

Supporting Information

Rec. Nat. Prod. 13:6 (2019) 462-467

Chemical Compounds from the Twigs and Leaves of *Caesalpinia cucullata* Roxb

Xuesong Liang, Dewen Bi, Fengqiu Li and Liqin Wang*

Faculty of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming

650050, China

Table of Contents	Page
Figure S1: MS Spectrum of Compound 1	2
Figure S2: HR-ESI-MS Spectrum of Compound 1	3
Figure S3: ¹ H-NMR (500 MHz, CD ₃ COCD ₃) Spectrum of Compound 1	4
Figure S4: ¹³ C-NMR + DEPT (125 MHz, CD ₃ COCD ₃) Spectrum of Compound 1	5
Figure S5: HSQC Spectrum of Compound 1	6
Figure S6: HMBC Spectrum of Compound 1	7
Figure S7: ¹ H- ¹ H COSY Spectrum of Compound 1	8
Figure S8: ROESY Spectrum of Compound 1	9
Figure S9: Experimental ECD Spectrum of Compound 1	10
Figure S10: Experimental and Calculated ECD Spectrum of Compound 1	11
S11. ECD Calculation Details of Compound 1	12
S11. 1. Methods	12
S11. 2. Results	12

Generic Display Report (all)

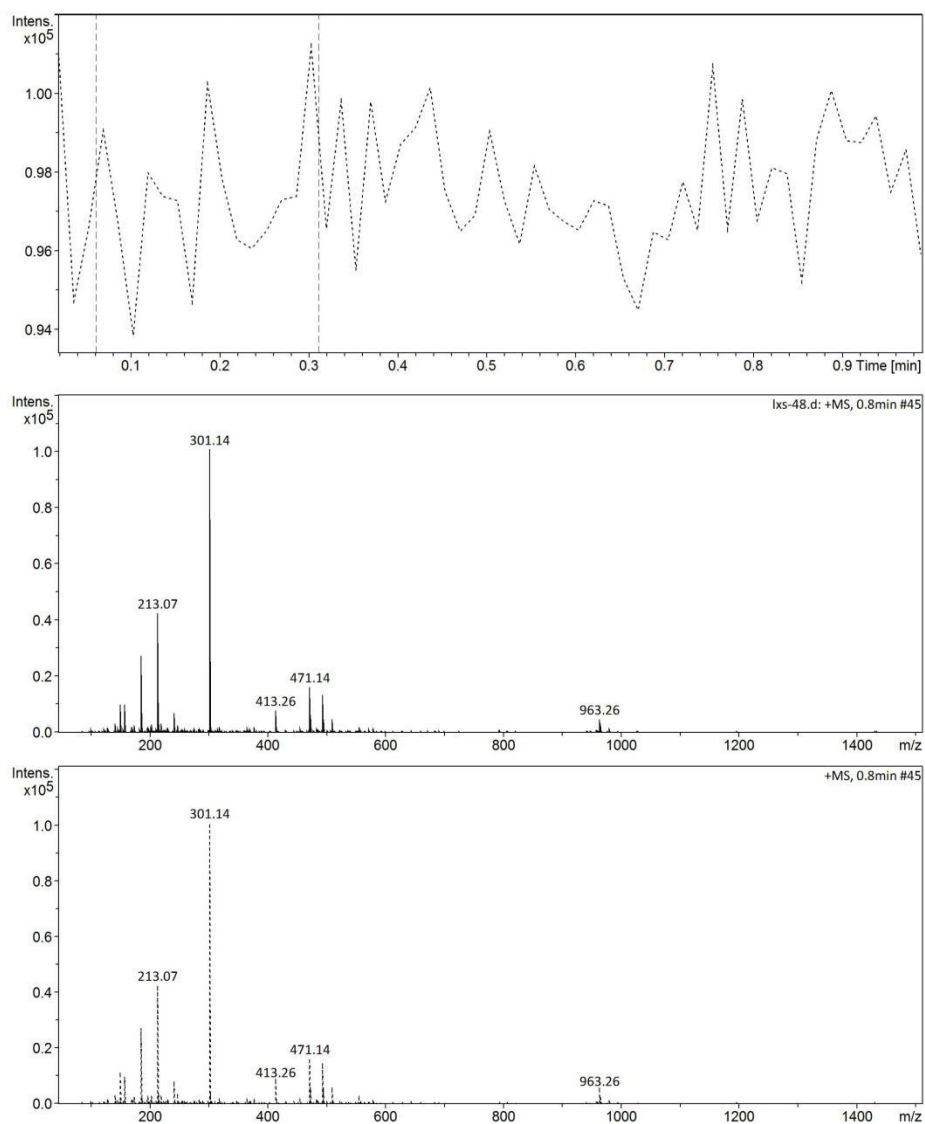


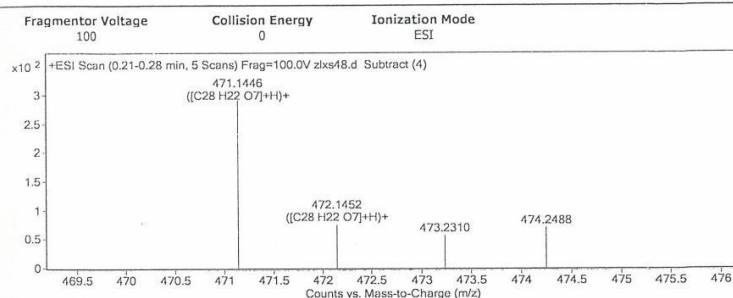
Figure S1: MS Spectrum of Compound 1

Qualitative Analysis Report

Data Filename	zlx48.d	Sample Name	zlx48
Sample Type	Sample	Position	P1-E9
Instrument Name	Instrument 1	User Name	
Acq Method	s.m	Acquired Time	12/28/2018 2:34:24 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
60.081	1	792.74		
88.1121		325.79		
102.1276	1	627.75		
116.1065		205.63		
223.096		215.15		
260.1937		281.68		
300.158		266.13		
314.3424		311.22		
374.1328		310.33		
471.1446	1	291.93	C28 H22 O7	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C28 H22 O7	470.1366	471.1438	471.1446	-0.80	-1.70	18.0000

