

Supporting Information

T-shaped donor-acceptor-donor type tetraphenylethylene substituted quinoxaline derivatives: Aggregation induced emission and mechanochromism

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Thermogravimetric analysis.

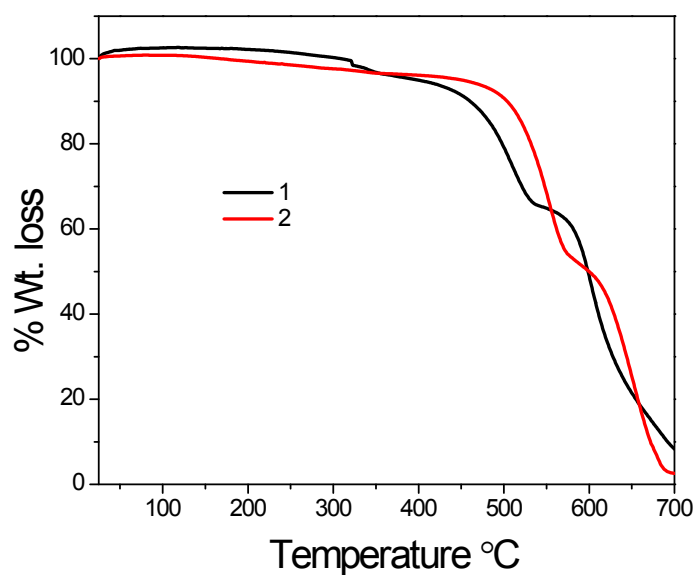


Fig. S1 Thermogravimetric analysis of luminophores **1** and **2** measured at a heating rate of 10 °C/min under nitrogen atmosphere.

Photophysical properties.

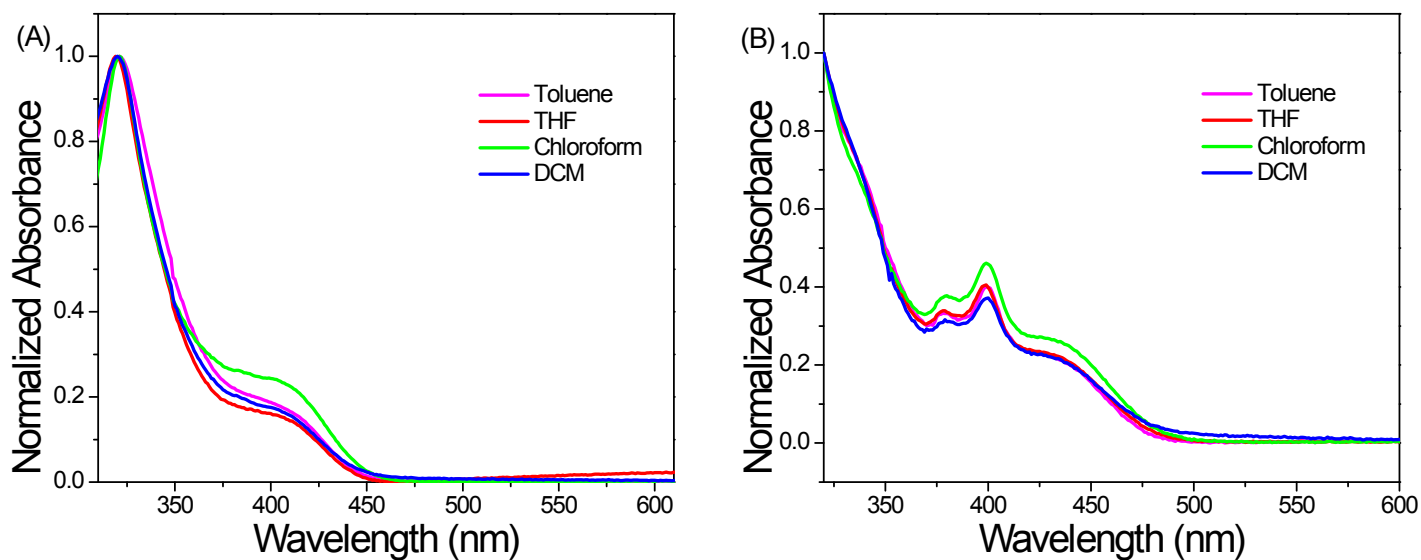


Fig. S2 UV-vis absorption spectra of **1** (A) and **2** (B) in different solvents of varying polarities

