158	-1.45926	-0.15722
C	3.67858	0.81849	-0.3486
C	3.53867	-0.61505	-3.15916
C	3.73078	-2.10762	-3.17181
C	4.82325	-2.81186	-2.81405
C	4.83377	-4.31532	-2.92861
C	6.10531	-2.23325	-2.2809
H	-2.7336	0.77595	-1.81418
H	-1.24164	-1.8815	-1.91227
H	-1.66204	-0.93192	-3.32952
H	-0.04494	-2.29851	1.30216
H	0.43204	0.86254	4.20866
H	1.52921	-0.73398	5.74084
H	1.8342	-3.10327	5.06523
H	1.03794	-3.86984	2.84486

H	-2.23705	-2.42923	0.27158
H	-2.5612	-1.57983	1.78943
H	-3.84978	-1.78593	0.6415
H	-3.27946	0.85213	1.74818
H	-3.05609	1.83586	0.29208
H	-4.37692	0.66762	0.39528
H	-4.13941	-0.54436	-3.03902
H	-4.81721	-0.47945	-1.44193
H	-3.26717	-2.86541	-2.6726
H	-4.02955	-5.00303	-2.35608
H	-4.85741	-5.22617	-0.81072
H	-5.7955	-5.07649	-2.31388
H	-6.18786	-3.25598	0.21292
H	-6.26557	-1.71021	-0.62623
H	-7.12259	-3.09913	-1.28828
H	0.90227	-0.61941	-3.82617
H	1.00943	-1.75056	-2.48851
H	2.29931	1.00053	-2.61566
H	0.45709	2.56278	-1.16082
H	0.96182	3.00009	-2.7847
H	-1.34586	3.91058	-3.23115
H	-1.87831	3.3897	-1.65611
H	-0.07596	5.72104	-2.40611
H	0.33767	7.39312	-0.84069
H	-0.84344	7.41834	0.47475
H	0.77417	6.72967	0.73917
H	-1.39044	3.64513	0.47184
H	-0.3301	4.54935	1.54567
H	-1.96885	5.14464	1.20444
H	1.9087	-2.15422	-0.41948
H	3.66614	-1.90367	-0.44297
H	2.71696	-1.38531	0.93544
H	4.64445	0.42197	-0.67411
H	3.5646	1.83304	-0.74769
H	3.70652	0.92264	0.74289
H	4.45407	-0.0886	-2.87987
H	3.36472	-0.32496	-4.20527
H	2.88095	-2.6645	-3.56689
H	3.8903	-4.71059	-3.31958
H	5.63415	-4.63869	-3.60218
H	5.00082	-4.76807	-1.94567
H	6.08356	-1.14837	-2.16585

H	6.32621	-2.65722	-1.29548
H	6.93458	-2.47572	-2.95368
Z-matrix:2b-1			
C	7.69772	0.29011	1.44591
C	6.41968	-0.10666	3.58713
C	6.42292	-0.19668	2.08637
C	5.41236	-0.66114	1.32515
C	3.54207	1.88026	0.66718
C	2.58484	1.23638	2.88724
C	-0.25288	4.613	-0.48271
C	0.44109	3.3955	-0.47396
C	0.89816	2.85985	-1.6859
C	0.65162	3.52787	-2.88814
C	-0.04787	4.73366	-2.88724
C	-0.49862	5.27771	-1.68572
C	0.67772	2.73066	0.84406
C	1.10489	1.29415	0.86724
C	2.51847	0.95739	1.36856
C	2.85136	-0.55266	1.04856
C	1.6209	-1.44865	1.34469
C	0.39444	-1.09429	0.45652
C	0.16271	0.39609	0.50927
O	0.5239	3.34846	1.89352
C	4.07533	-1.18541	1.76803
C	0.70076	-1.56218	-1.00309
C	-0.18142	-1.1069	-2.15667
O	1.60834	-2.3725	-1.23026
C	0.63701	-0.94386	-3.43725
C	-0.19685	-0.34993	-4.54036
C	-0.601	-0.93865	-5.68268
C	-1.41404	-0.17081	-6.6931
C	-0.31564	-2.36177	-6.07713
C	-0.81345	-1.88918	1.00015
C	-2.19408	-1.30709	0.62079
C	-2.21137	0.22995	0.86326
O	-1.10074	0.83021	0.15529
C	-3.28123	-2.13276	1.35342
C	-4.66864	-1.97473	0.7974
C	-5.79827	-1.64396	1.45393
C	-7.10857	-1.54343	0.71468
C	-5.90337	-1.3429	2.92372
C	-3.43767	0.90378	0.2256