--- End Of Report ---

Figure S2: HRESI-MS Spectrum of Compound 1

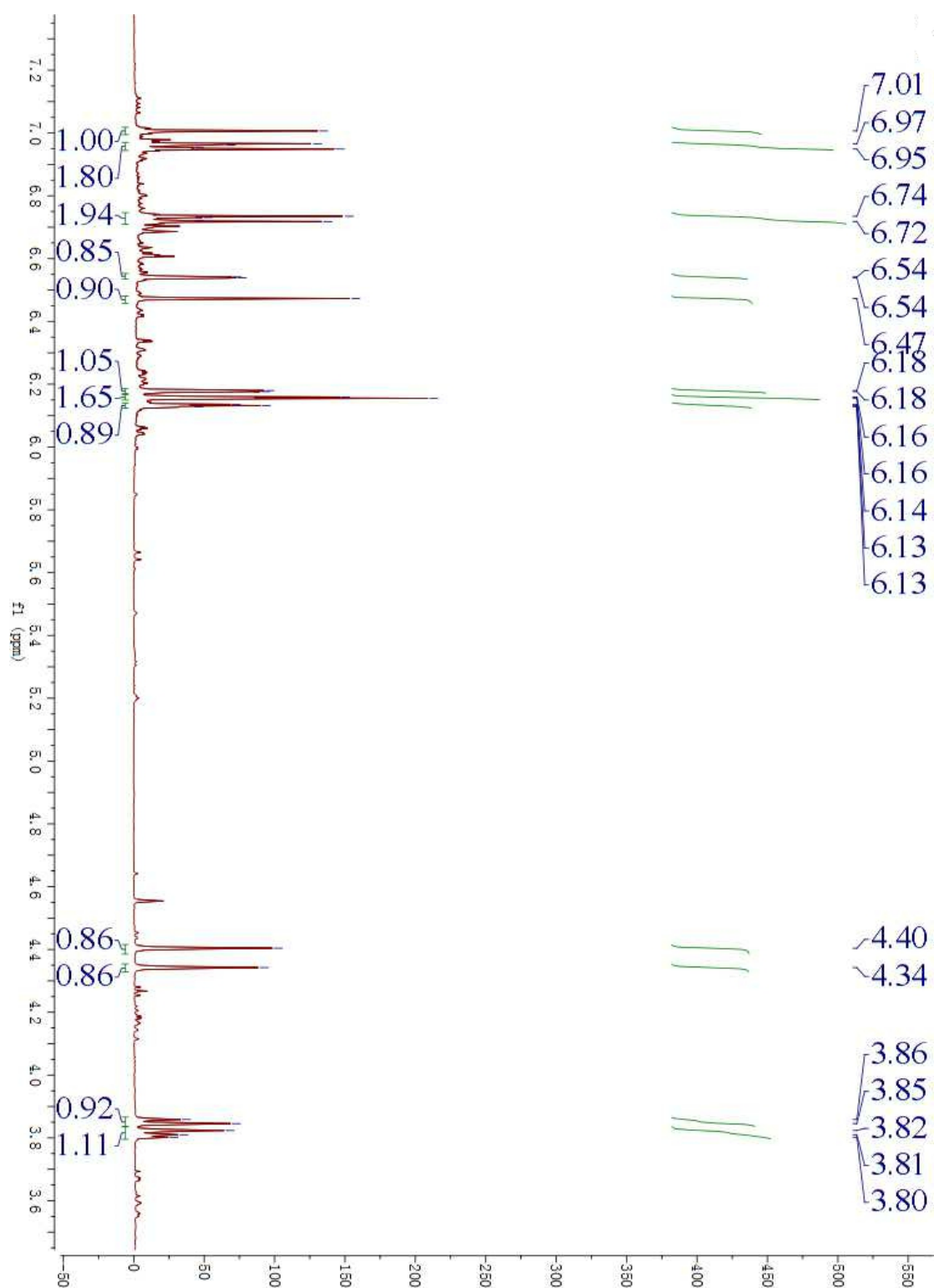


Figure S3: ¹H-NMR Spectrum of Compound **1**

