Supplementary Material

Antifungal Prenylated Diphenyl Ethers from *Arthrinium arundinis*, an Endophytic Fungus Isolated from the Leaves of Tobacco (*Nicotiana tabacum* L.)

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Table of Contents

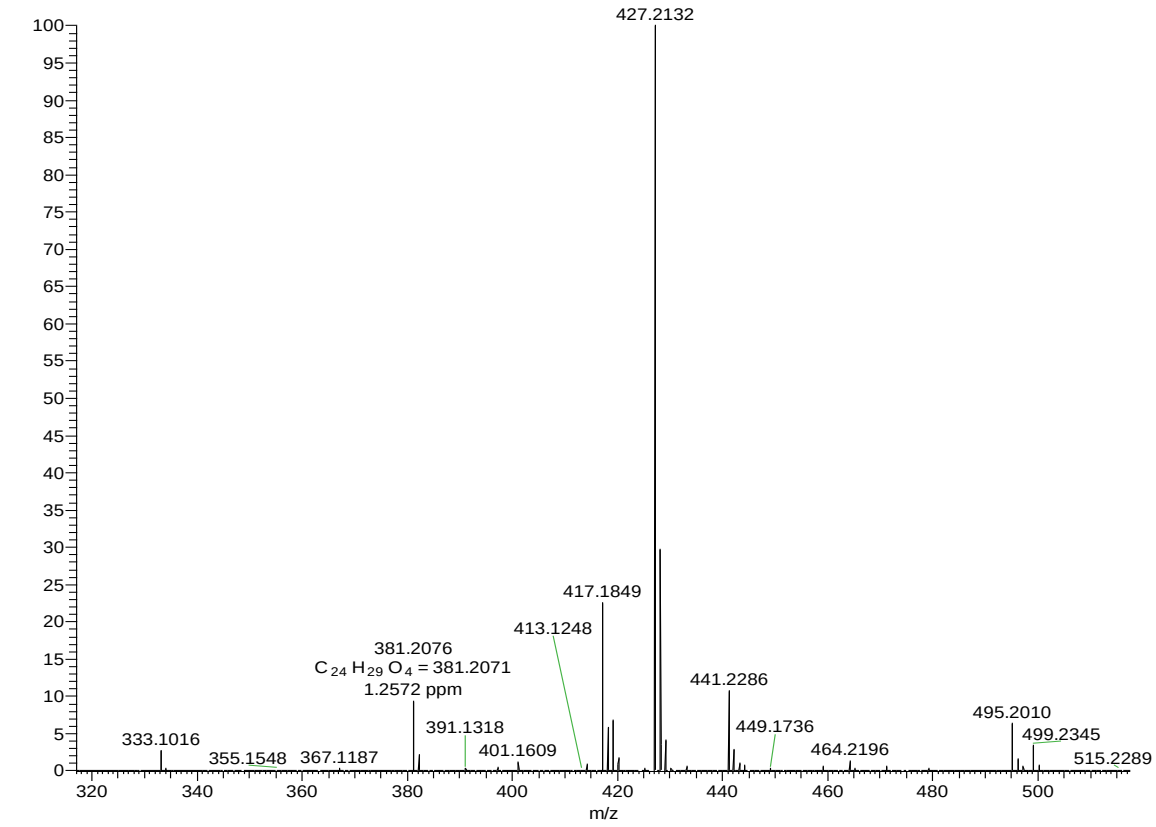

Figure S1. HRESIMS spectrum of compound **1**

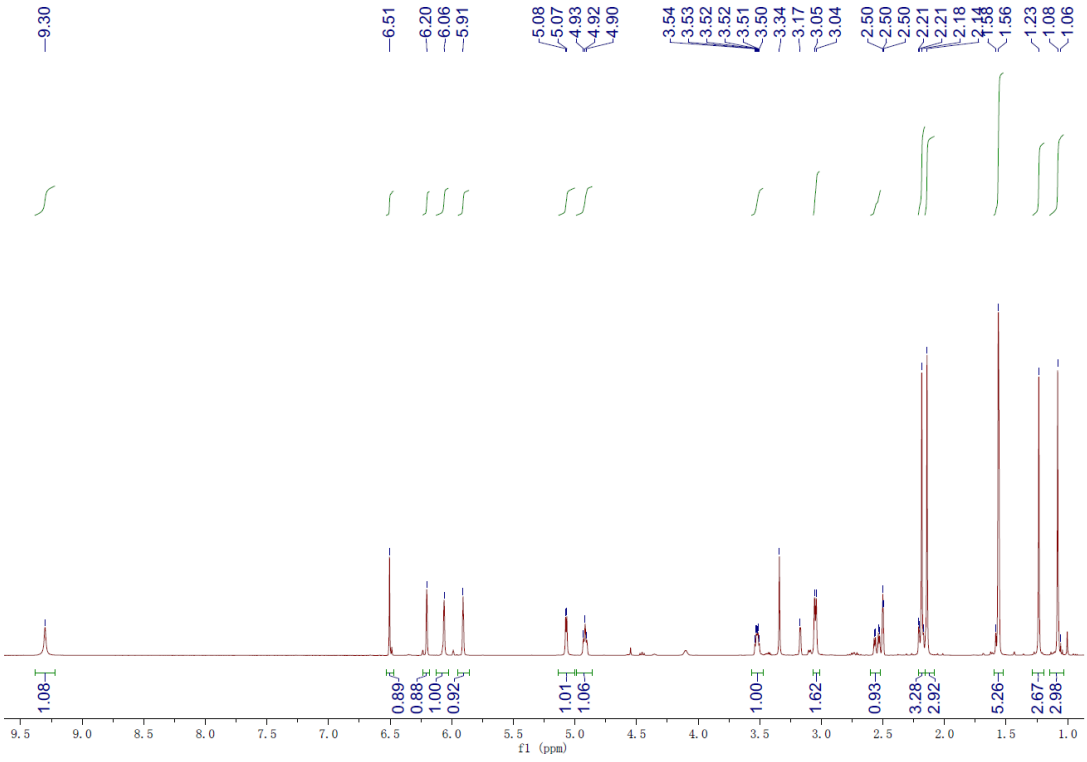

Figure S2. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**

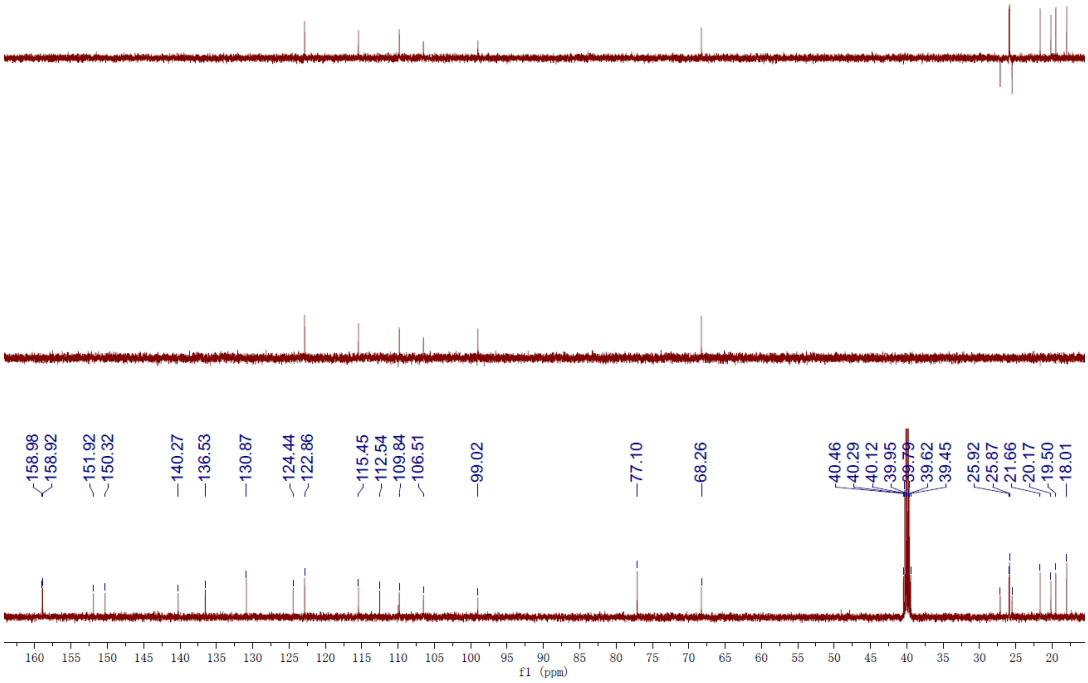

Figure S3. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **1**

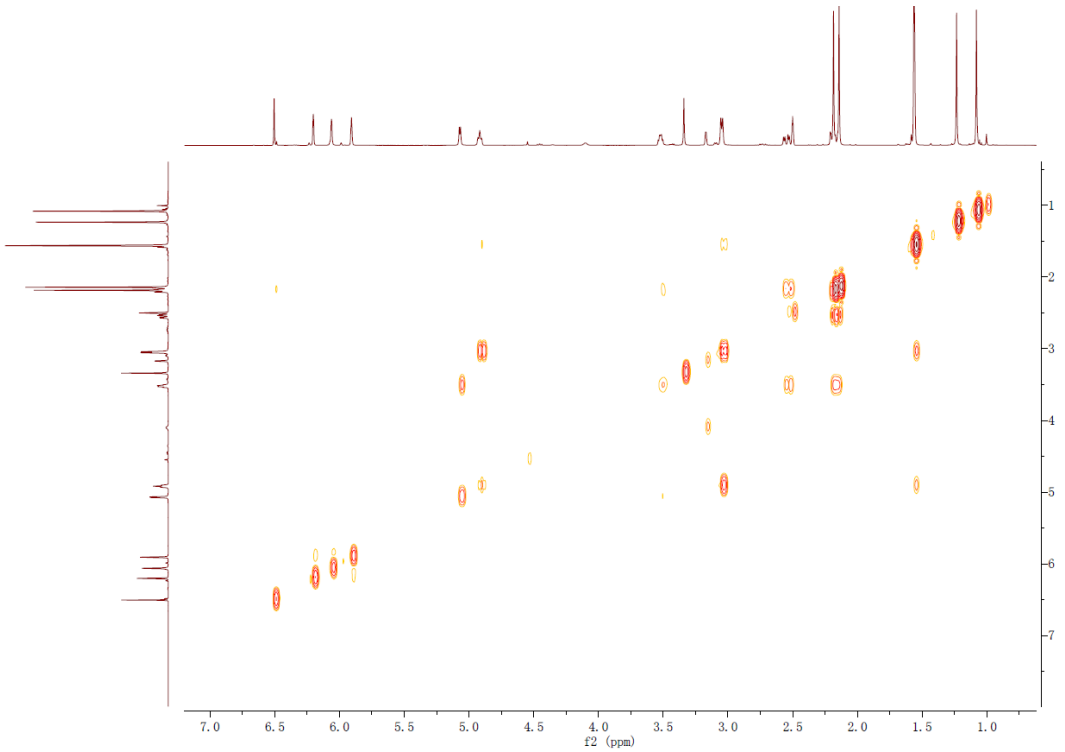

Figure S4. COSY spectrum of compound **1**

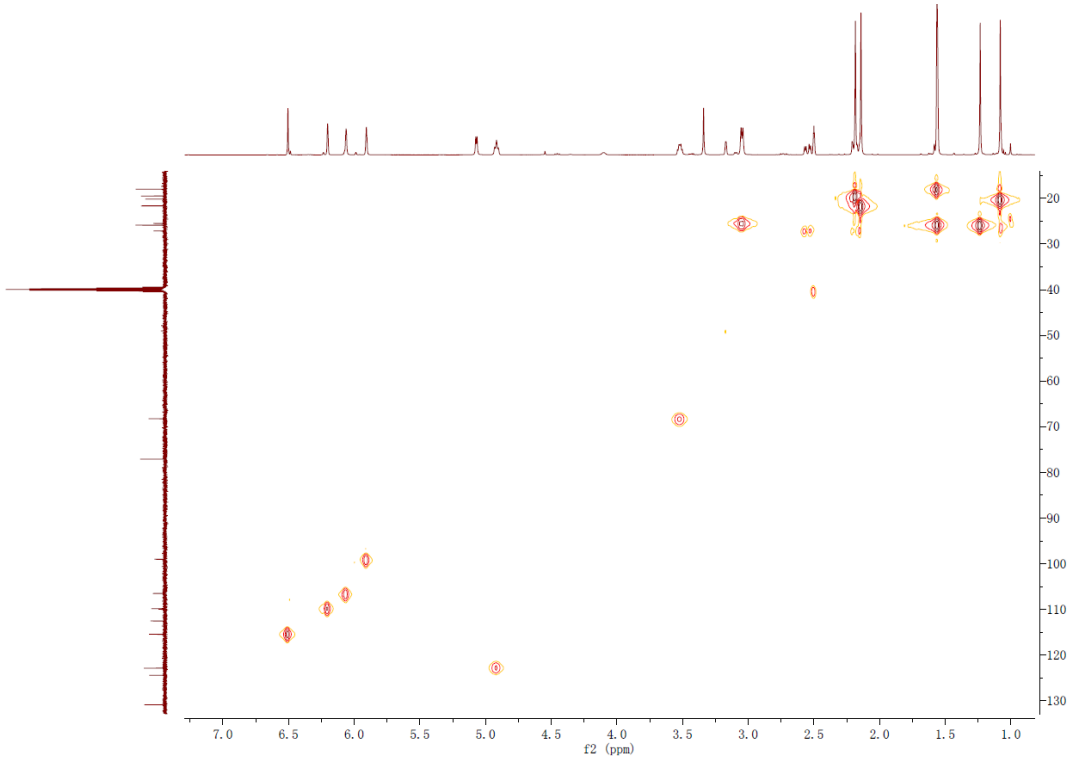

Figure S5. HSQC spectrum of compound **1**

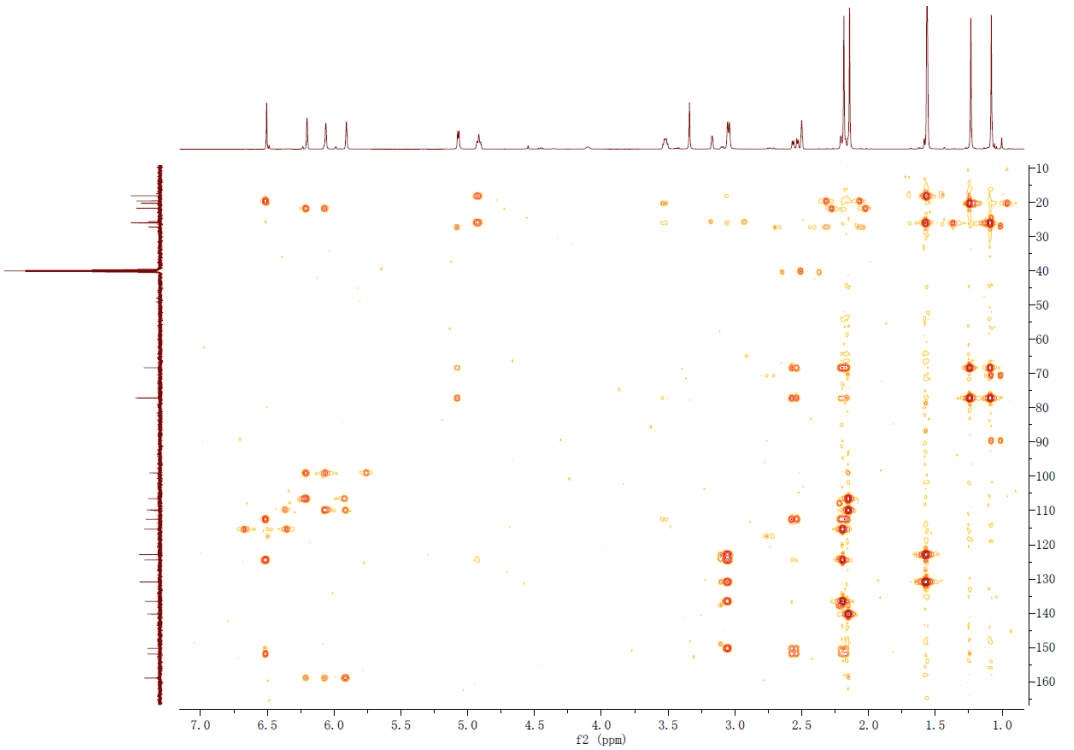

Figure S6. HMBC spectrum of compound **1**

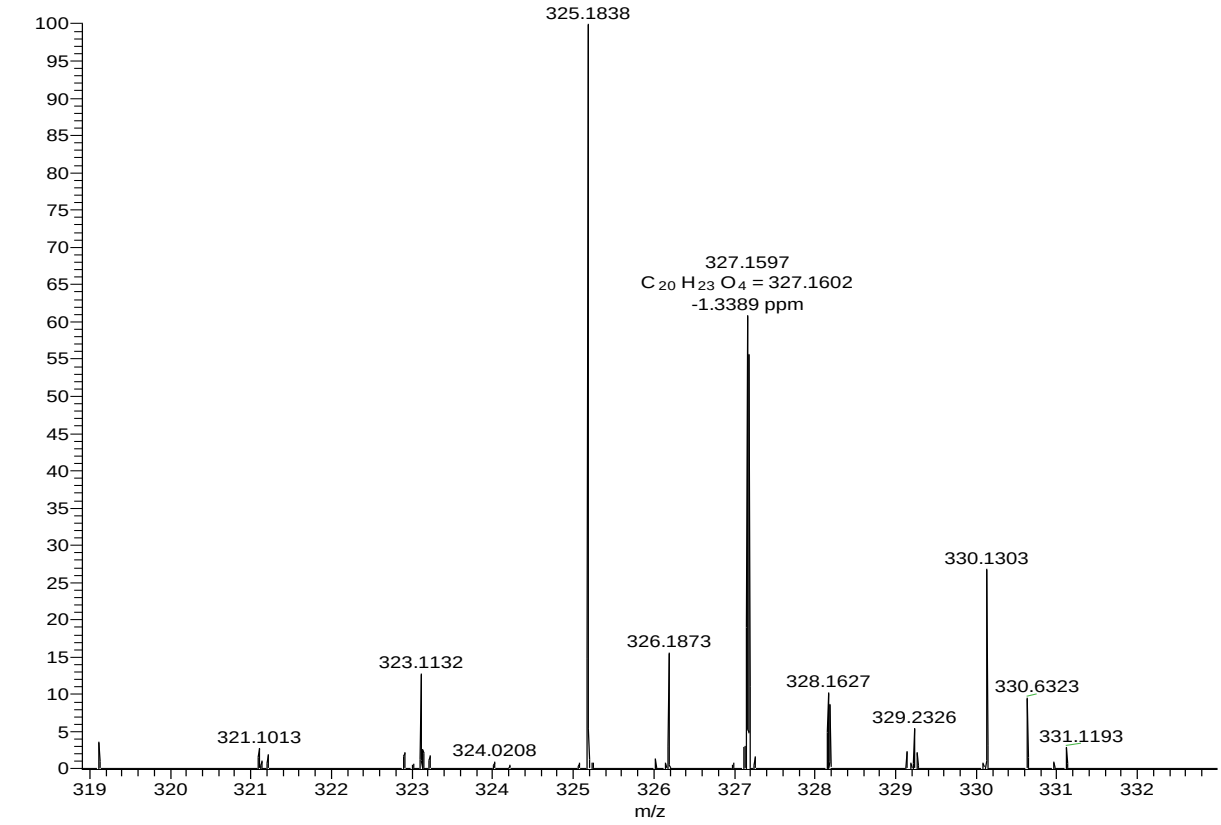

Figure S7. HRESIMS spectrum of compound **2**

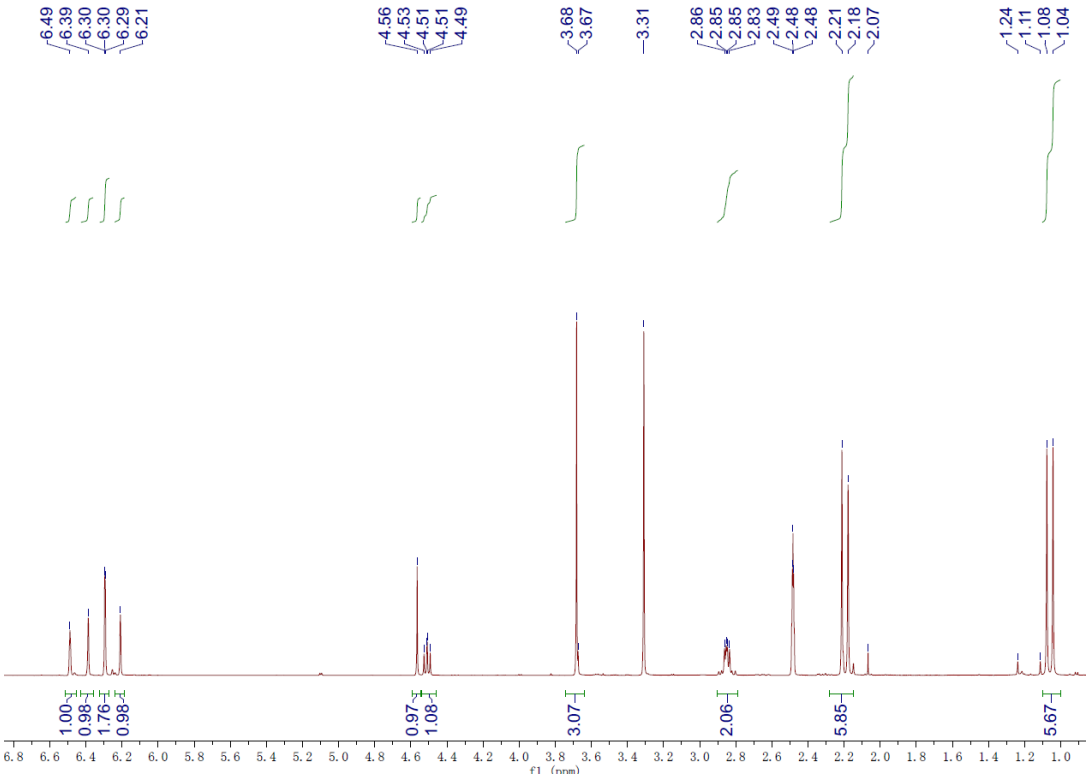

Figure S8. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **2**

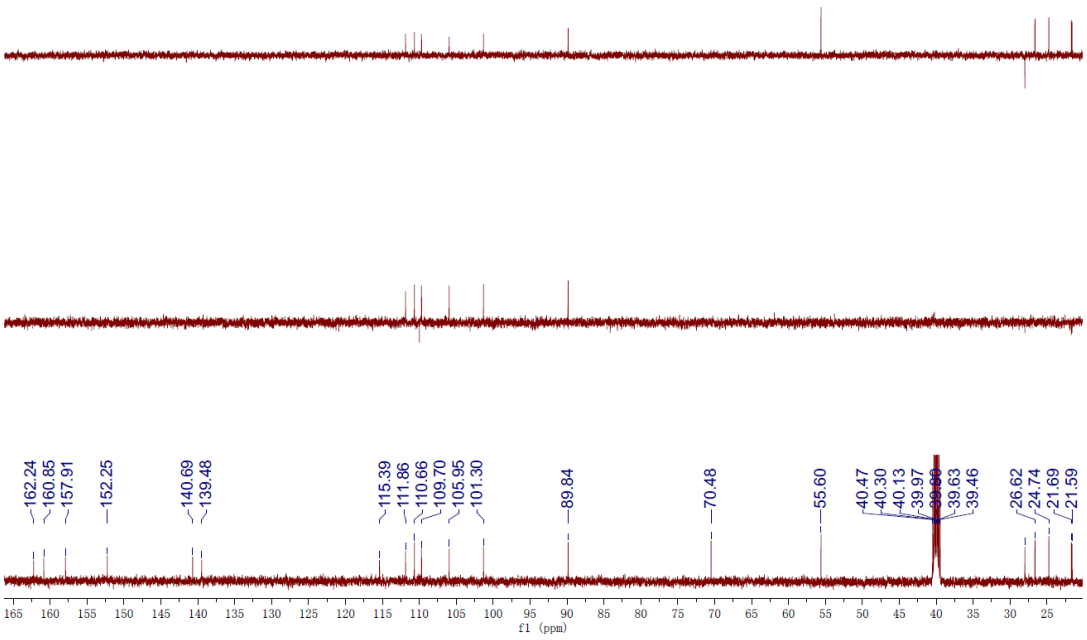

Figure S9. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **2**

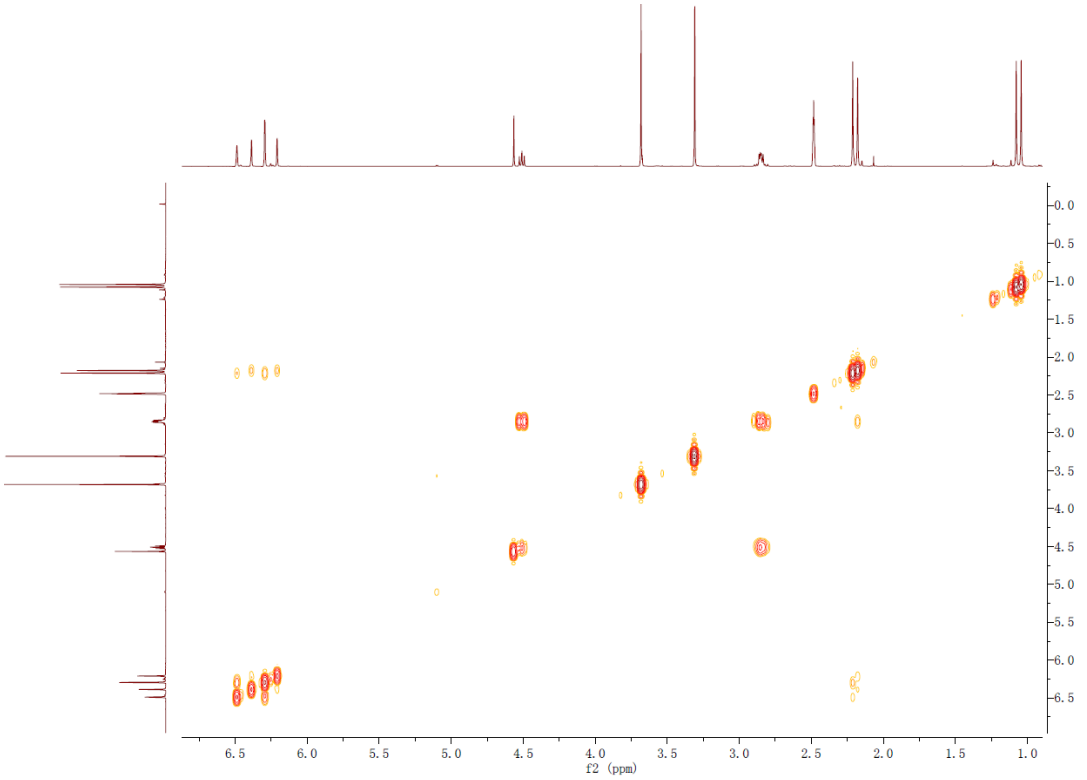

Figure S10. COSY spectrum of compound **2**

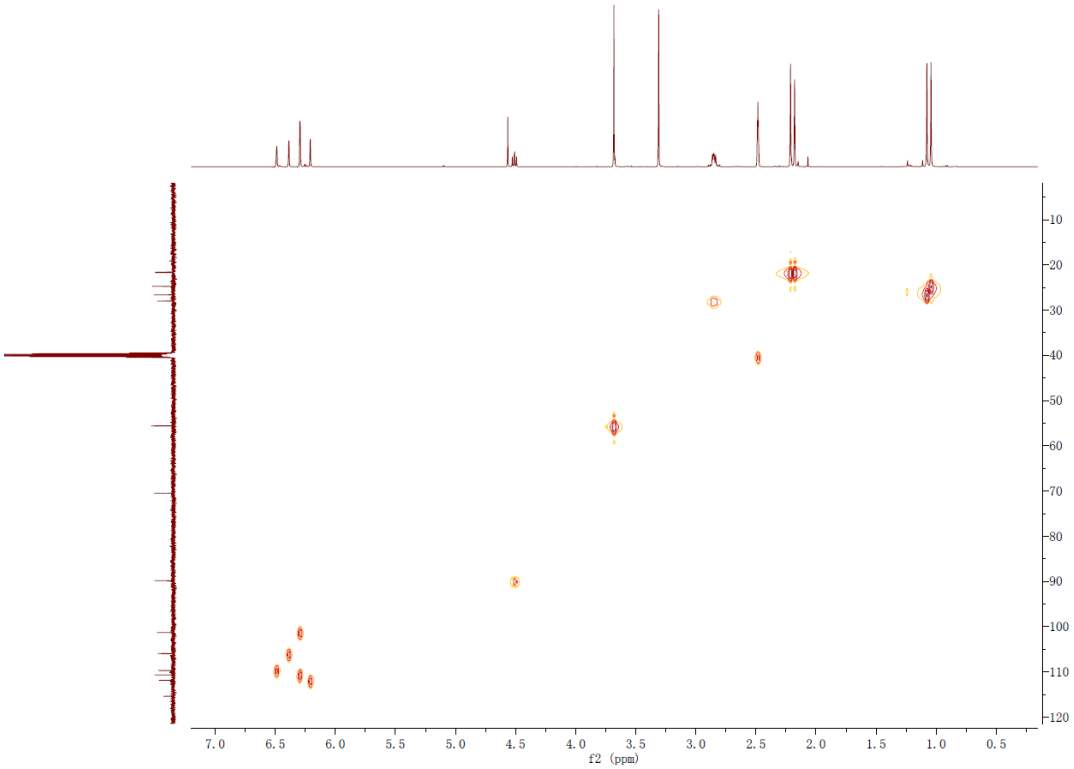

Figure S11. HSQC spectrum of compound **2**

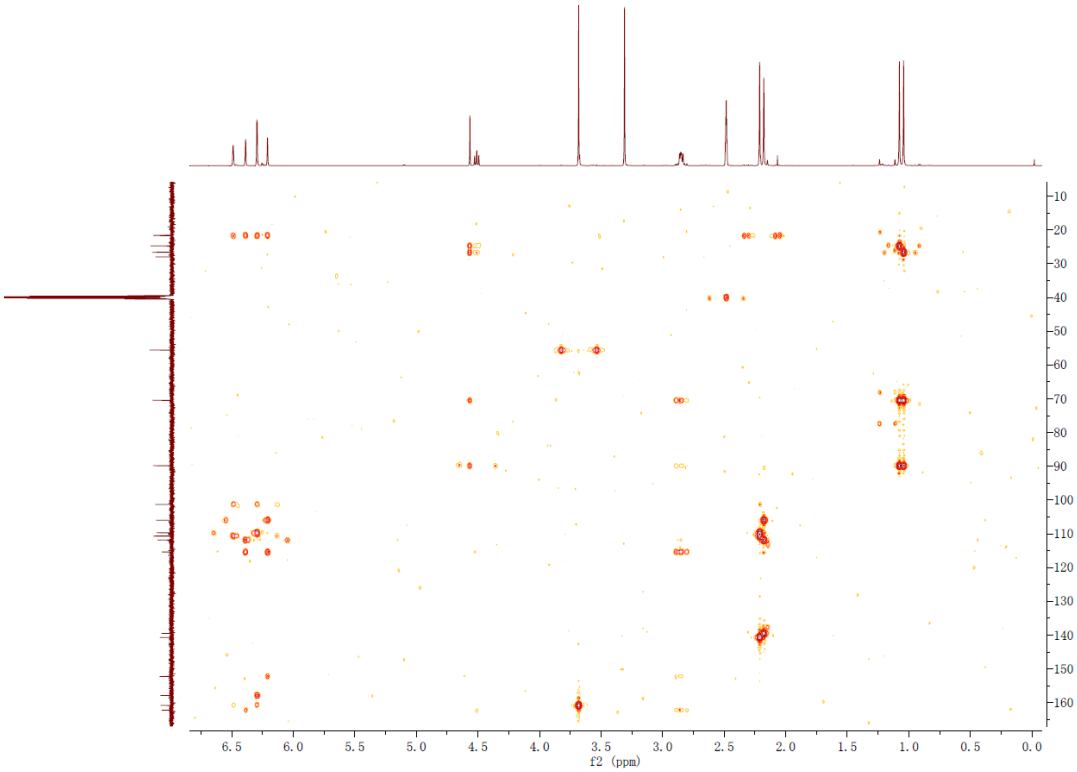

Figure S12. HMBC spectrum of compound **2**

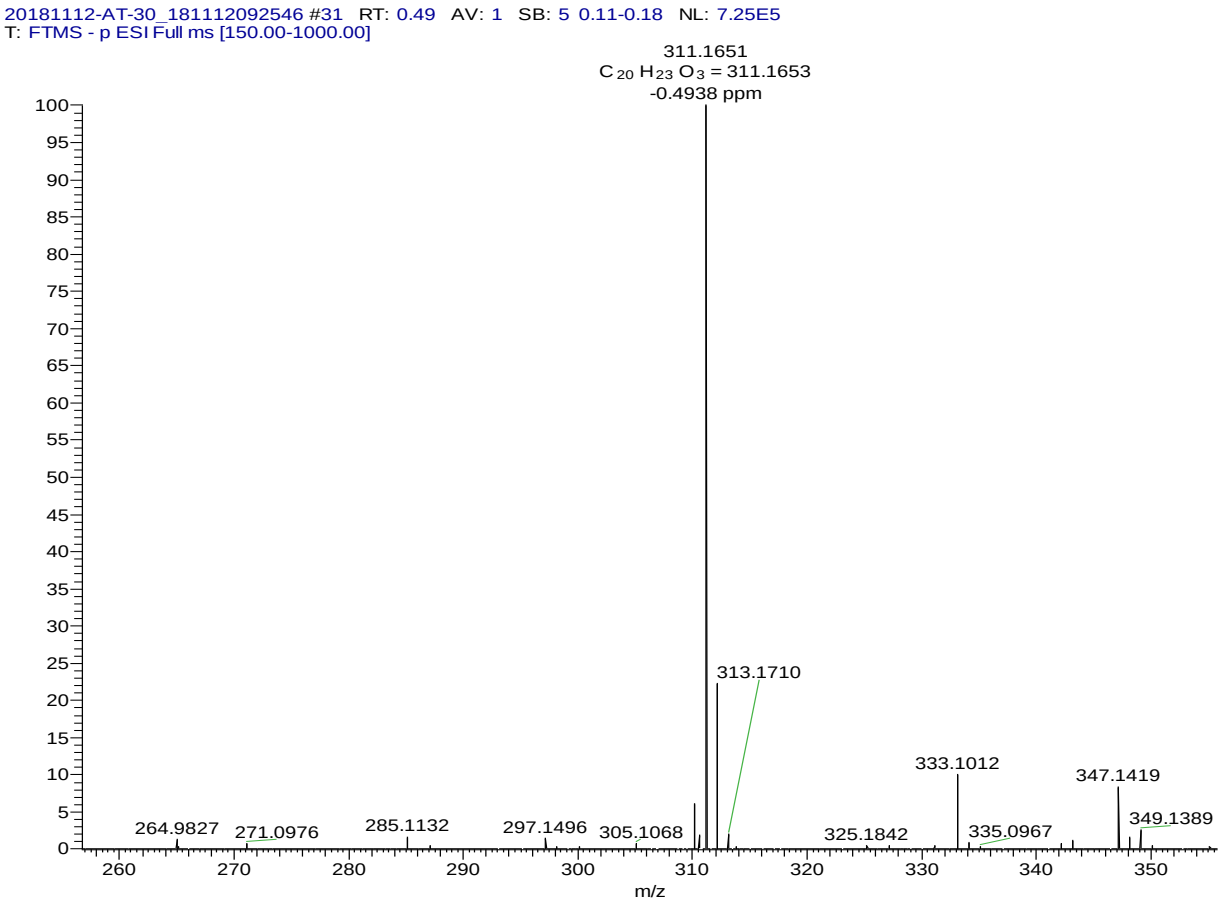

