Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Quenching of fluorescence as an indicator of donor-strength in *meso* arylethynyl BODIPYs

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Single Crystal X-ray Diffraction Studies.

Single crystal X-ray structural studies of **2d** and **2e** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 150(2) K using graphite-monochromated CuK\α radiation (λ_α = 1.5418 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on $F^{2.1}$. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2U_{eq} of their parent atoms. The crystal structure, and dat refinement parameters are summarized in Table 1. The CCDC numbers 967406, and 967407 contain the supplementary crystallographic data for **2d** and **3e** respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S1. Crystal structure and data refinement parameters

BODIPY	**2d**	**2e**
Empirical formula	C_{21} H_{13} B F_2 N_2	C_{21} H_{13} B F_2 N_2
Formula weight	342.14	342.14
Temperature/K	150(2)	150(2)
Crystal system	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$P2/c$
Unit cell dimensions		
a/Å	a = 5.5995(2)	a = 10.1059(3)
α/°	90	90
b/ Å	13.5098(4)	b = 10.4411(3)
β/°	90	100.699(3)
c/ Å	22.2683(8)	15.6091(5)
γ/°	90	90
Volume/ $Å^3$	1684.56(10)	1618.39(8)
Z	4	4
Calculated density/ Mg/m^3	1.349	1.404
Absorption coefficient/mm^{-1}	0.779	0.811
F(000)	704	704
Crystal size/mm	0.21 x 0.18 x 0.13	0.33 x 0.26 x 0.19
θ range from data collection/°	3.83 to 72.10	4.23 to 72.16
Reflections collected/unique	11102 / 3269 [R(int) = 0.0166]	10226 / 3147 [R(int) = 0.0239]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Data/restraints/parameters	3269 / 0 / 236	3147 / 0 / 236
Goodness-of-fit on F^2	1.023	1.090
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0281, wR_2 = 0.0735	R_1 = 0.0427, wR_2 = 0.1244
R indices (all data)	R_1 = 0.0336, wR_2 = 0.0788	R_1 = 0.0519, wR_2 = 0.1387
Largest diff. peak and hole/e $Å^{-3}$	0.081 and -0.099	0.198 and -0.207
Absolute structure parameter	0.10(14)	-
CCDC number	967406	967407

Table S2. Selected torsional angles obtained from crystal structure and theoretical calculations

BODIPY	**2d**	**2e**
Torsional angle	4.97	2.68
Theoretical torsional angle	0.23	13.43

Table S3. Distance and angle of intermolecular of interactions in the crystal structures.

Interaction	Distance (Å)	Angle of Interaction (°)
2d		
F(1)---H(7)-C(7)	2.355	131.08
F(1)---H(21)-C(21)	2.285	128.27
F(2)---H(9)-C(9)	2.627	119.94
C(17)-H(17)---π (pyrrolic)	3.044	
π---π between two BODIPY units	3.383	
2e		
F(1)---H(9)-C(9)	2.467	160.18
F(2)---H(18)-C(18)	2.527	156.97
π---π between two BODIPY units	3.384	

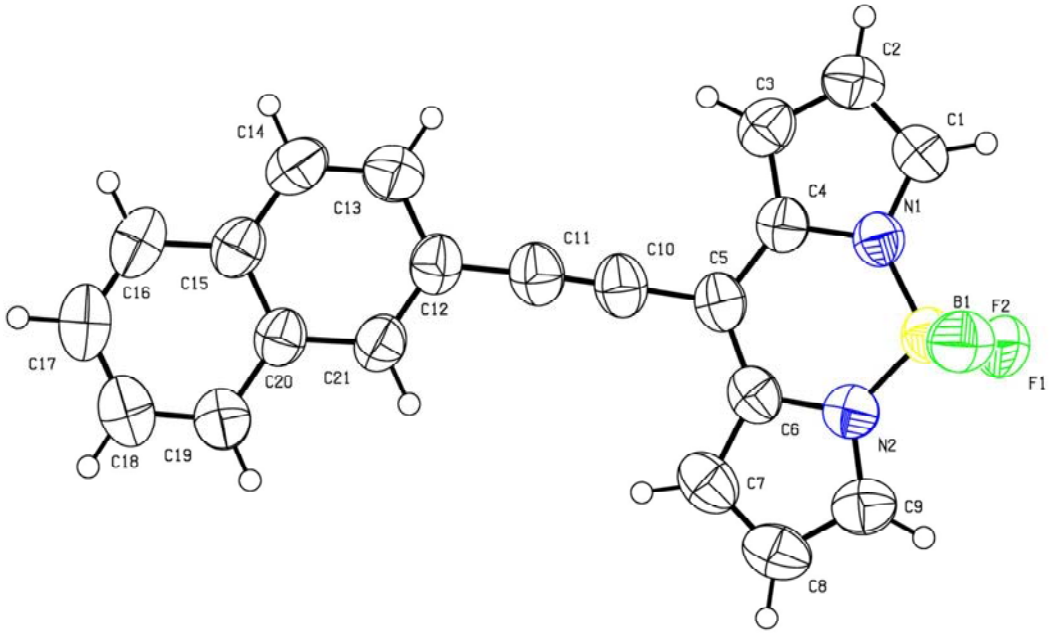


Figure S1. Crystal structure of **2d**

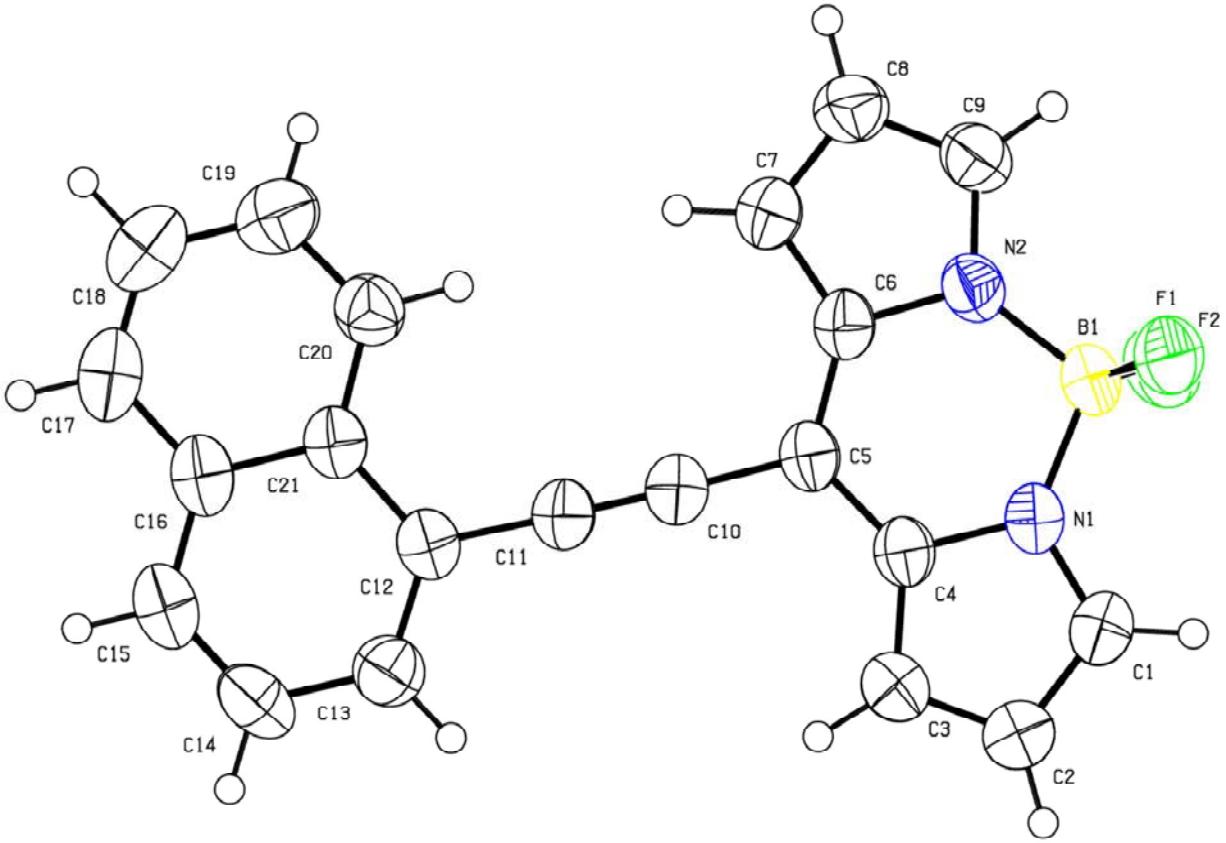


Figure S2. Crystal structure of **2e**

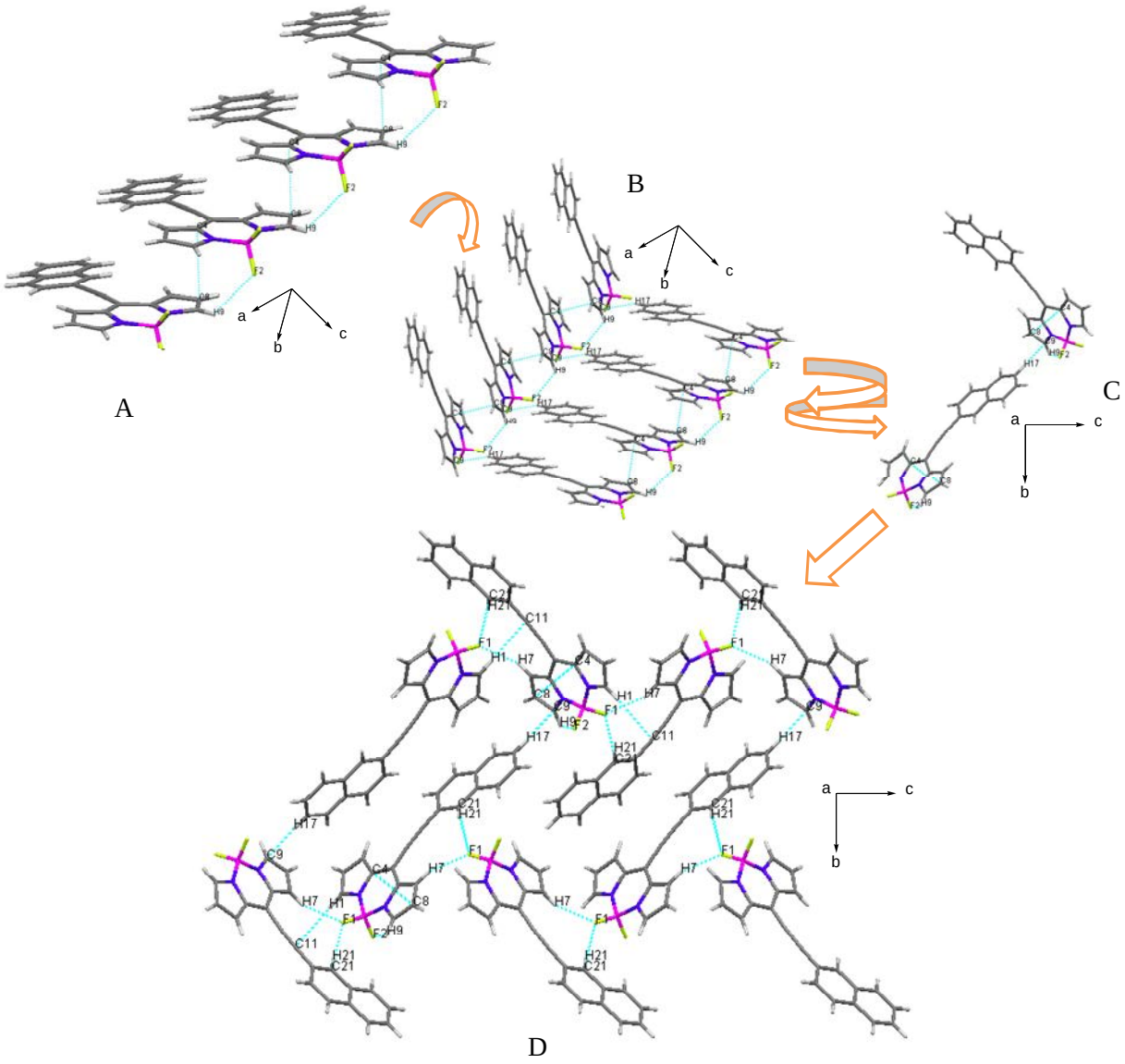


Figure S3. Crystal structure packing of **2d.**

The fluorescence quantum yields (ϕ_F)

The fluorescence quantum yields (ϕ_F) of compounds **2-6** were calculated by the steady-state comparative method using Rhodamine 6G as a standard (ϕ_{st} = 0.88, ethanol).[1]

$$\phi_F = \phi_{st} \times S_u/S_{st} \times A_{st} / A_u \times n^2_{Du}/n^2_{Dst} \ldots\ldots\ldots\ldots\ldots\ldots \text{(Eq. 1)}$$

Where ϕ_F is the emission quantum yield of the sample, ϕ_{st} is the emission quantum yield of the standard, A_{st} and A_u represent the absorbance of the standard and sample at the excitation wavelength, respectively, while S_{st} and S_u are the integrated emission band areas of the standard and sample, respectively, and n_{Dst} and n_{Du} the solvent refractive index of the standard and sample, u and st refer to the unknown and standard, respectively.