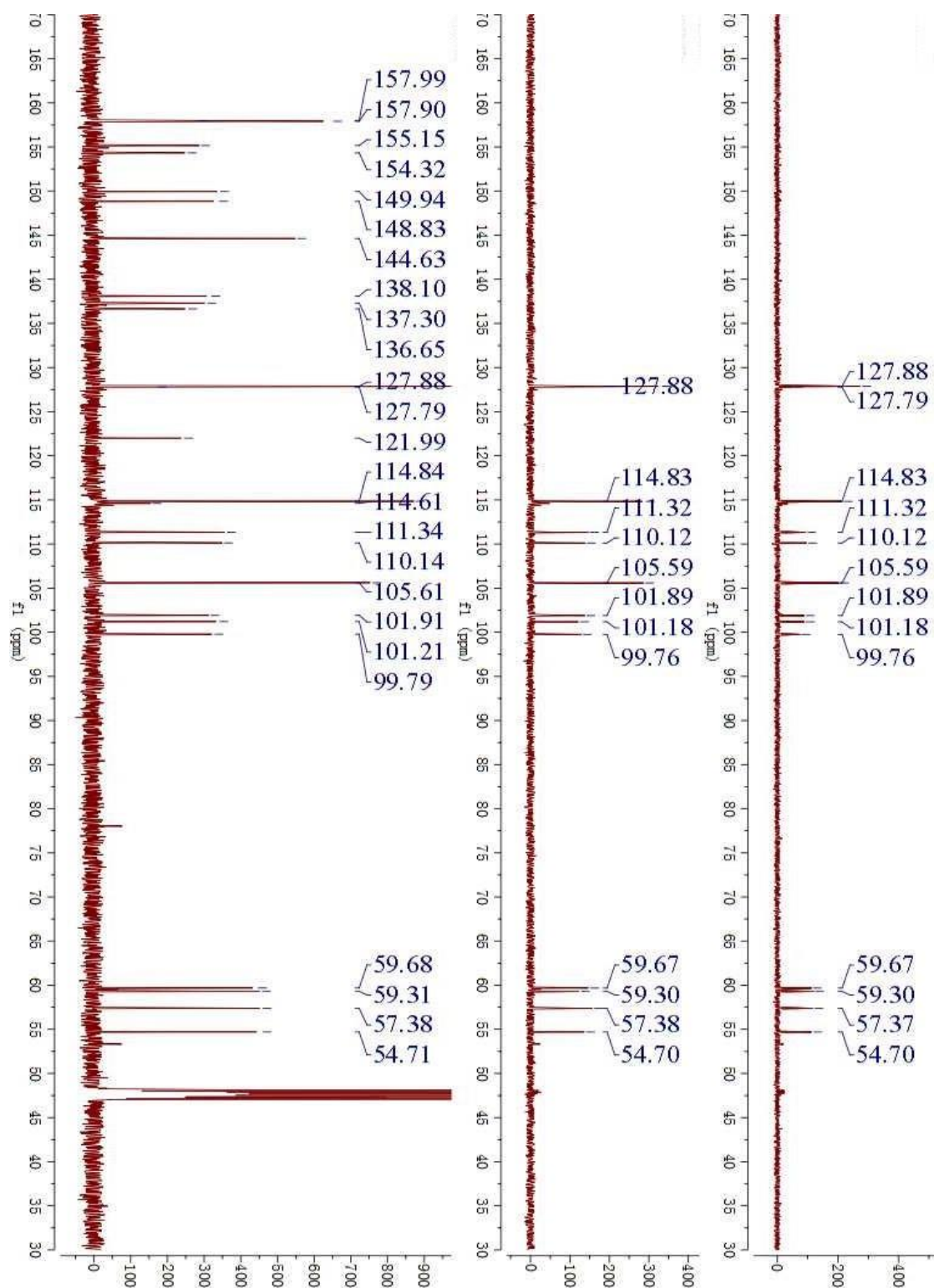


Figure S4: ^{13}C -NMR and DEPT Spectrum of Compound 1

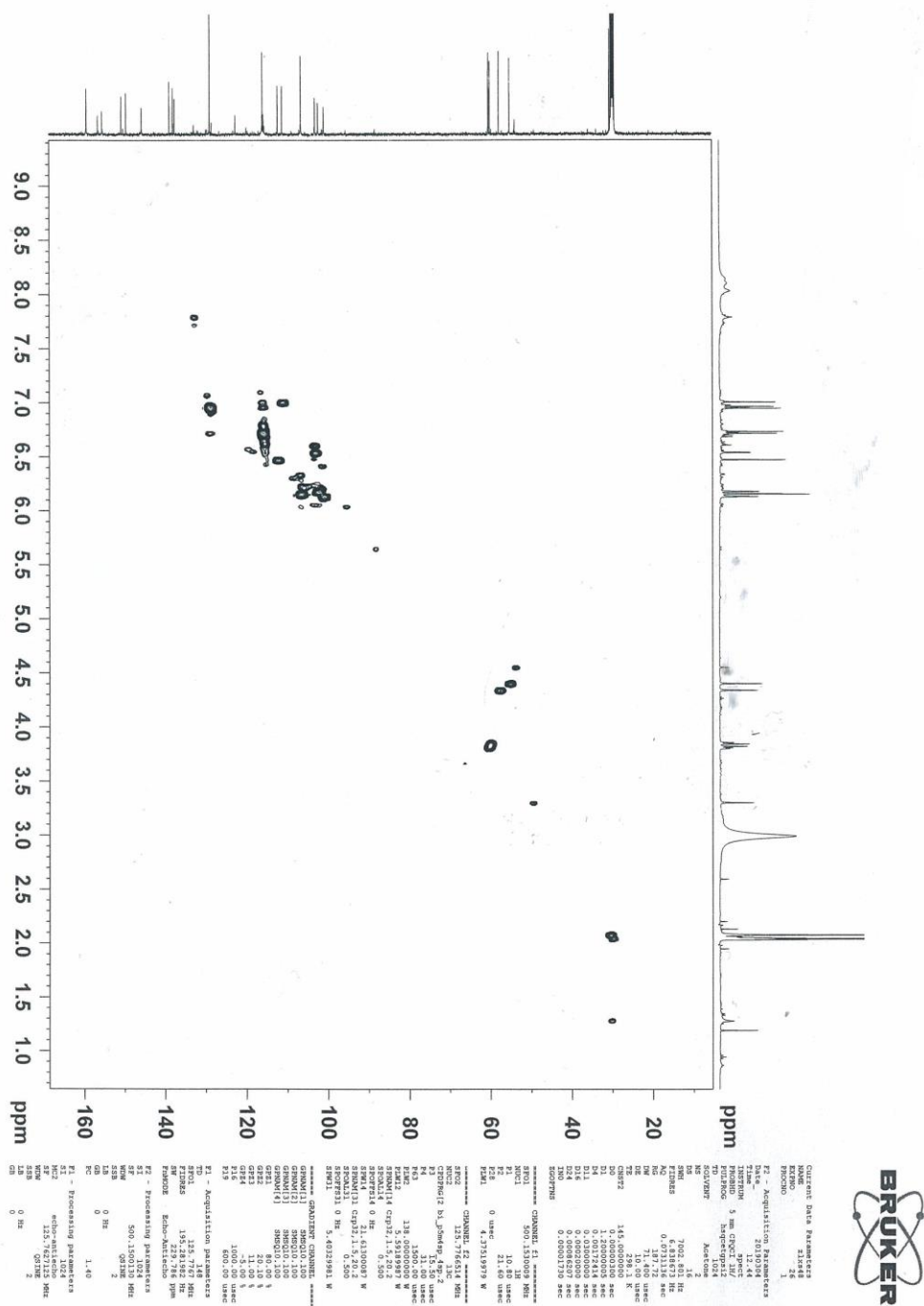


Figure S5: HSQC Spectrum of Compound 1