Figure S13. HRESIMS spectrum of compound **3**

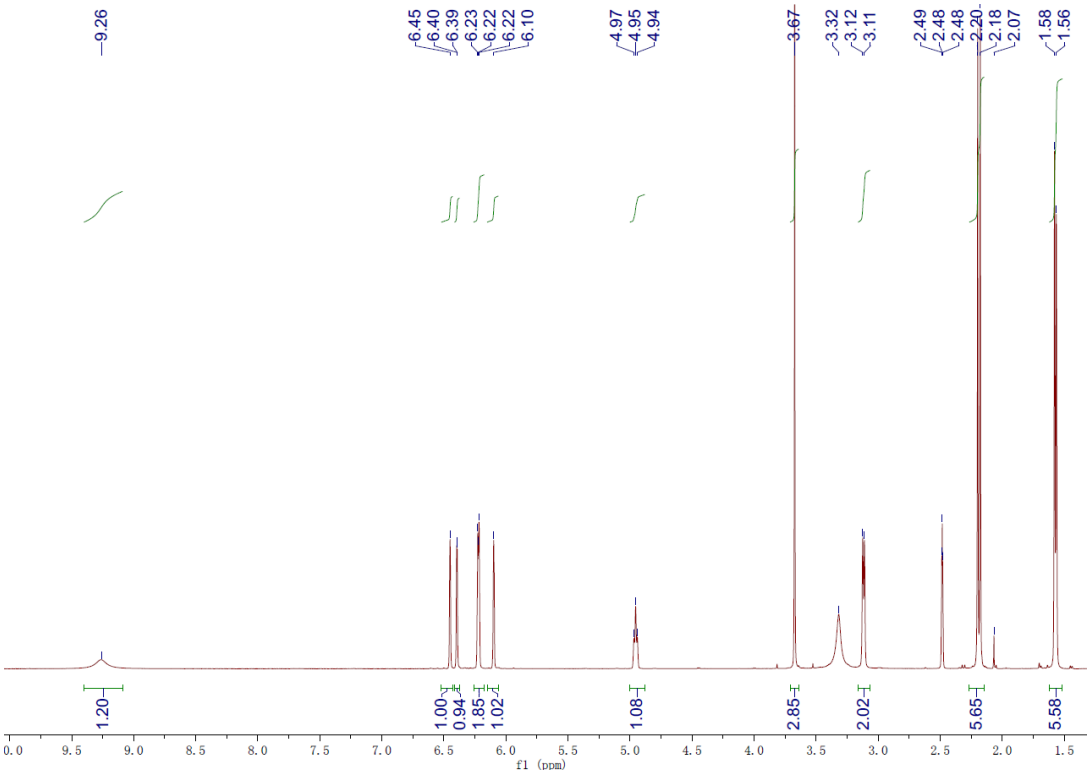

Figure S14. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **3**

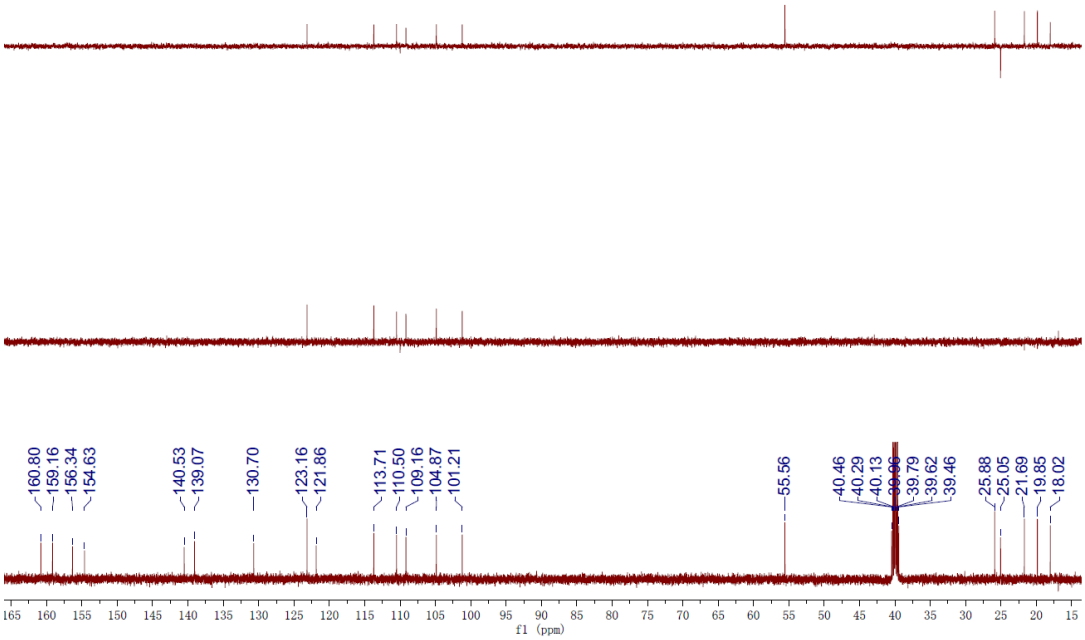

Figure S15. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **3**

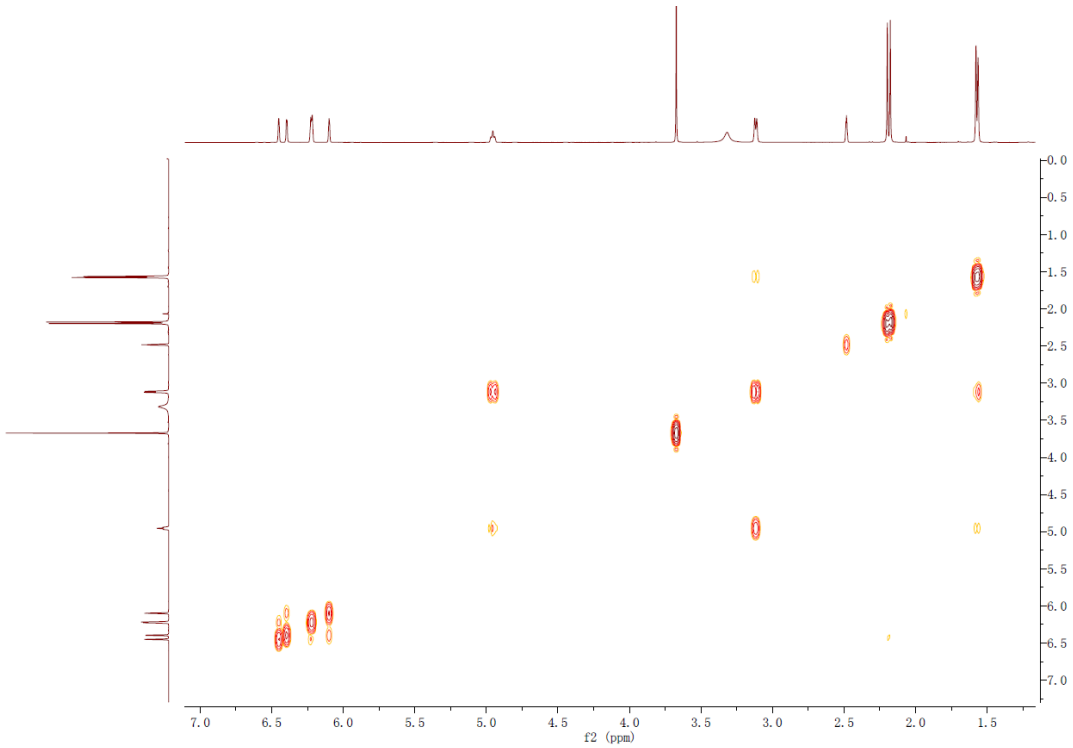

Figure S16. COSY spectrum of compound **3**

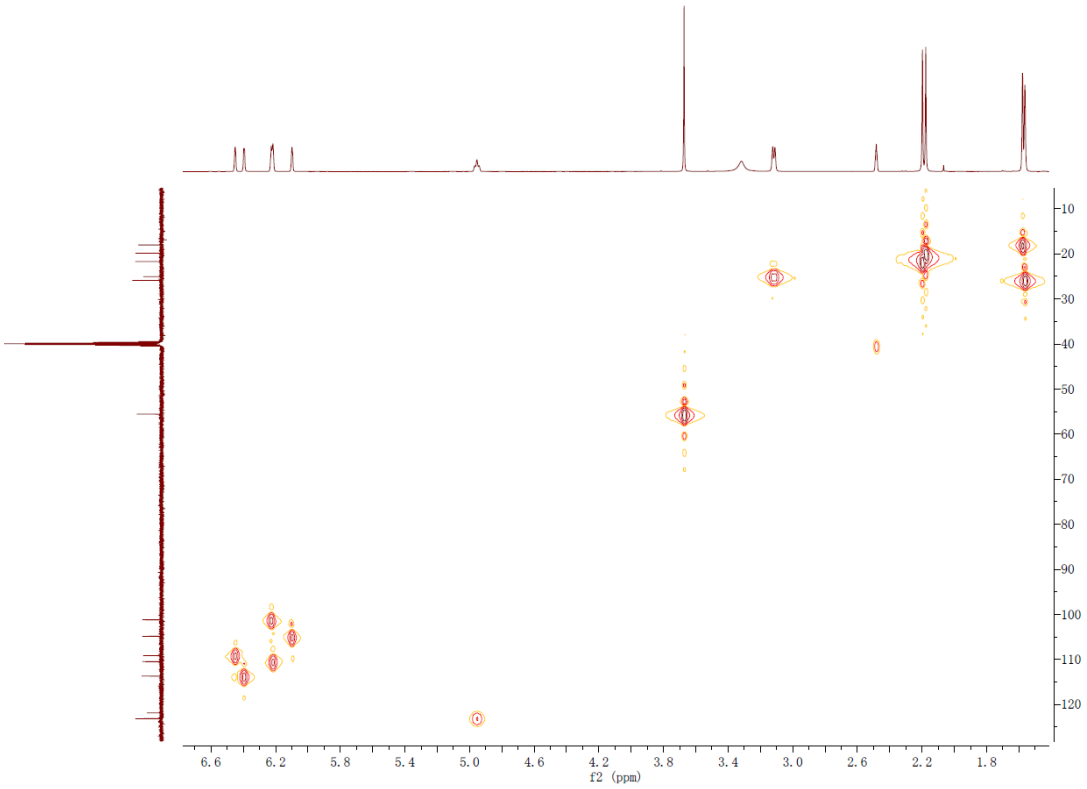

Figure S17. HSQC spectrum of compound **3**

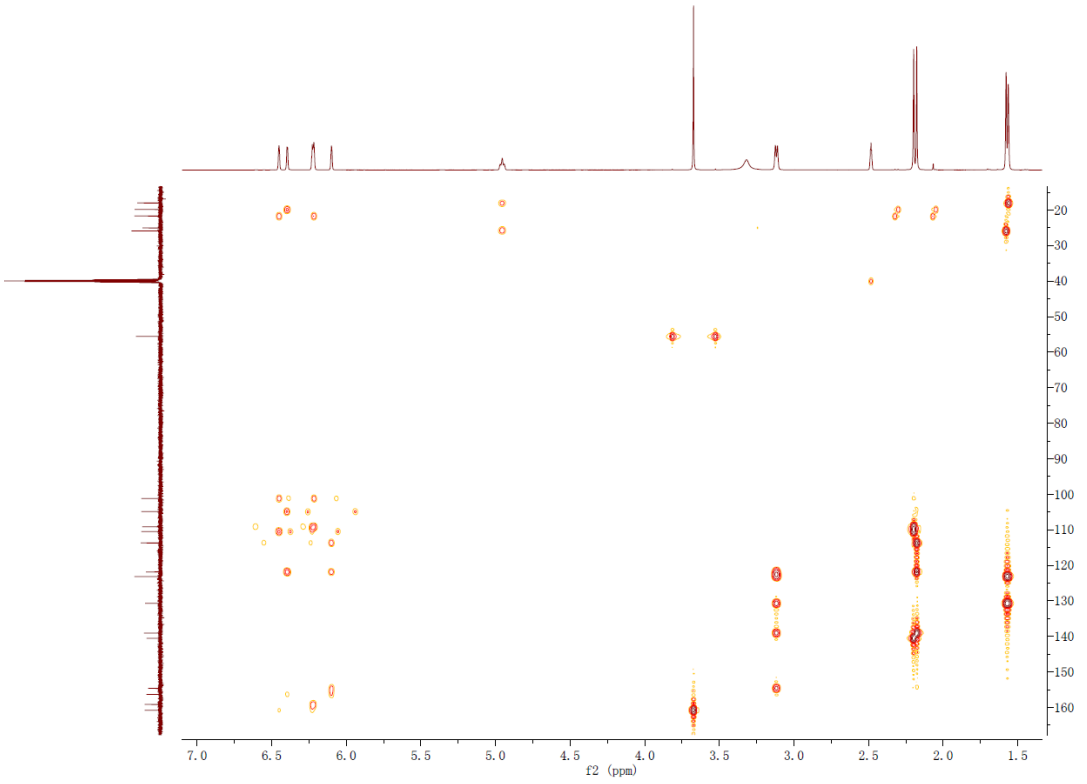

Figure S18. HMBC spectrum of compound **3**

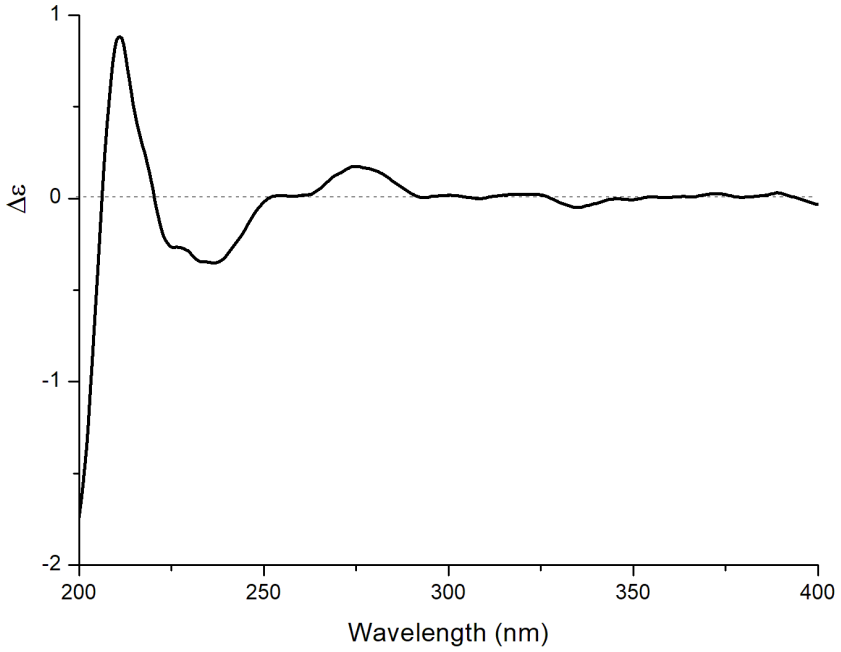

Figure S19. ECD spectrum of compound **2**

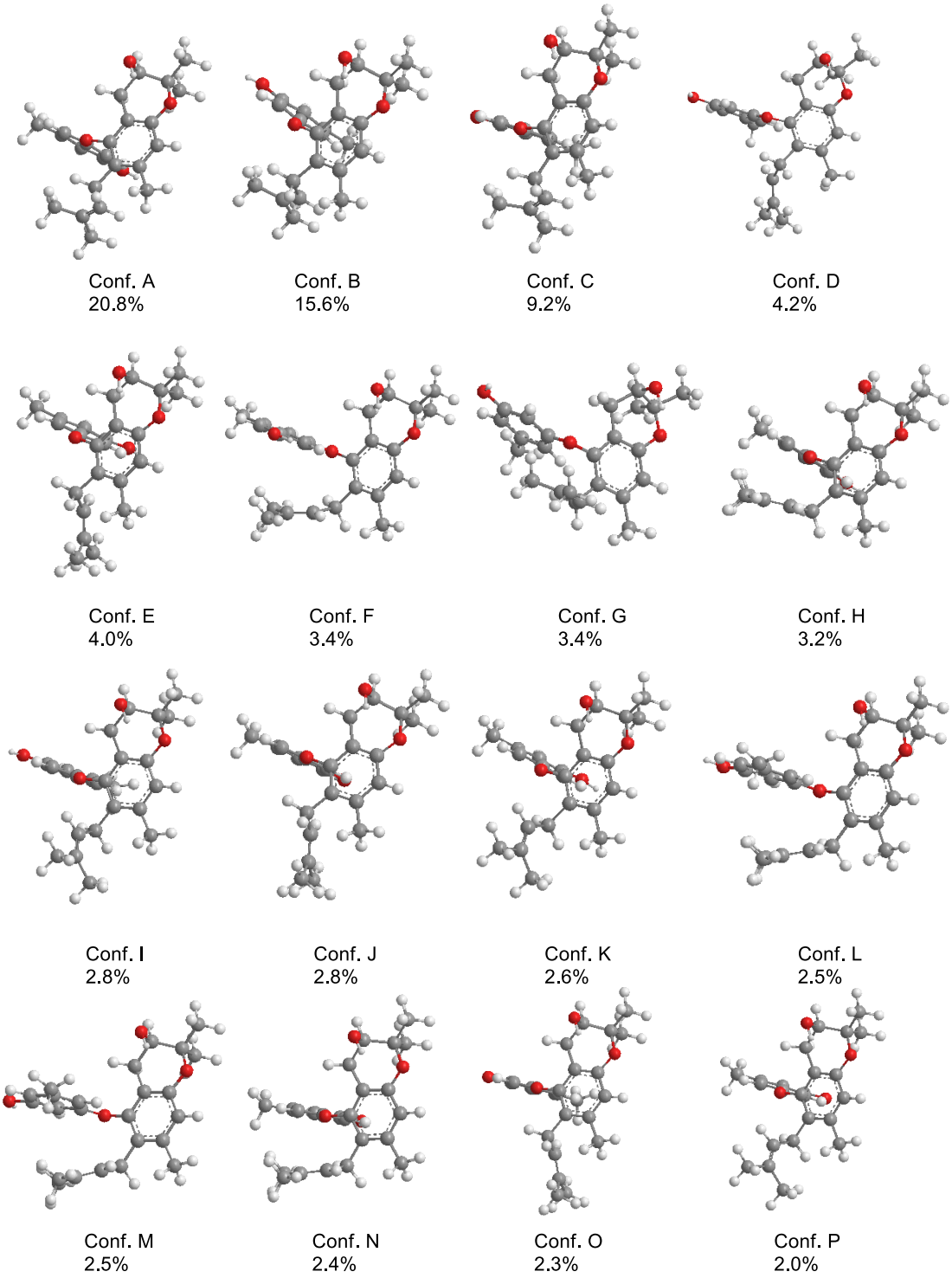

Figure S20. Structure and population of the low-energy conformers (>2%) of 8*R*-**1**

Table S1. Cartesian coordinates of the low-energy conformers (≥2%) of **1**

(8*R*)-**1**,Conf. A		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.255	-2.126	3.725
2	C	-4.7047	-3.1605	2.8974
3	C	-3.8038	-3.8515	2.0932
4	C	-2.4492	-3.5336	2.093
5	C	-1.9895	-2.5061	2.9203
6	C	-2.8886	-1.8167	3.742
7	O	-0.6699	-2.1142	3.0347
8	C	0.1899	-2.4334	2.0028
9	C	0.1638	-1.6703	0.8182
10	C	1.0407	-2.0137	-0.2094
11	C	1.9639	-3.0456	-0.0374
12	C	2.0296	-3.7767	1.1593
13	C	1.1371	-3.4636	2.2081
14	C	-5.2099	-1.4042	4.6278
15	O	-4.2944	-4.8571	1.3116
16	C	1.1681	-4.2165	3.5285
17	C	0.2954	-5.4455	3.5177
18	C	3.078	-4.8493	1.2867
19	O	1.1045	-1.372	-1.4166
20	C	0.0134	-0.489	-1.7477
21	C	-0.4	0.3677	-0.5311
