



Supporting Information

for

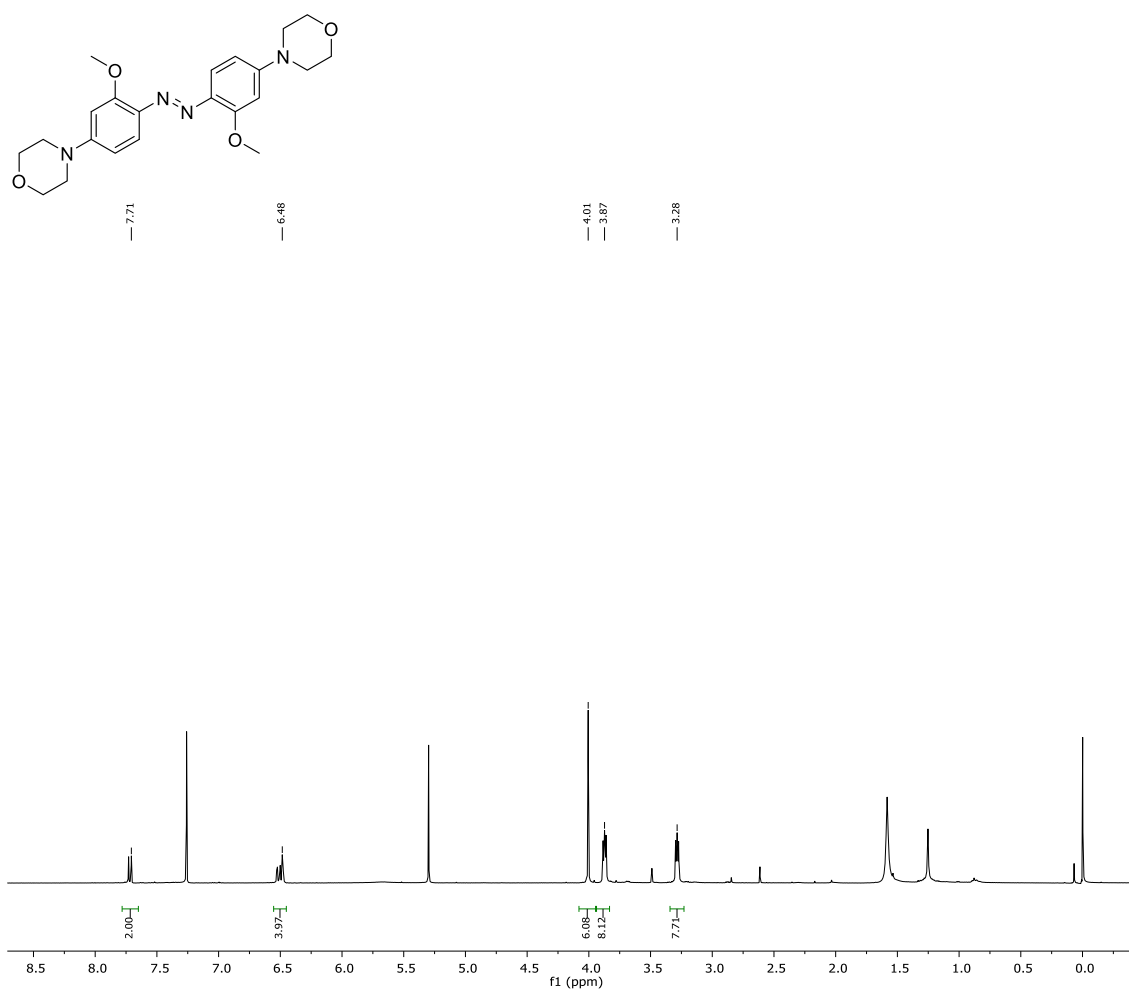
Synthesis and characterization of bis(4-amino-2-bromo-6-methoxy)azobenzene derivatives