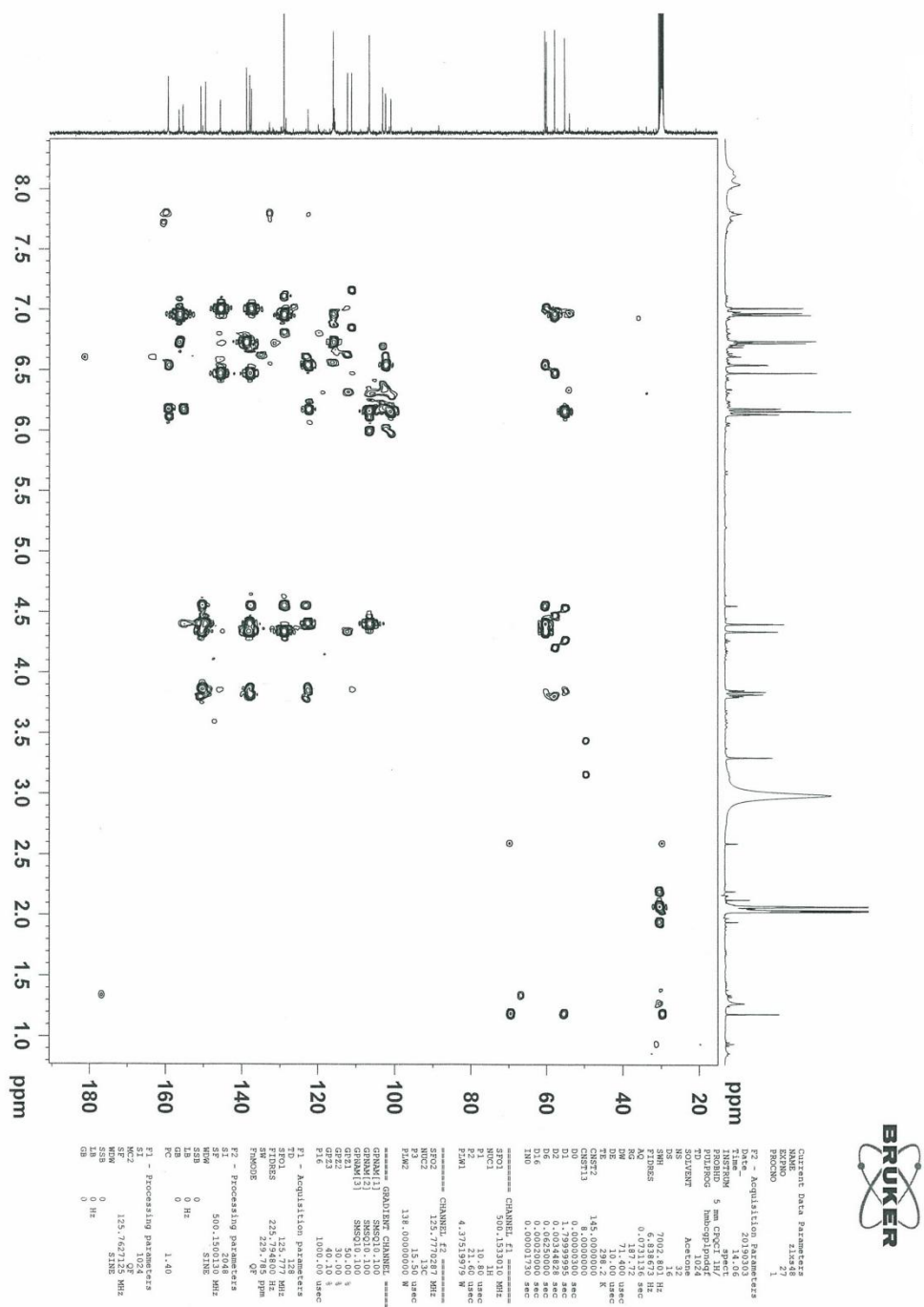


Figure S6: HMBC Spectrum of Compound 1

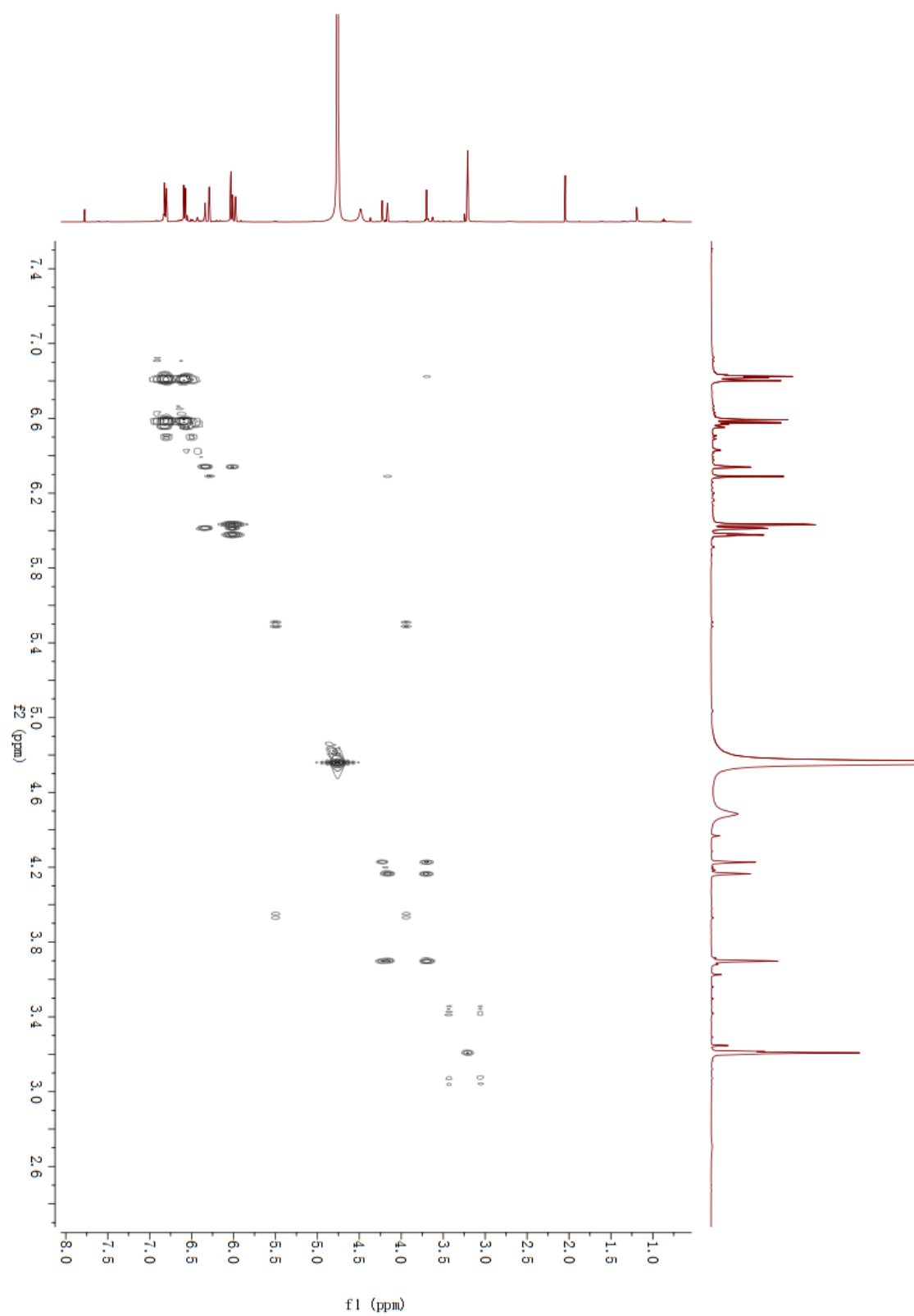
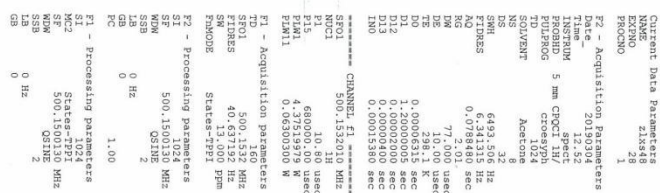