Electrochemical Characterizations

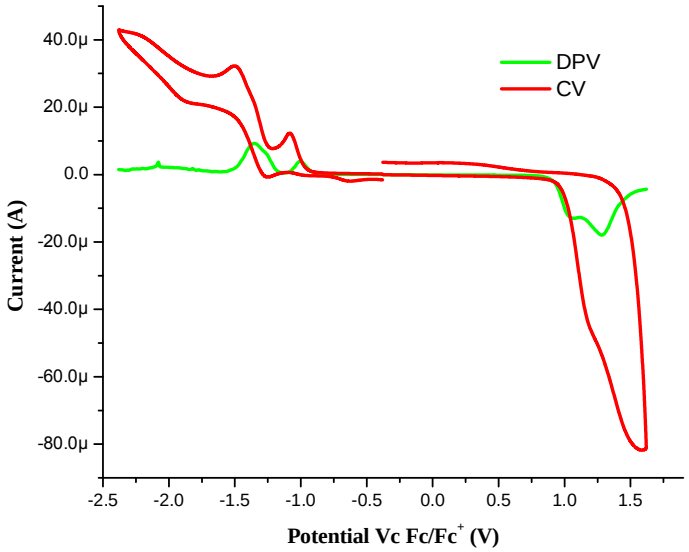


Figure S4. CV and DPV plots of of *meso*-arylethynyl BODIPY **2a.**

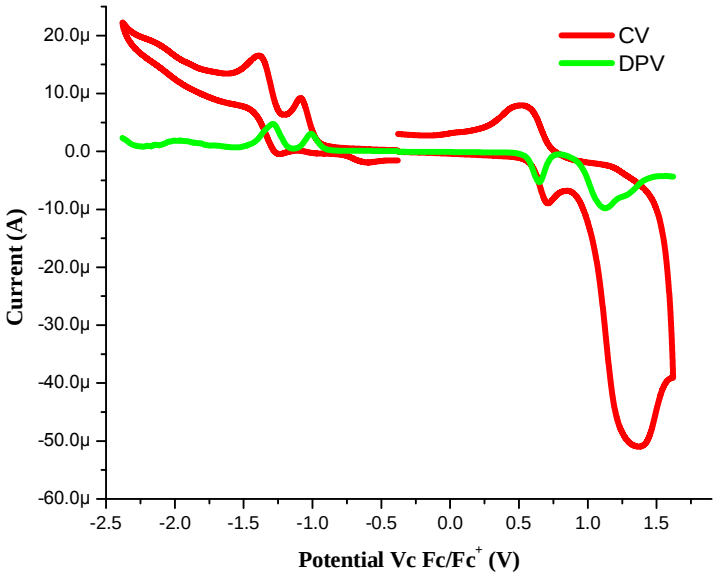


Figure S5. CV and DPV plots of of *meso*-arylethynyl BODIPY **2b.**

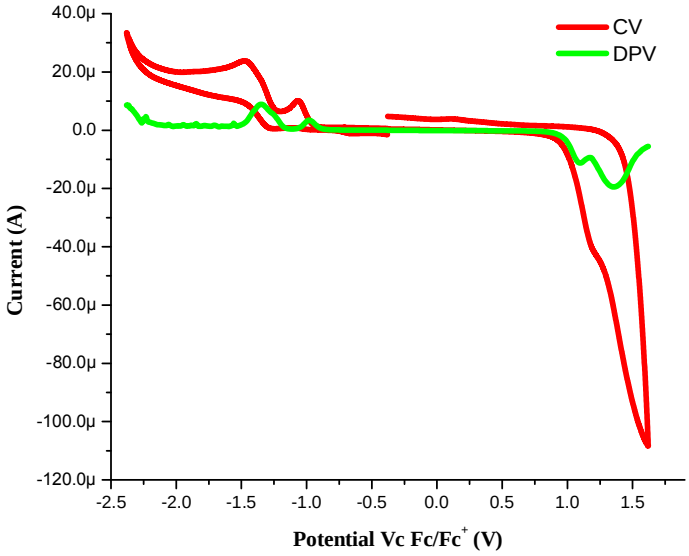


Figure S6. CV and DPV plots of of *meso*-arylethynyl BODIPY **2c.**

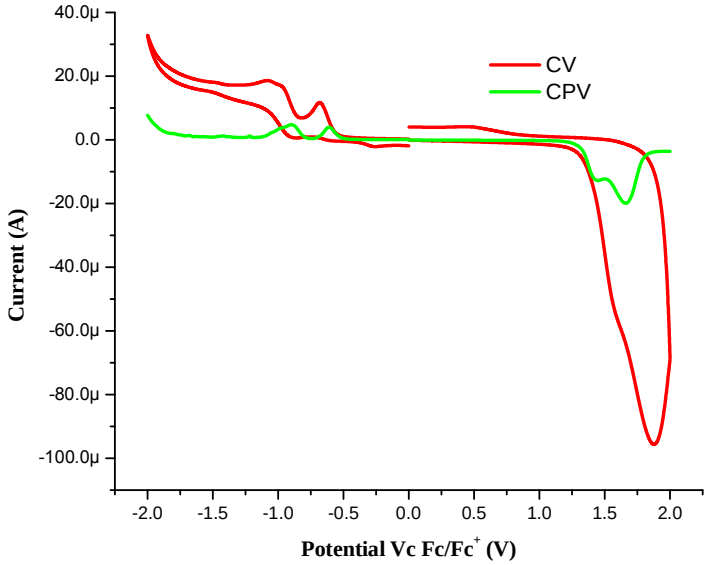


Figure S7. CV and DPV plots of of *meso*-arylethynyl BODIPY **2d.**

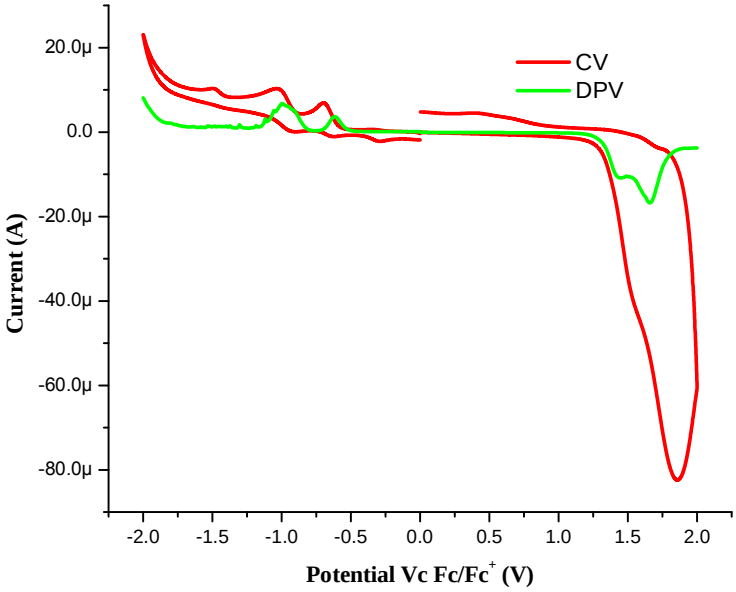


Figure S8. CV and DPV plots of of *meso*-arylethynyl BODIPY **2e.**

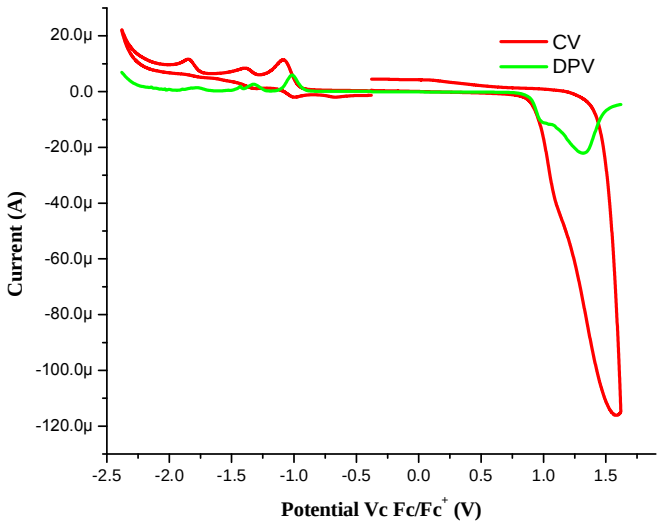


Figure S9. CV and DPV plots of of *meso*-arylethynyl BODIPY **2f.**

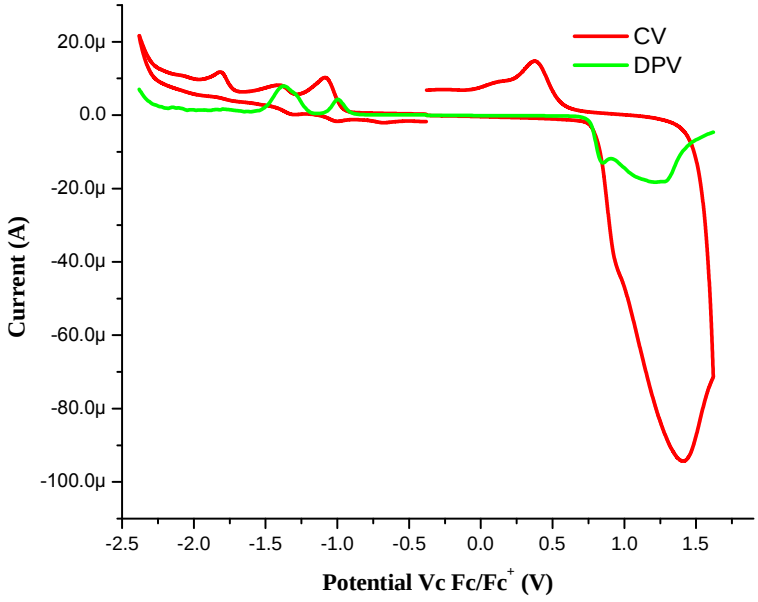


Figure S10. CV and DPV plots of *meso*-arylethynyl BODIPY **2g.**

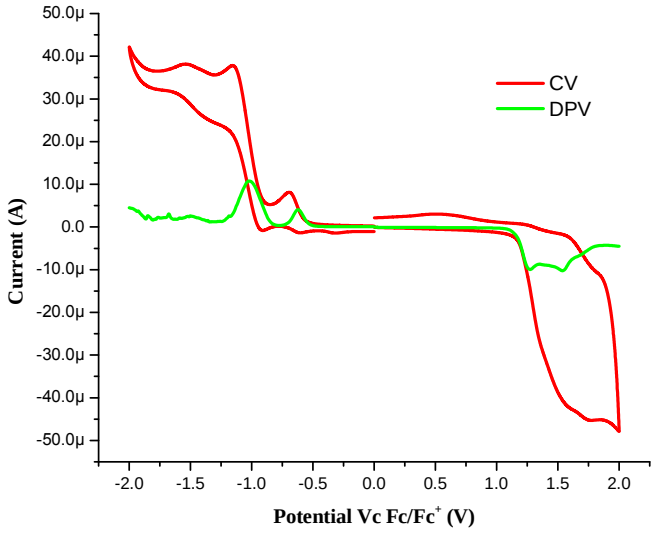
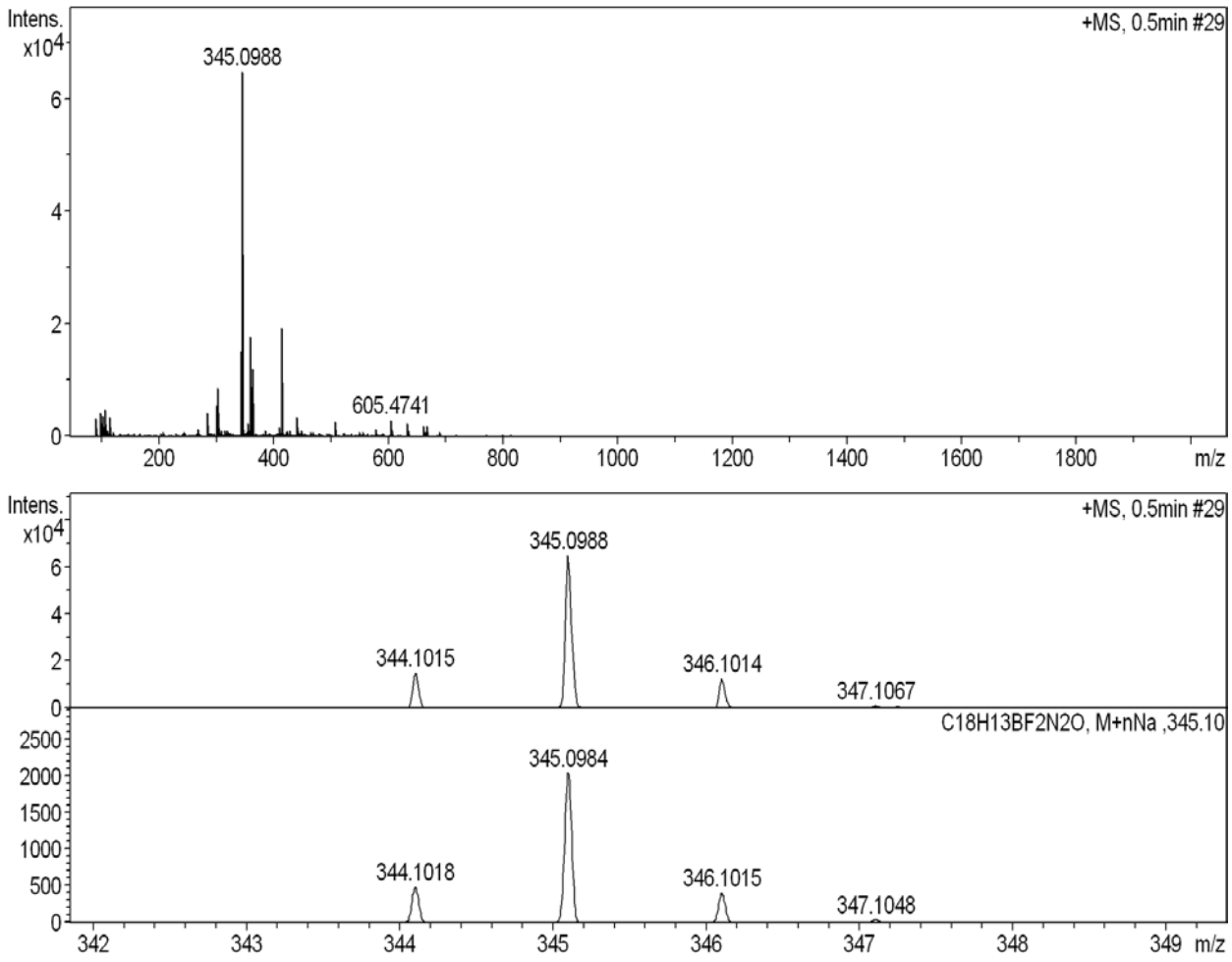
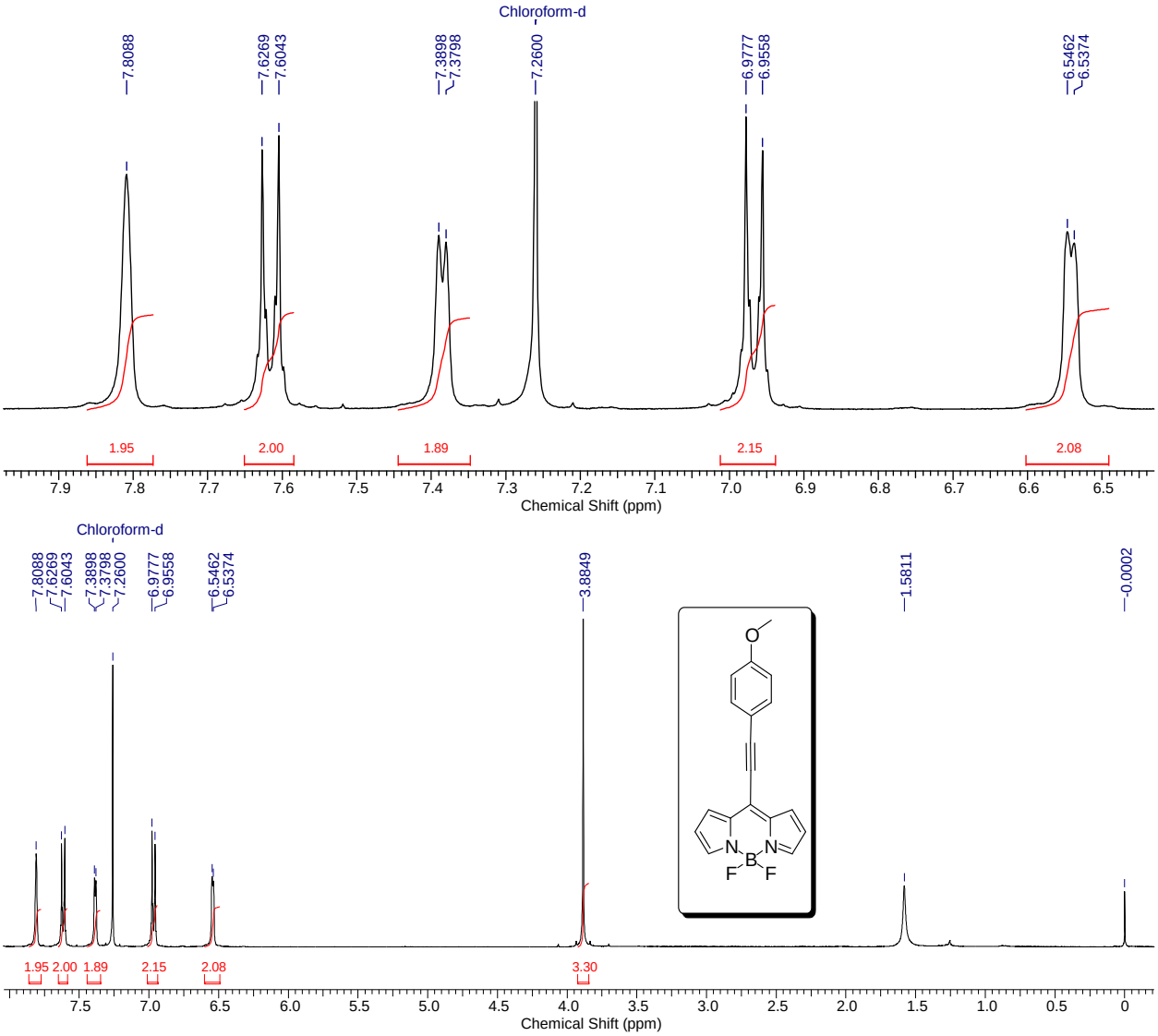


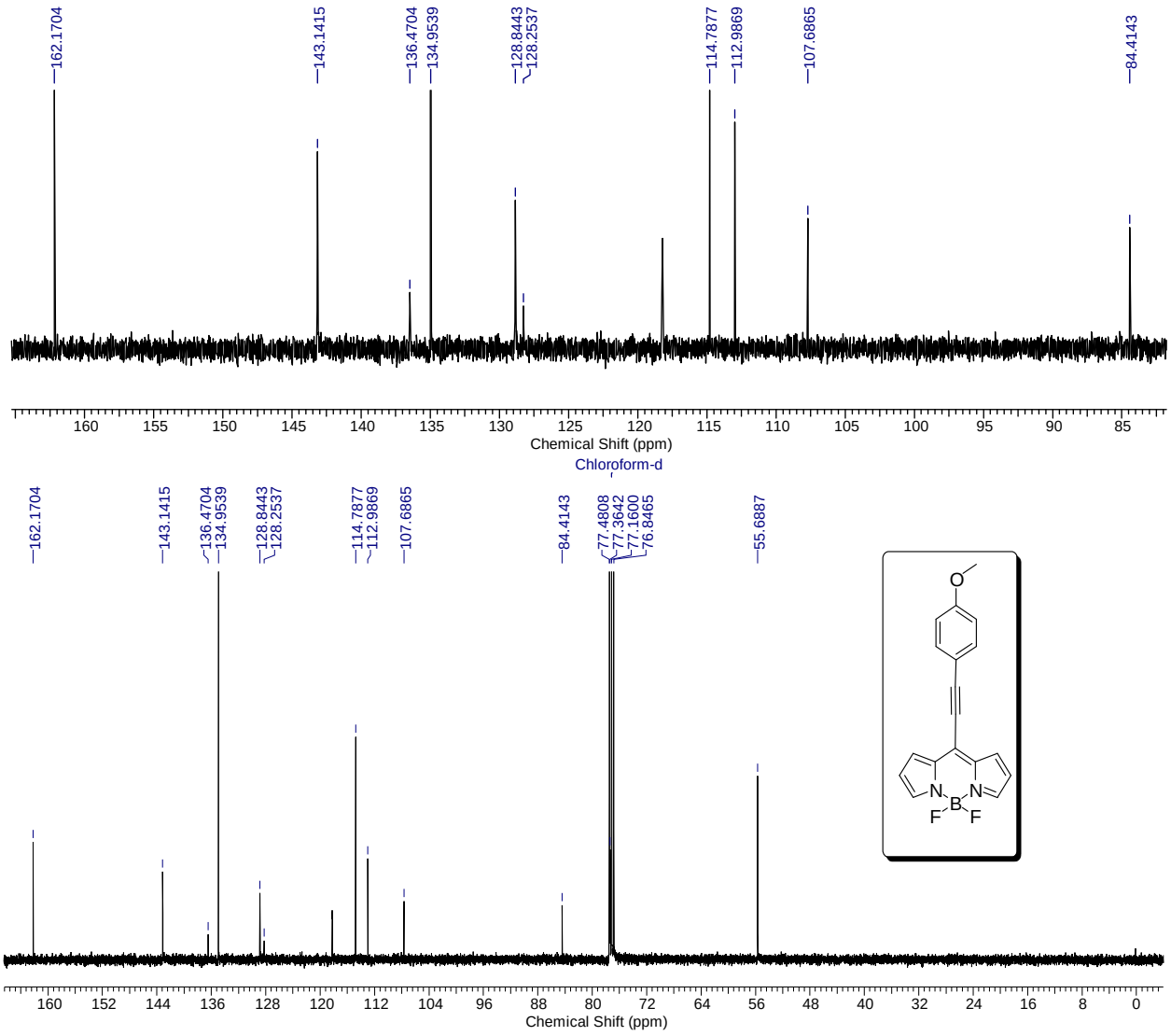
Figure S11. CV and DPV plots of *meso*-arylethynyl BODIPY **2h.**