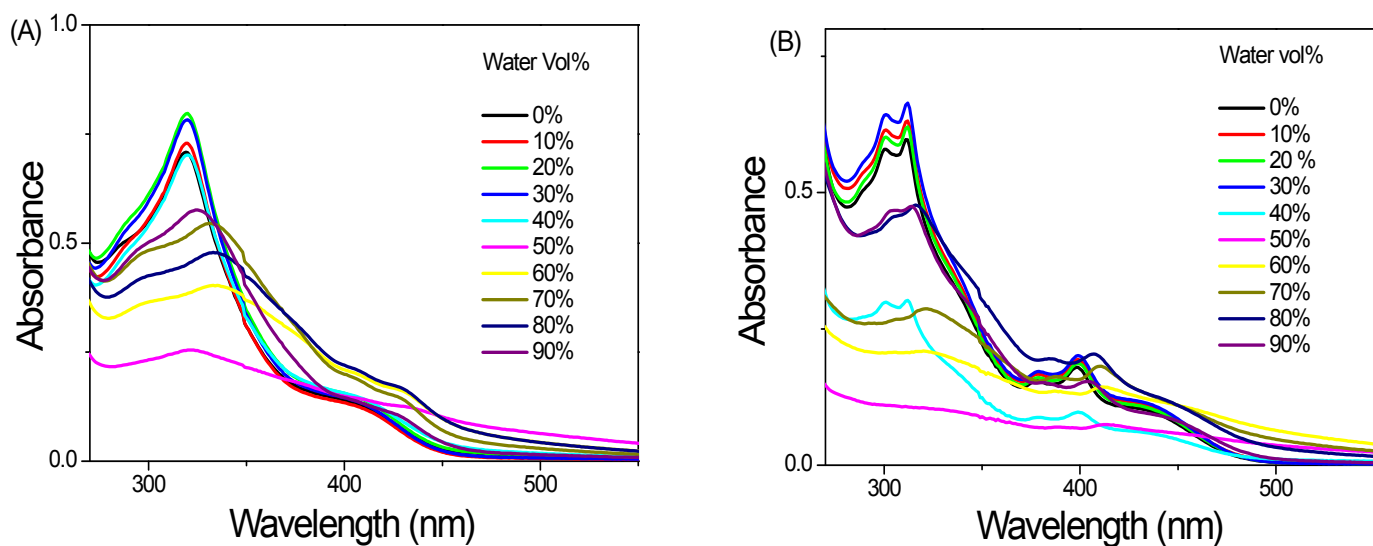


Fig. S3 UV-vis absorption spectra of **1** (A) and **2** (B) in THF–water mixtures with different water fractions.

Mechanochromism.

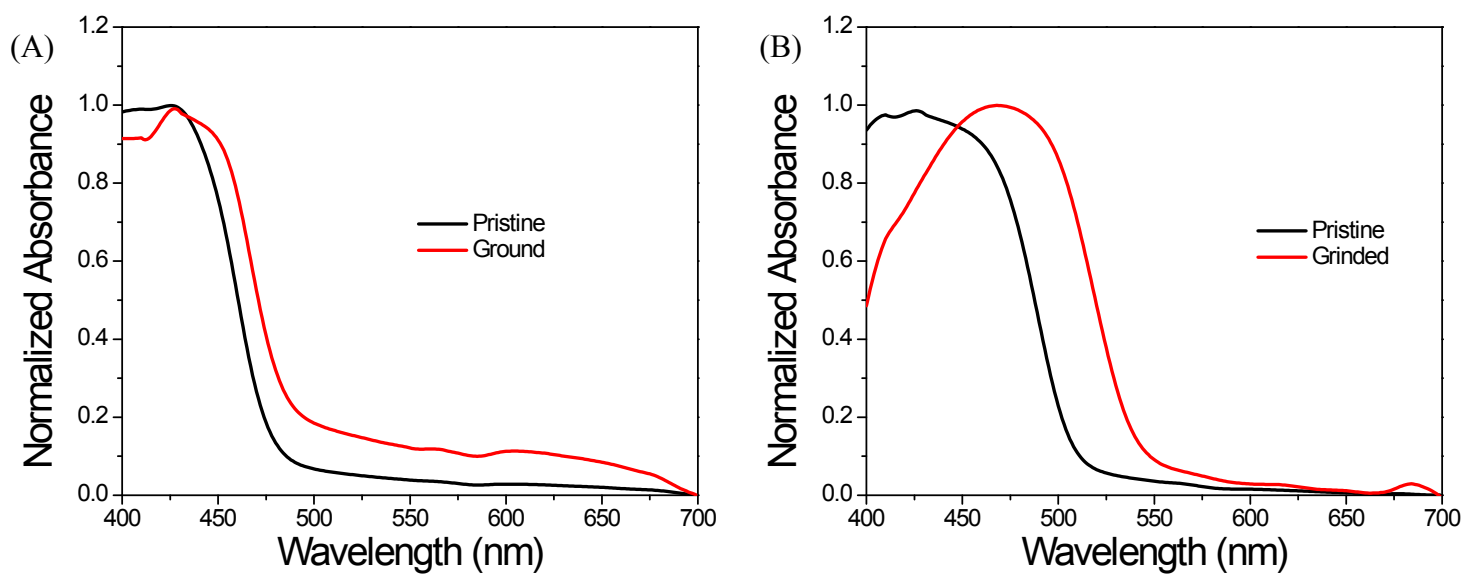


Fig. S4 Solid state absorption spectra of **1** (A) and **2** (B) in pristine and its ground form