C	-2.16247	0.64071	2.34565
H	8.54842	-0.30449	1.79453
H	7.66863	0.21994	0.35346
H	7.87481	1.33889	1.70591
H	7.27627	-0.6521	3.99755
H	6.49602	0.93998	3.89987
H	5.52397	-0.52464	4.04981
H	5.55928	-0.69282	0.24454
H	3.60607	1.66501	-0.40517
H	3.28556	2.93999	0.77728
H	4.54338	1.77962	1.09104
H	2.39146	2.28908	3.11862
H	1.85462	0.64007	3.44431
H	3.57665	1.02366	3.29641
H	-0.60824	5.04608	0.45045
H	1.45447	1.9288	-1.71763
H	1.00932	3.10918	-3.8259
H	-0.23824	5.25304	-3.82328
H	-1.04028	6.22024	-1.68266
H	3.05659	-0.61907	-0.0293
H	1.3621	-1.35281	2.40792
H	1.88235	-2.50599	1.20355
H	4.09295	-2.25871	1.53284
H	3.93751	-1.13489	2.85042
H	-0.96621	-1.8584	-2.29603
H	-0.66328	-0.15641	-1.93181
H	1.48257	-0.26938	-3.25047
H	1.08317	-1.89951	-3.72659
H	-0.47988	0.68961	-4.37034
H	-1.60146	0.86147	-6.37905
H	-0.88898	-0.13558	-7.65329
H	-2.38521	-0.6533	-6.84418
H	0.16532	-2.94534	-5.2896
H	-1.24972	-2.87636	-6.32719
H	0.33528	-2.38411	-6.95733
H	-0.75872	-1.94329	2.09606
H	-0.75585	-2.92918	0.65016
H	-2.31931	-1.47576	-0.45622
H	-3.2345	-1.93557	2.42687
H	-3.03758	-3.19868	1.24456
H	-4.74239	-2.18173	-0.27118
H	-7.00339	-1.76552	-0.35249

H	-7.83396	-2.24998	1.13115
H	-7.51655	-0.53121	0.80413
H	-4.95844	-1.43925	3.46095
H	-6.26025	-0.31806	3.07122
H	-6.61607	-2.02694	3.39663
H	-3.56962	0.57733	-0.81224
H	-4.35991	0.71211	0.77739
H	-3.30261	1.99208	0.18631
H	-3.06846	0.34171	2.88119
H	-1.30348	0.20612	2.86637
H	-2.05837	1.7281	2.44027
Z-matrix:2b-2			
C	5.89688	-3.42902	1.83102
C	4.95922	-1.79607	3.51514
C	5.297	-2.06773	2.07547
C	5.09173	-1.21864	1.04943
C	2.95975	2.69079	1.29485
C	3.51624	2.28892	-1.10533
C	-0.66809	5.12769	-0.85333
C	-0.10683	4.05373	-0.14729
C	-0.25778	4.00486	1.24398
C	-0.959	5.01132	1.9149
C	-1.51374	6.07261	1.20223
C	-1.36925	6.13155	-0.18193
C	0.64341	3.02405	-0.92584
C	1.17972	1.80894	-0.23591
C	2.68375	1.7632	0.09123
C	3.14787	0.28498	0.38829
C	2.07367	-0.47281	1.19778
C	0.73494	-0.56861	0.43009
C	0.31089	0.7842	-0.08496
O	0.84044	3.17139	-2.12996
C	4.52568	0.17744	1.09255
C	0.92855	-1.61391	-0.71268
C	0.83797	-1.1618	-2.16499
O	1.15332	-2.79782	-0.43446
C	1.22613	-2.27795	-3.13304
C	1.15303	-1.81011	-4.56127
C	0.20818	-2.10636	-5.47502
C	0.3092	-1.57707	-6.88194
C	-1.01107	-2.94816	-5.21651
C	-0.33909	-1.1098	1.3906

C	-1.73725	-1.10846	0.73991
C	-2.0781	0.32558	0.23501
O	-0.99043	0.90067	-0.53198
C	-2.73186	-1.75372	1.73767
C	-4.06277	-2.12527	1.14759
C	-5.29354	-1.79684	1.58788
C	-6.51897	-2.27411	0.85029
C	-5.59835	-0.96158	2.80041
C	-3.24216	0.30938	-0.77173
C	-2.44118	1.30413	1.36099
H	5.19809	-4.21269	2.1417
H	6.13507	-3.5962	0.77528
H	6.82412	-3.54195	2.40235
H	4.31352	-2.5903	3.90521
H	5.87342	-1.76899	4.11702
H	4.42996	-0.85377	3.66963
H	5.3726	-1.54808	0.04807
H	2.63972	3.71889	1.09296
H	2.44146	2.34945	2.19712
H	4.02856	2.752	1.52618
H	3.29942	1.72321	-2.01891
H	3.31529	3.34699	-1.30845
H	4.59226	2.21463	-0.9206
H	-0.56151	5.18623	-1.93539
H	0.15419	3.18962	1.82898
H	-1.07425	4.96572	2.99508
H	-2.05934	6.85435	1.72502
H	-1.80036	6.95784	-0.74165
H	3.24991	-0.22581	-0.58025
H	1.92543	0.0322	2.16186
H	2.4229	-1.48375	1.4397
H	4.45254	0.54513	2.11963
H	5.25828	0.82176	0.59487
H	-0.19247	-0.84883	-2.36376
H	1.50805	-0.30918	-2.31374
H	2.25557	-2.60182	-2.93237
H	0.60468	-3.16344	-2.96554
H	1.98367	-1.17118	-4.86294
H	1.21153	-0.97616	-7.03706
H	0.33585	-2.40635	-7.59651
H	-0.55471	-0.9453	-7.11291
H	-1.15507	-3.19061	-4.1611