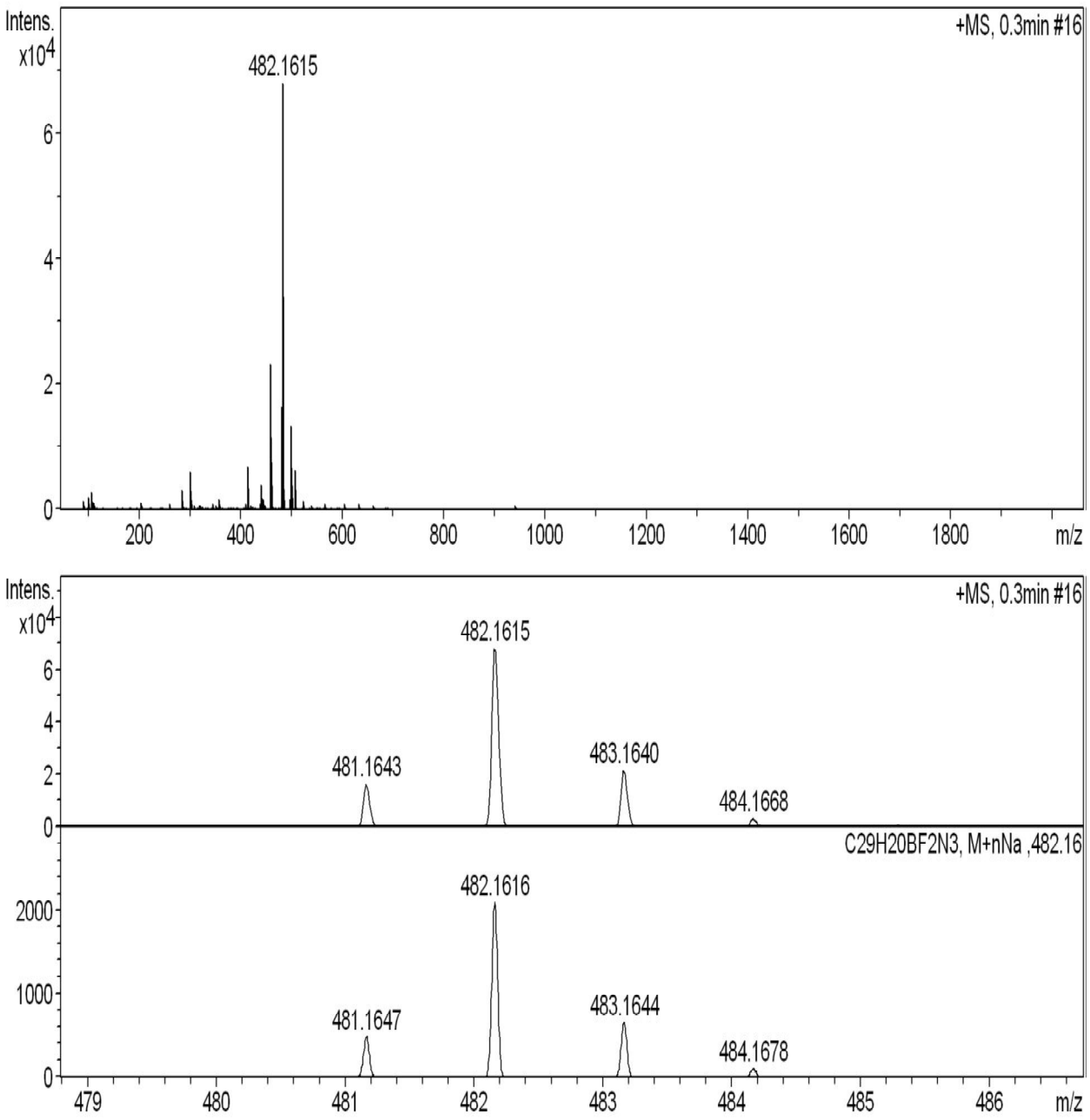
HRMS spectra of **2a**



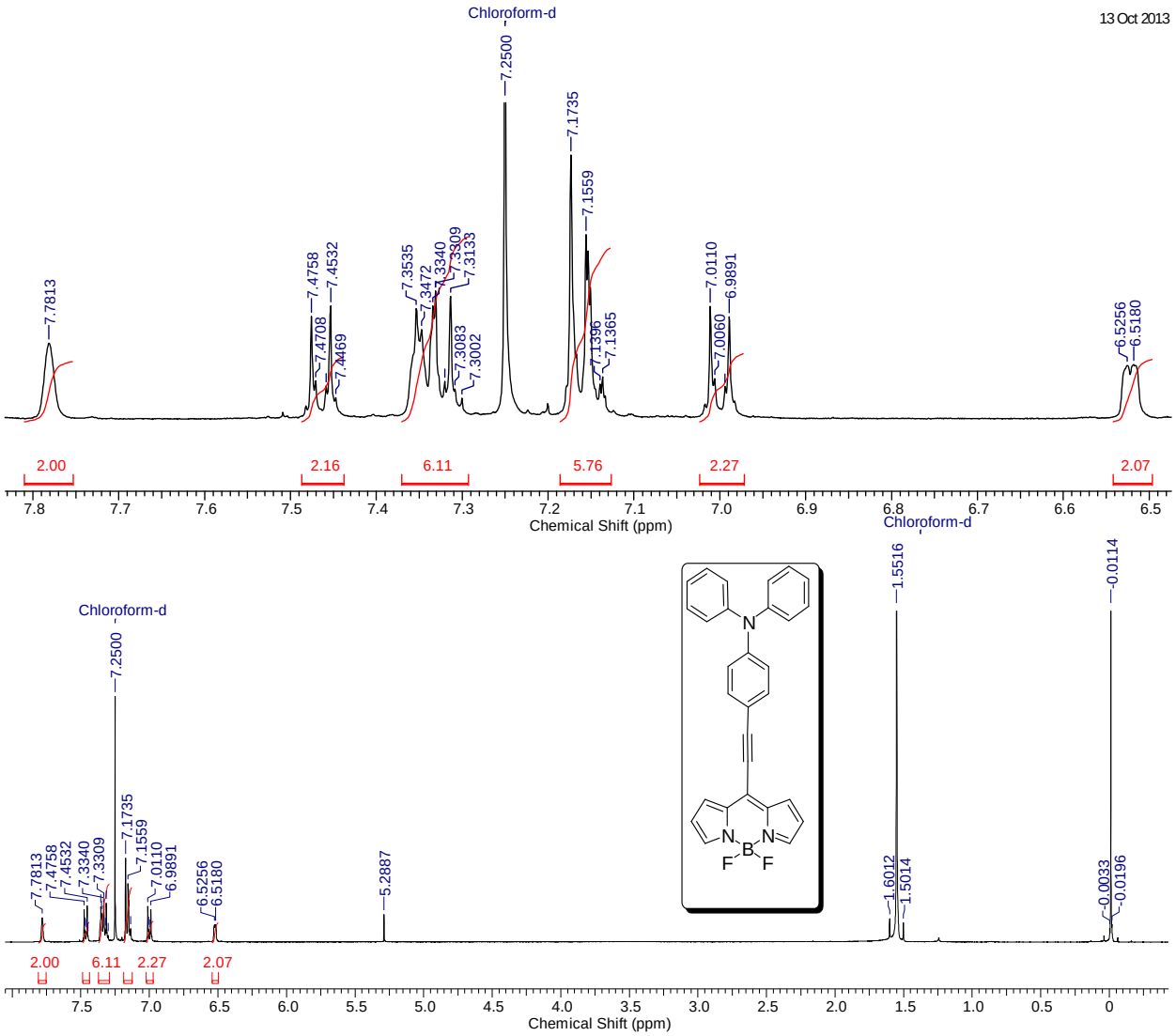
^{1}H NMR spectra of **2a**



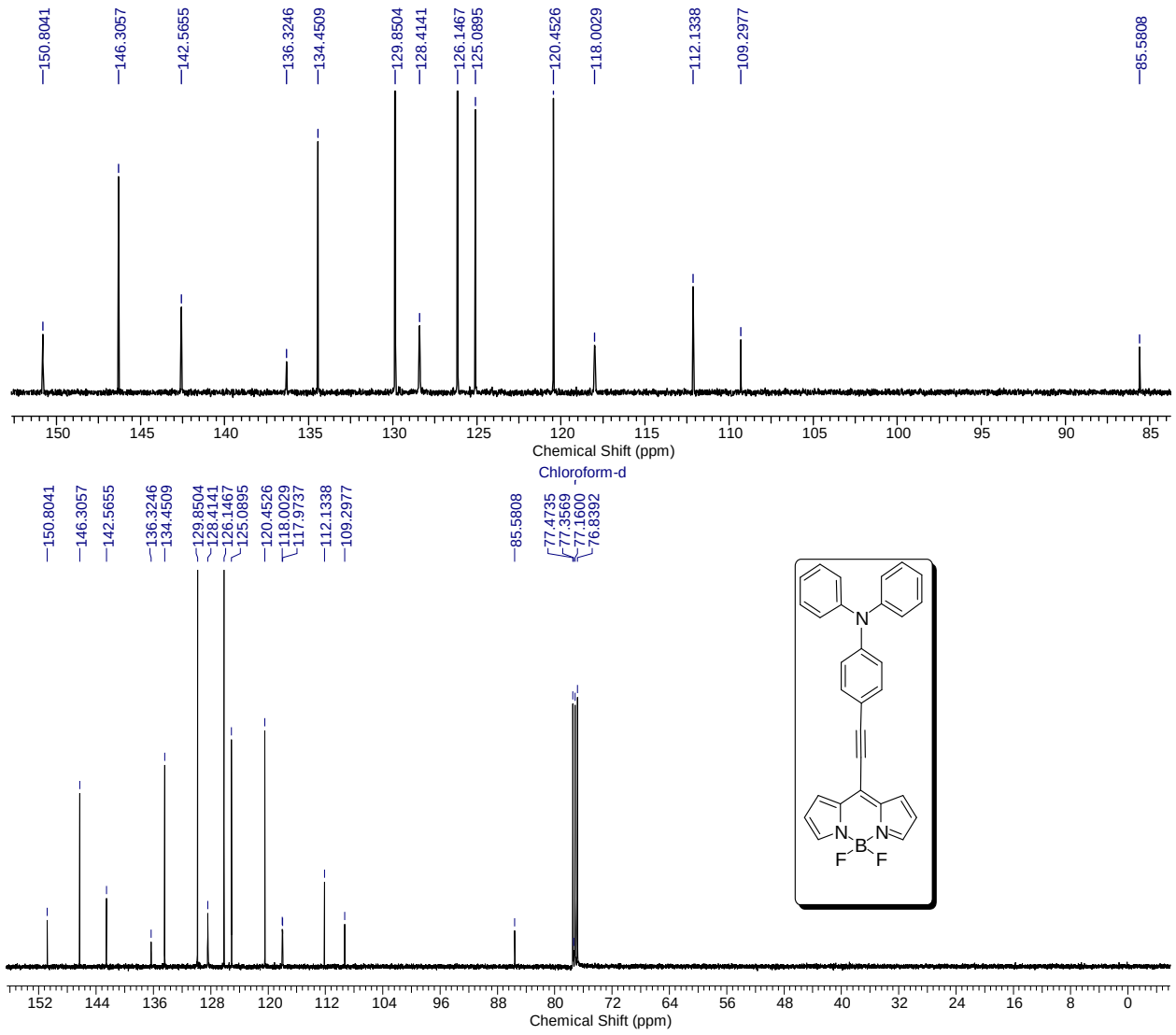
^{13}C NMR spectra of **2a**



HRMS spectra of **2b**



^{1}H NMR spectra of **2b**



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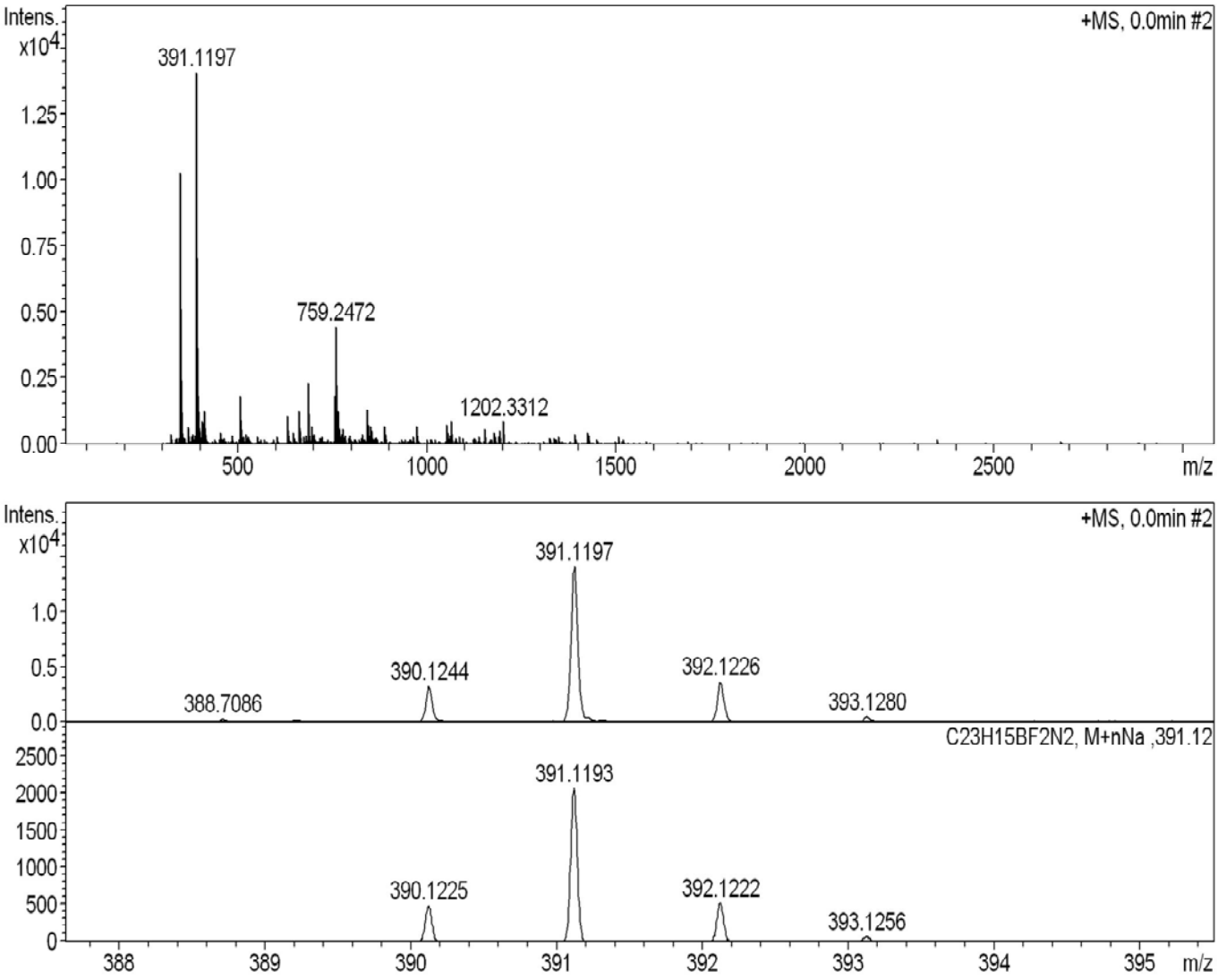
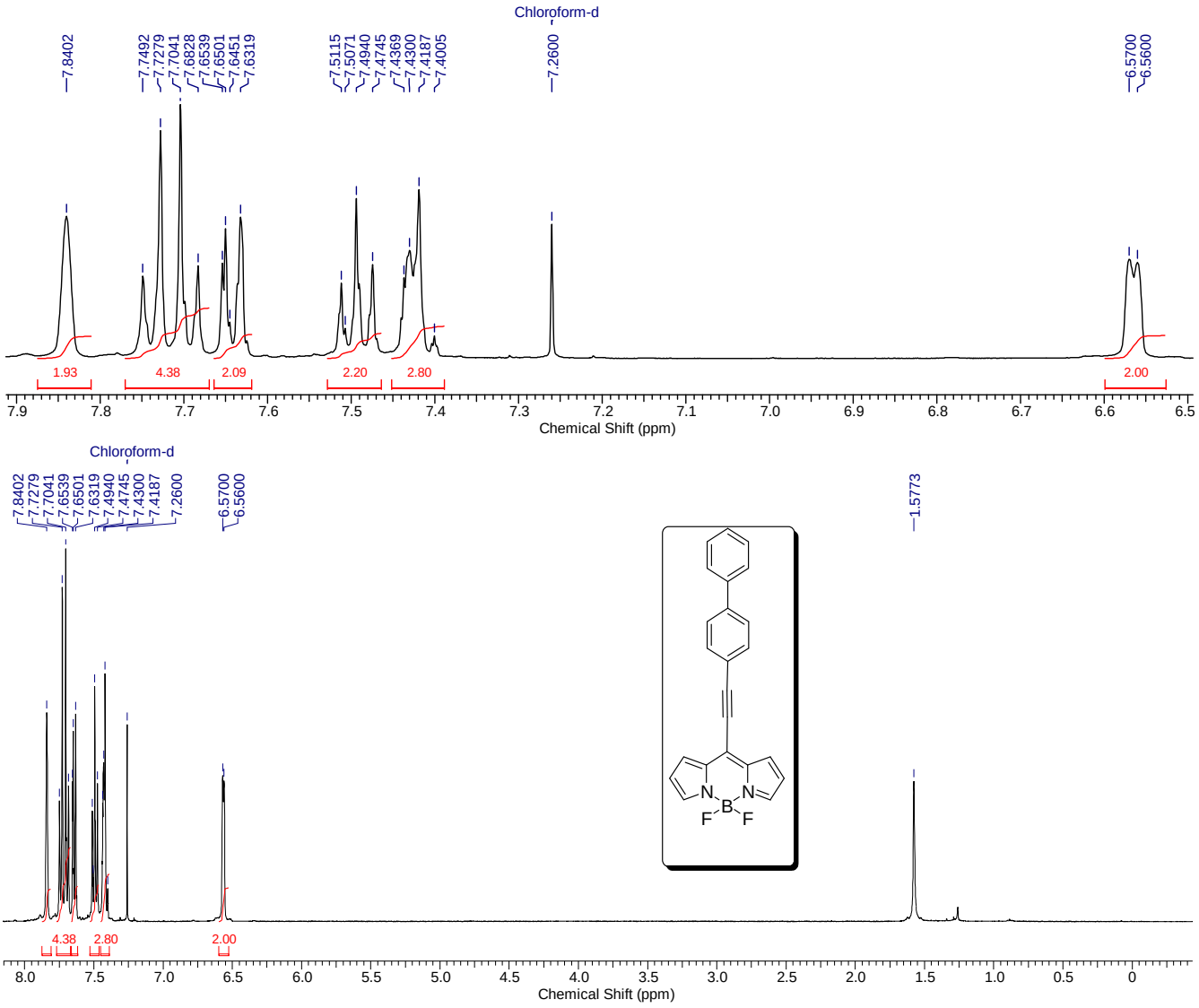