22	C	-0.787	-0.5124	0.6555
23	O	0.6663	1.2436	-0.1299
24	C	0.5418	0.4132	-2.8752
25	C	-1.1541	-1.3213	-2.3046
26	C	-0.7023	-5.7726	4.3637
27	C	-1.1655	-4.9464	5.5322
28	C	-1.4711	-7.0558	4.1808
29	H	-5.7557	-3.4379	2.8792
30	H	-1.7596	-4.0936	1.472
31	H	-2.5145	-1.0319	4.3959
32	H	2.6481	-3.2718	-0.8537
33	H	-4.8844	-0.3722	4.7952
34	H	-6.2102	-1.3609	4.1841
35	H	-5.2726	-1.9168	5.5926
36	H	-3.5503	-5.2767	0.8486
37	H	0.9201	-3.5289	4.3419
38	H	2.1955	-4.5279	3.7514

39	H	0.5277	-6.1453	2.7157
40	H	2.6255	-5.8049	1.5661
41	H	3.605	-5.0104	0.3399
42	H	3.8238	-4.5619	2.0345
43	H	-1.2438	1.0183	-0.788
44	H	-1.7969	-0.9077	0.4998
45	H	-0.7867	0.0939	1.5692
46	H	1.4565	0.685	-0.0034
47	H	-0.2085	1.1464	-3.1887
48	H	0.8282	-0.1835	-3.7493
49	H	1.4473	0.9484	-2.5679
50	H	-1.9916	-0.6823	-2.603
51	H	-0.8328	-1.9007	-3.1782
52	H	-1.5232	-2.0544	-1.5803
53	H	-2.2292	-4.7083	5.4268
54	H	-0.6306	-4.0015	5.642
55	H	-1.0315	-5.5078	6.4629
56	H	-2.5325	-6.8412	4.0176
57	H	-1.1149	-7.6364	3.3234
58	H	-1.3753	-7.6854	5.0714

(8*R*)-**1**,Conf. B		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-3.6738	-4.2476	1.6862
2	C	-4.6751	-3.6611	2.4683
3	C	-4.3589	-2.6303	3.3469
4	C	-3.0525	-2.1708	3.4691
5	C	-2.044	-2.7509	2.6962
6	C	-2.353	-3.7943	1.8156
7	O	-0.7775	-2.242	2.9082
8	C	0.1846	-2.4784	1.9469
9	C	0.1866	-1.7101	0.7656
10	C	1.1701	-1.9663	-0.1887
11	C	2.163	-2.9157	0.0547
12	C	2.1951	-3.6505	1.2505
13	C	1.1982	-3.4248	2.2251