H	-1.91136	-2.41622	-5.54312
H	-0.94479	-3.88779	-5.77453
H	-0.36176	-0.51176	2.3115
H	-0.08383	-2.13105	1.70396
H	-1.67916	-1.76681	-0.13859
H	-2.82746	-1.12209	2.62398
H	-2.29442	-2.69417	2.10024
H	-3.98941	-2.75794	0.26151
H	-6.26826	-2.87612	-0.0294
H	-7.14149	-2.88984	1.50771
H	-7.11161	-1.41902	0.50896
H	-4.71245	-0.67224	3.36825
H	-6.11382	-0.04268	2.50199
H	-6.25062	-1.5157	3.48385
H	-3.06278	-0.42575	-1.56459
H	-4.20569	0.09656	-0.30546
H	-3.33206	1.28095	-1.27386
H	-3.34782	1.00289	1.89296
H	-1.63208	1.39925	2.09094
H	-2.61861	2.30646	0.95605
Z-matrix:2b-3			
C	5.16908	-3.6984	2.32844
C	4.42354	-1.83702	3.86511
C	4.74843	-2.25662	2.45852
C	4.67422	-1.46723	1.36895
C	3.08329	2.69237	1.25907
C	3.63064	2.04556	-1.0898
C	-0.19627	5.41645	-1.10133
C	0.22677	4.32949	-0.32243
C	0.03935	4.37568	1.06438
C	-0.56264	5.48852	1.6594
C	-0.9817	6.56134	0.87469
C	-0.79941	6.52609	-0.50568
C	0.87676	3.18225	-1.02264
C	1.23414	1.94464	-0.25984
C	2.71101	1.72381	0.11486
C	2.96804	0.22316	0.52754
C	1.7753	-0.33433	1.33457
C	0.47004	-0.32216	0.50342
C	0.23509	1.05067	-0.08447
O	1.13257	3.24751	-2.22294
C	4.29491	-0.01054	1.29572

C	0.60493	-1.43012	-0.58921
C	0.45353	-1.05404	-2.05752
O	0.82858	-2.60076	-0.25931
C	0.65197	-2.25668	-2.9775
C	0.49853	-1.86471	-4.42194
C	-0.57322	-2.0608	-5.21429
C	-0.5494	-1.63042	-6.65763
C	-1.86799	-2.68667	-4.77476
C	-0.69867	-0.71678	1.42582
C	-2.05429	-0.54443	0.71711
C	-2.19097	0.91138	0.19194
O	-1.03198	1.32278	-0.56679
C	-3.21854	-0.99138	1.62901
C	-3.21132	-2.47224	1.90309
C	-3.84061	-3.43042	1.19521
C	-3.74915	-4.87648	1.60721
C	-4.65282	-3.18975	-0.04754
C	-3.34939	1.00533	-0.81916
C	-2.44425	1.94456	1.29982
H	4.36714	-4.35968	2.67277
H	5.4046	-3.97268	1.29473
H	6.0616	-3.88793	2.93376
H	3.69057	-2.52409	4.30187
H	5.32758	-1.86059	4.48229
H	3.99631	-0.83461	3.93422
H	4.92634	-1.90457	0.4018
H	2.90236	3.73602	0.97918
H	2.50911	2.48472	2.1682
H	4.14678	2.63274	1.51415
H	3.35313	1.45378	-1.96993
H	3.58412	3.10463	-1.36762
H	4.68172	1.83451	-0.8701
H	-0.05819	5.40184	-2.18132
H	0.34645	3.55512	1.70394
H	-0.7066	5.51724	2.73676
H	-1.45068	7.4256	1.33852
H	-1.12452	7.36091	-1.12145
H	3.03687	-0.36129	-0.40184
H	1.64931	0.2575	2.25132
H	1.98453	-1.35844	1.66576
H	4.23547	0.43522	2.2923
H	5.12162	0.49771	0.78774

H	-0.55181	-0.64825	-2.20969
H	1.19487	-0.2856	-2.30074
H	1.6596	-2.6695	-2.83969
H	-0.03341	-3.06623	-2.70527
H	1.37722	-1.37871	-4.84675
H	0.40963	-1.18551	-6.9433
H	-0.72397	-2.49098	-7.3117
H	-1.33008	-0.88593	-6.84493
H	-1.92036	-2.86447	-3.69809
H	-2.70763	-2.03011	-5.02752
H	-2.01462	-3.64488	-5.28349
H	-0.68243	-0.10958	2.34047
H	-0.5768	-1.75642	1.75447
H	-2.04596	-1.20833	-0.15916
H	-4.18503	-0.70611	1.20379
H	-3.16253	-0.47461	2.59545
H	-2.63277	-2.76914	2.77799
H	-3.14884	-5.01386	2.51278
H	-4.74847	-5.27677	1.80717
H	-3.28886	-5.46958	0.81019
H	-5.69935	-3.45861	0.12901
H	-4.62671	-2.15134	-0.38682
H	-4.2722	-3.80451	-0.87031
H	-3.20973	0.28899	-1.6372
H	-4.32524	0.82289	-0.36092
H	-3.37708	1.9979	-1.28515
H	-3.37859	1.75289	1.83634
H	-1.62881	1.96482	2.02886
H	-2.51046	2.95268	0.87612
Z-matrix:2b-4			
C	5.2784	-3.66294	-0.32362
C	4.71421	-2.47004	1.8321
C	4.87351	-2.3715	0.34041
C	4.67563	-1.25979	-0.39441
C	3.09265	2.66687	1.00626
C	3.19889	2.71801	-1.48975
C	-0.83754	5.58266	0.31425
C	-0.13923	4.40354	0.61084
C	-0.04743	3.98514	1.94431
C	-0.65091	4.73101	2.96128
C	-1.3487	5.89774	2.65385
C	-1.44274	6.32424	1.33088