HRMS spectra of **2c**



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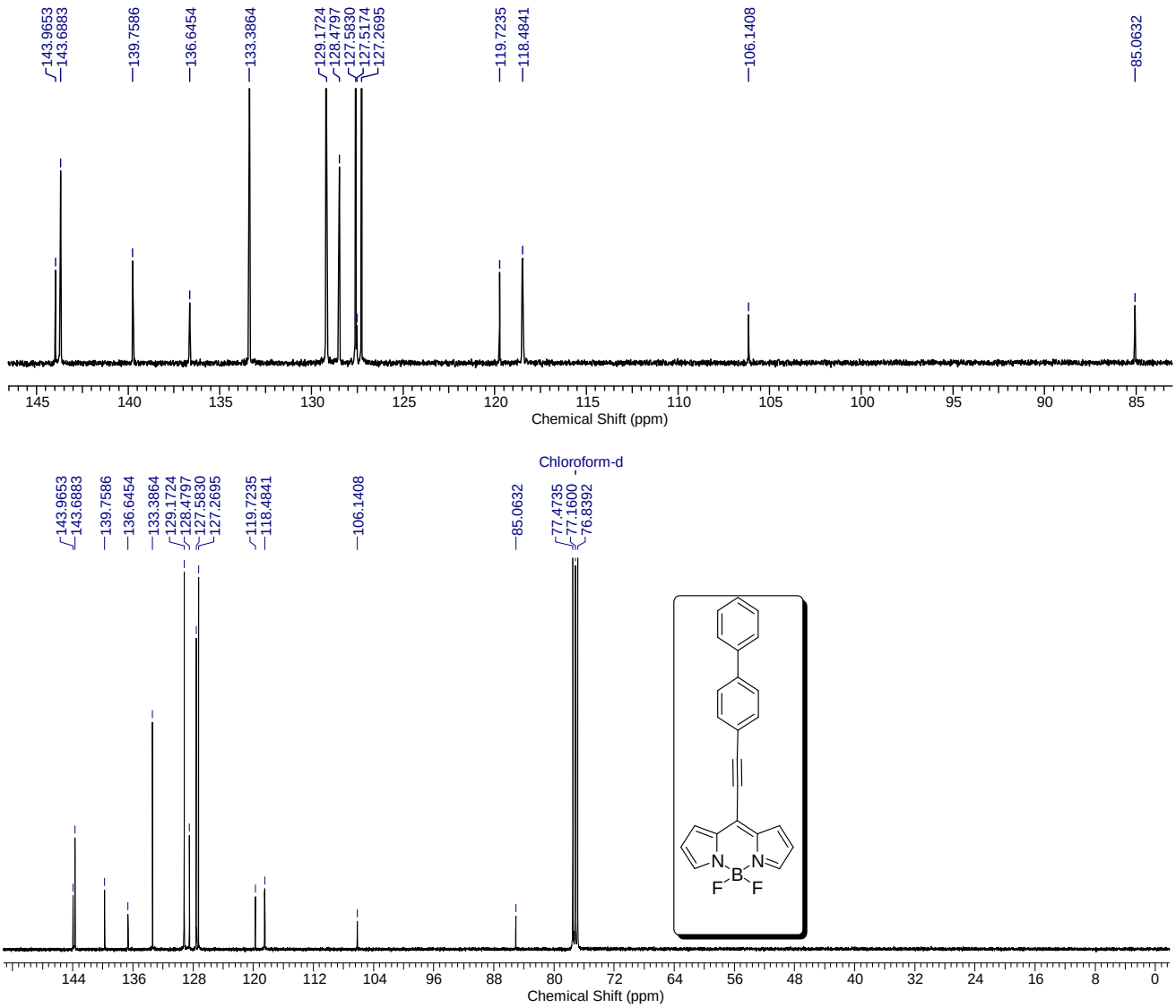

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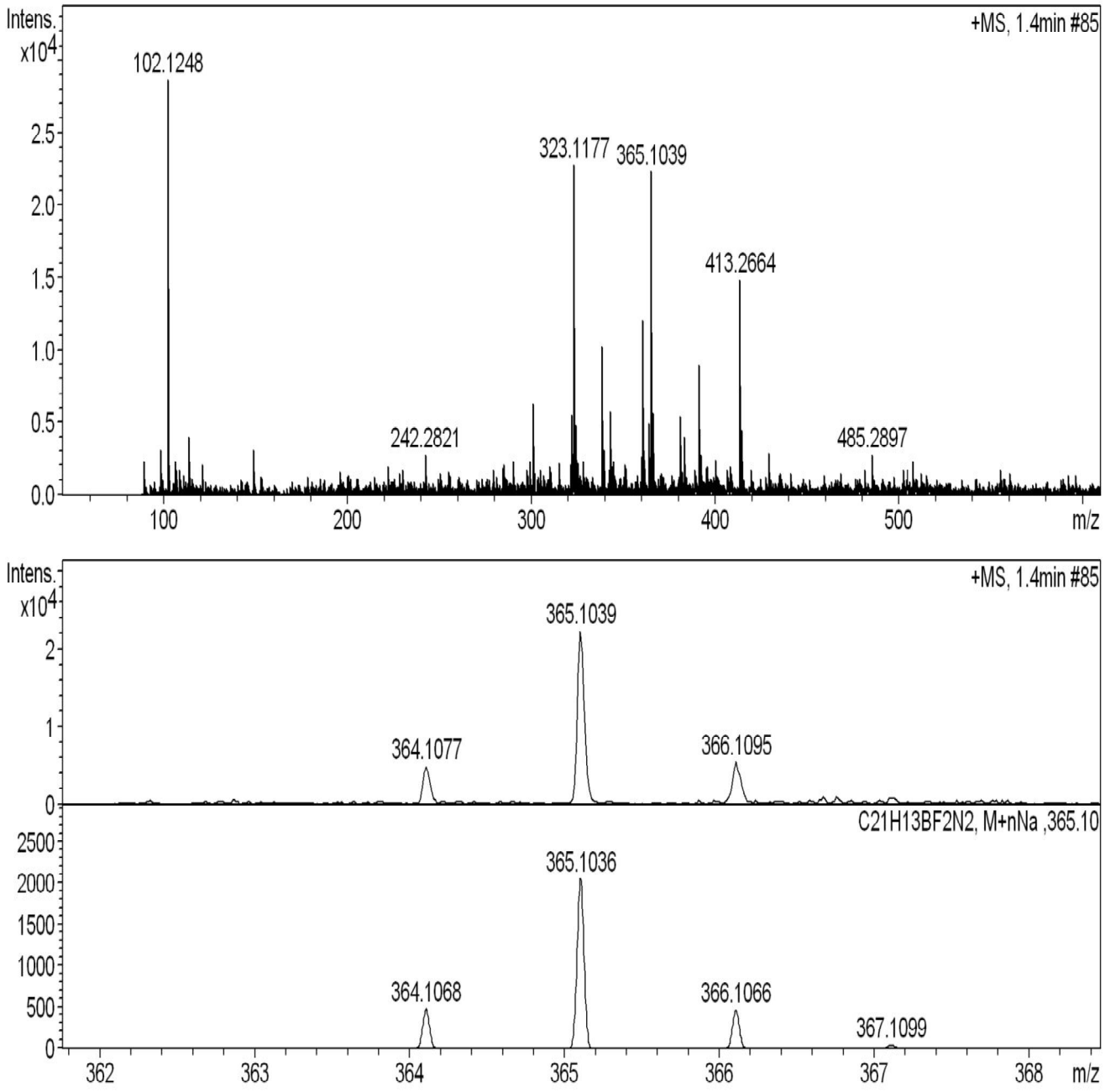

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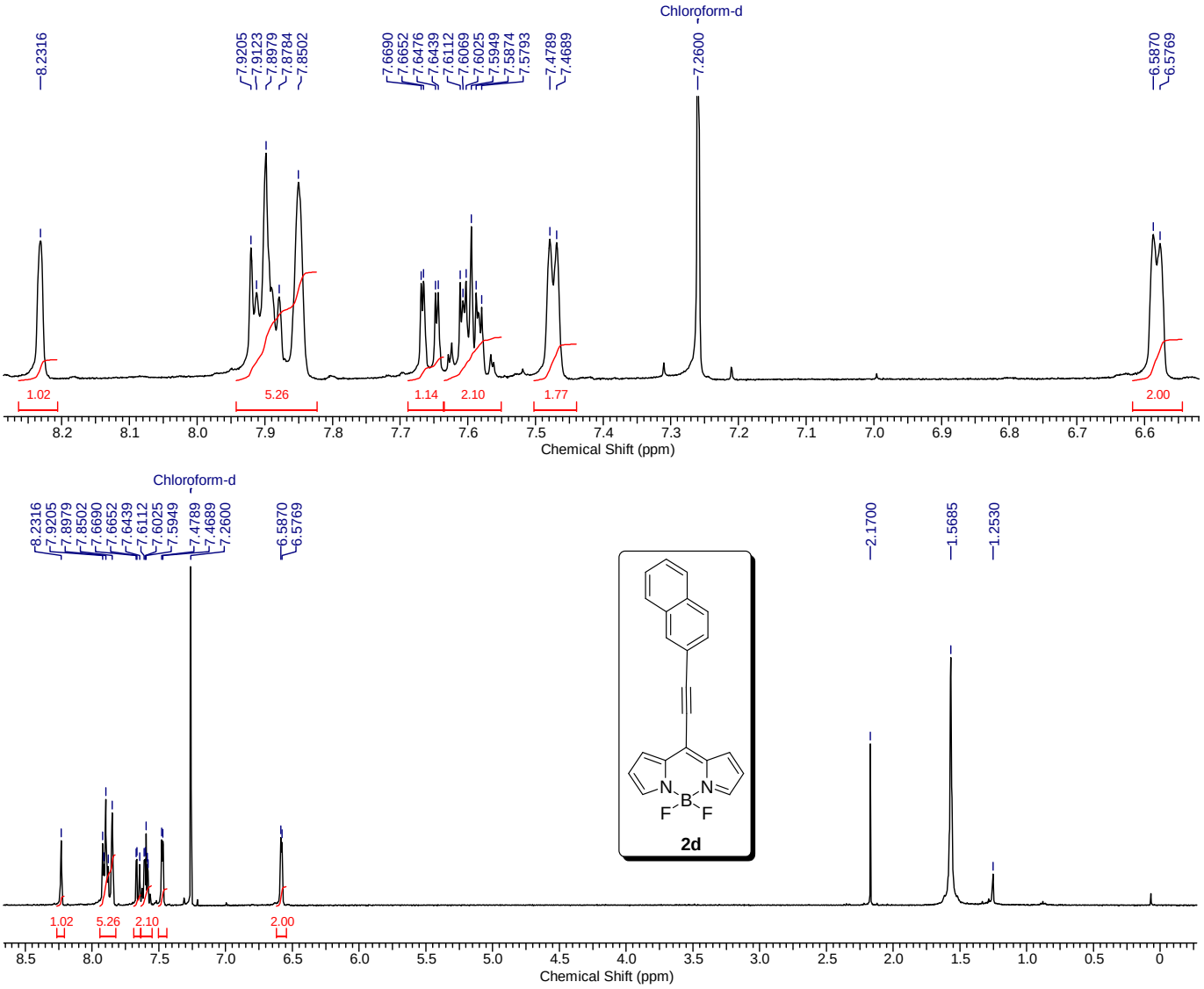

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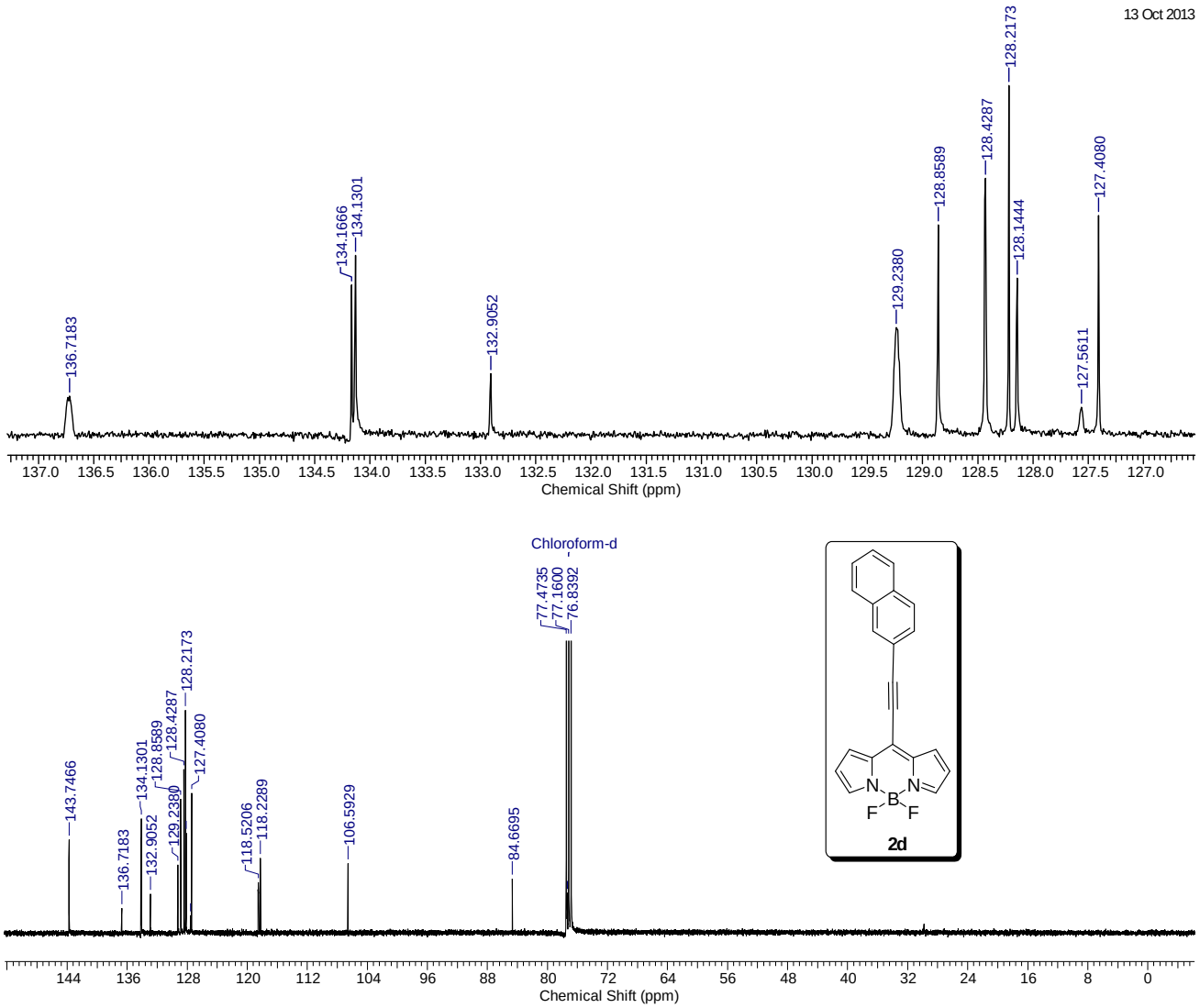