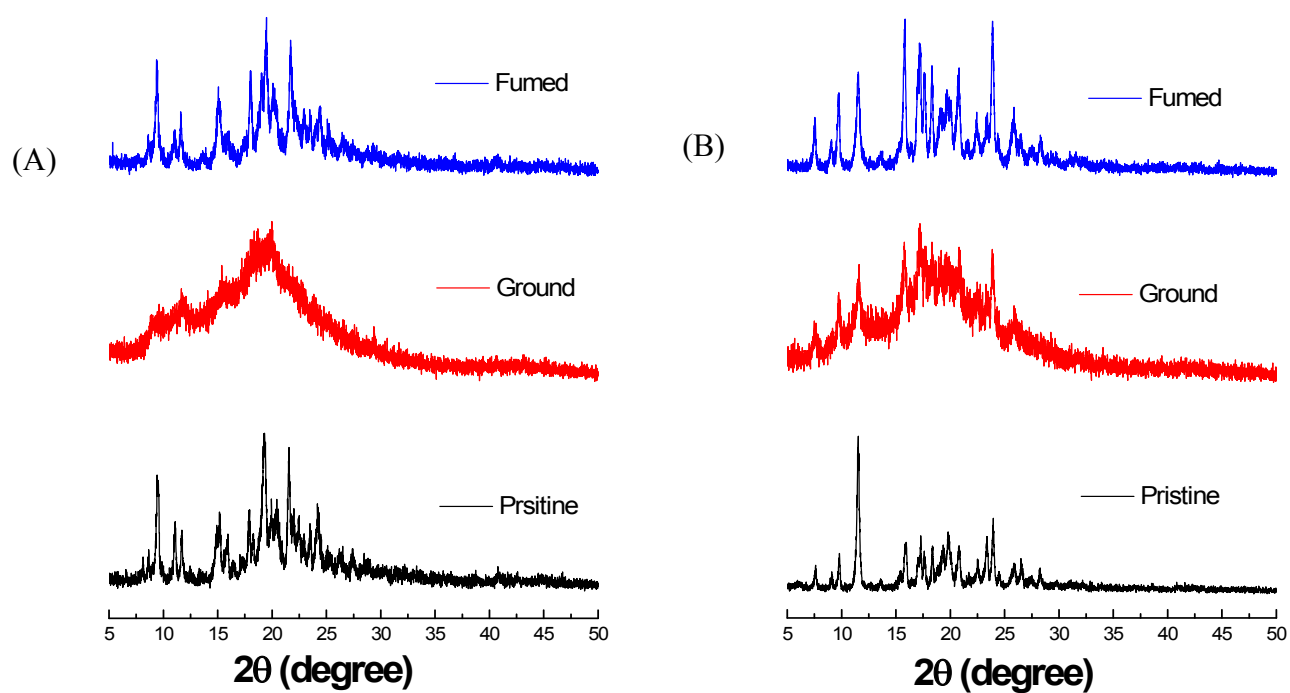


Fig. S5 PXRD curves of **1** (A) and **2** (B) in pristine, ground, and fumed form.

Electrochemical study

Table S1. Electrochemical properties of **1** and **2**.

Compounds	HOMO ^a eV	LUMO ^a eV	Electrochemical band gap eV
1	-5.50	-3.57	1.93
2	-5.52	-3.54	1.88

^a Calculated from CV: Reference electrode- Ag/AgCl.

DFT calculation data of 1 and 2.