14	C	-3.994	-5.3938	0.7738
15	O	-5.3726	-2.0929	4.085
16	C	1.1876	-4.1862	3.541
17	C	0.4171	-5.4787	3.4577
18	C	3.3163	-4.6332	1.4578

19	O	1.2739	-1.3099	-1.3853
20	C	0.1361	-0.5289	-1.8037
21	C	-0.449	0.2786	-0.6245
22	C	-0.8481	-0.6409	0.5276
23	O	0.4982	1.2441	-0.1387
24	C	0.6677	0.4251	-2.8861
25	C	-0.9023	-1.4607	-2.4514
26	C	-0.602	-5.8988	4.2343
27	C	-1.1969	-5.1366	5.386
28	C	-1.2594	-7.2304	3.9782
29	H	-5.7036	-4.007	2.4016
30	H	-2.7999	-1.3707	4.1571
31	H	-1.5715	-4.2772	1.2348
32	H	2.9267	-3.0752	-0.7047
33	H	-3.8543	-6.3421	1.3018
34	H	-5.0285	-5.3355	0.4193
35	H	-3.347	-5.3804	-0.1096
36	H	-5.0067	-1.3937	4.6515
37	H	0.8239	-3.5273	4.3343
38	H	2.216	-4.4188	3.8413
39	H	0.748	-6.1398	2.6572
40	H	2.9245	-5.6253	1.6994
41	H	3.927	-4.7423	0.555
42	H	3.9747	-4.291	2.2623
43	H	-1.3249	0.8523	-0.9484
44	H	-1.803	-1.1238	0.292
45	H	-0.9748	-0.0435	1.4384
46	H	1.3248	0.7584	0.044
47	H	-0.1195	1.0882	-3.2597
48	H	1.0768	-0.1372	-3.7338
49	H	1.4925	1.0393	-2.5079
50	H	-1.768	-0.8987	-2.8168
51	H	-0.4607	-2.0031	-3.2956
52	H	-1.26	-2.2286	-1.7581
53	H	-2.2656	-4.9696	5.2149
54	H	-0.7377	-4.1604	5.551
55	H	-1.0844	-5.7107	6.3118
56	H	-2.3221	-7.091	3.7539
57	H	-0.8095	-7.7618	3.1329
58	H	-1.1703	-7.8731	4.8601

(8*R*)-**1**,Conf. C		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-3.6346	-4.2169	1.7237
2	C	-4.6365	-3.6386	2.5129
3	C	-4.3161	-2.604	3.3882
4	C	-3.0118	-2.1382	3.4977
5	C	-2.0042	-2.7097	2.7203