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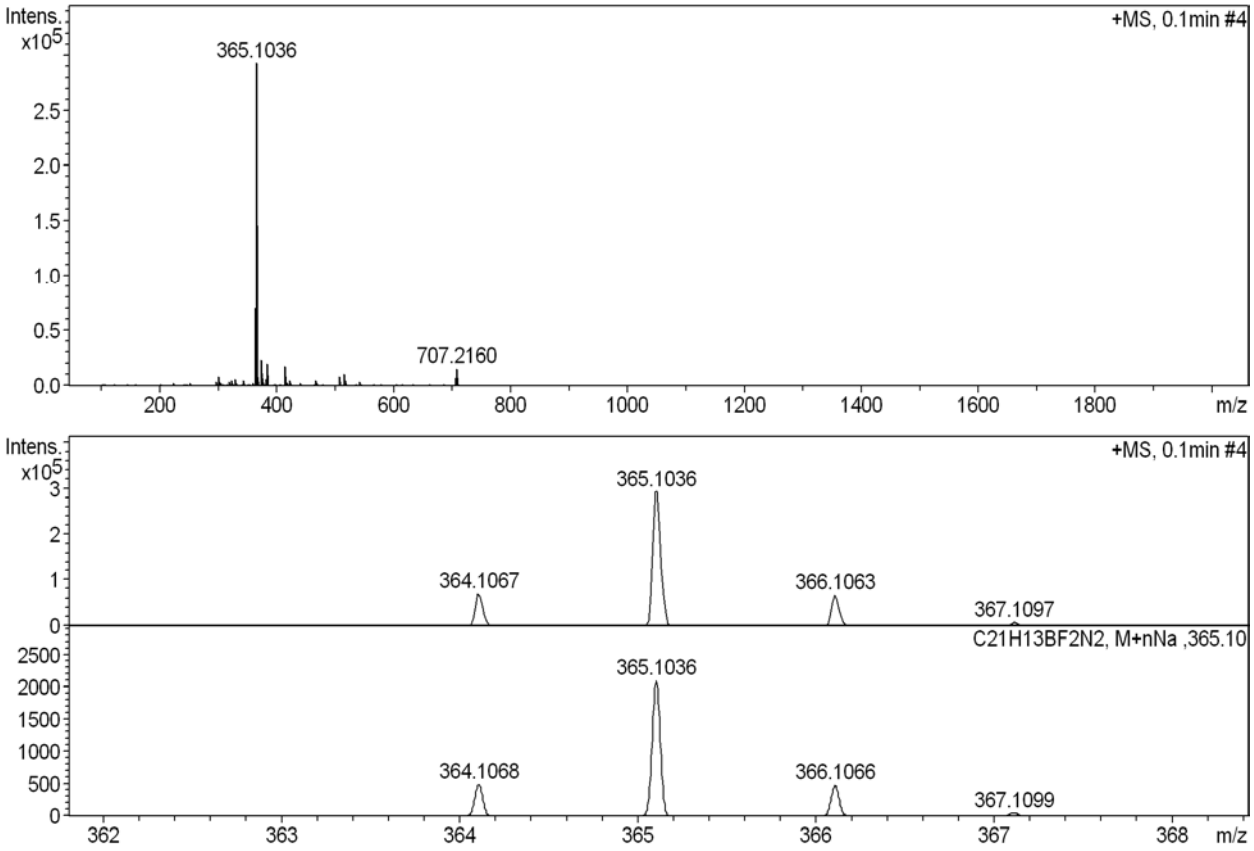

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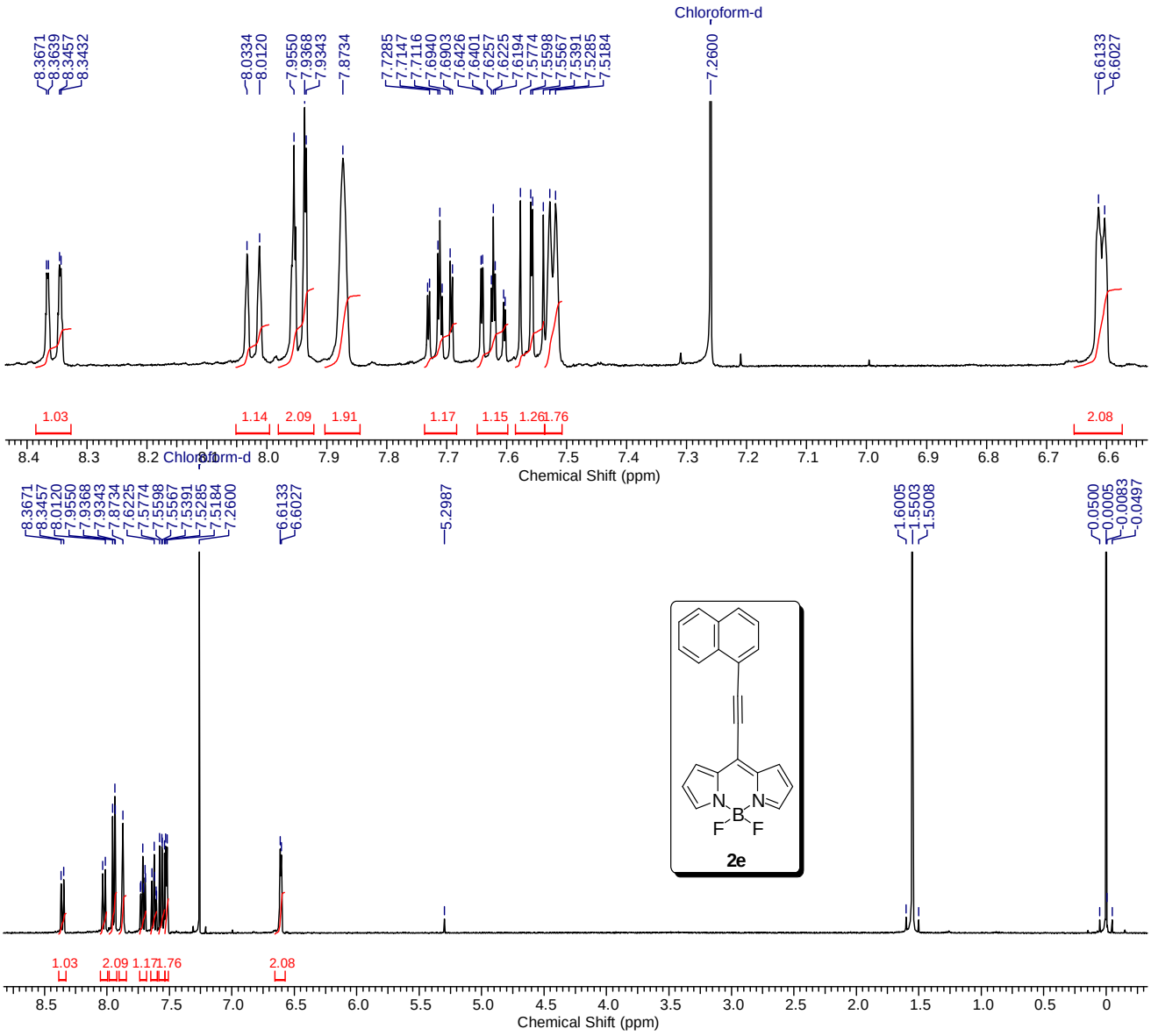

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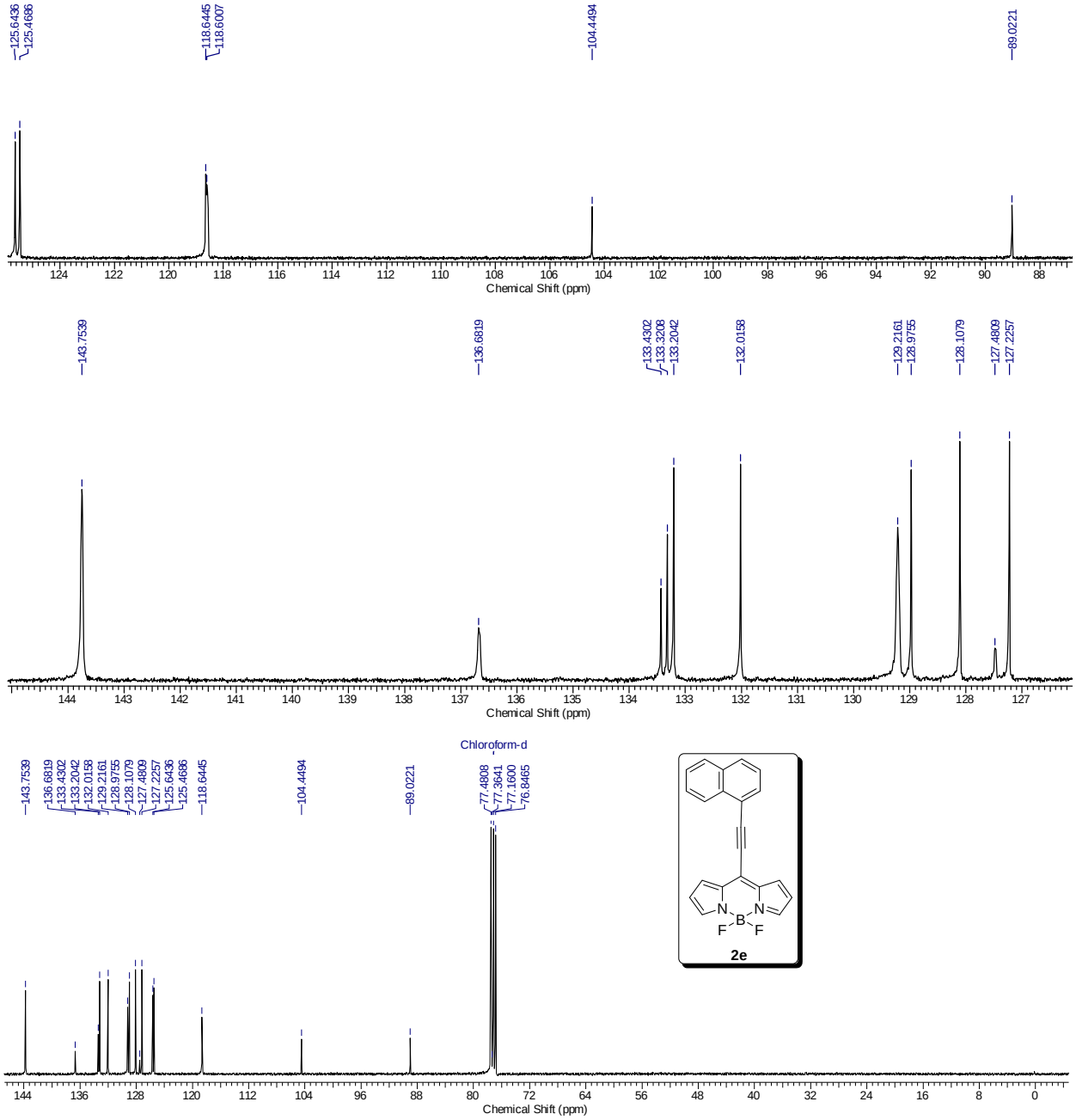

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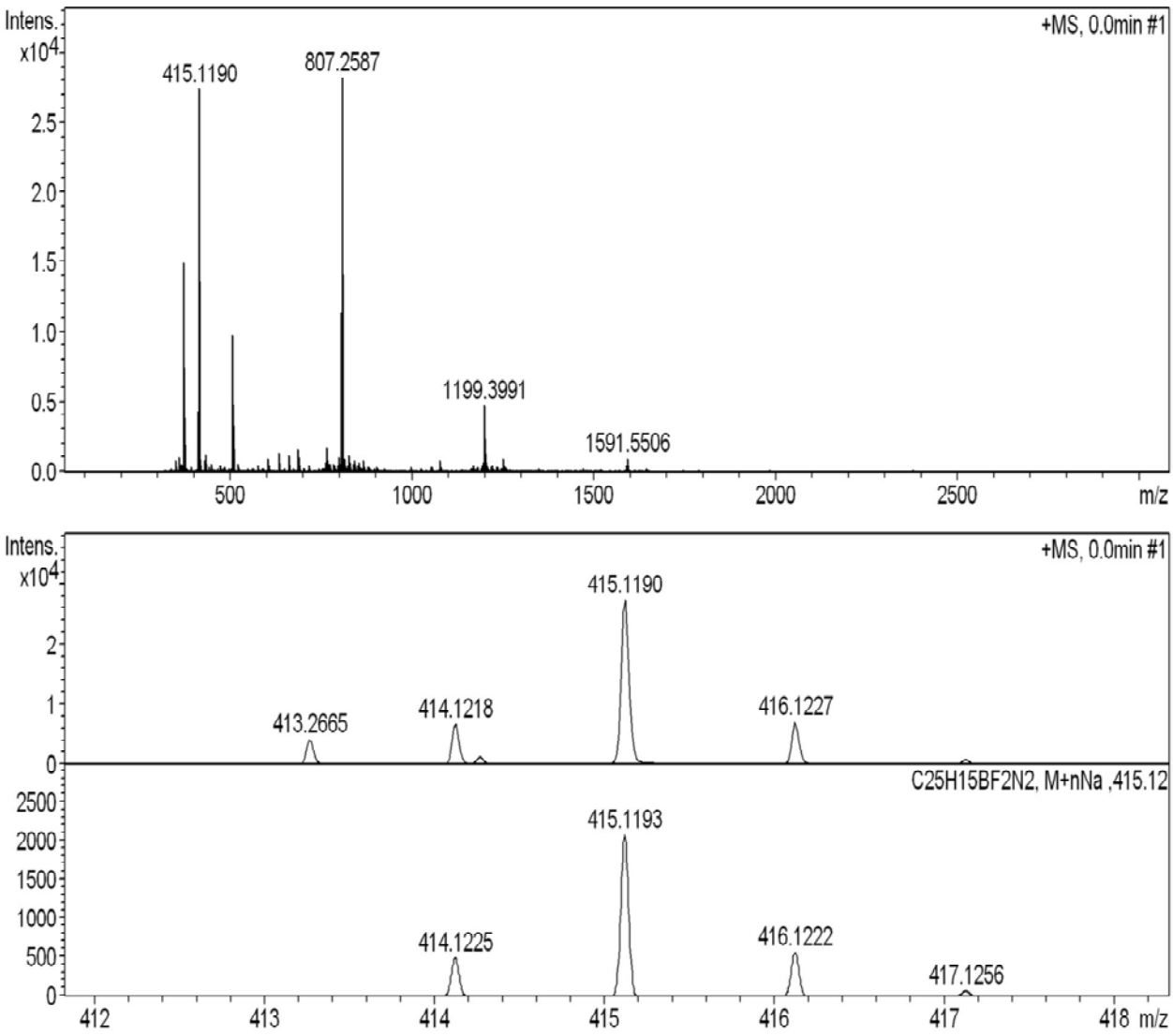
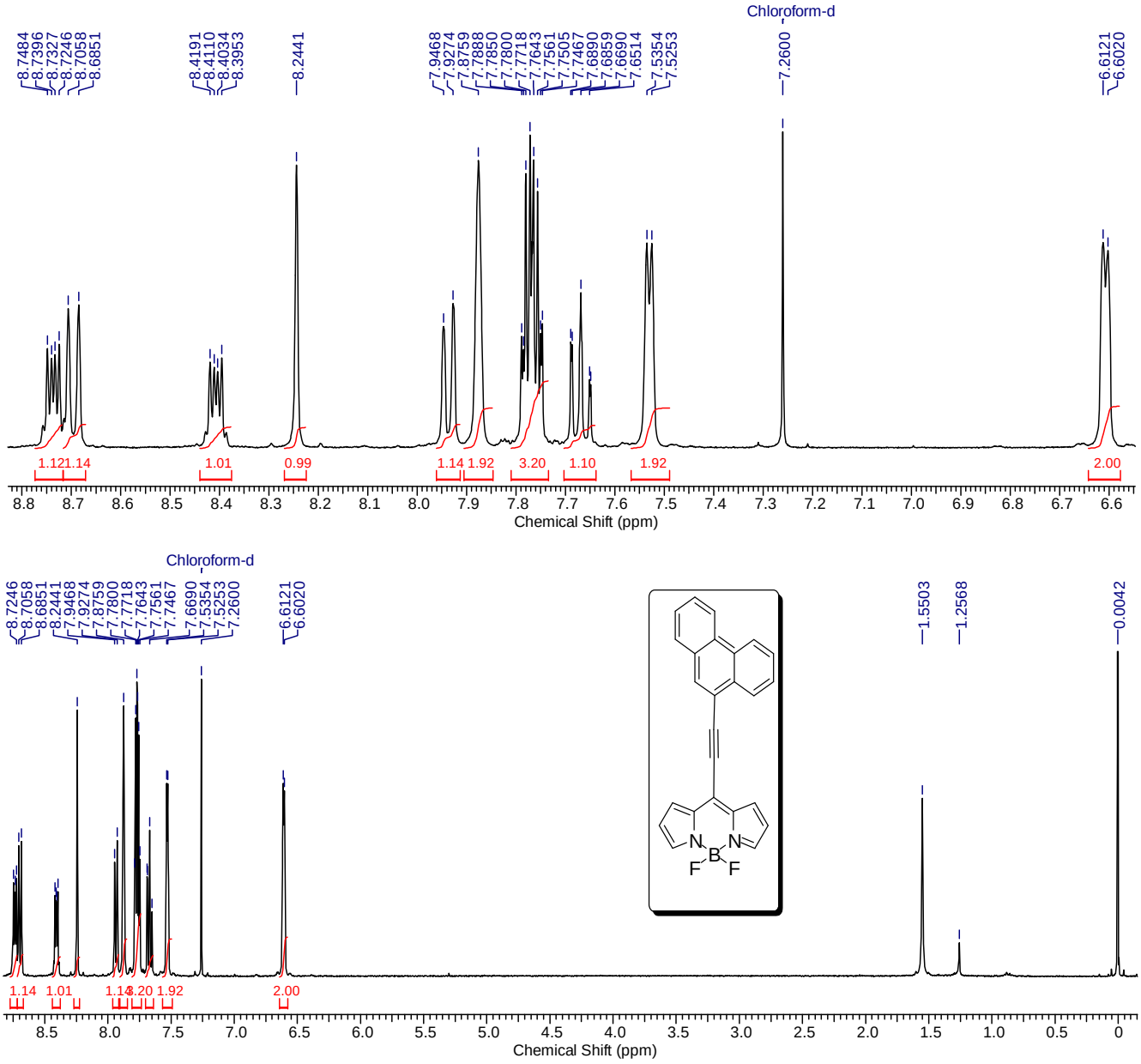


