

N[1,3]-Sigmatropic Shift in the Benzidine Rearrangement: Experimental and Theoretical Investigation

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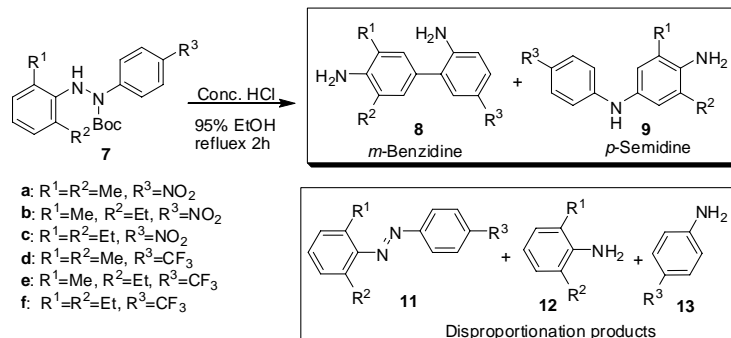
Electronic Supporting Information

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1. Details of Rearrangement Reactions

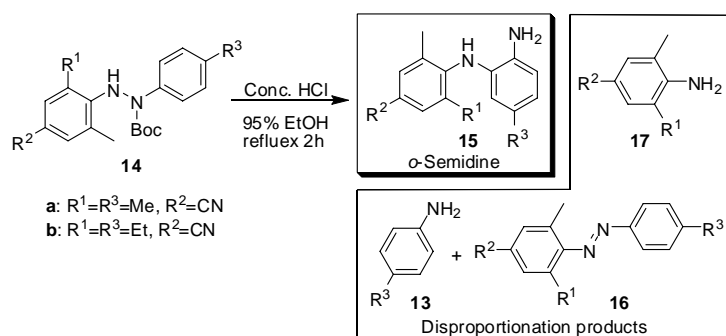
Table S1. Acid-catalyzed rearrangement of 2,4,6-trisubstituted N,N' -diaryl hydrazines **7**



Entry	7	Isolated yield (%)				
		8	9	11	12	13
1	a	5	5	24	10	18
2	b	3	3 ^a	26	11	20
3	c	4 ^a	4	27	10	25
4	d	21	18	10	6	9
5	e	10	18	12	6	10
6	f	14	16	15	8	12

^a The crude product was reacted with Ac_2O to afford the *N*-acetylated product.

Table S2. Acid-catalyzed rearrangement of 2,4,4',6-tetrasubstituted N,N' -diaryl hydrazines



Entry	14	Isolated yield (%)			
		15	16	17	13
1	a	35	22	17	8
2	b	16	38	29	17

2. Analytical Data of Unknown azobenzenes 11

1-(2-Ethyl-6-methylphenyl)-2-(4-nitrophenyl)diazene (IIb): Red oil, 70 mg, yield 26%, ^1H NMR (300 MHz, CDCl_3) δ : 1.20 (t, $J = 7.5$ Hz, 3 H), 2.40 (s, 3 H), 2.83 (q, $J = 7.5$ Hz, 2 H), 7.13-7.28 (m, 3 H), 7.97 (m, 2 H), 8.37 (m, 2 H). ^{13}C NMR (75 MHz, CDCl_3) δ : 155.7, 150.1, 148.7, 139.5, 130.6, 129.9, 129.6, 127.8, 124.8, 123.0, 25.5, 19.8, 15.8. IR (KBr) ν (cm^{-1}): 2968, 2929, 2871, 1524, 1344. HRMS (ESI) calcd. for $\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ m/z : 270.1237, found 270.1251.

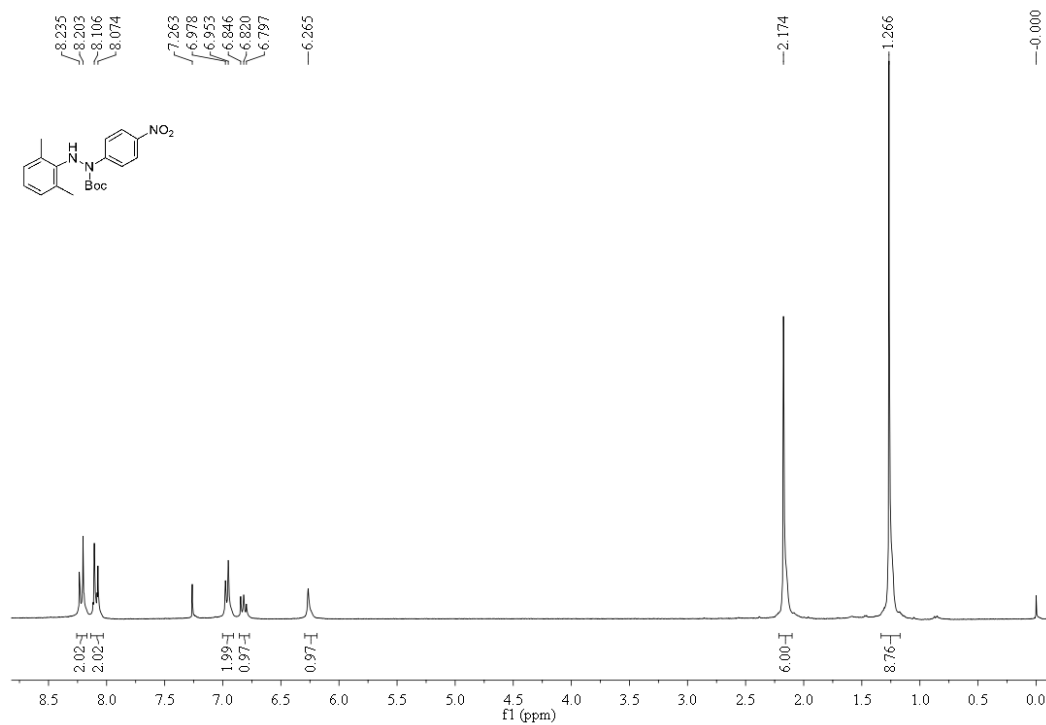
1-(2,6-Diethylphenyl)-2-(4-nitrophenyl)diazene (IIc): Red oil, 76 mg, yield 27%, ^1H NMR (300 MHz, CDCl_3) δ : 1.19 (t, $J = 7.5$ Hz, 6 H), 2.77 (q, $J = 7.5$ Hz, 4 H), 7.18-7.32 (m, 3 H), 7.99 (m, 2 H), 8.41 (m, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ : 155.7, 150.1, 148.7, 137.7, 129.8, 127.9, 124.8, 123.0, 25.6, 15.7. IR (KBr) ν (cm^{-1}): 2967, 2931, 2871, 1525, 1344. HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{17}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ m/z : 284.1394, found 284.1405.

1-(2-Ethyl-6-methylphenyl)-2-(4-(trifluoromethyl)phenyl)diazene (IIe): Red oil, 35 mg, yield 12%, ^1H NMR (300 MHz, CDCl_3) δ : 1.18 (t, $J_1 = 7.5$ Hz, 3 H), 2.36 (s, 3 H), 2.78 (q, $J_1 = 7.5$ Hz, 2 H), 7.13-7.25 (m, 3 H), 7.79 (d, $J_2 = 8.2$ Hz, 2 H), 7.97 (d, $J_2 = 8.2$ Hz, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ : 154.6, 150.7, 138.5, 132.3 (q, $J_1 = 32.8$ Hz), 123, 130.0, 129.1, 127.7, 126.4 (q, $J_2 = 3.8$ Hz), 123.9 (q, $J_3 = 273.4$ Hz), 122.7, 25.3, 19.4, 15.7. IR (KBr) ν (cm^{-1}): 2925, 2853, 1322. HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{15}\text{F}_3\text{N}_2$ $[\text{M}+\text{H}]^+$ m/z : 293.1260, found 293.1273.

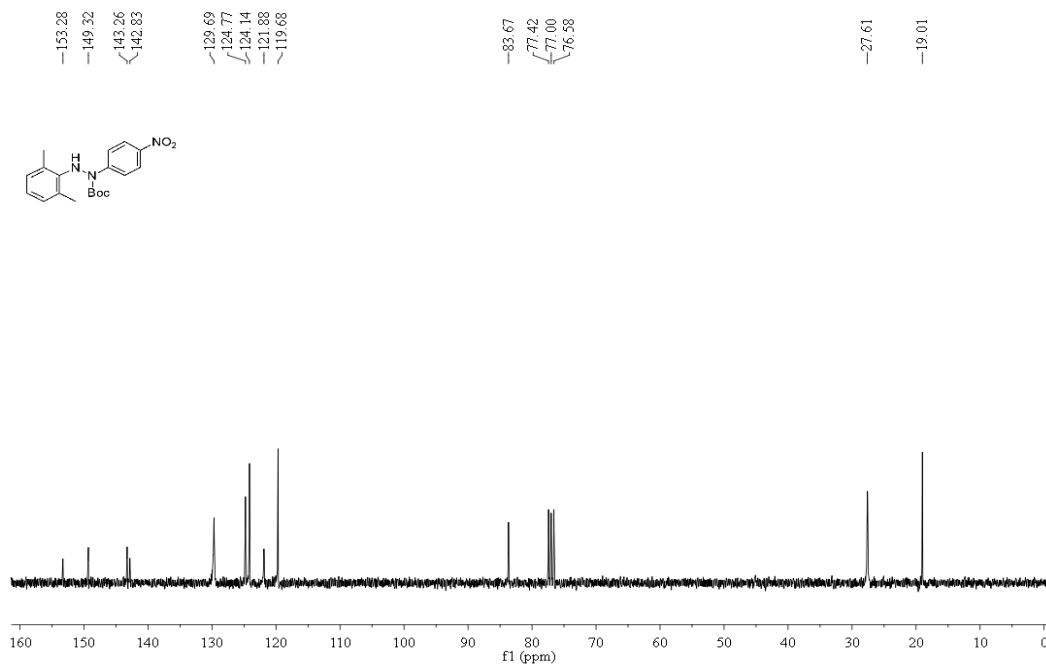
1-(2,6-Diethylphenyl)-2-(4-(trifluoromethyl)phenyl)diazene (IIf): Red oil, 46 mg, yield 15%, ^1H NMR (300 MHz, CDCl_3) δ : 1.17 (t, $J_1 = 7.5$ Hz, 6 H), 2.72 (q, $J_1 = 7.5$ Hz, 4 H), 7.16-7.26 (m, 3 H), 7.80 (d, $J_2 = 8.2$ Hz, 2 H), 7.97 (d, $J_2 = 8.2$ Hz, 2 H). ^{13}C NMR (126 MHz, CDCl_3) δ : 154.5, 150.7, 137.0, 132.4 (q, $J_1 = 32.8$ Hz), 129.1, 127.7, 126.4 (q, $J_2 = 3.8$ Hz), 123.9 (q, $J_3 = 272.2$ Hz), 122.7, 25.3, 15.6. IR (KBr) ν (cm^{-1}): 2967, 2929, 2872, 1322. HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{17}\text{F}_3\text{N}_2$ $[\text{M}+\text{H}]^+$ m/z : 307.1417, found 307.1431.