6	C	-2.3151	-3.7547	1.8426
7	O	-0.7395	-2.194	2.9233
8	C	0.2207	-2.4369	1.962
9	C	0.2222	-1.6729	0.7781
10	C	1.2002	-1.9379	-0.1792
11	C	2.1901	-2.8905	0.0646
12	C	2.2243	-3.6195	1.2639
13	C	1.2316	-3.3859	2.241
14	C	-3.9492	-5.366	0.8121
15	O	-5.2674	-2.0176	4.1706
16	C	1.2235	-4.1398	3.5611
17	C	0.4547	-5.4342	3.4869
18	C	3.3438	-4.6038	1.4726
19	O	1.301	-1.2882	-1.3796
20	C	0.1654	-0.5024	-1.7949
21	C	-0.4094	0.3137	-0.6166
22	C	-0.8074	-0.5982	0.5421
23	O	0.5454	1.2774	-0.1425
24	C	0.6964	0.4437	-2.8846
25	C	-0.8817	-1.4312	-2.4329
26	C	-0.5623	-5.8507	4.2682
27	C	-1.1567	-5.0804	5.4151
28	C	-1.2166	-7.1858	4.0239
29	H	-5.6563	-4.005	2.4407
30	H	-2.779	-1.3345	4.19
31	H	-1.5348	-4.2327	1.2561
32	H	2.9503	-3.0562	-0.697
33	H	-4.9865	-5.318	0.4646
34	H	-3.3084	-5.3452	-0.0758
35	H	-3.7962	-6.3132	1.3384
36	H	-6.1218	-2.4438	3.9937
37	H	0.8607	-3.4769	4.3516
38	H	2.2528	-4.3693	3.8608
39	H	0.7861	-6.1001	2.6908
40	H	4.0058	-4.259	2.273

41	H	2.9507	-5.5938	1.7206
42	H	3.9512	-4.719	0.5683
43	H	-1.2843	0.89	-0.9388
44	H	-1.7666	-1.0762	0.3146
45	H	-0.9247	0.0037	1.4512
46	H	1.3646	0.7861	0.0574
47	H	-0.089	1.1096	-3.2568
48	H	1.0976	-0.1248	-3.732
49	H	1.5268	1.0549	-2.5137
50	H	-1.7463	-0.8659	-2.7962
51	H	-0.4478	-1.9799	-3.2771
52	H	-1.24	-2.194	-1.7344
53	H	-0.7018	-4.1006	5.5696
54	H	-1.0382	-5.6456	6.3457
55	H	-2.2268	-4.9203	5.2463
56	H	-2.2801	-7.0509	3.8008
57	H	-0.7672	-7.7226	3.1818
58	H	-1.124	-7.8213	4.9106

