Syntheses and Properties of the V-shaped Dimeric Xanthene Dyes

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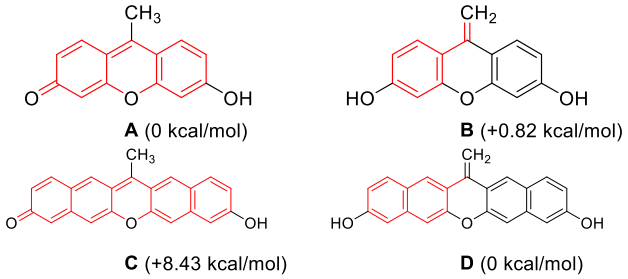
Electronic Supplementary Information (ESI)

Table of Contests

Figure S1. The DFT calculation of corresponding compounds with *exo*- and *endo*-double bonds. (B3LYP/6-31+G level)[a)]



A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.278407	0.757613	0.000007
2	6	0	-1.252057	-0.700848	-0.000079
3	6	0	-2.366259	-1.481496	-0.000020
4	6	0	-3.688241	-0.881017	0.000307
5	6	0	-3.734649	0.588251	-0.000072
6	6	0	-2.607025	1.347117	-0.000089
7	6	0	-0.093323	1.478496	0.000047
8	6	0	1.172187	0.762105	0.000065
9	6	0	1.170508	-0.654571	-0.000022
10	8	0	-0.017073	-1.360435	-0.000135
11	6	0	2.438575	1.394718	0.000153
12	6	0	3.619999	0.660453	0.000153
13	6	0	3.562825	-0.746777	0.000052
14	6	0	2.338491	-1.412053	-0.000033
15	6	0	-0.047996	2.986072	0.000068
16	8	0	-4.751307	-1.571402	-0.000328
17	8	0	4.701257	-1.540828	0.000048
18	1	0	-2.285114	-2.561235	-0.000142
19	1	0	-4.720694	1.040503	-0.000218
20	1	0	-2.698645	2.426457	-0.000190
21	1	0	2.497815	2.476339	0.000227
22	1	0	4.578663	1.170804	0.000229

23	1	0	2.292830	-2.493006	-0.000110
24	1	0	-1.037433	3.439778	-0.000073
25	1	0	0.486141	3.358914	-0.883283
26	1	0	0.485890	3.358896	0.883582
27	1	0	5.529763	-1.024514	0.000066

B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.829021	0.008736	1.251518
2	6	0	0.573552	0.092154	1.205433
3	6	0	1.375299	0.070020	2.350487
4	6	0	0.762170	-0.053023	3.595539
5	6	0	-0.633623	-0.161014	3.693509
6	6	0	-1.403018	-0.131432	2.535579
7	6	0	-1.623862	0.083252	0.000000
8	6	0	-0.829021	0.008736	-1.251518
9	6	0	0.573552	0.092154	-1.205433
10	8	0	1.271486	0.210564	0.000000
11	6	0	-1.403018	-0.131432	-2.535579
12	6	0	-0.633623	-0.161014	-3.693509
13	6	0	0.762170	-0.053023	-3.595539
14	6	0	1.375299	0.070020	-2.350487
15	6	0	-2.970110	0.232914	0.000000
16	8	0	1.479592	-0.085960	4.789961
17	8	0	1.479592	-0.085960	-4.789961
18	1	0	2.451890	0.144033	2.238138
19	1	0	-1.086637	-0.271283	4.671381
20	1	0	-2.478463	-0.227408	2.627022
21	1	0	-2.478463	-0.227408	-2.627022
22	1	0	-1.086637	-0.271283	-4.671381
23	1	0	2.451890	0.144033	-2.238138
24	1	0	-3.543255	0.307691	0.915751
25	1	0	-3.543255	0.307691	-0.915751

26	1	0	2.443543	-0.008752	4.656501
27	1	0	2.443543	-0.008752	-4.656501

C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.641899	0.712086	0.000038
2	6	0	-3.594482	-0.729137	0.000022
3	6	0	-2.326554	-1.367366	0.000008
4	6	0	-1.173665	-0.615177	0.000013
5	6	0	-1.181396	0.817331	0.000036
6	6	0	-2.433284	1.443748	0.000045
7	6	0	-4.918275	1.356164	0.000048
8	6	0	-6.084848	0.626538	0.000044
9	6	0	-6.022818	-0.792970	0.000030
10	6	0	-4.813382	-1.462187	0.000019
11	8	0	0.027761	-1.311413	-0.000009
12	6	0	1.252796	-0.636578	-0.000004
13	6	0	1.272387	0.820518	0.000017
14	6	0	0.080050	1.539871	0.000045
15	6	0	2.378125	-1.399680	-0.000023
16	6	0	3.685545	-0.792389	-0.000028
17	6	0	3.744049	0.674630	-0.000022
18	6	0	2.585308	1.416143	0.000000
19	6	0	4.853031	-1.525926	-0.000034
20	6	0	6.160060	-0.895967	0.000010
21	6	0	6.193689	0.576334	-0.000083
22	6	0	5.051538	1.309025	-0.000071
23	8	0	7.237147	-1.569941	-0.000167
24	8	0	-7.255236	-1.439850	0.000027
25	6	0	0.030129	3.046556	0.000075
26	1	0	-2.249604	-2.448880	-0.000007
27	1	0	-2.494652	2.526375	0.000056
28	1	0	-4.957020	2.441659	0.000059

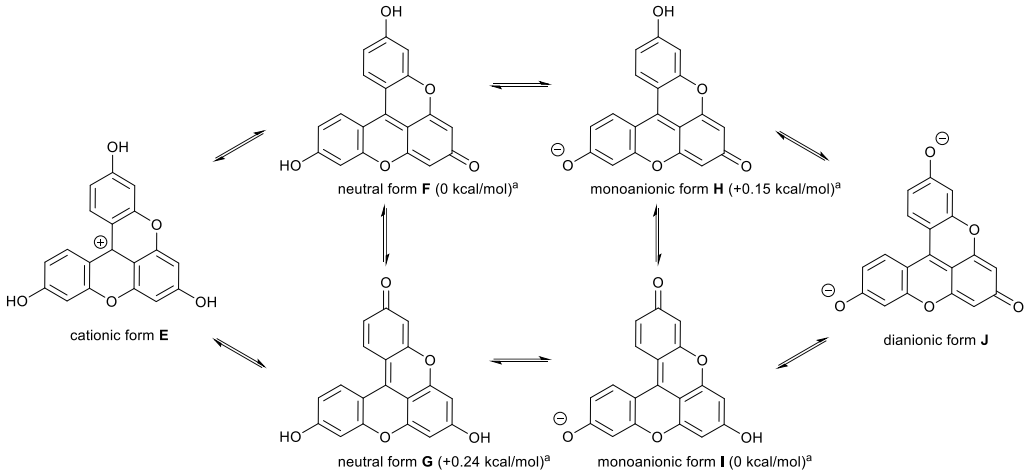
29	1	0	-7.059204	1.100343	0.000052
30	1	0	-4.778515	-2.548671	0.000007
31	1	0	2.287583	-2.480009	-0.000034
32	1	0	2.672276	2.496260	-0.000009
33	1	0	4.831315	-2.611059	-0.000053
34	1	0	7.175046	1.038731	-0.000137
35	1	0	5.087928	2.396024	-0.000107
36	1	0	-7.175923	-2.413206	0.000020
37	1	0	1.017517	3.505141	0.000211
38	1	0	-0.505477	3.418733	0.883062
39	1	0	-0.505262	3.418776	-0.883028

D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.689218	0.717925	-0.126224
2	6	0	-3.613931	-0.707851	0.059512
3	6	0	-2.341005	-1.294145	0.271801
4	6	0	-1.211049	-0.504229	0.312550
5	6	0	-1.254095	0.913791	0.168706
6	6	0	-2.500211	1.485268	-0.068733
7	6	0	-4.967134	1.311095	-0.361844
8	6	0	-6.111644	0.546760	-0.406894
9	6	0	-6.023293	-0.857988	-0.217950
10	6	0	-4.811296	-1.479005	0.008106
11	8	0	0.000000	-1.173274	0.522634
12	6	0	1.211049	-0.504229	0.312550
13	6	0	1.254095	0.913791	0.168706
14	6	0	0.000000	1.698313	0.296040
15	6	0	2.341005	-1.294145	0.271801
16	6	0	3.613931	-0.707851	0.059512
17	6	0	3.689218	0.717925	-0.126224
18	6	0	2.500211	1.485268	-0.068733
19	6	0	4.811296	-1.479005	0.008106

20	6	0	6.023293	-0.857988	-0.217950
21	6	0	6.111644	0.546760	-0.406894
22	6	0	4.967134	1.311095	-0.361844
23	8	0	7.237295	-1.544981	-0.280085
24	8	0	-7.237295	-1.544981	-0.280085
25	6	0	0.000000	3.027238	0.553642
26	1	0	-2.237468	-2.366386	0.397385
27	1	0	-2.576257	2.556654	-0.225390
28	1	0	-5.026810	2.386317	-0.504779
29	1	0	-7.087502	0.983781	-0.582857
30	1	0	-4.754384	-2.555821	0.148463
31	1	0	2.237468	-2.366386	0.397385
32	1	0	2.576257	2.556654	-0.225390
33	1	0	4.754384	-2.555821	0.148463
34	1	0	7.087502	0.983781	-0.582857
35	1	0	5.026810	2.386317	-0.504779
36	1	0	7.133691	-2.506429	-0.144941
37	1	0	-7.133691	-2.506429	-0.144941
38	1	0	0.918278	3.588434	0.679053
39	1	0	-0.918278	3.588434	0.679053

Figure S2. The protonation and deprotonation sequences of dye **3**. [a)] The energy difference between two tautomers from DFT calculations at the B3LYP/6-31+G(d,p) level.



E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.772204	-2.845816	0.391058
2	6	0	3.890017	-2.039052	0.079160
3	6	0	3.726431	-0.679065	-0.179317
4	6	0	2.443524	-0.142193	-0.151879
5	6	0	1.280492	-0.933435	0.061598
6	6	0	1.508415	-2.301450	0.380733
7	8	0	2.377935	1.206287	-0.341669
8	6	0	1.205883	1.866235	-0.160674
9	6	0	0.005280	1.131160	0.000826
10	6	0	-0.003516	-0.286321	0.000774
11	6	0	1.233061	3.248990	-0.176287
12	6	0	0.023413	3.941225	0.000772
13	6	0	-1.194820	3.263939	0.177305
14	6	0	-1.186730	1.883233	0.161678
15	8	0	-2.367090	1.236400	0.343639
16	6	0	-2.448803	-0.110852	0.153080
17	6	0	-1.295693	-0.916901	-0.059964
18	6	0	-3.738202	-0.632194	0.179430

19	6	0	-3.918624	-1.989906	-0.080365
20	6	0	-2.810793	-2.810474	-0.391736
21	6	0	-1.540433	-2.281715	-0.380202
22	8	0	-5.132084	-2.578959	-0.088323
23	8	0	-0.034892	5.289099	0.012155
24	8	0	5.096166	-2.642938	0.085291
25	1	0	2.929125	-3.885702	0.653663
26	1	0	4.572434	-0.027748	-0.371061
27	1	0	0.680660	-2.928731	0.677619
28	1	0	2.172651	3.771363	-0.315931
29	1	0	-2.117389	3.814091	0.314949
30	1	0	-4.575960	0.029802	0.371054
31	1	0	-2.980464	-3.848118	-0.655232
32	1	0	-0.720288	-2.918904	-0.677046
33	1	0	-5.835144	-1.944358	0.119027
34	1	0	0.841133	5.683437	-0.118334
35	1	0	5.806321	-2.016695	-0.123391

F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.347305	2.804566	-2.793232
2	6	0	-0.010173	3.909400	-1.988594
3	6	0	0.261771	3.732660	-0.632718
4	6	0	0.221083	2.446515	-0.098199
5	6	0	-0.024331	1.296588	-0.889407
6	6	0	-0.352707	1.534686	-2.247585
7	8	0	0.429145	2.370879	1.248694
8	6	0	0.192213	1.200093	1.921386
9	6	0	0.000000	0.000000	1.159938
10	6	0	0.000000	0.000000	-0.233539
11	6	0	0.208468	1.219071	3.286337
12	6	0	0.000000	0.000000	4.047557
13	6	0	-0.208468	-1.219071	3.286337

14	6	0	-0.192213	-1.200093	1.921386
15	8	0	-0.429145	-2.370879	1.248694
16	6	0	-0.221083	-2.446515	-0.098199
17	6	0	0.024331	-1.296588	-0.889407
18	6	0	-0.261771	-3.732660	-0.632718
19	6	0	0.010173	-3.909400	-1.988594
20	6	0	0.347305	-2.804566	-2.793232
21	6	0	0.352707	-1.534686	-2.247585
22	8	0	0.000000	-5.128412	-2.584930
23	8	0	0.000000	5.128412	-2.584930
24	8	0	0.000000	0.000000	5.309393
25	1	0	-0.613576	2.964938	-3.831900
26	1	0	0.475305	4.572398	0.020664
27	1	0	-0.665138	0.713809	-2.876891
28	1	0	0.380519	2.147066	3.820453
29	1	0	-0.380519	-2.147066	3.820453
30	1	0	-0.475305	-4.572398	0.020664
31	1	0	0.613576	-2.964938	-3.831900
32	1	0	0.665138	-0.713809	-2.876891
33	1	0	-0.227883	-5.823604	-1.949798
34	1	0	0.227883	5.823604	-1.949798

G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.923243	-2.682584	-0.403421
2	6	0	-3.983271	-1.811469	-0.086172
3	6	0	-3.727265	-0.468922	0.186437
4	6	0	-2.409497	-0.015604	0.170553
5	6	0	-1.304774	-0.875290	-0.050132
6	6	0	-1.623423	-2.215543	-0.387487
7	8	0	-2.265228	1.330837	0.372754
8	6	0	-1.051350	1.918123	0.165854
9	6	0	0.097806	1.118792	-0.011017

10	6	0	0.037113	-0.314560	0.006639
11	6	0	-1.001535	3.302508	0.175679
12	6	0	0.240775	3.925990	-0.010000
13	6	0	1.414934	3.180107	-0.186181
14	6	0	1.324958	1.795082	-0.169688
15	8	0	2.471505	1.085815	-0.333813
16	6	0	2.488716	-0.275362	-0.127946
17	6	0	1.259867	-1.007669	0.073253
18	6	0	3.724190	-0.866999	-0.157994
19	6	0	3.878833	-2.282149	0.074884
20	6	0	2.650564	-3.008467	0.383905
21	6	0	1.428061	-2.404708	0.375833
22	8	0	5.001781	-2.856749	0.050814
23	8	0	-5.235565	-2.332855	-0.099593
24	8	0	0.245123	5.283242	-0.003673
25	1	0	-3.142383	-3.708917	-0.675684
26	1	0	-4.527421	0.237648	0.381947
27	1	0	-0.836152	-2.891808	-0.688077
28	1	0	-1.900029	3.889626	0.321402
29	1	0	2.378235	3.659136	-0.322652
30	1	0	4.606309	-0.262200	-0.340101
31	1	0	2.743952	-4.057841	0.647510
32	1	0	0.563225	-2.985449	0.667205
33	1	0	-5.896821	-1.657348	0.112586
34	1	0	1.141410	5.627183	-0.134042

H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.876360	-2.696883	-0.408261
2	6	0	-3.951802	-1.849566	-0.089554
3	6	0	-3.721556	-0.504426	0.191943
4	6	0	-2.412028	-0.022157	0.181059
5	6	0	-1.292542	-0.858870	-0.044005

6	6	0	-1.583981	-2.201139	-0.387158
7	8	0	-2.292501	1.322503	0.392375
8	6	0	-1.086885	1.946682	0.167421
9	6	0	0.079252	1.147602	-0.006250
10	6	0	0.041806	-0.262779	0.007221
11	6	0	-1.062386	3.317516	0.175045
12	6	0	0.180250	4.036362	-0.013741
13	6	0	1.370532	3.231965	-0.185526
14	6	0	1.302748	1.861324	-0.166591
15	8	0	2.459670	1.152091	-0.353030
16	6	0	2.494019	-0.207692	-0.141928
17	6	0	1.285353	-0.955044	0.059489
18	6	0	3.745098	-0.782232	-0.159660
19	6	0	3.927415	-2.188423	0.082854
20	6	0	2.713665	-2.929288	0.382695
21	6	0	1.476211	-2.340741	0.366016
22	8	0	5.070338	-2.743857	0.070497
23	8	0	-5.199372	-2.393602	-0.106708
24	8	0	0.222708	5.306382	-0.022799
25	1	0	-3.072617	-3.727286	-0.683344
26	1	0	-4.536444	0.184748	0.390233
27	1	0	-0.782524	-2.861333	-0.686145
28	1	0	-1.977930	3.878764	0.329233
29	1	0	2.324856	3.728123	-0.328060
30	1	0	4.615717	-0.158823	-0.337943
31	1	0	2.816338	-3.978281	0.646535
32	1	0	0.621596	-2.939831	0.651673
33	1	0	-5.868561	-1.727477	0.108730

I

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.769397	-2.890643	-0.385802
2	6	0	-3.956734	-2.111083	-0.077426