3. Copies of ^1H NMR and ^{13}C NMR Spectra

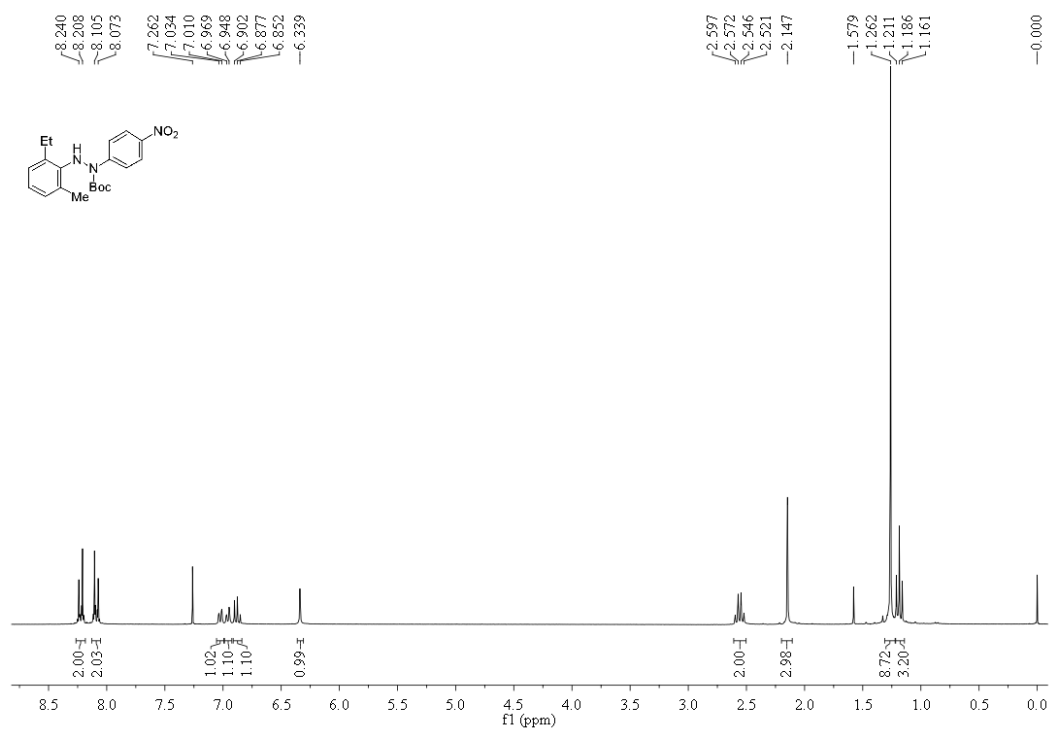
7a ^1H NMR, 300 MHz, CDCl_3



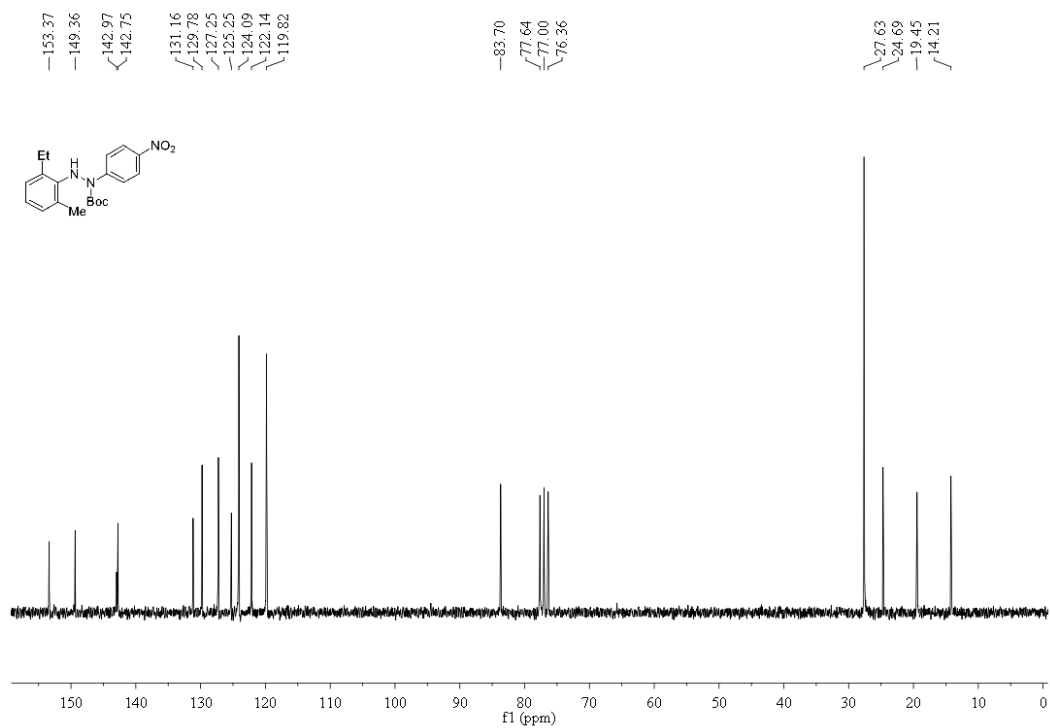
7a ^{13}C NMR, 75 MHz, CDCl_3



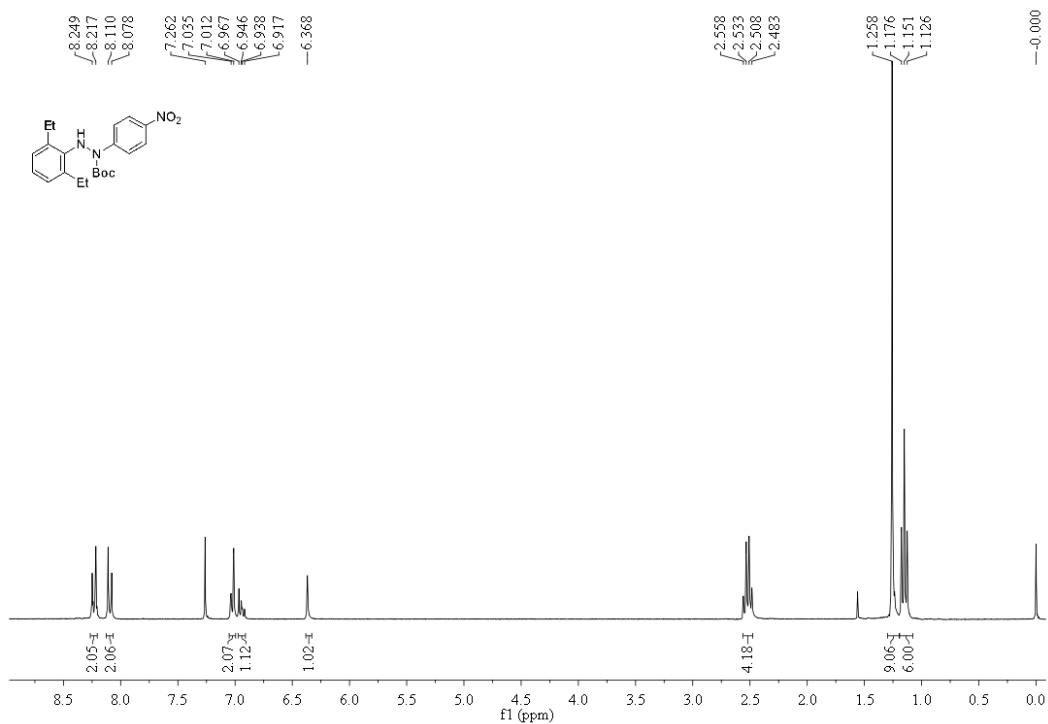
7b ^1H NMR, 300 MHz, CDCl_3



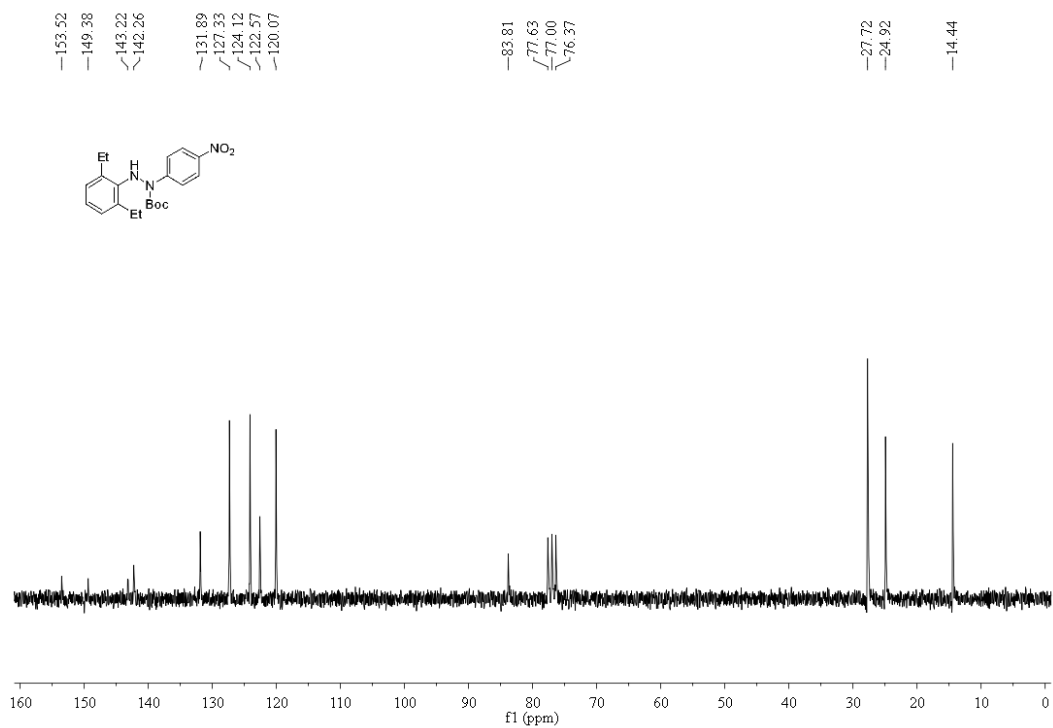
7b ^{13}C NMR, 50 MHz, CDCl_3



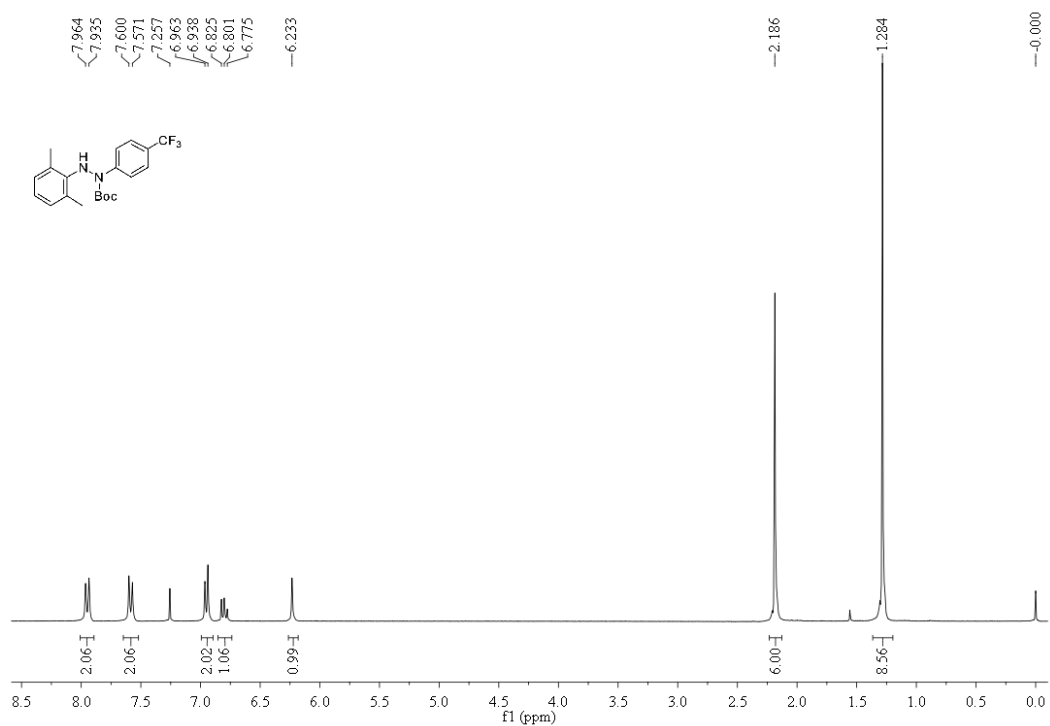
