Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Methyl ketone bridged molecule as multi-stimuli-responsive color switch for electrochromic device

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1. Structure identification of M5

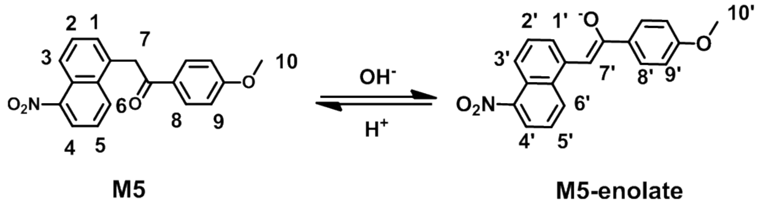


Figure S1: The chemical structures of **M5** and **M5-enolate**.

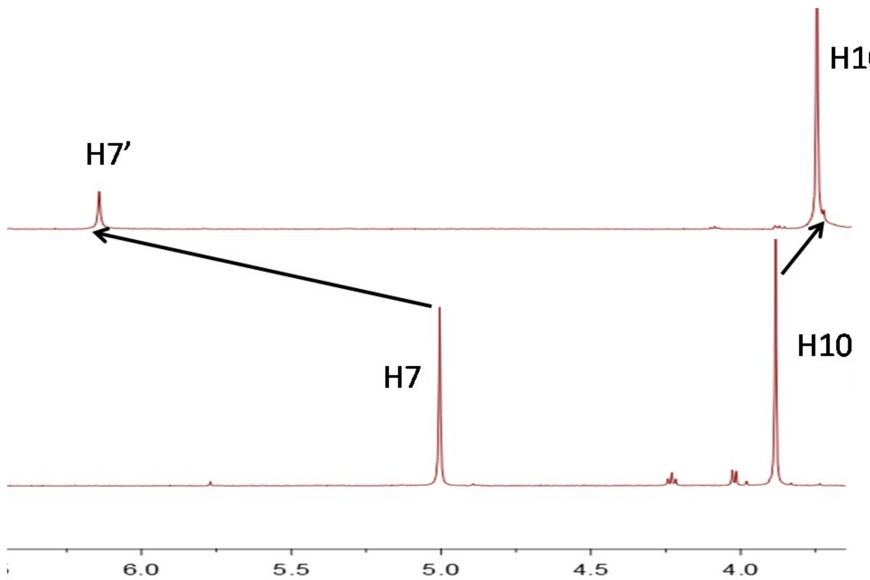


Figure S2: Partial ^{1}H NMR spectra of **M5** (bottom) and **M5-enolate** (top) obtained by adding potassium *tert*-butoxide to **M5** in DMSO-d^6.

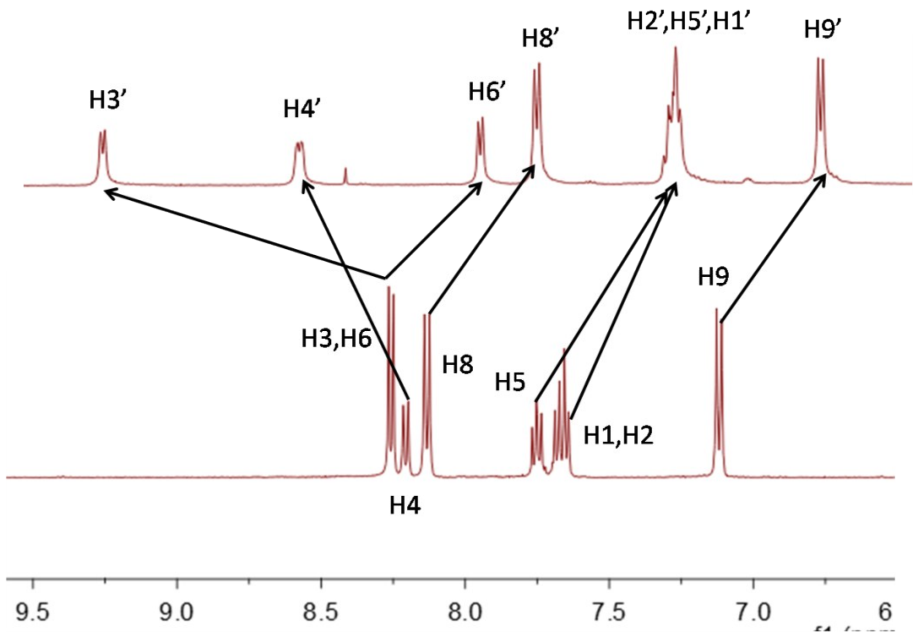


Figure S3: Partial ^{1}H NMR spectra of **M5** (bottom) and **M5-enolate** (top) obtained by adding potassium *tert*-butoxide to **M5** in DMSO-d^6.

2. Basochromic and electrochromic properties of M5

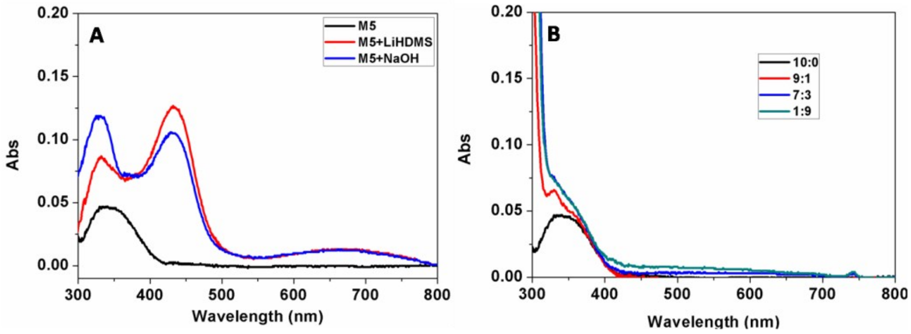


Figure S4: (a) Absorption spectra of **M5** (1.0×10^{-5} M, black curve), treated with 10eq Lithium bis(trimethylsilyl)amide (red curve) and 25 eq NaOH (blue curve) in DMF. (b) Absorption spectra of M5 (1.0×10^{-5} M) in different DMF/ triethylamine.

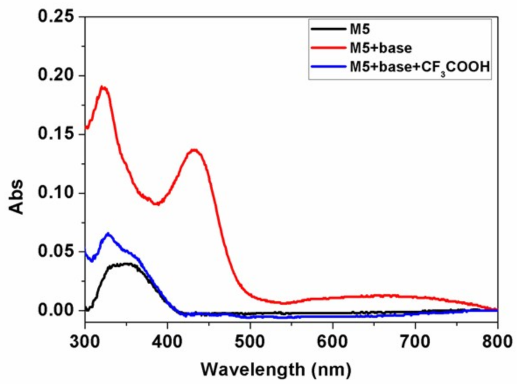


Figure S5: Absorption spectra of **M5** (1.0×10^{-5} M, black curve), treated with 50eq potassium *tert*-butoxide (red curve), then neutralized with CF_3COOH (blue curve) in DMF.

