Supplementary Information

Two Antimicrobial Heterodimeric Tetrahydroxanthones with a 7,7′-Linkage from Mangrove Endophytic Fungus *Aspergillus flavus* QQYZ

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Content

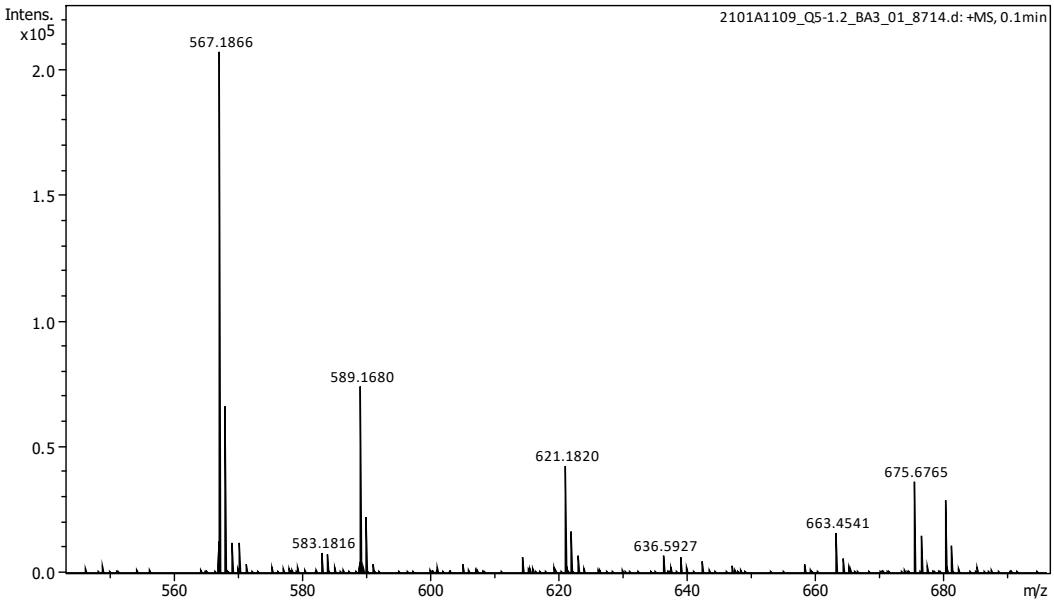

Figure S1. HRESIMS of aflaxanthone A (**1**).

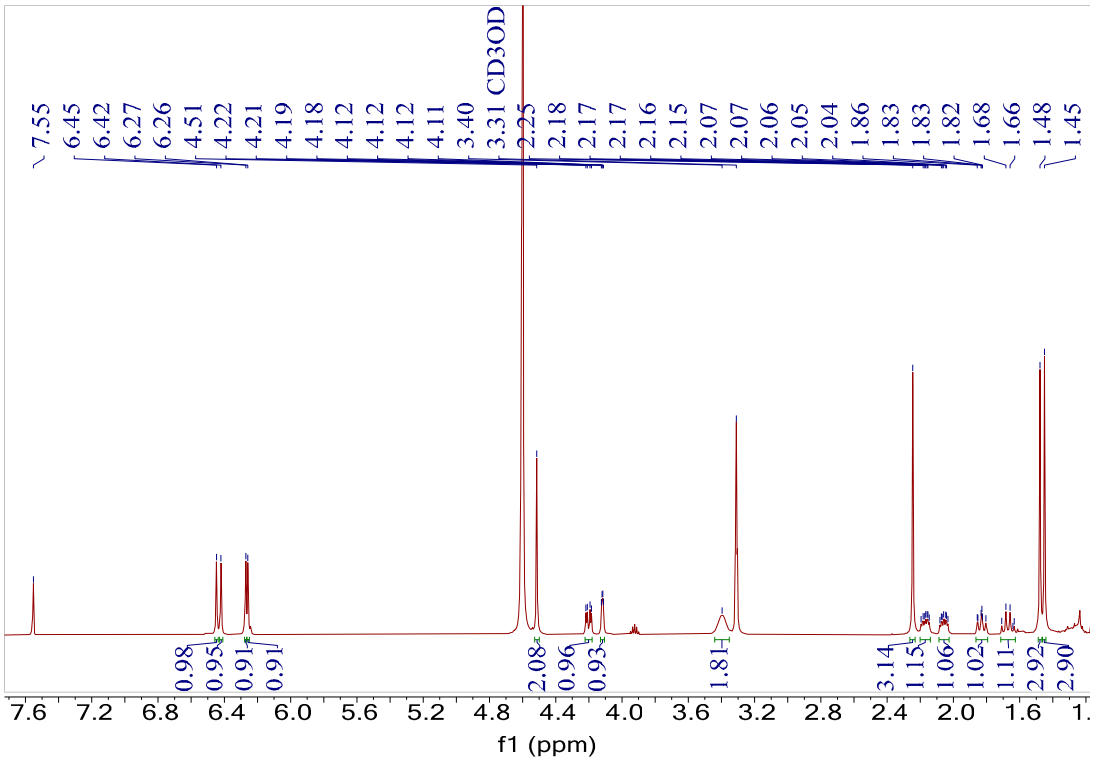

Figure S2. ^{1}H NMR spectrum of aflaxanthone A (**1**) in MeOD-d_4 and $CDCl_3$ at 500 MHz.

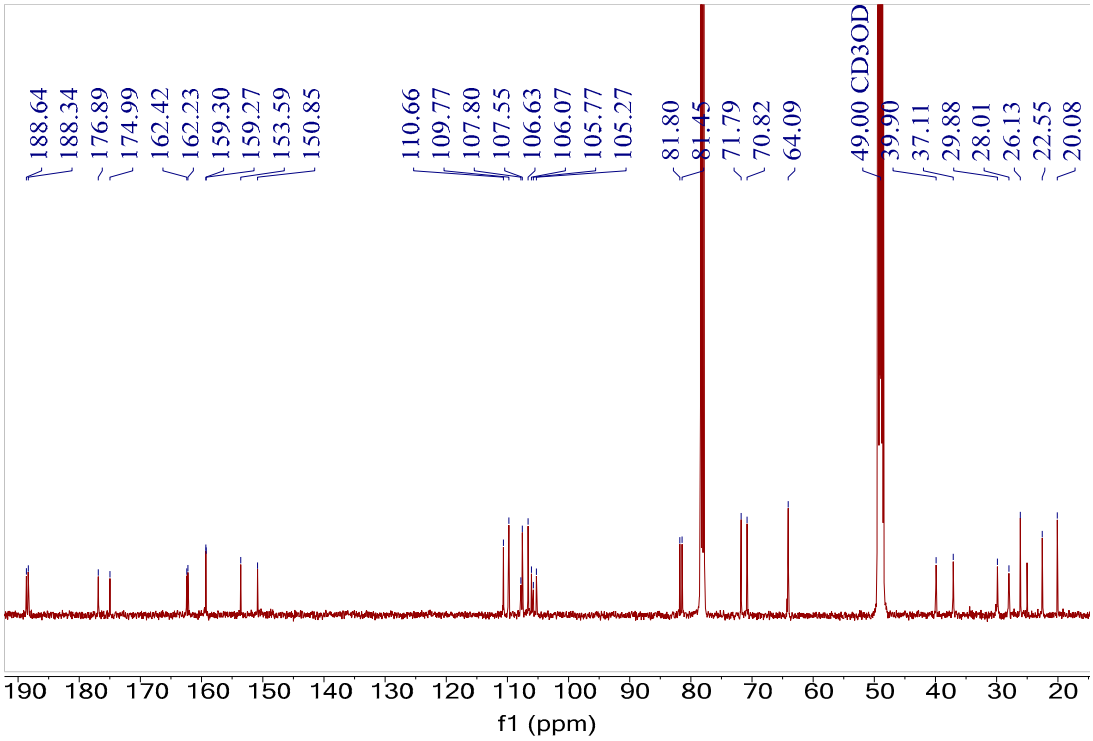

Figure S3. ^{13}C NMR spectrum of aflaxanthone A (**1**) in MeOD-d_4 and $CDCl_3$ at 125 MHz.

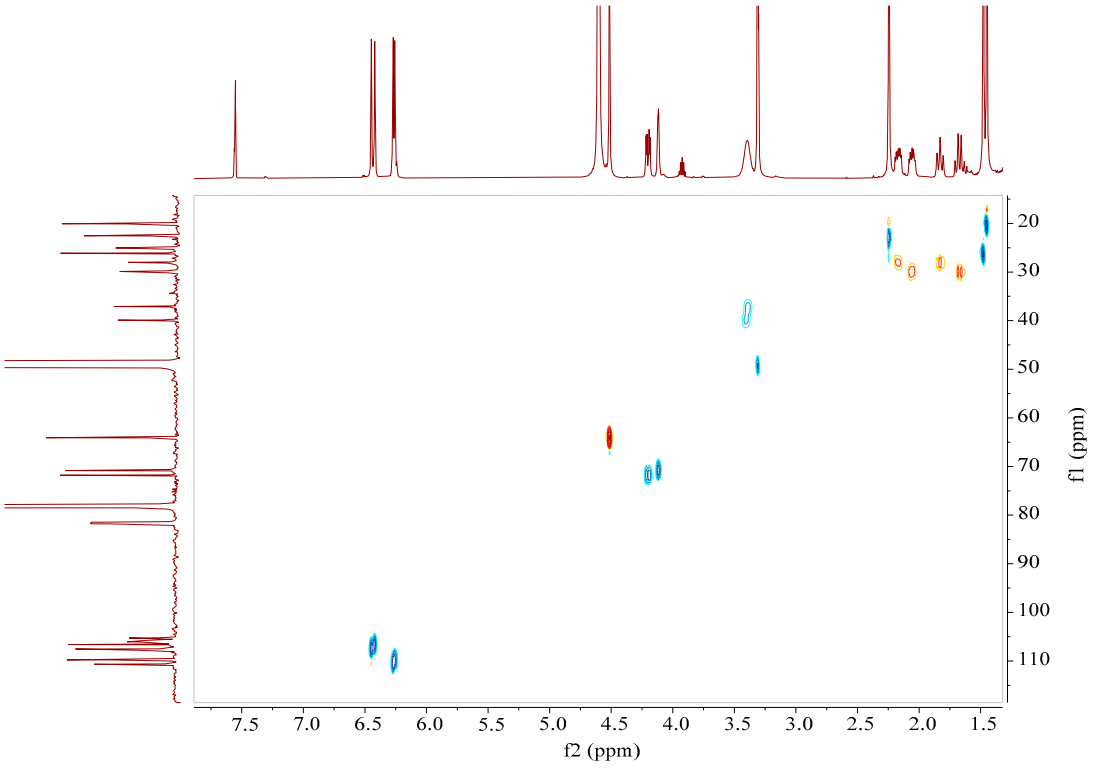

Figure S4. HSQC spectrum of aflaxanthone A (**1**) in MeOD-d_4 and $CDCl_3$ at 500 MHz and 125 MHz.

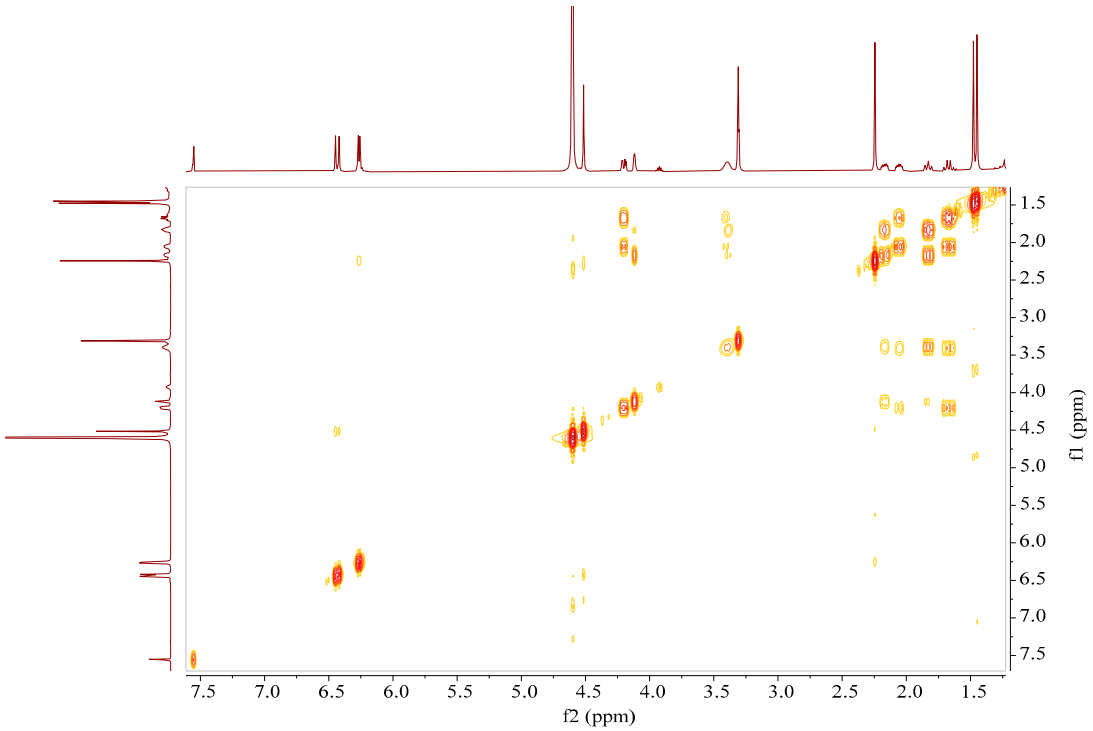

Figure S5. ^{1}H-^{1}H COSY spectrum of aflaxanthone A (**1**) in MeOD-d_4 and $CDCl_3$ at 500 MHz.