7c ¹H NMR, 300 MHz, CDCl₃



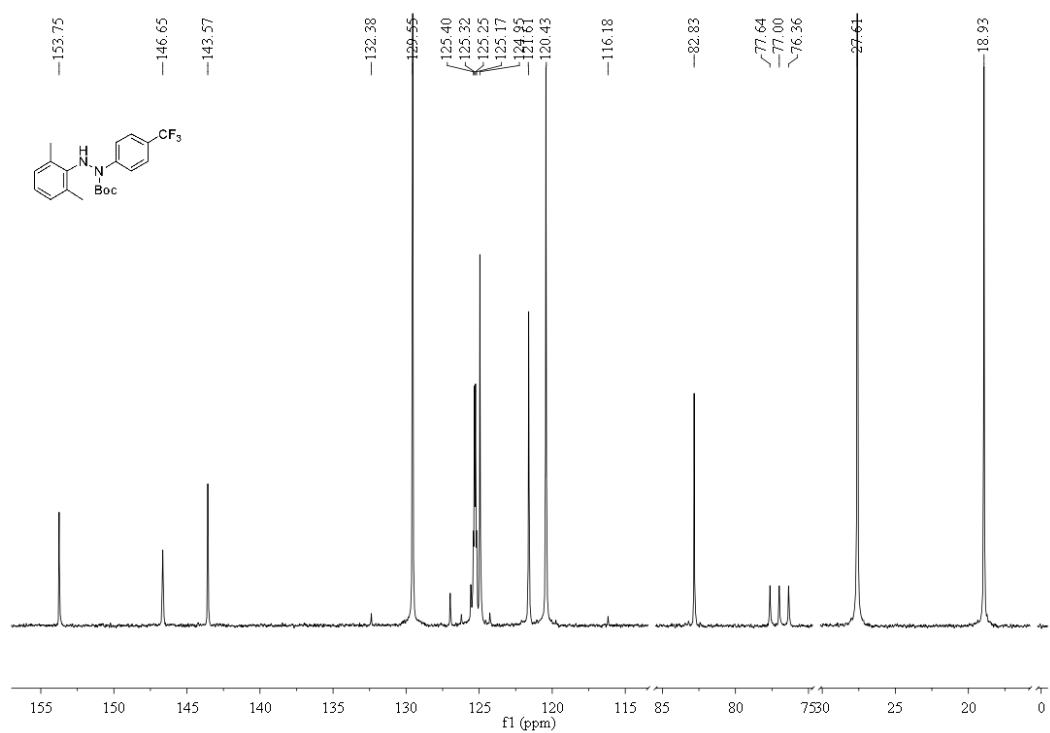
7c ¹³C NMR, 75 MHz, CDCl₃



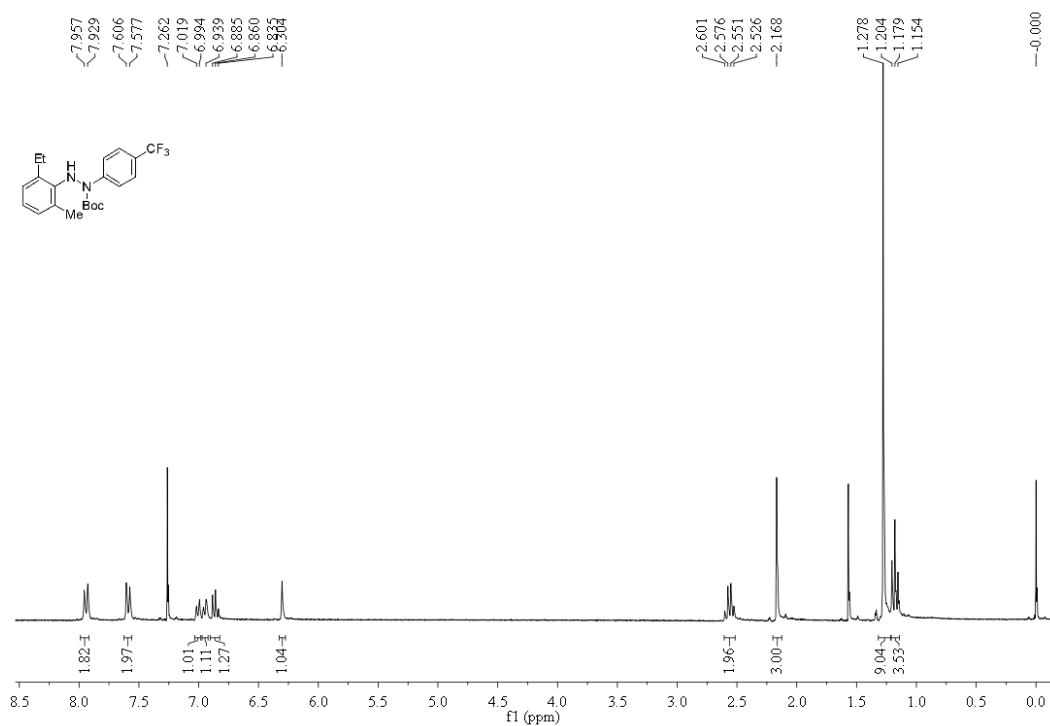
7d ¹H NMR, 300 MHz, CDCl₃



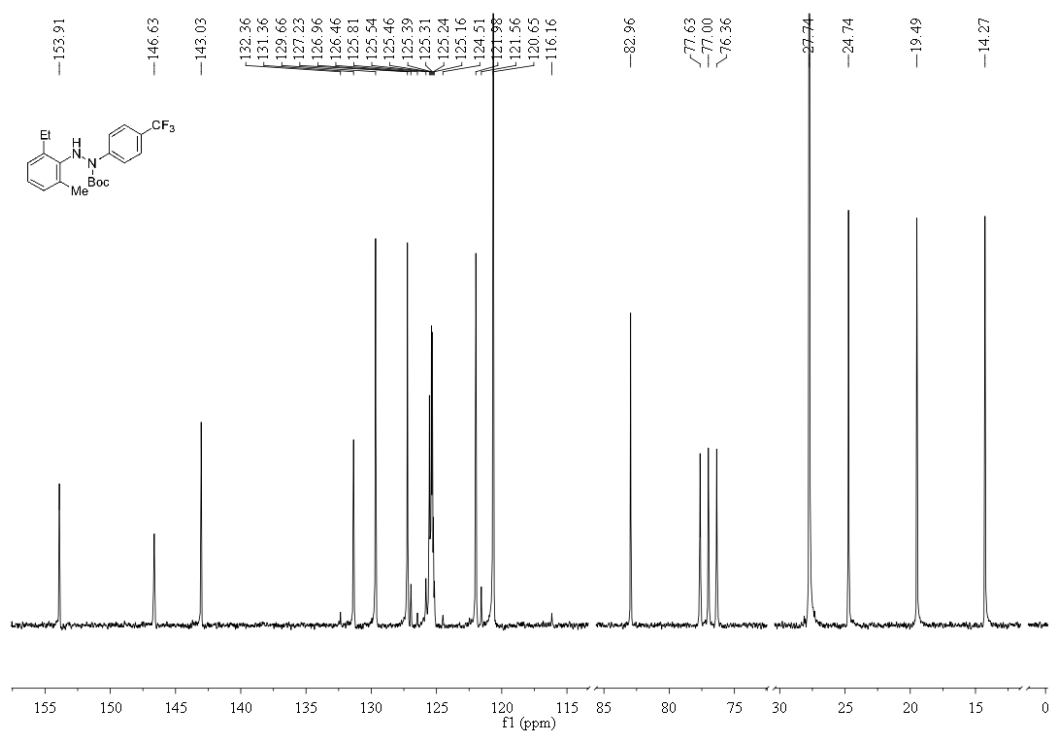
7d ¹³C NMR, 50 MHz, CDCl₃



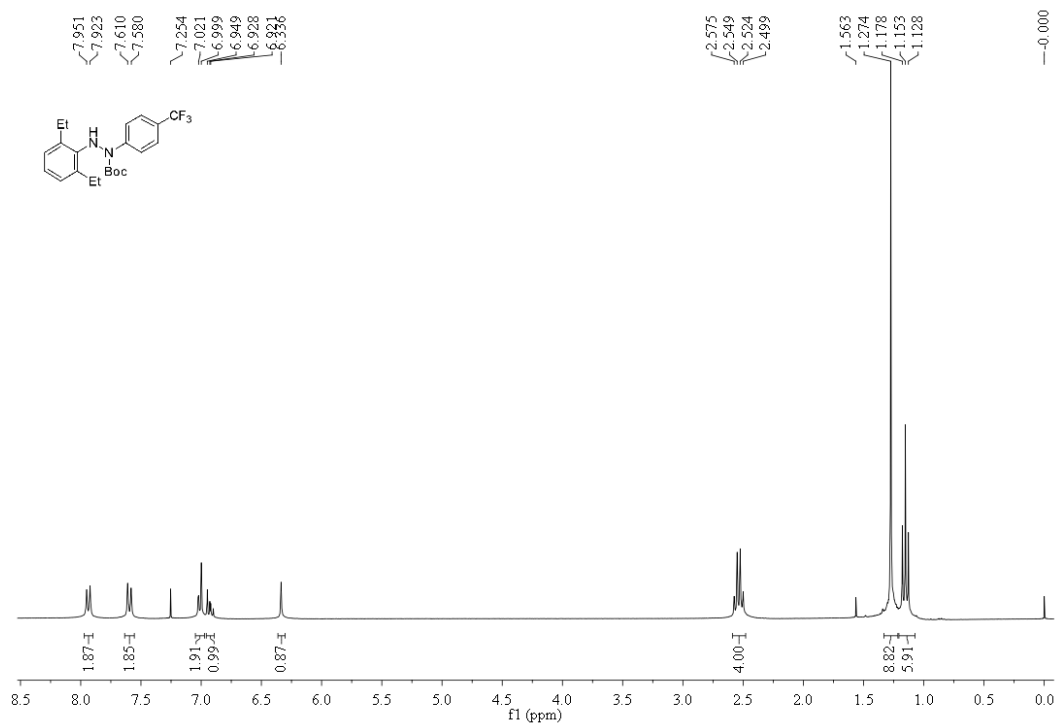
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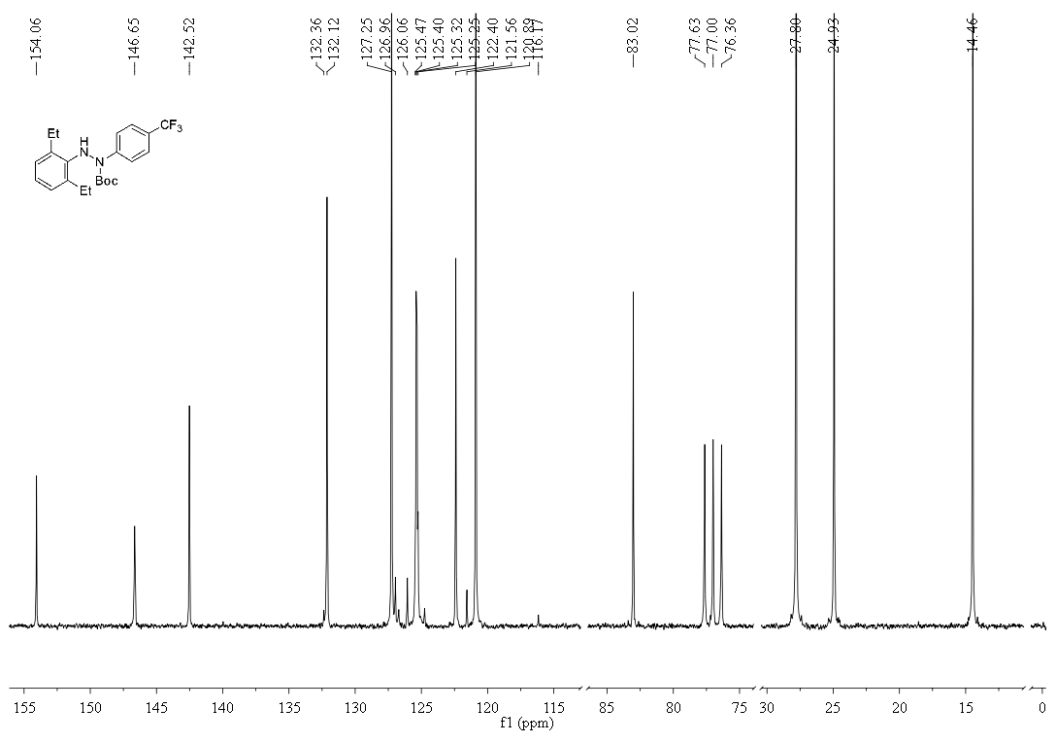
7e ^{13}C NMR, 50 MHz, CDCl_3