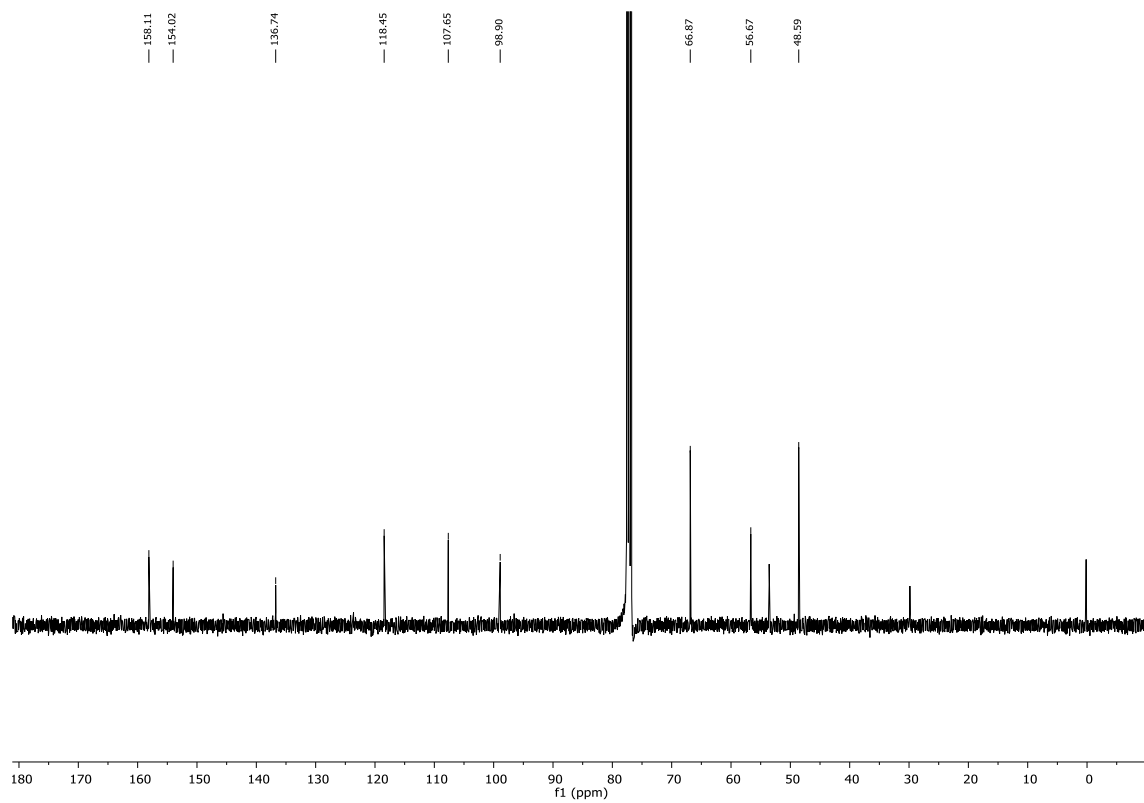
David Martínez-López, Amirhossein Babalhavaeji, Diego Sampedro
and G. Andrew Woolley

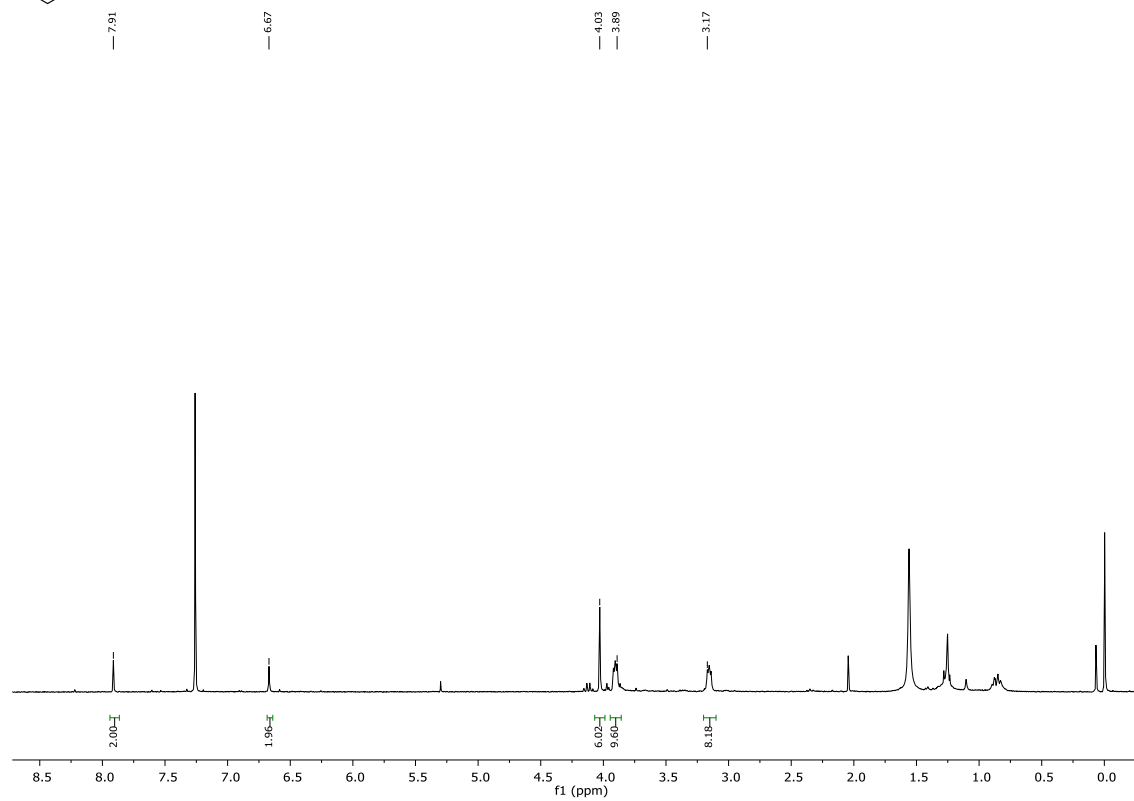
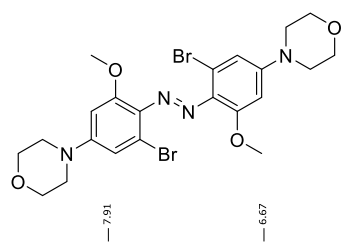
Beilstein J. Org. Chem. **2019**, *15*, 3000–3008. doi:10.3762/bjoc.15.296