(8*R*)-**1**,Conf. D		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-3.9847	-3.9304	1.5029
2	C	-4.9951	-3.4085	2.3182
3	C	-4.6942	-2.4309	3.2604
4	C	-3.3939	-1.9629	3.4144
5	C	-2.374	-2.4823	2.6132
6	C	-2.6695	-3.4704	1.6656
7	O	-1.1202	-1.9543	2.8567
8	C	-0.0886	-2.3108	2.0131
9	C	0.0681	-1.6181	0.7963
10	C	1.0992	-2.0051	-0.0573
11	C	1.9908	-3.0089	0.3212
12	C	1.8777	-3.6592	1.5609
13	C	0.8251	-3.3048	2.4332
14	C	-4.2912	-5.0139	0.512
15	O	-5.7168	-1.9529	4.0264
16	C	0.6682	-3.9663	3.7933
17	C	0.0012	-5.3146	3.7207
18	C	2.8797	-4.7294	1.9014
19	O	1.3434	-1.4375	-1.2783
20	C	0.3036	-0.606	-1.8327

21	C	-0.3079	0.3156	-0.7545
22	C	-0.8624	-0.4965	0.414
23	O	0.6694	1.2413	-0.2515
24	C	0.9873	0.236	-2.9227
25	C	-0.7499	-1.5017	-2.5066
26	C	0.4452	-6.4991	4.1871
27	C	1.7472	-6.7247	4.9039
28	C	-0.385	-7.7453	4.0136
29	H	-6.0193	-3.7612	2.2257
30	H	-3.1555	-1.2011	4.1497
31	H	-1.8859	-3.9	1.0466
32	H	2.7912	-3.2795	-0.3655
33	H	-4.1424	-5.9951	0.9731
34	H	-5.3256	-4.942	0.1598
35	H	-3.6429	-4.9322	-0.3667
36	H	-5.3606	-1.2913	4.6422
37	H	0.0688	-3.3308	4.4564
38	H	1.6468	-4.0025	4.2791
39	H	-0.9747	-5.2948	3.2368
40	H	2.3968	-5.7104	1.9194
41	H	3.6849	-4.7739	1.1598
42	H	3.3516	-4.5285	2.8676
43	H	-1.1106	0.9274	-1.1818
44	H	-1.8307	-0.9251	0.1327
45	H	-1.0123	0.1653	1.2754
46	H	1.4415	0.712	0.0247
47	H	0.2837	0.928	-3.397
48	H	1.416	-0.4076	-3.7
49	H	1.8251	0.813	-2.5156
50	H	-1.54	-0.9044	-2.9735
51	H	-0.2874	-2.1276	-3.2788
52	H	-1.217	-2.1958	-1.8006
53	H	1.5615	-7.1632	5.8902
54	H	2.3248	-5.8122	5.061
55	H	2.3748	-7.4167	4.3324
56	H	-0.6351	-8.1732	4.9899
57	H	-1.3245	-7.5506	3.4857
58	H	0.1704	-8.4926	3.4373

(8*R*)-**1**,Conf. E		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z

1	C	-4.5784	-1.8931	3.6624
2	C	-5.0098	-2.8887	2.7795
3	C	-4.095	-3.5268	1.9481
4	C	-2.7431	-3.1973	1.9788
5	C	-2.2995	-2.2102	2.8638
6	C	-3.2155	-1.5706	3.7071
7	O	-0.9894	-1.7933	3.0068
8	C	-0.0612	-2.2445	2.0916
9	C	0.0474	-1.5901	0.8485
10	C	0.9659	-2.0785	-0.0783
11	C	1.8003	-3.1471	0.2499
12	C	1.7421	-3.7611	1.5118
13	C	0.8025	-3.3016	2.4606
14	C	-5.5493	-1.2267	4.5905
15	O	-4.5702	-4.4898	1.1058
16	C	0.7145	-3.9149	3.8494
17	C	-0.0778	-5.1952	3.882
18	C	2.6809	-4.9024	1.796
19	O	1.1512	-1.5564	-1.3295
20	C	0.1466	-0.6418	-1.8136
21	C	-0.2903	0.3453	-0.7089
22	C	-0.8139	-0.3985	0.5181
23	O	0.8017	1.1887	-0.3081
24	C	0.8089	0.1208	-2.973
25	C	-1.0338	-1.4489	-2.3804
26	C	0.3032	-6.4101	4.3257
27	C	1.6509	-6.7494	4.8991
28	C	-0.6546	-7.5732	4.2785
29	H	-6.058	-3.1743	2.7366
30	H	-2.0476	-3.7132	1.3265
31	H	-2.8578	-0.813	4.4015
32	H	2.5145	-3.4965	-0.4941
33	H	-5.2361	-0.201	4.8121
34	H	-6.5458	-1.1713	4.1398
35	H	-5.6155	-1.7871	5.5281
36	H	-3.8248	-4.8641	0.6077
37	H	0.2417	-3.2098	4.544
38	H	1.7266	-4.0324	4.2456
39	H	-1.0971	-5.0885	3.5133
40	H	2.123	-5.8375	1.8968
41	H	3.4033	-5.0384	0.9836
42	H	3.2595	-4.7134	2.705
43	H	-1.0702	1.019	-1.0821

44	H	-1.8347	-0.7463	0.3254
45	H	-0.8357	0.2866	1.374
46	H	1.5441	0.5984	-0.0782
47	H	0.132	0.8665	-3.4026
48	H	1.1132	-0.5689	-3.7692
49	H	1.7252	0.6259	-2.6477
50	H	-1.8049	-0.79	-2.7929
51	H	-0.694	-2.1235	-3.175
52	H	-1.4989	-2.0895	-1.6243
53	H	1.5377	-7.1499	5.9121
54	H	2.3272	-5.8953	4.9641
55	H	2.1405	-7.5096	4.2814
56	H	-0.8308	-7.9604	5.2875
57	H	-1.6258	-7.297	3.8544
58	H	-0.2412	-8.3789	3.663

(8*R*)-**1**,Conf. F		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.6707	-3.4038	2.9454
2	C	-4.2041	-2.5644	3.9618
3	C	-2.8847	-2.1231	3.9498
4	C	-2.0044	-2.5092	2.9426
5	C	-2.4543	-3.3638	1.9334
6	C	-3.7824	-3.8083	1.9402
7	O	-1.6913	-3.8436	0.8862
8	C	-0.3822	-3.4223	0.7783
9	C	-0.1052	-2.2692	0.0172
10	C	1.227	-1.8979	-0.1608
11	C	2.2538	-2.6335	0.4309
12	C	1.9861	-3.7908	1.1788
13	C	0.6477	-4.2149	1.3383
14	C	-6.0797	-3.915	2.9677
15	O	-2.4837	-1.3037	4.9653
16	C	0.3085	-5.4884	2.0982
17	C	0.1451	-5.2586	3.5789
18	C	3.1498	-4.5659	1.7371
19	O	1.6339	-0.8135	-0.8904
20	C	0.6717	-0.2483	-1.8044
21	C	-0.7147	-0.1254	-1.1374
22	C	-1.2113	-1.4802	-0.6352
23	O	-0.6683	0.7866	-0.0269

24	C	1.2139	1.1458	-2.1617
25	C	0.6349	-1.0924	-3.0896
26	C	-0.8446	-5.691	4.386
27	C	-2.0131	-6.5366	3.9612
28	C	-0.8516	-5.3299	5.8492
29	H	-4.863	-2.2495	4.767
30	H	-0.9791	-2.1595	2.9588
31	H	-4.1202	-4.4796	1.1536
32	H	3.2814	-2.3069	0.2793
33	H	-6.4481	-4.0883	1.9511
34	H	-6.1277	-4.8546	3.5266
35	H	-6.7518	-3.189	3.437
36	H	-1.5529	-1.0672	4.8193
37	H	1.106	-6.2258	1.9491
38	H	-0.5735	-5.9492	1.6446
39	H	0.9365	-4.6599	4.0284
40	H	4.0892	-4.013	1.6276
41	H	3.0171	-4.7558	2.8058
42	H	3.2598	-5.5162	1.2054
43	H	-1.4462	0.29	-1.8399
44	H	-1.6025	-2.0685	-1.4734
45	H	-2.026	-1.3125	0.0768
46	H	0.0804	0.5072	0.5325
47	H	0.5367	1.68	-2.8362
48	H	2.1947	1.0695	-2.6459
49	H	1.3692	1.7569	-1.2655
50	H	-0.0563	-0.6673	-3.8248
51	H	1.6314	-1.1482	-3.5434
52	H	0.3358	-2.1277	-2.898
53	H	-2.0155	-7.4778	4.5213
54	H	-2.0069	-6.7926	2.9003
55	H	-2.9523	-6.0138	4.1687
56	H	-0.8198	-6.2356	6.4635
57	H	0.0051	-4.7079	6.1291
58	H	-1.7608	-4.772	6.0969

(8*R*)-**1**,Conf. G		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.1737	-4.0593	0.9126
2	C	-5.1095	-3.6344	1.8628
3	C	-4.6854	-2.9817	3.0154

4	C	-3.3351	-2.7462	3.2468
5	C	-2.3914	-3.1695	2.3079
6	C	-2.8093	-3.8368	1.1501
7	O	-1.0781	-2.9005	2.6406
8	C	-0.1256	-2.9945	1.6468
9	C	0.0497	-1.9166	0.7579
10	C	1.0172	-2.0324	-0.2387
11	C	1.8345	-3.1615	-0.3044
12	C	1.7023	-4.2147	0.6146
13	C	0.7018	-4.1406	1.6072
14	C	-4.6196	-4.8004	-0.3129
15	O	-5.6385	-2.5859	3.9073
16	C	0.5242	-5.2364	2.6441
17	C	1.2474	-4.9275	3.9289
18	C	2.6286	-5.3944	0.4938
19	O	1.2717	-1.073	-1.181
20	C	0.291	-0.0261	-1.3297
21	C	-0.2057	0.4735	0.0449
22	C	-0.7908	-0.6715	0.8689
23	O	0.862	1.0814	0.7901
24	C	1.0112	1.1088	-2.0765
25	C	-0.856	-0.5354	-2.2191
26	C	0.7332	-4.8017	5.1689
27	C	-0.7182	-4.9539	5.5316
28	C	1.6273	-4.4727	6.3364
29	H	-6.1715	-3.8118	1.7119
30	H	-2.9983	-2.2396	4.1455
31	H	-2.0847	-4.1946	0.4235
32	H	2.5924	-3.2096	-1.0846
33	H	-3.9485	-4.6006	-1.1549
34	H	-4.6305	-5.8767	-0.1157
35	H	-5.6235	-4.486	-0.6168
36	H	-5.2005	-2.148	4.6558
37	H	0.9052	-6.1894	2.2599
38	H	-0.5426	-5.4236	2.791
39	H	2.3219	-4.7917	3.8053
40	H	3.4003	-5.2242	-0.2649
41	H	3.1452	-5.5778	1.4409
42	H	2.0675	-6.2871	0.2003
43	H	-0.9663	1.2525	-0.0813
44	H	-1.8011	-0.8991	0.5108
45	H	-0.855	-0.3642	1.9196
46	H	1.5889	0.4307	0.8208

47	H	0.3557	1.9736	-2.2226
48	H	1.359	0.7689	-3.0592
49	H	1.9076	1.4361	-1.5379
50	H	-1.6048	0.2452	-2.3887
51	H	-0.4729	-0.8644	-3.1923
52	H	-1.3603	-1.4059	-1.7875
53	H	-1.1075	-4.0086	5.9241
54	H	-0.8327	-5.7207	6.3053
55	H	-1.3525	-5.2479	4.6939
56	H	1.5786	-5.2683	7.0871
57	H	2.6755	-4.3596	6.04
58	H	1.3112	-3.5337	6.8025

(8*R*)-**1**,Conf. H		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.6501	-2.5319	3.4274
2	C	-5.1588	-3.2642	2.3495
3	C	-4.2929	-3.8128	1.4083
4	C	-2.9147	-3.653	1.5188
5	C	-2.3969	-2.926	2.5939
6	C	-3.2627	-2.3811	3.5492
7	O	-1.0541	-2.7045	2.8313
8	C	-0.1692	-2.9265	1.7962
9	C	0.0057	-1.9306	0.8162
10	C	0.8978	-2.1781	-0.2255
11	C	1.6474	-3.3549	-0.2511
12	C	1.5205	-4.3253	0.7558
13	C	0.5924	-4.1178	1.7986
14	C	-5.5711	-1.9711	4.469
15	O	-4.8444	-4.5161	0.3769
16	C	0.4276	-5.1174	2.9307
17	C	1.2533	-4.7534	4.1366
18	C	2.3751	-5.5613	0.6747
19	O	1.1404	-1.3101	-1.2552
20	C	0.2137	-0.2176	-1.4228
21	C	-0.162	0.4113	-0.063
22	C	-0.7553	-0.6321	0.8815
23	O	0.985	1.0064	0.5652
24	C	0.9466	0.8126	-2.2979
25	C	-1.0168	-0.7189	-2.1978
26	C	0.8318	-4.4863	5.3891