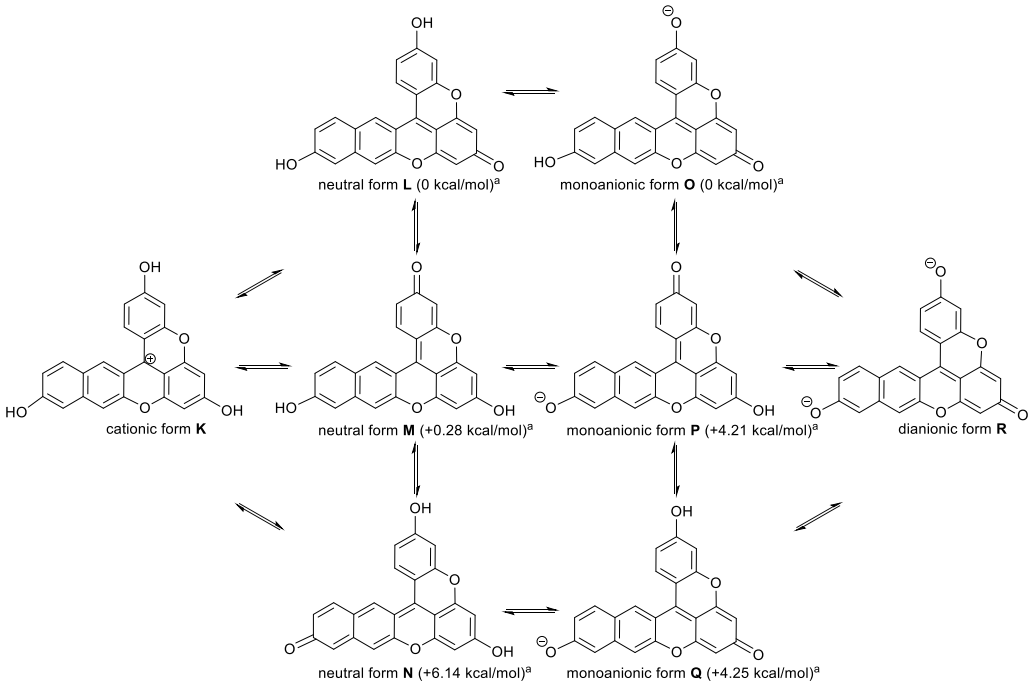
3	6	0	-3.725447	-0.711318	0.161415
4	6	0	-2.455191	-0.182287	0.140851
5	6	0	-1.271660	-0.966635	-0.061562
6	6	0	-1.513407	-2.343925	-0.373239
7	8	0	-2.381509	1.181983	0.344948
8	6	0	-1.202498	1.835499	0.163678
9	6	0	-0.007695	1.109394	0.000444
10	6	0	0.005041	-0.333532	0.001272
11	6	0	-1.235313	3.225800	0.174175
12	6	0	-0.032617	3.922199	-0.001696
13	6	0	1.182095	3.246996	-0.176098
14	6	0	1.174906	1.858461	-0.163411
15	8	0	2.364938	1.224013	-0.345076
16	6	0	2.462076	-0.138489	-0.140473
17	6	0	1.292712	-0.943550	0.064041
18	6	0	3.741037	-0.646021	-0.163070
19	6	0	3.996797	-2.041601	0.075770
20	6	0	2.823879	-2.841163	0.388177
21	6	0	1.558771	-2.316006	0.377408
22	8	0	5.165384	-2.538511	0.053454
23	8	0	-5.116828	-2.627746	-0.058615
24	8	0	0.017865	5.283029	-0.013271
25	1	0	-2.908783	-3.934261	-0.654265
26	1	0	-4.573012	-0.056939	0.339012
27	1	0	-0.678916	-2.968231	-0.663908
28	1	0	-2.178840	3.743091	0.310579
29	1	0	2.106949	3.794716	-0.311604
30	1	0	4.577011	0.022556	-0.342656
31	1	0	2.981936	-3.881768	0.657949
32	1	0	0.735559	-2.953897	0.670717
33	1	0	-0.864850	5.660010	0.115931

J

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.348510	2.808016	-2.831725
2	6	0	-0.027946	3.983359	-2.046333
3	6	0	0.213846	3.735704	-0.652691
4	6	0	0.184284	2.457906	-0.129637
5	6	0	-0.034224	1.287856	-0.921734
6	6	0	-0.346051	1.544161	-2.291988
7	8	0	0.392475	2.373428	1.230412
8	6	0	0.177895	1.190171	1.891696
9	6	0	0.000000	0.000000	1.136724
10	6	0	0.000000	0.000000	-0.284795
11	6	0	0.191144	1.211602	3.267716
12	6	0	0.000000	0.000000	4.030002
13	6	0	-0.191144	-1.211602	3.267716
14	6	0	-0.177895	-1.190171	1.891696
15	8	0	-0.392475	-2.373428	1.230412
16	6	0	-0.184284	-2.457906	-0.129637
17	6	0	0.034224	-1.287856	-0.921734
18	6	0	-0.213846	-3.735704	-0.652691
19	6	0	0.027946	-3.983359	-2.046333
20	6	0	0.348510	-2.808016	-2.831725
21	6	0	0.346051	-1.544161	-2.291988
22	8	0	0.000000	-5.154080	-2.554008
23	8	0	0.000000	5.154080	-2.554008
24	8	0	0.000000	0.000000	5.306771
25	1	0	-0.615751	2.954455	-3.875126
26	1	0	0.401162	4.575239	0.010066
27	1	0	-0.644653	0.719054	-2.925165
28	1	0	0.347270	2.147745	3.794297
29	1	0	-0.347270	-2.147745	3.794297
30	1	0	-0.401162	-4.575239	0.010066
31	1	0	0.615751	-2.954455	-3.875126
32	1	0	0.644653	-0.719054	-2.925165

Figure S3. The protonation and deprotonation sequences of dye **4**. [a)] The energy difference between three tautomers from DFT calculations at the B3LYP/6-31+G(d,p) level.



K

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.996855	0.662952	-0.204397
2	6	0	3.480635	-0.655468	0.117359
3	6	0	2.534977	-1.687921	0.326014
4	6	0	1.189105	-1.417623	0.258743
5	6	0	0.673655	-0.093679	0.041230
6	6	0	1.617495	0.906952	-0.236519
7	8	0	0.353163	-2.496920	0.406279
8	6	0	-0.973561	-2.372948	0.164374
9	6	0	-1.545559	-1.082109	-0.000611
10	6	0	-0.758693	0.093604	0.053209
11	6	0	-1.736975	-3.523005	0.132792
12	6	0	-3.119588	-3.407860	-0.094031
13	6	0	-3.736641	-2.159297	-0.277890
14	6	0	-2.946854	-1.025983	-0.213352

15	8	0	-3.549103	0.176224	-0.394080
16	6	0	-2.867285	1.331267	-0.155816
17	6	0	-1.469537	1.341286	0.114001
18	6	0	-3.636852	2.489158	-0.194289
19	6	0	-3.030806	3.707154	0.109013
20	6	0	-1.666805	3.753129	0.479840
21	6	0	-0.915803	2.600645	0.481255
22	6	0	3.946358	1.696899	-0.478640
23	6	0	5.291276	1.449734	-0.417437
24	6	0	5.759051	0.143872	-0.084182
25	6	0	4.876449	-0.888888	0.174278
26	8	0	-3.698701	4.878595	0.107280
27	8	0	-3.816793	-4.561742	-0.122348
28	8	0	7.108788	-0.002170	-0.045374
29	1	0	2.860564	-2.706048	0.511048
30	1	0	1.288361	1.893362	-0.532556
31	1	0	-1.282683	-4.495408	0.277467
32	1	0	-4.802312	-2.070593	-0.455907
33	1	0	-4.693165	2.417701	-0.429158
34	1	0	-1.233991	4.700735	0.779354
35	1	0	0.106935	2.657130	0.824384
36	1	0	3.584820	2.689953	-0.727580
37	1	0	6.020291	2.227940	-0.616205
38	1	0	5.244915	-1.881941	0.416136
39	1	0	-4.628136	4.757807	-0.141661
40	1	0	-4.760716	-4.402419	-0.275716
41	1	0	7.350909	-0.911352	0.186671

L

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.773181	3.697354	0.497172
2	6	0	3.127915	3.630855	0.119265
3	6	0	3.705940	2.404109	-0.203933

4	6	0	2.915216	1.257439	-0.175650
5	6	0	1.527178	1.291077	0.108425
6	6	0	1.001487	2.550761	0.491318
7	8	0	3.573829	0.091221	-0.438034
8	6	0	2.961296	-1.115485	-0.224710
9	6	0	1.542897	-1.132581	0.002831
10	6	0	0.793462	0.038189	0.060163
11	6	0	3.717061	-2.249129	-0.295749
12	6	0	3.108433	-3.555145	-0.113656
13	6	0	1.676103	-3.583660	0.133046
14	6	0	0.949107	-2.429640	0.173628
15	8	0	-0.386439	-2.510102	0.456464
16	6	0	-1.199691	-1.417015	0.289369
17	6	0	-0.657173	-0.109417	0.060706
18	6	0	-2.553159	-1.657393	0.348952
19	6	0	-3.477241	-0.608205	0.123655
20	6	0	-2.964565	0.693957	-0.202639
21	6	0	-1.572565	0.905218	-0.228369
22	8	0	3.828303	4.793190	0.122222
23	8	0	3.789605	-4.614571	-0.163346
24	6	0	-4.880776	-0.811905	0.172300
25	6	0	-5.740193	0.235193	-0.099799
26	6	0	-5.242580	1.526313	-0.435701
27	6	0	-3.889135	1.743733	-0.486874
28	8	0	-7.098308	0.113885	-0.070901
29	1	0	1.353224	4.648751	0.803781
30	1	0	4.759273	2.315807	-0.448644
31	1	0	-0.020418	2.623809	0.834968
32	1	0	4.781764	-2.189257	-0.492359
33	1	0	1.192916	-4.541395	0.292407
34	1	0	-2.901280	-2.667032	0.541088
35	1	0	-1.220710	1.884658	-0.522603
36	1	0	4.749152	4.645612	-0.140655
37	1	0	-5.270966	-1.795803	0.419392
38	1	0	-5.951563	2.320331	-0.645291
39	1	0	-3.506114	2.728288	-0.739016

40	1	0	-7.354390	-0.790479	0.163216

M

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.607069	3.812856	0.484190
2	6	0	3.017785	3.851060	0.106035
3	6	0	3.623485	2.572491	-0.178142
4	6	0	2.889080	1.417184	-0.135724
5	6	0	1.467854	1.387297	0.128835
6	6	0	0.887750	2.655531	0.487384
7	8	0	3.579108	0.255635	-0.395672
8	6	0	2.985831	-0.954977	-0.227299
9	6	0	1.593860	-1.029562	-0.012928
10	6	0	0.792542	0.157145	0.061028
11	6	0	3.792269	-2.082771	-0.294451
12	6	0	3.194324	-3.337331	-0.108984
13	6	0	1.818340	-3.465074	0.132253
14	6	0	1.043541	-2.317140	0.171318
15	8	0	-0.282741	-2.463551	0.442748
16	6	0	-1.137099	-1.396323	0.284544
17	6	0	-0.650006	-0.067018	0.054198
18	6	0	-2.479038	-1.694916	0.347687
19	6	0	-3.448015	-0.687417	0.124455
20	6	0	-2.991779	0.633770	-0.209927
21	6	0	-1.611116	0.903574	-0.241624
22	8	0	3.664552	4.932599	0.069953
23	8	0	3.911288	-4.489012	-0.145008
24	6	0	-4.841443	-0.950158	0.179876
25	6	0	-5.745041	0.058723	-0.092818
26	6	0	-5.303379	1.367987	-0.438478
27	6	0	-3.960978	1.642137	-0.497302
28	8	0	-7.096402	-0.118407	-0.056258
29	1	0	1.147573	4.747764	0.790975

30	1	0	4.682351	2.530077	-0.410478
31	1	0	-0.137785	2.682615	0.830481
32	1	0	4.856997	-1.978989	-0.472373
33	1	0	1.372577	-4.440093	0.287135
34	1	0	-2.782105	-2.718799	0.540936
35	1	0	-1.301072	1.894511	-0.544623
36	1	0	4.849545	-4.308765	-0.305247
37	1	0	-5.188663	-1.948364	0.433014
38	1	0	-6.046186	2.130166	-0.649088
39	1	0	-3.620420	2.640267	-0.756716
40	1	0	-7.314263	-1.030906	0.185139

N

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.621444	3.764888	0.483876
2	6	0	2.979499	3.723761	0.108940
3	6	0	3.582202	2.506669	-0.203078
4	6	0	2.814049	1.345150	-0.170997
5	6	0	1.422543	1.350926	0.105849
6	6	0	0.873727	2.604724	0.483593
7	8	0	3.507436	0.192735	-0.418294
8	6	0	2.909672	-1.015190	-0.214630
9	6	0	1.517031	-1.082466	0.011951
10	6	0	0.701593	0.093124	0.053106
11	6	0	3.711951	-2.142245	-0.273967
12	6	0	3.112038	-3.395483	-0.086019
13	6	0	1.732601	-3.521935	0.139954
14	6	0	0.959131	-2.371113	0.172730
15	8	0	-0.371096	-2.511477	0.397547
16	6	0	-1.222502	-1.436733	0.237583
17	6	0	-0.701868	-0.101124	0.038113
18	6	0	-2.558488	-1.713362	0.300683
19	6	0	-3.532862	-0.681974	0.112108

20	6	0	-3.036286	0.652251	-0.191038
21	6	0	-1.675335	0.902813	-0.217787
22	8	0	3.654665	4.898746	0.108615
23	8	0	3.932542	-4.473187	-0.138356
24	6	0	-4.902363	-0.917314	0.165295
25	6	0	-5.868396	0.115974	-0.078265
26	6	0	-5.335772	1.445399	-0.401391
27	6	0	-3.999525	1.691273	-0.458420
28	8	0	-7.119431	-0.082196	-0.029927
29	1	0	1.183456	4.708880	0.788042
30	1	0	4.638036	2.436520	-0.442095
31	1	0	-0.148444	2.658033	0.829806
32	1	0	4.776333	-2.058340	-0.455920
33	1	0	1.266310	-4.491462	0.278447
34	1	0	-2.878172	-2.735770	0.475185
35	1	0	-1.351863	1.896103	-0.499192
36	1	0	4.580782	4.770170	-0.146432
37	1	0	3.438827	-5.293192	0.011084
38	1	0	-5.273239	-1.915024	0.386080
39	1	0	-6.059191	2.232859	-0.594610
40	1	0	-3.630275	2.686182	-0.696209

O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.712016	3.763149	0.481373
2	6	0	3.118438	3.777830	0.113730
3	6	0	3.691405	2.490825	-0.178895
4	6	0	2.930443	1.344202	-0.148195
5	6	0	1.519363	1.340667	0.116532
6	6	0	0.968278	2.612606	0.476568
7	8	0	3.602916	0.173171	-0.413571
8	6	0	2.999718	-1.041765	-0.225022
9	6	0	1.590066	-1.080468	-0.006601

10	6	0	0.823884	0.100081	0.064499
11	6	0	3.776253	-2.170354	-0.297793
12	6	0	3.191690	-3.482519	-0.124622
13	6	0	1.764980	-3.527438	0.124773
14	6	0	1.022454	-2.376339	0.170492
15	8	0	-0.315107	-2.485175	0.463707
16	6	0	-1.145474	-1.405327	0.297092
17	6	0	-0.630537	-0.087660	0.063505
18	6	0	-2.495711	-1.672919	0.357239
19	6	0	-3.442827	-0.646236	0.127336
20	6	0	-2.957579	0.662634	-0.208326
21	6	0	-1.567791	0.900860	-0.236479
22	8	0	3.796158	4.851962	0.087649
23	8	0	3.891749	-4.540387	-0.180203
24	6	0	-4.843372	-0.877764	0.179753
25	6	0	-5.724111	0.149257	-0.097470
26	6	0	-5.253255	1.446849	-0.443637
27	6	0	-3.903385	1.690454	-0.498572
28	8	0	-7.081908	-0.000039	-0.064112
29	1	0	1.261949	4.703860	0.786356
30	1	0	4.750359	2.422789	-0.407573
31	1	0	-0.058981	2.664522	0.812586
32	1	0	4.842151	-2.088825	-0.482862
33	1	0	1.289628	-4.489154	0.286784
34	1	0	-2.821777	-2.689439	0.553084
35	1	0	-1.235477	1.885383	-0.536655
36	1	0	-5.212947	-1.867895	0.434438
37	1	0	-5.977809	2.225609	-0.657784
38	1	0	-3.540670	2.680812	-0.758689
39	1	0	-7.316573	-0.907663	0.178873

P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.720055	3.706514	0.493982
2	6	0	3.073025	3.644985	0.114508
3	6	0	3.652820	2.419973	-0.209708
4	6	0	2.865888	1.268850	-0.182593
5	6	0	1.478849	1.297564	0.101930
6	6	0	0.953029	2.554898	0.488383
7	8	0	3.534343	0.106728	-0.443212
8	6	0	2.924044	-1.103785	-0.220620
9	6	0	1.513887	-1.130206	0.008621
10	6	0	0.740325	0.040485	0.055902
11	6	0	3.694174	-2.233496	-0.284414
12	6	0	3.101103	-3.542479	-0.098255
13	6	0	1.671166	-3.579744	0.136900
14	6	0	0.932680	-2.426893	0.172935
15	8	0	-0.406680	-2.522704	0.432506
16	6	0	-1.232463	-1.431285	0.264212
17	6	0	-0.688434	-0.113929	0.056034
18	6	0	-2.579219	-1.680611	0.319063
19	6	0	-3.530559	-0.634448	0.116542
20	6	0	-3.006760	0.682263	-0.189344
21	6	0	-1.630416	0.902192	-0.210411
22	8	0	3.773375	4.810731	0.117157
23	8	0	3.796322	-4.600779	-0.141110
24	6	0	-4.913403	-0.843712	0.162499
25	6	0	-5.855724	0.199137	-0.091070
26	6	0	-5.292107	1.511640	-0.413646
27	6	0	-3.946691	1.733717	-0.462499
28	8	0	-7.120567	0.028562	-0.051824
29	1	0	1.295881	4.655590	0.802481
30	1	0	4.706540	2.334531	-0.454551
31	1	0	-0.068568	2.623484	0.833854
32	1	0	4.758439	-2.160554	-0.480732
33	1	0	1.189647	-4.540193	0.287328
34	1	0	-2.918390	-2.696830	0.495719
35	1	0	-1.287305	1.889355	-0.491501
36	1	0	4.693562	4.661762	-0.146507

37	1	0	-5.298909	-1.835394	0.388738
38	1	0	-5.995912	2.315461	-0.615191
39	1	0	-3.560943	2.722707	-0.701489

Q

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.565995	3.820627	0.479799
2	6	0	2.971235	3.863639	0.100718
3	6	0	3.571871	2.586723	-0.187237
4	6	0	2.835277	1.427577	-0.147253
5	6	0	1.422823	1.393098	0.121780
6	6	0	0.847776	2.657159	0.483596
7	8	0	3.536516	0.268268	-0.405954
8	6	0	2.948287	-0.944146	-0.222496
9	6	0	1.560018	-1.028893	-0.000597
10	6	0	0.738499	0.152123	0.062151
11	6	0	3.764903	-2.067279	-0.287498
12	6	0	3.178707	-3.325936	-0.100571
13	6	0	1.804193	-3.464238	0.136185
14	6	0	1.019266	-2.320621	0.174979
15	8	0	-0.307220	-2.479524	0.429220
16	6	0	-1.173765	-1.413956	0.267464
17	6	0	-0.681599	-0.077351	0.054548
18	6	0	-2.508483	-1.719233	0.326676
19	6	0	-3.502683	-0.714239	0.122596
20	6	0	-3.032443	0.620668	-0.193660
21	6	0	-1.667209	0.895897	-0.219034
22	8	0	3.623142	4.949434	0.066339
23	8	0	3.908230	-4.473625	-0.135598
24	6	0	-4.875302	-0.979117	0.172213
25	6	0	-5.858990	0.023531	-0.087861
26	6	0	-5.349177	1.355779	-0.420729
27	6	0	-4.014339	1.631624	-0.473918