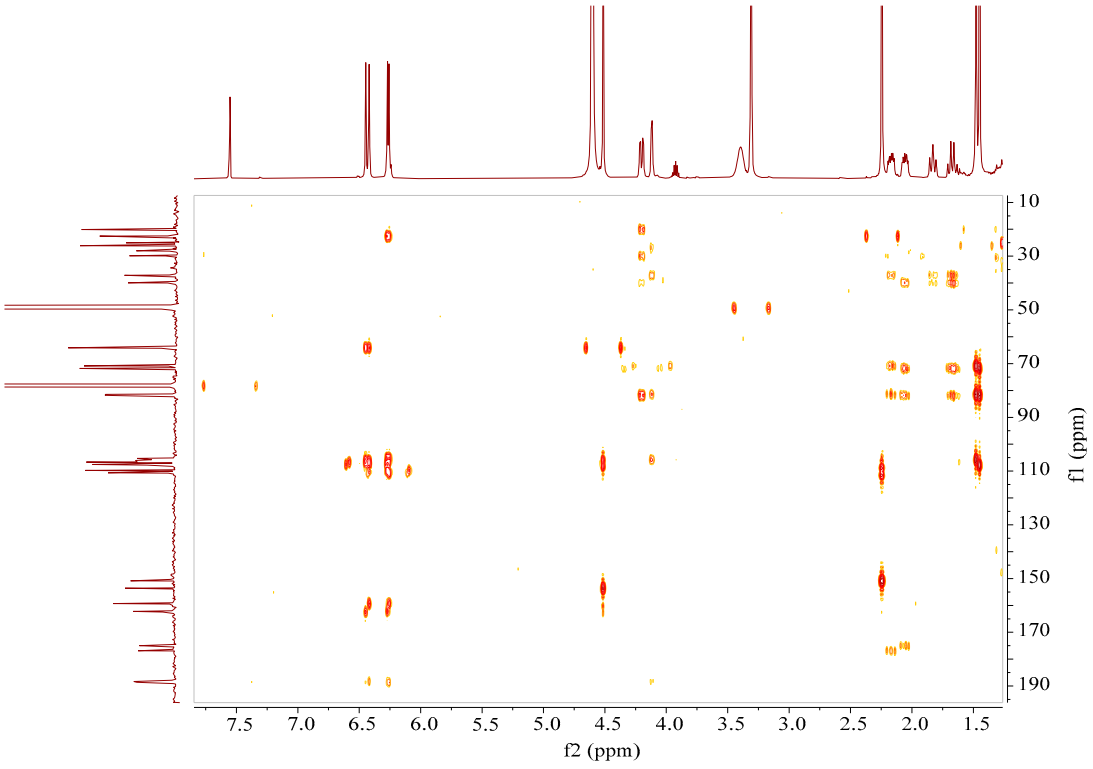

Figure S6. HMBC spectrum of aflaxanthone A (**1**) in MeOD-d_4 and $CDCl_3$ at 500 MHz and 125 MHz.

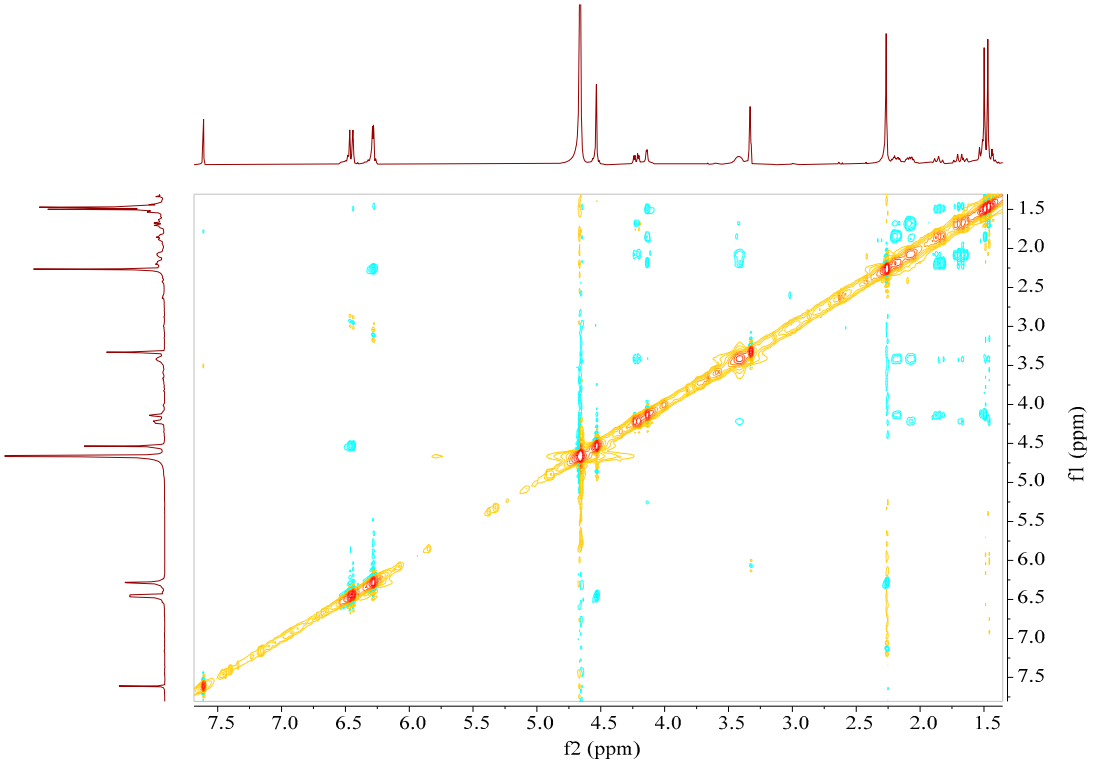

Figure S7. NOESY spectrum of aflaxanthone A (**1**) in MeOD-d_4 and $CDCl_3$ at 500 MHz.

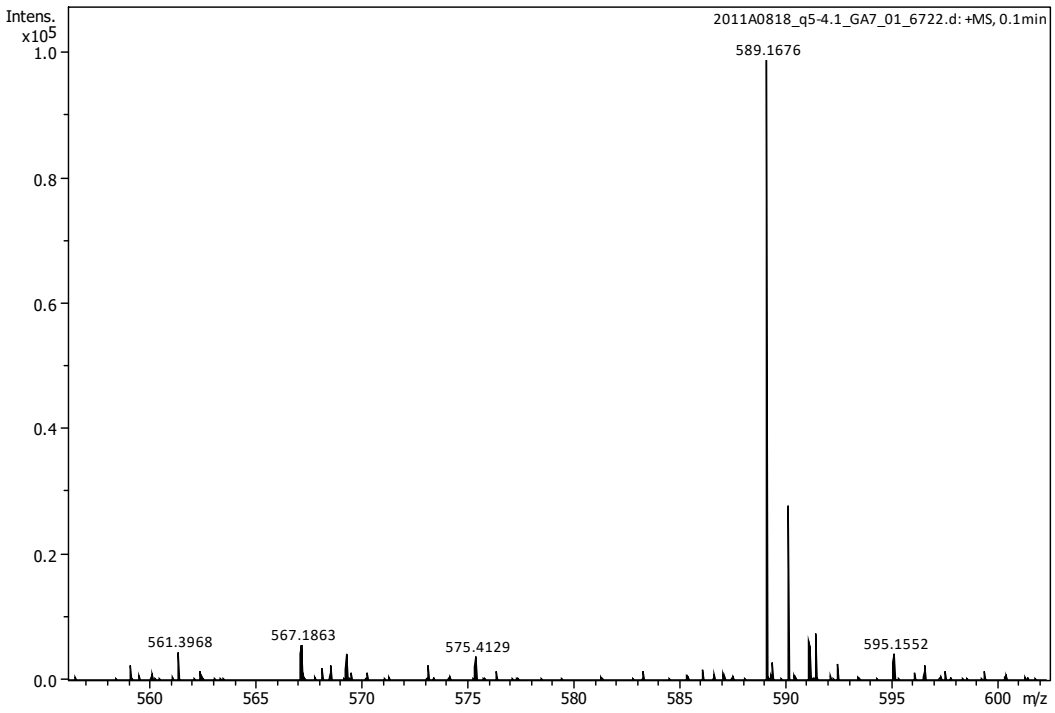

Figure S8. HRESIMS of aflaxanthone B (**2**).

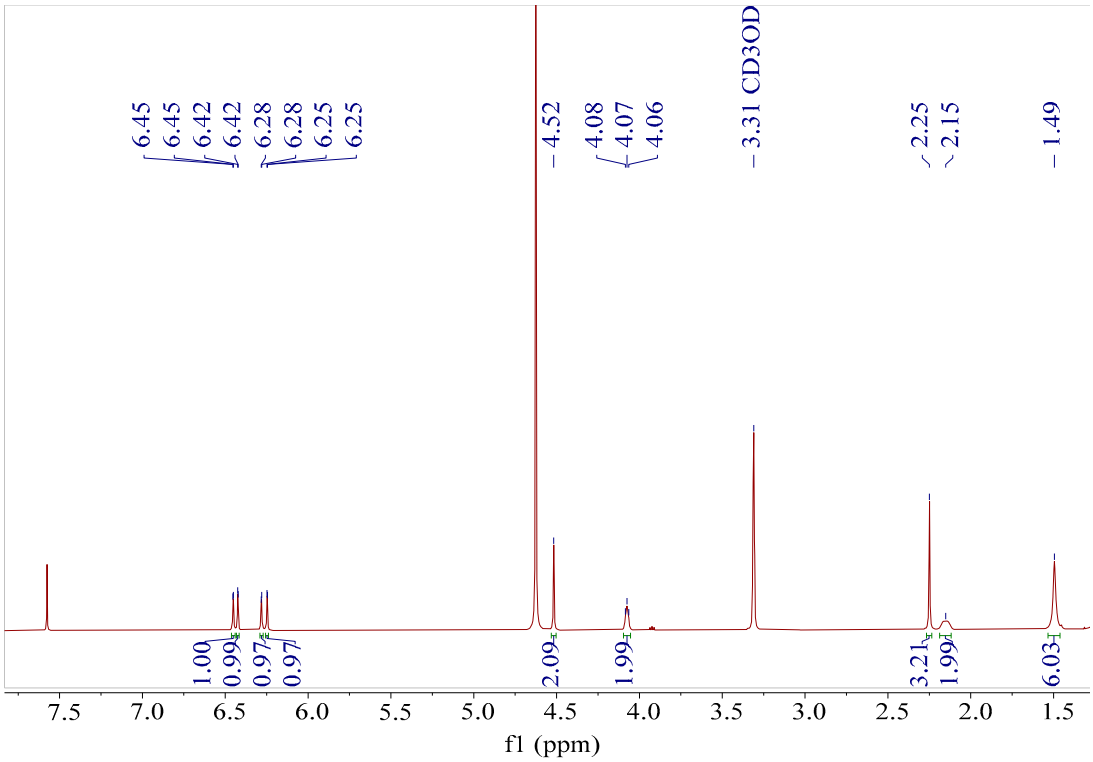

Figure S9. ^{1}H NMR spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500 MHz, 298K.

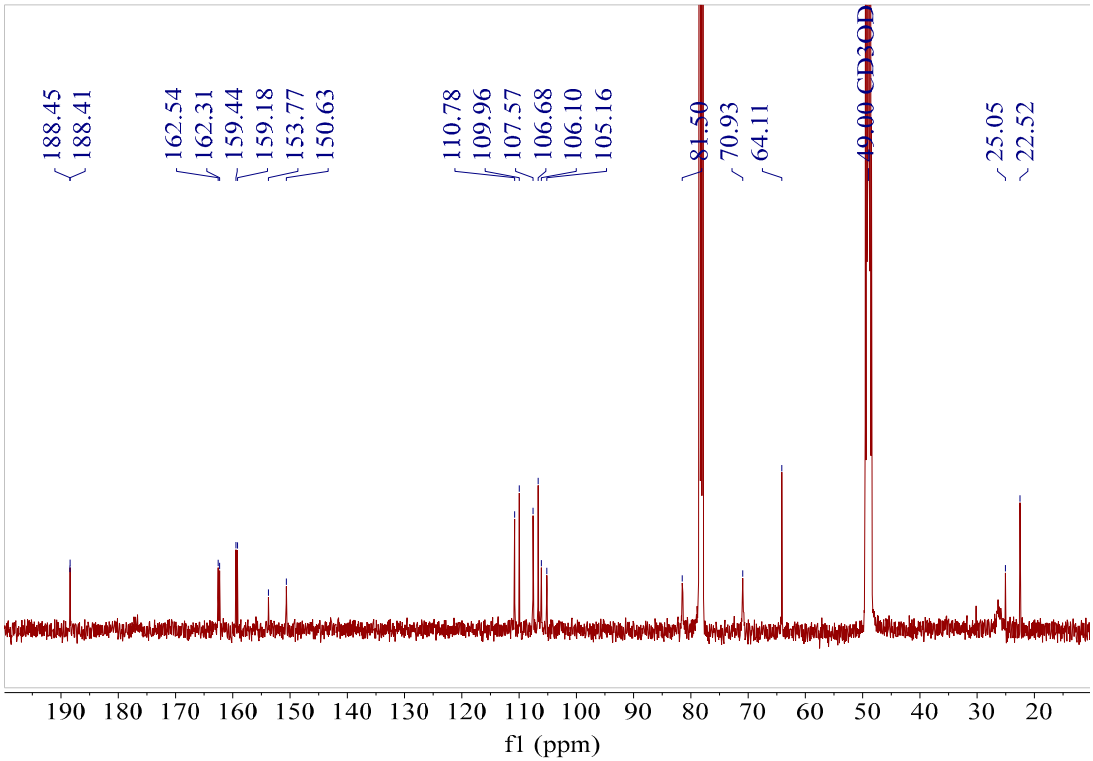

Figure S10. ^{13}C NMR spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 125 MHz, 298K.