27	C	-0.5994	-4.5007	5.8507
28	C	1.821	-4.1246	6.4669
29	H	-6.2299	-3.4141	2.2385
30	H	-2.2572	-4.0969	0.7802
31	H	-2.8449	-1.8323	4.3908
32	H	2.3497	-3.5059	-1.0693
33	H	-5.7237	-2.7039	5.2672
34	H	-5.1573	-1.0549	4.9034
35	H	-6.5426	-1.7137	4.0341
36	H	-4.1294	-4.8504	-0.1895
37	H	0.729	-6.1183	2.6014
38	H	-0.6348	-5.2297	3.1612
39	H	2.3239	-4.706	3.9372
40	H	2.9442	-5.6981	1.5994
41	H	1.7505	-6.4413	0.4919
42	H	3.1015	-5.4955	-0.1425
43	H	-0.8844	1.2238	-0.2021
44	H	-1.798	-0.824	0.6044
45	H	-0.7334	-0.2449	1.9072
46	H	1.6728	0.3154	0.6083
47	H	0.3337	1.7036	-2.4691
48	H	1.208	0.3808	-3.2713
49	H	1.8943	1.1217	-1.8429
50	H	-1.7299	0.0918	-2.3798
51	H	-0.7184	-1.1406	-3.1648
52	H	-1.5395	-1.5231	-1.6704
53	H	-0.8974	-3.4993	6.1787
54	H	-0.7137	-5.1878	6.6959
55	H	-1.3061	-4.8188	5.0826
56	H	1.7691	-4.848	7.2872
57	H	2.8525	-4.1128	6.0993
58	H	1.5995	-3.129	6.8654

(8*R*)-**1**,Conf. I		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.4266	-3.7593	0.9454
2	C	-5.381	-3.1699	1.7825
3	C	-4.9761	-2.4207	2.8822
4	C	-3.6273	-2.248	3.1714
5	C	-2.6655	-2.8339	2.345
6	C	-3.0651	-3.6004	1.2433

7	O	-1.3554	-2.612	2.7248
8	C	-0.3638	-2.865	1.7987
9	C	-0.0822	-1.9009	0.8113
10	C	0.9246	-2.1754	-0.1127
11	C	1.6762	-3.3467	-0.0137
12	C	1.434	-4.2875	1
13	C	0.3947	-4.0516	1.9254
14	C	-4.8552	-4.6033	-0.2181
15	O	-5.947	-1.8666	3.6639
16	C	0.1134	-5.019	3.0635
17	C	0.926	-4.7058	4.2925
18	C	2.3041	-5.5133	1.0665
19	O	1.2824	-1.3382	-1.1347
20	C	0.3748	-0.2619	-1.4467
21	C	-0.1577	0.4089	-0.1615
22	C	-0.8513	-0.6072	0.7434
23	O	0.9069	1.0325	0.5751
24	C	1.1976	0.7451	-2.2672
25	C	-0.7555	-0.801	-2.34
26	C	1.7476	-5.5183	4.987
27	C	2.026	-6.9608	4.6677
28	C	2.4809	-5.0049	6.1997
29	H	-6.4429	-3.294	1.5851
30	H	-3.3069	-1.6652	4.0289
31	H	-2.3289	-4.0842	0.6068
32	H	2.4704	-3.5176	-0.7384
33	H	-4.1277	-4.54	-1.0342
34	H	-4.9499	-5.6483	0.0925
35	H	-5.8177	-4.2634	-0.6148
36	H	-5.522	-1.389	4.3954
37	H	0.2559	-6.0432	2.7108
38	H	-0.9472	-4.9805	3.3377
39	H	0.8038	-3.6804	4.6441
40	H	1.6994	-6.4194	0.9624
41	H	3.0447	-5.5249	0.2593
42	H	2.8543	-5.5407	2.0112
43	H	-0.8624	1.2108	-0.4099
44	H	-1.854	-0.8168	0.3545
45	H	-0.9498	-0.1853	1.7508
46	H	1.5961	0.353	0.7019
47	H	0.6032	1.6236	-2.5389
48	H	1.5721	0.283	-3.1883
49	H	2.0846	1.079	-1.7172

50	H	-1.4472	-0.0037	-2.631
51	H	-0.3454	-1.2528	-3.2509
52	H	-1.3312	-1.5917	-1.8484
53	H	1.7656	-7.5918	5.5241
54	H	3.0906	-7.0979	4.4504
55	H	1.4659	-7.3356	3.8091
56	H	3.5624	-5.0955	6.0544
57	H	2.2608	-3.9521	6.4056
58	H	2.1986	-5.5826	7.0861

(8*R*)-**1**,Conf. J		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.5648	-2.0458	3.6659
2	C	-4.9735	-3.0276	2.7559
3	C	-4.0449	-3.5912	1.8841
4	C	-2.7091	-3.2034	1.9044
5	C	-2.2881	-2.2343	2.8165
6	C	-3.2159	-1.6655	3.6969
7	O	-0.9967	-1.7637	2.9532
8	C	-0.0409	-2.214	2.0665
9	C	0.0953	-1.5619	0.8252
10	C	1.0536	-2.0346	-0.0692
11	C	1.8992	-3.0841	0.2901
12	C	1.8094	-3.6975	1.5503
13	C	0.8266	-3.2573	2.4643
14	C	-5.5411	-1.4523	4.6378
15	O	-4.4124	-4.5468	0.9816
16	C	0.6951	-3.881	3.8447
17	C	-0.0322	-5.1998	3.8278
18	C	2.756	-4.8241	1.8663
19	O	1.2676	-1.5129	-1.3163
20	C	0.2471	-0.6394	-1.8413
21	C	-0.2494	0.348	-0.7624
22	C	-0.7843	-0.3944	0.4603
23	O	0.8068	1.2282	-0.3435
24	C	0.9163	0.1284	-2.9934
25	C	-0.8916	-1.4909	-2.4283
26	C	0.3693	-6.3875	4.3239
27	C	1.6722	-6.6454	5.0278
28	C	-0.5139	-7.6023	4.1987
29	H	-6.0125	-3.3436	2.7366

30	H	-2.0201	-3.6749	1.211
31	H	-2.8767	-0.918	4.4114
32	H	2.643	-3.4223	-0.4293
33	H	-5.5586	-2.0434	5.5585
34	H	-5.2685	-0.4206	4.8838
35	H	-6.5501	-1.4286	4.213
36	H	-5.3602	-4.7286	1.0893
37	H	0.151	-3.2068	4.5169
38	H	1.6911	-3.9509	4.29
39	H	-1.0128	-5.1533	3.3542
40	H	3.2741	-4.6453	2.8131
41	H	2.2153	-5.7736	1.9114
42	H	3.5303	-4.9229	1.0975
43	H	-1.0377	0.994	-1.1657
44	H	-1.7917	-0.7686	0.2472
45	H	-0.8433	0.2992	1.3077
46	H	1.5578	0.6606	-0.0854
47	H	0.2281	0.8461	-3.4516
48	H	1.2638	-0.562	-3.7711
49	H	1.807	0.667	-2.6509
50	H	-1.6699	-0.8621	-2.8729
51	H	-0.5088	-2.1666	-3.2021
52	H	-1.3592	-2.1339	-1.6758
53	H	2.2836	-5.7509	5.1595
54	H	2.2667	-7.3706	4.4623
55	H	1.4848	-7.0572	6.0252
56	H	-0.767	-7.9909	5.1906
57	H	-1.4525	-7.3842	3.6782
58	H	0.0015	-8.3885	3.6374

(8*R*)-**1**,Conf. K		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.9011	-1.9313	3.2866
2	C	-5.4092	-2.7357	2.261
3	C	-4.5411	-3.4339	1.4272
4	C	-3.1617	-3.354	1.595
5	C	-2.6447	-2.5546	2.6183
6	C	-3.5136	-1.8594	3.4673
7	O	-1.301	-2.397	2.9008
8	C	-0.3918	-2.7634	1.9293
9	C	-0.1187	-1.8733	0.8724

10	C	0.7998	-2.2638	-0.1002
11	C	1.4789	-3.4773	0.0144
12	C	1.2497	-4.3448	1.0944
13	C	0.2963	-3.9903	2.073
14	C	-5.8282	-1.2077	4.2166
15	O	-5.0919	-4.2023	0.4429
16	C	0.0375	-4.8729	3.2831
17	C	0.9541	-4.5477	4.4329
18	C	2.0443	-5.6203	1.1739
19	O	1.138	-1.5076	-1.1895
20	C	0.288	-0.3836	-1.4965
21	C	-0.1067	0.3851	-0.2163
22	C	-0.8031	-0.5338	0.7853
23	O	1.0465	0.9667	0.4133
24	C	1.1198	0.5205	-2.4213
25	C	-0.9361	-0.8813	-2.2838
26	C	1.7729	-5.3733	5.1153
27	C	1.9405	-6.8455	4.8615
28	C	2.6202	-4.8441	6.2441
29	H	-6.4819	-2.826	2.1083
30	H	-2.5036	-3.9136	0.9405
31	H	-3.0991	-1.255	4.2716
32	H	2.2081	-3.7393	-0.7506
33	H	-6.0656	-1.8416	5.0764
34	H	-5.3733	-0.2786	4.576
35	H	-6.7596	-0.9373	3.7082
36	H	-4.3769	-4.6407	-0.0473
37	H	0.0897	-5.9222	2.9832
38	H	-0.9962	-4.7488	3.6262
39	H	0.9191	-3.4994	4.7331
40	H	2.7182	-5.728	0.317
41	H	2.6626	-5.6295	2.0759
42	H	1.3782	-6.4885	1.171
43	H	-0.7711	1.2221	-0.4602
44	H	-1.8419	-0.6916	0.4748
45	H	-0.8035	-0.0568	1.7727
46	H	1.6928	0.2461	0.5382
47	H	0.5705	1.4259	-2.6991
48	H	1.3965	-0.0112	-3.3395
49	H	2.0639	0.8147	-1.9493
50	H	-1.5896	-0.0508	-2.5702
51	H	-0.6226	-1.4048	-3.1947
52	H	-1.5295	-1.6036	-1.7142

53	H	1.7019	-7.412	5.7679
54	H	2.9772	-7.0624	4.5831
55	H	1.3009	-7.2284	4.0643
56	H	3.6813	-5.0114	6.0314
57	H	2.4792	-3.7699	6.4035
58	H	2.3675	-5.3545	7.1792

(8*R*)-**1**,Conf. L		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-3.1589	-2.2634	3.6315
2	C	-4.3733	-2.9391	3.4593
3	C	-4.494	-3.8977	2.4571
4	C	-3.4218	-4.2039	1.6283
5	C	-2.2017	-3.5474	1.7982
6	C	-2.072	-2.5809	2.802
7	O	-1.2042	-3.9411	0.9278
8	C	0.0039	-3.2764	0.9698
9	C	0.1731	-2.1266	0.1728
10	C	1.4231	-1.5087	0.1606
11	C	2.4665	-2.0017	0.9443
12	C	2.3094	-3.1557	1.7279
13	C	1.066	-3.8264	1.7261
14	C	-2.9959	-1.2576	4.7326
15	O	-5.6634	-4.5717	2.2581
16	C	0.8569	-5.1063	2.5209
17	C	0.4235	-4.8485	3.9413
18	C	3.497	-3.6612	2.5027
19	O	1.7265	-0.3978	-0.5795
20	C	0.8281	-0.0727	-1.6599
21	C	-0.6435	-0.1985	-1.2121
22	C	-0.9467	-1.6013	-0.6882
23	O	-0.9472	0.7545	-0.1791
24	C	1.1458	1.3848	-2.0339
25	C	1.1522	-0.9608	-2.8732
26	C	-0.5913	-5.4196	4.6211
27	C	-1.516	-6.4777	4.0856
28	C	-0.8895	-5.0067	6.0391
29	H	-5.2119	-2.7114	4.1105
30	H	-3.5339	-4.9575	0.8547
31	H	-1.1259	-2.0711	2.9612
32	H	3.4248	-1.4857	0.9183