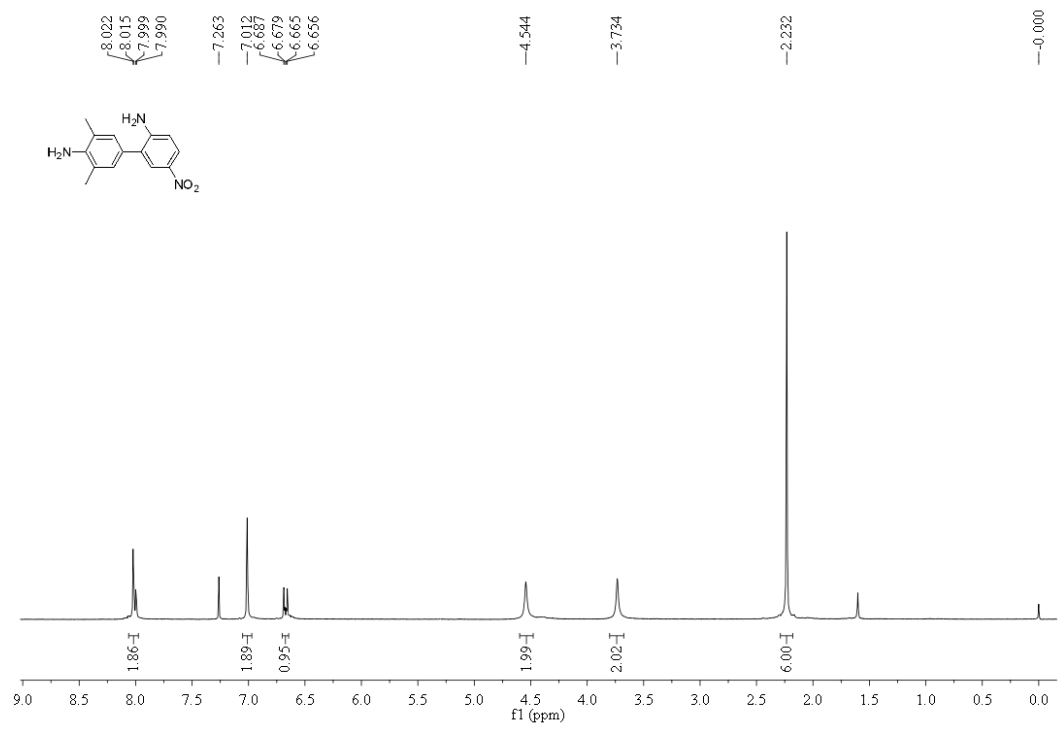
7f ^1H NMR, 300 MHz, CDCl_3



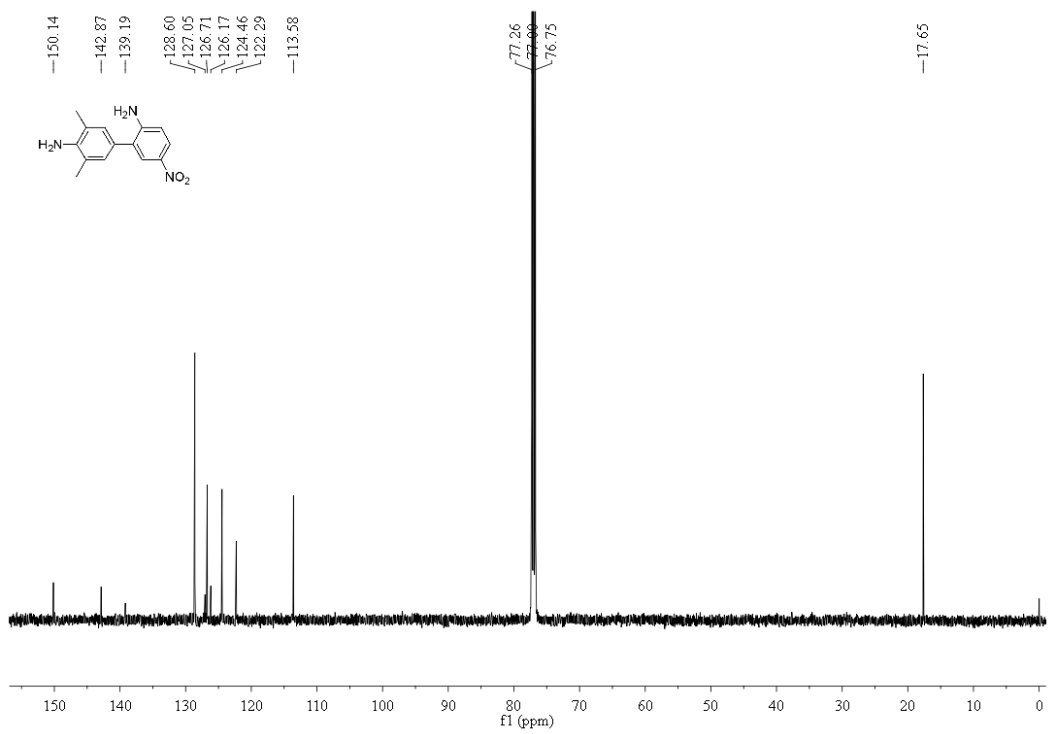
7f ^{13}C NMR, 50 MHz, CDCl_3



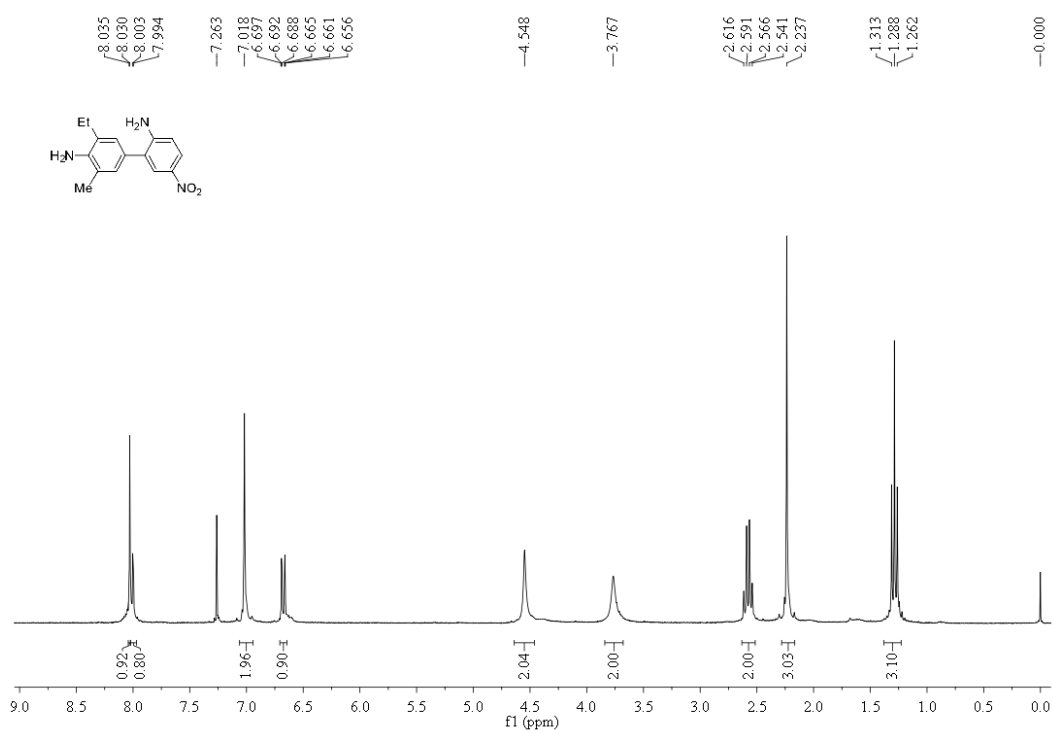
8a ^1H NMR, 300 MHz, CDCl_3



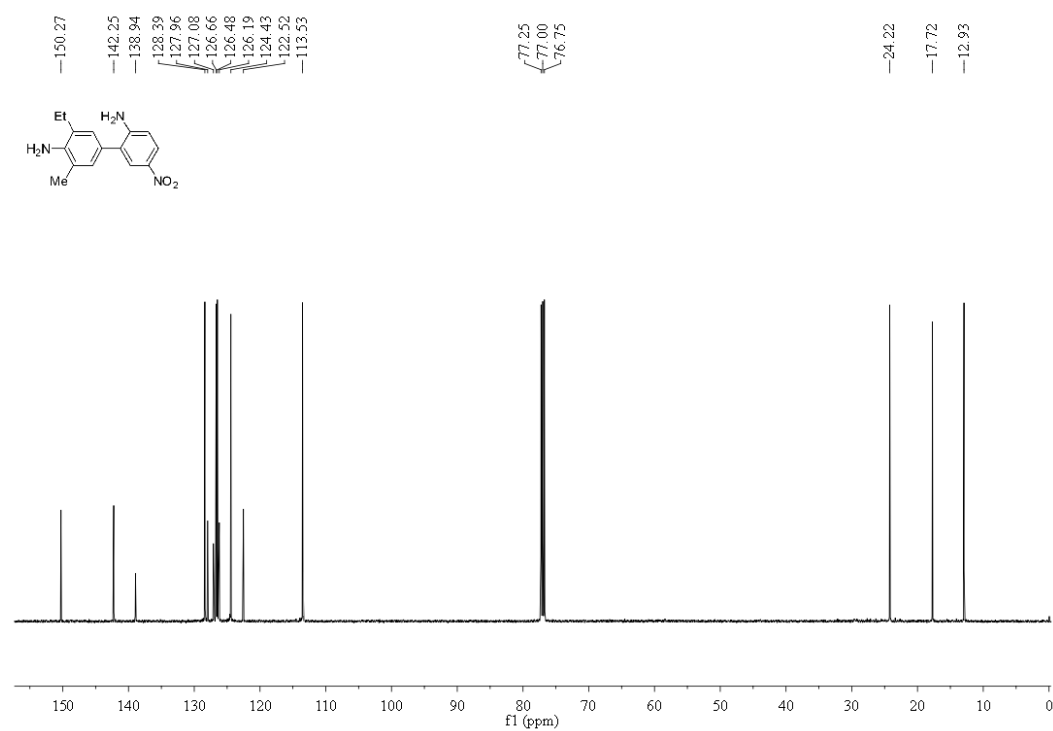
8a ^{13}C NMR, 126 MHz, CDCl_3



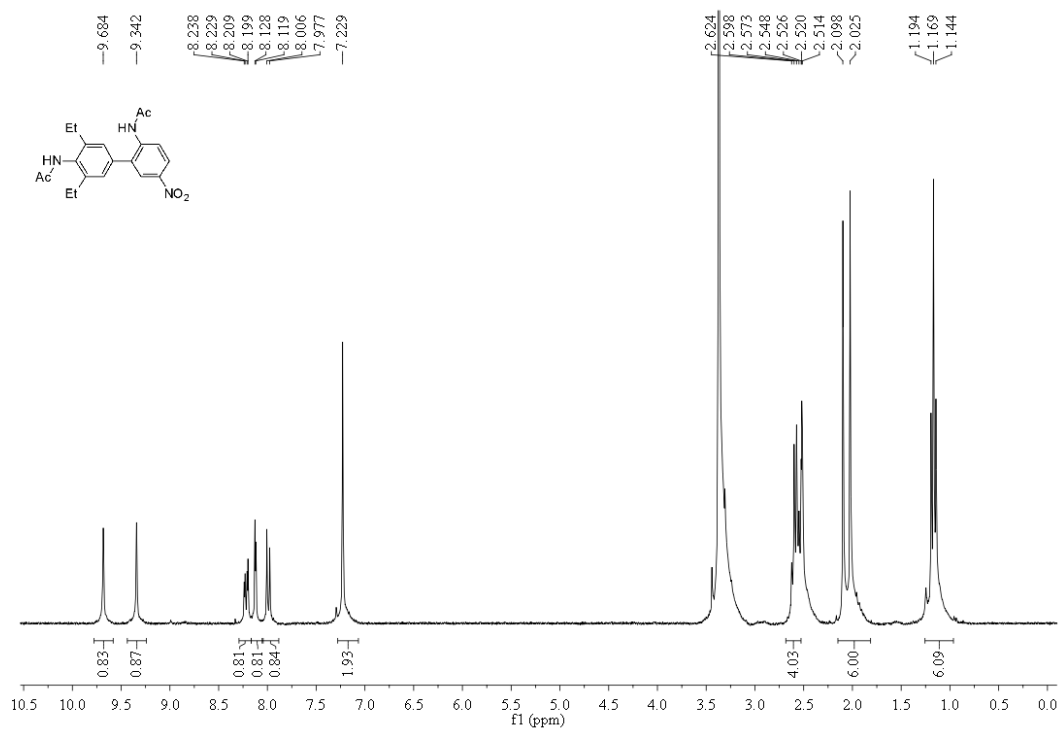