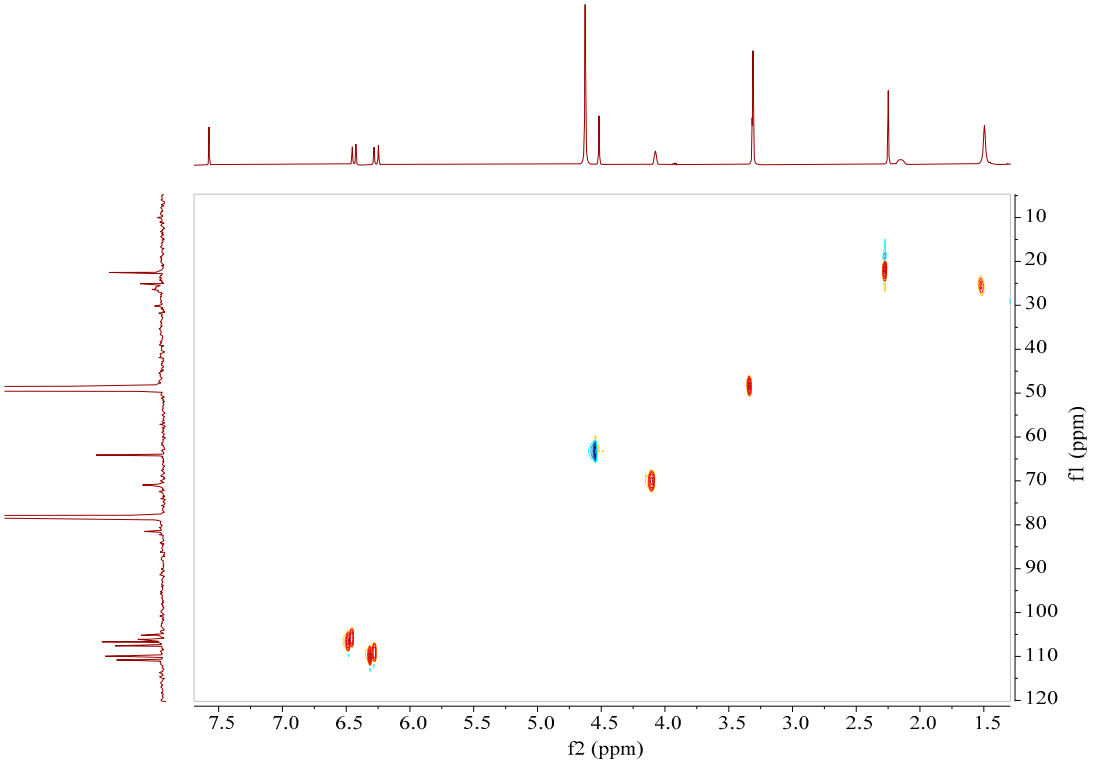

Figure S11. HSQC spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500 MHz and 125MHz, 298K.

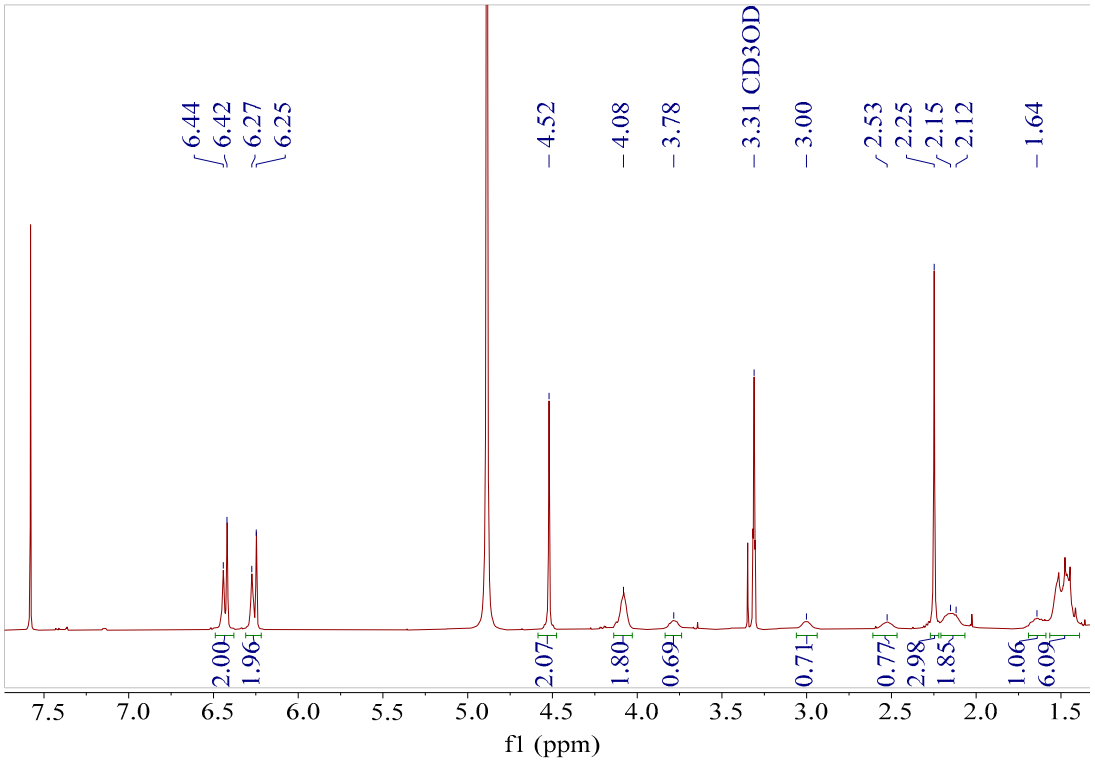

Figure S12. ^1H NMR spectrum of aflaxanthone B **(2)** in MeOD-d_4 and $CDCl_3$ at 500 MHz, 273K.

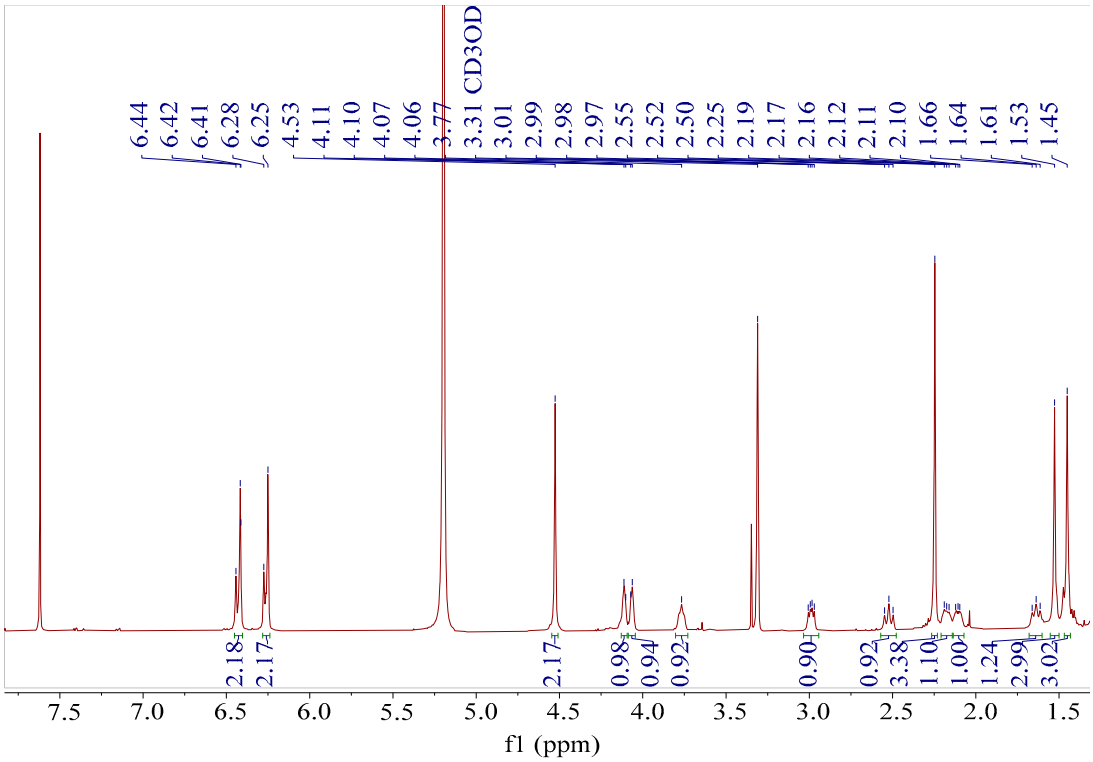

Figure S13. ^{1}H NMR spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500 MHz, 243K.

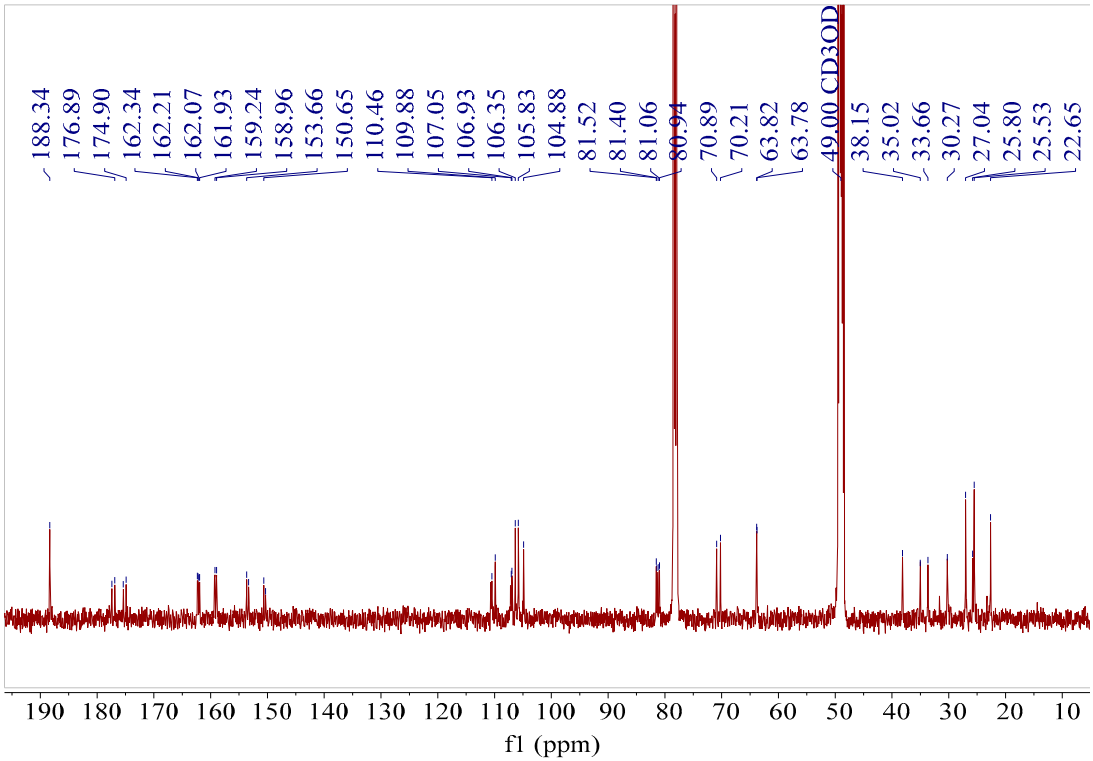

Figure S14. ^{13}C NMR spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 125 MHz, 243K.

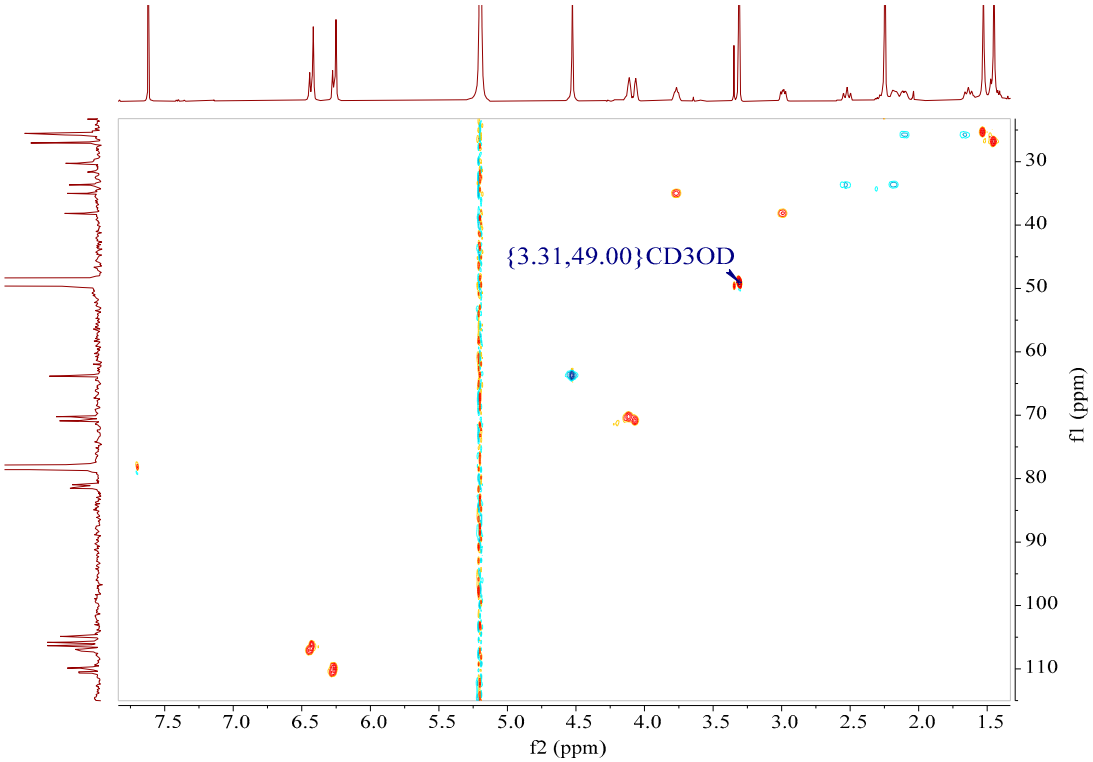

Figure S15. HSQC spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500MHz and 125 MHz, 243K.