28	8	0	-7.115261	-0.197431	-0.046437
29	1	0	1.100872	4.752636	0.788245
30	1	0	4.631054	2.540651	-0.419104
31	1	0	-0.177660	2.684779	0.827575
32	1	0	4.828193	-1.954339	-0.469311
33	1	0	1.363664	-4.442892	0.283955
34	1	0	-2.804264	-2.748387	0.506034
35	1	0	-1.362922	1.893588	-0.507829
36	1	0	4.843569	-4.281669	-0.297801
37	1	0	-5.220873	-1.983973	0.404633
38	1	0	-6.085377	2.128746	-0.627028
39	1	0	-3.668666	2.633271	-0.721035

R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.999360	0.652662	-0.192400
2	6	0	-3.497343	-0.668396	0.124145
3	6	0	-2.525745	-1.691716	0.334339
4	6	0	-1.180923	-1.416305	0.279351
5	6	0	-0.663361	-0.092693	0.063657
6	6	0	-1.622517	0.897367	-0.214938
7	8	0	-0.339702	-2.496740	0.445086
8	6	0	0.998549	-2.376111	0.170075
9	6	0	1.558255	-1.078329	-0.000800
10	6	0	0.774151	0.099138	0.062263
11	6	0	1.751378	-3.524701	0.127683
12	6	0	3.176628	-3.471978	-0.112783
13	6	0	3.750118	-2.157446	-0.289446
14	6	0	2.963819	-1.032135	-0.221657
15	8	0	3.564249	0.184560	-0.420139
16	6	0	2.883532	1.352650	-0.156651
17	6	0	1.476591	1.344877	0.111046
18	6	0	3.643561	2.503128	-0.187470

19	6	0	3.071949	3.788372	0.107187
20	6	0	1.669025	3.768956	0.478699
21	6	0	0.927604	2.614050	0.475100
22	8	0	3.751021	4.865869	0.081686
23	8	0	3.887371	-4.527748	-0.162588
24	6	0	-3.958665	1.681297	-0.473385
25	6	0	-5.301530	1.432542	-0.423727
26	6	0	-5.841330	0.114014	-0.092412
27	6	0	-4.880458	-0.904669	0.170892
28	8	0	-7.107675	-0.079340	-0.054879
29	1	0	-2.843214	-2.714666	0.514253
30	1	0	-1.297476	1.889004	-0.502324
31	1	0	1.278557	-4.489183	0.282480
32	1	0	4.815235	-2.066817	-0.476073
33	1	0	4.702590	2.434607	-0.416929
34	1	0	1.215299	4.707463	0.786099
35	1	0	-0.099107	2.663605	0.813377
36	1	0	-3.593454	2.676490	-0.720097
37	1	0	-6.019611	2.222194	-0.632530
38	1	0	-5.244483	-1.902964	0.405800

[a)] Gaussian 09w, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Figure S4. HOMOs, LUMOs and energy gaps in the four states (five species) of dye **4** from DFT calculations at the B3LYP/6-31+G(d,p) level.

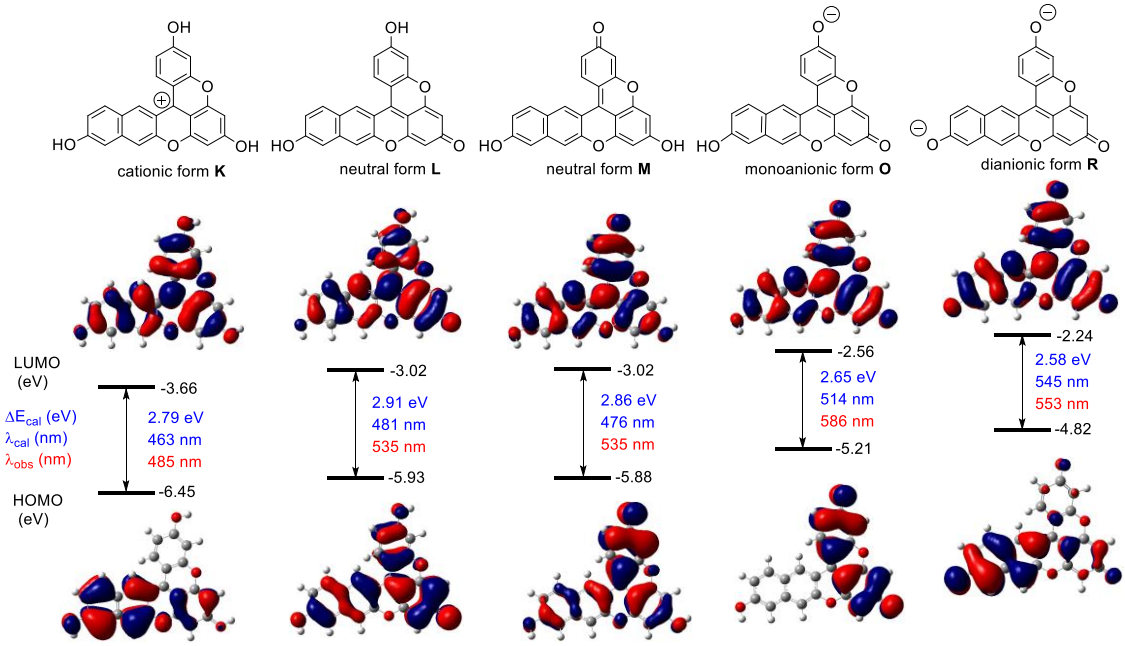
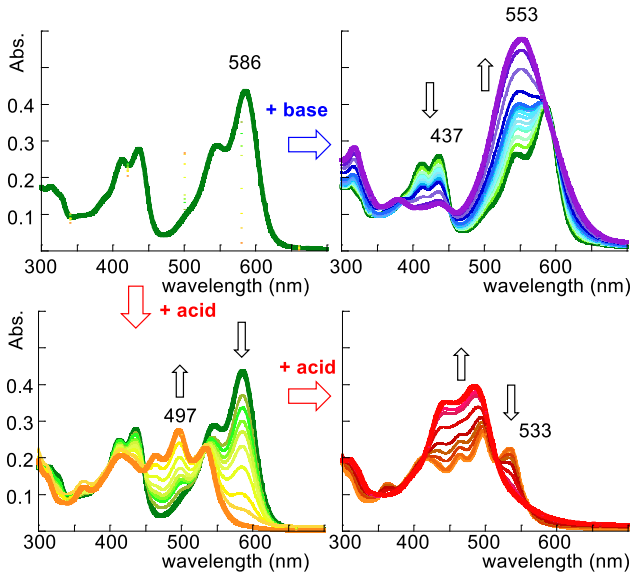
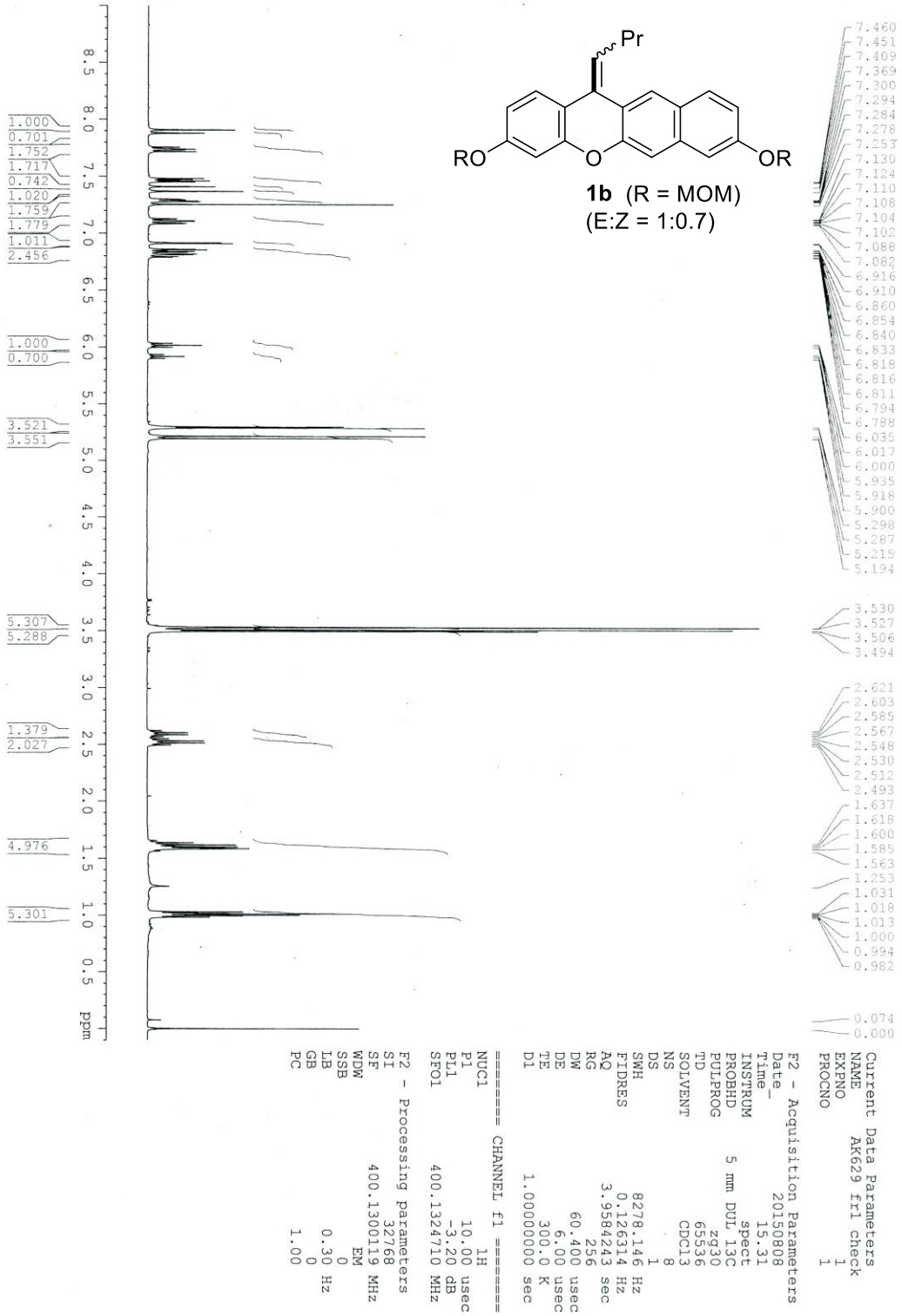


Figure S5. Titration UV-vis spectra of V-shaped dye **4** with acid and base.



Titration UV-vis spectra of V-shaped dye **4** with acid or base. (a) UV-vis spectrum of monoanionic **4**. (b) UV-vis spectra for the conversion of monoanionic **4** to the corresponding dianionic material. (c) UV-vis spectra for the conversion of monoanionic **4** to the corresponding neutral material. (d) UV-vis spectra for the conversion of neutral **4** to the corresponding monocationic material. Conditions; [**4**] = $1x10^{-5}$ M in DMSO at 25 °C.

^{1}H NMR and ^{13}C NMR spectra for all new compounds.

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PROCNO                           1

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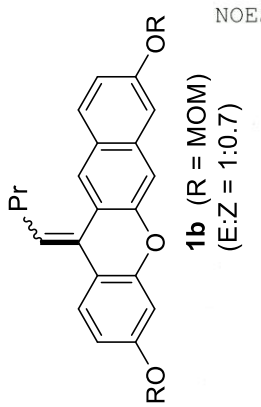
Time_                         3.53
INSTRUM                       spect
PROBHD                5 mm DUL 13C
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                            5500
DS                               2
SWH                      23980.814 Hz
FIDRES                       0.365918 Hz
AQ                        1.3664756 sec
RG                           32768
DW                          20.850 usec
DE                           6.00 usec
TE                          300.0 K
D1                       2.00000000 sec
d11                      0.03000000 sec
d12                      0.00002000 sec

======== CHANNEL f1 ========
NUC1                           13C
P1                            8.40 usec
PL1                           1.00 dB
SFO1                100.6228298 MHz

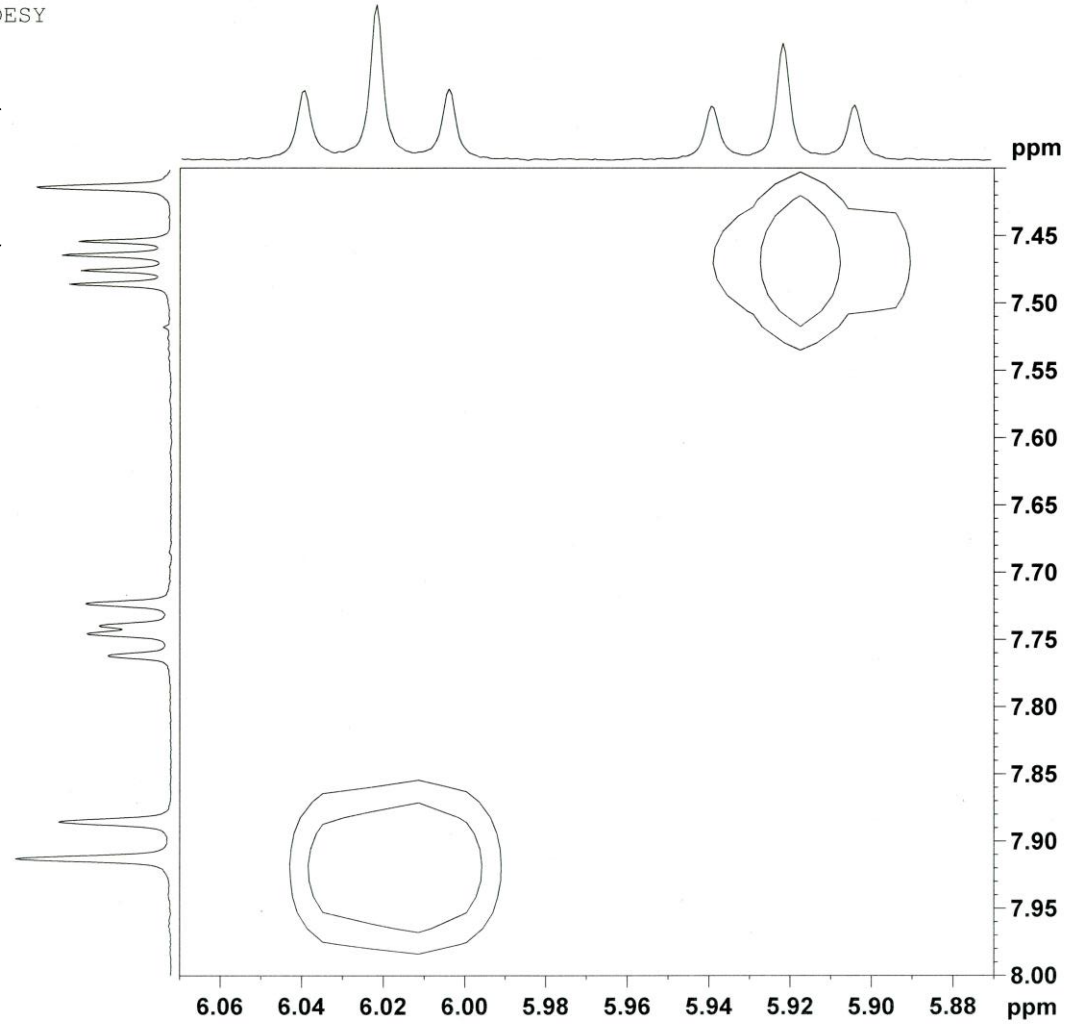
======== CHANNEL f2 ========
CPDPRG2                    waltz16
NUC2                           1H
PCPD2                        80.00 usec
PL2                          -3.20 dB
PL12                         15.00 dB
PL13                         15.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                           32768
SF                  100.6127695 MHz
WDW                             EM
SSB                              0
LB                            1.00 Hz
GB                               0
PC                            1.00
```



1b (R = MOM)
(E:Z = 1:0.7)

NOESY



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```
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EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
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INSTRUM           spect
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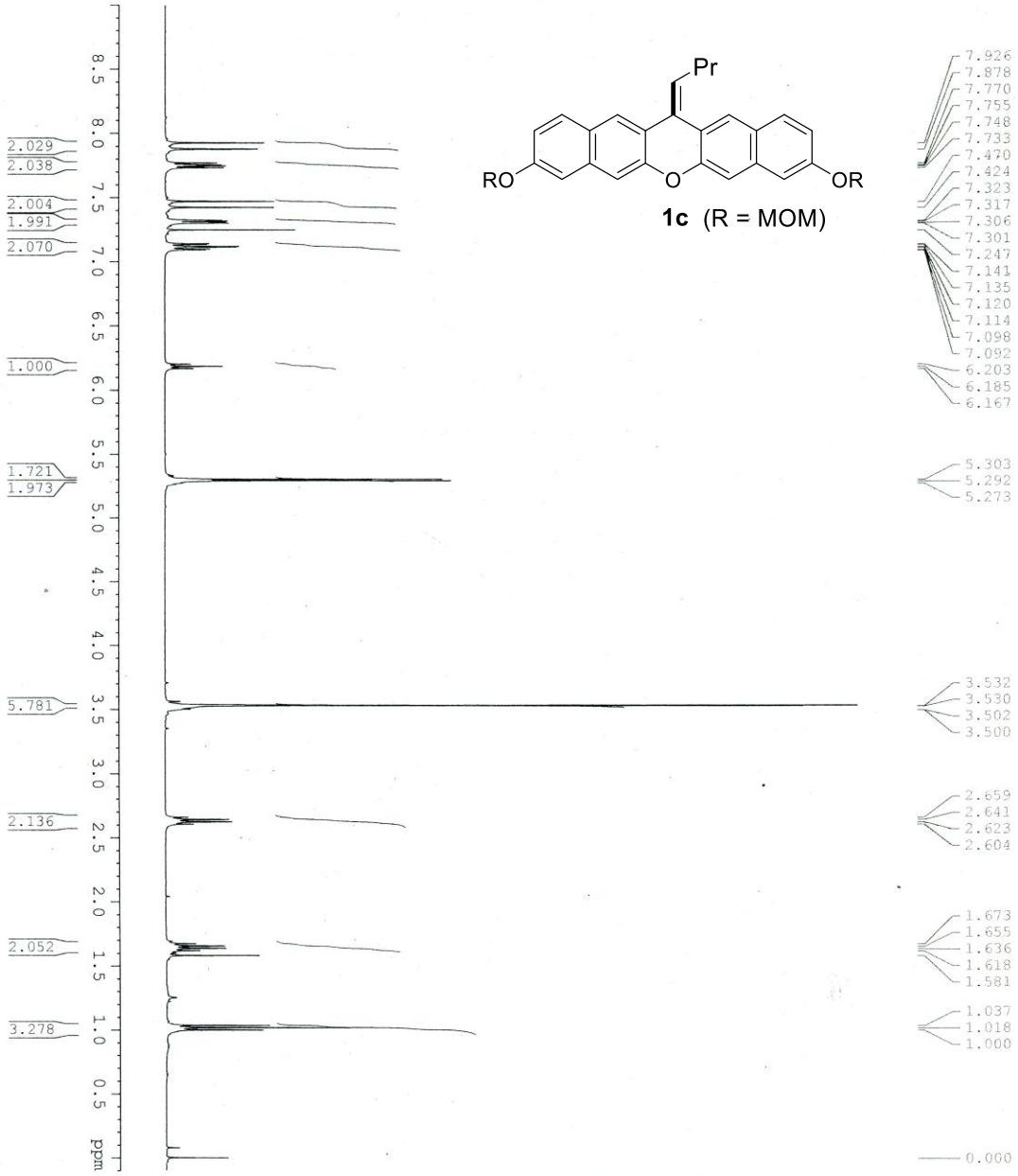
PULPROG         noesyph
TD                2048
SOLVENT           CDC13
NS                   16
DS                    4
SWH            4789.272 Hz
FIDRES         2.338512 Hz
AQ            0.2138612 sec
RG                287.4
DW              104.400 usec
DE                6.00 usec
TE                300.0 K
d0           0.00000300 sec
D1           2.00000000 sec
D8           0.75000000 sec
IN0          0.00020880 sec
MCREST       0.00000000 sec
MCWRK        1.00000000 sec
ST1CNT               45

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1               -3.20 dB
SFO1       400.1320007 MHz

F1 - Acquisition parameters
ND0                   1
TD                  256
SFO1           400.132 MHz
FIDRES       18.708094 Hz
SW              11.969 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                 1024
SF         400.1300095 MHz
WDW               QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2          States-TPPI
SF         400.1300095 MHz
WDW               QSINE
SSB                   2
LB                 0.00 Hz
GB                    0
```