8b ^1H NMR, 300 MHz, CDCl_3



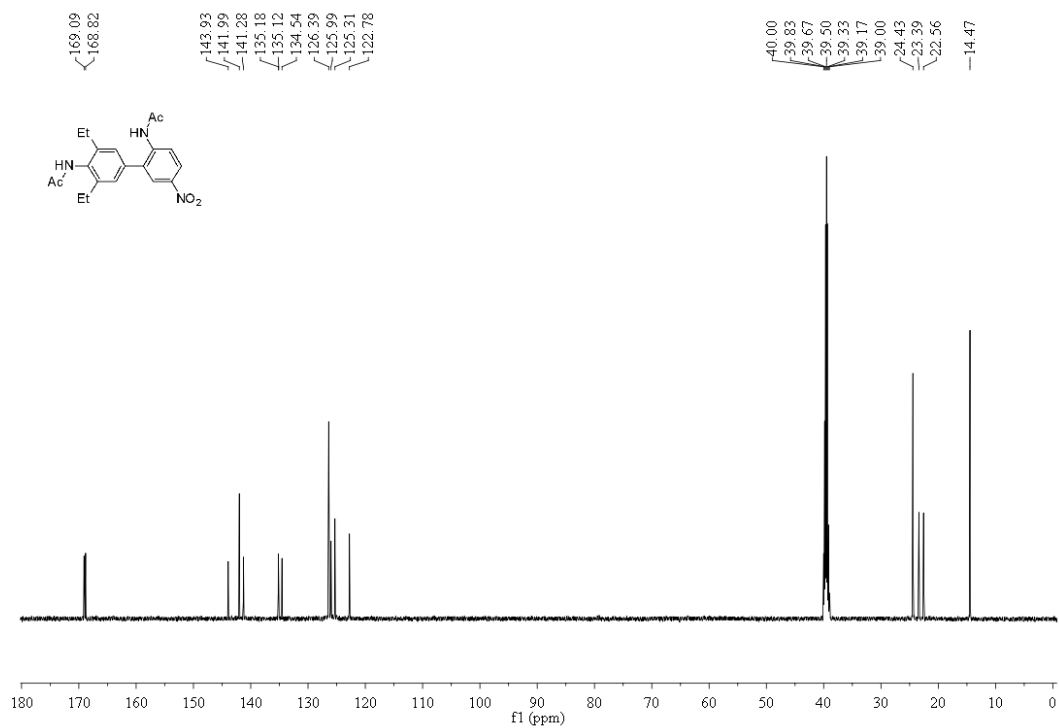
8b ^{13}C NMR, 126 MHz, CDCl_3



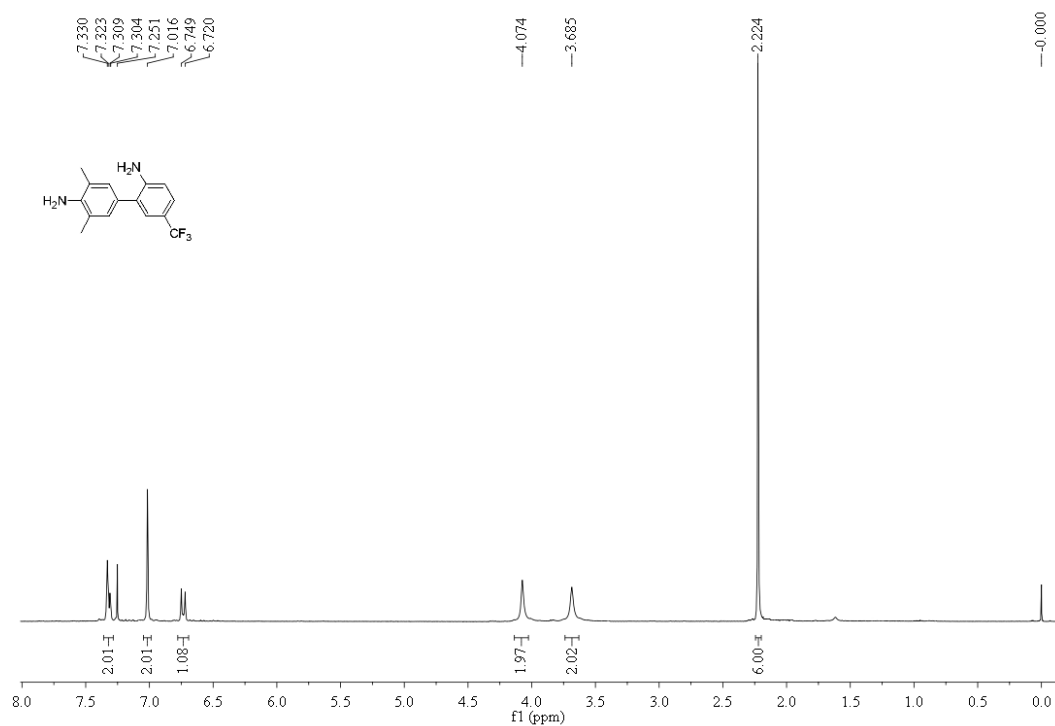
8c ^1H NMR, 300 MHz, $\text{DMSO-}d_6$



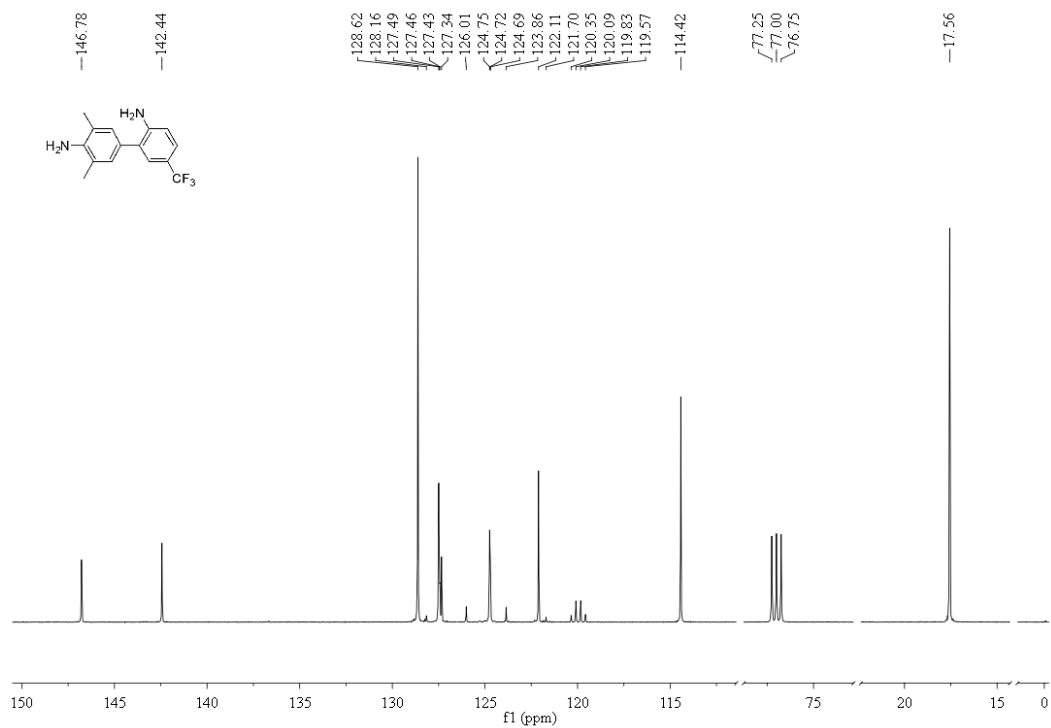
8c ^{13}C NMR, 126 MHz, $\text{DMSO-}d_6$



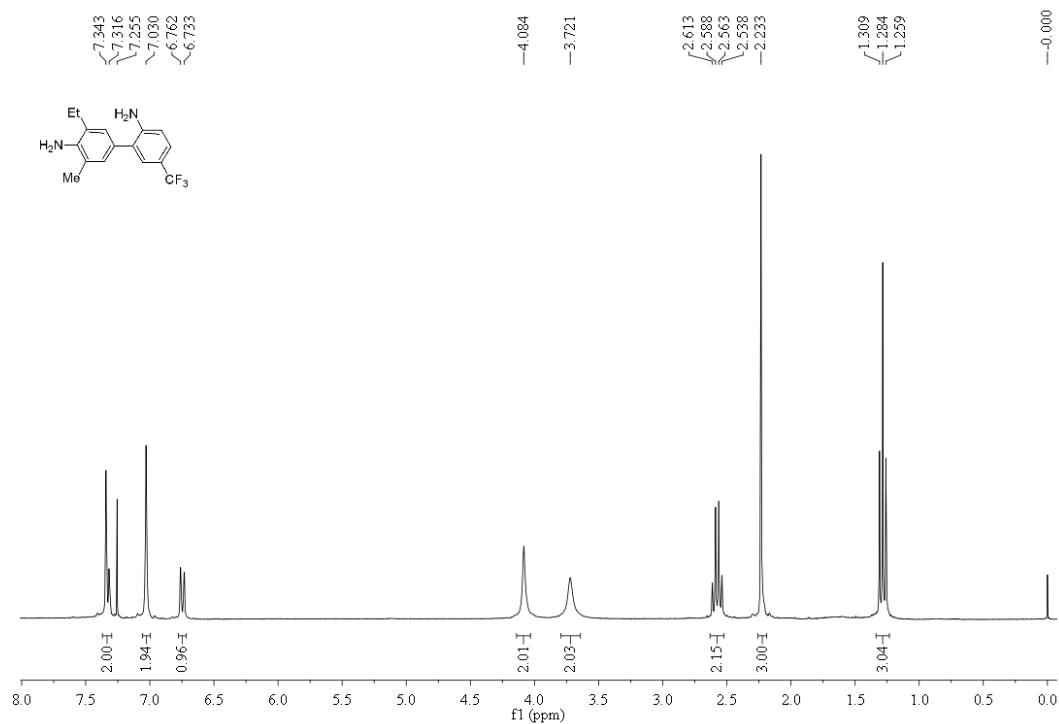
8d ^1H NMR, 300 MHz, CDCl_3