Figure S7: ^1H - ^1H COSY Spectrum of Compound **1**



9

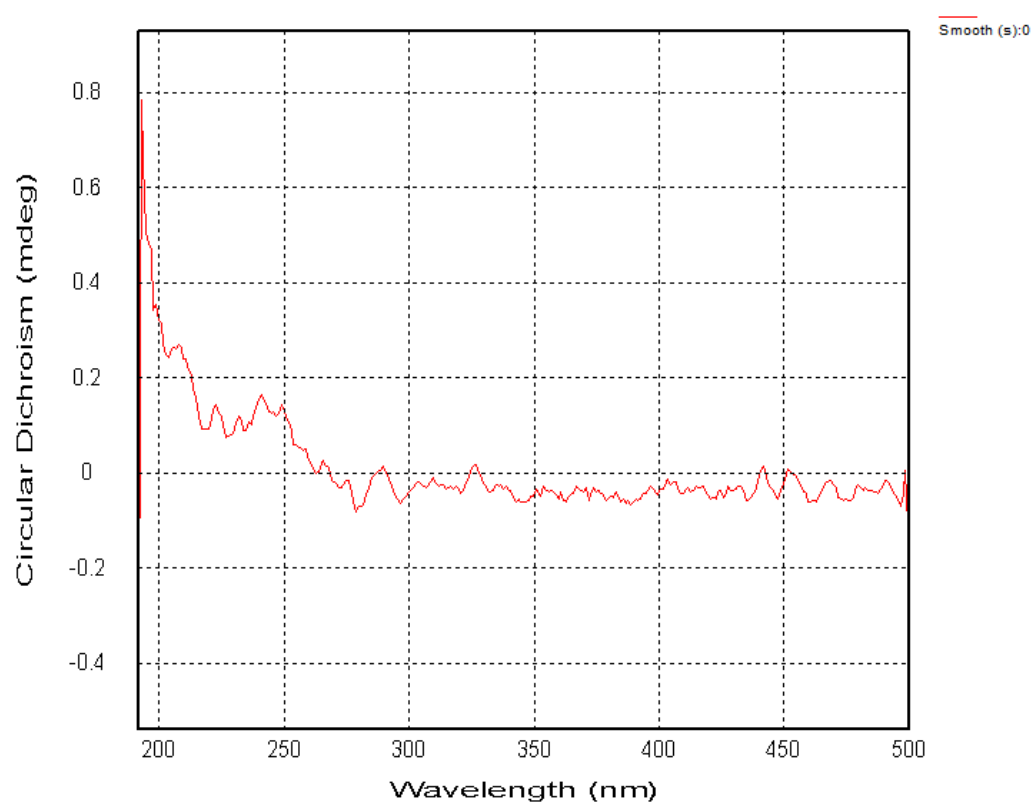
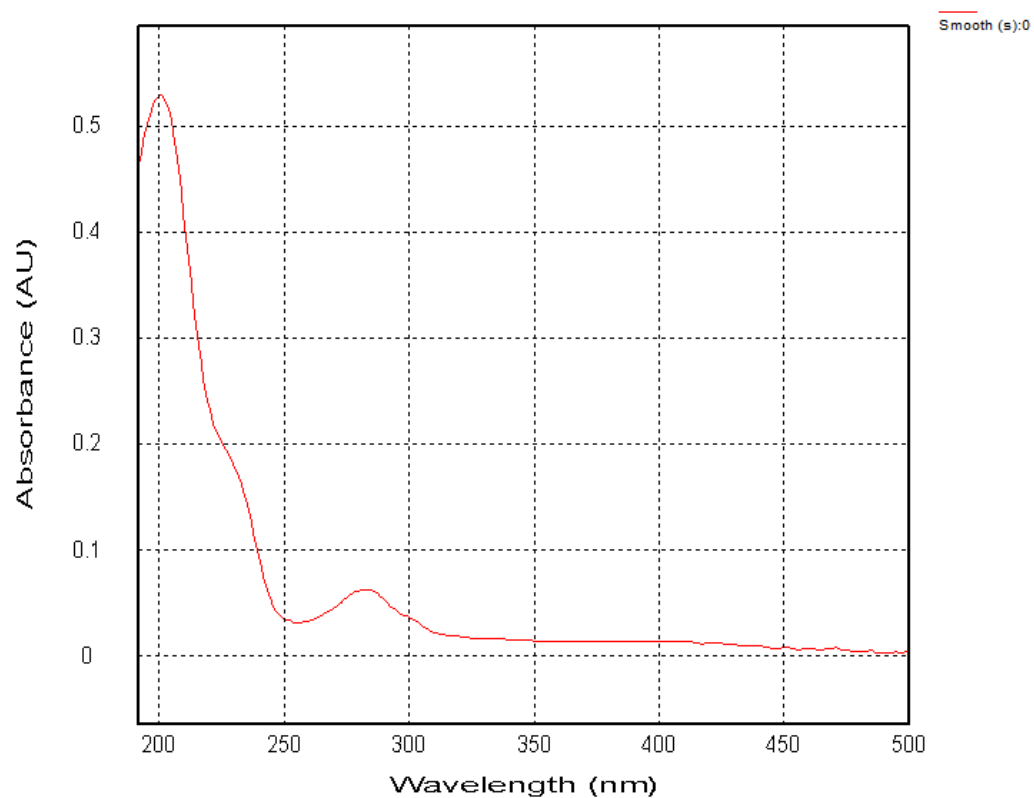