Pr
RO
O
OR
1c (R = MOM)
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7.770
7.755
7.748
7.733
7.470
7.424
7.323
7.317
7.306
7.301
7.247
7.141
7.135
7.120
7.114
7.098
7.092
6.203
6.185
6.167
5.303
5.292
5.273
3.532
3.530
3.502
3.500
2.659
2.641
2.623
2.604
1.673
1.655
1.636
1.618
1.581
1.037
1.018
1.000
0.000
2.029
2.038
2.004
1.991
2.070
1.000
1.721
1.973
5.781
2.136
2.052
3.278
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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NAME AK551 fr2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150417
Time_ 20.18
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


Pr
RO
O
OR
1c (R = MOM)
155.76
155.42
151.93
150.90
134.58
134.56
129.90
129.58
129.32
127.05
126.95
126.71
125.84
125.75
122.05
121.99
117.71
117.65
111.10
110.88
108.76
108.72
94.47
94.45
77.32
77.20
77.00
76.68
56.12
32.26
23.66
14.03
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME AK551 13C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150418
Time_ 15.13
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.40 usec
PL1 1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.20 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
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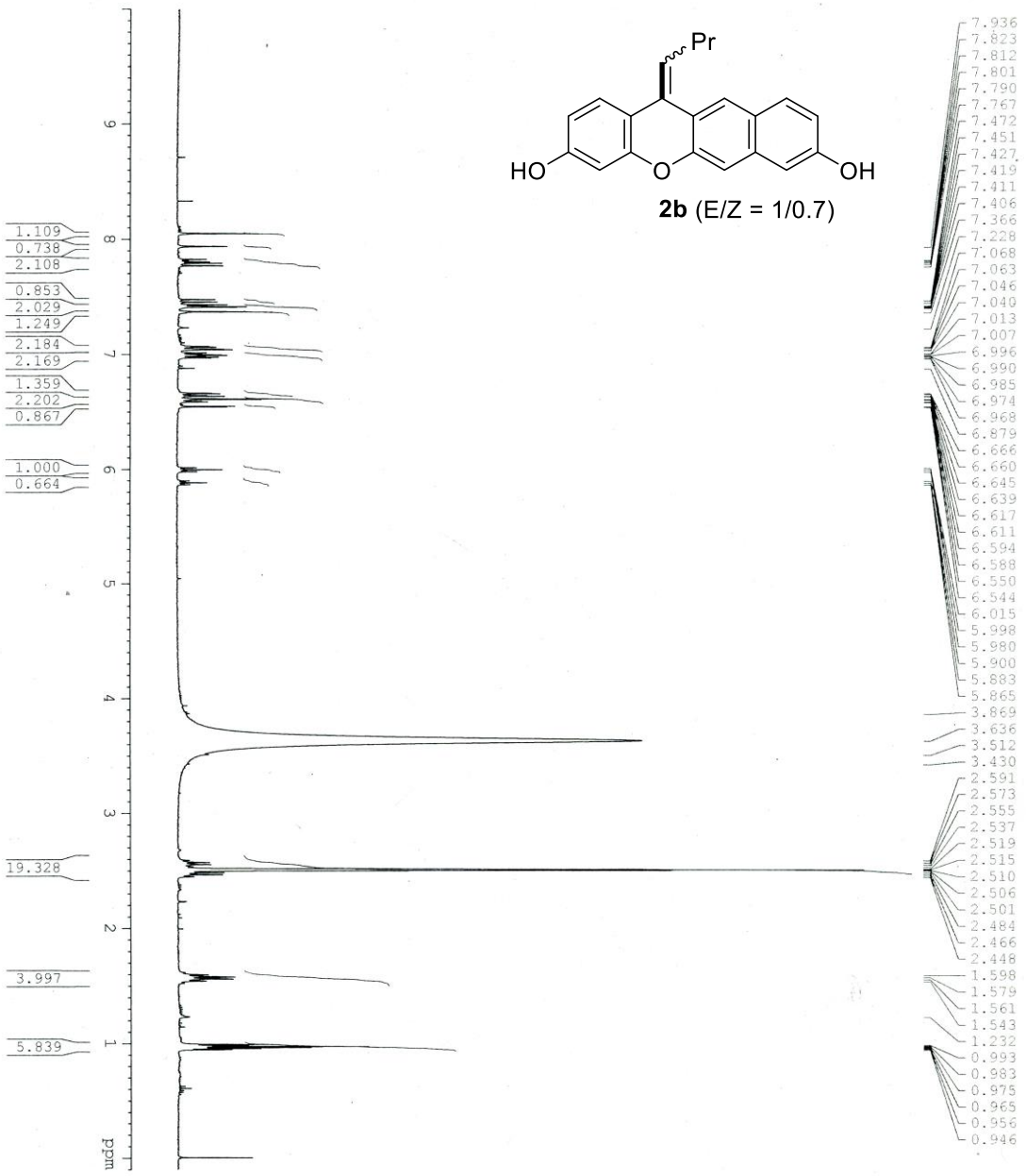
SF 100.6127725 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Pr
HO
O
OH
2b (E/Z = 1/0.7)
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7.812
7.801
7.790
7.767
7.472
7.451
7.427
7.419
7.411
7.406
7.366
7.228
7.068
7.063
7.046
7.040
7.013
7.007
6.996
6.990
6.985
6.974
6.968
6.879
6.666
6.660
6.645
6.639
6.617
6.611
6.594
6.588
6.550
6.544
6.015
5.998
5.980
5.900
5.883
5.865
3.869
3.636
3.512
3.430
2.591
2.573
2.555
2.537
2.519
2.515
2.510
2.506
2.501
2.484
2.466
2.448
1.598
1.579
1.561
1.543
1.232
0.993
0.983
0.975
0.965
0.956
0.946
1.109
0.738
2.108
0.853
2.029
1.249
2.184
2.169
1.359
2.202
0.867
1.000
0.664
19.328
3.997
5.839
ppm
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NAME AK601 DMSO
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150628
Time_ 18.17
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1299981 MHz
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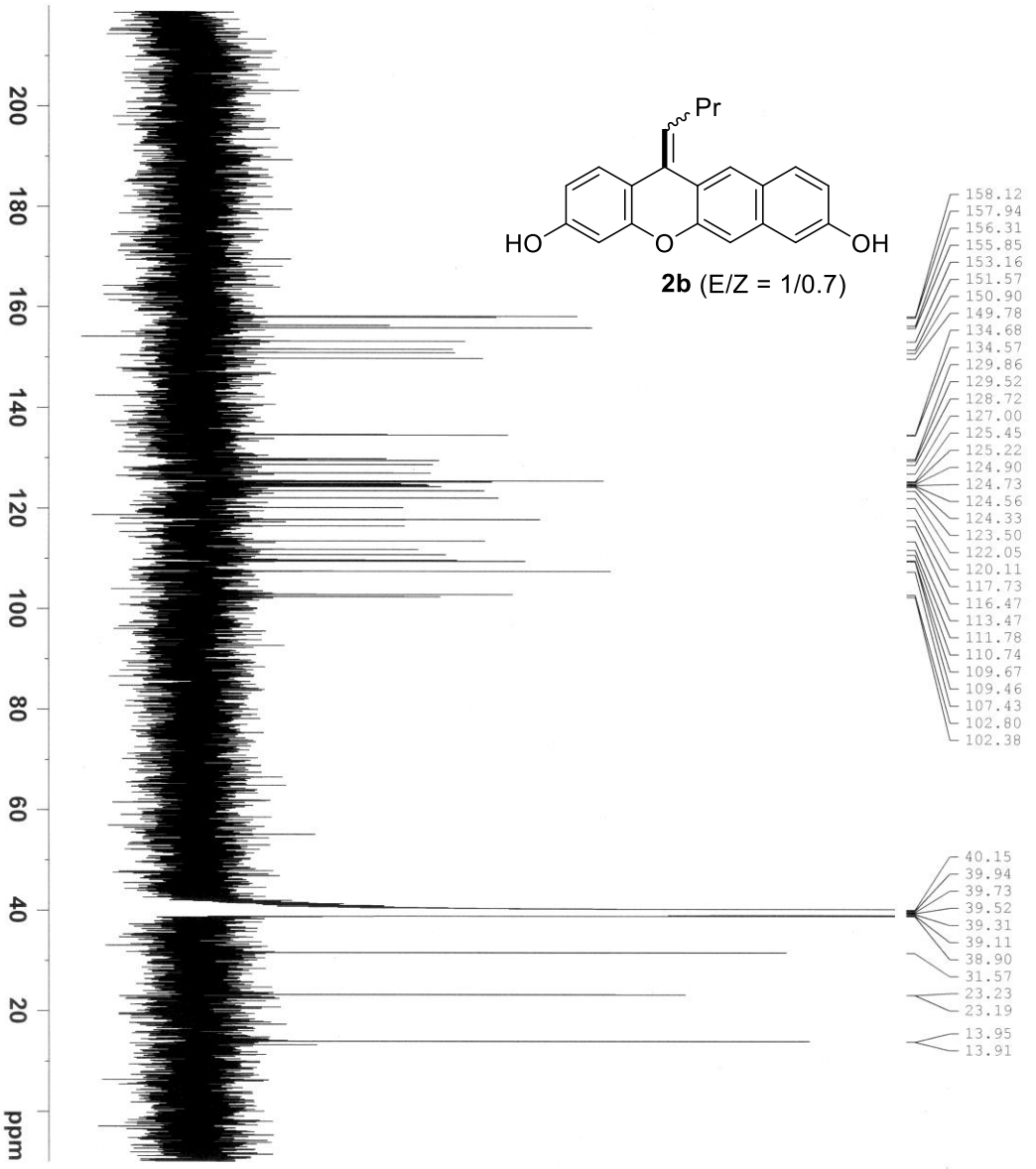
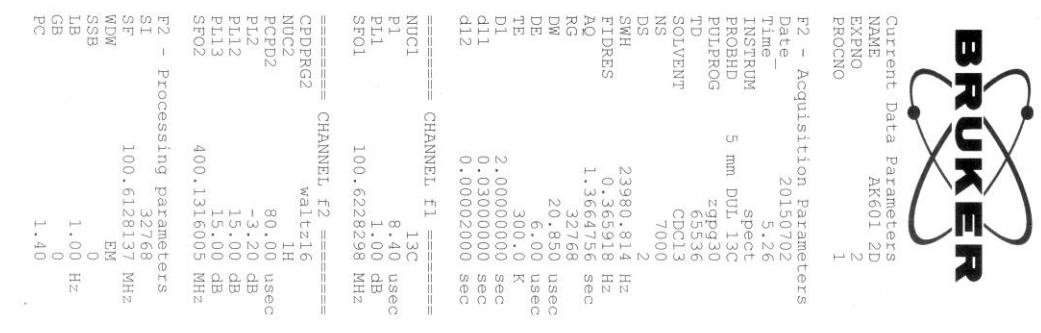
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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EXPNO                        2
PROCNO                       1

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Time_                   5.26
INSTRUM                 spect
PROBHD     5 mm DUL 13C
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    7000
DS                       2
SWH                23980.814 Hz
FIDRES             0.365918 Hz
AQ                 1.3664756 sec
RG                     32768
DW                    20.850 usec
DE                     6.00 usec
TE                    300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
d12                0.00002000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       8.40 usec
PL1                     1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -3.20 dB
PL12                   15.00 dB
PL13                   15.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF             100.6128137 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```
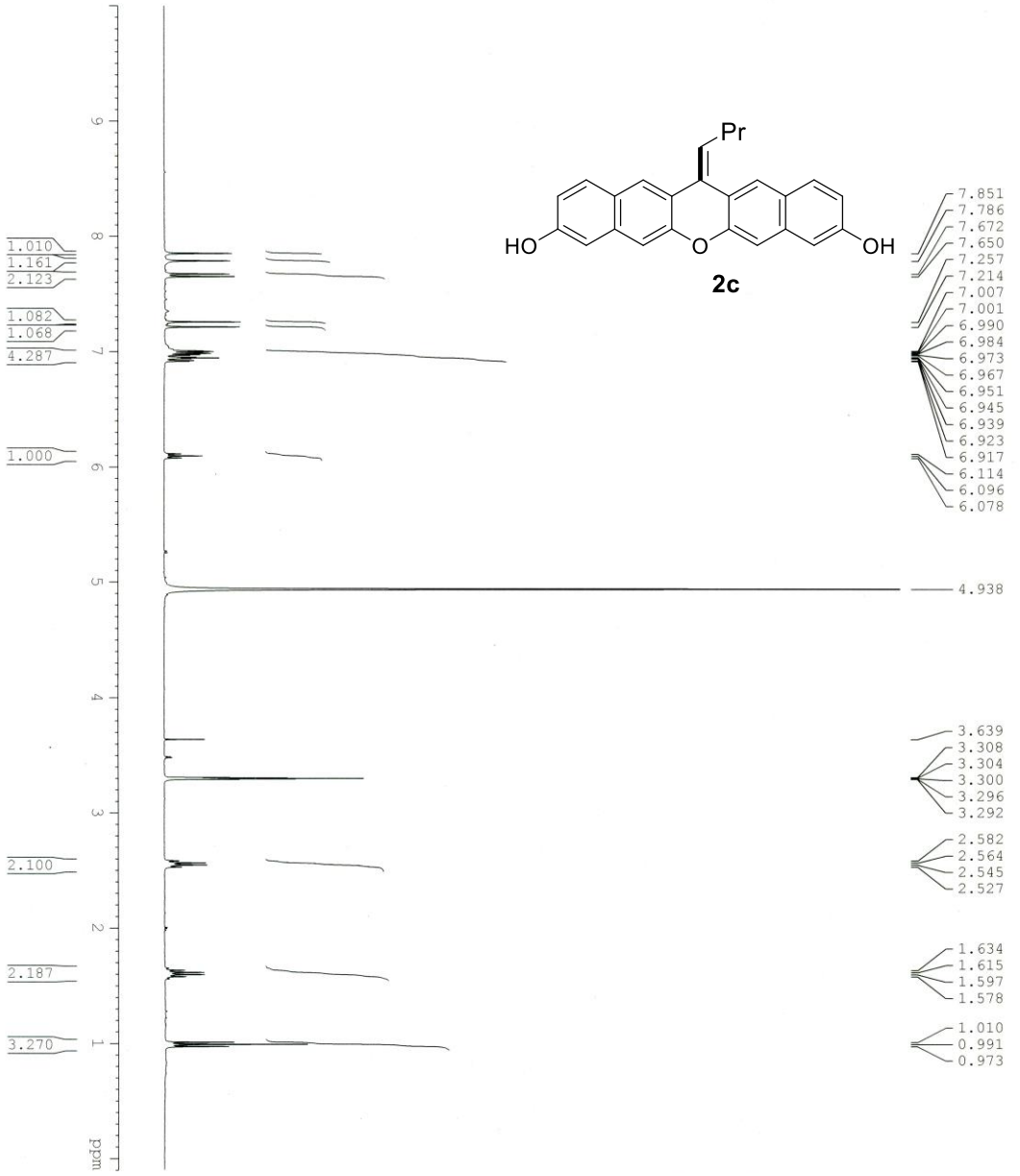

Pr
NOESY
HO
O
OH
2b (E/Z = 1/0.7)
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
6.10
6.05
6.00
5.95
5.90
5.85
ppm
BRUKER

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NAME                  AK553 bussei
EXPNO                            1
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20150812
Time_                     17.38
INSTRUM                     spect
PROBHD     5 mm DUL 13C
PULPROG                     zg30
TD                         65536
SOLVENT                     MeOD
NS                             8
DS                             1
SWH                     8278.146 Hz
FIDRES                  0.126314 Hz
AQ                      3.9584243 sec
RG                         287.4
DW                      60.400 usec
DE                       6.00 usec
TE                        300.0 K
D1                      1.00000000 sec