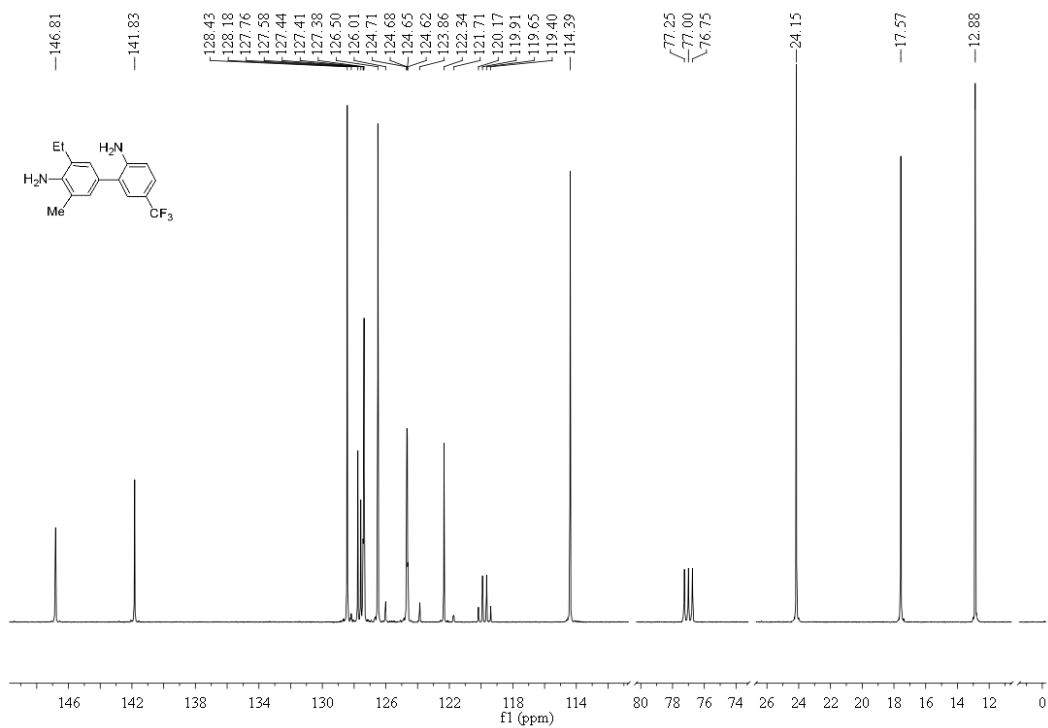
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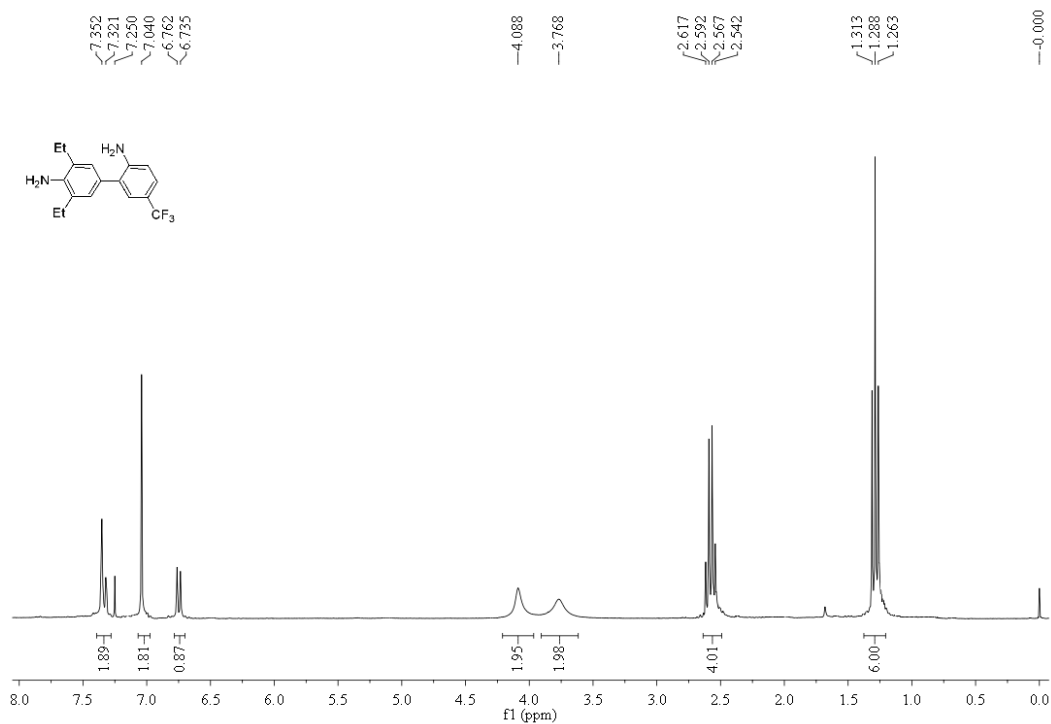
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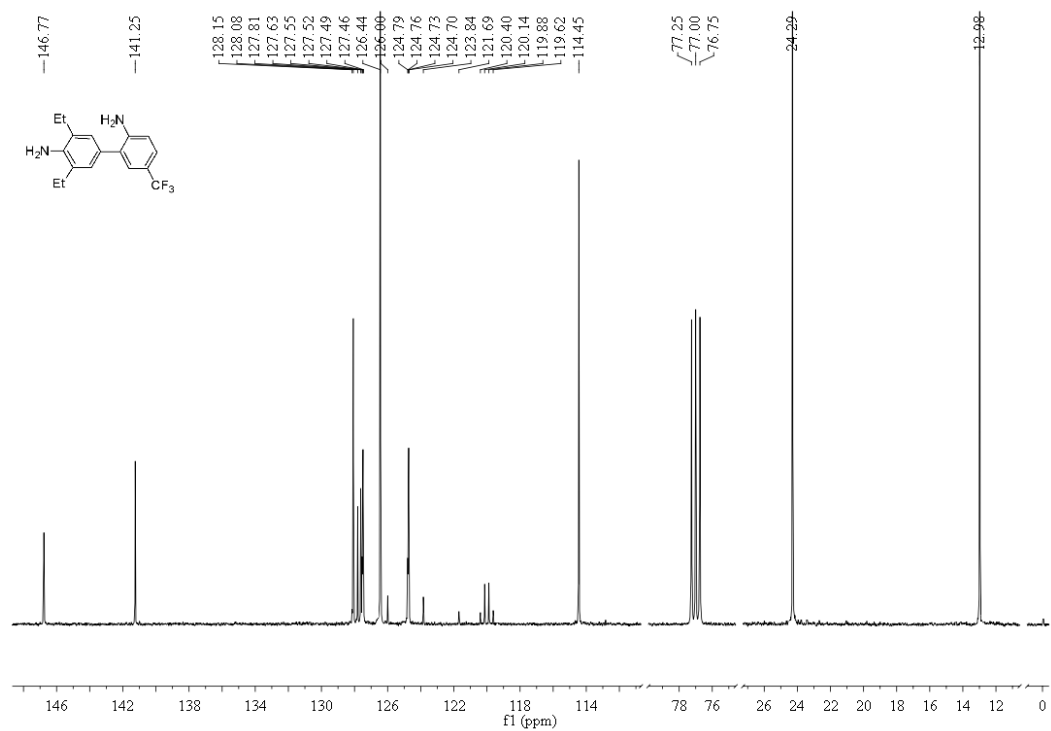
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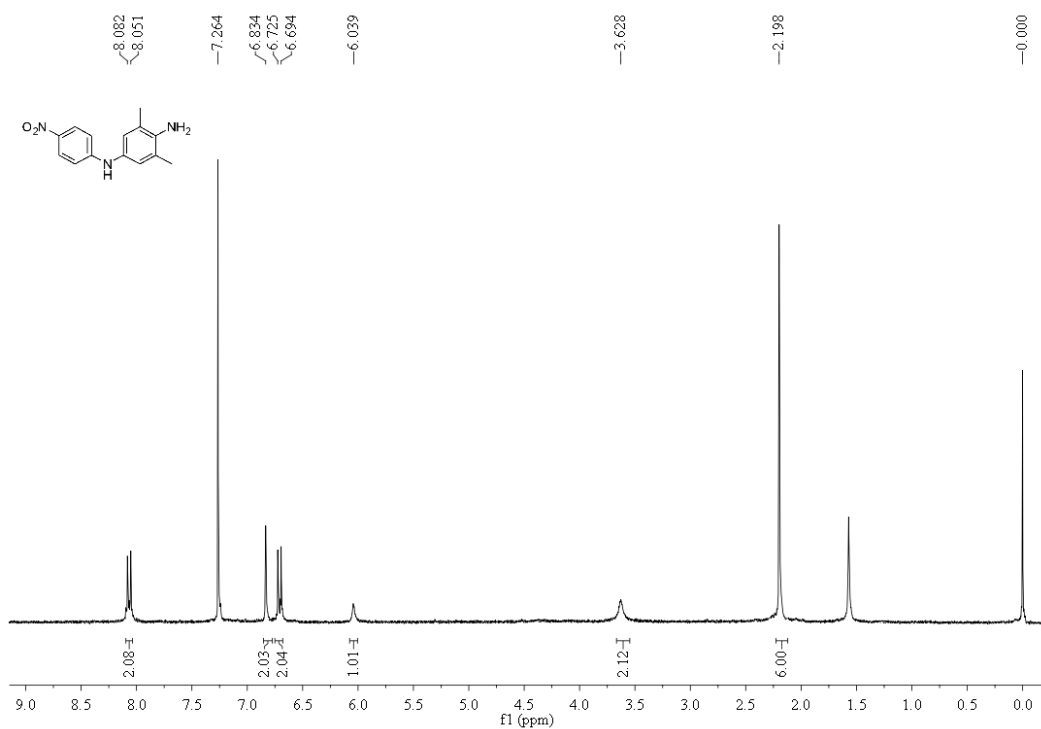
8f ^1H NMR, 300 MHz, CDCl_3