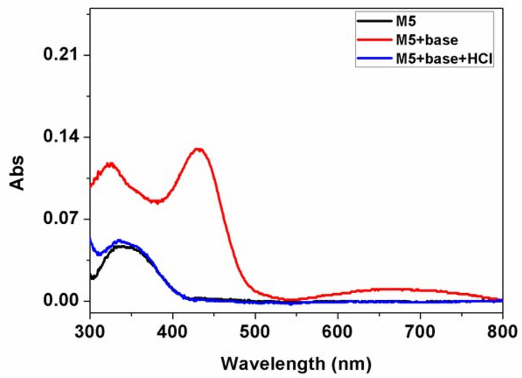


Figure S6: Absorption spectra of **M5** (1.0×10^{-5} M, black curve), treated with 50eq potassium *tert*-butoxide (red curve), then neutralized with HCl (blue curve) in DMF.

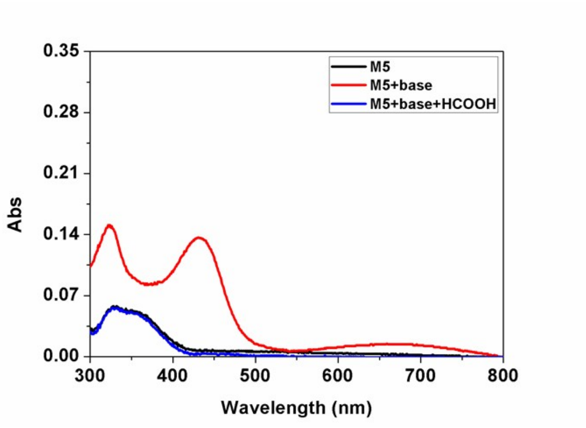


Figure S7: Absorption spectra of **M5** (1.0×10^{-5} M, black curve), treated with 50eq potassium *tert*-butoxide (red curve), then neutralized with HCOOH (blue curve) in DMF.

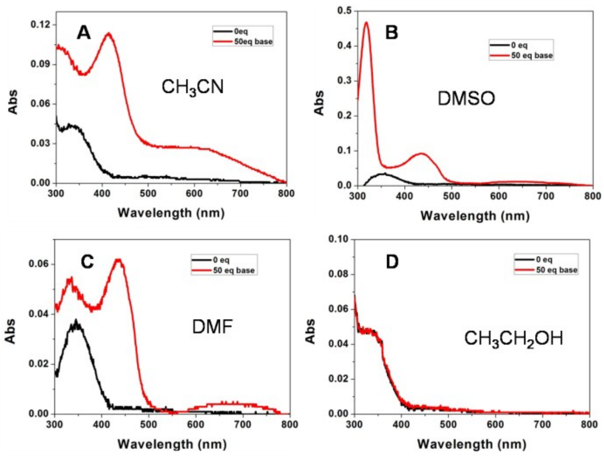


Figure S8: Absorption spectra of **M5** (1.0×10^{-5} M) in different solvents.

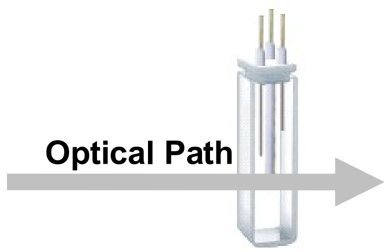


Figure S9*:* Illustration of *in-situ* Spectroelectrochemical Characterization.

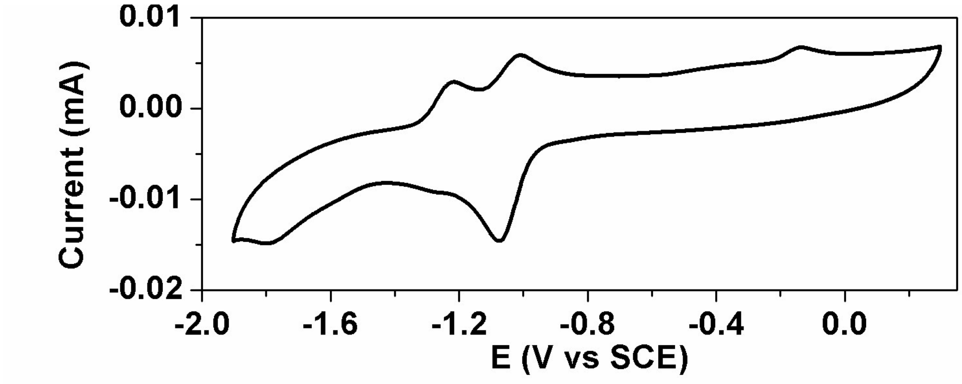


Figure S10: The cyclic voltammogram of **M5** (1.0×10^{-3} M) in DMF with 0.1 M $TBAPF_6$. Scan rate: 50 mV s^{-1}.

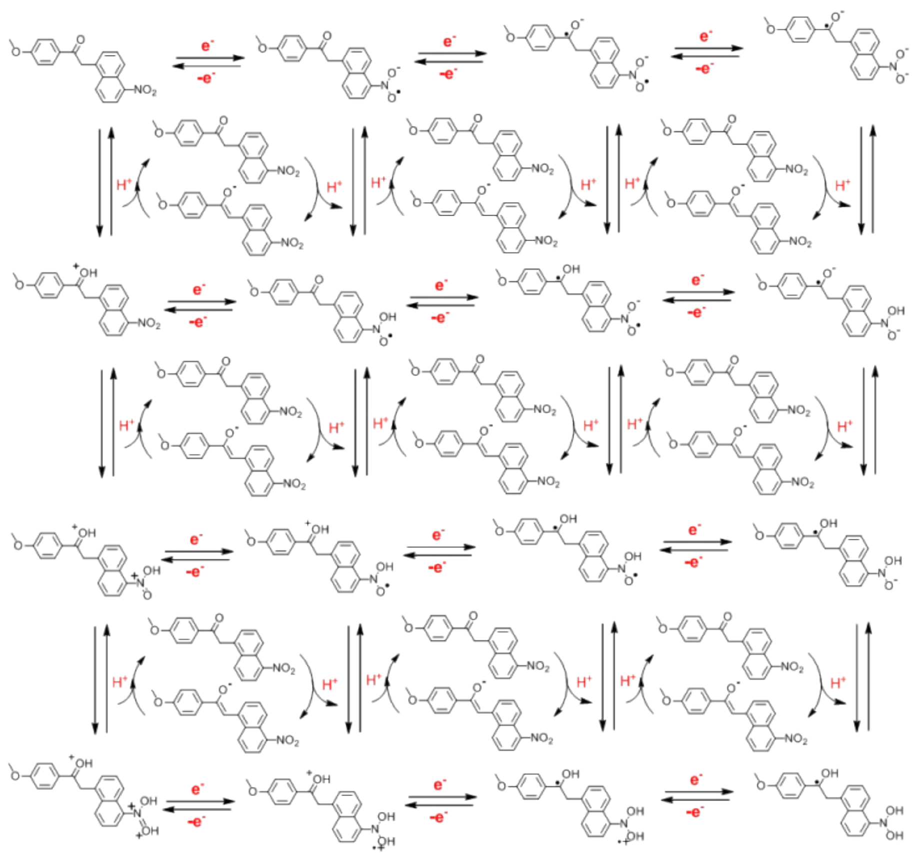


Figure S11. The electrochromic mechanism of **M5** with three-electron reduction mechanism.