========== CHANNEL f1 ========
NUC1                         1H
P1                       10.00 usec
PL1                      -3.20 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                         32768
SF              400.1300114 MHz
WDW                           EM
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PC                          1.00
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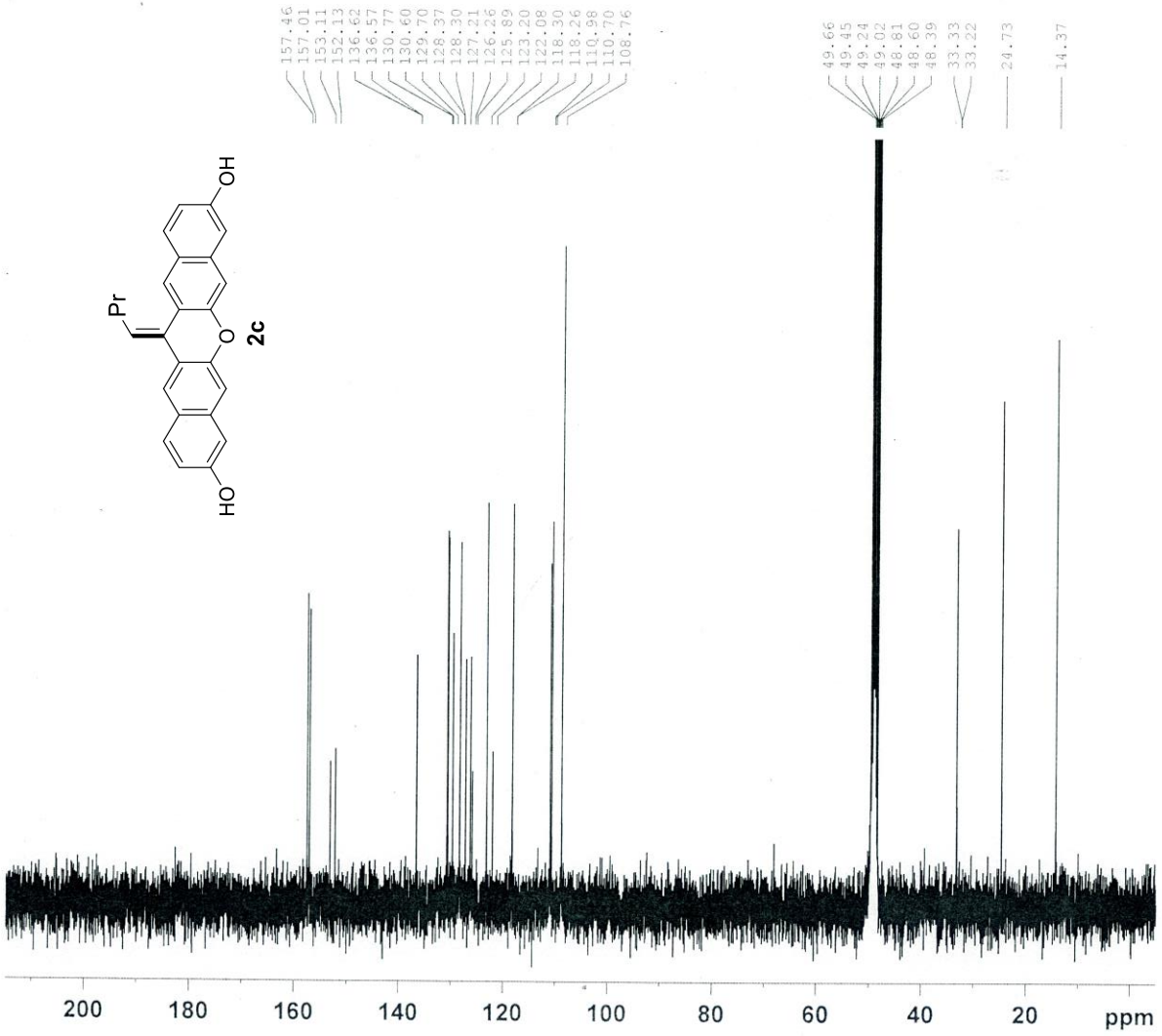

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Current Data Parameters

NAME	AK553 bussei
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20150812	
Time	18.52	
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PROBHD	5 mm DUL 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	1200	
DS	2	
SWH	23980.814	Hz
FIDRES	0.365918	Hz
AQ	1.3664756	sec
RG	32768	
DW	20.850	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
d12	0.00002000	sec

======== CHANNEL f1 ========

NUC1	13C	
P1	8.40	usec
PL1	1.00	dB
SFO1	100.6228298	MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.20	dB
PL12	15.00	dB
PL13	15.00	dB
SFO2	400.1316005	MHz

F2 - Processing parameters

SI	32768	
SF	100.6126262	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
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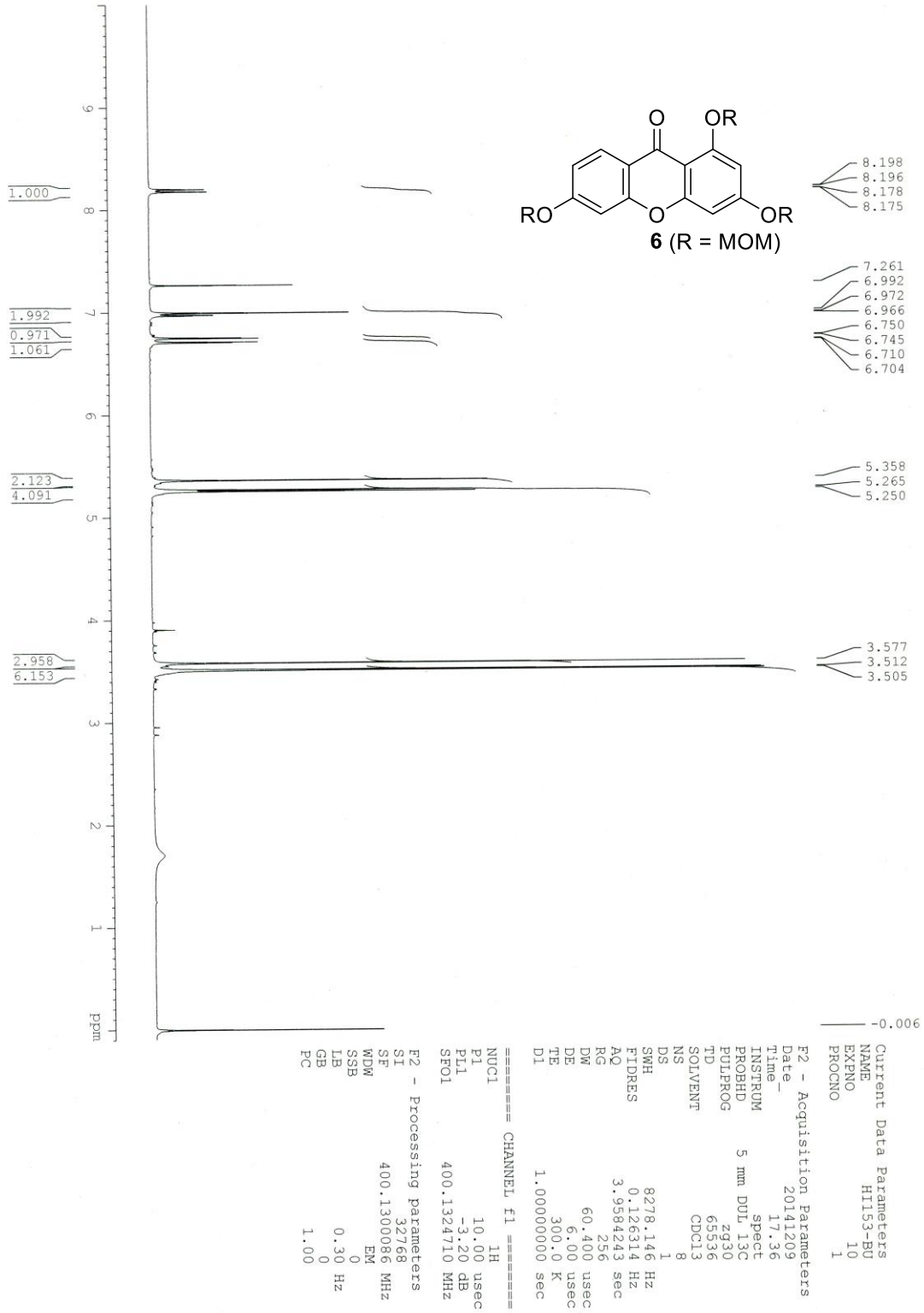
PC	1.00	


O
OR
RO
O
OR
6 (R = MOM)
8.198
8.196
8.178
8.175
7.261
6.992
6.972
6.966
6.750
6.745
6.710
6.704
5.358
5.265
5.250
3.577
3.512
3.505
1.000
1.992
0.971
1.061
2.123
4.091
2.958
6.153
ppm
-0.006
Current Data Parameters
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EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141209
Time_ 17.36
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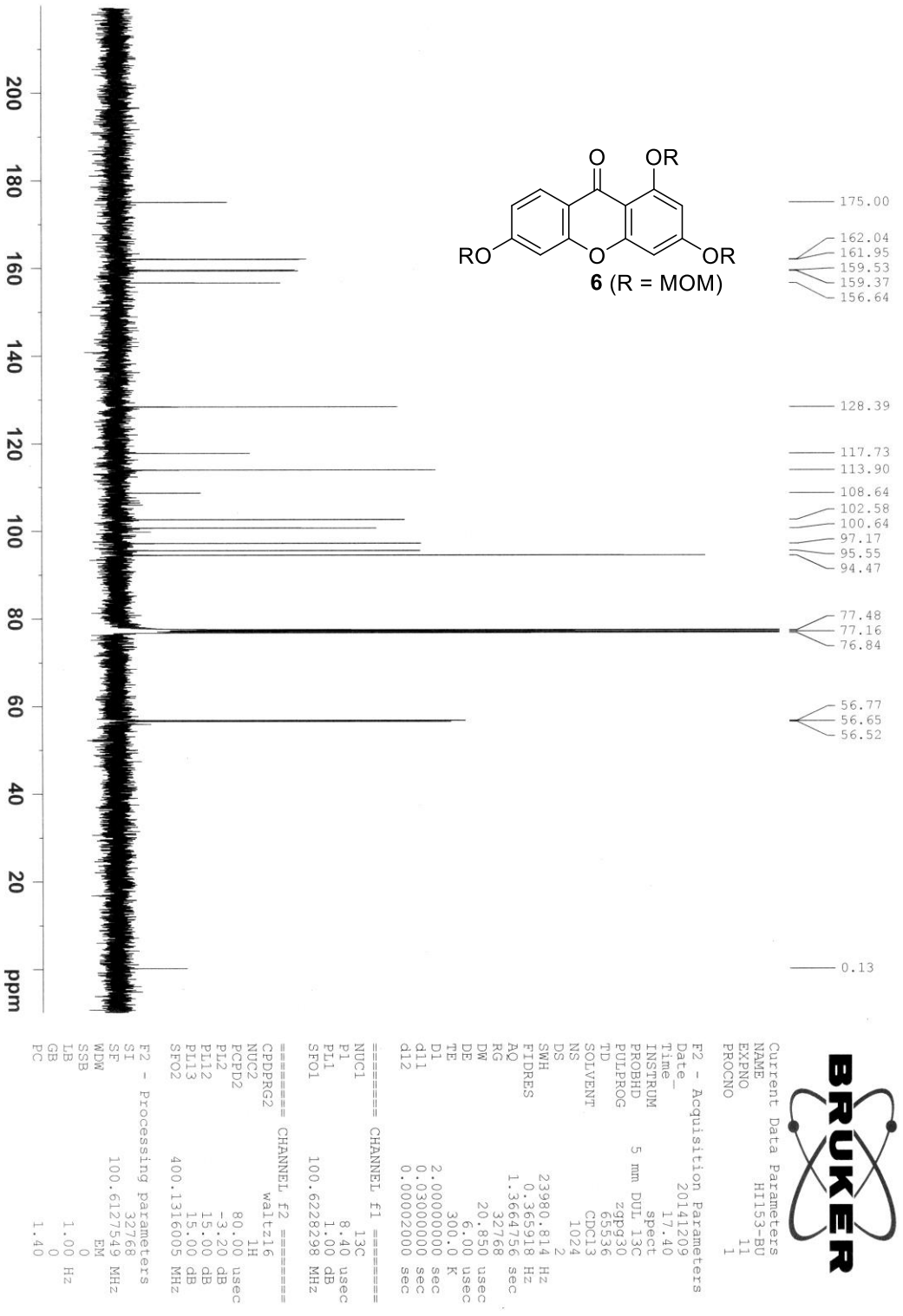
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


O
OR
RO
O
OR
6 (R = MOM)
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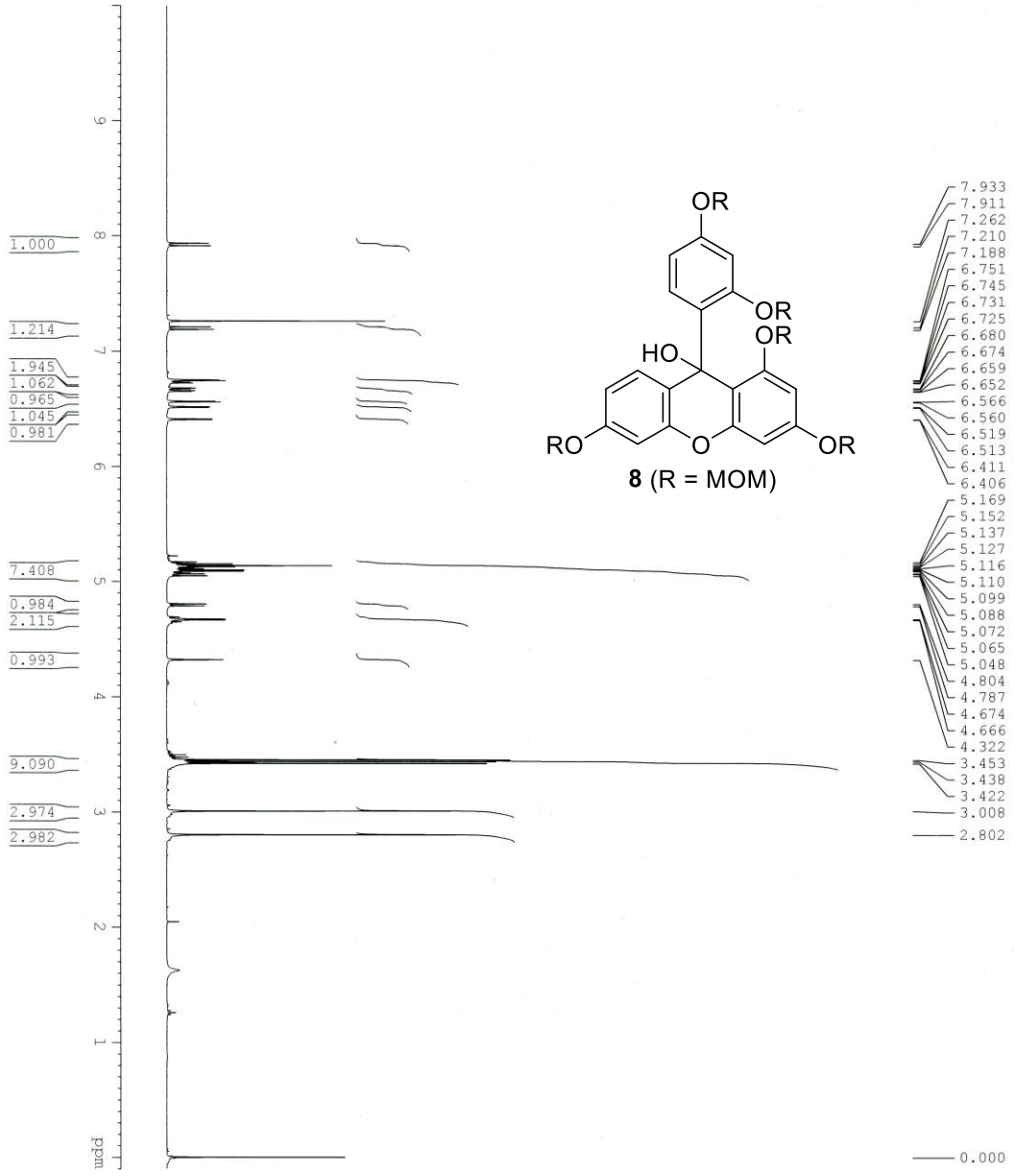
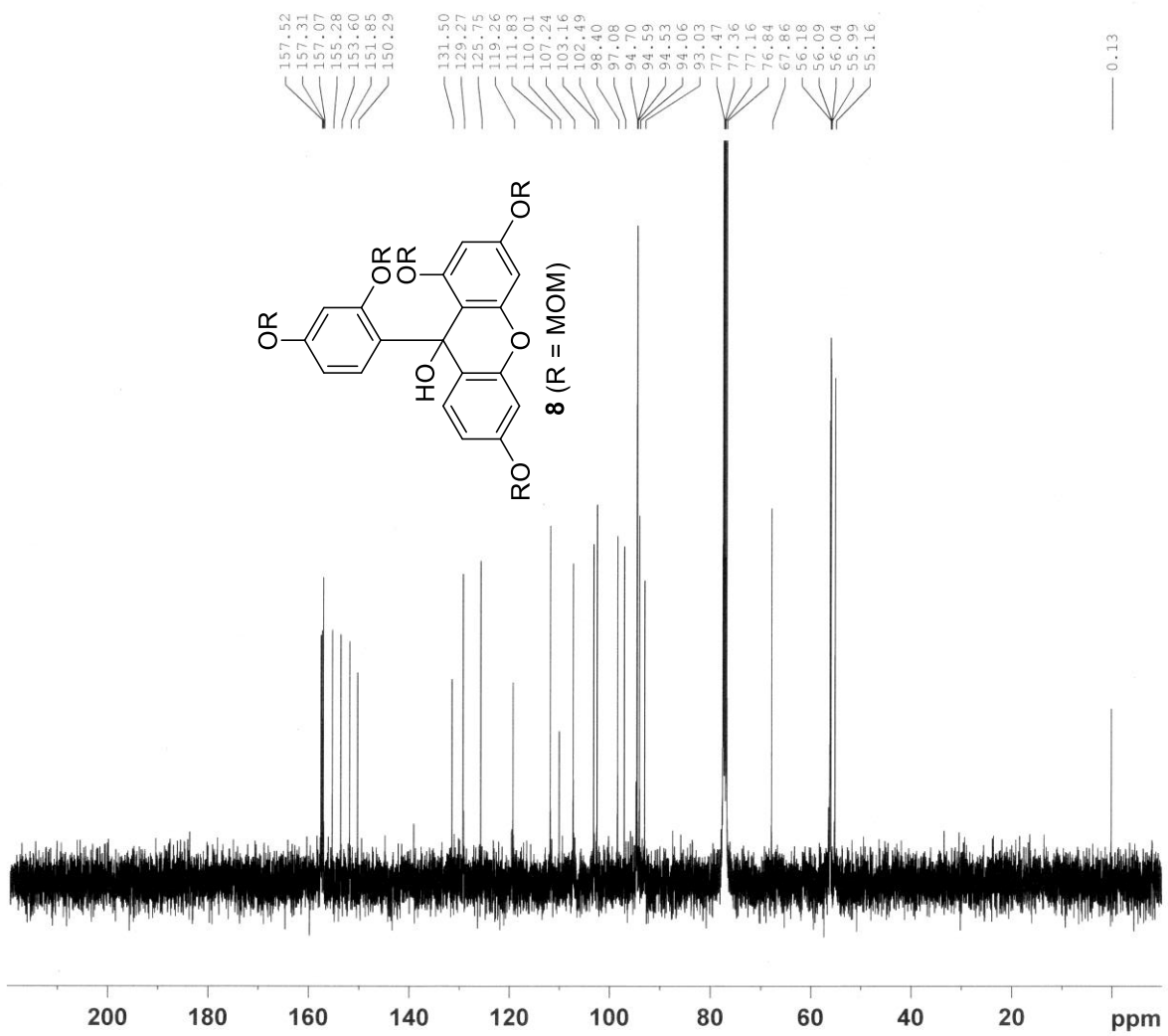
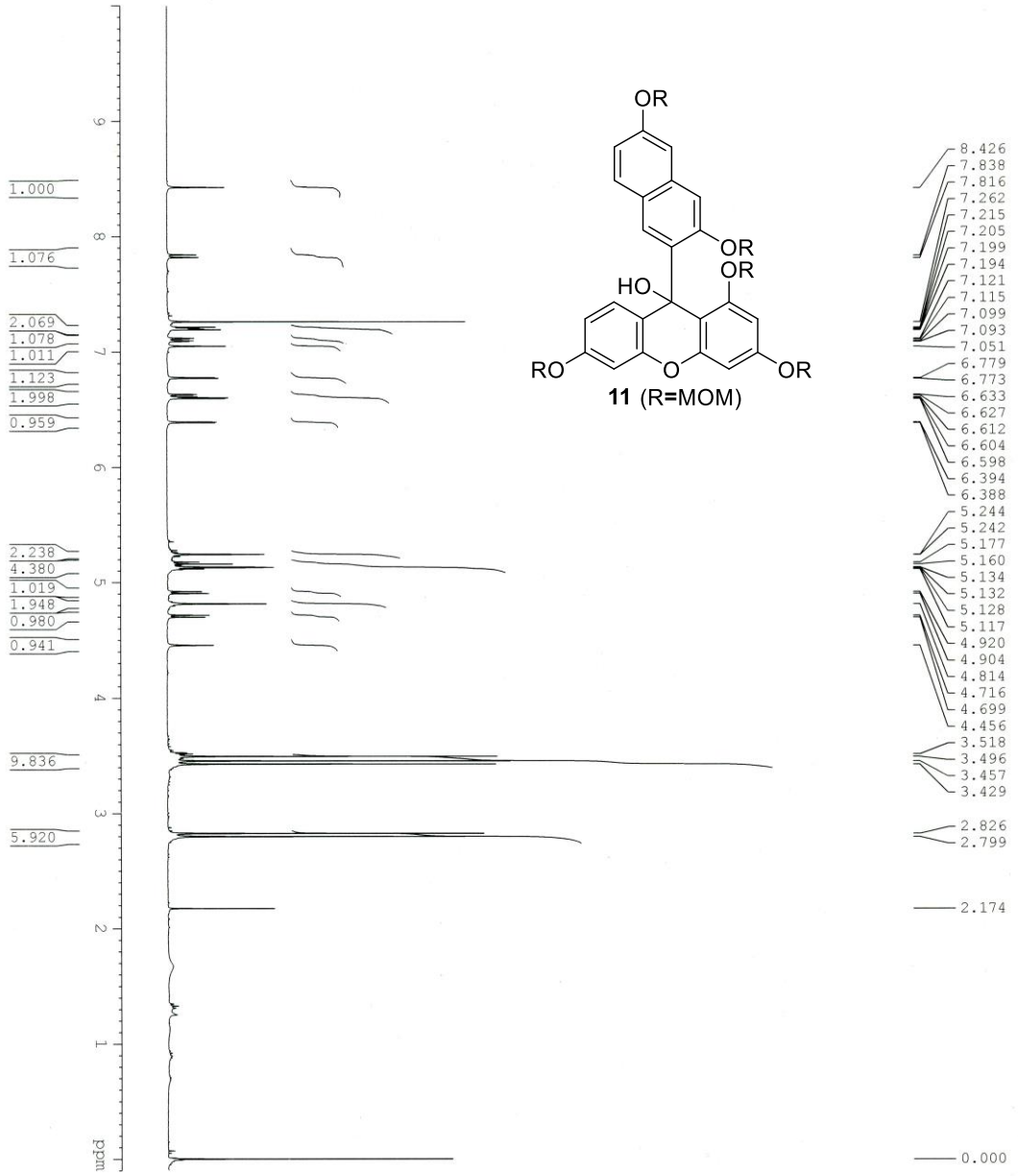
161.95
159.53
159.37
156.64
128.39
117.73
113.90
108.64
102.58
100.64
97.17
95.55
94.47
77.48
77.16
76.84
56.77
56.65
56.52
0.13
200
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME HI153-BU
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141209
Time 17.40
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.40 usec
PL1 1.00 dB
SFO1 100.6228298 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.20 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127549 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