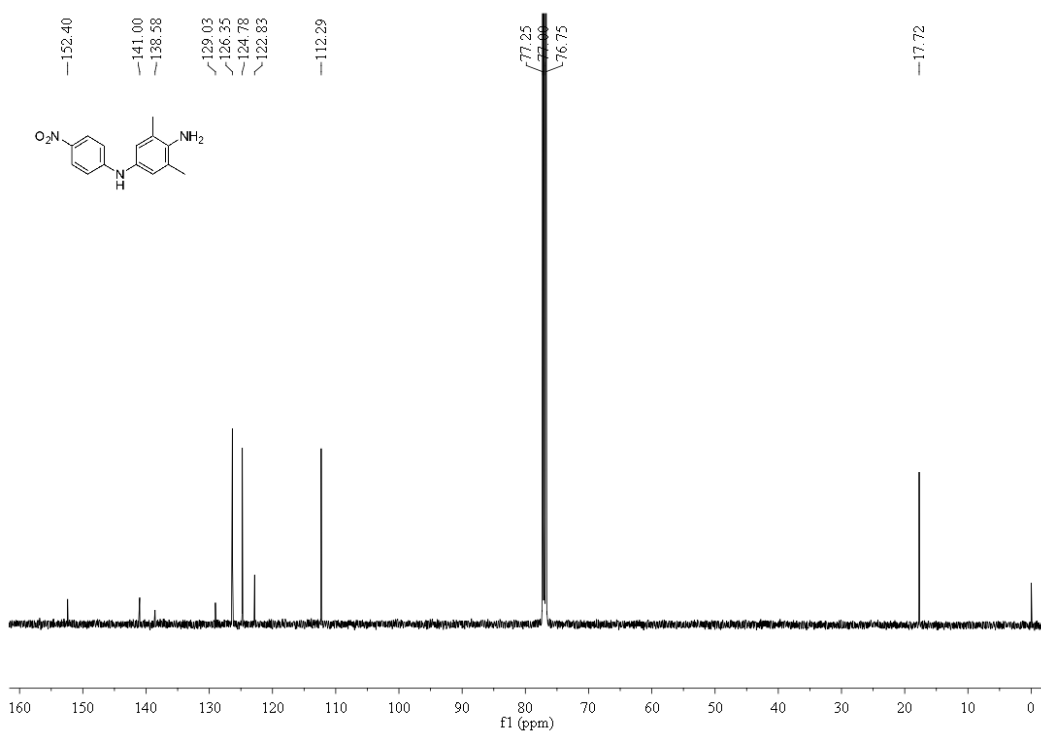
8f ^{13}C NMR, 126 MHz, CDCl_3



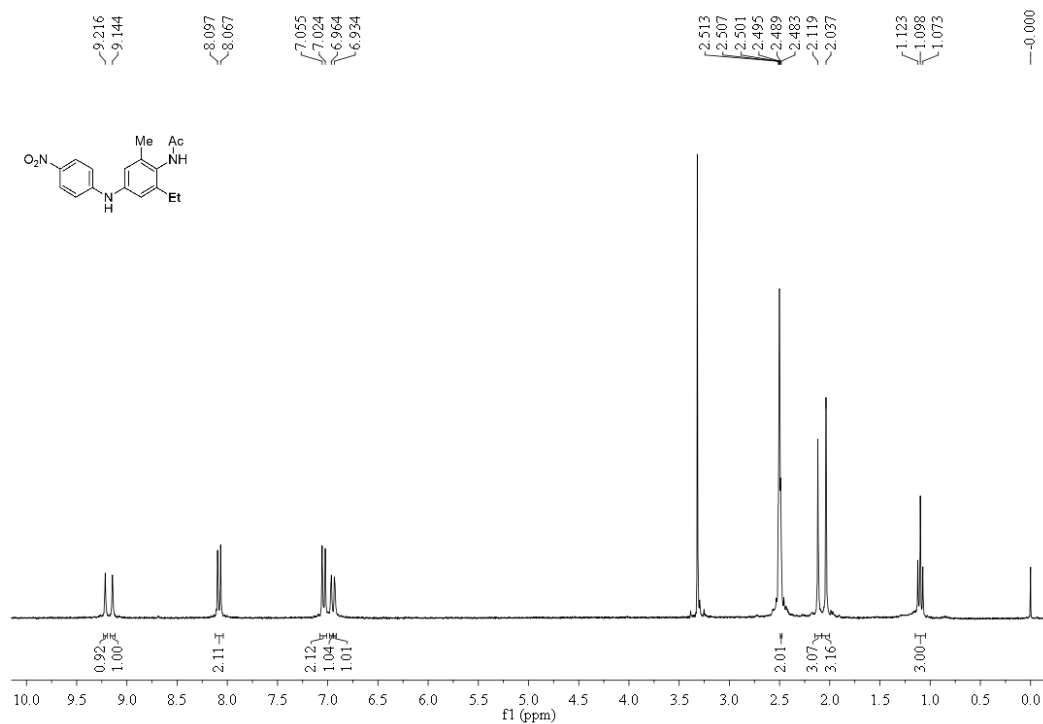
9a ¹H NMR, 300 MHz, CDCl₃



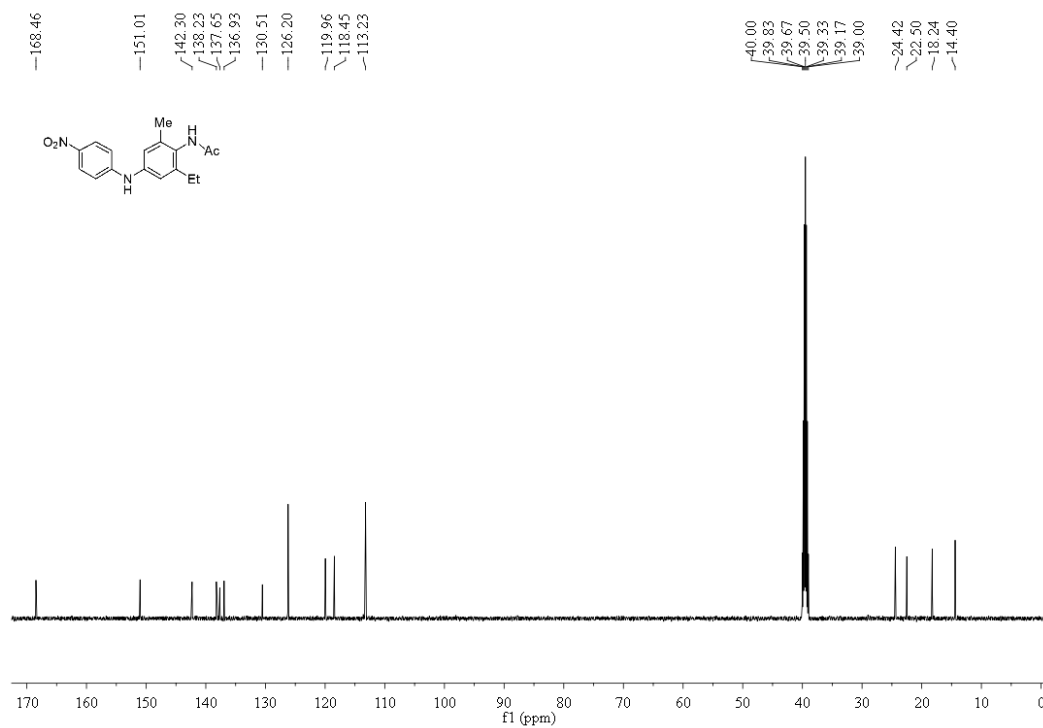
9a ¹³C NMR, 126 MHz, CDCl₃



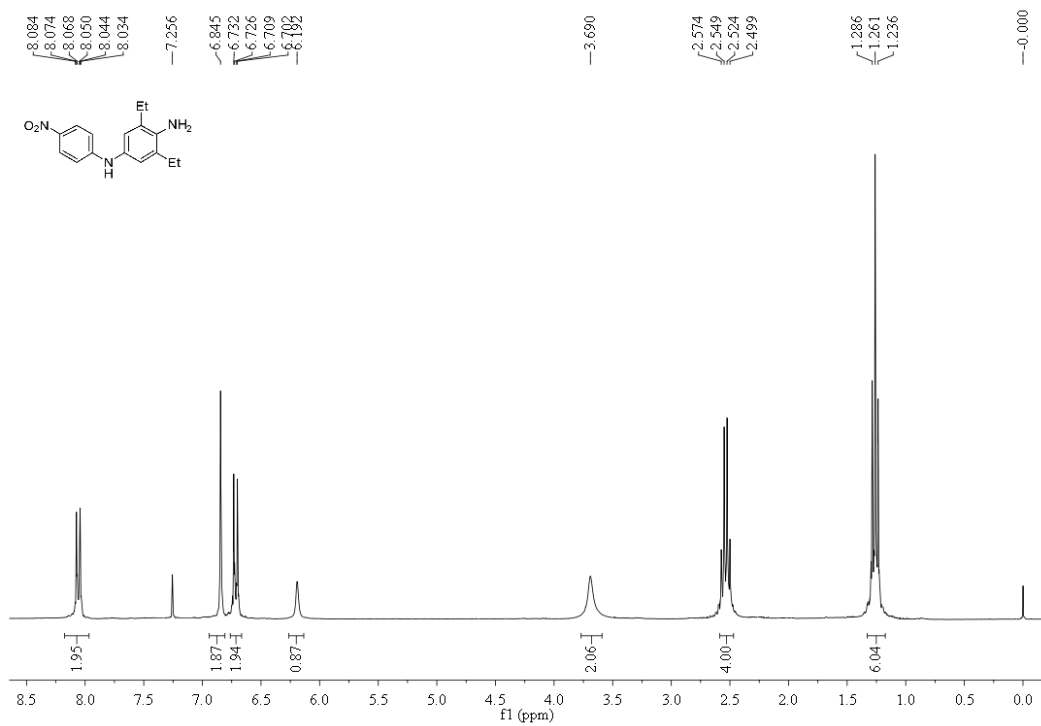
9b ^1H NMR, 300 MHz, $\text{DMSO-}d_6$