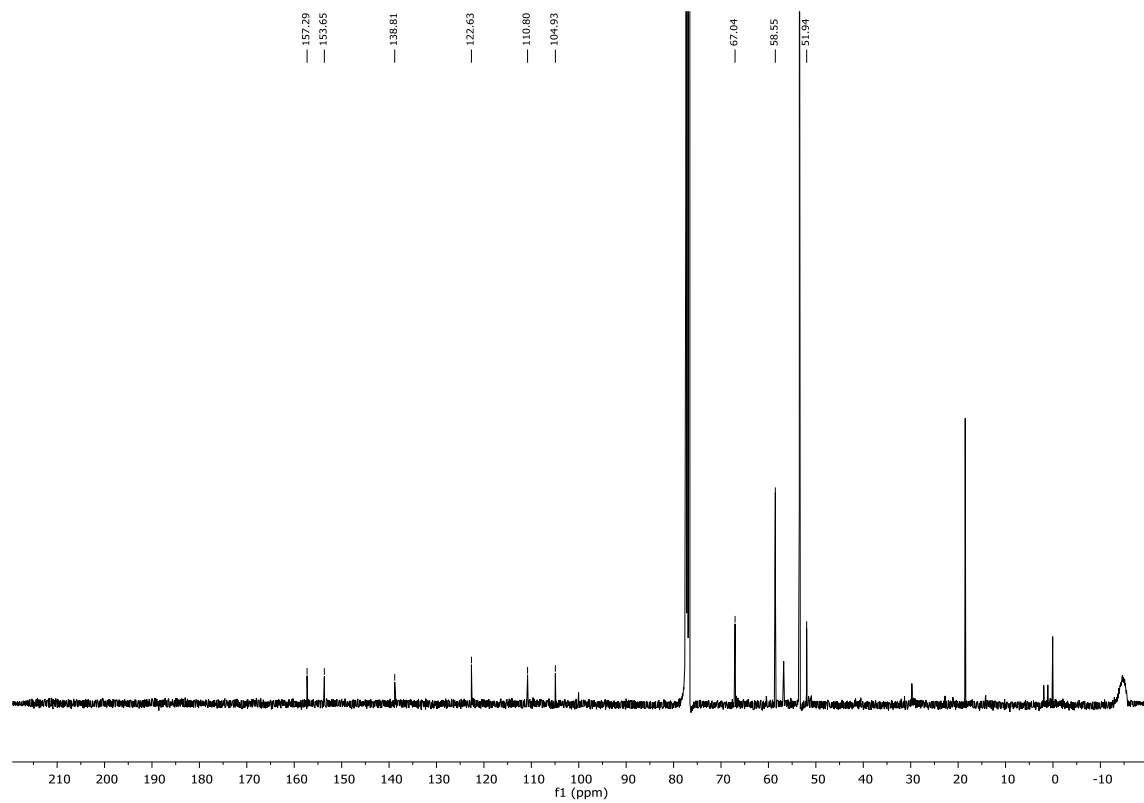
NMR spectra and further computational data