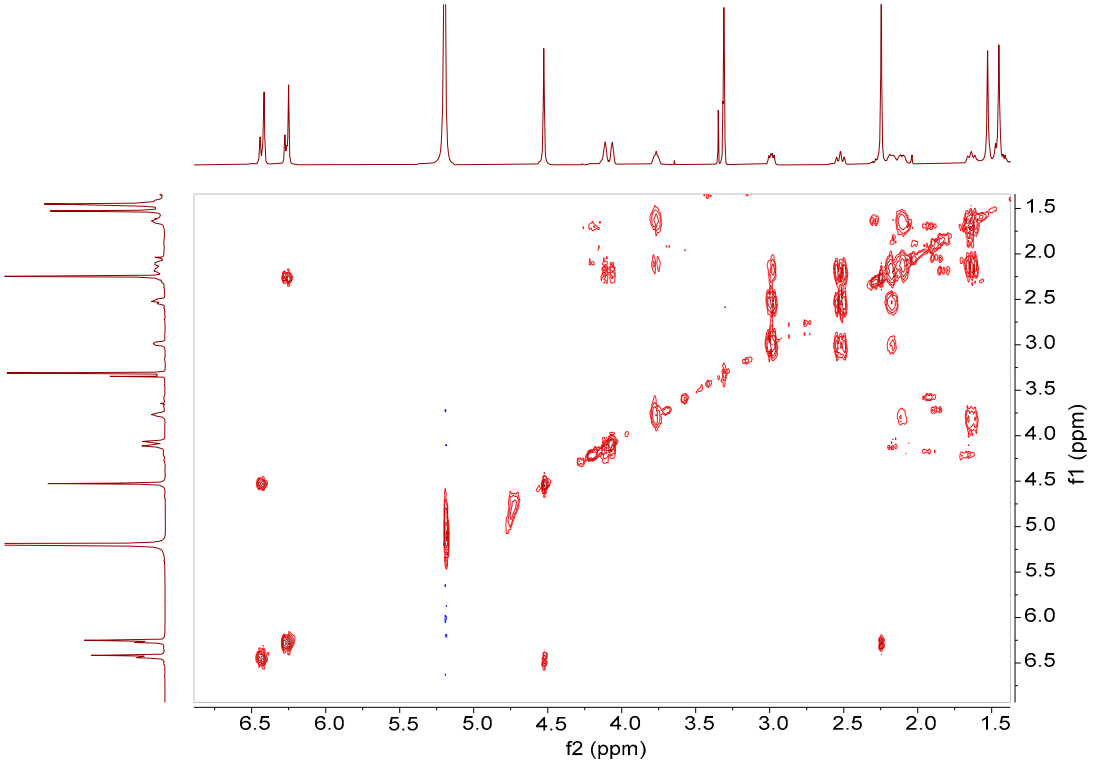

Figure S16. ^{1}H-^{1}H COSY spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500 MHz, 243K.

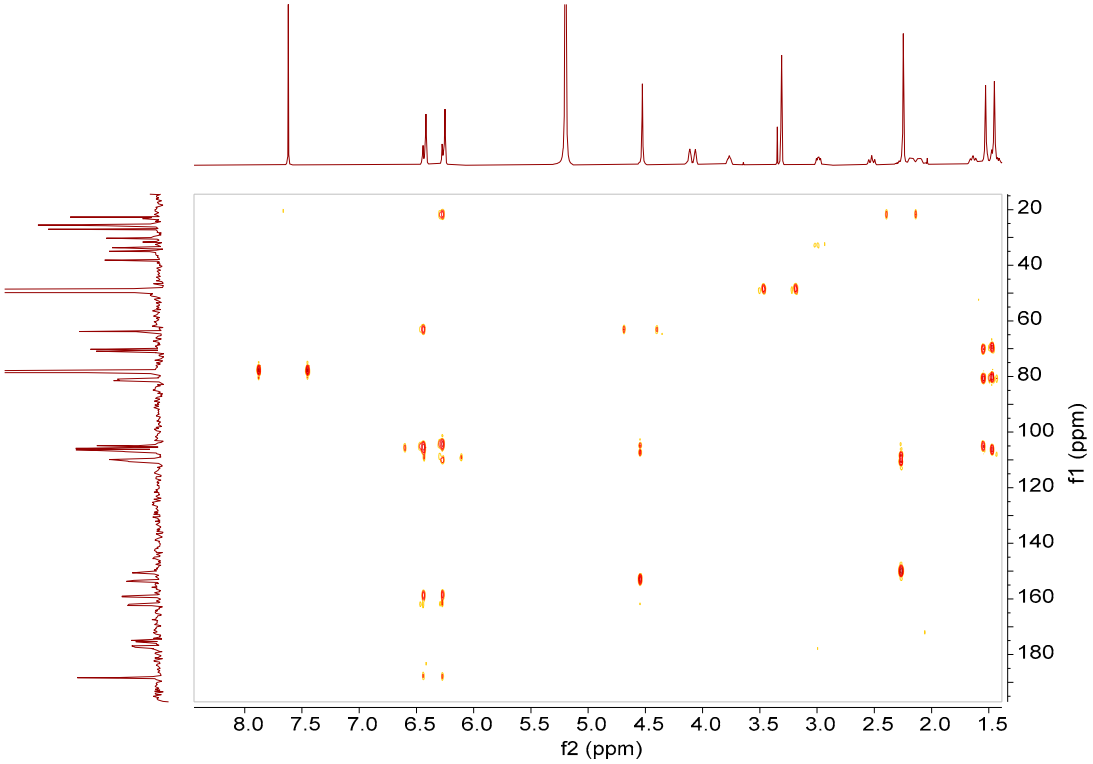

Figure S17. HMBC spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500MHz and 125 MHz, 243K.

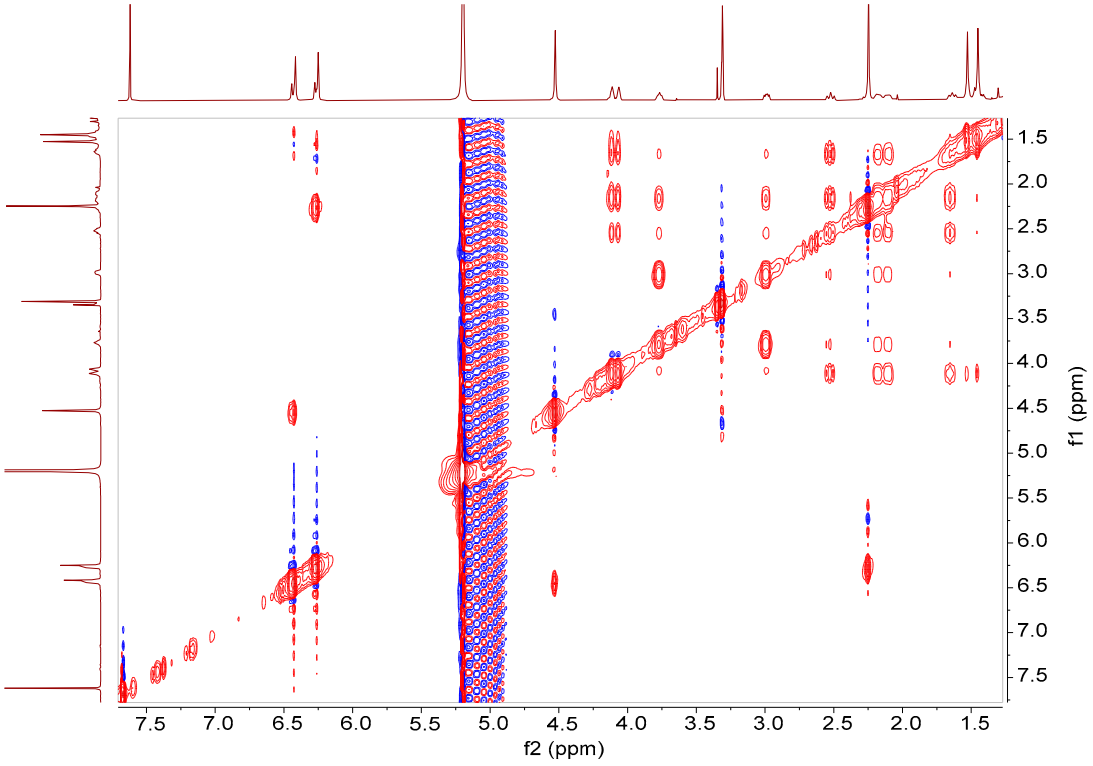

Figure S18. NOESY spectrum of aflaxanthone B (**2**) in MeOD-d_4 and $CDCl_3$ at 500MHz and 125 MHz, 243K.

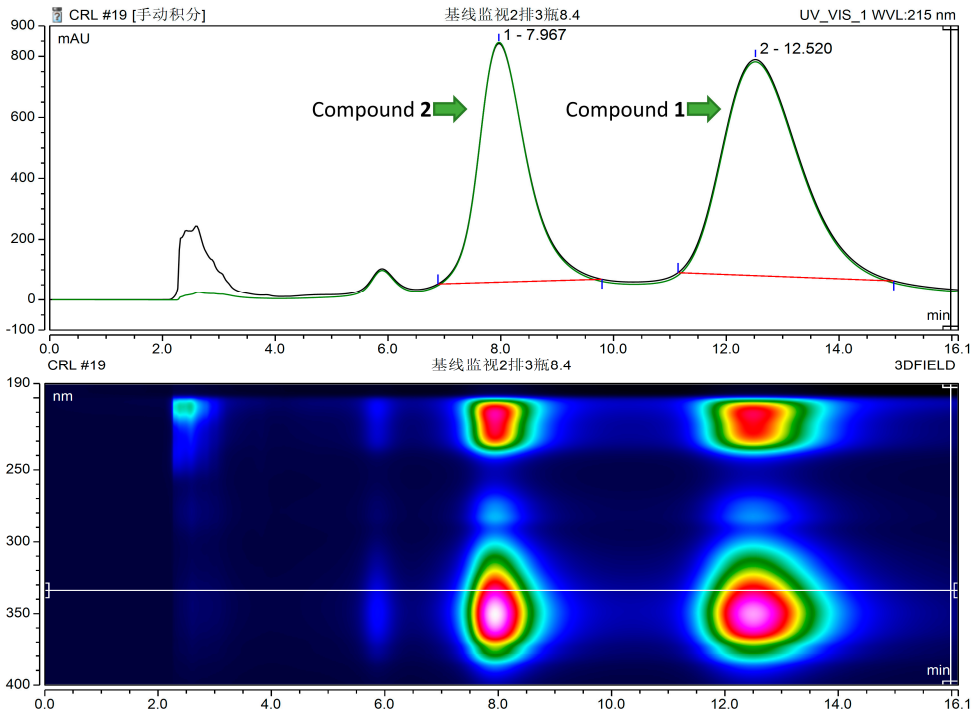

Figure S19. Chiral HPLC separation profile of **1** and **2**.

Table S1. Gibbs free energy and Boltzmann population of low energy of 5*S*,7*R*,10a*R*,5'*S*,7'*S*,10a'*S*-**1** in CH_3CN.