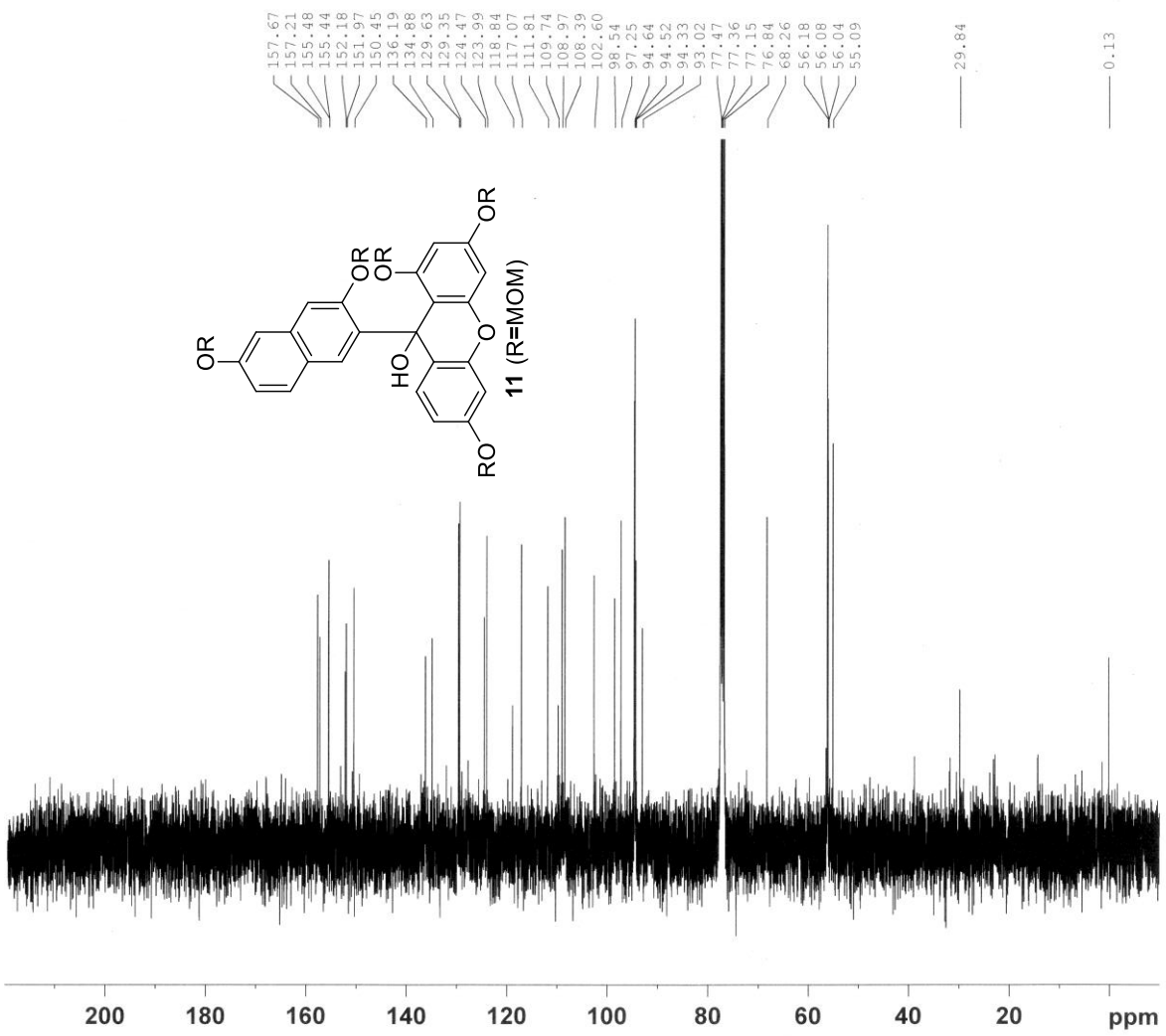

OR
OR
OR
HO
RO
O
OR
8 (R = MOM)
7.933
7.911
7.262
7.210
7.188
6.751
6.745
6.731
6.725
6.680
6.674
6.659
6.652
6.566
6.560
6.519
6.513
6.411
6.406
5.169
5.152
5.137
5.127
5.116
5.110
5.099
5.088
5.072
5.065
5.048
4.804
4.787
4.674
4.666
4.322
3.453
3.438
3.422
3.008
2.802
0.000
1.000
1.214
1.945
1.062
0.965
1.045
0.981
7.408
0.984
2.115
0.993
9.090
2.974
2.982
ppm
Current Data Parameters
NAME AY51 fr3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150331
Time_ 20.12
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

```
Current Data Parameters
NAME                  HI177-BU
EXPNO                       11
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20141224
Time                     10.16
INSTRUM                  spect
PROBHD     5 mm DUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           2
SWH                  23980.814 Hz
FIDRES               0.365918 Hz
AQ                   1.3664756 sec
RG                       32768
DW                     20.850 usec
DE                      6.00 usec
TE                      300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
d12                0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                        8.40 usec
PL1                       1.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -3.20 dB
PL12                     15.00 dB
PL13                     15.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6127556 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```


OR
OR
OR
HO
RO
O
OR
11 (R=MOM)
8.426
7.838
7.816
7.262
7.215
7.205
7.199
7.194
7.121
7.115
7.099
7.093
7.051
6.779
6.773
6.633
6.627
6.612
6.604
6.598
6.394
6.388
5.244
5.242
5.177
5.160
5.134
5.132
5.128
5.117
4.920
4.904
4.814
4.716
4.699
4.456
3.518
3.496
3.457
3.429
2.826
2.799
2.174
0.000
1.000
1.076
2.069
1.078
1.011
1.123
1.998
0.959
2.238
4.380
1.019
1.948
0.980
0.941
9.836
5.920
ppm
Current Data Parameters
NAME HI209 fr3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150325
Time_ 17.34
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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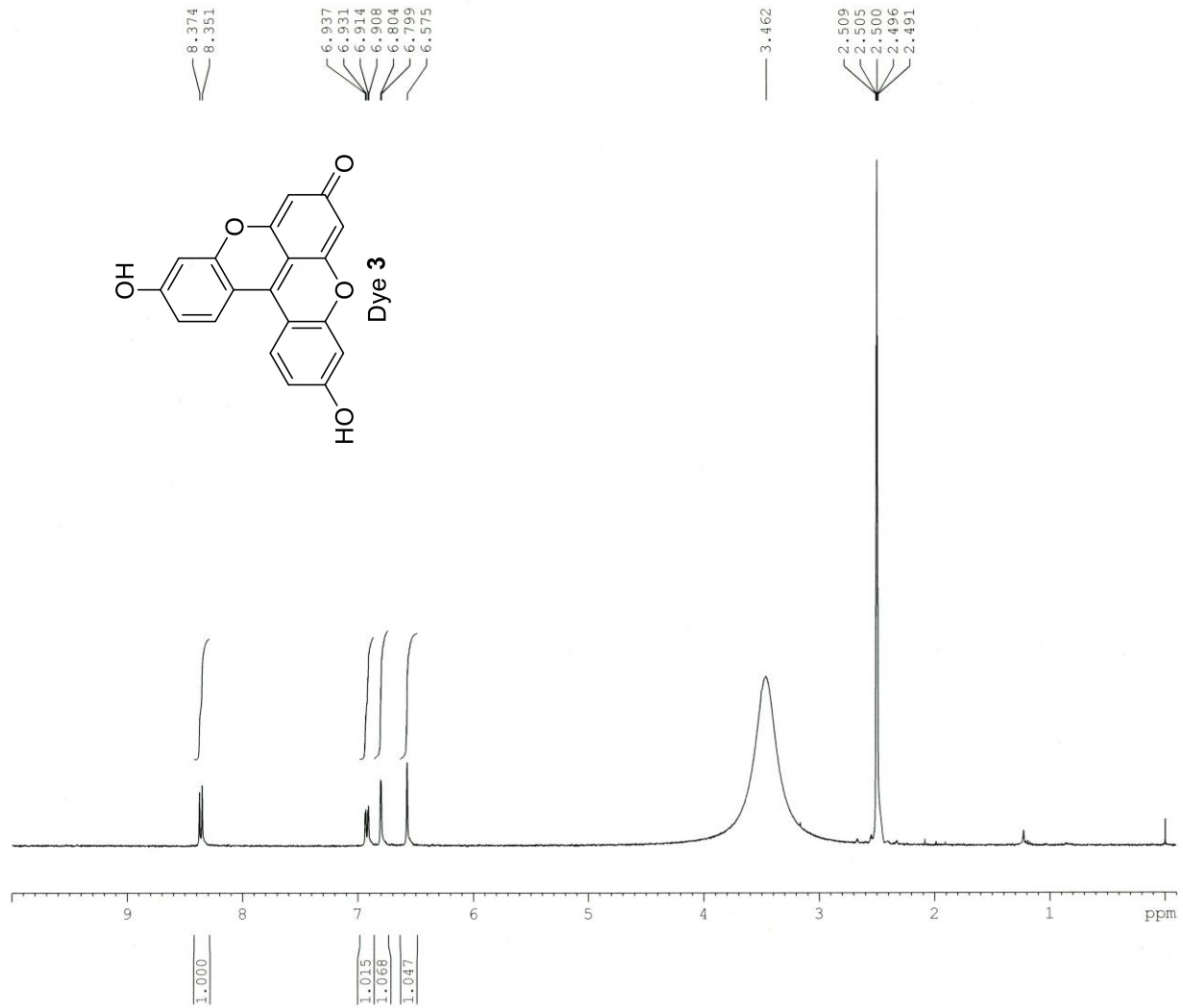
Current Data Parameters
NAME HI176-BU
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141224
Time 12.45
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 8.40 usec
PL1 1.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.20 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127556 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

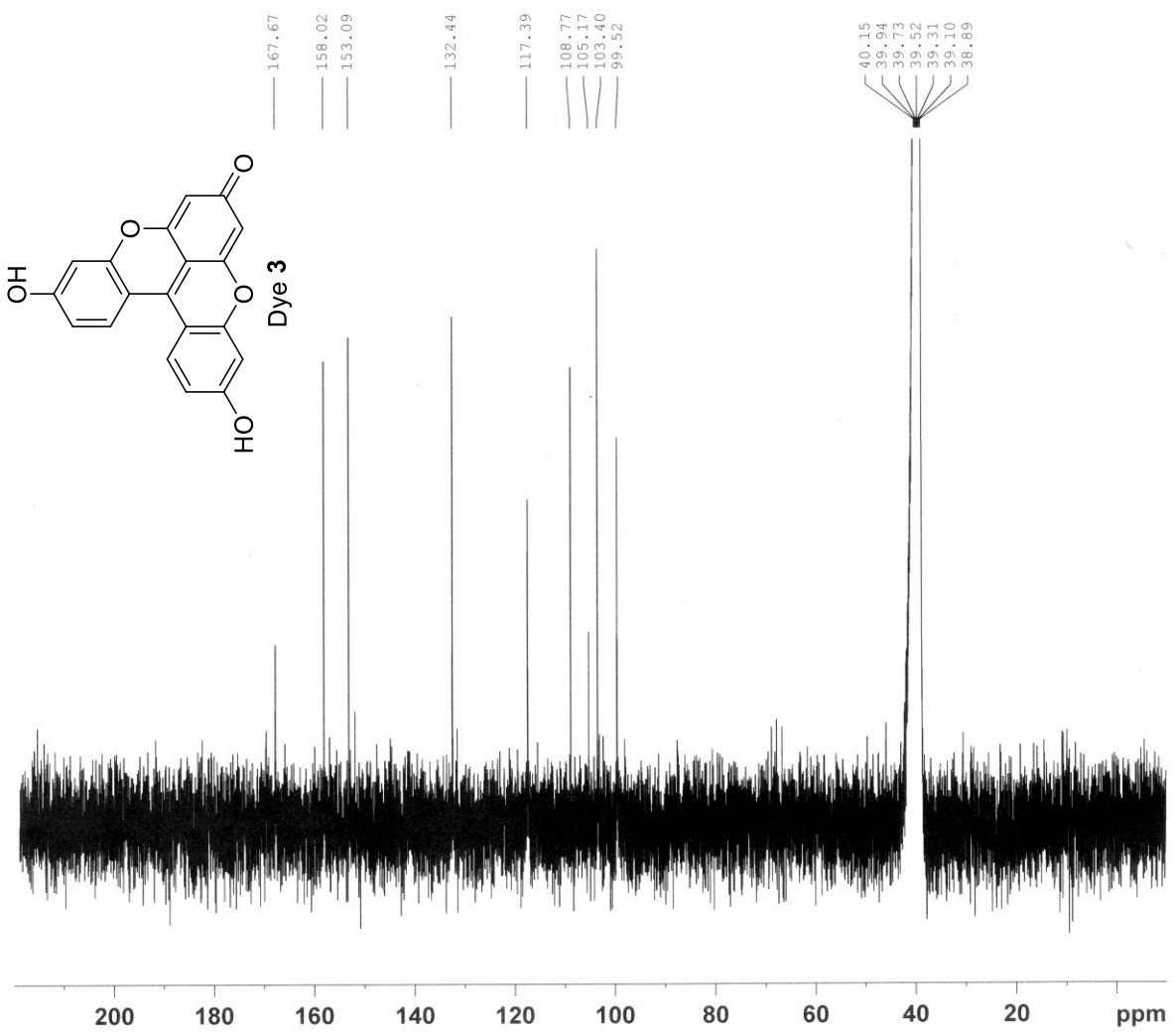