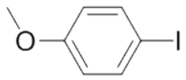
The calculation method of the coloration efficiency:

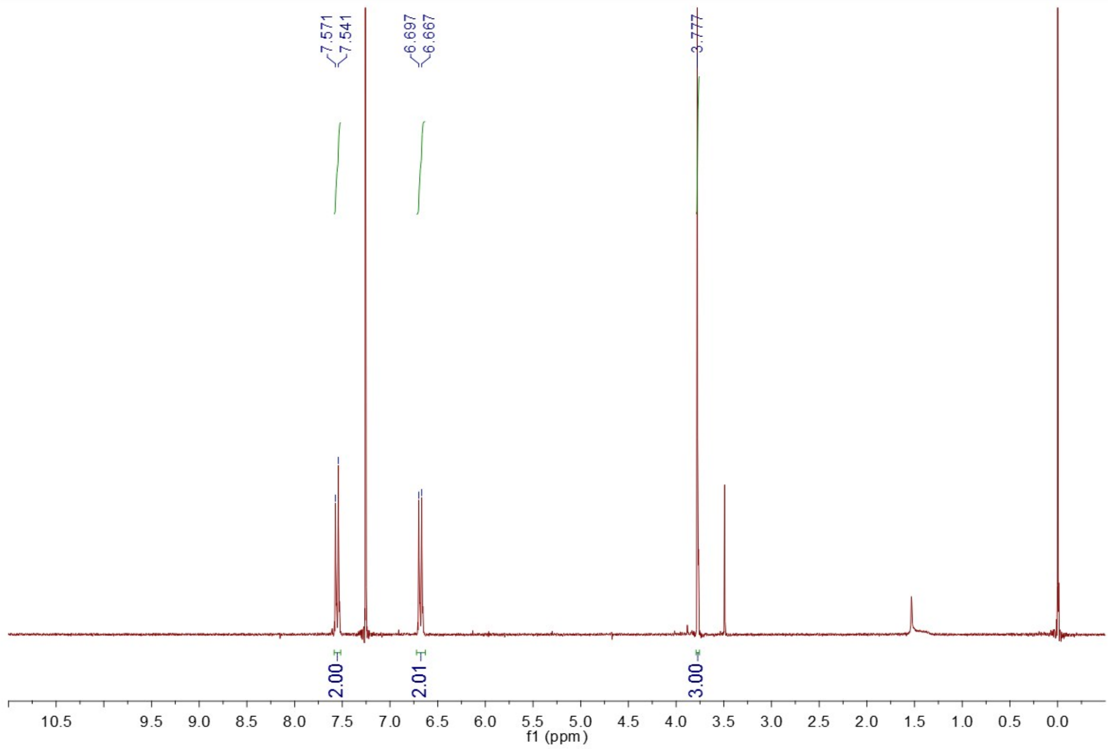
Although the coloration efficiency has been defined in several ways, all definitions are suitable only for an electrochromic polymer. We have modified the definition of the coloration efficiency of the device by eliminating the background interference of electrolytes for small organic electrochromic materials, in our earlier work (Light: Science & Applications, 2015, 4, e249).

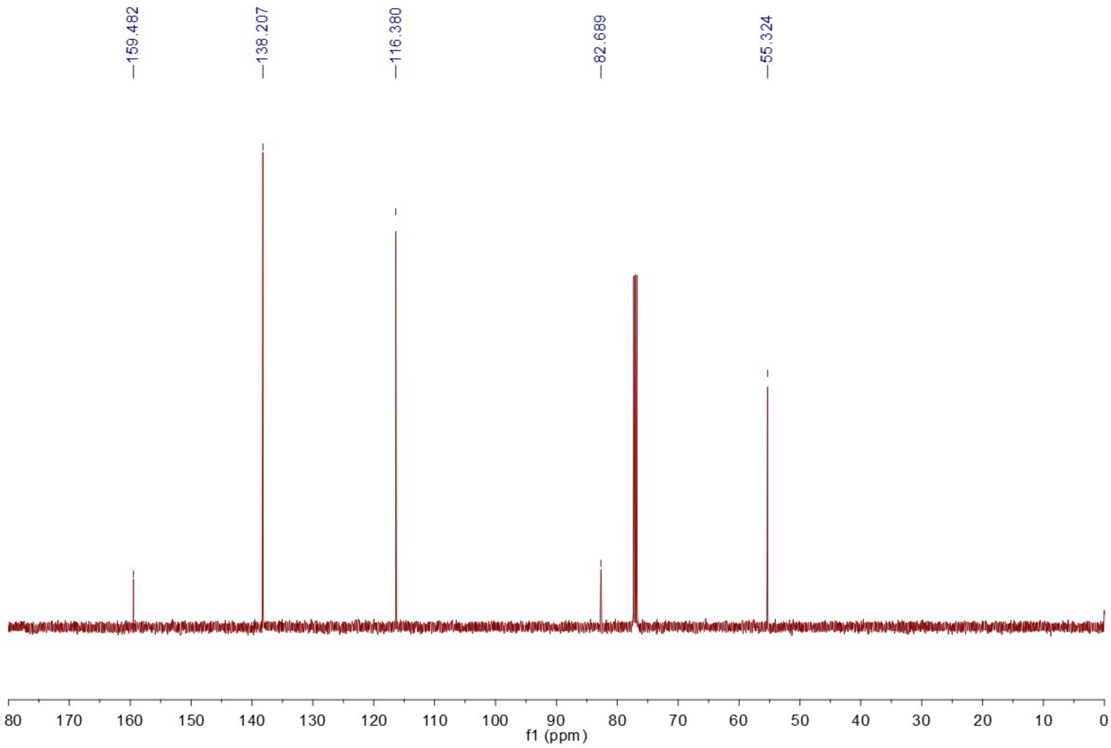
The newly defined coloration efficiency η is given by the optical absorbance change (ΔA) obtained for the change in injected charges per unit area (ΔQ) only, where (ΔQ) is calculated by subtracting the injected charge per unit area (Q2) of a blank device with no switchable molecules from the injected charge per unit area (Q1) of electrochromic device subtracts.