Conformers of 5*S*,7*R*,10a*R*,5'*S*,7'*S*,10a'*S*-1	**ΔG（kcal/mol）**	**P**
1a	0	0.266
1b	0.52	0.216
1c	0.62	0.207
1d	2.32	0.104
1e	3.38	0.068
1f	3.50	0.065
1g	6.44	0.020
1h	6.96	0.016
1i	7.01	0.016
1j	7.12	0.015

Table S2. Cartesian coordinates for the low-energy optimized conformer of **1**a at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1a			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.836900	−2.763597	−0.219150
2	6	0	7.655909	−1.645137	−0.019158
3	6	0	7.062497	−0.389368	0.166795
4	6	0	5.673525	−0.247430	0.117251
5	6	0	4.864602	−1.363147	−0.080341
6	6	0	5.450526	−2.622572	−0.246482
7	8	0	5.191647	1.018512	0.300799
8	6	0	3.873174	1.282584	−0.235470
9	6	0	2.888530	0.184734	0.078742
10	6	0	3.405454	−1.198271	−0.054110
11	6	0	3.423812	2.602042	0.458651
12	6	0	1.955429	2.910965	0.183189
13	6	0	1.030577	1.791545	0.704982
14	6	0	1.617877	0.398039	0.481716
15	8	0	4.724796	−3.769330	−0.431533
16	6	0	9.146127	−1.801349	0.057487
17	8	0	2.659419	−2.173443	−0.121602
18	8	0	0.742061	−0.637694	0.763020
19	6	0	4.004765	1.474184	−1.762587
20	1	0	3.580723	2.524269	1.543258
21	8	0	4.209582	3.717092	0.022991
22	6	0	−0.425197	2.011120	0.161962
23	1	0	1.008907	1.918103	1.797754
24	6	0	−0.545650	1.649067	−1.340289
25	6	0	−1.993415	1.458316	−1.779646
26	6	0	−2.729968	0.377992	−0.933379

27	6	0	−2.521889	0.639066	0.536468
28	6	0	−1.497921	1.362382	1.032230
29	8	0	−4.118440	0.488131	−1.330796
30	6	0	−5.027756	−0.119471	−0.512565
31	6	0	−4.809488	−0.361908	0.839512
32	6	0	−3.547430	0.077577	1.447077
33	6	0	−6.247179	−0.469391	−1.097081
34	6	0	−7.248448	−1.104490	−0.346433
35	6	0	−7.017779	−1.344000	1.016019
36	6	0	−5.809401	−0.972617	1.603248
37	8	0	−5.679896	−1.230290	2.941579
38	8	0	−3.375272	−0.011770	2.661690
39	8	0	−1.355120	1.633633	2.384753
40	8	0	−2.659960	2.728472	−1.691154
41	1	0	−2.022753	1.183606	−2.841659
42	6	0	−2.224838	−1.025766	−1.323391
43	6	0	−8.576577	−1.466048	−0.956666
44	8	0	−8.417078	−1.828784	−2.321647
45	1	0	−0.633735	3.089603	0.239846
46	1	0	7.272638	−3.752355	−0.344767
47	1	0	7.683563	0.486077	0.343844
48	1	0	1.687642	3.861390	0.663541
49	1	0	1.811634	3.088304	−0.887831
50	1	0	3.770288	−3.543646	−0.371687
51	1	0	9.485098	−2.628206	−0.576159
52	1	0	9.652222	−0.896189	−0.293003
53	1	0	9.448125	−1.999801	1.090321
54	1	0	1.180415	−1.494395	0.564642
55	1	0	4.753681	2.237880	−2.001784
56	1	0	4.346601	0.558078	−2.258336
57	1	0	3.056228	1.758473	−2.228199
58	1	0	5.136473	3.505217	0.243446
59	1	0	0.020620	0.743025	−1.578567
60	1	0	−0.098817	2.458302	−1.931295
61	1	0	−6.414081	−0.261441	−2.153066
62	1	0	−7.780733	−1.815059	1.631867
63	1	0	−4.813019	−0.873963	3.238993
64	1	0	−2.004366	1.088412	2.882514
65	1	0	−3.612036	2.546121	−1.803942
66	1	0	−2.767745	−1.814939	−0.791590
67	1	0	−2.389176	−1.210227	−2.391658
68	1	0	−1.160361	−1.161624	−1.112165
69	1	0	−9.256718	−0.611350	−0.893288

70	1	0	−9.020557	−2.320225	−0.433792
71	1	0	−9.295273	−2.089997	−2.643541

Table S3. Cartesian coordinates for the low-energy optimized conformer of **1**b at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1b			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.912036	−2.656698	−0.386926
2	6	0	7.706833	−1.544110	−0.089158
3	6	0	7.087502	−0.316818	0.188486
4	6	0	5.697414	−0.196476	0.131170
5	6	0	4.911920	−1.308254	−0.162882
6	6	0	5.523119	−2.539433	−0.420936
7	8	0	5.188685	1.041100	0.408217
8	6	0	3.872207	1.323850	−0.122862
9	6	0	2.905431	0.186967	0.092497
10	6	0	3.449693	−1.172202	−0.143398
11	6	0	3.389796	2.575954	0.666203
12	6	0	1.919271	2.878761	0.398291
13	6	0	1.010143	1.705044	0.819954
14	6	0	1.625864	0.344002	0.494103
15	8	0	4.822034	−3.680694	−0.705663
16	6	0	9.199051	−1.678786	−0.006131
17	8	0	2.722962	−2.151687	−0.297167
18	8	0	0.766873	−0.725904	0.681223
19	6	0	4.017586	1.636914	−1.628406
20	1	0	3.536788	2.417104	1.743359
21	8	0	4.158331	3.736249	0.328442
22	6	0	−0.444259	1.939655	0.279197
23	1	0	0.975613	1.744988	1.918549
24	6	0	−0.542648	1.696386	−1.248100
25	6	0	−1.982807	1.512138	−1.717891
26	6	0	−2.704999	0.353469	−0.967925
27	6	0	−2.517793	0.502183	0.520707
28	6	0	−1.512346	1.203984	1.083588
29	8	0	−4.091335	0.464245	−1.373820
30	6	0	−4.999129	−0.214527	−0.611206
31	6	0	−4.789126	−0.557541	0.720278
32	6	0	−3.538864	−0.148255	1.373168
33	6	0	−6.208272	−0.532700	−1.232417
34	6	0	−7.209219	−1.226876	−0.535465
35	6	0	−6.986588	−1.579652	0.801518
36	6	0	−5.786773	−1.239780	1.425206

37	8	0	−5.662535	−1.602198	2.739344
38	8	0	−3.375403	−0.333834	2.578552
39	8	0	−1.388993	1.370644	2.453924
40	8	0	−2.674675	2.757270	−1.536236
41	1	0	−1.995326	1.321465	−2.797987
42	6	0	−2.165909	−1.004615	−1.459707
43	6	0	−8.506582	−1.566507	−1.216949
44	8	0	−9.236065	−0.381372	−1.499157
45	1	0	−0.674684	3.004697	0.439911
46	1	0	7.367485	−3.624766	−0.585276
47	1	0	7.690071	0.552225	0.441695
48	1	0	1.627466	3.784007	0.946938
49	1	0	1.782905	3.136309	−0.658082
50	1	0	3.863375	−3.478151	−0.639981
51	1	0	9.560913	−2.446128	−0.697257
52	1	0	9.691466	−0.738948	−0.276831
53	1	0	9.493352	−1.952149	1.012452
54	1	0	1.225703	−1.555507	0.424315
55	1	0	4.754322	2.429941	−1.797895
56	1	0	4.382146	0.768746	−2.189931
57	1	0	3.069132	1.939828	−2.083028
58	1	0	5.085794	3.525588	0.544219
59	1	0	0.044237	0.823208	−1.551829
60	1	0	−0.106673	2.558094	−1.767942
61	1	0	−6.374556	−0.243108	−2.269581
62	1	0	−7.746719	−2.110098	1.370684
63	1	0	−4.803930	−1.257958	3.074142
64	1	0	−2.028295	0.774274	2.900995
65	1	0	−3.621402	2.570857	−1.683993
66	1	0	−2.699632	−1.844141	−0.998443
67	1	0	−2.315727	−1.107865	−2.540490
68	1	0	−1.102167	−1.136112	−1.245774
69	1	0	−9.130806	−2.210066	−0.588760
70	1	0	−8.318833	−2.099056	−2.154721
71	1	0	−9.066359	0.245689	−0.774762

Table S4. Cartesian coordinates for the low-energy optimized conformer of **1**c at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1c			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.810195	−2.794750	−0.176221
2	6	0	7.636233	−1.682886	0.025192
3	6	0	7.050819	−0.421907	0.201831

4	6	0	5.663856	−0.268979	0.140222
5	6	0	4.847960	−1.379274	−0.056756
6	6	0	5.425327	−2.644273	−0.213343
7	8	0	5.189315	1.000805	0.314298
8	6	0	3.878226	1.273021	−0.232045
9	6	0	2.882496	0.184496	0.080120
10	6	0	3.390254	−1.203426	−0.042918
11	6	0	3.432470	2.599236	0.451330
12	6	0	1.968598	2.917698	0.164333
13	6	0	1.033180	1.807284	0.686120
14	6	0	1.610406	0.408767	0.472888
15	8	0	4.693227	−3.785522	−0.399355
16	6	0	9.124717	−1.848949	0.113838
17	8	0	2.636696	−2.173291	−0.111922
18	8	0	0.725088	−0.618646	0.752197
19	6	0	4.022278	1.455979	−1.760235
20	1	0	3.582003	2.526966	1.536795
21	8	0	4.229595	3.707084	0.015161
22	6	0	−0.419225	2.035129	0.133216
23	1	0	1.005603	1.940449	1.777051
24	6	0	−0.531759	1.667817	−1.367832
25	6	0	−1.979701	1.483339	−1.815587
26	6	0	−2.727455	0.412492	−0.968286
27	6	0	−2.526839	0.679262	0.501477
28	6	0	−1.499889	1.398283	1.000596
29	8	0	−4.112281	0.524828	−1.376941
30	6	0	−5.033935	−0.060891	−0.557133
31	6	0	−4.824479	−0.298995	0.797861
32	6	0	−3.560684	0.128755	1.409841
33	6	0	−6.255517	−0.398634	−1.144600
34	6	0	−7.272013	−0.998474	−0.386780
35	6	0	−7.045643	−1.254701	0.972017
36	6	0	−5.834394	−0.897787	1.560328
37	8	0	−5.707615	−1.161748	2.896858
38	8	0	−3.393704	0.037674	2.624410
39	8	0	−1.364351	1.673908	2.351564
40	8	0	−2.636995	2.758617	−1.735993
41	1	0	−2.004549	1.204655	−2.875640
42	6	0	−2.227063	−0.996706	−1.347697
43	6	0	−8.574298	−1.378255	−1.037055
44	8	0	−8.376243	−2.474971	−1.917405
45	1	0	−0.619110	3.115378	0.205922
46	1	0	7.239728	−3.787520	−0.294125

47	1	0	7.677599	0.450772	0.378910
48	1	0	1.704652	3.872940	0.637246
49	1	0	1.833766	3.090261	−0.909041
50	1	0	3.739791	−3.553359	−0.346503
51	1	0	9.462104	−2.681525	−0.512920
52	1	0	9.639968	−0.948491	−0.236601
53	1	0	9.417948	−2.044708	1.149731
54	1	0	1.159732	−1.479165	0.563664
55	1	0	4.779011	2.212150	−1.997707
56	1	0	4.360391	0.534460	−2.248738
57	1	0	3.079211	1.744623	−2.234537
58	1	0	5.152629	3.489886	0.243253
59	1	0	0.028564	0.757612	−1.600070
60	1	0	−0.076792	2.471535	−1.959294
61	1	0	−6.414895	−0.202305	−2.204061
62	1	0	−7.814360	−1.722284	1.584943
63	1	0	−4.841649	−0.807937	3.200359
64	1	0	−2.017199	1.135141	2.849352
65	1	0	−3.589910	2.585015	−1.859478
66	1	0	−2.779951	−1.779064	−0.815837
67	1	0	−2.385730	−1.185256	−2.415656
68	1	0	−1.165851	−1.138467	−1.127226
69	1	0	−8.980120	−0.535132	−1.605752
70	1	0	−9.323177	−1.666387	−0.291674
71	1	0	−7.695988	−3.046159	−1.523676

Table S5. Cartesian coordinates for the low-energy optimized conformer of **1**d at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1d			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	−7.402831	−1.581902	−0.819087
2	6	0	−7.586386	−1.438501	0.561329
3	6	0	−6.601578	−0.787504	1.315850
4	6	0	−5.433616	−0.321654	0.707600
5	6	0	−5.256912	−0.466503	−0.665402
6	6	0	−6.246944	−1.095282	−1.428235
7	8	0	−4.532369	0.297225	1.525651
8	6	0	−3.155033	0.301671	1.070654
9	6	0	−3.026775	0.661317	−0.386953
10	6	0	−4.055858	0.097510	−1.292418
11	6	0	−2.477627	1.410030	1.928005
12	6	0	−1.051359	1.699035	1.472113
13	6	0	−0.983483	2.115677	−0.013433

14	6	0	−2.068158	1.476936	−0.874305
15	8	0	−6.157214	−1.261527	−2.784626
16	6	0	−8.849969	−1.919073	1.211874
17	8	0	−3.934217	0.104375	−2.516172
18	8	0	−2.012824	1.856726	−2.204910
19	6	0	−2.556949	−1.088624	1.368206
20	1	0	−3.067321	2.334479	1.869305
21	8	0	−2.441345	1.056377	3.317086
22	6	0	0.463160	1.952691	−0.607045
23	1	0	−1.218493	3.191850	−0.040877
24	6	0	1.385751	3.054895	−0.031213
25	6	0	2.861765	2.780587	−0.307039
26	6	0	3.316220	1.412021	0.278819
27	6	0	2.342797	0.326745	−0.105983
28	6	0	1.065459	0.553352	−0.481904
29	8	0	4.641142	1.197743	−0.259519
30	6	0	5.134285	−0.071669	−0.155915
31	6	0	4.336199	−1.206265	−0.045718
32	6	0	2.875982	−1.055942	−0.071672
33	6	0	6.524824	−0.197905	−0.199357
34	6	0	7.135946	−1.456818	−0.092045
35	6	0	6.322967	−2.593451	0.020987
36	6	0	4.935011	−2.467805	0.040533
37	8	0	4.220828	−3.632530	0.137403
38	8	0	2.141927	−2.043633	−0.079708
39	8	0	0.197668	−0.470187	−0.823664
40	8	0	3.074958	2.832413	−1.725518
41	1	0	3.472163	3.589268	0.113679
42	6	0	3.423077	1.517946	1.814805
43	6	0	8.632500	−1.608057	−0.159481
44	8	0	9.272164	−0.500642	0.460752
45	1	0	0.405877	2.145168	−1.688499
46	1	0	−8.162508	−2.063513	−1.431749
47	1	0	−6.737995	−0.648588	2.386095
48	1	0	−0.634316	2.496016	2.102219
49	1	0	−0.422568	0.827005	1.681852
50	1	0	−5.330482	−0.826019	−3.092593
51	1	0	−9.249011	−2.796044	0.690145
52	1	0	−8.665518	−2.215694	2.250221
53	1	0	−9.603118	−1.125691	1.198539
54	1	0	−2.626501	1.288040	−2.720166
55	1	0	−2.728535	−1.375570	2.411510
56	1	0	−3.029857	−1.869728	0.760795