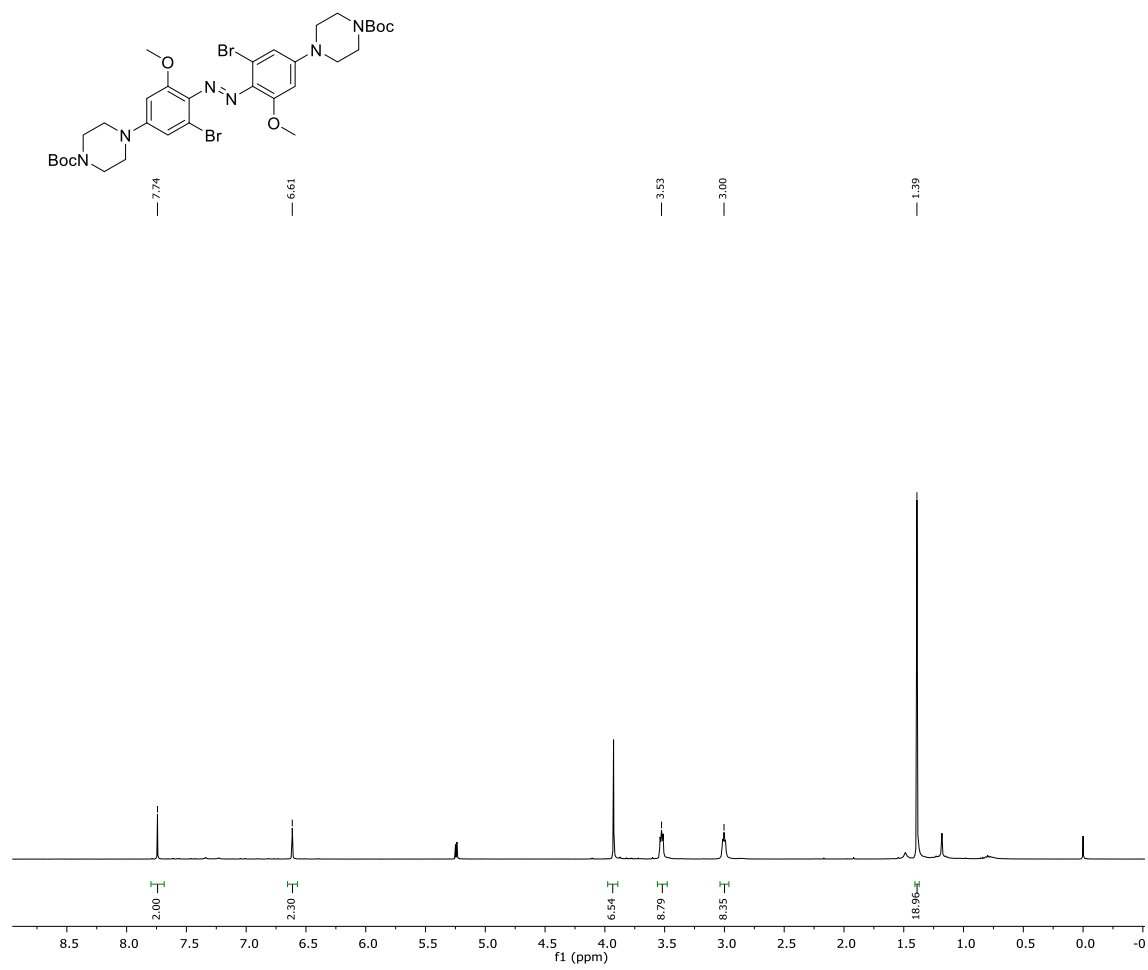
Synthesis/Characterization Data:

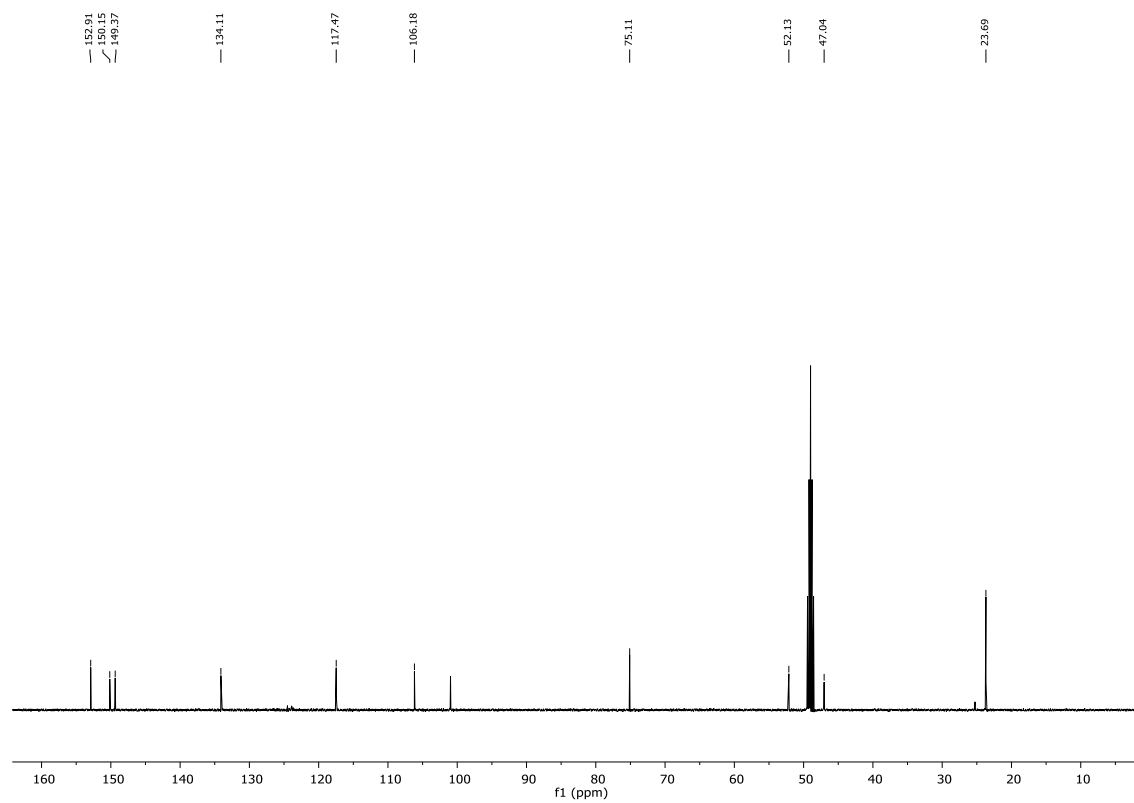


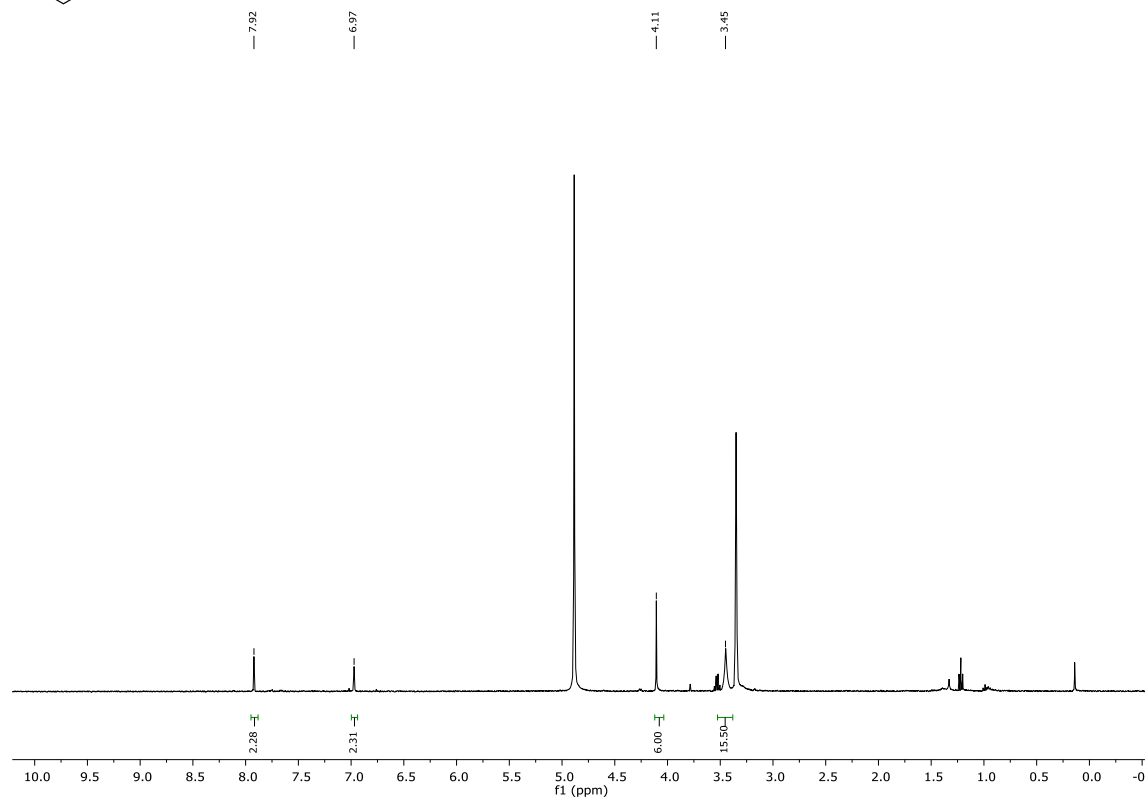
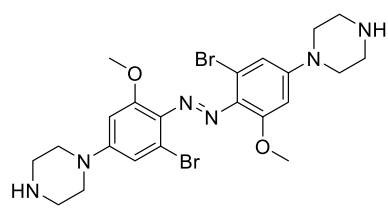