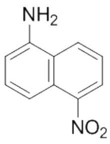
$$\eta = \Delta A/\Delta Q = \Delta A/(Q1-Q2)$$

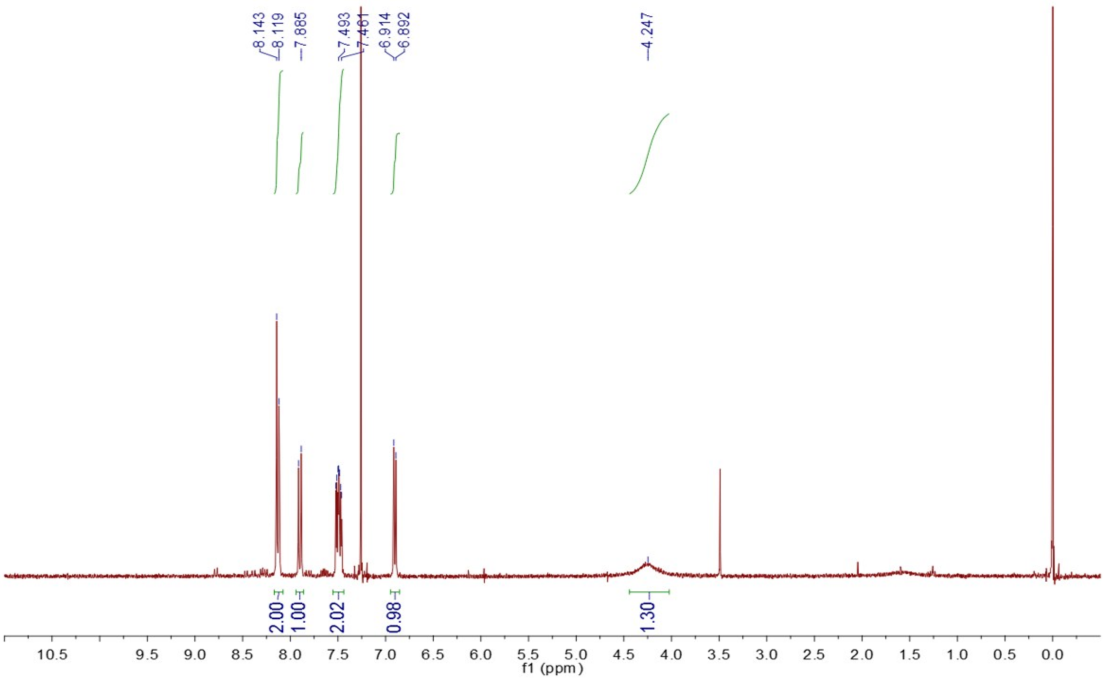
3. ^{1}H NMR and ^{13}C NMR








NH2
NO2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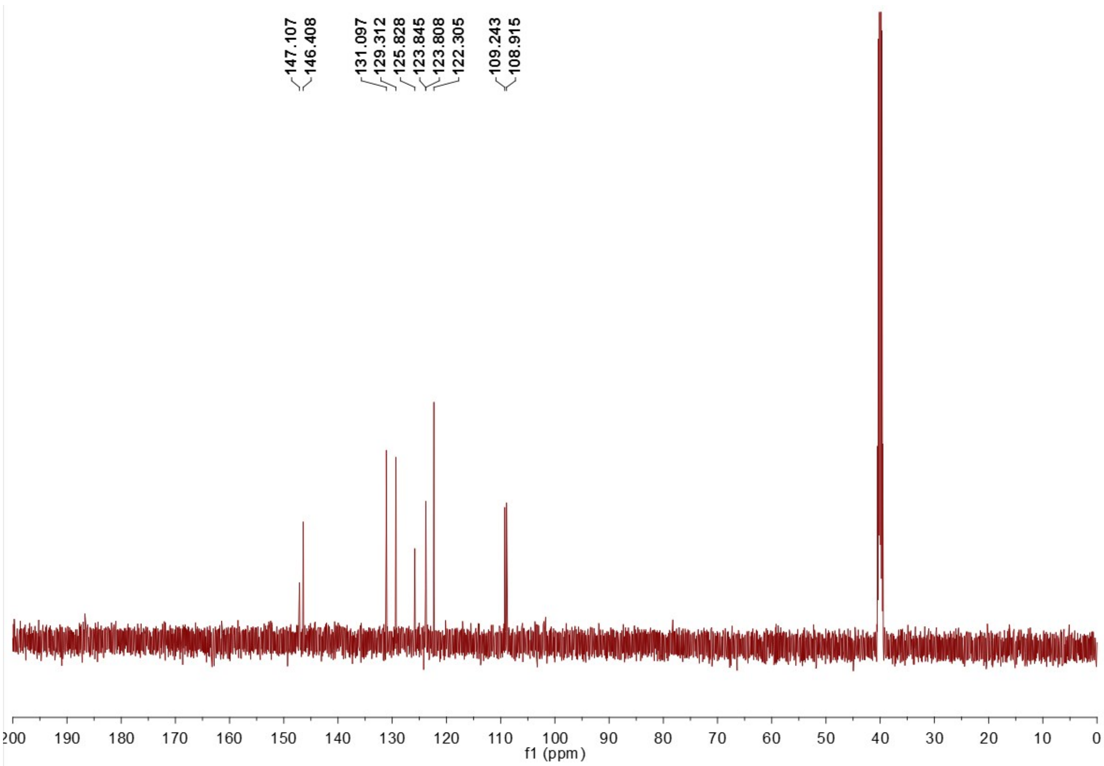
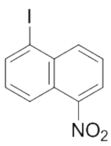
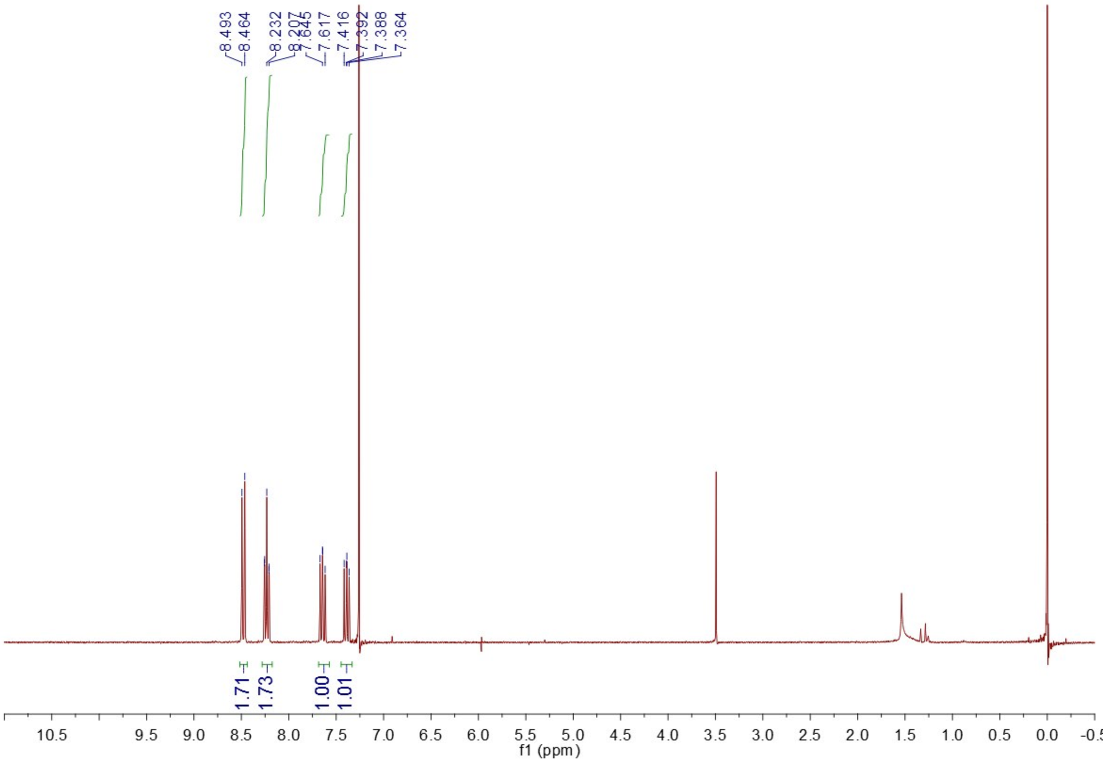
8.119
7.885
7.493
7.461
6.914
6.892
4.247
2.00
1.00
2.02
0.98
1.30
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.107
146.408
131.097
129.312
125.828
123.845
123.808
122.305
109.243
108.915
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