Calculation method: B3LYP/6-31G(d,p) with Gaussian 09

1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.757177	5.869155	-0.270586
2	6	0	1.647549	6.697222	-0.332536
3	6	0	0.336400	6.142976	-0.363330
4	6	0	0.259356	4.739849	-0.329798
5	6	0	1.393772	3.889350	-0.267420
6	6	0	2.653019	4.451659	-0.235817
7	1	0	-0.915780	7.922551	-0.451480
8	1	0	3.746423	6.316967	-0.247818
9	1	0	1.777343	7.775880	-0.357039
10	6	0	-0.905691	6.836284	-0.422708
11	6	0	-0.962033	4.017152	-0.351048
12	1	0	3.546639	3.837164	-0.182340
13	6	0	-2.150836	4.713822	-0.407085
14	6	0	-2.100305	6.133910	-0.443085
15	1	0	-3.105466	4.197521	-0.422963
16	1	0	-3.034647	6.685723	-0.487909
17	6	0	0.862050	2.517658	-0.252536
18	6	0	-0.585622	2.595506	-0.303034
19	6	0	0.732553	0.247570	-0.195472
20	6	0	-0.706844	0.323803	-0.243412
21	7	0	1.505023	1.381150	-0.195741
22	7	0	-1.350492	1.534850	-0.293152
23	6	0	1.387065	-1.022317	-0.110731
24	6	0	0.585632	-2.154674	-0.055922
25	1	0	1.058078	-3.131088	-0.012448
26	6	0	-0.815956	-2.081030	-0.103792
27	1	0	-1.387569	-3.003693	-0.097817
28	6	0	-1.493488	-0.872298	-0.206030
29	6	0	2.865145	-1.152295	-0.064455
30	6	0	3.464103	-2.026135	0.858366
31	6	0	3.706855	-0.459768	-0.951497
32	6	0	4.845097	-2.191741	0.903305
33	1	0	2.838835	-2.563705	1.565314
34	6	0	5.086047	-0.622199	-0.902551
35	1	0	3.272869	0.205818	-1.687563
36	6	0	5.688651	-1.475689	0.037607
37	1	0	5.279836	-2.871626	1.629676
38	1	0	5.712462	-0.080624	-1.603466
39	6	0	7.169744	-1.656483	0.090335
40	6	0	8.039015	-0.601304	0.094540
41	6	0	7.624952	-3.079464	0.144735
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44	6	0	7.080845	-4.035447	-0.731007

45	6	0	8.556203	-3.512997	1.103460
46	6	0	10.428061	-0.126849	0.737386
47	6	0	10.015398	-1.513891	-1.191503
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49	6	0	6.753661	1.154355	1.382913
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54	6	0	11.801279	-0.256551	0.538176
55	1	0	10.056788	0.471568	1.563884
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66	1	0	12.492153	0.236140	1.216530
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68	6	0	6.825254	3.487631	0.746838
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70	1	0	5.727775	2.720463	2.438036
71	1	0	8.715963	-6.824876	0.332141
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73	1	0	6.533929	4.519915	0.919456
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84	6	0	-7.309877	-1.021153	-0.451103
85	6	0	-8.120294	-0.964192	0.648226
86	6	0	-7.847787	-1.144886	-1.841218
87	6	0	-9.580339	-1.281335	0.590447
88	6	0	-7.620296	-0.576719	2.002901
89	6	0	-7.311289	-2.090075	-2.732937
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94	6	0	-6.839131	0.575926	2.192199
95	6	0	-7.790070	-2.197092	-4.037468
96	1	0	-6.515553	-2.746640	-2.393997
97	6	0	-9.327719	-0.386511	-3.619765
98	1	0	-9.271191	0.459263	-1.642810
99	6	0	-11.880841	-0.725188	1.168612
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118	1	0	-6.411667	0.465499	5.567660