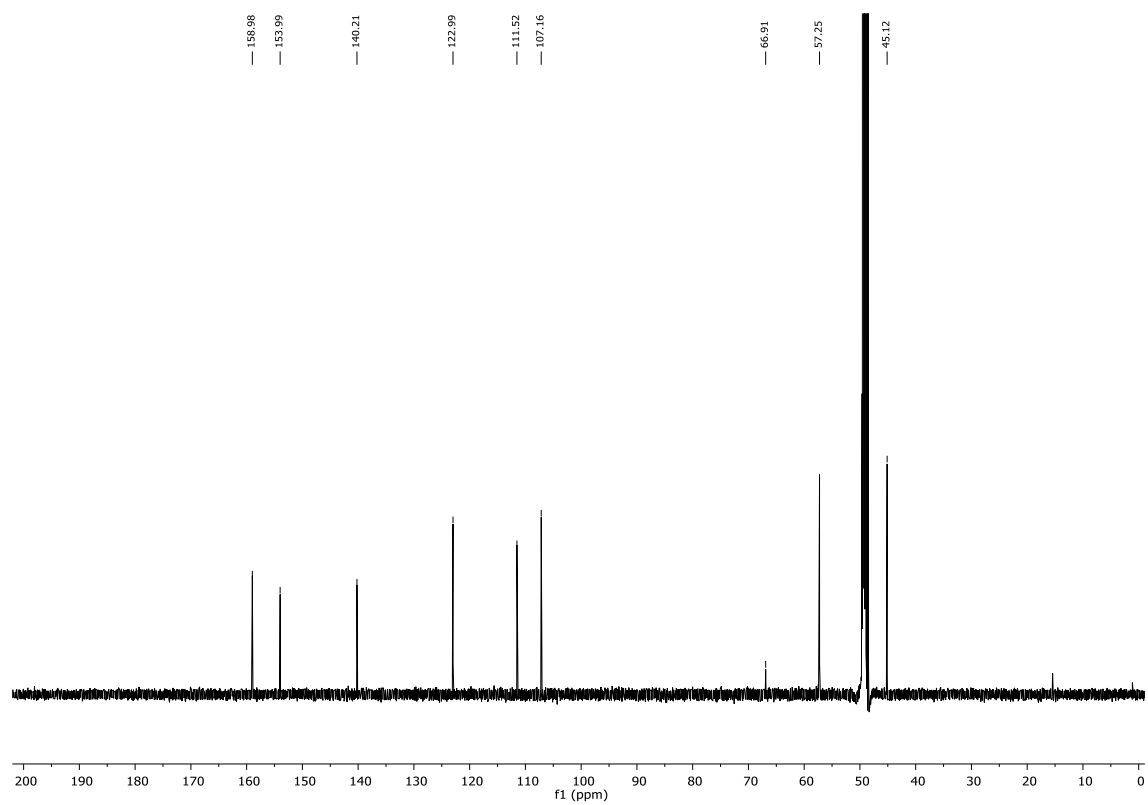






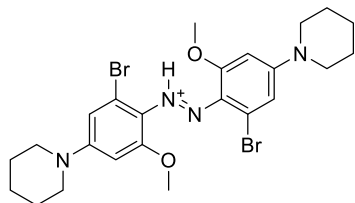






Computational Chemistry

Cartesian coordinates for:



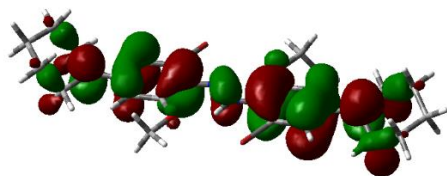
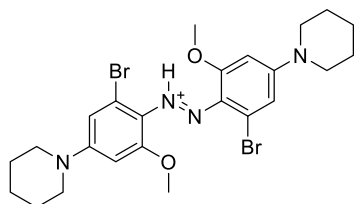
63

protonated_6 mem 0.000000

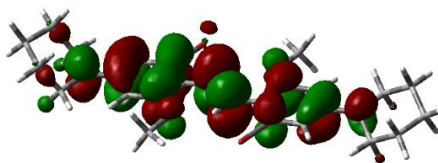
C	-2.4550	-1.0500	-0.2060
C	-4.0790	1.2300	-0.2700
C	-1.8190	0.2440	-0.1950
C	-3.8250	-1.1950	-0.2430
C	-4.6940	-0.0610	-0.2800
C	-2.7150	1.3610	-0.2300
H	-4.2370	-2.1900	-0.2220
N	0.4020	-0.3810	-0.1250
C	1.7760	-0.1570	-0.0830
C	4.6350	0.0990	0.0010
C	2.3990	1.1270	-0.0570
C	2.6390	-1.2760	-0.0640
C	4.0110	-1.1780	-0.0220
C	3.7880	1.2340	-0.0190
H	4.2200	2.2200	-0.0470
N	-6.0440	-0.2020	-0.3270
C	-7.0020	0.9100	-0.1840
H	-7.6350	0.9220	-1.0820
H	-6.4840	1.8640	-0.1430
C	-6.7430	-1.4940	-0.4410
H	-6.0380	-2.2970	-0.6400
H	-7.3980	-1.4260	-1.3210
N	6.0040	0.2140	0.0760
C	6.6480	1.5210	0.2680
H	5.9750	2.1690	0.8290
H	6.8370	1.9930	-0.7110
C	6.8910	-0.7940	-0.5370
H	6.3690	-1.7450	-0.6230
H	7.1250	-0.4660	-1.5640
C	8.1910	-0.9740	0.2510
H	8.8230	-1.6940	-0.2800
H	7.9610	-1.4040	1.2340
C	7.9620	1.3900	1.0530
H	7.7270	1.0890	2.0820
H	8.4290	2.3800	1.1050
C	8.9120	0.3670	0.4220
H	9.8080	0.2480	1.0400
H	9.2510	0.7300	-0.5590
C	-7.5870	-1.7790	0.8100

H	-8.1130	-2.7310	0.6720
H	-6.9200	-1.8990	1.6740
C	-7.8680	0.7200	1.0720
H	-7.2260	0.8010	1.9590
H	-8.5930	1.5400	1.1240
C	-8.5830	-0.6380	1.0600
H	-9.1160	-0.7960	2.0040
H	-9.3430	-0.6420	0.2670
N	-0.5020	0.5360	-0.1590
H	0.1160	-1.3670	-0.1290
O	-1.5990	-2.1050	-0.1660
O	1.5800	2.1940	-0.0920
C	2.1330	3.5130	-0.0640
H	2.7070	3.6790	0.8540
H	2.7610	3.6960	-0.9430
H	1.2740	4.1820	-0.0840
C	-2.1060	-3.4490	-0.1770
H	-2.7250	-3.6330	0.7060
H	-2.6740	-3.6370	-1.0930
H	-1.2260	-4.0890	-0.1500
H	4.5920	-2.0860	0.0320
H	-4.6710	2.1300	-0.3130
Br	1.8990	-3.0400	-0.0830
Br	-1.9990	3.1130	-0.2330

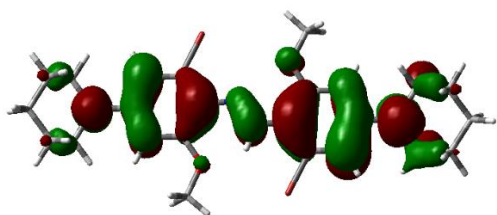
Calculated HOMO/LUMO for:



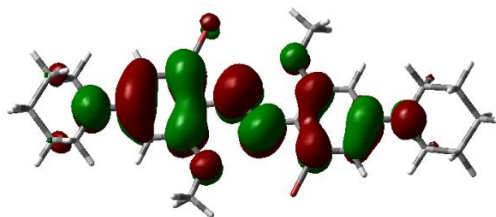
HOMO (sideview)



LUMO (sideview)