HRMS spectra of **2f**



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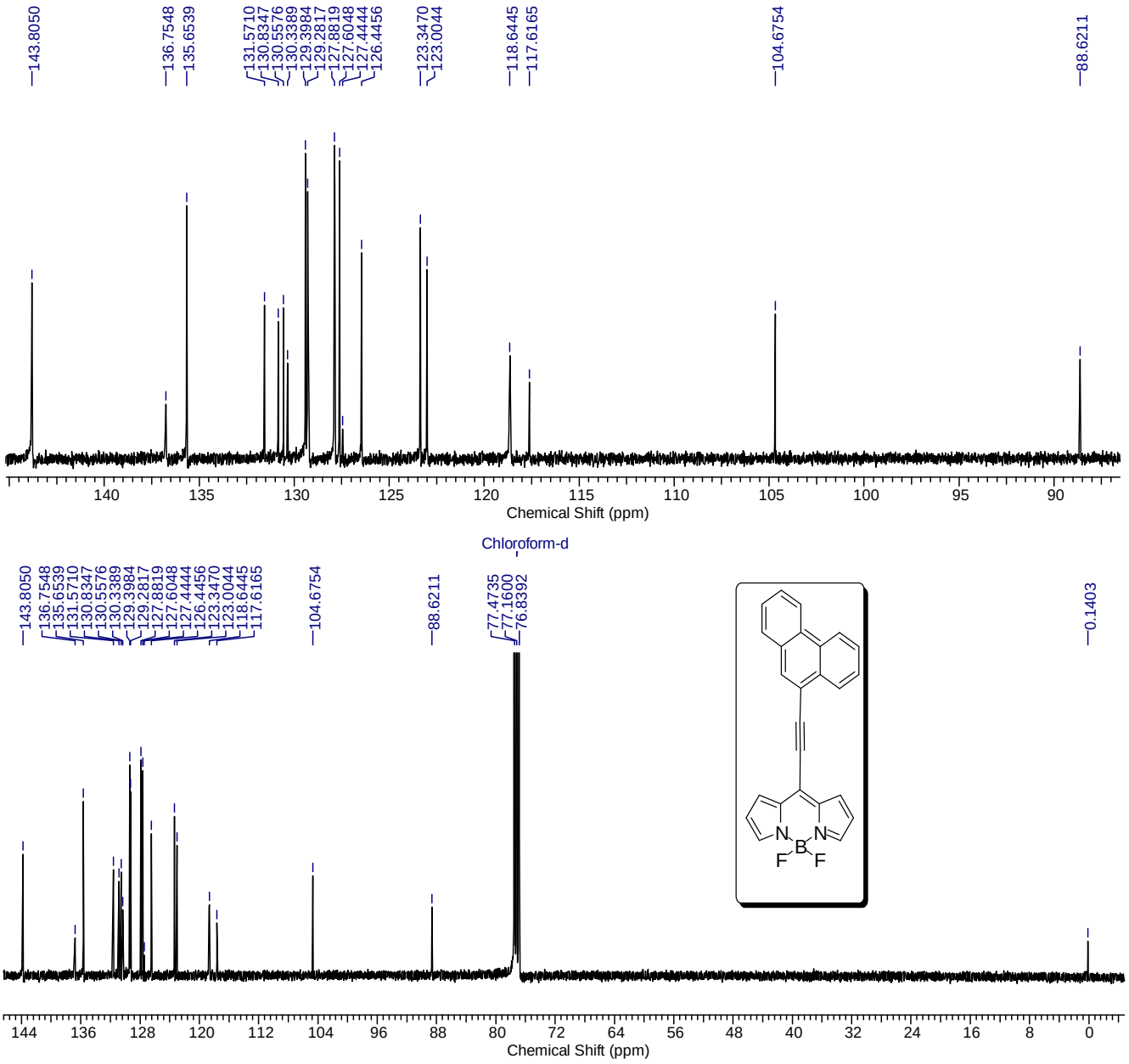

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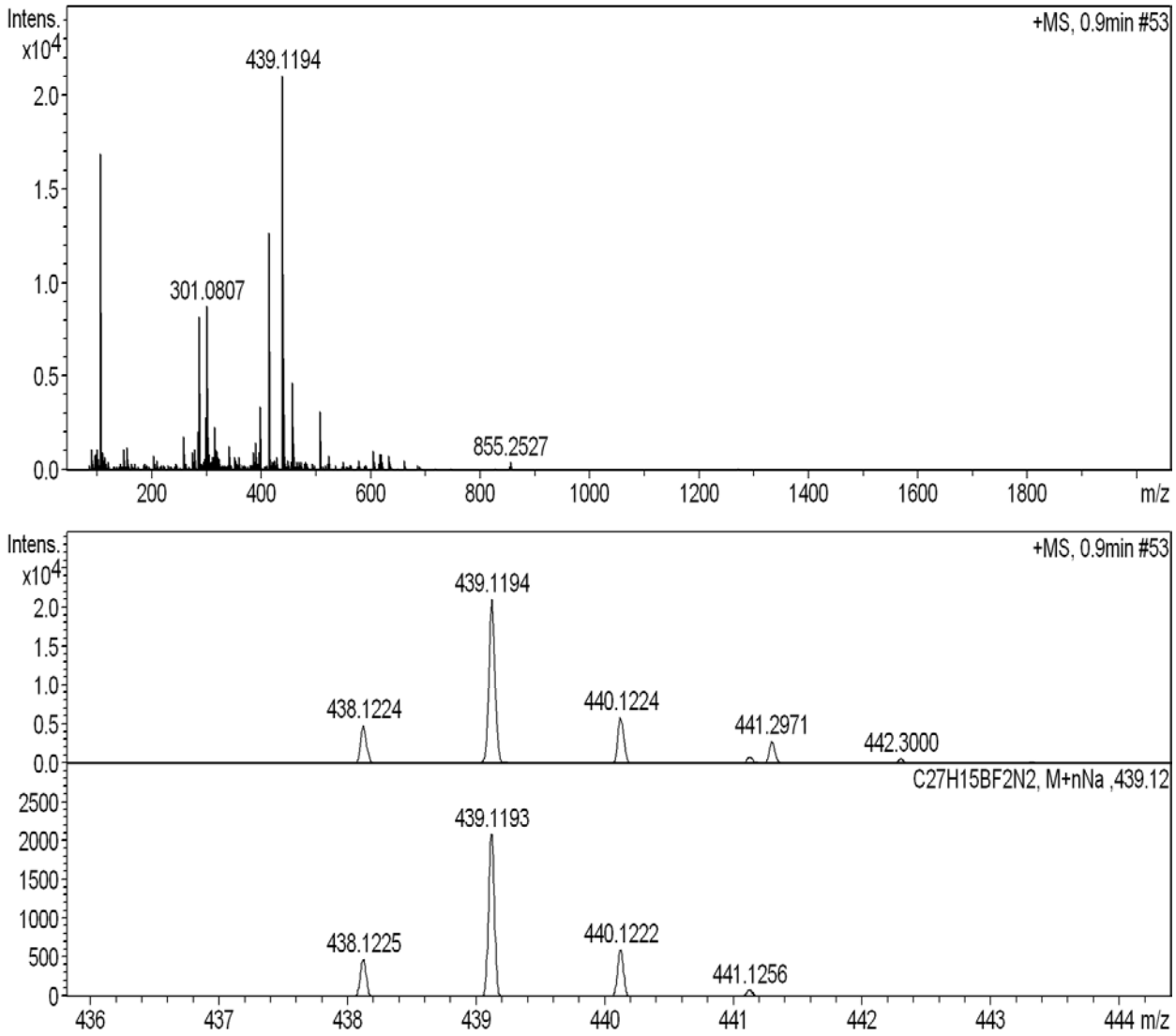
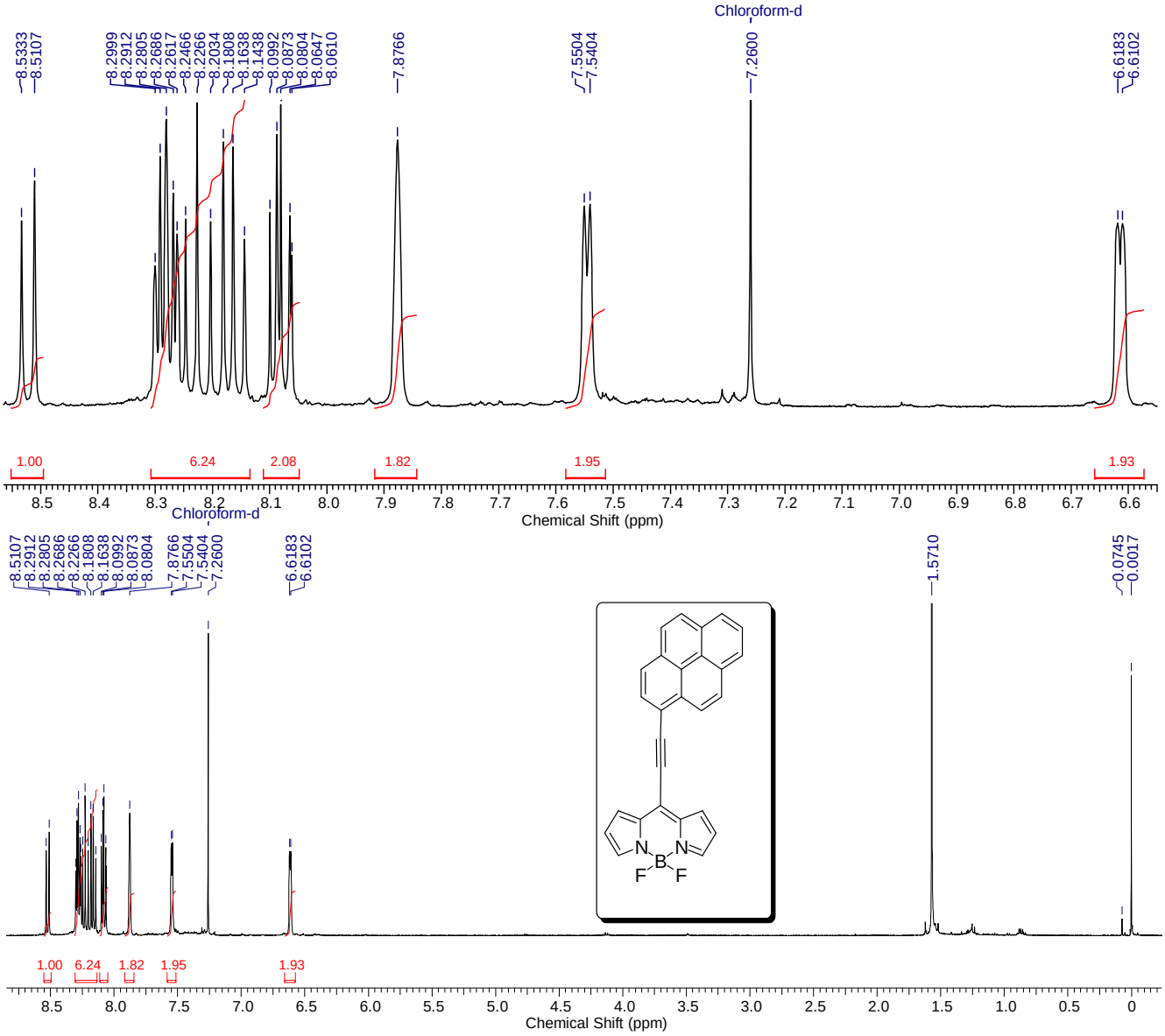