33	H	-2.2922	-0.4708	4.4409
34	H	-3.9494	-0.7708	4.9628
35	H	-2.6232	-1.7501	5.636
36	H	-6.3217	-4.2423	2.8914
37	H	1.7921	-5.6782	2.5446
38	H	0.1605	-5.7522	1.979
39	H	1.0179	-4.0968	4.4595
40	H	3.2403	-3.8165	3.5543
41	H	3.8589	-4.599	2.0697
42	H	4.325	-2.9442	2.4805
43	H	-1.3204	0.031	-2.043
44	H	-1.0842	-2.2918	-1.5286
45	H	-1.8796	-1.566	-0.1166
46	H	-0.2774	0.6311	0.5196
47	H	0.4935	1.7456	-2.8359
48	H	2.1866	1.4836	-2.3645
49	H	1.0411	2.0516	-1.1708
50	H	0.5169	-0.7116	-3.7295
51	H	2.1998	-0.8383	-3.1724
52	H	1.0271	-2.0257	-2.6532
53	H	-2.5516	-6.1238	4.1165
54	H	-1.4453	-7.381	4.701
55	H	-1.2997	-6.7704	3.0567
56	H	-0.8012	-5.8667	6.7109
57	H	-0.206	-4.231	6.4001
58	H	-1.9078	-4.6105	6.1117

(8*R*)-**1**,Conf. M		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-3.1185	-2.178	3.7306
2	C	-4.338	-2.8538	3.6131
3	C	-4.5077	-3.8158	2.6238
4	C	-3.4742	-4.1297	1.748
5	C	-2.2455	-3.4743	1.8655
6	C	-2.0698	-2.5014	2.8564
7	O	-1.2872	-3.8766	0.9549
8	C	-0.057	-3.2525	0.9769
9	C	0.1341	-2.1089	0.176
10	C	1.4023	-1.5305	0.1405
11	C	2.4436	-2.056	0.9055
12	C	2.2641	-3.2035	1.6937

13	C	1.0005	-3.8351	1.7149
14	C	-2.9108	-1.1678	4.8193
15	O	-5.7176	-4.4417	2.5482
16	C	0.7668	-5.1062	2.5172
17	C	0.3658	-4.8308	3.9437
18	C	3.4486	-3.7443	2.4494
19	O	1.7268	-0.4294	-0.605
20	C	0.8179	-0.0723	-1.6662
21	C	-0.648	-0.1535	-1.1902
22	C	-0.9849	-1.5472	-0.6626
23	O	-0.9031	0.806	-0.1507
24	C	1.174	1.3757	-2.0424
25	C	1.0899	-0.9663	-2.8879
26	C	-0.6327	-5.3949	4.6527
27	C	-1.5611	-6.4671	4.1542
28	C	-0.9064	-4.9578	6.0687
29	H	-5.1598	-2.6348	4.2901
30	H	-3.6015	-4.8833	0.978
31	H	-1.1177	-1.991	2.9718
32	H	3.417	-1.5701	0.8622
33	H	-2.4892	-1.6541	5.7045
34	H	-2.2296	-0.3758	4.4907
35	H	-3.856	-0.6889	5.0956
36	H	-5.6946	-5.0708	1.8086
37	H	1.6841	-5.7066	2.5257
38	H	0.0392	-5.7297	1.9901
39	H	0.9666	-4.068	4.438
40	H	3.2035	-3.8954	3.5044
41	H	3.7772	-4.6907	2.0087
42	H	4.2959	-3.0506	2.4166
43	H	-1.3331	0.0983	-2.0078
44	H	-1.1597	-2.2314	-1.5013
45	H	-1.9051	-1.4851	-0.0726
46	H	-0.2237	0.6634	0.535
47	H	0.5176	1.7596	-2.8302
48	H	2.2106	1.4428	-2.3933
49	H	1.1075	2.0424	-1.1754
50	H	0.446	-0.6945	-3.7309
51	H	2.1348	-0.876	-3.2074
52	H	0.9355	-2.0274	-2.6681
53	H	-1.3515	-6.7881	3.1323
54	H	-2.5966	-6.113	4.1837
55	H	-1.4848	-7.3535	4.7931

56	H	-0.7978	-5.8043	6.7546
57	H	-0.2224	-4.1701	6.4015
58	H	-1.9262	-4.5682	6.154

(8*R*)-**1**,Conf. N		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.6248	-2.6794	3.3943
2	C	-5.1081	-3.3993	2.2953
3	C	-4.2175	-3.8821	1.3387
4	C	-2.8479	-3.6696	1.4567
5	C	-2.356	-2.9584	2.5519
6	C	-3.2437	-2.4766	3.5208
7	O	-1.0241	-2.6908	2.7996
8	C	-0.1184	-2.9048	1.7811
9	C	0.0589	-1.9093	0.8013
10	C	0.9798	-2.1421	-0.2187
11	C	1.7528	-3.3038	-0.2235
12	C	1.62	-4.2746	0.7821
13	C	0.6644	-4.0821	1.8031
14	C	-5.5627	-2.1847	4.4551
15	O	-4.6578	-4.5844	0.2545
16	C	0.4911	-5.0838	2.9318
17	C	1.2896	-4.709	4.1533
18	C	2.4952	-5.497	0.7209
19	O	1.2285	-1.2719	-1.2455
20	C	0.2739	-0.2095	-1.4455
21	C	-0.149	0.4209	-0.1004
22	C	-0.734	-0.6293	0.8415
23	O	0.9679	1.0528	0.5467
24	C	0.996	0.8333	-2.3147
25	C	-0.9243	-0.753	-2.2424
26	C	0.8432	-4.4579	5.4004
27	C	-0.5942	-4.5073	5.8391
28	C	1.8073	-4.0792	6.4948
29	H	-6.1749	-3.5782	2.1971
30	H	-2.1896	-4.0715	0.6935
31	H	-2.8468	-1.9371	4.3784
32	H	2.4747	-3.4444	-1.0261
33	H	-5.6817	-2.9449	5.2332
34	H	-5.1838	-1.2649	4.9131
35	H	-6.5459	-1.9548	4.0314

36	H	-5.6239	-4.6674	0.3087
37	H	0.812	-6.0804	2.608
38	H	-0.5737	-5.2102	3.1426
39	H	2.3618	-4.6367	3.9704
40	H	3.0438	-5.6264	1.6589
41	H	1.889	-6.3864	0.522
42	H	3.2403	-5.4189	-0.0782
43	H	-0.8897	1.2123	-0.263
44	H	-1.7662	-0.8488	0.5463
45	H	-0.7413	-0.2337	1.8642
46	H	1.6714	0.3791	0.6112
47	H	0.3616	1.7045	-2.5082
48	H	1.2912	0.4002	-3.2778
49	H	1.924	1.1742	-1.8422
50	H	-1.6549	0.0357	-2.4497
51	H	-0.5924	-1.1768	-3.1976
52	H	-1.4372	-1.5655	-1.7179
53	H	-0.7051	-5.197	6.6828
54	H	-1.2805	-4.8433	5.0602
55	H	-0.922	-3.5136	6.162
56	H	1.7598	-4.808	7.3106
57	H	2.8437	-4.0417	6.143
58	H	1.5569	-3.0912	6.8948

(8*R*)-**1**,Conf. O		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-3.9484	-3.9039	1.5506
2	C	-4.9598	-3.3798	2.3652
3	C	-4.6537	-2.3915	3.2969
4	C	-3.3541	-1.9207	3.4388
5	C	-2.3349	-2.4418	2.6409
6	C	-2.6332	-3.4383	1.7034
7	O	-1.0816	-1.9099	2.8753
8	C	-0.0524	-2.2727	2.0316
9	C	0.1018	-1.5868	0.8107
10	C	1.1279	-1.9817	-0.0451
11	C	2.0185	-2.9855	0.3357
12	C	1.9094	-3.6278	1.5799
13	C	0.8607	-3.2663	2.4541
14	C	-4.2509	-4.9974	0.5685
15	O	-5.6147	-1.855	4.1026

16	C	0.7075	-3.9186	3.8192
17	C	0.0454	-5.2701	3.7565
18	C	2.9111	-4.6972	1.9231
19	O	1.3677	-1.4226	-1.2708
20	C	0.3282	-0.5901	-1.8243
21	C	-0.275	0.3399	-0.7487
22	C	-0.8263	-0.4633	0.4277
23	O	0.7078	1.2663	-0.2582
24	C	1.0096	0.243	-2.9225
25	C	-0.7319	-1.4858	-2.4879
26	C	0.4954	-6.4505	4.2276
27	C	1.8008	-6.6669	4.9411
28	C	-0.3304	-7.7007	4.064
29	H	-5.9763	-3.7491	2.2658
30	H	-3.1347	-1.1508	4.173
31	H	-1.8505	-3.8704	1.0848
32	H	2.8155	-3.2619	-0.3526
33	H	-3.6053	-4.9187	-0.3125
34	H	-4.0952	-5.974	1.0371
35	H	-5.2865	-4.9343	0.2184
36	H	-6.4638	-2.2813	3.9018
37	H	0.1066	-3.281	4.4788
38	H	1.6871	-3.948	4.3036
39	H	-0.9327	-5.2555	3.2769
40	H	2.428	-5.6781	1.9433
41	H	3.7165	-4.7434	1.1818
42	H	3.3831	-4.4942	2.8888
43	H	-1.0782	0.9512	-1.176
44	H	-1.798	-0.8894	0.1544
45	H	-0.9682	0.2039	1.2863
46	H	1.4729	0.7358	0.0344
47	H	0.3063	0.9349	-3.3973
48	H	1.432	-0.4067	-3.6983
49	H	1.8517	0.819	-2.5229
50	H	-1.5215	-0.8884	-2.9553
51	H	-0.2752	-2.1186	-3.258
52	H	-1.1987	-2.1734	-1.7755
53	H	1.6205	-7.1039	5.9291
54	H	2.3735	-5.7506	5.0945
55	H	2.4306	-7.3566	4.3695
56	H	-0.5758	-8.1239	5.0436
57	H	-1.2724	-7.5126	3.538
58	H	0.2259	-8.4491	3.4903

(8*R*)-**1**,Conf. P		Standard Orientation (Ångstroms)		
No.	Atom	X	Y	Z
1	C	-4.8878	-2.0885	3.2596
2	C	-5.3678	-2.8833	2.212
3	C	-4.469	-3.5201	1.359
4	C	-3.095	-3.3882	1.5311
5	C	-2.6067	-2.6021	2.576
6	C	-3.5033	-1.9665	3.4425
7	O	-1.2715	-2.3992	2.8666
8	C	-0.3409	-2.7539	1.9113
9	C	-0.0649	-1.8606	0.8581
10	C	0.883	-2.2328	-0.0936
11	C	1.5861	-3.4306	0.0385
12	C	1.3509	-4.3017	1.1142
13	C	0.3686	-3.9665	2.0709
14	C	-5.8385	-1.4265	4.2124
15	O	-4.9055	-4.2992	0.3269
16	C	0.0986	-4.856	3.2733
17	C	0.98	-4.5133	4.446
18	C	2.166	-5.5628	1.2101
19	O	1.2268	-1.4712	-1.1777
20	C	0.3467	-0.3792	-1.5132
21	C	-0.0942	0.3894	-0.2483
22	C	-0.7811	-0.5398	0.7502
23	O	1.0303	1.0107	0.3962
24	C	1.1661	0.5413	-2.4328
25	C	-0.8468	-0.923	-2.3169
26	C	1.7981	-5.3228	5.1481
27	C	2.0009	-6.7912	4.8976
28	C	2.6075	-4.7777	6.2967
29	H	-6.4387	-2.9998	2.073
30	H	-2.4313	-3.9093	0.849
31	H	-3.1118	-1.3695	4.2637
32	H	2.3353	-3.6792	-0.7112
33	H	-6.0546	-2.0959	5.0507
34	H	-5.4151	-0.495	4.6025
35	H	-6.7784	-1.1708	3.7119
36	H	-5.8764	-4.3147	0.3375
37	H	0.1802	-5.9035	2.9737
38	H	-0.9455	-4.7542	3.5911

39	H	0.9168	-3.466	4.7444
40	H	2.7582	-5.5662	2.1295
41	H	1.5162	-6.4429	1.1835
42	H	2.8666	-5.6533	0.3728
43	H	-0.7781	1.2043	-0.5123
44	H	-1.8107	-0.7265	0.4252
45	H	-0.8092	-0.0558	1.7339
46	H	1.6933	0.3088	0.5395
47	H	0.5936	1.4262	-2.7298
48	H	1.4755	0.0095	-3.3404
49	H	2.092	0.87	-1.9477
50	H	-1.52	-0.116	-2.6244
51	H	-0.5005	-1.4461	-3.216
52	H	-1.4286	-1.6569	-1.7503
53	H	1.3868	-7.1864	4.0866
54	H	1.7539	-7.3631	5.7984
55	H	3.0476	-6.9869	4.6422
56	H	3.6764	-4.9236	6.1094
57	H	2.4414	-3.7065	6.4529
58	H	2.3428	-5.2935	7.2256