C	0.50688	3.67115	-0.51895
C	0.99308	2.26736	-0.31227
C	2.51566	2.03386	-0.27945
C	2.84485	0.49487	-0.3535
C	1.81286	-0.31684	0.45993
C	0.39441	-0.17144	-0.13516
C	0.0474	1.30046	-0.2552
O	0.66457	4.23018	-1.60145
C	4.28519	0.11854	0.07705
C	0.32511	-0.85206	-1.54637
C	0.92382	-2.24889	-1.69305
O	-0.21831	-0.31136	-2.51242
C	0.60128	-2.88038	-3.04483
C	1.15653	-4.27699	-3.13073
C	2.33155	-4.65382	-3.67162
C	2.73154	-6.10527	-3.70972
C	3.34428	-3.7145	-4.26707
C	-0.60675	-0.86237	0.80293
C	-2.06153	-0.61667	0.3602
C	-2.33263	0.91532	0.2866
O	-1.28444	1.63336	-0.40494
C	-2.99348	-1.44902	1.27744
C	-4.40736	-1.57474	0.78586
C	-5.55037	-1.33063	1.45685
C	-6.88473	-1.50944	0.7776
C	-5.64929	-0.87201	2.88525
C	-3.58405	1.22616	-0.55402
C	-2.51472	1.56984	1.66376
H	4.51795	-4.43185	-0.15203
H	5.40169	-3.5539	-1.40616
H	6.23099	-4.01621	0.08447
H	4.00711	-3.26856	2.08149
H	5.67676	-2.70394	2.29848
H	4.3351	-1.55486	2.29141
H	4.82109	-1.32606	-1.47397
H	2.84914	3.73302	1.07629
H	2.70841	2.17695	1.90697
H	4.18589	2.60525	1.0348
H	2.73969	2.40353	-2.43428
H	3.13731	3.81025	-1.43054
H	4.2651	2.47788	-1.54766
H	-0.91442	5.92599	-0.71615

H	0.48326	3.07922	2.21559
H	-0.57829	4.39981	3.99419
H	-1.81901	6.47619	3.44515
H	-1.98456	7.23455	1.08693
H	2.74569	0.19825	-1.40803
H	1.82398	0.02654	1.50373
H	2.09128	-1.37443	0.50469
H	4.39527	0.21844	1.16069
H	5.01054	0.81147	-0.36285
H	2.00984	-2.17234	-1.58802
H	0.53836	-2.88669	-0.8922
H	-0.4858	-2.93238	-3.18603
H	0.97258	-2.25351	-3.863
H	0.50393	-5.04476	-2.71528
H	1.96777	-6.75851	-3.27474
H	2.89345	-6.42635	-4.7439
H	3.65874	-6.25804	-3.14767
H	3.09827	-2.66072	-4.11556
H	4.32547	-3.88046	-3.80961
H	3.43245	-3.88976	-5.34411
H	-0.47117	-0.50421	1.8323
H	-0.41272	-1.94096	0.83828
H	-2.15973	-1.02438	-0.65552
H	-2.93623	-1.0727	2.30152
H	-2.6027	-2.47487	1.32445
H	-4.48649	-1.92035	-0.24626
H	-6.78276	-1.83665	-0.26249
H	-7.48127	-2.26078	1.30528
H	-7.4372	-0.56405	0.77485
H	-4.6852	-0.80564	3.39244
H	-6.11495	0.11812	2.92946
H	-6.26738	-1.56904	3.46121
H	-3.534	0.72551	-1.52771
H	-4.51288	0.93849	-0.05816
H	-3.64918	2.30038	-0.76844
H	-3.38439	1.17687	2.19764
H	-1.63225	1.43151	2.29537
H	-2.65964	2.65076	1.5592
Z-matrix:2b-5			
C	5.84833	-3.0336	-0.95323
C	5.81667	-0.70097	-1.93316
C	5.46628	-1.58844	-0.76989