I
NO2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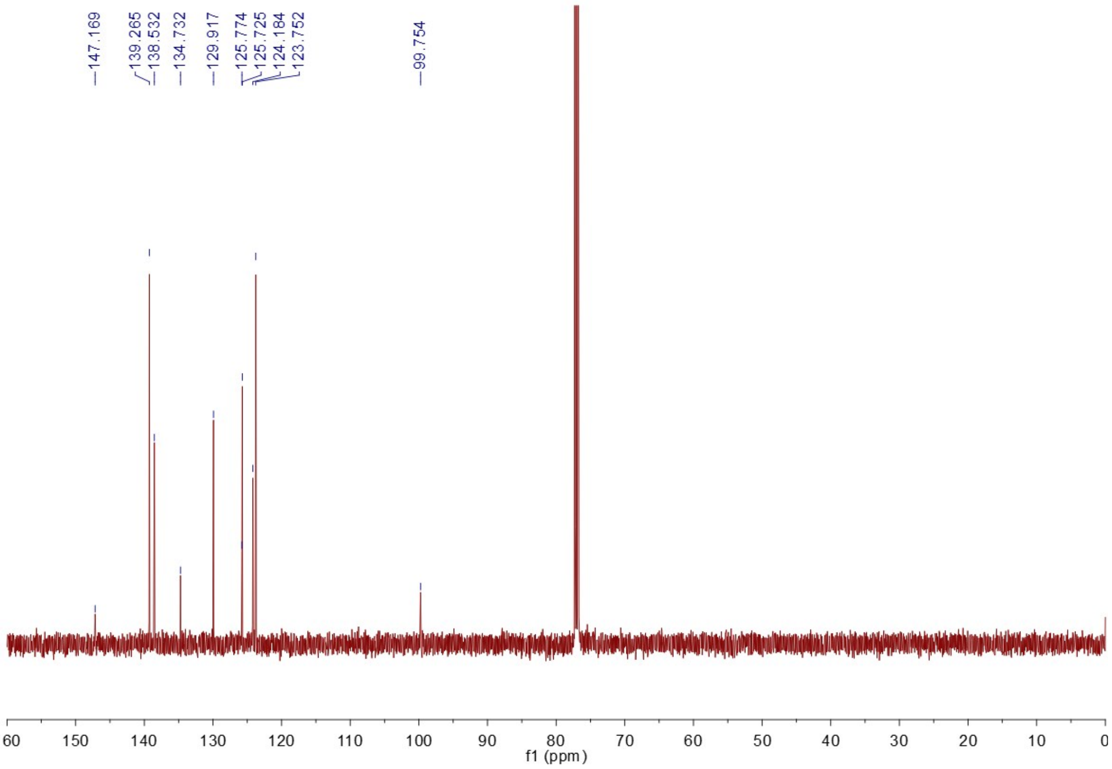
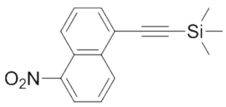
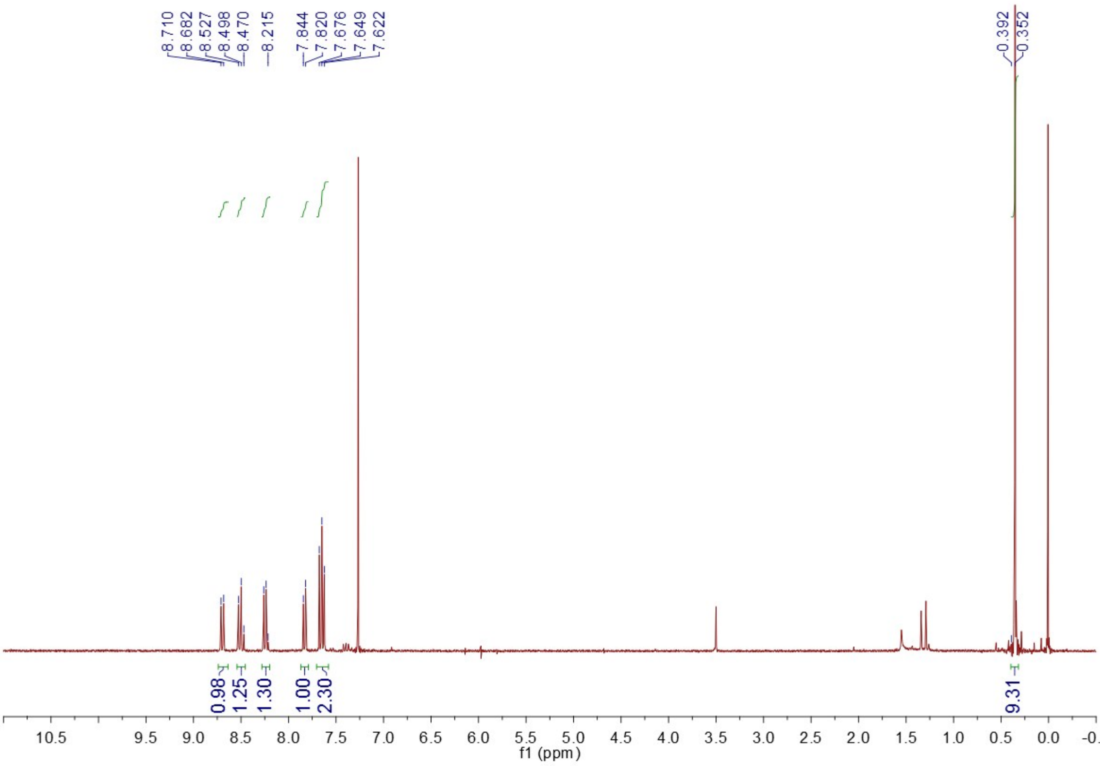
8.464
8.232
8.207
7.645
7.617
7.416
7.392
7.388
7.364
1.71
1.73
1.00
1.01
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.169
139.265
138.532
134.732
129.917
125.774
125.725
124.184
123.752
99.754
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