Figure S9: Experimental ECD Spectrum of Compound **1**

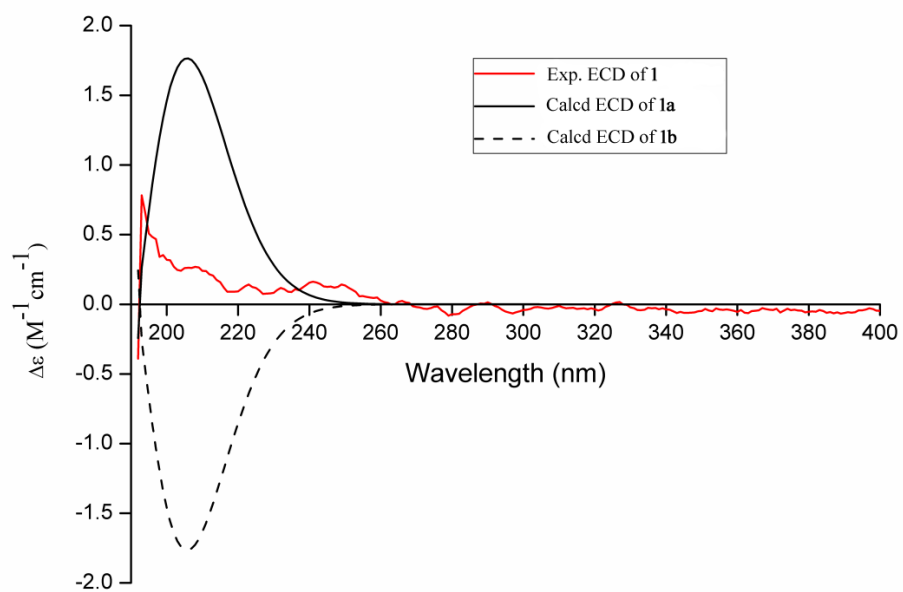


Figure S10: Experimental ECD Spectrum (200–400 nm) of Compound **1** in MeOH and the Calculated ECD Spectrum of the Model Molecules of Compound **1** at the B3LYP/6-311+G(d, p) level.

S11. ECD Calculation Details

S11. 1. Methods

Monte Carlo conformational searches were carried out by means of the Spartan's 10 software using Merck Molecular Force Field (MMFF). The conformers with Boltzmann-population of over 5% were chosen for ECD calculations, and then the conformers were initially optimized at B3LYP/6-31+g (d, p) level in MeOH using the CPCM polarizable conductor calculation model. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-31+g (d, p) level for all conformers of compounds **1**. Rotatory strengths for a total of 30 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.

S11. 2. Results

Table S1. Gibbs free energies^a and equilibrium populations^b of low-energy conformers of compound **1**.

Conformers	In MeOH	
	ΔG	P (%) / 100
Compound 1-1	0.00	0.290
Compound 1-2	0.10	0.123
Compound 1-3	0.23	0.098
Compound 1-4	0.47	0.066

^aB3LYP/6-31+G(d,p), in kcal/mol. ^bFrom ΔG values at 298.15K.

Table S2. Cartesian coordinates for the low-energy reoptimized MMFF conformers of compound **1** at B3LYP/6-311+G(d,p) level of theory in CH₃OH.

Compound 1-1		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-0.954310	-3.113766	0.169501
2.	6.	0.	-0.223409	-4.305167	0.037068
3.	6.	0.	1.118439	-4.288792	-0.344482
4.	6.	0.	1.768904	-3.072523	-0.603382
5.	6.	0.	1.068348	-1.872554	-0.452778
6.	6.	0.	-0.293698	-1.920056	-0.073371
7.	6.	0.	1.542242	-0.424167	-0.688589
8.	6.	0.	0.467470	0.306172	0.153761
9.	6.	0.	-0.806137	-0.503552	-0.132036
10.	6.	0.	-0.052051	1.720127	0.092683
11.	6.	0.	-1.412466	1.674775	0.459947

12.	6.	0.	-1.886677	0.228298	0.699295
13.	6.	0.	0.585810	2.934090	-0.147406
14.	6.	0.	-0.148942	4.116184	-0.037978
15.	6.	0.	-1.505446	4.069624	0.332079
16.	6.	0.	-2.141325	2.855872	0.586373
17.	6.	0.	-3.327421	-0.078096	0.344220
18.	6.	0.	2.978573	-0.102045	-0.311028
19.	6.	0.	3.505983	-0.521905	0.921735
20.	6.	0.	4.812977	-0.177573	1.273855
21.	6.	0.	5.611628	0.577569	0.408959
22.	6.	0.	5.086309	0.983030	-0.817313
23.	6.	0.	3.776490	0.642790	-1.183348
24.	6.	0.	-4.150682	-0.771127	1.237925
25.	6.	0.	-5.470120	-1.092959	0.916002
26.	6.	0.	-5.993809	-0.717355	-0.323307
27.	6.	0.	-5.189445	-0.017857	-1.230534
28.	6.	0.	-3.876926	0.294022	-0.893856
29.	8.	0.	-0.886259	-5.473224	0.297431
30.	8.	0.	3.074926	-3.148537	-0.989404
31.	8.	0.	5.377523	-0.556814	2.456988
32.	8.	0.	5.808837	1.714826	-1.713462
33.	8.	0.	-2.124370	5.300799	0.407274
34.	8.	0.	0.450901	5.315047	-0.289755
35.	8.	0.	-7.277505	-0.996682	-0.703276
36.	1.	0.	-1.071140	-0.310665	-1.185801
37.	1.	0.	0.741439	0.105700	1.203866
38.	1.	0.	-2.002369	-3.151792	0.443219
39.	1.	0.	1.685630	-5.210055	-0.447031
40.	1.	0.	1.404316	-0.160458	-1.748069
41.	1.	0.	-1.737922	-0.020920	1.761721
42.	1.	0.	1.633992	2.990638	-0.421703
43.	1.	0.	-3.194603	2.836261	0.858657
44.	1.	0.	2.897243	-1.117898	1.597219
45.	1.	0.	6.626144	0.826645	0.706039
46.	1.	0.	3.397867	0.974623	-2.144313
47.	1.	0.	-3.756031	-1.068987	2.206247
48.	1.	0.	-6.089245	-1.633347	1.629243
49.	1.	0.	-5.608988	0.270448	-2.188735
50.	1.	0.	-3.266751	0.844559	-1.604417
51.	1.	0.	-0.285049	-6.214362	0.146823
52.	1.	0.	3.455087	-2.257403	-1.002584
53.	1.	0.	4.735354	-1.075060	2.959871
54.	1.	0.	6.684199	1.894384	-1.345745