C	4.84968	-1.17419	0.35417
C	3.03333	2.70116	1.56125
C	3.45778	2.87041	-0.89464
C	-0.83745	5.57181	0.49541
C	-0.16108	4.38914	0.82729
C	-0.23291	3.91131	2.14166
C	-0.97496	4.60209	3.10448
C	-1.64874	5.7731	2.76154
C	-1.58084	6.25856	1.45752
C	0.63842	3.71816	-0.24093
C	1.13244	2.31738	-0.03081
C	2.6443	2.11514	0.18565
C	3.02397	0.58845	0.08934
C	1.91988	-0.28729	0.71893
C	0.58476	-0.13876	-0.0457
C	0.21368	1.3291	-0.13618
O	0.91406	4.32526	-1.27267
C	4.4111	0.23112	0.68076
C	0.71536	-0.7395	-1.4867
C	1.36903	-2.10962	-1.63241
O	0.30159	-0.15056	-2.48829
C	0.94111	-2.80646	-2.92071
C	1.53487	-4.18622	-3.00864
C	0.93462	-5.3543	-2.70757
C	1.66209	-6.66093	-2.88855
C	-0.46396	-5.49191	-2.1716
C	-0.50851	-0.9049	0.71459
C	-1.90168	-0.66311	0.10369
C	-2.20264	0.86461	0.08351
O	-1.09796	1.64029	-0.43657
C	-2.9167	-1.56823	0.8471
C	-4.25744	-1.68896	0.18091
C	-5.47822	-1.51183	0.72376
C	-6.71752	-1.67227	-0.12015
C	-5.75792	-1.14984	2.15602
C	-3.35251	1.20017	-0.88304
C	-2.56419	1.43424	1.46298
H	6.92927	-3.12427	-1.10167
H	5.57839	-3.64759	-0.08758
H	5.33929	-3.45131	-1.82821
H	6.90031	-0.69611	-2.08966
H	5.33669	-1.07083	-2.8454

H	5.49808	0.33534	-1.79745
H	4.63971	-1.90778	1.13241
H	2.75051	3.75645	1.64595
H	2.55237	2.1598	2.38266
H	4.11549	2.6659	1.727
H	3.13779	2.58526	-1.90363
H	3.3533	3.95689	-0.80041
H	4.52963	2.66277	-0.81897
H	-0.78818	5.96133	-0.52008
H	0.27569	3.00083	2.43903
H	-1.02866	4.22493	4.12259
H	-2.22645	6.30885	3.51062
H	-2.1032	7.17253	1.18631
H	3.06924	0.33999	-0.9805
H	1.78839	-0.00281	1.77204
H	2.22229	-1.33953	0.73938
H	4.38836	0.32154	1.77411
H	5.1797	0.93319	0.34283
H	2.45487	-1.97301	-1.62136
H	1.09226	-2.73569	-0.77943
H	-0.15125	-2.833	-2.99778
H	1.281	-2.23133	-3.79136
H	2.56031	-4.20678	-3.37847
H	2.67332	-6.52237	-3.28537
H	1.75002	-7.18238	-1.92979
H	1.11652	-7.3042	-3.5867
H	-0.92952	-4.53446	-1.92561
H	-1.10006	-5.99872	-2.9044
H	-0.45683	-6.08622	-1.25145
H	-0.51429	-0.60742	1.77176
H	-0.29302	-1.98	0.71237
H	-1.85975	-1.01132	-0.93779
H	-2.99289	-1.25613	1.89135
H	-2.50815	-2.58775	0.87938
H	-4.20359	-1.96774	-0.87278
H	-7.35174	-2.46764	0.28485
H	-7.29125	-0.73966	-0.13042
H	-6.48453	-1.92952	-1.15882
H	-4.86268	-1.09569	2.77786
H	-6.25433	-0.17505	2.20604
H	-6.41873	-1.89638	2.60952
H	-3.17455	0.75741	-1.86971

H	-4.32614	0.86749	-0.5187
H	-3.41872	2.28362	-1.04431
H	-3.47786	0.99029	1.86778
H	-1.75782	1.28162	2.18634
H	-2.72869	2.51564	1.40078
Z-matrix:2b-6			
C	7.63656	0.99166	-0.04149
C	6.79586	0.00844	2.12665
C	6.51848	0.27611	0.67307
C	5.39301	-0.06128	0.01242
C	3.40778	2.41469	0.38346
C	2.80216	1.19584	2.4828
C	-0.31224	5.23758	0.29659
C	0.22033	3.9832	-0.03451
C	0.38284	3.64793	-1.38496
C	0.00848	4.54963	-2.38499
C	-0.52405	5.79197	-2.04521
C	-0.68397	6.13731	-0.70482
C	0.61066	3.07018	1.08372
C	1.03896	1.66948	0.7778
C	2.51526	1.29449	0.96805
C	2.81828	-0.07161	0.23111
C	1.70155	-1.1068	0.51832
C	0.29596	-0.63637	0.07803
C	0.05993	0.8171	0.41338
O	0.60127	3.46372	2.24793
C	4.17638	-0.76254	0.54604
C	0.22077	-0.78787	-1.474
C	-0.18814	-2.13972	-2.04842
O	0.56248	0.12793	-2.22986
C	-0.08436	-2.17165	-3.57235
C	-0.56252	-3.48971	-4.11903
C	0.18269	-4.49653	-4.6149
C	-0.47308	-5.73798	-5.16255
C	1.68495	-4.51187	-4.68
C	-0.75557	-1.484	0.82562
C	-2.20044	-0.95147	0.67112
C	-2.24959	0.56547	1.02258
O	-1.23909	1.26489	0.26014
C	-3.14365	-1.87726	1.47759
C	-4.59924	-1.7445	1.12941
C	-5.6392	-1.5281	1.95898