O2N
Si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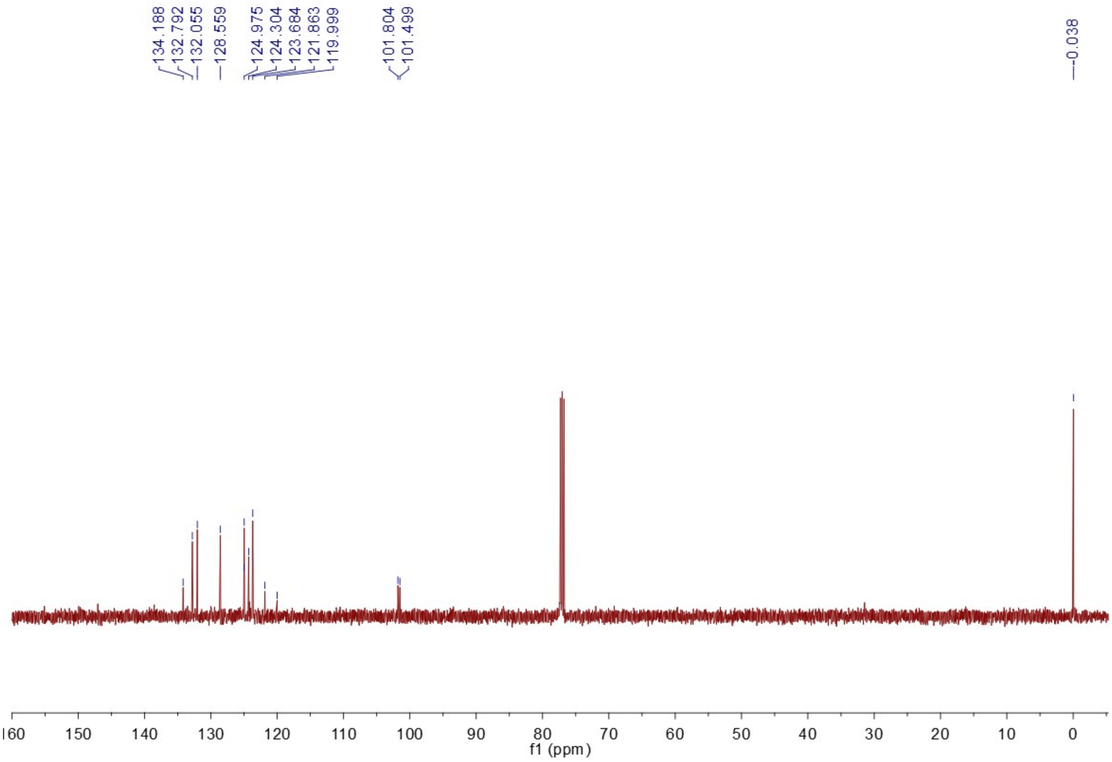
8.527
8.498
8.470
8.215
7.844
7.820
7.676
7.649
7.622
0.392
0.352
0.98
1.25
1.30
1.00
2.30
9.31
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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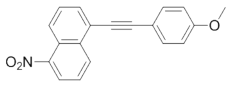
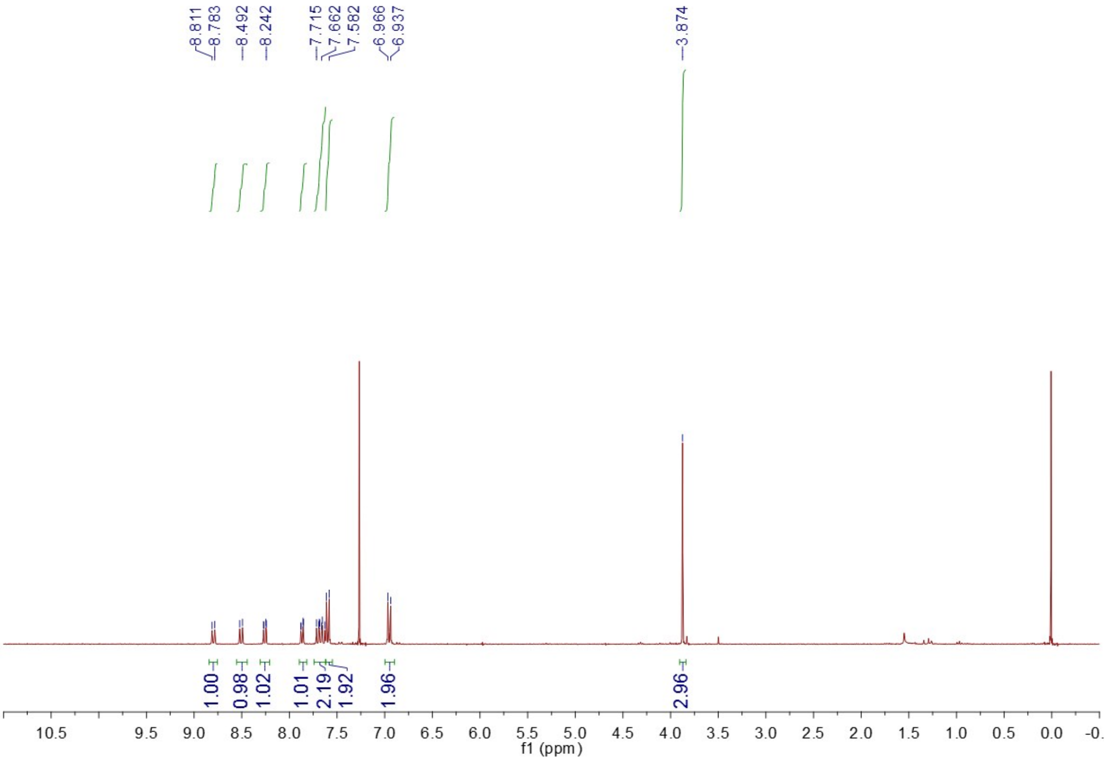
132.792
132.055
128.559
124.975
124.304
123.684
121.863
119.999
101.804
101.499
0.038
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O2N
O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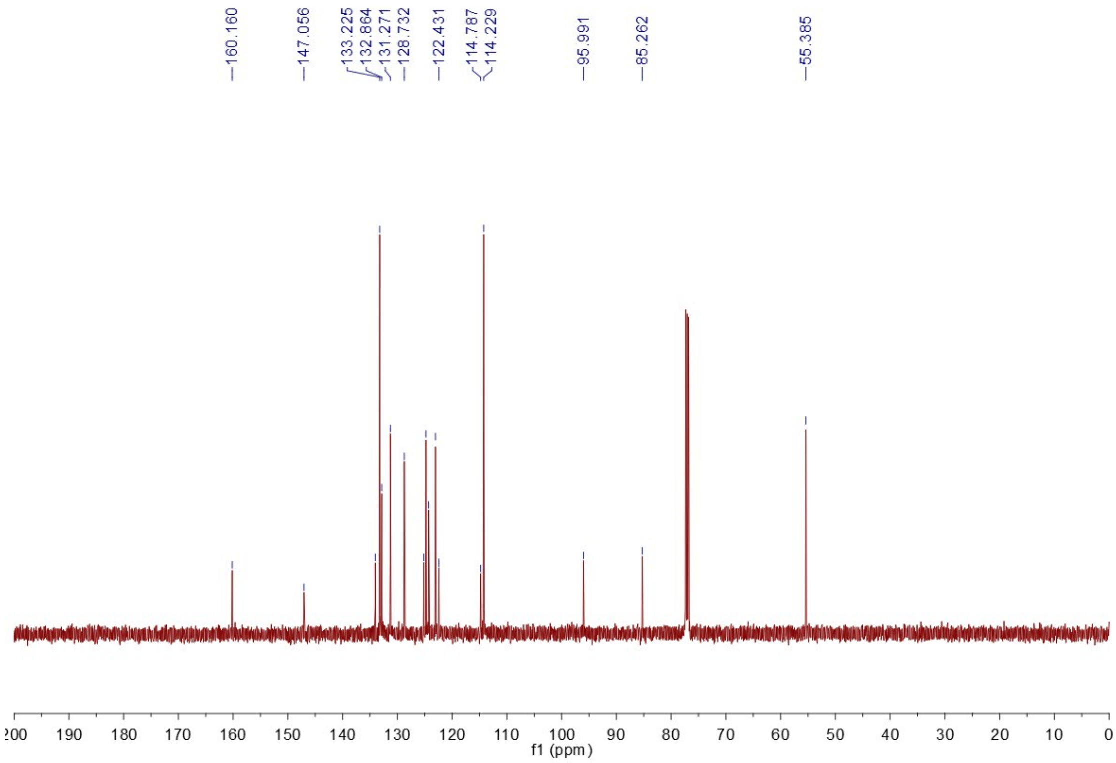
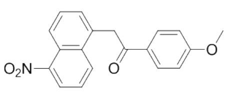
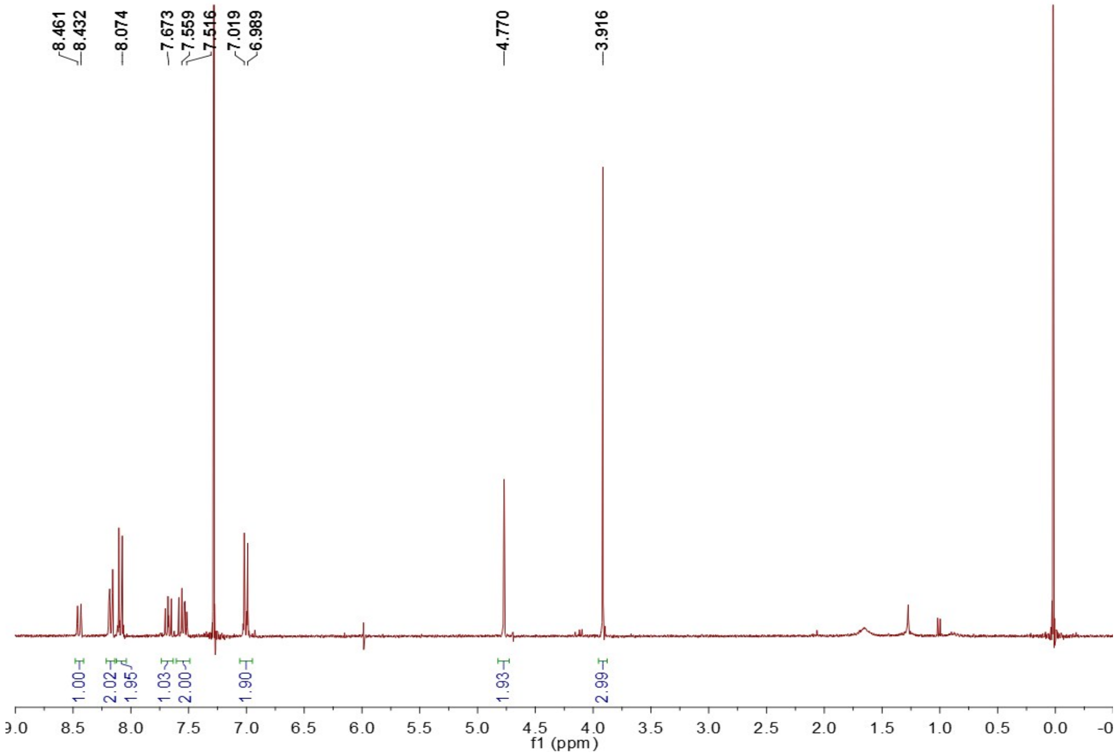
8.242
7.715
7.662
7.582
6.966
6.937
3.874
1.00
0.98
1.02