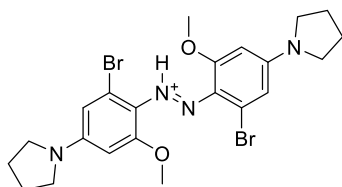


HOMO (topview)



LUMO (topview)

Cartesian coordinates for:



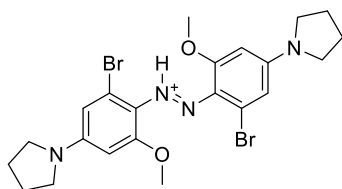
57

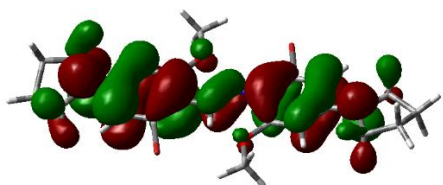
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Molecule Name  0.000000
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C -4.0657  1.1590  0.0093
C -1.7956  0.1964  0.0073
C -3.7794 -1.2735 -0.0133
C -4.6471 -0.1433 -0.0049
C -2.7021  1.3071  0.0131
H -4.2005 -2.2674 -0.0090
N  0.4361 -0.3984  0.0081
C  1.8074 -0.1569  0.0042
C  4.6519  0.1373 -0.0067
C  2.4124  1.1409 -0.0085
C  2.6835 -1.2670  0.0093
C  4.0549 -1.1530  0.0051
C  3.7966  1.2680 -0.0150
H  4.2291  2.2566 -0.0108
N -5.9874 -0.2984 -0.0103
C -6.9489  0.8183  0.0940
H -6.9595  1.3939 -0.8415
H -6.6675  1.4917  0.9089
C -6.6705 -1.6013 -0.1221
H -6.5567 -2.1683  0.8125
H -6.2398 -2.1916 -0.9373
  
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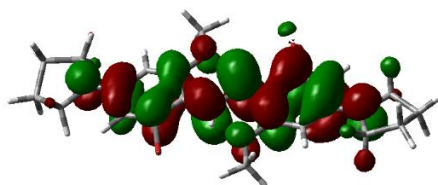
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C	6.6935	1.5706	-0.1231
H	6.5811	2.1465	0.8069
H	6.2739	2.1629	-0.9435
C	6.9445	-0.8497	0.0976
H	6.6560	-1.5185	0.9151
H	6.9539	-1.4323	-0.8347
C	8.2960	-0.1679	0.3509
H	9.1337	-0.7672	-0.0135
H	8.4387	-0.0097	1.4256
C	8.1571	1.1807	-0.3732
H	8.8531	1.9392	-0.0071
H	8.3310	1.0554	-1.4476
C	-8.1360	-1.2256	-0.3802
H	-8.3054	-1.1017	-1.4554
H	-8.8252	-1.9920	-0.0181
C	-8.2919	0.1202	0.3446
H	-8.4358	-0.0394	1.4188
H	-9.1347	0.7105	-0.0221
N	-0.4804	0.5058	0.0106
H	0.1633	-1.3884	0.0069
O	-1.5369	-2.1518	-0.0019
O	1.5741	2.1935	-0.0091
C	2.1089	3.5200	-0.0215
H	2.7123	3.7090	0.8732
H	2.7048	3.6952	-0.9239
H	1.2405	4.1772	-0.0228
C	-2.0295	-3.5015	-0.0121
H	-2.6270	-3.6974	0.8832
H	-2.6166	-3.6875	-0.9164
H	-1.1424	-4.1324	-0.0105
H	4.6623	-2.0463	-0.0033
H	-4.6924	2.0390	0.0019
Br	-2.0052	3.0652	0.0213
Br	1.9653	-3.0389	0.0178

Calculated HOMO/LUMO for:

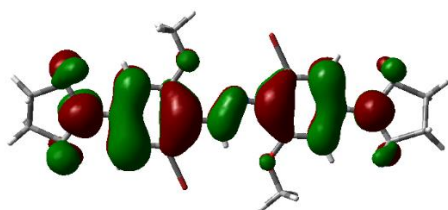




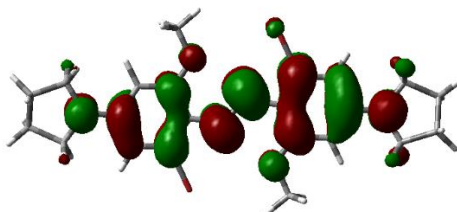
HOMO (sideview)



LUMO (sideview)



HOMO (topview)



LUMO (topview)