```
Current Data Parameters
NAME                 AY53 roka
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150413
Time                   13.37
INSTRUM                spect
PROBHD     5 mm DUL 13C
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                         8
DS                         1
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                     574.7
DW                    60.400 usec
DE                     6.00 usec
TE                     300.0 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                    10.00 usec
PL1                   -3.20 dB
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                         32768
SF                 400.1300018 MHz
WDW                           EM
SSB                            0
LB                      0.30 Hz
GB                             0
PC                          1.00
```



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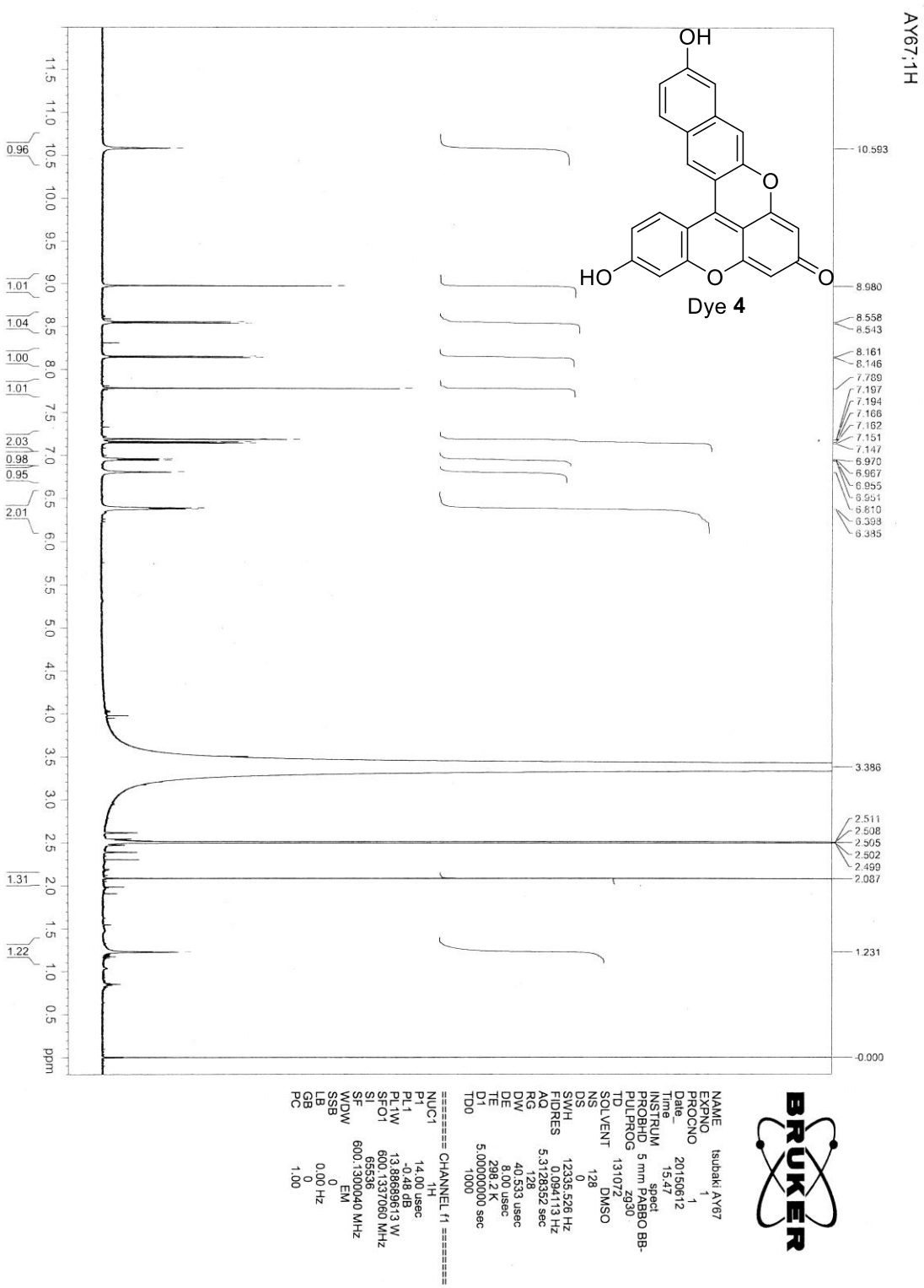
Current Data Parameters
NAME AY53
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150425
Time 18.11
INSTRUM spect
PROBHD 5 mm DUL 13C
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 41278
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

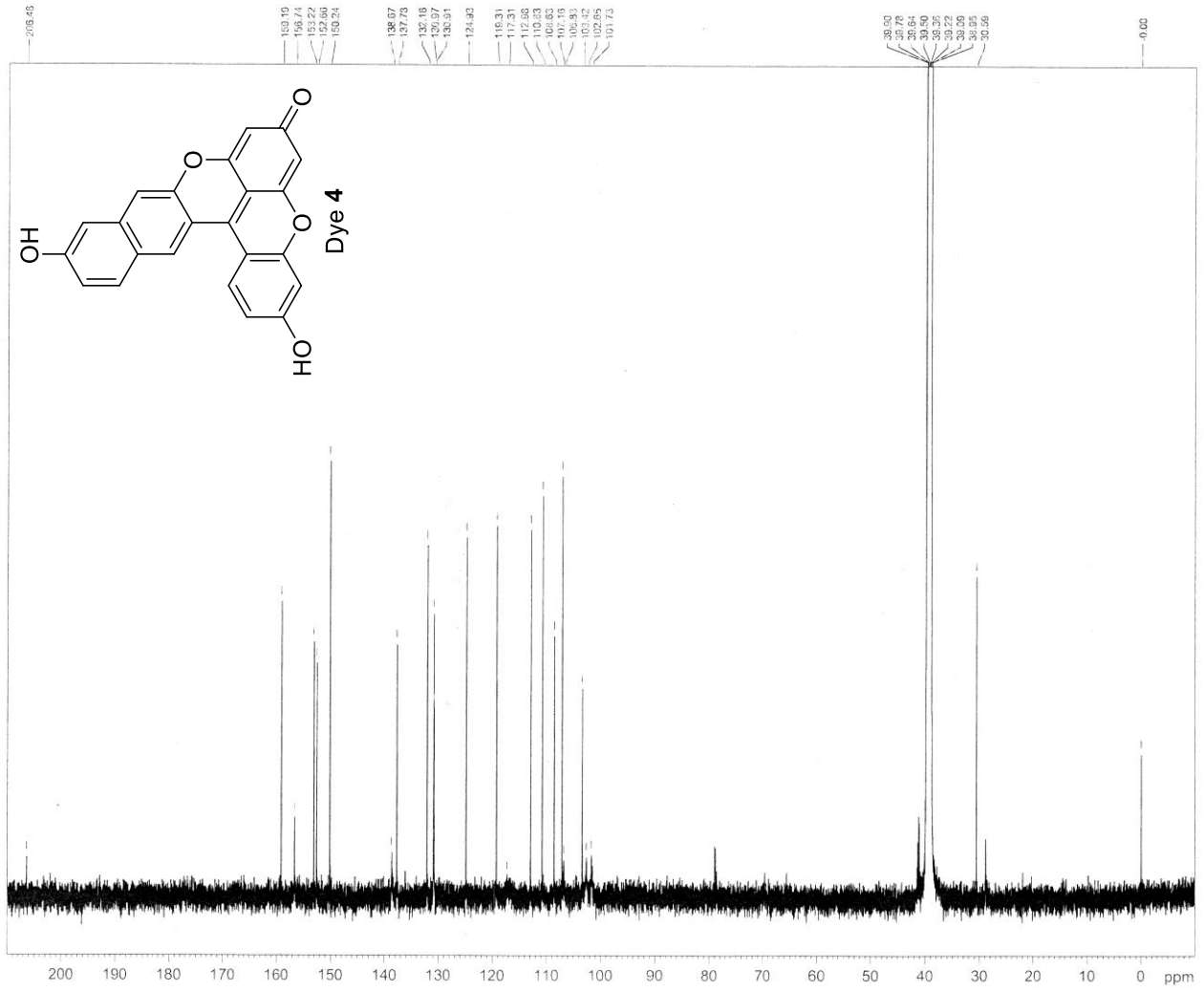
======== CHANNEL f1 ========
NUC1 13C
P1 8.40 usec
PL1 1.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.20 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128125 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


AY67;1H
OH
HO
O
O
O
Dye 4
10.593
8.980
8.558
8.543
8.161
8.146
7.789
7.197
7.194
7.166
7.162
7.151
7.147
6.970
6.967
6.955
6.951
6.810
6.398
6.385
3.386
2.511
2.508
2.505
2.502
2.499
2.087
1.231
-0.000
0.96
1.01
1.04
1.00
1.01
2.03
0.98
0.95
2.01
1.31
1.22
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
NAME tsubaki AY67
EXPNO 1
PROCNO 1
Date_ 20150612
Time 15.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 131072
SOLVENT DMSO
NS 128
DS 0
SWH 12335.526 Hz
FIDRES 0.094113 Hz
AQ 5.312352 sec
RG 128
DW 40.533 usec
DE 8.00 usec
TE 298.2 K
D1 5.00000000 sec
TD0 1000
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 -0.48 dB
PL1W 13.88689613 W
SFO1 600.1337060 MHz
SI 65536
SF 600.1300040 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
BRUKER

AY67;13C



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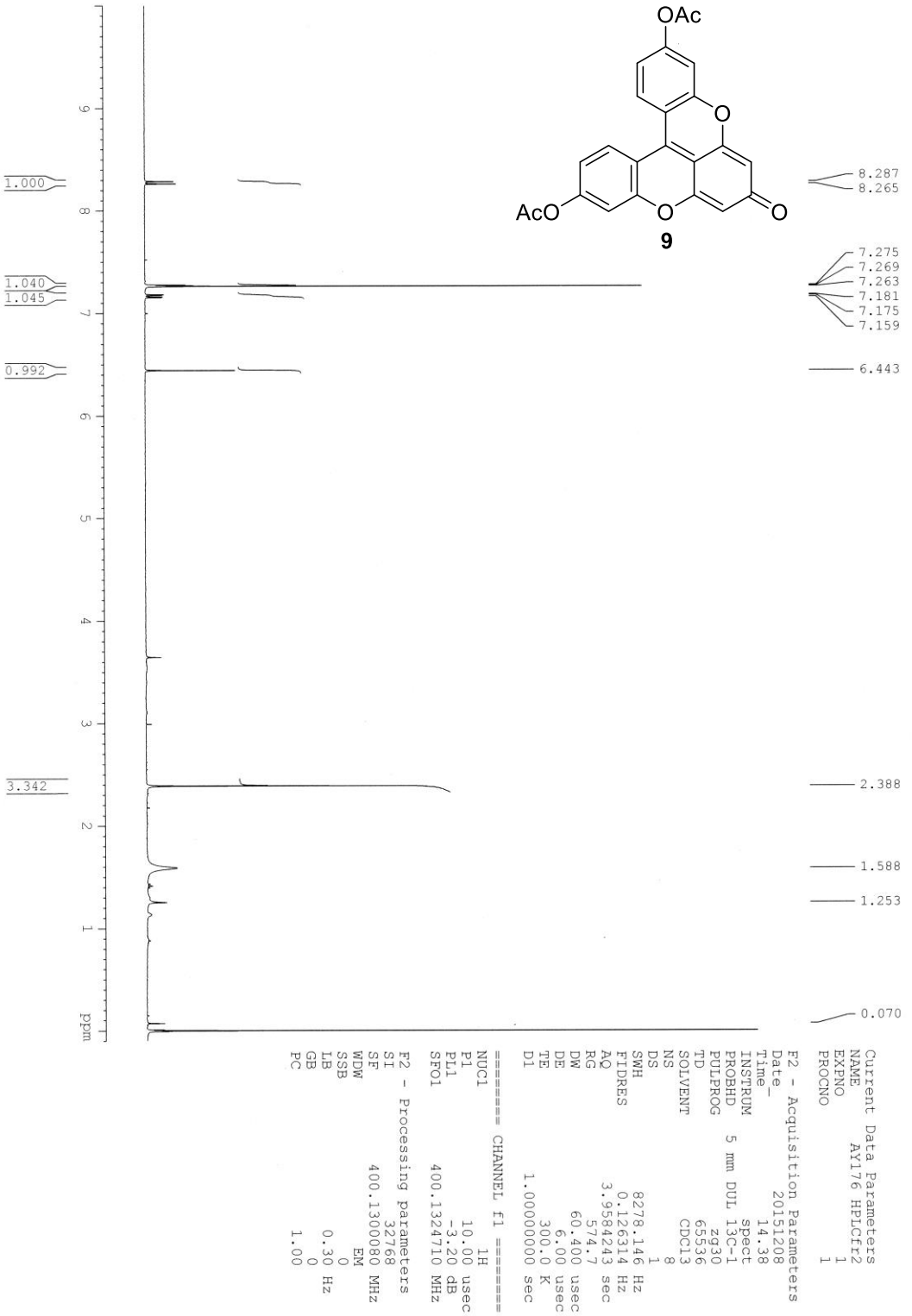
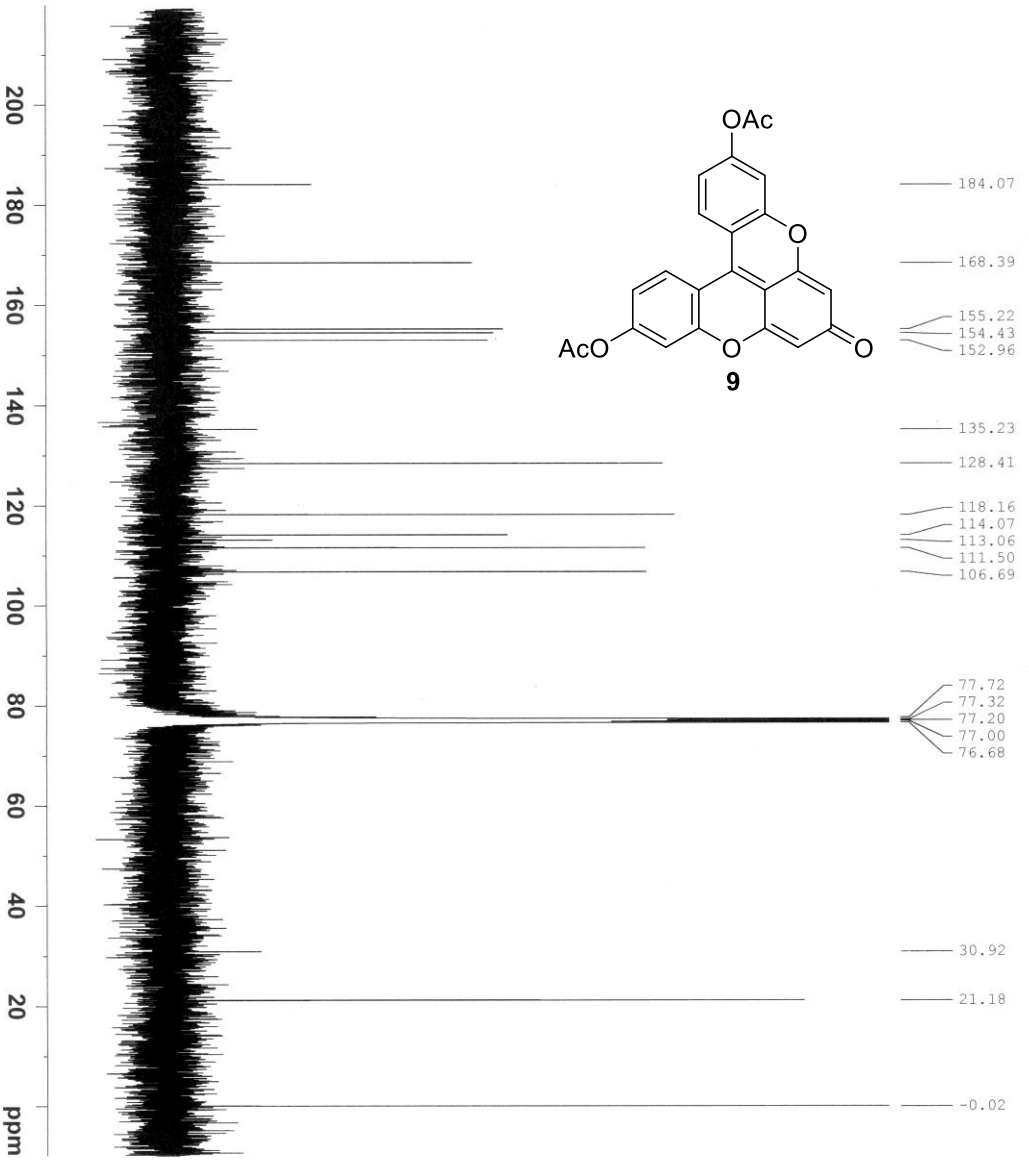
NAME tsubaki AY67
EXPNO 2
PROCNO 1
Date_ 20150613
Time 7.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg45
TD 131072
SOLVENT DMSO
NS * 200000
DS 4
SWH 48076.922 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 10.400 usec
DE 8.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10000

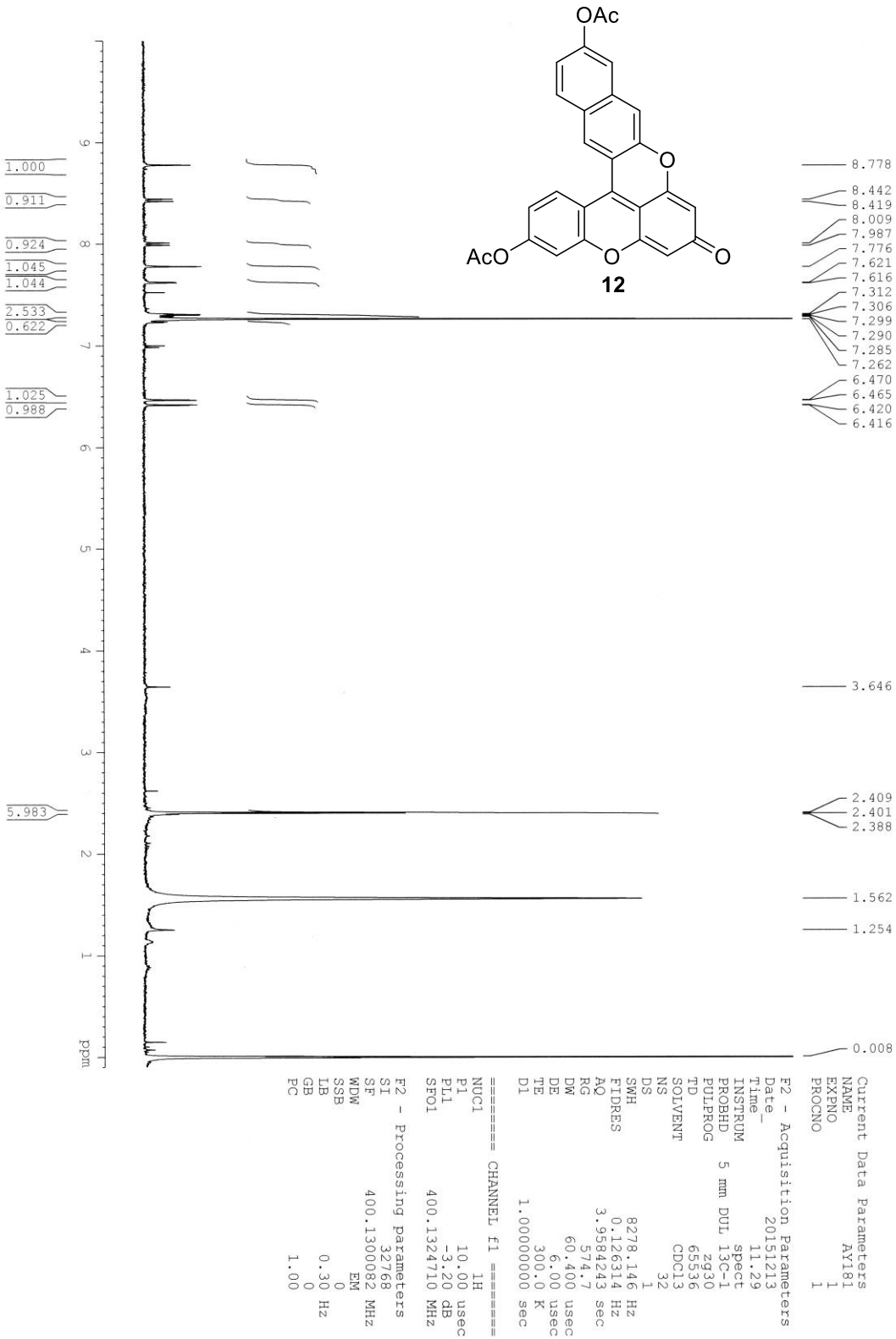
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PL1 -1.30 dB
PL1W 118.93429565 W
SFO1 150.9178988 MHz

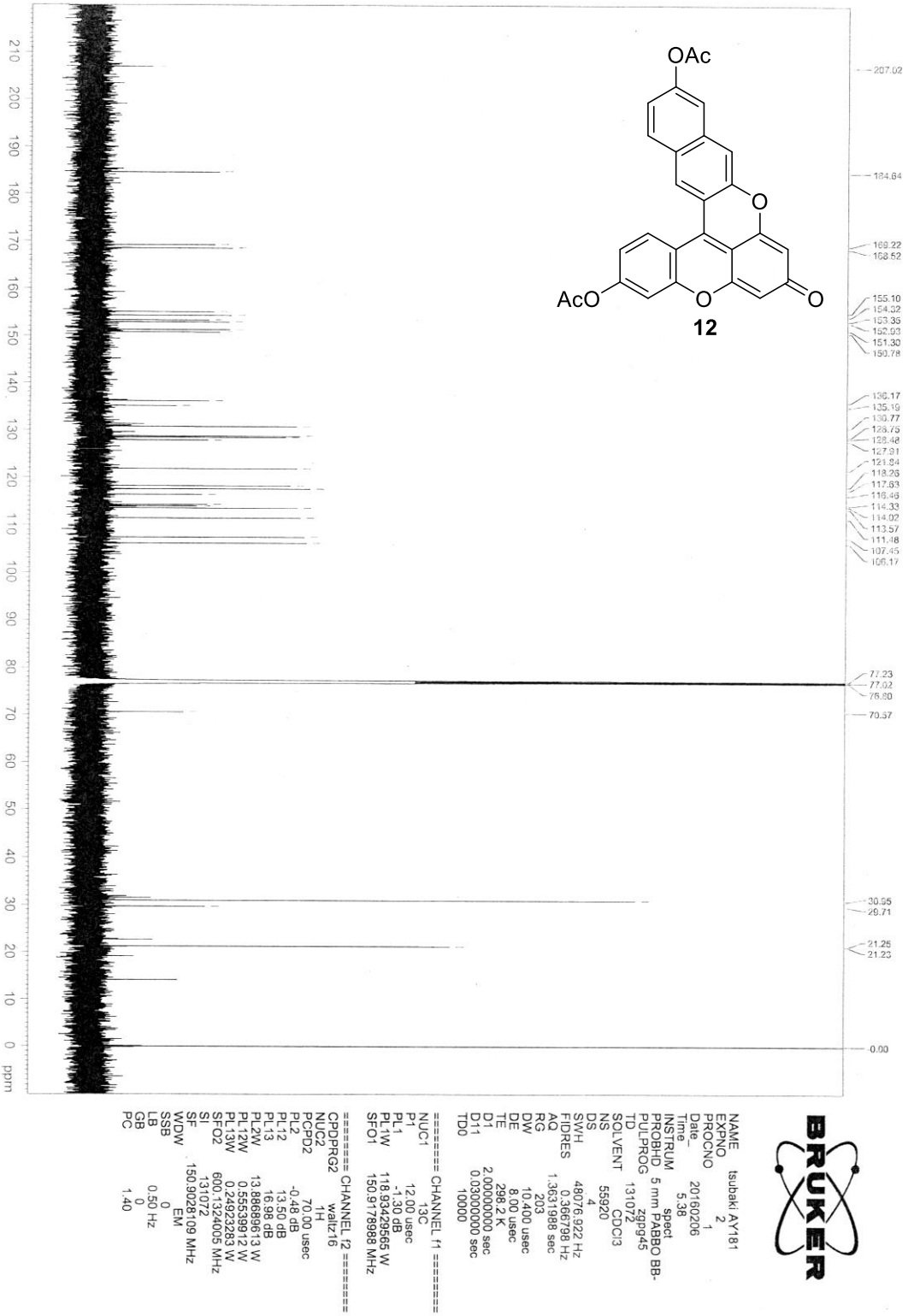
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -0.48 dB
PL12 13.50 dB
PL13 16.98 dB
PL2W 13.88689613 W
PL12W 0.55539912 W
PL13W 0.24923283 W
SFO2 600.1324005 MHz
SI 65536
SF 150.9028970 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


OAc
AcO
O
O
O
9
8.287
8.265
7.275
7.269
7.263
7.181
7.175
7.159
6.443
2.388
1.588
1.253
0.070
1.000
1.040
1.045
0.992
3.342
ppm
Current Data Parameters
NAME AY176 HELCfr2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20151208
Time 14.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

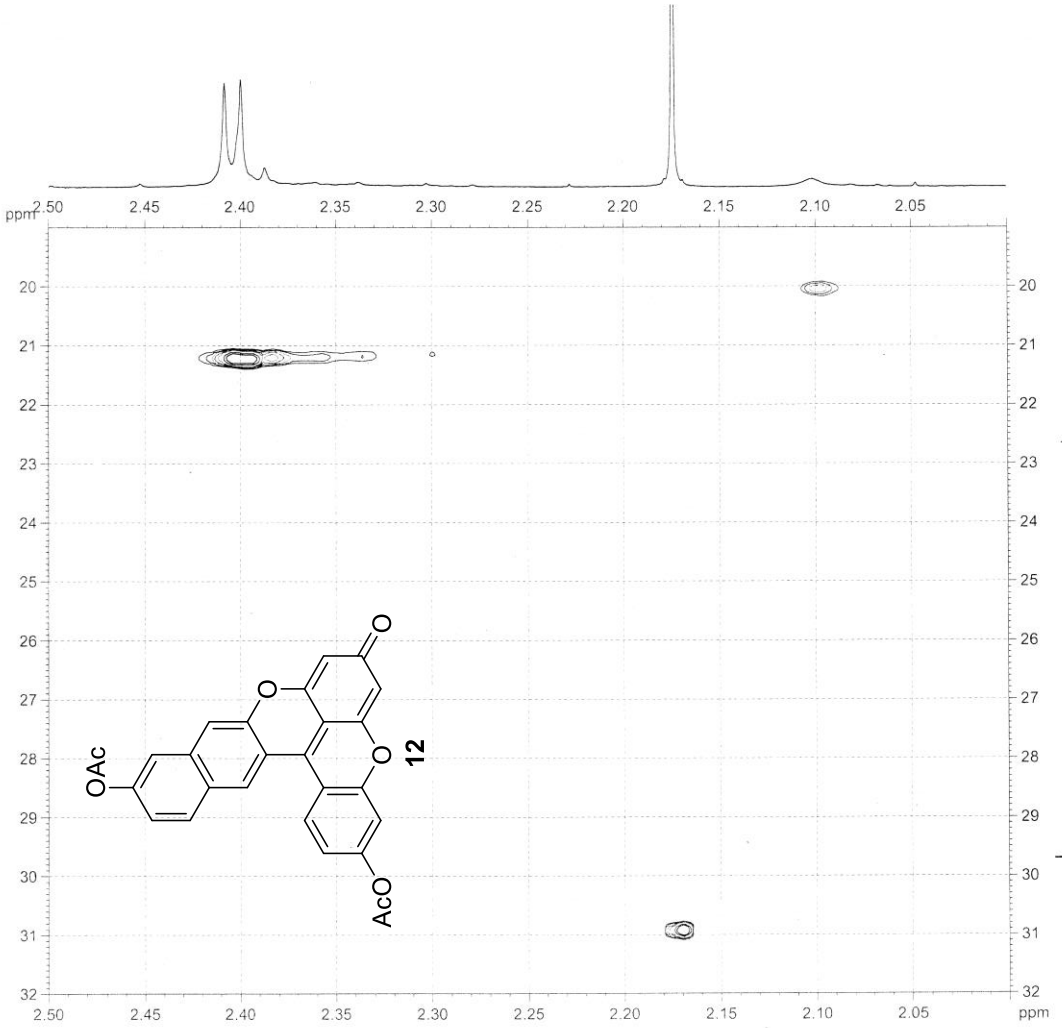


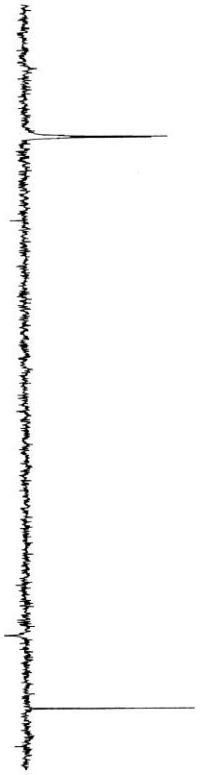