1.01
2.19
1.92
1.96
2.96
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.160
147.056
133.225
132.864
131.271
128.732
122.431
114.787
114.229
95.991
85.262
55.385
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O2N
O
O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8.074
7.673
7.559
7.516
7.019
6.989
4.770
3.916
1.00
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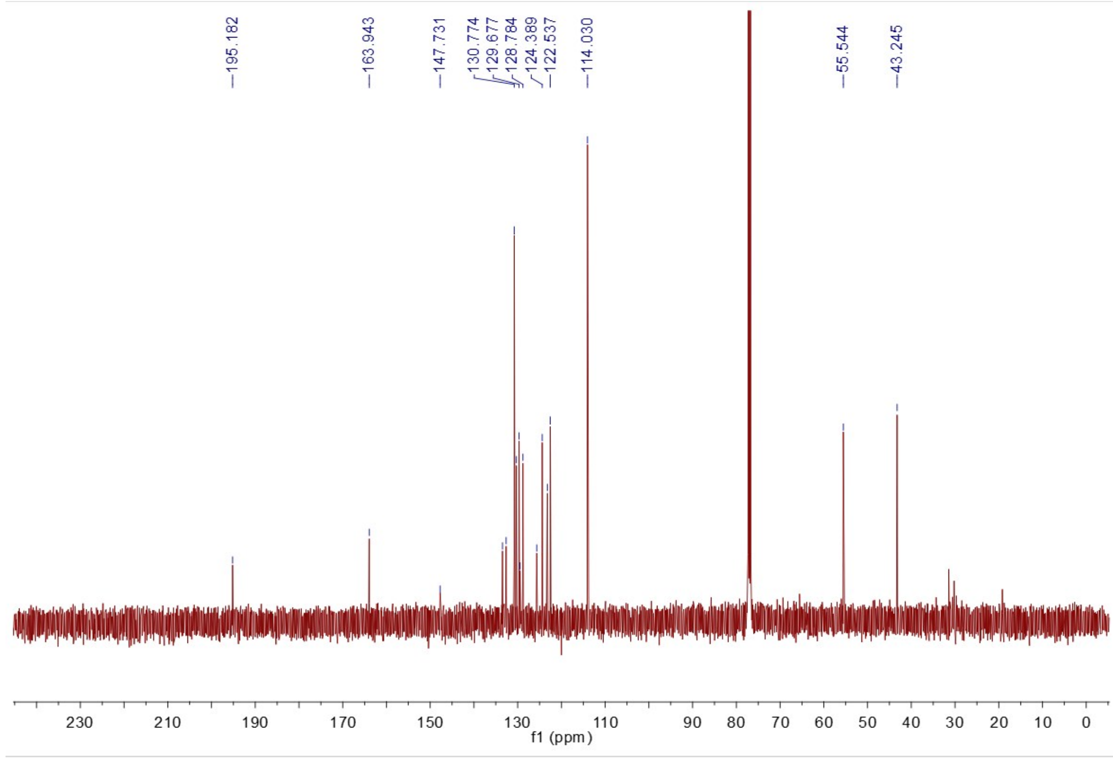
1.95
1.03
2.00
1.90
1.93
2.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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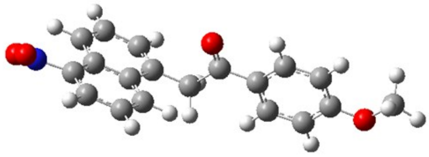
163.943
147.731
130.774
129.677
128.784
124.389
122.537
114.030
55.544
43.245
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4. The Cartesian Coordinate