C	-7.0416	-1.42916	1.41396
C	-5.55203	-1.36062	3.451
C	-3.56063	1.22188	0.5585
C	-2.06712	0.87916	2.51793
H	7.83138	1.95856	0.43416
H	8.55344	0.3942	-0.00549
H	7.40436	1.18122	-1.09473
H	7.7282	-0.55656	2.23284
H	6.90337	0.95437	2.66781
H	6.01456	-0.56877	2.62385
H	5.33181	0.18159	-1.04942
H	3.31362	2.47309	-0.7066
H	3.15656	3.40029	0.79133
H	4.46196	2.26838	0.62608
H	2.61432	2.14569	2.99498
H	2.17961	0.43686	2.96825
H	3.8496	0.95095	2.68243
H	-0.44128	5.51775	1.34019
H	0.79314	2.688	-1.6859
H	0.13189	4.27609	-3.43012
H	-0.81508	6.49021	-2.82574
H	-1.0982	7.10565	-0.43659
H	2.80881	0.12487	-0.85053
H	1.70783	-1.33971	1.59119
H	1.94156	-2.05066	0.01133
H	4.17695	-1.74979	0.06316
H	4.24521	-0.97077	1.61604
H	0.463	-2.90926	-1.62017
H	-1.22098	-2.34934	-1.75605
H	-0.70861	-1.37993	-4.00616
H	0.93848	-1.94386	-3.88849
H	-1.64737	-3.60021	-4.12198
H	-1.5657	-5.69147	-5.10489
H	-0.20181	-5.87664	-6.2143
H	-0.14813	-6.61889	-4.59938
H	2.15038	-3.667	-4.16766
H	2.07207	-5.4212	-4.20772
H	2.01612	-4.49804	-5.72349
H	-0.51187	-1.50964	1.89704
H	-0.70956	-2.53	0.49868
H	-2.45942	-1.04822	-0.39188
H	-2.95425	-1.7563	2.54663

H	-2.87943	-2.91985	1.25321
H	-4.81224	-1.86107	0.06588
H	-7.07574	-1.55053	0.32617
H	-7.67524	-2.20574	1.85478
H	-7.47186	-0.45085	1.65213
H	-4.5406	-1.46606	3.84689
H	-5.91461	-0.36794	3.73806
H	-6.17385	-2.11174	3.94966
H	-3.77934	0.96693	-0.48469
H	-4.41563	0.94283	1.17722
H	-3.47717	2.31552	0.59227
H	-2.8984	0.49896	3.11902
H	-1.1393	0.45841	2.91761
H	-2.00447	1.96203	2.67846
Z-matrix:2b-7			
C	7.60655	0.91452	-0.19839
C	6.80741	-0.06744	1.98615
C	6.49672	0.21194	0.54175
C	5.35034	-0.10672	-0.09151
C	3.39719	2.38903	0.34555
C	2.81503	1.15937	2.44468
C	-0.29523	5.25346	0.3759
C	0.21543	3.99854	0.01267
C	0.34784	3.68537	-1.34629
C	-0.03368	4.60989	-2.32264
C	-0.5437	5.85276	-1.95085
C	-0.67405	6.17603	-0.60189
C	0.61586	3.06184	1.10738
C	1.02771	1.66294	0.77111
C	2.50361	1.27285	0.93566
C	2.78206	-0.08973	0.18291
C	1.65948	-1.11518	0.47991
C	0.25518	-0.62816	0.0535
C	0.03644	0.82393	0.40811
O	0.62815	3.43469	2.27845
C	4.13858	-0.79562	0.46897
C	0.16808	-0.76573	-1.49901
C	-0.22599	-2.11912	-2.07982
O	0.47964	0.16383	-2.25084
C	-0.01881	-2.17634	-3.5919
C	-0.42811	-3.5149	-4.14388
C	0.37551	-4.53555	-4.50089

C	-0.20157	-5.80097	-5.08042
C	1.87354	-4.54362	-4.36777
C	-0.80035	-1.47641	0.79538
C	-2.23993	-0.92658	0.65652
C	-2.27022	0.58429	1.03524
O	-1.25967	1.28641	0.27592
C	-3.18998	-1.85529	1.45169
C	-4.64541	-1.70004	1.11196
C	-5.67955	-1.48727	1.94969
C	-7.08247	-1.35985	1.41191
C	-5.58494	-1.35027	3.44434
C	-3.57853	1.26238	0.59586
C	-2.07006	0.87033	2.534
H	7.82997	1.87499	0.27755
H	8.51415	0.30212	-0.19115
H	7.3491	1.11463	-1.24382
H	7.73605	-0.64278	2.06595
H	6.93811	0.87393	2.53014
H	6.03256	-0.63993	2.49892
H	5.26578	0.14247	-1.15016
H	3.28362	2.45927	-0.74193
H	3.16377	3.37301	0.76757
H	4.45395	2.22828	0.5675
H	2.64678	2.10729	2.96708
H	2.1922	0.40394	2.93513
H	3.86304	0.90168	2.62466
H	-0.40137	5.51655	1.4265
H	0.73915	2.72545	-1.67211
H	0.06576	4.35373	-3.37474
H	-0.84063	6.56845	-2.71305
H	-1.07079	7.14433	-0.30855
H	2.75665	0.11589	-0.89688
H	1.67296	-1.34999	1.5523
H	1.88553	-2.06022	-0.03086
H	4.11852	-1.78231	-0.01473
H	4.22834	-1.00571	1.53706
H	0.38292	-2.89361	-1.60135
H	-1.27919	-2.30615	-1.84889
H	-0.62695	-1.40587	-4.08303
H	1.01866	-1.9341	-3.845
H	-1.50397	-3.6302	-4.27894
H	-1.29216	-5.75799	-5.17003