Total Energy (HF) = -2804.7661982Hartree

2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.005257	3.566913	4.858408
2	6	0	0.010707	2.856196	3.670094
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7	6	0	-0.005257	0.716481	2.406717
8	6	0	-0.001087	-0.736762	4.900411
9	6	0	-0.003756	-1.448790	3.673302
10	6	0	0.005257	-0.716481	2.406717
11	6	0	-0.010707	-2.856196	3.670094
12	1	0	-0.022787	-3.367591	2.714482
13	6	0	-0.005257	-3.566913	4.858408
14	6	0	0.002356	-2.874787	6.076954
15	6	0	0.002356	-1.488031	6.093798
16	1	0	0.006542	4.652115	4.838462
17	1	0	0.022787	3.367591	2.714482
18	1	0	-0.007118	0.983660	7.052727
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20	1	0	-0.006542	-4.652115	4.838462
21	1	0	0.007315	-3.421757	7.015408
22	1	0	0.007118	-0.983660	7.052727
23	6	0	-0.031724	0.719992	0.098197
24	6	0	0.031724	-0.719992	0.098197
25	7	0	-0.030250	1.395332	1.267148
26	7	0	0.030250	-1.395332	1.267148
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28	6	0	-0.040507	0.704072	-2.308816
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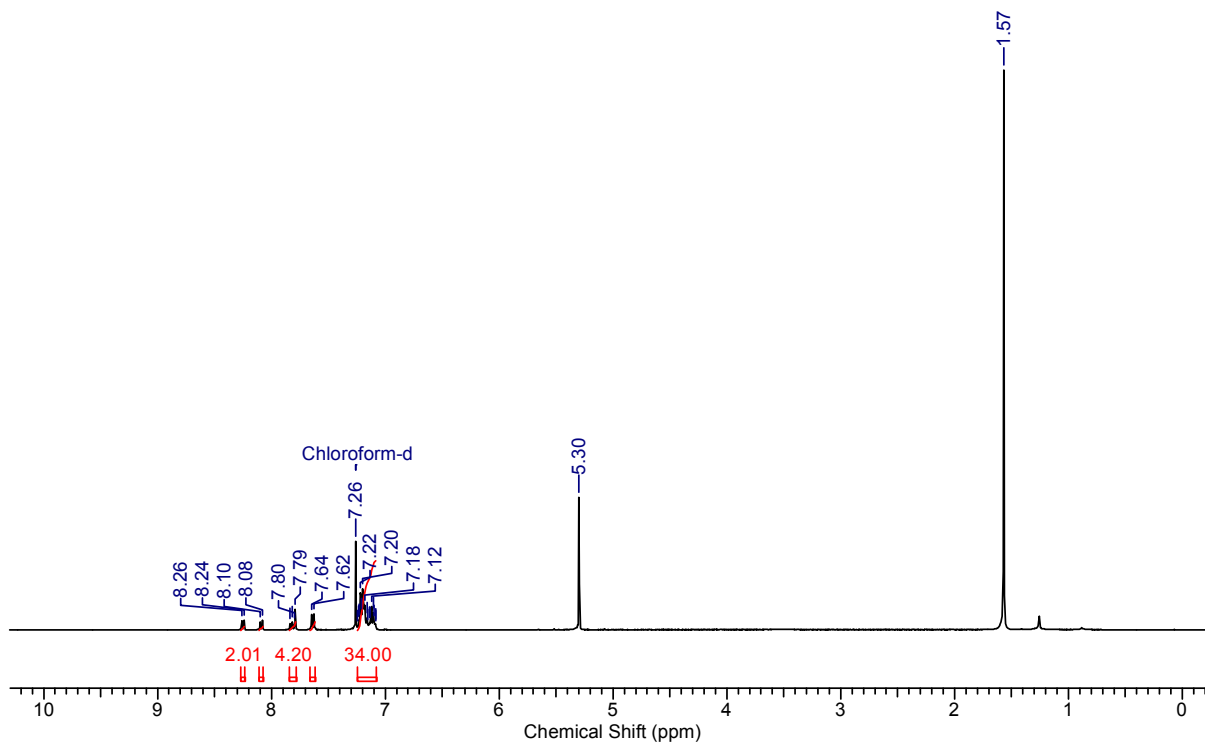
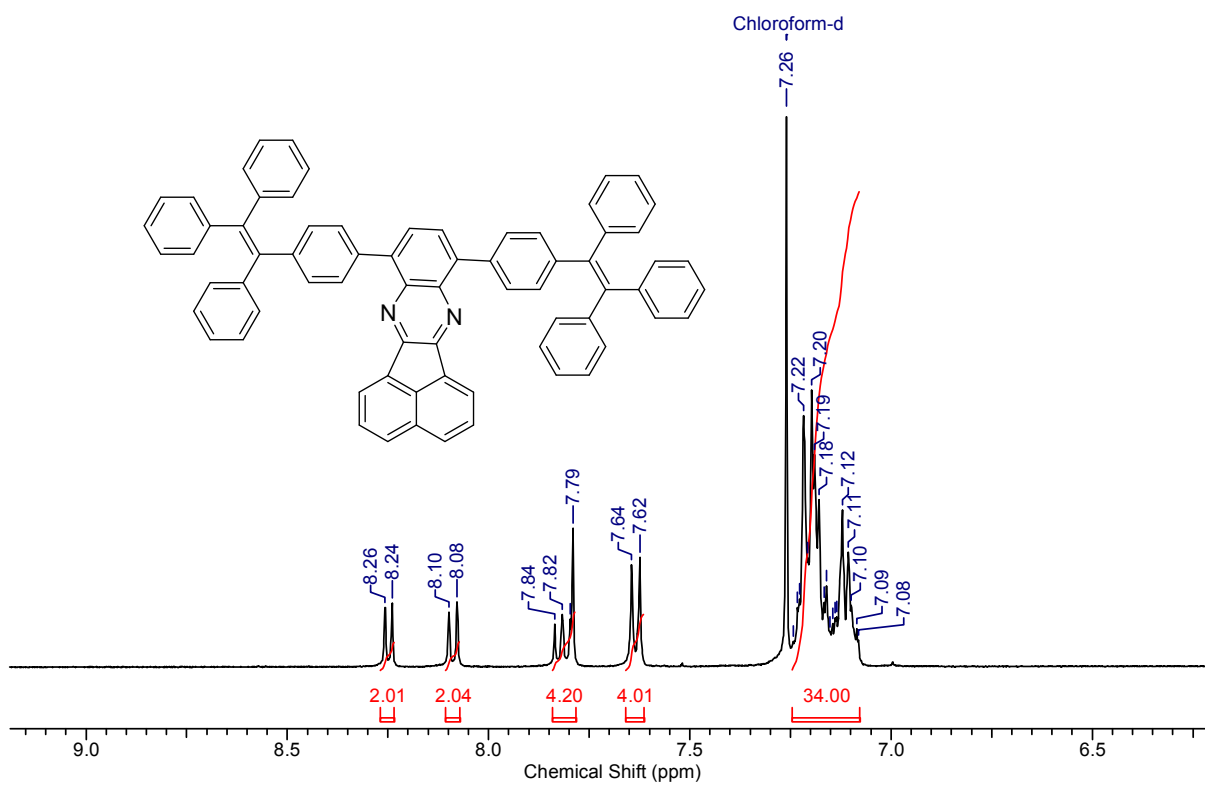
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54	6	0	1.744985	-7.430727	-5.201509
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58	6	0	0.271585	-11.916818	-0.366174
59	1	0	-1.029821	-10.305900	0.215412
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71	1	0	3.296537	-11.535604	-1.868487
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75	1	0	1.071257	-8.729803	-6.787520
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81	6	0	0.536417	5.004036	-2.288366
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83	6	0	-1.079914	5.066234	-0.509779
84	1	0	-1.621273	3.177331	0.345174
85	6	0	-0.309114	5.759547	-1.458695
86	1	0	1.137574	5.509509	-3.038106
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88	6	0	-0.428218	7.237059	-1.637746