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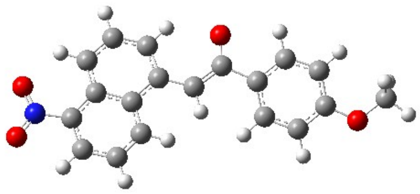
C	-1.92297909	0.12531074	-0.36707630
C	-3.31360985	0.34613894	-0.05119765
C	-4.17266874	-0.79893587	-0.10801512
C	-3.71551684	-2.06227185	-0.42029507
H	-2.00326852	-3.24366639	-1.00034262
H	-0.44635140	-1.35315715	-0.94891073
C	-1.00358748	1.22542941	-0.31775574
C	-3.73067789	1.64927310	0.33723943
H	-4.41375436	-2.89019089	-0.42551078
C	-2.82027768	2.67977707	0.39296746
C	-1.46569646	2.47079564	0.05575666
H	-4.76814735	1.83109970	0.57719378
H	-3.15001425	3.66971584	0.69363472
H	-0.77340024	3.30758045	0.09725832
C	0.45620306	1.05743586	-0.66973758
H	0.57982414	0.48866709	-1.60008558
H	0.88705756	2.04475248	-0.87466975
C	1.31345233	0.39585203	0.42400515
O	0.81222906	0.03478596	1.47980607
C	2.77069724	0.21557484	0.15822463
C	3.39927929	0.62489131	-1.03517519
C	3.55945938	-0.39100613	1.14826070
C	4.76030406	0.43521697	-1.22783768
H	2.82834710	1.09939417	-1.82636911
C	4.92624252	-0.58897899	0.97039329
H	3.07723151	-0.70610769	2.06782367
C	5.53480259	-0.17318649	-0.22532905
H	5.24946650	0.74967226	-2.14371714
H	5.50320468	-1.06062663	1.75671724
O	6.85691237	-0.31309740	-0.50558284
C	7.70961456	-0.91409027	0.46703985
H	7.40562520	-1.94611701	0.67792893
H	8.70637722	-0.91182322	0.02566000
H	7.72018160	-0.33420094	1.39743141
N	-5.61840646	-0.70140764	0.16216412
O	-6.17286224	-1.68747616	0.65400649
O	-6.20739899	0.34025802	-0.13864134



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C	3.41868436	0.28383030	0.00058066
C	4.44433421	-0.74159877	-0.05538784
C	4.13183565	-2.09636037	-0.16314456
H	2.56708138	-3.56448280	-0.31273292
H	0.76486892	-1.91311864	-0.21427857
C	0.90966407	0.77066698	0.02422302
C	3.65408024	1.66924600	0.08289329
H	4.94466041	-2.80908717	-0.20372400
C	2.57365800	2.55569857	0.11749283
C	1.24916474	2.14541700	0.08886293
H	4.66202533	2.04556412	0.11500971
H	2.78730726	3.62185928	0.17406637
H	0.43808040	2.86101430	0.12016145
C	-0.44545996	0.33814124	0.03036683
H	-0.63494489	-0.72501774	0.00193129
C	-1.60775273	1.15723253	0.04353846
O	-1.64026380	2.41734648	0.00695204
C	-2.95616182	0.44983443	0.07272751
C	-3.16891959	-0.86979654	0.51494108
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H	-4.59632227	-2.45522952	0.87941796
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N	5.86562129	-0.45481510	-0.00893043
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