H	0.20689	-5.97952	-6.08052
H	0.04613	-6.65714	-4.44446
H	2.26545	-3.67674	-3.83093
H	2.19661	-5.43188	-3.81421
H	2.3392	-4.56673	-5.35829
H	-0.55018	-1.521	1.86456
H	-0.76881	-2.51763	0.45267
H	-2.50358	-1.00338	-0.4072
H	-2.99504	-1.75355	2.52169
H	-2.93852	-2.89696	1.20934
H	-4.86395	-1.7934	0.04723
H	-7.12124	-1.45548	0.32168
H	-7.72362	-2.13909	1.83688
H	-7.50073	-0.3824	1.67383
H	-4.57466	-1.48347	3.83487
H	-5.92729	-0.35649	3.75172
H	-6.21991	-2.09855	3.93061
H	-3.81191	1.02586	-0.44846
H	-4.42971	0.98362	1.22
H	-3.48217	2.35433	0.64561
H	-2.89822	0.48668	3.13709
H	-1.14159	0.43576	2.91695
H	-1.9968	1.94975	2.71229
Z-matrix:2b-8			
C	6.35259	-3.08726	0.85604
C	5.35009	-2.1269	2.96653
C	5.62666	-1.9342	1.50072
C	5.27062	-0.85716	0.77328
C	2.58698	2.44114	2.31089
C	3.25925	2.94581	-0.05017
C	-1.29183	4.37439	-1.32883
C	-0.24972	3.44623	-1.20564
C	0.23878	2.80559	-2.35039
C	-0.32939	3.06944	-3.5988
C	-1.37686	3.98267	-3.71143
C	-1.8559	4.63845	-2.57822
C	0.31427	3.19853	0.15192
C	1.0139	1.90402	0.43828
C	2.48904	1.94826	0.84965
C	3.12873	0.51641	0.67833
C	2.22427	-0.57063	1.30281
C	0.78975	-0.59454	0.72245

C	0.26286	0.78371	0.40803
O	0.21025	4.05106	1.02942
C	4.56903	0.39224	1.2425
C	0.80548	-1.51452	-0.53693
C	0.86556	-0.87685	-1.91799
O	0.81693	-2.7444	-0.41398
C	0.92586	-1.91215	-3.03768
C	1.04817	-1.24871	-4.38396
C	0.04093	-0.85476	-5.18756
C	0.32158	-0.23106	-6.52924
C	-1.42088	-0.97611	-4.85272
C	-0.14708	-1.22757	1.77946
C	-1.63877	-1.1557	1.37446
C	-2.0185	0.30946	0.99736
O	-1.06726	0.83724	0.03897
C	-2.47629	-1.8183	2.49571
C	-3.88388	-2.16766	2.10118
C	-5.03331	-1.83438	2.72099
C	-6.3584	-2.29029	2.165
C	-5.14769	-1.01099	3.97405
C	-3.35428	0.37888	0.23842
C	-2.10342	1.27024	2.19623
H	7.32111	-3.24378	1.34222
H	5.76355	-4.00564	0.9483
H	6.53943	-2.91839	-0.20966
H	4.81314	-3.06825	3.12612
H	6.29129	-2.16847	3.52435
H	4.73792	-1.33554	3.40351
H	5.52459	-0.84799	-0.28725
H	2.18406	3.45272	2.42752
H	2.03492	1.79218	2.99895
H	3.62546	2.49019	2.6539
H	2.83457	3.95491	-0.00354
H	4.30568	3.04736	0.25284
H	3.24628	2.62796	-1.09878
H	-1.67139	4.88908	-0.44835
H	1.06365	2.10411	-2.29373
H	0.04737	2.56293	-4.48403
H	-1.81745	4.18747	-4.684
H	-2.66824	5.35542	-2.66535
H	3.19297	0.31323	-0.3991
H	2.19239	-0.41308	2.38884