HRMS spectra of **2g**



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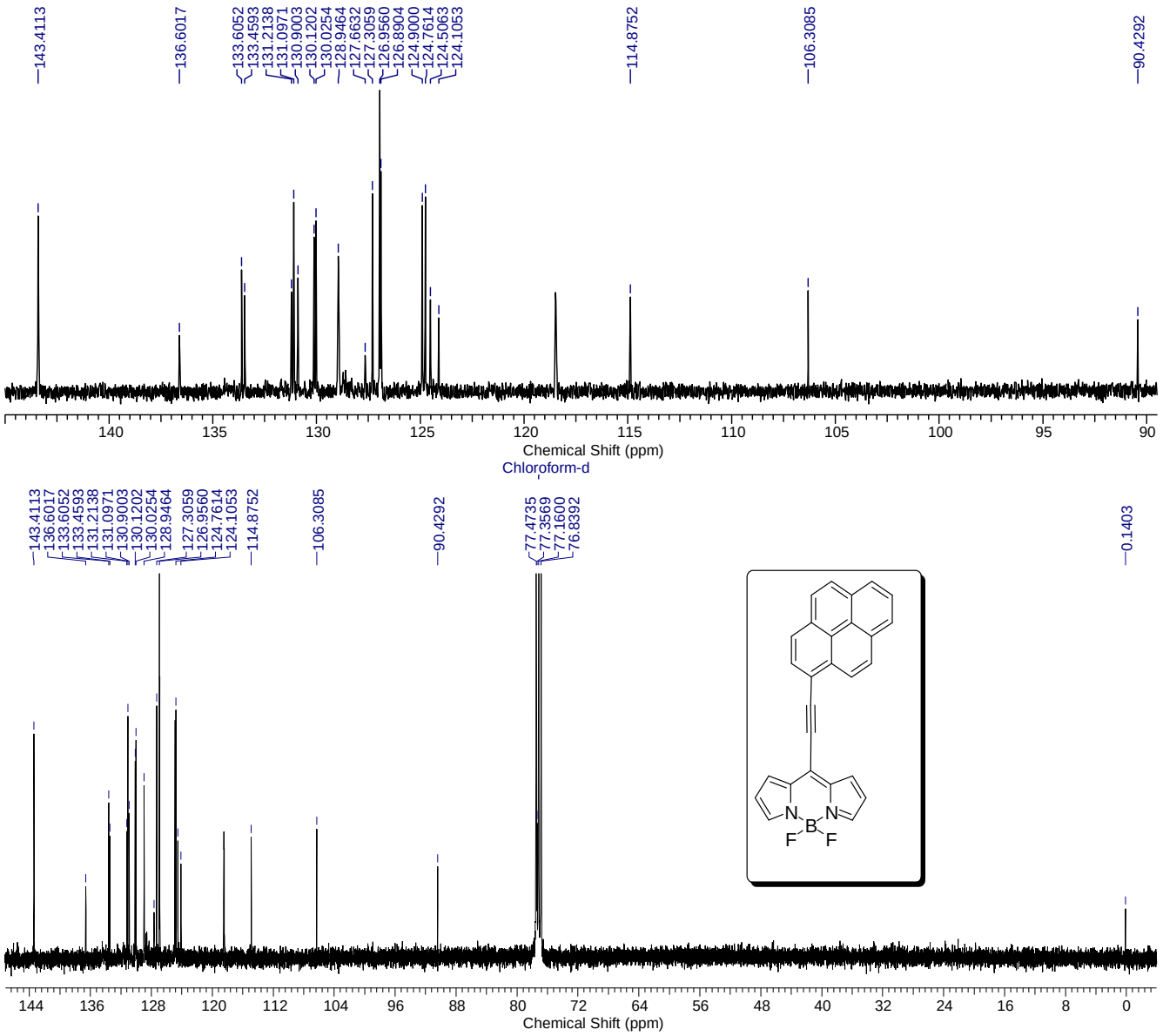
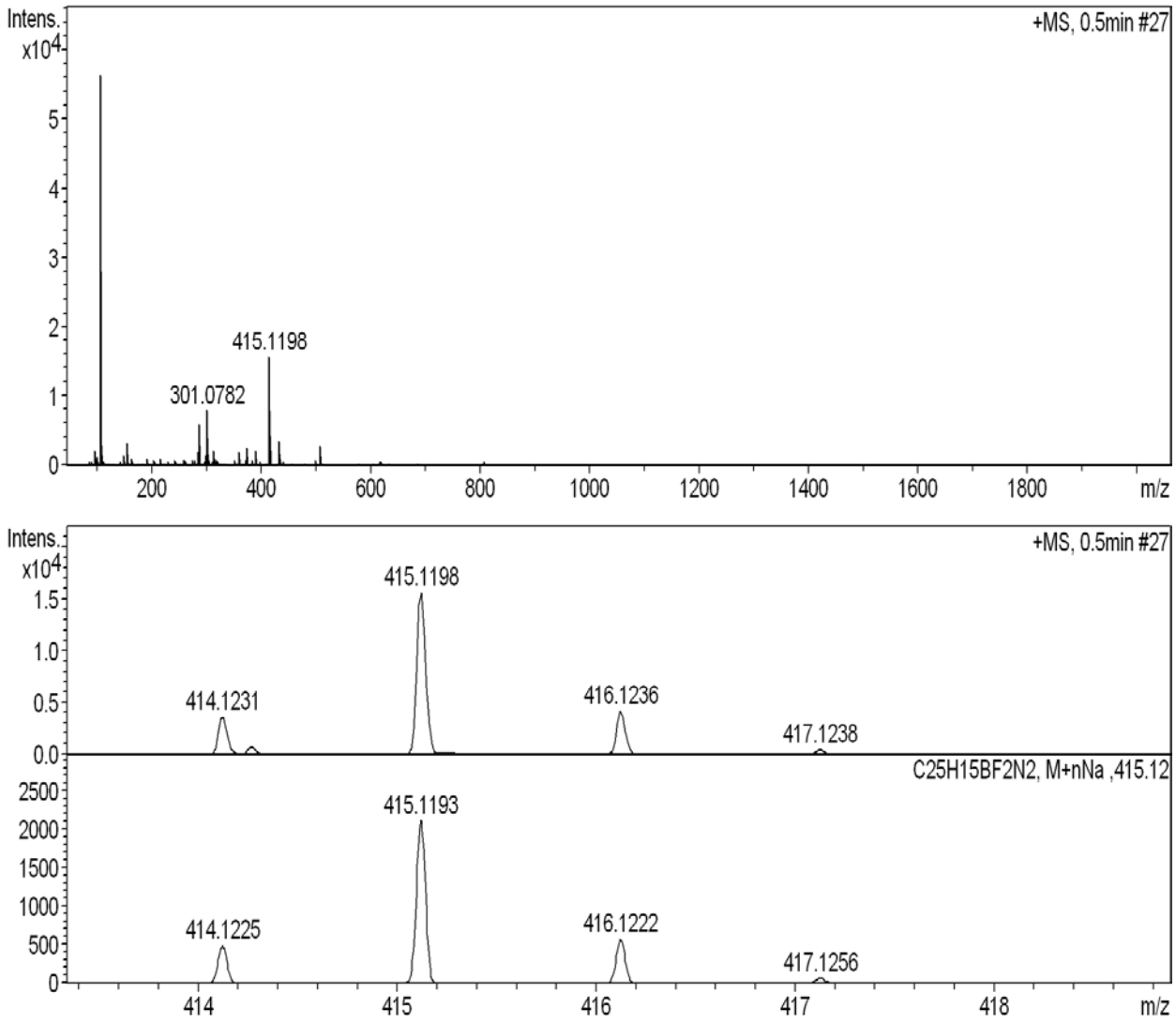
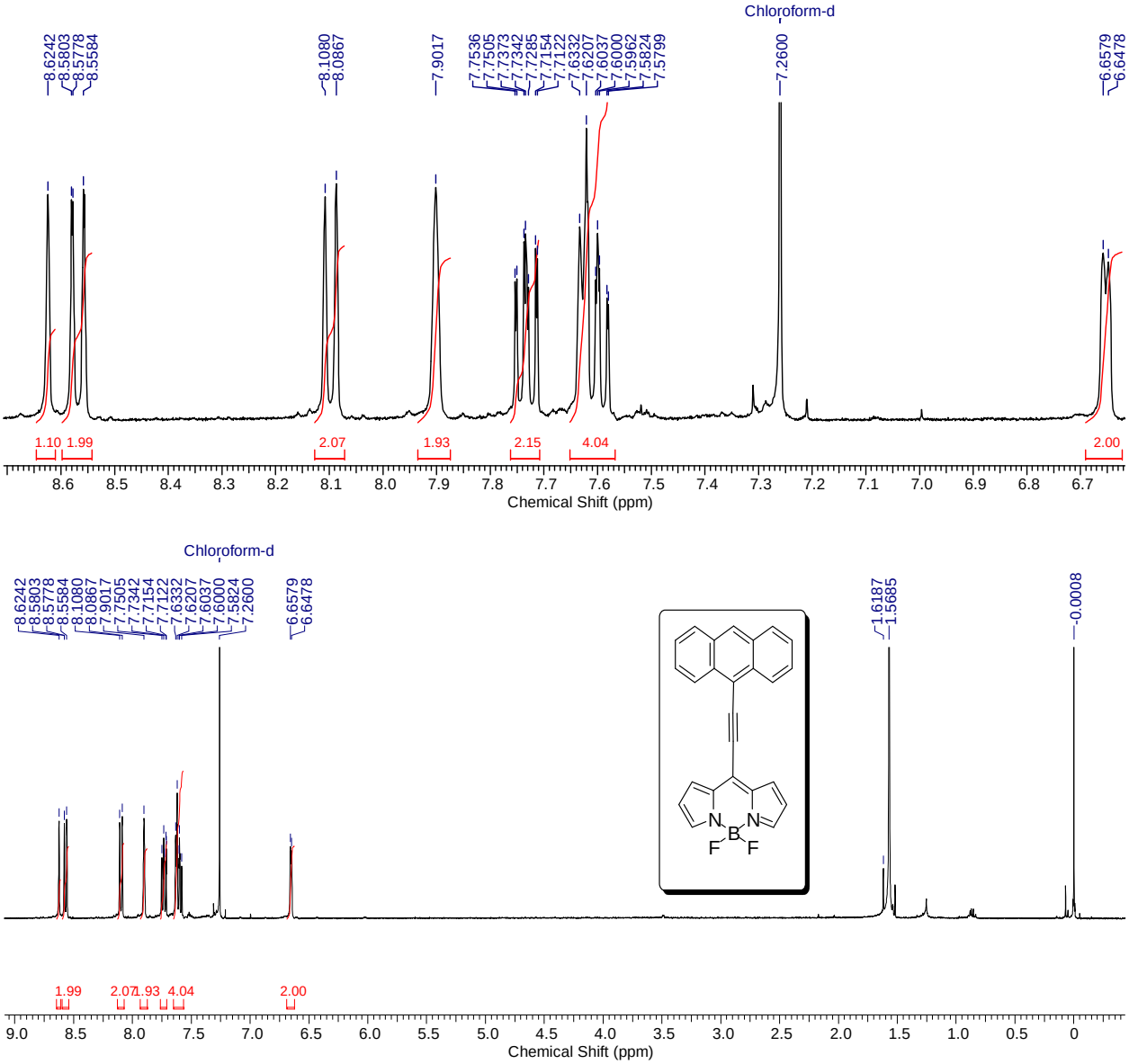


^{13}C NMR spectra of **2g**



HRMS spectra of **2h**



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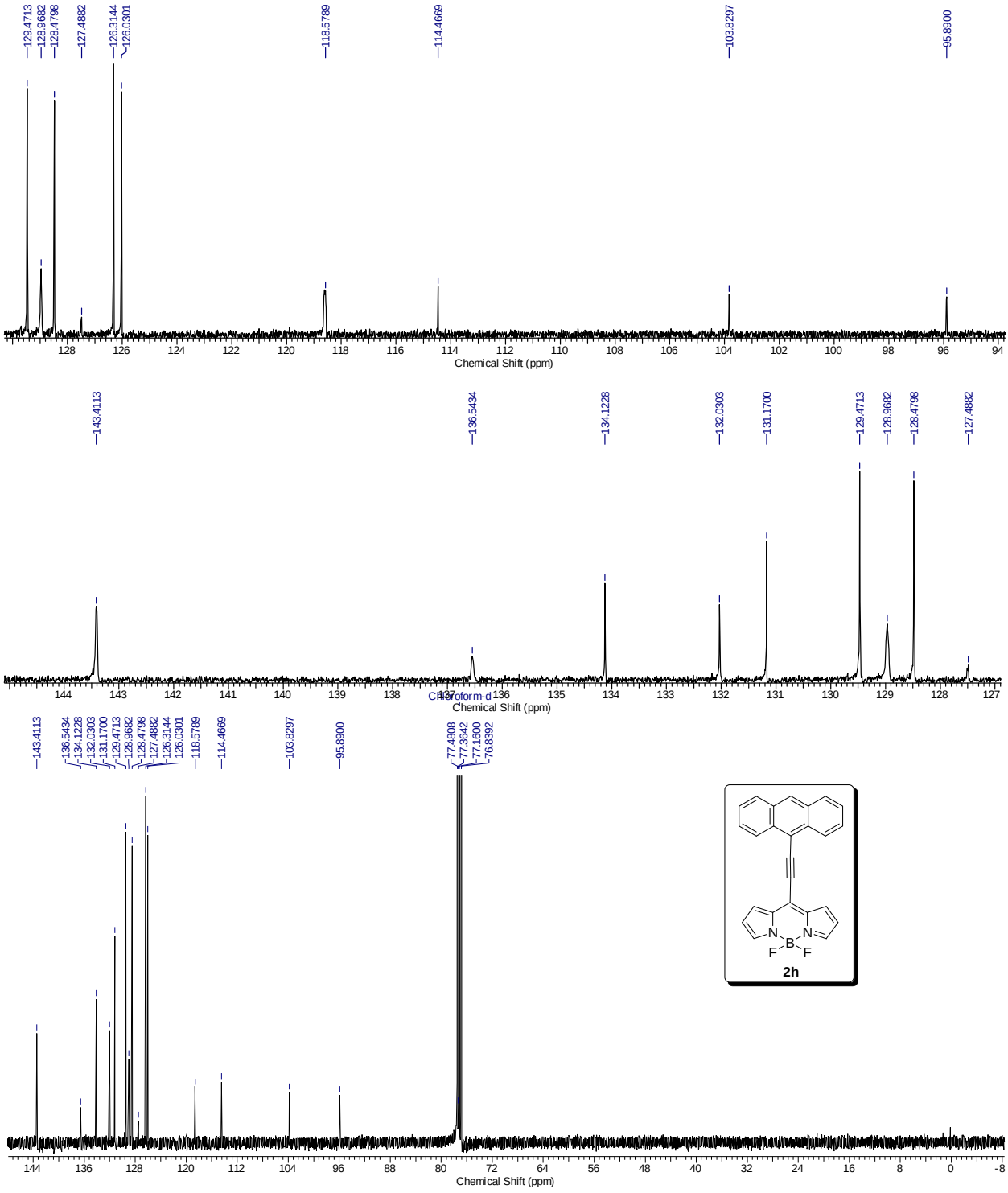
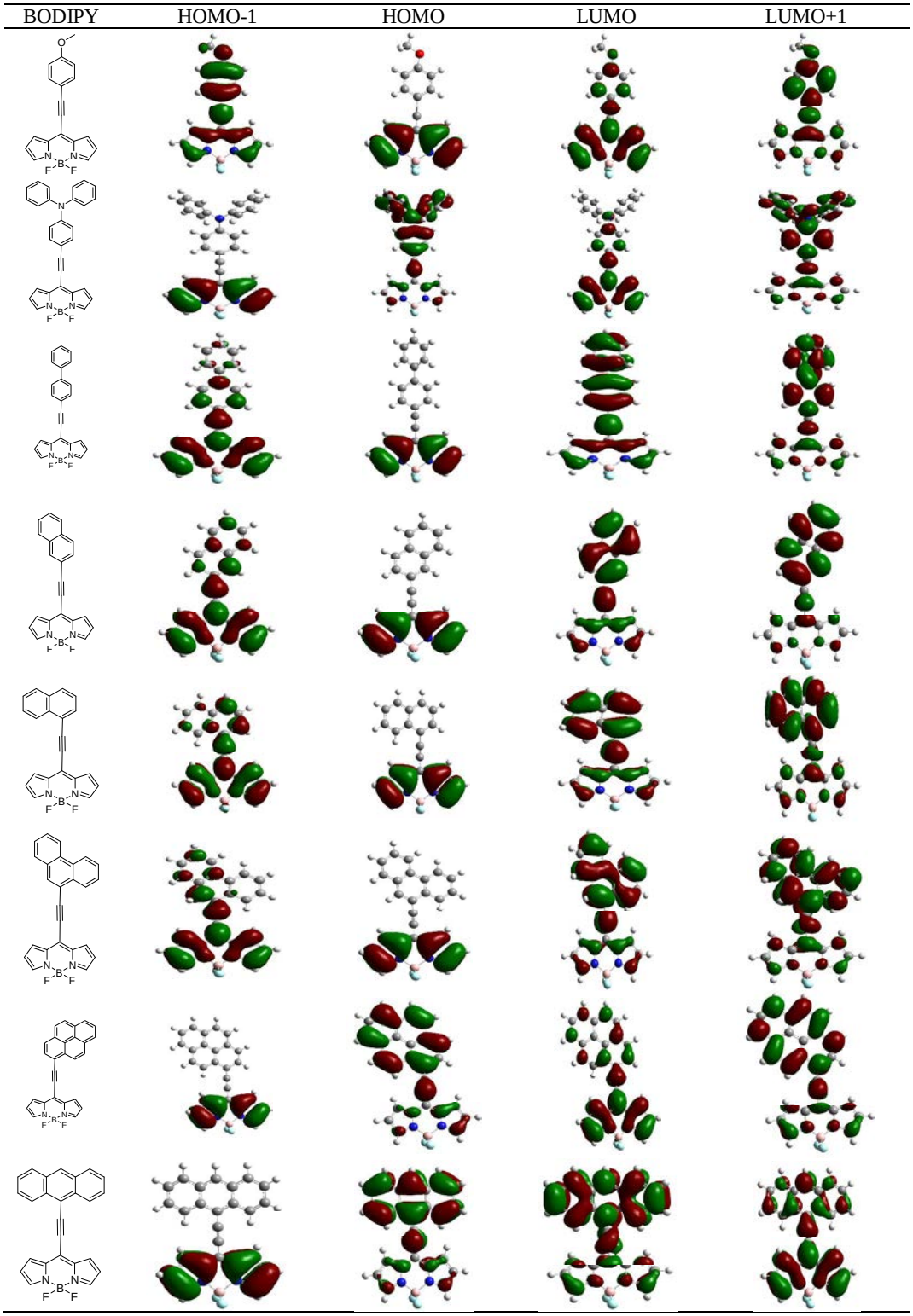


^{13}C NMR spectra of **2h**

DFT calculation data

Calculation method: B3LYP/6-31G(d) with Gaussian 09.[2]



The HOMO-1, HOMO, LUMO. LUMO+1 energy levels of the BODIPY dimmers

DFT Data for meso-arylethynyl BODIPY **2a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.423410	2.546303	-0.084649
2	1	0	0.373736	2.804655	-0.104308
3	6	0	2.516227	3.405004	-0.120820
4	1	0	2.504050	4.485052	-0.171706
5	6	0	3.668252	2.594270	-0.085738
6	1	0	4.710645	2.883147	-0.096311
7	7	0	3.323711	1.296967	-0.031347
8	5	0	4.312519	0.085600	0.101503
9	6	0	2.750879	-3.350862	-0.116326
10	6	0	1.601084	-2.570271	-0.081152
11	1	0	0.571999	-2.901411	-0.100030
12	6	0	2.020657	-1.219076	-0.028890
13	6	0	1.274508	-0.020201	-0.017372
14	6	0	1.935914	1.227758	-0.030535
15	7	0	3.410059	-1.191605	-0.029821
16	9	0	5.243621	0.117453	-0.918490
17	6	0	3.843832	-2.461859	-0.082434
18	1	0	4.903804	-2.677441	-0.092742
19	9	0	4.918299	0.107312	1.344634

20	1	0	2.813741	-4.429209	-0.165670
21	6	0	-0.135853	-0.068359	-0.014120
22	6	0	-1.354545	-0.107030	-0.006997
23	6	0	-2.771236	-0.152929	0.000978
24	6	0	-3.457285	-1.390005	0.006248
25	6	0	-3.531043	1.032224	0.004184
26	6	0	-4.839272	-1.432106	0.014196
27	1	0	-2.886372	-2.313112	0.004257
28	6	0	-4.921580	0.996852	0.012176
29	1	0	-3.019153	1.989455	0.000596
30	6	0	-5.585032	-0.239525	0.017155
31	1	0	-5.374405	-2.376124	0.018367
32	1	0	-5.476542	1.927575	0.014468
33	8	0	-6.932913	-0.391383	0.024920
34	6	0	-7.751444	0.772348	0.028916
35	1	0	-7.584530	1.381629	-0.868131
36	1	0	-8.780524	0.410509	0.035051
37	1	0	-7.574248	1.382714	0.923243

Total Energy= -1103.1147262 HF

DFT data for *meso*-arylethynyl BODIPY **2b**

Standard orientation:

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

1	6	0	-4.118253	-2.376357	-0.950875
2	1	0	-3.078004	-2.645663	-1.070740
3	6	0	-5.240062	-3.136649	-1.263282
4	1	0	-5.264518	-4.134683	-1.678775
5	6	0	-6.363444	-2.350585	-0.939891
6	1	0	-7.415145	-2.585039	-1.034957
7	7	0	-5.974510	-1.160598	-0.451491
8	5	0	-6.921601	-0.035552	0.094921
9	6	0	-5.246198	3.215547	1.049914
10	6	0	-4.122862	2.434624	0.800206
11	1	0	-3.083129	2.719339	0.883294
12	6	0	-4.587436	1.161817	0.391442
13	6	0	-3.880922	0.007703	-0.015967
14	6	0	-4.585321	-1.139991	-0.444755
15	7	0	-5.976672	1.179400	0.399002
16	9	0	-7.850947	0.312917	-0.866571
17	6	0	-6.368003	2.403720	0.791072
18	1	0	-7.420200	2.642147	0.869090
19	9	0	-7.532586	-0.459809	1.261411
20	1	0	-5.272629	4.246696	1.374483
21	6	0	-2.471439	0.008149	-0.014343
22	6	0	-1.251157	0.006686	-0.010149
23	6	0	0.163593	0.004515	-0.005799
24	6	0	0.890896	-1.147836	-0.376616
25	6	0	0.892432	1.154450	0.369382
26	6	0	2.275435	-1.150976	-0.375857

27	1	0	0.351350	-2.039791	-0.679808
28	6	0	2.276976	1.153192	0.376232
29	1	0	0.354088	2.047906	0.670284
30	6	0	2.999660	0.000047	0.001978
31	1	0	2.810999	-2.043979	-0.678089
32	1	0	2.813689	2.044402	0.681717
33	7	0	4.403421	-0.001982	0.005358
34	6	0	5.136019	1.195848	-0.256831
35	6	0	6.206533	1.562027	0.571472
36	6	0	4.807291	2.005004	-1.354639
37	6	0	6.936216	2.718555	0.300998
38	1	0	6.461522	0.936649	1.421294
39	6	0	5.531496	3.168807	-1.607483
40	1	0	3.987338	1.716730	-2.005201
41	6	0	6.600751	3.529928	-0.784873
42	1	0	7.763526	2.991215	0.950604
43	1	0	5.266787	3.786830	-2.461167
44	1	0	7.167835	4.433528	-0.989067
45	6	0	5.131265	-1.202123	0.270352
46	6	0	6.203893	-1.571531	-0.553760
47	6	0	4.795554	-2.010392	1.366688
48	6	0	6.928844	-2.730419	-0.280618
49	1	0	6.464297	-0.946840	-1.402443
50	6	0	5.515079	-3.176522	1.622170
51	1	0	3.973900	-1.719649	2.014010
52	6	0	6.586457	-3.540891	0.803747

53	1	0	7.757867	-3.005585	-0.926976
54	1	0	5.245004	-3.793890	2.474641
55	1	0	7.149785	-4.446356	1.010070

Total Energy = -1506.0416803 HF

DFT data for *meso*-arylethynyl BODIPY **2c**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.699110	-2.549335	-0.248511
2	1	0	-1.659089	-2.842054	-0.288743
3	6	0	-3.820621	-3.365202	-0.336889
4	1	0	-3.846034	-4.439374	-0.457964
5	6	0	-4.944349	-2.518784	-0.245727
6	1	0	-5.996073	-2.770503	-0.272128
7	7	0	-4.555533	-1.240697	-0.108267
8	5	0	-5.501829	-0.006614	0.106262
9	6	0	-3.819996	3.380703	0.101241
10	6	0	-2.698653	2.560070	0.081984
11	1	0	-1.658584	2.855371	0.081383
12	6	0	-3.165734	1.223314	0.048809
13	6	0	-2.463135	0.001111	-0.018031
14	6	0	-3.165924	-1.219565	-0.107331

15	7	0	-4.555344	1.244679	0.051194
16	9	0	-6.436023	0.058199	-0.908739
17	6	0	-4.943888	2.529835	0.081971
18	1	0	-5.995551	2.783074	0.089656
19	9	0	-6.102987	-0.085784	1.348870
20	1	0	-3.845210	4.461487	0.121576
21	6	0	-1.050207	0.001009	-0.017200
22	6	0	0.168387	0.000699	-0.012385
23	6	0	1.587791	0.000304	-0.006867
24	6	0	2.309054	1.211840	0.014933
25	6	0	2.308494	-1.211660	-0.022752
26	6	0	3.696903	1.205410	0.020180
27	1	0	1.767121	2.152146	0.037353
28	6	0	3.696343	-1.206027	-0.016753
29	1	0	1.766197	-2.151663	-0.048877
30	6	0	4.422475	-0.000521	0.004643
31	1	0	4.231582	2.149466	0.064584
32	1	0	4.230807	-2.150409	-0.056539
33	6	0	5.905180	-0.000938	0.010894
34	6	0	6.629831	0.973535	-0.697137
35	6	0	6.623199	-0.975780	0.725156
36	6	0	8.023444	0.972325	-0.692015
37	1	0	6.096434	1.719415	-1.279630
38	6	0	8.016800	-0.975238	0.732121
39	1	0	6.084419	-1.721342	1.303077
40	6	0	8.722948	-0.001626	0.023104

41	1	0	8.563740	1.729022	-1.254463
42	1	0	8.551827	-1.732152	1.299289
43	1	0	9.809417	-0.001868	0.027836

Total Energy= -1219.6478668 HF

DFT data for *meso*-arylethynyl BODIPY **2d**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.121916	-2.597946	-0.070808
2	1	0	-1.114658	-2.990482	-0.087768
3	6	0	-3.316376	-3.307509	-0.099042
4	1	0	-3.444654	-4.380343	-0.140477
5	6	0	-4.353985	-2.353524	-0.069308
6	1	0	-5.424987	-2.505457	-0.076169
7	7	0	-3.844708	-1.111611	-0.025749
8	5	0	-4.669868	0.219273	0.088762

9	6	0	-2.669109	3.423010	-0.104128
10	6	0	-1.631858	2.498690	-0.074556
11	1	0	-0.568224	2.691694	-0.092083
12	6	0	-2.225311	1.213453	-0.028205
13	6	0	-1.643000	-0.072080	-0.017509
14	6	0	-2.459384	-1.223036	-0.026381
15	7	0	-3.606380	1.368270	-0.027624
16	9	0	-5.578109	0.305976	-0.948045
17	6	0	-3.869530	2.684462	-0.073294
18	1	0	-4.891915	3.037801	-0.080705
19	9	0	-5.294728	0.280060	1.320528
20	1	0	-2.590485	4.500557	-0.147249
21	6	0	-0.236316	-0.206555	-0.015463
22	6	0	0.977354	-0.314805	-0.009397
23	6	0	2.390697	-0.453565	-0.001825
24	6	0	3.211833	0.669281	-0.002123
25	6	0	2.983436	-1.755729	0.006904
26	6	0	4.621059	0.546401	0.006080

27	1	0	2.765513	1.659596	-0.008411
28	6	0	4.347250	-1.897188	0.015006
29	1	0	2.335191	-2.626071	0.007424
30	6	0	5.475628	1.683309	0.006058
31	6	0	5.206454	-0.762973	0.014904
32	1	0	4.791402	-2.889412	0.021822
33	6	0	6.843390	1.533554	0.014427
34	1	0	5.028476	2.674255	-0.000555
35	6	0	6.619944	-0.881601	0.023376
36	6	0	7.420616	0.239606	0.023171
37	1	0	7.487225	2.408533	0.014421
38	1	0	7.062336	-1.874718	0.030126
39	1	0	8.502001	0.135221	0.029762

Total Energy = -1142.2341676HF

DFT data for *meso*-arylethynyl BODIPY **2e**

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.058509	2.696533	-0.074515
2	1	0	1.096740	3.188910	-0.090135
3	6	0	3.319303	3.280556	-0.113173
4	1	0	3.555662	4.333886	-0.162398
5	6	0	4.254795	2.226123	-0.083921
6	1	0	5.335205	2.268755	-0.097670
7	7	0	3.621089	1.042721	-0.030716
8	5	0	4.303930	-0.363521	0.107868
9	6	0	1.996310	-3.347885	-0.149356
10	6	0	1.056266	-2.324980	-0.102814
11	1	0	-0.020789	-2.410369	-0.121710
12	6	0	1.775547	-1.106407	-0.039181
13	6	0	1.325122	0.231754	-0.017144
14	6	0	2.254748	1.294630	-0.024820
15	7	0	3.133904	-1.398322	-0.044832
16	9	0	5.233227	-0.543240	-0.898426

17	6	0	3.264831	-2.733746	-0.110831
18	1	0	4.246127	-3.187733	-0.126424
19	9	0	4.876839	-0.485026	1.361120
20	1	0	1.810270	-4.410697	-0.209499
21	6	0	-0.059705	0.507855	-0.011444
22	6	0	-1.255465	0.745369	-0.004689
23	6	0	-2.765932	1.045394	0.003844
24	6	0	-3.677305	-0.046174	0.011484
25	6	0	-3.227473	2.338432	0.003377
26	6	0	-3.227505	-1.395172	0.012157
27	6	0	-5.071685	0.216198	0.018724
28	6	0	-4.619143	2.600909	0.010692
29	1	0	-2.525302	3.185074	-0.002501
30	6	0	-4.129029	-2.430443	0.019353
31	1	0	-2.144466	-1.589404	0.006571
32	6	0	-5.982982	-0.875025	0.026254
33	6	0	-5.520653	1.565549	0.018160
34	1	0	-4.964591	3.645218	0.009977

35	6	0	-5.520536	-2.168163	0.026442
36	1	0	-3.783596	-3.474792	0.019809
37	1	0	-7.062141	-0.660905	0.031627
38	1	0	-6.603639	1.760176	0.023777
39	1	0	-6.222787	-3.014748	0.032240

Total Energy = -1142.2335905 HF

DFT data for *meso*-arylethynyl BODIPY **2f**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.348991	-2.685926	0.321721
2	1	0	-1.307306	-2.973245	0.357634
3	6	0	-3.465696	-3.507336	0.418492
4	1	0	-3.484797	-4.580580	0.548599
5	6	0	-4.594391	-2.669836	0.307102
6	1	0	-5.644713	-2.926831	0.337913

7	7	0	-4.212905	-1.392463	0.145869
8	5	0	-5.163370	-0.144276	0.094492
9	6	0	-3.508365	3.144483	-0.768879
10	6	0	-2.380843	2.353548	-0.582407
11	1	0	-1.343849	2.645097	-0.676481
12	6	0	-2.837812	1.048962	-0.272694
13	6	0	-2.127763	-0.149483	-0.043447
14	6	0	-2.823439	-1.362563	0.148116
15	7	0	-4.227507	1.060765	-0.273982
16	9	0	-6.123550	-0.316170	-0.882864
17	6	0	-4.625847	2.308798	-0.569211
18	1	0	-5.679447	2.547324	-0.625340
19	9	0	-5.731145	0.063893	1.337972
20	1	0	-3.541318	4.193919	-1.027203
21	6	0	-0.714705	-0.141744	-0.027783
22	6	0	0.504071	-0.146533	-0.005628
23	6	0	1.923610	-0.171857	0.005577
24	6	0	2.574229	-1.372448	-0.163019

25	6	0	2.690003	1.052841	0.178791
26	6	0	3.996109	-1.463735	-0.192359
27	1	0	1.992327	-2.280892	-0.289228
28	6	0	4.114562	0.995675	0.152252
29	6	0	2.045057	2.292346	0.381524
30	6	0	4.627628	-2.718049	-0.376384
31	6	0	4.785470	-0.284562	-0.040437
32	6	0	4.827562	2.205882	0.321222
33	1	0	0.960558	2.314714	0.417917
34	6	0	2.771511	3.455784	0.545198
35	6	0	6.002812	-2.820425	-0.411964
36	1	0	4.005474	-3.602317	-0.490331
37	6	0	6.191139	-0.424917	-0.082672
38	6	0	4.175909	3.410121	0.511620
39	1	0	5.911593	2.199410	0.305710
40	1	0	2.258827	4.400568	0.701812
41	6	0	6.787211	-1.660695	-0.263726
42	1	0	6.478513	-3.786512	-0.553758

43	1	0	6.827713	0.445757	0.027430
44	1	0	4.753381	4.321443	0.639178
45	1	0	7.870849	-1.734079	-0.291517

Total Energy = -1295.8790759 HF

DFT data for *meso*-arylethynyl BODIPY **2g**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.347029	-2.349957	-0.356413
2	1	0	-1.270948	-2.404794	-0.445485
3	6	0	-3.261808	-3.393274	-0.442051
4	1	0	-3.051709	-4.442159	-0.599796
5	6	0	-4.541109	-2.821495	-0.294475
6	1	0	-5.511385	-3.299555	-0.302232
7	7	0	-4.440566	-1.492594	-0.126204
8	5	0	-5.629928	-0.506943	0.150286

9	6	0	-4.757986	3.171344	0.135598
10	6	0	-3.481114	2.624247	0.086919
11	1	0	-2.534730	3.146723	0.070314
12	6	0	-3.635690	1.217216	0.045308
13	6	0	-2.676505	0.184923	-0.054093
14	6	0	-3.091434	-1.161751	-0.158903
15	7	0	-4.993967	0.925296	0.073447
16	9	0	-6.600680	-0.650269	-0.821705
17	6	0	-5.661538	2.089686	0.127276
18	1	0	-6.742754	2.098931	0.159325
19	9	0	-6.139552	-0.727310	1.416941
20	1	0	-5.025040	4.218626	0.168134
21	6	0	-1.302494	0.506415	-0.069487
22	6	0	-0.117300	0.797200	-0.070116
23	6	0	1.249214	1.168251	-0.077977
24	6	0	2.283115	0.190577	0.001294
25	6	0	1.587831	2.535656	-0.170905
26	6	0	3.643469	0.621835	-0.024603

27	6	0	2.009020	-1.211673	0.112330
28	6	0	2.908842	2.946882	-0.194314
29	1	0	0.787893	3.266908	-0.228556
30	6	0	4.697133	-0.338510	0.049672
31	6	0	3.958808	2.012132	-0.124380
32	6	0	3.016314	-2.127174	0.183638
33	1	0	0.972944	-1.532041	0.147201
34	1	0	3.145229	4.004990	-0.269016
35	6	0	4.393848	-1.729025	0.152762
36	6	0	6.059835	0.088332	0.022302
37	6	0	5.335608	2.411541	-0.149101
38	1	0	2.785819	-3.186234	0.268570
39	6	0	5.446859	-2.656398	0.223759
40	6	0	7.079012	-0.875200	0.095632
41	6	0	6.339856	1.492629	-0.079490
42	1	0	5.563677	3.471592	-0.225594
43	6	0	6.773495	-2.231623	0.194824
44	1	0	5.214525	-3.715448	0.302722

45	1	0	8.116281	-0.550366	0.074296
46	1	0	7.378762	1.812482	-0.099735
47	1	0	7.575403	-2.962352	0.250574

Total Energy = -1372.1153225 HF

DFT data for *meso*-arylethynyl BODIPY **2h**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.004628	-2.420783	-0.810645
2	1	0	-0.964612	-2.689306	-0.935439
3	6	0	-3.124070	-3.202512	-1.071836
4	1	0	-3.146101	-4.221693	-1.432334
5	6	0	-4.249908	-2.403614	-0.788480
6	1	0	-5.300932	-2.646541	-0.868599
7	7	0	-3.864384	-1.186586	-0.370467
8	5	0	-4.815163	-0.027555	0.093638

9	6	0	-3.148561	3.282050	0.840548
10	6	0	-2.023216	2.488649	0.649735
11	1	0	-0.985216	2.777211	0.742055
12	6	0	-2.483825	1.193455	0.308595
13	6	0	-1.775712	0.016100	-0.018366
14	6	0	-2.475236	-1.159420	-0.370462
15	7	0	-3.873270	1.210753	0.303000
16	9	0	-5.747910	0.243189	-0.888322
17	6	0	-4.268110	2.455191	0.619042
18	1	0	-5.321012	2.696312	0.676863
19	9	0	-5.418873	-0.363756	1.291413
20	1	0	-3.178410	4.329692	1.106484
21	6	0	-0.363957	0.017880	-0.013865
22	6	0	0.856473	0.013063	-0.006700
23	6	0	2.271904	0.002711	0.002090
24	6	0	2.966020	-1.223881	0.213777
25	6	0	2.988659	1.217585	-0.200659
26	6	0	2.291525	-2.459568	0.436491

27	6	0	4.406856	-1.223001	0.216986
28	6	0	4.429191	1.193275	-0.185096
29	6	0	2.337456	2.463952	-0.432399
30	6	0	2.994022	-3.621951	0.634716
31	1	0	1.206715	-2.464768	0.457567
32	6	0	5.101325	-2.454443	0.426708
33	6	0	5.095612	-0.020373	0.020436
34	6	0	5.146224	2.413247	-0.385782
35	1	0	1.253229	2.486226	-0.467528
36	6	0	3.061097	3.614748	-0.621718
37	6	0	4.416758	-3.623553	0.627892
38	1	0	2.459612	-4.552805	0.802891
39	1	0	6.188388	-2.440382	0.425179
40	1	0	6.183603	-0.029228	0.027623
41	6	0	4.483469	3.593262	-0.596105
42	1	0	6.232799	2.381604	-0.369941
43	1	0	2.544151	4.554149	-0.796866
44	1	0	4.954122	-4.554033	0.786968

45	1	0	5.037905	4.514869	-0.748073

Total Energy = -1295.8719177 HF

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