89	6	0	-0.368670	8.120013	-0.596519
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91	6	0	-0.750628	9.558507	-0.743274
92	6	0	0.089202	7.733319	0.772613
93	6	0	-1.575672	7.046779	-3.872533
94	6	0	0.182477	8.678681	-3.623123
95	6	0	0.087804	10.575056	-0.252866
96	6	0	-1.976353	9.930452	-1.320392
97	6	0	-0.618886	8.163784	1.908894
98	6	0	1.270052	6.996173	0.968122
99	6	0	-1.744985	7.430727	-5.201509
100	1	0	-2.190812	6.254948	-3.455823
101	6	0	0.022514	9.053685	-4.956005
102	1	0	0.936682	9.163004	-3.011803
103	6	0	-0.271585	11.916818	-0.366174
104	1	0	1.029821	10.305900	0.215412
105	6	0	-2.341674	11.271622	-1.422866
106	1	0	-2.643756	9.158209	-1.688247
107	6	0	-0.175140	7.850757	3.192359
108	1	0	-1.523513	8.749966	1.779358
109	6	0	1.719501	6.690103	2.251216
110	1	0	1.839702	6.668999	0.104930
111	6	0	-0.945460	8.435738	-5.749547
112	1	0	-2.498752	6.940760	-5.811393
113	1	0	0.658140	9.828067	-5.375974
114	6	0	-1.488739	12.271029	-0.951592
115	1	0	0.397756	12.686551	0.007561
116	1	0	-3.296537	11.535604	-1.868487
117	6	0	0.999046	7.115735	3.369540
118	1	0	-0.742058	8.189758	4.054835
119	1	0	2.639426	6.126774	2.378029
120	1	0	-1.071257	8.729803	-6.787520
121	1	0	-1.772837	13.316167	-1.033189
122	1	0	1.358199	6.888714	4.369268

Total Energy (HF) = -2882.2081542Hartree

Copies of NMR and HRMS spectra of the new compounds.