57	1	0	−1.482681	−1.131993	1.171429
58	1	0	−3.361525	0.853445	3.570374
59	1	0	1.237208	3.170664	1.047583
60	1	0	1.102245	4.011419	−0.488063
61	1	0	7.141443	0.693505	−0.301118
62	1	0	6.763299	−3.586401	0.086362
63	1	0	3.264574	−3.411842	0.086445
64	1	0	0.652635	−1.331338	−0.697436
65	1	0	3.974128	2.487558	−1.883483
66	1	0	3.831033	0.602965	2.259353
67	1	0	4.109997	2.323780	2.098231
68	1	0	2.453812	1.706803	2.288646
69	1	0	8.950295	−1.662523	−1.205587
70	1	0	8.953318	−2.515931	0.362936
71	1	0	10.227855	−0.672542	0.418210

Table S6. Cartesian coordinates for the low-energy optimized conformer of **1**e at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1e			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	7.362176	−1.669221	0.851049
2	6	0	7.580768	−1.450893	−0.515154
3	6	0	6.619655	−0.750322	−1.255845
4	6	0	5.440008	−0.309944	−0.650167
5	6	0	5.228872	−0.529598	0.707513
6	6	0	6.195123	−1.208345	1.458220
7	8	0	4.563059	0.361928	−1.454378
8	6	0	3.175807	0.351325	−1.033211
9	6	0	3.013798	0.631146	0.438595
10	6	0	4.015748	0.007457	1.335972
11	6	0	2.527298	1.511889	−1.843522
12	6	0	1.091948	1.787705	−1.406345
13	6	0	0.991035	2.122095	0.097625
14	6	0	2.049529	1.425546	0.947630
15	8	0	6.069258	−1.450360	2.799407
16	6	0	8.857039	−1.904548	−1.160250
17	8	0	3.862899	−0.053488	2.554748
18	8	0	1.963041	1.730025	2.295706
19	6	0	2.575454	−1.014833	−1.421910
20	1	0	3.122124	2.426317	−1.719623
21	8	0	2.521535	1.236434	−3.249944
22	6	0	−0.469969	1.939842	0.647002
23	1	0	1.234145	3.192048	0.191293

24	6	0	−1.369788	3.081808	0.111100
25	6	0	−2.854680	2.807994	0.336470
26	6	0	−3.305751	1.479019	−0.335949
27	6	0	−2.351804	0.363999	0.010222
28	6	0	−1.081955	0.556203	0.427771
29	8	0	−4.647496	1.248238	0.153541
30	6	0	−5.147339	−0.010171	−0.020987
31	6	0	−4.355551	−1.145143	−0.175971
32	6	0	−2.895373	−1.009330	−0.114512
33	6	0	−6.539160	−0.126364	−0.008106
34	6	0	−7.154620	−1.376174	−0.180691
35	6	0	−6.351890	−2.511381	−0.349063
36	6	0	−4.962551	−2.395526	−0.340364
37	8	0	−4.256044	−3.557861	−0.490016
38	8	0	−2.170583	−2.003124	−0.150155
39	8	0	−0.231136	−0.493306	0.732432
40	8	0	−3.101442	2.781357	1.749333
41	1	0	−3.447317	3.644350	−0.053048
42	6	0	−3.372025	1.670502	−1.867030
43	6	0	−8.655197	−1.486594	−0.170219
44	8	0	−9.160895	−1.145796	1.112415
45	1	0	−0.439215	2.071199	1.737645
46	1	0	8.103630	−2.190905	1.453529
47	1	0	6.783693	−0.552323	−2.312525
48	1	0	0.696290	2.621113	−1.999938
49	1	0	0.462570	0.933516	−1.679423
50	1	0	5.239458	−1.025864	3.111721
51	1	0	9.614689	−1.118772	−1.082382
52	1	0	9.236327	−2.811749	−0.679425
53	1	0	8.697529	−2.139692	−2.217377
54	1	0	2.561081	1.129143	2.792685
55	1	0	1.496109	−1.060042	−1.254555
56	1	0	2.770292	−1.244458	−2.476376
57	1	0	3.028645	−1.832235	−0.848881
58	1	0	3.446311	1.041220	−3.493154
59	1	0	−1.193752	3.256207	−0.955228
60	1	0	−1.088731	4.008382	0.629022
61	1	0	−7.152715	0.762005	0.132095
62	1	0	−6.799003	−3.494331	−0.478918
63	1	0	−3.298879	−3.351384	−0.409218
64	1	0	−0.688612	−1.342044	0.545288
65	1	0	−4.010948	2.448278	1.868133
66	1	0	−3.778543	0.786293	−2.370360

67	1	0	−4.043179	2.498911	−2.121963
68	1	0	−2.389671	1.872999	−2.304790
69	1	0	−8.981550	−2.504233	−0.406558
70	1	0	−9.092337	−0.813335	−0.914555
71	1	0	−8.525637	−1.471851	1.772937

Table S7. Cartesian coordinates for the low-energy optimized conformer of **1**f at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1f			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	−7.392929	−1.594754	−0.821999
2	6	0	−7.567762	−1.483609	0.563837
3	6	0	−6.581414	−0.843733	1.325640
4	6	0	−5.421062	−0.358271	0.720261
5	6	0	−5.252970	−0.471425	−0.656546
6	6	0	−6.244377	−1.088709	−1.427064
7	8	0	−4.516879	0.247375	1.545893
8	6	0	−3.143480	0.269515	1.082597
9	6	0	−3.026915	0.662832	−0.366555
10	6	0	−4.058059	0.113588	−1.278637
11	6	0	−2.465781	1.362561	1.960292
12	6	0	−1.045183	1.671475	1.501174
13	6	0	−0.990146	2.122482	0.025018
14	6	0	−2.076118	1.495304	−0.842017
15	8	0	−6.161358	−1.224518	−2.786599
16	6	0	−8.824255	−1.985856	1.210655
17	8	0	−3.943839	0.148048	−2.502417
18	8	0	−2.031216	1.904791	−2.164966
19	6	0	−2.535313	−1.123800	1.344192
20	1	0	−3.062770	2.284766	1.927445
21	8	0	−2.417048	0.977896	3.340742
22	6	0	0.452706	1.983012	−0.582012
23	1	0	−1.232505	3.196364	0.023479
24	6	0	1.371994	3.079140	0.012891
25	6	0	2.847416	2.822811	−0.279395
26	6	0	3.316467	1.445402	0.272635
27	6	0	2.348337	0.361346	−0.130207
28	6	0	1.067152	0.586272	−0.490830
29	8	0	4.641467	1.253599	−0.275437
30	6	0	5.142232	−0.016405	−0.216330
31	6	0	4.353150	−1.158037	−0.124919
32	6	0	2.892045	−1.018122	−0.129201
33	6	0	6.532425	−0.131920	−0.282270

34	6	0	7.149125	−1.390914	−0.234604
35	6	0	6.348825	−2.534540	−0.118673
36	6	0	4.961002	−2.418259	−0.074385
37	8	0	4.255801	−3.588005	0.015471
38	8	0	2.166016	−2.010588	−0.146895
39	8	0	0.204251	−0.436631	−0.848997
40	8	0	3.050338	2.906622	−1.697983
41	1	0	3.454628	3.626363	0.154234
42	6	0	3.430643	1.516648	1.810451
43	6	0	8.648107	−1.499569	−0.282801
44	8	0	9.209391	−1.022964	0.931267
45	1	0	0.388314	2.199133	−1.658244
46	1	0	−8.154387	−2.067036	−1.439587
47	1	0	−6.712239	−0.729437	2.400125
48	1	0	−0.628238	2.456062	2.145938
49	1	0	−0.408756	0.798321	1.686483
50	1	0	−5.340845	−0.777710	−3.090673
51	1	0	−9.221972	−2.852765	0.672237
52	1	0	−8.632619	−2.303333	2.241257
53	1	0	−9.582166	−1.196429	1.219368
54	1	0	−2.646784	1.344956	−2.688020
55	1	0	−2.698001	−1.434799	2.382922
56	1	0	−3.007825	−1.892795	0.722993
57	1	0	−1.461642	−1.155829	1.139582
58	1	0	−3.334243	0.765475	3.596240
59	1	0	1.229539	3.169910	1.093723
60	1	0	1.077354	4.043702	−0.422086
61	1	0	7.145132	0.766302	−0.361650
62	1	0	6.798695	−3.525700	−0.075461
63	1	0	3.297271	−3.375893	−0.025449
64	1	0	0.665102	−1.297575	−0.744000
65	1	0	3.953954	2.579560	−1.870866
66	1	0	3.850297	0.595707	2.230638
67	1	0	4.111269	2.322768	2.108294
68	1	0	2.463318	1.685025	2.294187
69	1	0	9.049735	−0.911648	−1.115010
70	1	0	8.968189	−2.536754	−0.425391
71	1	0	8.601625	−1.268502	1.649465

Table S8. Cartesian coordinates for the low-energy optimized conformer of **1**g at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1g			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.856004	−2.758031	−0.235102
2	6	0	7.667208	−1.649306	0.033181
3	6	0	7.067938	−0.401207	0.247182
4	6	0	5.682186	−0.255341	0.155168
5	6	0	4.880772	−1.361487	−0.111000
6	6	0	5.470775	−2.615379	−0.304348
7	8	0	5.189301	1.000298	0.371476
8	6	0	3.901460	1.294048	−0.220266
9	6	0	2.904015	0.188311	0.039422
10	6	0	3.422359	−1.192025	−0.127566
11	6	0	3.422770	2.611820	0.465344
12	6	0	1.950674	2.896943	0.178221
13	6	0	1.035965	1.766906	0.690611
14	6	0	1.626321	0.384589	0.430027
15	8	0	4.750627	−3.751874	−0.556069
16	6	0	9.154515	−1.808293	0.154257
17	8	0	2.675843	−2.161744	−0.252104
18	8	0	0.749088	−0.660034	0.663867
19	6	0	4.097661	1.505065	−1.738361
20	1	0	3.584708	2.536418	1.548773
21	8	0	4.189362	3.738283	0.019846
22	6	0	−0.427514	1.992866	0.165807
23	1	0	1.024939	1.872936	1.784738
24	6	0	−0.563685	1.660894	−1.340999
25	6	0	−2.017839	1.482383	−1.767056
26	6	0	−2.747288	0.387262	−0.934166
27	6	0	−2.520157	0.615957	0.538009
28	6	0	−1.488359	1.327960	1.036642
29	8	0	−4.140602	0.510018	−1.310931
30	6	0	−5.040885	−0.113503	−0.495350
31	6	0	−4.805270	−0.385632	0.848540
32	6	0	−3.535539	0.038642	1.449940
33	6	0	−6.268092	−0.447738	−1.071975
34	6	0	−7.261166	−1.096740	−0.321498
35	6	0	−7.014202	−1.367075	1.032442
36	6	0	−5.797786	−1.010928	1.611968
37	8	0	−5.651565	−1.297451	2.942353
38	8	0	−3.348357	−0.075286	2.661089

39	8	0	−1.329905	1.572815	2.391939
40	8	0	−2.678976	2.753132	−1.643656
41	1	0	−2.060869	1.229860	−2.833709
42	6	0	−2.251981	−1.010359	−1.360614
43	6	0	−8.597751	−1.444879	−0.922782
44	8	0	−8.459098	−1.764606	−2.300307
45	1	0	−0.635261	3.070047	0.267408
46	1	0	7.295831	−3.742637	−0.382643
47	1	0	7.679668	0.469801	0.476354
48	1	0	1.662563	3.843811	0.654214
49	1	0	1.814418	3.069186	−0.895864
50	1	0	3.796116	−3.524945	−0.520239
51	1	0	9.514837	−2.611743	−0.496623
52	1	0	9.670317	−0.891085	−0.146443
53	1	0	9.422932	−2.044106	1.189058
54	1	0	1.191513	−1.508163	0.438597
55	1	0	3.174570	1.824572	−2.233133
56	1	0	4.875883	2.251155	−1.935595
57	1	0	4.430688	0.589073	−2.239138
58	1	0	3.960465	4.491843	0.591225
59	1	0	−0.003168	0.758420	−1.604149
60	1	0	−0.121321	2.480653	−1.920890
61	1	0	−6.448221	−0.217243	−2.120843
62	1	0	−7.769923	−1.849738	1.647217
63	1	0	−4.779925	−0.949313	3.236602
64	1	0	−1.971437	1.015666	2.886191
65	1	0	−3.632093	2.575171	−1.752187
66	1	0	−2.790647	−1.808507	−0.837826
67	1	0	−2.433280	−1.171684	−2.429796
68	1	0	−1.186217	−1.154104	−1.168053
69	1	0	−9.278595	−0.592533	−0.822978
70	1	0	−9.031131	−2.314296	−0.418007
71	1	0	−9.341750	−2.021269	−2.616353

Table S9. Cartesian coordinates for the low-energy optimized conformer of **1**h at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1h			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.907165	−2.683360	−0.376023
2	6	0	7.703280	−1.579743	−0.045872
3	6	0	7.086341	−0.353214	0.233408
4	6	0	5.699363	−0.221194	0.146067
5	6	0	4.913717	−1.321836	−0.181530