55.	1.	0.	-3.052010	5.183586	0.645967
56.	1.	0.	-0.217767	6.005031	-0.162744
57.	1.	0.	-7.713659	-1.492610	0.001927

Compound 1-2		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-1.000317	-3.106253	0.172643
2.	6.	0.	-0.286605	-4.307776	0.035826
3.	6.	0.	1.054329	-4.309630	-0.349625
4.	6.	0.	1.720839	-3.102179	-0.608125
5.	6.	0.	1.038113	-1.892684	-0.453222
6.	6.	0.	-0.323975	-1.921571	-0.069673
7.	6.	0.	1.528878	-0.450451	-0.690941
8.	6.	0.	0.467725	0.292671	0.157609
9.	6.	0.	-0.817650	-0.497972	-0.124858
10.	6.	0.	-0.033085	1.711989	0.098025
11.	6.	0.	-1.393296	1.691862	0.468497
12.	6.	0.	-1.886804	0.250306	0.707201
13.	6.	0.	0.619491	2.919910	-0.137852
14.	6.	0.	-0.104809	4.105239	-0.020102
15.	6.	0.	-1.461163	4.092945	0.352553
16.	6.	0.	-2.106615	2.880637	0.601941
17.	6.	0.	-3.330722	-0.041726	0.353394
18.	6.	0.	2.968464	-0.137114	-0.319310
19.	6.	0.	3.509778	-0.589001	0.895618
20.	6.	0.	4.818483	-0.247535	1.246019
21.	6.	0.	5.603928	0.539441	0.397481
22.	6.	0.	5.064097	0.978207	-0.811010
23.	6.	0.	3.753886	0.639787	-1.175768
24.	6.	0.	-3.881173	0.350418	-0.874076
25.	6.	0.	-5.199216	0.044908	-1.207208
26.	6.	0.	-6.001603	-0.665560	-0.308069
27.	6.	0.	-5.473846	-1.062009	0.923713
28.	6.	0.	-4.154986	-0.747490	1.241001
29.	8.	0.	-0.965140	-5.466189	0.295535
30.	8.	0.	3.025199	-3.196334	-0.998447
31.	8.	0.	5.395963	-0.657797	2.411618
32.	8.	0.	5.773073	1.745999	-1.689289
33.	8.	0.	-2.151529	5.265076	0.463495
34.	8.	0.	0.419611	5.360328	-0.248587

35.	8.	0.	-7.302018	-0.993677	-0.576100
36.	1.	0.	-1.082341	-0.301032	-1.178060
37.	1.	0.	0.744045	0.085504	1.205919
38.	1.	0.	-2.047959	-3.130015	0.449532
39.	1.	0.	1.608231	-5.238551	-0.455426
40.	1.	0.	1.388003	-0.184288	-1.749604
41.	1.	0.	-1.740000	0.002017	1.769868
42.	1.	0.	1.671843	2.945250	-0.412421
43.	1.	0.	-3.155966	2.893162	0.878024
44.	1.	0.	2.909610	-1.206384	1.559406
45.	1.	0.	6.619643	0.786033	0.692612
46.	1.	0.	3.366093	0.991290	-2.126176
47.	1.	0.	-3.275574	0.912996	-1.578915
48.	1.	0.	-5.605991	0.362002	-2.165505
49.	1.	0.	-6.105779	-1.608036	1.616125
50.	1.	0.	-3.755766	-1.058580	2.203364
51.	1.	0.	-0.375115	-6.216132	0.144302
52.	1.	0.	3.419041	-2.311418	-1.006235
53.	1.	0.	4.764378	-1.199744	2.902962
54.	1.	0.	6.660571	1.894310	-1.336894
55.	1.	0.	-1.536490	5.983812	0.253005
56.	1.	0.	1.351070	5.283660	-0.489145
57.	1.	0.	-7.535689	-0.661334	-1.452642

Compound 1-3		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-1.005548	-3.103273	0.170659
2.	6.	0.	-0.293792	-4.306069	0.035912
3.	6.	0.	1.047690	-4.310564	-0.347395
4.	6.	0.	1.716632	-3.104416	-0.606017
5.	6.	0.	1.035742	-1.893613	-0.453136
6.	6.	0.	-0.326912	-1.919890	-0.071682
7.	6.	0.	1.529135	-0.452224	-0.691035
8.	6.	0.	0.468172	0.292931	0.156087
9.	6.	0.	-0.818116	-0.495577	-0.128198
10.	6.	0.	-0.030410	1.713071	0.096439
11.	6.	0.	-1.390990	1.694858	0.465621
12.	6.	0.	-1.886946	0.253931	0.702866
13.	6.	0.	0.624206	2.920184	-0.137849
14.	6.	0.	-0.098439	4.106493	-0.019834