H	2.67941	-1.55934	1.16676
H	4.5551	0.45353	2.33393
H	5.18625	1.23102	0.90558
H	-0.0313	-0.26639	-2.05678
H	1.74788	-0.23331	-1.968
H	1.79351	-2.56953	-2.89841
H	0.05115	-2.57164	-3.00223
H	2.07408	-1.10184	-4.72136
H	-0.10119	0.77789	-6.57493
H	1.39431	-0.15131	-6.73418
H	-0.12608	-0.83245	-7.32724
H	-1.6035	-1.36098	-3.84641
H	-1.90251	0.00574	-4.91327
H	-1.91521	-1.64751	-5.56229
H	-0.01746	-0.72064	2.74563
H	0.13294	-2.27504	1.95452
H	-1.74398	-1.76979	0.46846
H	-2.43358	-1.20578	3.39927
H	-1.99912	-2.76961	2.76843
H	-3.94744	-2.78806	1.20586
H	-6.24566	-2.87943	1.24885
H	-6.88305	-2.91241	2.8974
H	-6.98687	-1.42566	1.92764
H	-5.69725	-0.08688	3.76575
H	-5.6929	-1.56995	4.74209
H	-4.18508	-0.73027	4.40494
H	-3.37424	-0.34257	-0.58632
H	-4.21757	0.20274	0.88268
H	-3.48655	1.36714	-0.21975
H	-2.92274	1.00898	2.87219
H	-1.17585	1.28564	2.77688
H	-2.26635	2.29905	1.85377
Z-matrix:2b-9			
C	7.57495	0.69185	-0.6409
C	6.92782	-0.11865	1.66106
C	6.50685	0.08284	0.23164
C	5.30043	-0.22681	-0.28356
C	3.48417	2.37209	0.14654
C	3.0394	1.30086	2.36288
C	-0.07935	5.3866	0.29443
C	0.35078	4.09066	-0.02607
C	0.35632	3.68814	-1.36781

C	-0.07127	4.56515	-2.36853
C	-0.50082	5.84948	-2.03871
C	-0.50443	6.26151	-0.70772
C	0.80466	3.20676	1.0915
C	1.1352	1.77385	0.81393
C	2.6044	1.33309	0.88086
C	2.76739	-0.08432	0.19881
C	1.63548	-1.04029	0.65258
C	0.22044	-0.52117	0.30726
C	0.08624	0.95759	0.58646
O	0.92597	3.6494	2.23169
C	4.11587	-0.8283	0.418
C	0.00304	-0.7481	-1.22228
C	-0.48881	-2.11581	-1.68251
O	0.28929	0.11958	-2.05385
C	-0.41165	-2.27527	-3.19913
C	-0.9161	-3.6276	-3.62496
C	-0.18384	-4.7037	-3.97258
C	-0.85385	-5.97851	-4.41541
C	1.31873	-4.76761	-3.95732
C	-0.8038	-1.27891	1.17938
C	-2.22767	-0.67899	1.10883
C	-2.17346	0.84995	1.40011
O	-1.19746	1.46759	0.53069
C	-3.15476	-1.52575	2.01185
C	-4.62598	-1.31644	1.79421
C	-5.3945	-1.88771	0.84622
C	-6.86763	-1.58371	0.76338
C	-4.89871	-2.84539	-0.20218
C	-3.48482	1.55739	1.01888
C	-1.85043	1.20829	2.86142
H	7.87104	1.67045	-0.24885
H	8.45788	0.04485	-0.66697
H	7.23819	0.83637	-1.67285
H	7.83634	-0.72905	1.70215
H	7.14156	0.84827	2.1285
H	6.17722	-0.6219	2.27294
H	5.13623	-0.04093	-1.34597
H	3.28105	2.3786	-0.93013
H	3.32305	3.38951	0.52047
H	4.54959	2.18222	0.29019
H	2.95111	2.28565	2.83431

H	2.43392	0.60386	2.95171
H	4.0889	1.01134	2.47162
H	-0.08631	5.71899	1.33068
H	0.68224	2.69391	-1.66082
H	-0.07053	4.23971	-3.40599
H	-0.83372	6.52836	-2.81959
H	-0.83819	7.2625	-0.44724
H	2.65914	0.05488	-0.88644
H	1.72803	-1.20685	1.73383
H	1.7832	-2.02458	0.18966
H	4.01852	-1.84106	0.00254
H	4.28777	-0.97587	1.48645
H	0.12807	-2.885	-1.20568
H	-1.52529	-2.24341	-1.35632
H	-1.02969	-1.51171	-3.68862
H	0.60915	-2.09417	-3.55159
H	-2.00299	-3.70391	-3.66663
H	-1.94574	-5.89468	-4.42016
H	-0.53636	-6.24006	-5.43014
H	-0.58681	-6.80084	-3.74361
H	1.78528	-3.88627	-3.51119
H	1.65214	-5.6323	-3.37337
H	1.70128	-4.87277	-4.97769
H	-0.47515	-1.2684	2.22794
H	-0.8361	-2.33948	0.90223
H	-2.56536	-0.79803	0.07065
H	-2.92906	-1.3444	3.06949
H	-2.93536	-2.59157	1.8668
H	-5.10017	-0.64524	2.51008
H	-7.19051	-0.8776	1.53561
H	-7.10915	-1.14386	-0.20985
H	-7.45178	-2.50155	0.88589
H	-3.82294	-3.02902	-0.14545
H	-5.40435	-3.81105	-0.09814
H	-5.10888	-2.45111	-1.20194
H	-3.80431	1.27462	0.00942
H	-4.29728	1.34929	1.71816
H	-3.34373	2.64544	0.9988
H	-2.64314	0.88854	3.5447
H	-0.91041	0.76052	3.19847
H	-1.72731	2.29216	2.97299