```
Current Data Parameters
NAME                  AY207
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20160130
Time_                 20.23
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  15704
DS                      2
SWH             23980.814 Hz
FIDRES              0.365918 Hz
AQ                1.3664756 sec
RG                    32768
DW                 20.850 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec

========== CHANNEL f1 ==========
NUC1                    13C
P1                   8.40 usec
PL1                  1.00 dB
SFO1          100.6228298 MHz

========== CHANNEL f2 ==========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -3.20 dB
PL12                 15.00 dB
PL13                 15.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127688 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```


OAc
AcO
O
O
O
12
8.778
8.442
8.419
8.009
7.987
7.776
7.621
7.616
7.312
7.306
7.299
7.290
7.285
7.262
6.470
6.465
6.420
6.416
3.646
2.409
2.401
2.388
1.562
1.254
0.008
1.000
0.911
0.924
1.045
1.044
2.533
0.622
1.025
0.988
5.983
ppm
Current Data Parameters
NAME AY181
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151213
Time_ 11.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 1
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.20 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


OAc
AcO
O
O
O
12
207.02
184.64
169.22
168.52
155.10
154.32
153.35
152.93
151.30
150.78
136.17
135.19
130.77
128.75
128.48
127.91
121.84
118.23
117.53
116.46
114.33
114.02
113.57
111.48
107.45
106.17
77.23
77.02
76.80
70.37
30.55
29.71
21.25
21.23
0.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
NAME tsubaki AY181
EXPNO 2
PROCNO 1
Date_ 20160206
Time_ 5.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg45
TD 131072
SOLVENT CDCl3
NS 55920
DS 4
SWH 48076.922 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 10.400 usec
DE 8.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PL1 -1.30 dB
PL1W 118.93429565 W
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -0.48 dB
PL12 13.50 dB
PL13 16.98 dB
PL2W 13.88689613 W
PL12W 0.55539912 W
PL13W 0.24923283 W
SFO2 600.1324005 MHz
SI 131072
SF 150.9028109 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
BRUKER

AY181;HSQC

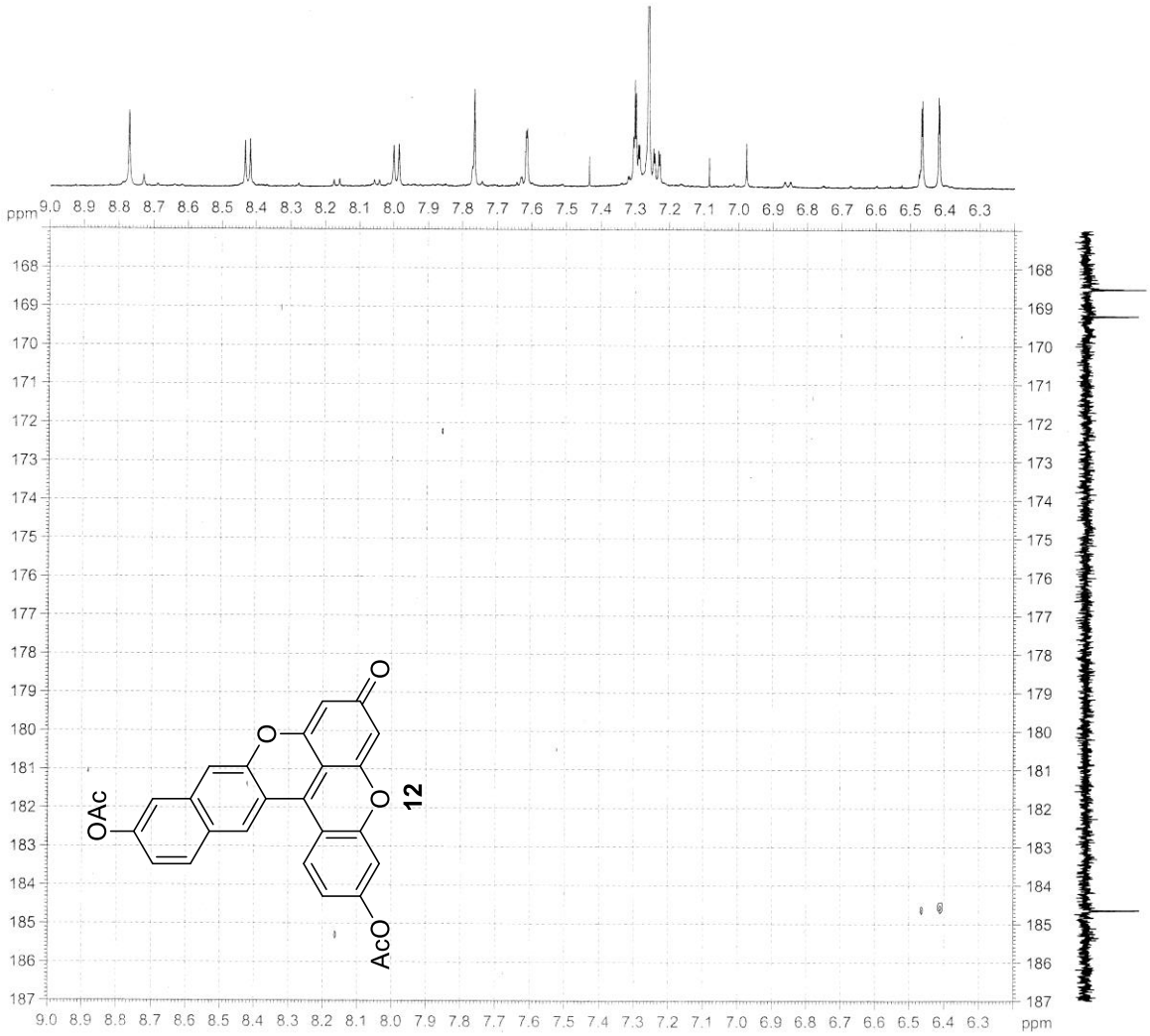




BRUKER

```
NAME        tsubaki AY181
EXPNO             6
PROCNO            1
Date_        20160203
Time             19.14
INSTRUM          spect
PROBHD  5 mm PABBO BB-
PULPROG     hsqcetgpsi2
TD               4096
SOLVENT          CDCl3
NS                 24
DS                 16
SWH          6410.256 Hz
FIDRES       1.565004 Hz
AQ           0.3195380 sec
RG                 161
DW             78.000 usec
DE              6.00 usec
TE             298.6 K
CNST2        145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D13          0.00000400 sec
D16          0.00010000 sec
D24          0.00086207 sec
IN0          0.00002000 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1               1H
P1              14.00 usec
P2              28.00 usec
P28              0.10 usec
PL1             -0.48 dB
PL1W        13.88689613 W
SFO1       600.1326335 MHz

======== CHANNEL f2 ========
CPDPRG2          garp
NUC2               13C
P3              12.00 usec
P4              24.00 usec
PCPD2           60.00 usec
PL2             -1.30 dB
PL12            12.88 dB
PL2W        118.93429565 W
PL12W        4.75671434 W
SFO2       150.9125742 MHz

====== GRADIENT CHANNEL =====
GPNAM1         SINE.100
GPNAM2         SINE.100
GPNAM3         SINE.100
GPNAM4         SINE.100
GPZ1            80.00 %
GPZ2            20.10 %
GPZ3            11.00 %
GPZ4            -5.00 %
P16           1000.00 usec
P19            600.00 usec
ND0                2
TD              1024
SFO1       150.9126 MHz
FIDRES      24.414063 Hz
SW          165.659 ppm
FnMODE     Echo-Antiecho
SI              2048
SF         600.1300157 MHz
WDW             QSINE
SSB                2
LB              0.00 Hz
GB                 0
PC              1.40
SI              4096
MC2        echo-antiecho
SF         150.9028109 MHz
WDW             QSINE
SSB                2
LB              0.00 Hz
GB                 0
```

AY181;HMBC



BRUKER

```
NAME      tsubaki AY181
EXPNO             7
PROCNO            1
Date_      20160205
Time_         3.16
INSTRUM       spect
PROBHD  5 mm PABBO BB-
PULPROG   hmbcgplpndqf
TD             4096
SOLVENT       CDCl3
NS               48
DS               16
SWH        6024.096 Hz
FIDRES     1.470727 Hz
AQ         0.3400180 sec
RG              181
DW           83.000 usec
DE            8.00 usec
TE           298.2 K
CNST2      145.0000000
CNST13      10.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D2         0.00344828 sec
D6         0.05000000 sec
D16        0.00010000 sec
IN0        0.00001400 sec

======== CHANNEL f1 ========
NUC1             1H
P1            14.00 usec
P2            28.00 usec
PL1           -0.48 dB
PL1W      13.88689613 W
SFO1     600.1326139 MHz

======== CHANNEL f2 ========
NUC2            13C
P3            12.00 usec
PL2           -1.30 dB
PL2W      118.93429565 W
SFO2     150.9175774 MHz

====== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GPNAM3       SINE.100
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16         1000.00 usec
ND0               2
TD             1024
SFO1     150.9176 MHz
FIDRES     34.877232 Hz
SW         236.648 ppm
FnMODE           QF
SI             2048
SF       600.1300165 MHz
WDW            SINE
SSB               0
LB           0.00 Hz
GB                0
PC             1.40
SI             4096
MC2              QF
SF       150.9028113 MHz
WDW            SINE
SSB               0
LB           0.00 Hz
GB                0
```