15.	6.	0.	-1.455200	4.096027	0.351516
16.	6.	0.	-2.102763	2.884490	0.599174
17.	6.	0.	-3.330694	-0.035466	0.346807
18.	6.	0.	2.968828	-0.141093	-0.318037
19.	6.	0.	3.508189	-0.593249	0.897683
20.	6.	0.	4.817053	-0.253689	1.249268
21.	6.	0.	5.604620	0.531656	0.401222
22.	6.	0.	5.066728	0.970703	-0.808053
23.	6.	0.	3.756375	0.634130	-1.174038
24.	6.	0.	-4.157471	-0.731774	1.234498
25.	6.	0.	-5.478696	-1.042921	0.909907
26.	6.	0.	-6.000289	-0.652468	-0.325658
27.	6.	0.	-5.192238	0.050895	-1.226410
28.	6.	0.	-3.877949	0.351876	-0.887317
29.	8.	0.	-0.974685	-5.463380	0.295833
30.	8.	0.	3.021397	-3.201190	-0.994050
31.	8.	0.	5.392652	-0.664392	2.415728
32.	8.	0.	5.777781	1.736951	-1.685926
33.	8.	0.	-2.143719	5.269013	0.463219
34.	8.	0.	0.428259	5.360958	-0.246240
35.	8.	0.	-7.285425	-0.921790	-0.708163
36.	1.	0.	-1.080921	-0.298518	-1.181762
37.	1.	0.	0.742891	0.085053	1.204723
38.	1.	0.	-2.053800	-3.124688	0.445322
39.	1.	0.	1.600187	-5.240500	-0.451646
40.	1.	0.	1.389694	-0.186508	-1.749962
41.	1.	0.	-1.741640	0.004699	1.765606
42.	1.	0.	1.676888	2.944226	-0.411255
43.	1.	0.	-3.152696	2.898402	0.872959
44.	1.	0.	2.906361	-1.209322	1.561193
45.	1.	0.	6.620411	0.776803	0.697292
46.	1.	0.	3.370116	0.985852	-2.124983
47.	1.	0.	-3.764798	-1.039783	2.200454
48.	1.	0.	-6.101218	-1.585382	1.618593
49.	1.	0.	-5.611260	0.353747	-2.180268
50.	1.	0.	-3.266181	0.908409	-1.591710
51.	1.	0.	-0.386287	-6.214262	0.142897
52.	1.	0.	3.416426	-2.316809	-1.003334
53.	1.	0.	4.759660	-1.205295	2.906391
54.	1.	0.	6.665098	1.884251	-1.332658
55.	1.	0.	-1.529027	5.986771	0.248452
56.	1.	0.	1.356977	5.282372	-0.496553
57.	1.	0.	-7.728460	-1.408647	-0.000965

Compound 1-4		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-1.019599	-3.097782	0.155293
2.	6.	0.	-0.318041	-4.306178	0.013645
3.	6.	0.	1.023430	-4.319963	-0.367947
4.	6.	0.	1.698479	-3.118433	-0.617553
5.	6.	0.	1.027369	-1.899098	-0.457288
6.	6.	0.	-0.332455	-1.914898	-0.077620
7.	6.	0.	1.531322	-0.460599	-0.693119
8.	6.	0.	0.474489	0.292179	0.152645
9.	6.	0.	-0.816415	-0.488546	-0.130020
10.	6.	0.	-0.017291	1.715017	0.092222
11.	6.	0.	-1.377540	1.703978	0.463544
12.	6.	0.	-1.878240	0.265616	0.705785
13.	6.	0.	0.642306	2.918703	-0.145370
14.	6.	0.	-0.074888	4.108550	-0.028916
15.	6.	0.	-1.431200	4.105050	0.344169
16.	6.	0.	-2.083818	2.897023	0.595768
17.	6.	0.	-3.324489	-0.022277	0.358693
18.	6.	0.	2.971732	-0.157054	-0.316564
19.	6.	0.	3.512409	-0.630771	0.890109
20.	6.	0.	4.821744	-0.297046	1.246304
21.	6.	0.	5.607065	0.505514	0.412532
22.	6.	0.	5.067303	0.966613	-0.787747
23.	6.	0.	3.757321	0.634947	-1.158897
24.	6.	0.	-3.877544	0.362371	-0.870100
25.	6.	0.	-5.197034	0.057252	-1.197821
26.	6.	0.	-5.999012	-0.644972	-0.291732
27.	6.	0.	-5.469271	-1.032886	0.942020
28.	6.	0.	-4.148723	-0.718812	1.253770
29.	8.	0.	-0.910424	-5.517923	0.240375
30.	8.	0.	3.002005	-3.217470	-1.007730
31.	8.	0.	5.399238	-0.729507	2.403628
32.	8.	0.	5.776571	1.750354	-1.651647
33.	8.	0.	-2.114532	5.281323	0.453770
34.	8.	0.	0.456783	5.359989	-0.259177
35.	8.	0.	-7.300159	-0.973781	-0.554424
36.	1.	0.	-1.081752	-0.287174	-1.182224
37.	1.	0.	0.748135	0.083807	1.201374

38.	1.	0.	-2.071510	-3.091458	0.429132
39.	1.	0.	1.547883	-5.262350	-0.473647
40.	1.	0.	1.395786	-0.193500	-1.752284
41.	1.	0.	-1.727810	0.017770	1.768130
42.	1.	0.	1.694756	2.937266	-0.419938
43.	1.	0.	-3.132759	2.916517	0.873096
44.	1.	0.	2.911787	-1.259399	1.542821
45.	1.	0.	6.623174	0.745590	0.711646
46.	1.	0.	3.370225	1.002462	-2.103517
47.	1.	0.	-3.272437	0.918551	-1.580346
48.	1.	0.	-5.605287	0.368413	-2.157385
49.	1.	0.	-6.102190	-1.569062	1.641346
50.	1.	0.	-3.748613	-1.020229	2.218981
51.	1.	0.	-1.834349	-5.371305	0.481545
52.	1.	0.	3.401940	-2.335459	-1.010056
53.	1.	0.	4.771407	-1.288982	2.879939
54.	1.	0.	6.664932	1.889615	-1.297739
55.	1.	0.	-1.495194	5.996263	0.242873
56.	1.	0.	1.388333	5.278029	-0.497725
57.	1.	0.	-7.538765	-0.640241	-1.429223