¹H NMR of 1



HRMS of **1**

Display Report

Analysis Info

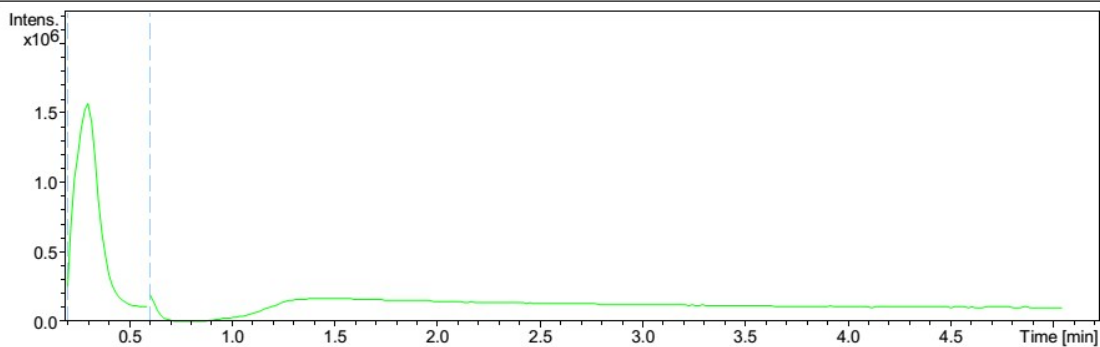
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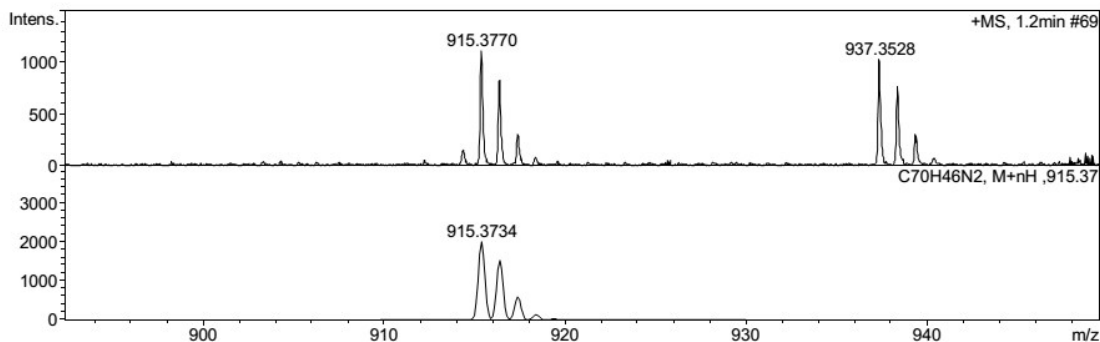
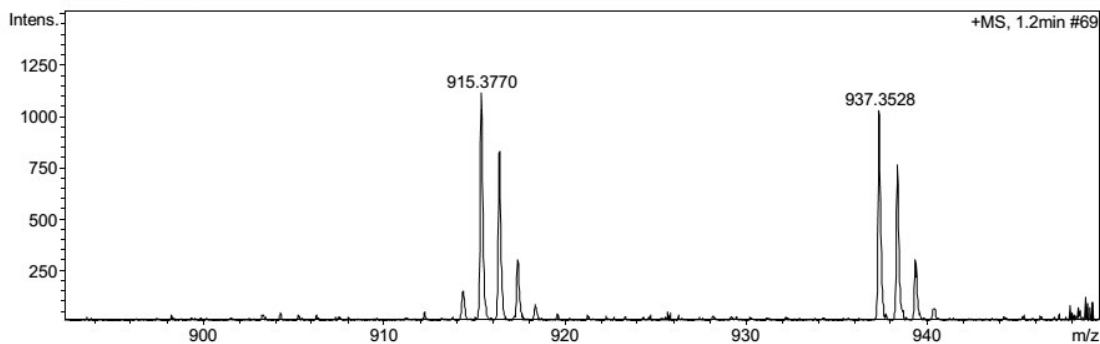
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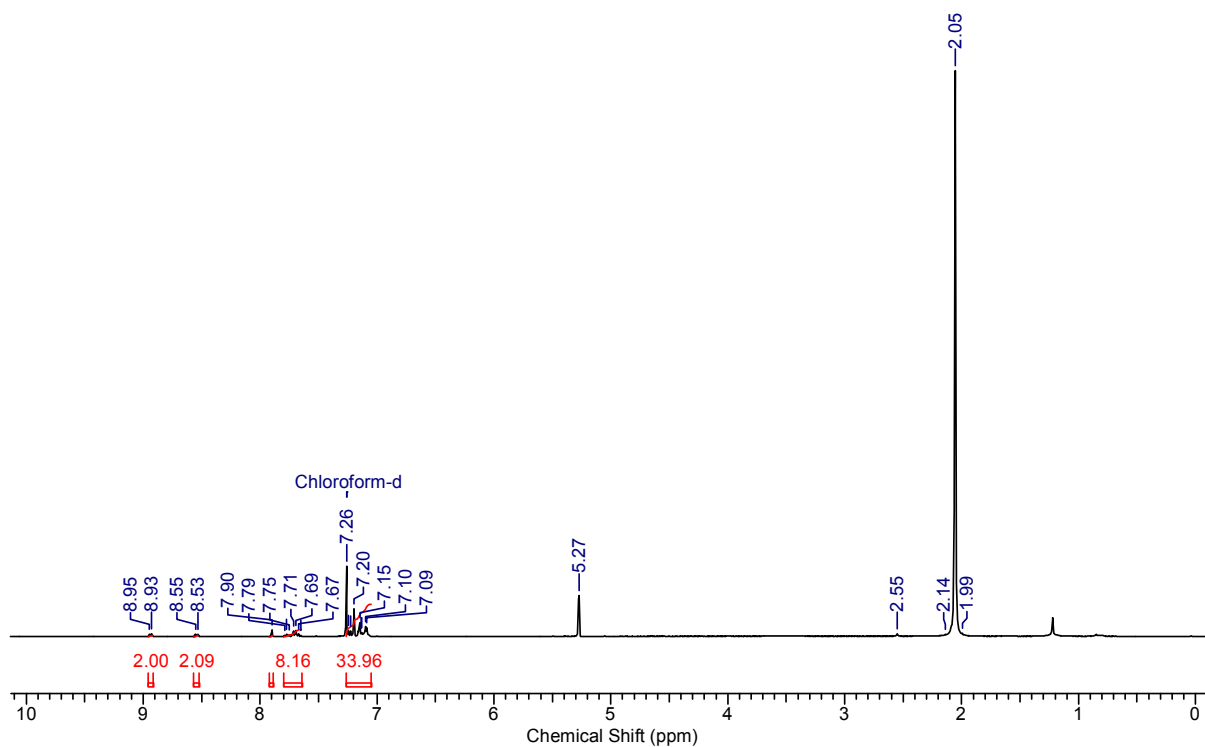