6	6	0	5.521417	−2.555292	−0.441095
7	8	0	5.189828	1.014501	0.428536
8	6	0	3.898054	1.321848	−0.149969
9	6	0	2.915628	0.190628	0.046925
10	6	0	3.453541	−1.171537	−0.192871
11	6	0	3.401296	2.594388	0.603844
12	6	0	1.925697	2.874438	0.329201
13	6	0	1.024559	1.706988	0.777341
14	6	0	1.635111	0.348895	0.444077
15	8	0	4.816933	−3.685949	−0.755199
16	6	0	9.192221	−1.725936	0.069871
17	8	0	2.719585	−2.142920	−0.371904
18	8	0	0.771399	−0.718589	0.618822
19	6	0	4.094562	1.617441	−1.653948
20	1	0	3.561709	2.462589	1.682819
21	8	0	4.154078	3.753184	0.222321
22	6	0	−0.439865	1.941460	0.261684
23	1	0	1.010595	1.752802	1.876148
24	6	0	−0.569202	1.688592	−1.261137
25	6	0	−2.019714	1.514630	−1.699659
26	6	0	−2.736916	0.366426	−0.928516
27	6	0	−2.515730	0.520303	0.554234
28	6	0	−1.493656	1.217066	1.093109
29	8	0	−4.129121	0.489050	−1.305766
30	6	0	−5.027922	−0.176277	−0.520745
31	6	0	−4.792417	−0.517836	0.806323
32	6	0	−3.524858	−0.117820	1.430611
33	6	0	−6.254009	−0.486283	−1.115633
34	6	0	−7.254014	−1.155838	−0.393175
35	6	0	−6.994256	−1.520834	0.935758
36	6	0	−5.778437	−1.192625	1.533141
37	8	0	−5.624441	−1.562839	2.842071
38	8	0	−3.334924	−0.301800	2.632966
39	8	0	−1.340365	1.389349	2.460012
40	8	0	−2.697180	2.767796	−1.509845
41	1	0	−2.058393	1.319982	−2.778952
42	6	0	−2.221839	−0.998722	−1.426381
43	6	0	−8.567041	−1.539665	−1.026491
44	8	0	−8.895404	−0.658518	−2.091349
45	1	0	−0.662837	3.008310	0.420654
46	1	0	7.361437	−3.652148	−0.575911
47	1	0	7.686201	0.511845	0.511230
48	1	0	1.623586	3.790714	0.854091

49	1	0	1.788645	3.103052	−0.733928
50	1	0	3.858914	−3.474180	−0.709652
51	1	0	9.461755	−2.012002	1.091364
52	1	0	9.564715	−2.487244	−0.621767
53	1	0	9.697226	−0.786379	−0.178748
54	1	0	1.227068	−1.547902	0.351416
55	1	0	3.168799	1.951587	−2.133011
56	1	0	4.863260	2.382723	−1.808099
57	1	0	4.441386	0.734582	−2.202548
58	1	0	3.912009	4.472537	0.832166
59	1	0	0.004167	0.809406	−1.570081
60	1	0	−0.136881	2.543591	−1.794637
61	1	0	−6.432527	−0.202998	−2.151901
62	1	0	−7.743625	−2.051525	1.519870
63	1	0	−4.760095	−1.218879	3.158015
64	1	0	−1.976639	0.798729	2.921568
65	1	0	−3.649481	2.584869	−1.627625
66	1	0	−2.752356	−1.831310	−0.949849
67	1	0	−2.395494	−1.105448	−2.503399
68	1	0	−1.154241	−1.139109	−1.235660
69	1	0	−9.373707	−1.487740	−0.287979
70	1	0	−8.499868	−2.559075	−1.420719
71	1	0	−9.770879	−0.928032	−2.415470

Table S10. Cartesian coordinates for the low-energy optimized conformer of **1**i at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1i			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.927965	−2.654575	−0.388355
2	6	0	7.715824	−1.554457	−0.027939
3	6	0	7.091177	−0.335208	0.269858
4	6	0	5.703702	−0.207665	0.171242
5	6	0	4.926000	−1.305753	−0.185472
6	6	0	5.541694	−2.530226	−0.463683
7	8	0	5.185579	1.019108	0.473833
8	6	0	3.899668	1.333196	−0.110629
9	6	0	2.919939	0.194818	0.054025
10	6	0	3.465689	−1.161140	−0.207900
11	6	0	3.388781	2.587848	0.663415
12	6	0	1.914187	2.866919	0.379640
13	6	0	1.014722	1.686594	0.795935
14	6	0	1.634669	0.338763	0.441627
15	8	0	4.846266	−3.658200	−0.808786

16	6	0	9.203639	−1.695613	0.099431
17	8	0	2.738173	−2.130777	−0.414331
18	8	0	0.773837	−0.736543	0.585850
19	6	0	4.108410	1.659305	−1.607171
20	1	0	3.540499	2.434944	1.741199
21	8	0	4.139256	3.757749	0.311240
22	6	0	−0.445763	1.924884	0.272501
23	1	0	0.991235	1.710616	1.895716
24	6	0	−0.559802	1.703715	−1.256893
25	6	0	−2.005172	1.528936	−1.712852
26	6	0	−2.720874	0.360803	−0.972854
27	6	0	−2.515284	0.484655	0.515397
28	6	0	−1.503366	1.177365	1.078649
29	8	0	−4.112025	0.481079	−1.359030
30	6	0	−5.010975	−0.209670	−0.597620
31	6	0	−4.785685	−0.576050	0.725630
32	6	0	−3.528205	−0.177755	1.369724
33	6	0	−6.228217	−0.516720	−1.209554
34	6	0	−7.221012	−1.222558	−0.512730
35	6	0	−6.983154	−1.596808	0.816004
36	6	0	−5.775893	−1.269427	1.430942
37	8	0	−5.635824	−1.654134	2.736850
38	8	0	−3.349458	−0.381938	2.569442
39	8	0	−1.364354	1.322776	2.450107
40	8	0	−2.692956	2.774163	−1.502392
41	1	0	−2.031727	1.356514	−2.795487
42	6	0	−2.192007	−0.990583	−1.494224
43	6	0	−8.527485	−1.549617	−1.183551
44	8	0	−9.261840	−0.358715	−1.429904
45	1	0	−0.676271	2.987603	0.451056
46	1	0	7.388372	−3.616829	−0.603373
47	1	0	7.684300	0.525508	0.571103
48	1	0	1.604309	3.771964	0.920094
49	1	0	1.787244	3.116442	−0.679175
50	1	0	3.886272	−3.451337	−0.768053
51	1	0	9.464542	−2.002012	1.117148
52	1	0	9.586947	−2.442270	−0.604478
53	1	0	9.707441	−0.749241	−0.125244
54	1	0	1.236612	−1.558286	0.307580
55	1	0	3.185823	1.998943	−2.087986
56	1	0	4.875704	2.431215	−1.737925
57	1	0	4.464599	0.788533	−2.169753
58	1	0	3.893186	4.461866	0.935870

59	1	0	0.021699	0.835065	−1.578829
60	1	0	−0.128727	2.573197	−1.768405
61	1	0	−6.406865	−0.210044	−2.239433
62	1	0	−7.736281	−2.137322	1.385135
63	1	0	−4.772741	−1.316588	3.066419
64	1	0	−1.997520	0.717487	2.894220
65	1	0	−3.640760	2.590600	−1.645647
66	1	0	−2.719590	−1.836172	−1.038680
67	1	0	−2.356882	−1.075775	−2.573926
68	1	0	−1.125063	−1.127036	−1.297927
69	1	0	−9.142455	−2.207645	−0.561425
70	1	0	−8.351139	−2.061187	−2.135897
71	1	0	−9.085023	0.250843	−0.692498

Table S11. Cartesian coordinates for the low-energy optimized conformer of **1**j at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 1j			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.826985	−2.792852	−0.187271
2	6	0	7.645764	−1.688204	0.078917
3	6	0	7.054582	−0.432522	0.279451
4	6	0	5.670666	−0.277174	0.177617
5	6	0	4.862156	−1.379268	−0.084964
6	6	0	5.443973	−2.637966	−0.265568
7	8	0	5.187481	0.983679	0.381114
8	6	0	3.905328	1.283242	−0.219875
9	6	0	2.897421	0.188164	0.041774
10	6	0	3.406164	−1.197635	−0.112474
11	6	0	3.432403	2.609963	0.452559
12	6	0	1.964731	2.904132	0.153495
13	6	0	1.037840	1.785403	0.669209
14	6	0	1.619377	0.397088	0.422595
15	8	0	4.716980	−3.771620	−0.514438
16	6	0	9.130880	−1.857809	0.209893
17	8	0	2.652177	−2.162385	−0.235520
18	8	0	0.731814	−0.639617	0.657356
19	6	0	4.112606	1.482133	−1.739364
20	1	0	3.588095	2.541202	1.537062
21	8	0	4.210867	3.726657	0.002415
22	6	0	−0.420541	2.019560	0.134166
23	1	0	1.021748	1.899910	1.762338
24	6	0	−0.550974	1.677914	−1.370429
25	6	0	−2.003102	1.505109	−1.804511

26	6	0	−2.744057	0.420470	−0.968460
27	6	0	−2.524727	0.659160	0.503973
28	6	0	−1.490988	1.367805	1.003271
29	8	0	−4.134636	0.545399	−1.357211
30	6	0	−5.046370	−0.055700	−0.537268
31	6	0	−4.820768	−0.319292	0.809964
32	6	0	−3.548235	0.094282	1.414406
33	6	0	−6.276180	−0.379047	−1.116256
34	6	0	−7.284249	−0.992480	−0.356797
35	6	0	−7.041797	−1.274938	0.992688
36	6	0	−5.821539	−0.931629	1.572818
37	8	0	−5.679104	−1.220834	2.903284
38	8	0	−3.366497	−0.018435	2.625271
39	8	0	−1.339117	1.620492	2.357610
40	8	0	−2.656581	2.780602	−1.692924
41	1	0	−2.041862	1.246019	−2.869480
42	6	0	−2.254070	−0.982915	−1.380400
43	6	0	−8.595494	−1.356756	−0.998764
44	8	0	−8.408306	−2.424752	−1.915544
45	1	0	−0.622130	3.098120	0.226946
46	1	0	7.260626	−3.780838	−0.325086
47	1	0	7.672088	0.433891	0.506121
48	1	0	1.681384	3.857152	0.619522
49	1	0	1.835835	3.069172	−0.922159
50	1	0	3.763647	−3.536684	−0.485478
51	1	0	9.488773	−2.669028	−0.432662
52	1	0	9.656115	−0.946597	−0.093203
53	1	0	9.390228	−2.087699	1.248374
54	1	0	1.171303	−1.492980	0.444717
55	1	0	4.898313	2.218541	−1.936977
56	1	0	4.442359	0.558851	−2.230212
57	1	0	3.194980	1.805099	−2.241476
58	1	0	3.987194	4.485437	0.568595
59	1	0	0.006552	0.770549	−1.624734
60	1	0	−0.100161	2.490779	−1.953691
61	1	0	−6.448337	−0.162181	−2.168922
62	1	0	−7.803299	−1.752434	1.606496
63	1	0	−4.808564	−0.875163	3.202418
64	1	0	−1.984868	1.070556	2.852830
65	1	0	−3.610931	2.611024	−1.812968
66	1	0	−2.801002	−1.774540	−0.855951
67	1	0	−2.427834	−1.151547	−2.449962
68	1	0	−1.189700	−1.131379	−1.178460

69	1	0	−9.012285	−0.497782	−1.534533
70	1	0	−9.330811	−1.670624	−0.250997
71	1	0	−7.724776	−3.009756	−1.546137

Table S12. Gibbs free energy and Boltzmann population of low energy of 5*S*,7*R*,10a*R*,5'*S*,7'*R*,10a'*R*-**2** in CH_3CN.

Conformers of 5*S*,7*R*,10a*R*,5'*S*,7'*R*,10a'*R*-2	**Δ*G*（kcal/mol）**	**P**
2a	0	0.288
2b	0.47	0.239
2c	0.49	0.237
2d	0.58	0.228

Table S13. Cartesian coordinates for the low-energy optimized conformer of **2**a at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 2a			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.494229	−2.684530	−0.787475
2	6	0	7.301673	−1.816132	−0.043099
3	6	0	6.755296	−0.615927	0.432791
4	6	0	5.412465	−0.307151	0.201518
5	6	0	4.615423	−1.173937	−0.539666
6	6	0	5.161147	−2.363448	−1.036370
7	8	0	4.972448	0.881461	0.711646
8	6	0	3.545952	0.985425	0.945657
9	6	0	2.728444	0.455270	−0.206733
10	6	0	3.228594	−0.791443	−0.832387
11	6	0	3.286536	2.507515	1.136203
12	6	0	1.798103	2.836561	1.157346
13	6	0	1.074203	2.369973	−0.131363
14	6	0	1.620832	1.058528	−0.689397
15	8	0	4.448267	−3.259826	−1.785307
16	8	0	2.532475	−1.477250	−1.581285
17	8	0	0.906714	0.555081	−1.764910
18	6	0	3.215577	0.232464	2.249769
19	6	0	8.749539	−2.137347	0.186754
20	6	0	−6.111143	−2.369567	0.988859
21	6	0	−6.886605	−1.509354	0.196932
22	6	0	−6.284181	−0.357753	−0.334074
23	6	0	−4.931639	−0.091739	−0.114319
24	6	0	−4.171774	−0.952110	0.672443
25	6	0	−4.766755	−2.089948	1.226429
26	8	0	−4.440775	1.050869	−0.681039

27	6	0	−3.012656	1.078690	−0.922055
28	6	0	−2.216096	0.574809	0.256378
29	6	0	−2.769807	−0.613612	0.948260
30	6	0	−2.687422	2.576265	−1.192917
31	6	0	−1.185372	2.837549	−1.230496
32	6	0	−0.480508	2.409365	0.080988
33	6	0	−1.083163	1.153665	0.708225
34	8	0	−4.093325	−2.975914	2.024275
35	8	0	−2.105640	−1.286625	1.734829
36	8	0	−0.389437	0.677422	1.809338
37	6	0	−2.719127	0.244408	−2.185300
38	6	0	−8.349481	−1.797831	−0.011879
39	8	0	3.902079	3.270231	0.084816
40	8	0	−3.266812	3.419748	−0.182823
41	8	0	−8.771291	−1.337519	−1.288346
42	1	0	−0.688130	3.217822	0.799874
43	1	0	1.315258	3.129751	−0.891071
44	1	0	−3.141741	2.892961	−2.139344
45	1	0	3.755512	2.853874	2.065858
46	1	0	6.900917	−3.611072	−1.186993
47	1	0	7.374663	0.078742	0.995988
48	1	0	1.342777	2.403377	2.052459
49	1	0	1.668661	3.923745	1.243656
50	1	0	3.549326	−2.891601	−1.933365
51	1	0	1.278611	−0.323218	−2.002776
52	1	0	2.159986	0.312505	2.524913
53	1	0	3.453452	−0.835173	2.176156
54	1	0	3.817450	0.619434	3.079854
55	1	0	9.098531	−1.710282	1.133002
56	1	0	8.905350	−3.219457	0.241554
57	1	0	9.356033	−1.732320	−0.629458
58	1	0	−6.551971	−3.260739	1.432206
59	1	0	−6.874383	0.329299	−0.939617
60	1	0	−0.750994	2.337855	−2.100540
61	1	0	−1.008181	3.912013	−1.374135
62	1	0	−3.178699	−2.639247	2.151752
63	1	0	−0.799971	−0.169491	2.092481
64	1	0	−1.661536	0.265001	−2.464535
65	1	0	−3.001126	−0.806329	−2.054819
66	1	0	−3.305909	0.613102	−3.033980
67	1	0	−8.938070	−1.293730	0.760142
68	1	0	−8.539294	−2.875261	0.034062
69	1	0	4.806415	2.917119	−0.015032

70	1	0	−4.188818	3.117113	−0.074173
71	1	0	−9.705445	−1.589161	−1.379792

Table S14. Cartesian coordinates for the low-energy optimized conformer of **2**b at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 2b			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.538642	−2.625115	−0.789089
2	6	0	7.328251	−1.765583	−0.015038
3	6	0	6.764672	−0.581973	0.479878
4	6	0	5.421865	−0.280589	0.236913
5	6	0	4.642720	−1.138260	−0.534302
6	6	0	5.206967	−2.310758	−1.048841
7	8	0	4.964178	0.892536	0.766193
8	6	0	3.533333	0.978225	0.982691
9	6	0	2.735719	0.465912	−0.190846
10	6	0	3.256310	−0.762262	−0.837406
11	6	0	3.257123	2.494105	1.202945
12	6	0	1.765045	2.808107	1.211776
13	6	0	1.062965	2.364002	−0.095537
14	6	0	1.630142	1.069295	−0.676059
15	8	0	4.512114	−3.198241	−1.827283
16	8	0	2.577238	−1.436587	−1.610505
17	8	0	0.934065	0.583231	−1.771805
18	6	0	3.193012	0.193436	2.266508
19	6	0	8.775694	−2.079227	0.227560
20	6	0	−6.096477	−2.457036	0.841538
21	6	0	−6.876851	−1.572062	0.084988
22	6	0	−6.270953	−0.419284	−0.440621
23	6	0	−4.920649	−0.150174	−0.205479
24	6	0	−4.162950	−1.020809	0.571716
25	6	0	−4.754226	−2.176725	1.093041
26	8	0	−4.431558	1.002039	−0.750730
27	6	0	−3.000650	1.050438	−0.968358
28	6	0	−2.214890	0.528675	0.209256
29	6	0	−2.765452	−0.679340	0.866607
30	6	0	−2.686193	2.557035	−1.202130
31	6	0	−1.187360	2.833399	−1.213929
32	6	0	−0.494944	2.383257	0.097055
33	6	0	−1.092814	1.107819	0.687613
34	8	0	−4.077688	−3.081825	1.865434
35	8	0	−2.101870	−1.368718	1.640789

36	8	0	−0.408065	0.613177	1.786790
37	6	0	−2.680091	0.247127	−2.245335
38	6	0	−8.319226	−1.903365	−0.194517
39	8	0	3.879035	3.285252	0.176670
40	8	0	−3.286841	3.371328	−0.180930
41	8	0	−9.079212	−0.721939	−0.409371
42	1	0	−0.719083	3.172644	0.830561
43	1	0	1.306378	3.141676	−0.836143
44	1	0	−3.131963	2.890668	−2.146905
45	1	0	3.709278	2.823836	2.145812
46	1	0	6.959435	−3.539161	−1.203165
47	1	0	7.369418	0.106641	1.066575
48	1	0	1.302744	2.351046	2.091123
49	1	0	1.624125	3.891631	1.319966
50	1	0	3.611950	−2.833109	−1.978705
51	1	0	1.318701	−0.285452	−2.023438
52	1	0	2.134061	0.258864	2.528601
53	1	0	3.441817	−0.868864	2.172993
54	1	0	3.780474	0.568934	3.113169
55	1	0	9.107902	−1.669880	1.187310
56	1	0	8.940904	−3.160272	0.261837
57	1	0	9.389154	−1.651289	−0.570888
58	1	0	−6.530877	−3.365479	1.253229
59	1	0	−6.858006	0.274855	−1.039505
60	1	0	−0.737329	2.357249	−2.089333
61	1	0	−1.019052	3.912215	−1.332315
62	1	0	−3.169351	−2.738455	2.016462
63	1	0	−0.815447	−0.243395	2.046137
64	1	0	−1.619554	0.281611	−2.507267
65	1	0	−2.956871	−0.808985	−2.141488
66	1	0	−3.257157	0.629113	−3.095004
67	1	0	−8.760033	−2.434286	0.656129
68	1	0	−8.385247	−2.531773	−1.087856
69	1	0	4.788288	2.943378	0.082298
70	1	0	−4.206620	3.057234	−0.086923
71	1	0	−10.001602	−1.002848	−0.530866

Table S15. Cartesian coordinates for the low-energy optimized conformer of **2**c at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 2c			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	−6.541433	−2.624778	0.760211
2	6	0	−7.323310	−1.773280	−0.030003

3	6	0	−6.755078	−0.593517	−0.529160
4	6	0	−5.415657	−0.287792	−0.274016
5	6	0	−4.644669	−1.137558	0.514342
6	6	0	−5.212468	−2.306883	1.032549
7	8	0	−4.953044	0.881342	−0.808412
8	6	0	−3.520474	0.966734	−1.008965
9	6	0	−2.735971	0.466470	0.177635
10	6	0	−3.261895	−0.756666	0.829366
11	6	0	−3.242881	2.481528	−1.240443
12	6	0	−1.751550	2.796602	−1.233576
13	6	0	−1.064168	2.364862	0.086724
14	6	0	−1.636294	1.075458	0.670720
15	8	0	−4.525847	−3.185329	1.826258
16	8	0	−2.591010	−1.424194	1.615899
17	8	0	−0.952633	0.598910	1.778166
18	6	0	−3.163926	0.171276	−2.281984
19	6	0	−8.767127	−2.090078	−0.285943
20	6	0	6.110999	−2.456309	−0.711647
21	6	0	6.871404	−1.572145	0.064122
22	6	0	6.265568	−0.407151	0.558357
23	6	0	4.918986	−0.141313	0.301598
24	6	0	4.172780	−1.018780	−0.478479
25	6	0	4.773407	−2.176513	−0.986023
26	8	0	4.423232	1.018755	0.826475
27	6	0	2.988559	1.067698	1.024653
28	6	0	2.219569	0.533873	−0.158227
29	6	0	2.779673	−0.680362	−0.797572
30	6	0	2.669675	2.575920	1.239349
31	6	0	1.169805	2.850705	1.228538
32	6	0	0.495609	2.387016	−0.087217
33	6	0	1.103797	1.106770	−0.658624
34	8	0	4.112310	−3.082577	−1.770531
35	8	0	2.129388	−1.374371	−1.577989
36	8	0	0.434815	0.601585	−1.761935
37	6	0	2.651923	0.275859	2.304561
38	6	0	8.322711	−1.847372	0.349681
39	8	0	−3.876559	3.280375	−0.227451
40	8	0	3.282910	3.381326	0.219007
41	8	0	9.142263	−0.911023	−0.333751
42	1	0	0.728116	3.169761	−0.825152
43	1	0	−1.318466	3.149495	0.816128
44	1	0	3.101564	2.918743	2.187664
45	1	0	−3.685299	2.802164	−2.190463

46	1	0	−6.966478	−3.535487	1.176929
47	1	0	−7.354701	0.089820	−1.127962
48	1	0	−1.277548	2.332108	−2.102871
49	1	0	−1.609360	3.879254	−1.350965
50	1	0	−3.628324	−2.819606	1.985193
51	1	0	−1.339997	−0.267549	2.034548
52	1	0	−2.101903	0.235230	−2.532388
53	1	0	−3.412990	−0.891129	−2.181972
54	1	0	−3.742224	0.538323	−3.138326
55	1	0	−9.089805	−1.689030	−1.253457
56	1	0	−8.931067	−3.171667	−0.313112
57	1	0	−9.390096	−1.655825	0.501259
58	1	0	6.555978	−3.363504	−1.117537
59	1	0	6.849105	0.294611	1.153568
60	1	0	0.709112	2.382276	2.102761
61	1	0	0.998180	3.930283	1.333950
62	1	0	3.202796	−2.745960	−1.931025
63	1	0	0.843434	−0.257815	−2.007455
64	1	0	1.588187	0.313022	2.553773
65	1	0	2.930346	−0.780138	2.214770
66	1	0	3.218826	0.667042	3.157895
67	1	0	8.608662	−2.853617	0.024047
68	1	0	8.521799	−1.777344	1.424212
69	1	0	−4.788113	2.939973	−0.140925
70	1	0	4.207574	3.077880	0.149736
71	1	0	8.700707	−0.691362	−1.171871

Table S16. Cartesian coordinates for the low-energy optimized conformer of **2**d at B3LYP/6–311+g (d,p) level of theory in CH_3CN.

Conformer of 2d			**Standard Orientation (Å)**		
Number	Atom	Type	X	Y	Z
1	6	0	6.454829	−2.738907	−0.743018
2	6	0	7.271573	−1.865052	−0.014337
3	6	0	6.737606	−0.651910	0.441983
4	6	0	5.398108	−0.334283	0.206812
5	6	0	4.591152	−1.206562	−0.519278
6	6	0	5.124168	−2.408415	−0.995464
7	8	0	4.969309	0.867119	0.695977
8	6	0	3.544850	0.988290	0.930856
9	6	0	2.719969	0.447324	−0.211411
10	6	0	3.206839	−0.815151	−0.816035
11	6	0	3.299742	2.517276	1.095874
12	6	0	1.814592	2.859813	1.113231

13	6	0	1.085457	2.378709	−0.166973
14	6	0	1.618533	1.052914	−0.703880
15	8	0	4.401274	−3.311243	−1.727987
16	8	0	2.503668	−1.506474	−1.551728
17	8	0	0.897300	0.537427	−1.768822
18	6	0	3.208879	0.260742	2.248142
19	6	0	8.716757	−2.196485	0.219409
20	6	0	−6.148578	−2.265445	1.045090
21	6	0	−6.916613	−1.397556	0.257602
22	6	0	−6.302163	−0.273508	−0.313853
23	6	0	−4.945028	−0.021133	−0.105504
24	6	0	−4.193477	−0.875326	0.695791
25	6	0	−4.798975	−1.999386	1.268170
26	8	0	−4.442843	1.101436	−0.699660
27	6	0	−3.012993	1.114646	−0.936254
28	6	0	−2.222208	0.623075	0.249696
29	6	0	−2.786749	−0.548772	0.960382
30	6	0	−2.673802	2.604544	−1.231814
31	6	0	−1.170276	2.851945	−1.273156
32	6	0	−0.469514	2.438038	0.045854
33	6	0	−1.083852	1.198933	0.692614
34	8	0	−4.129895	−2.884413	2.069379
35	8	0	−2.126593	−1.219733	1.753545
36	8	0	−0.394594	0.733423	1.800878
37	6	0	−2.725443	0.257661	−2.185646
38	6	0	−8.374860	−1.671454	0.005868
39	8	0	3.920418	3.255946	0.030121
40	8	0	−3.244930	3.469058	−0.234887
41	8	0	−8.570831	−2.062521	−1.344727
42	1	0	−0.667772	3.259311	0.750840
43	1	0	1.333094	3.122994	−0.939657
44	1	0	−3.125132	2.911619	−2.183114
45	1	0	3.773060	2.874423	2.018416
46	1	0	6.851050	−3.675681	−1.127207
47	1	0	7.364435	0.047190	0.992050
48	1	0	1.356043	2.445440	2.015080
49	1	0	1.694435	3.949478	1.181780
50	1	0	3.505875	−2.935876	−1.882030
51	1	0	1.263078	−0.346651	−1.993649
52	1	0	2.155305	0.356418	2.522366
53	1	0	3.436309	−0.809458	2.192467
54	1	0	3.815182	0.657629	3.071026
55	1	0	8.861539	−3.279499	0.292293

56	1	0	9.326087	−1.812061	−0.604741
57	1	0	9.071060	−1.756188	1.156592
58	1	0	−6.596648	−3.147204	1.498005
59	1	0	−6.886479	0.403835	−0.935818
60	1	0	−0.740270	2.333682	−2.135072
61	1	0	−0.982321	3.921884	−1.433724
62	1	0	−3.212560	−2.555075	2.195725
63	1	0	−0.811469	−0.105830	2.098159
64	1	0	−1.668403	0.262209	−2.462882
65	1	0	−3.019495	−0.787795	−2.039009
66	1	0	−3.307104	0.618255	−3.042257
67	1	0	−8.973481	−0.777244	0.207576
68	1	0	−8.747393	−2.472401	0.653415
69	1	0	4.822224	2.894225	−0.062895
70	1	0	−4.172433	3.183580	−0.125662
71	1	0	−7.787218	−2.568788	−1.619286