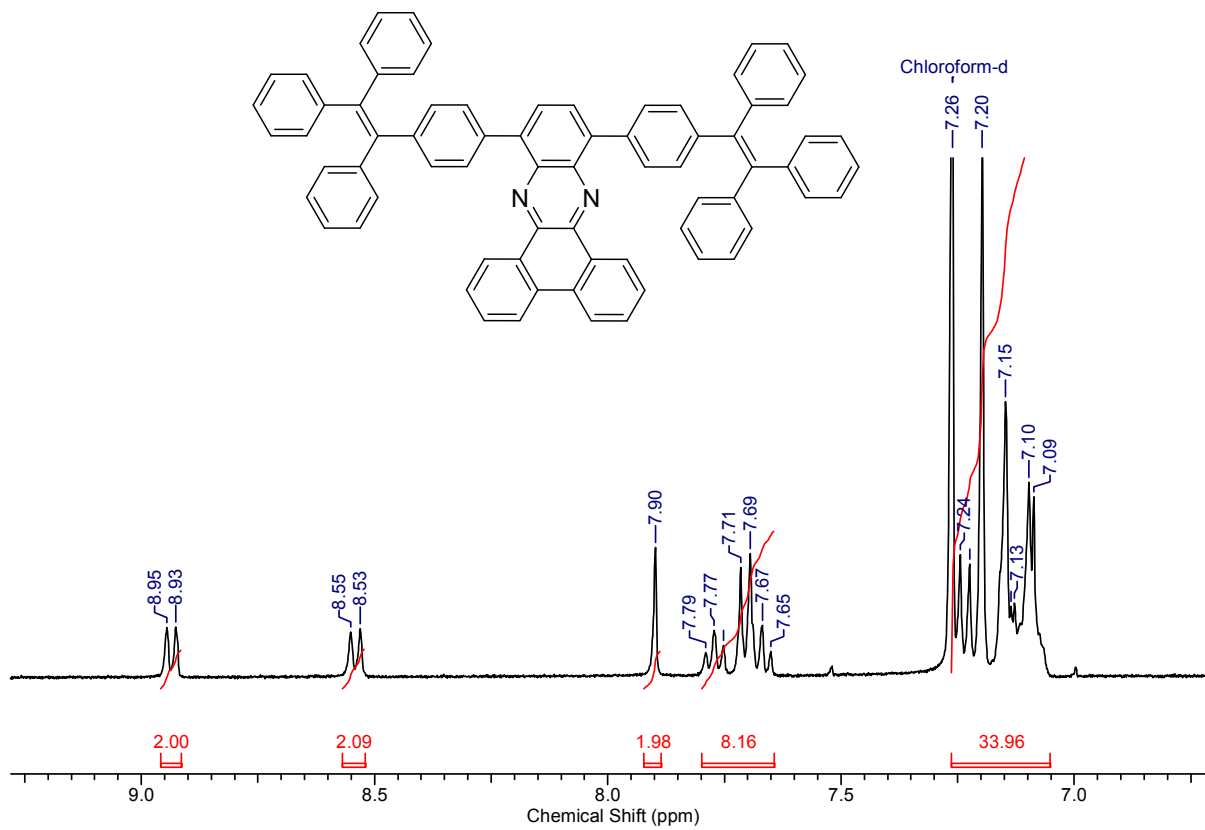
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TIC +All MS



^1H NMR of 2



Display Report

Analysis Info

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Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	21 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste