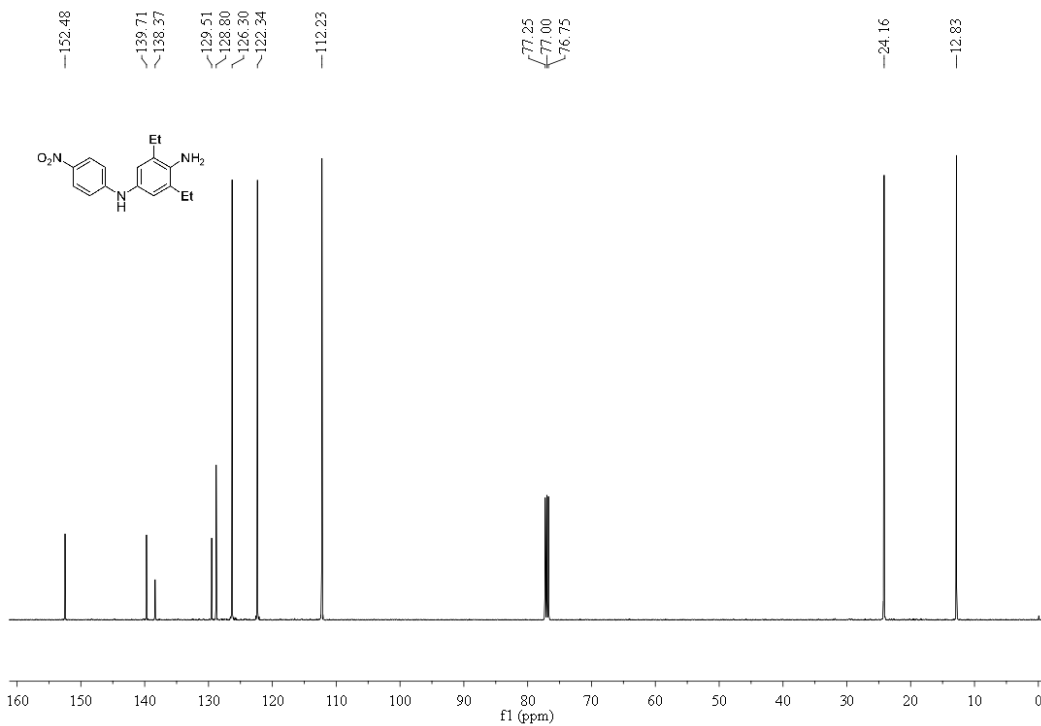
9b ^{13}C NMR, 126 MHz, $\text{DMSO-}d_6$



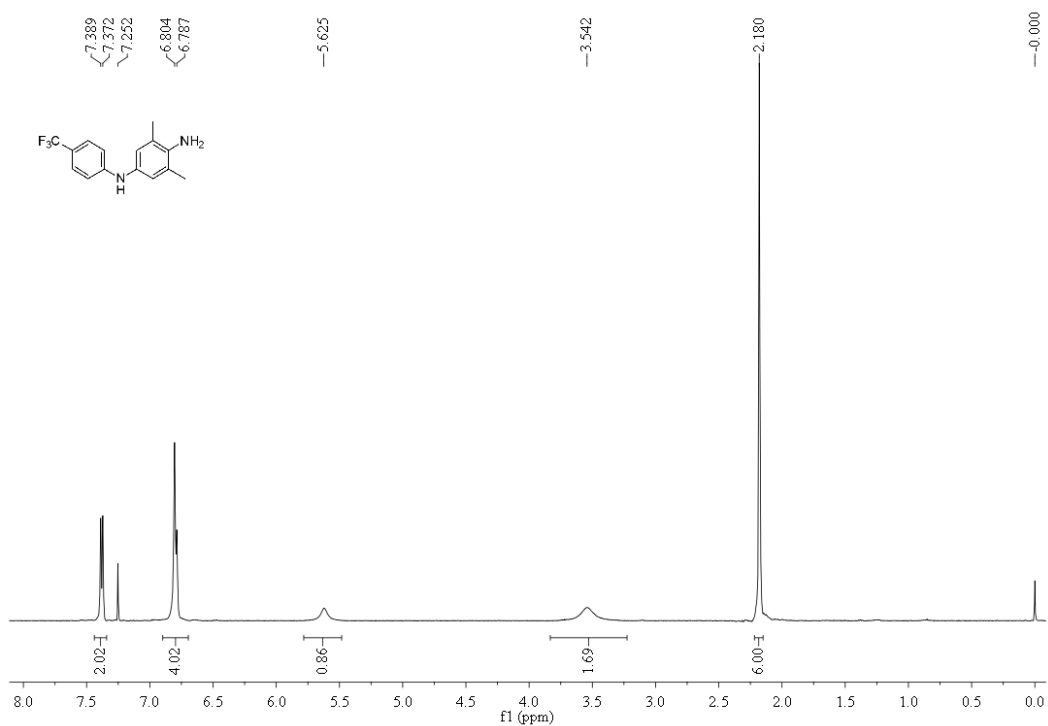
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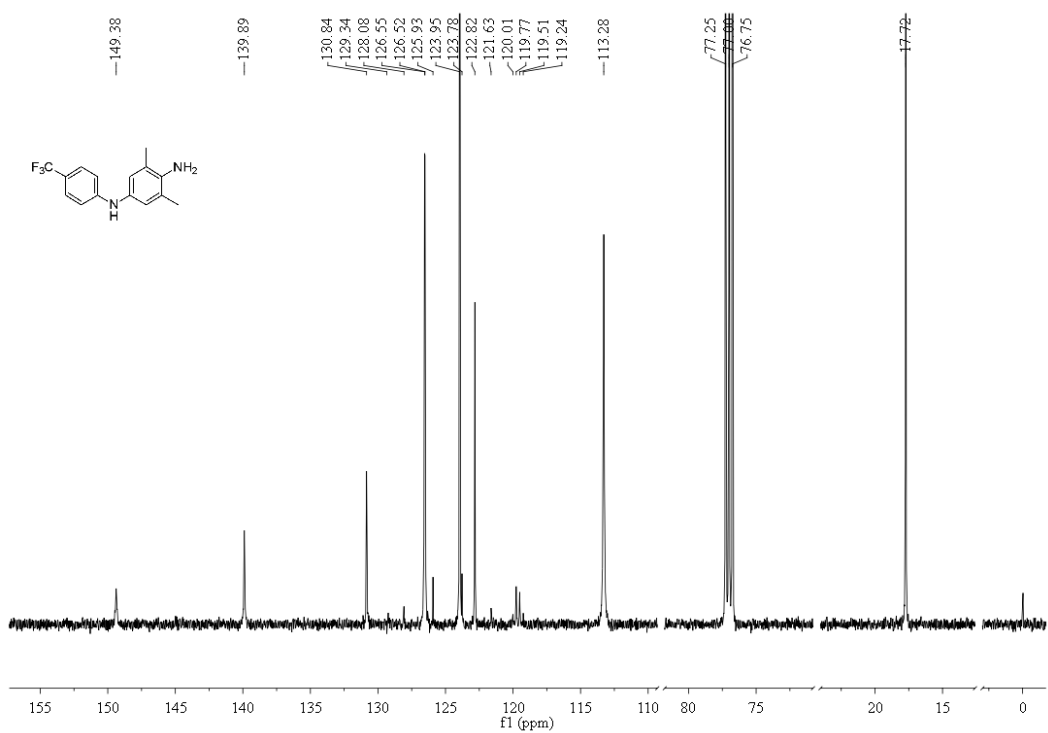
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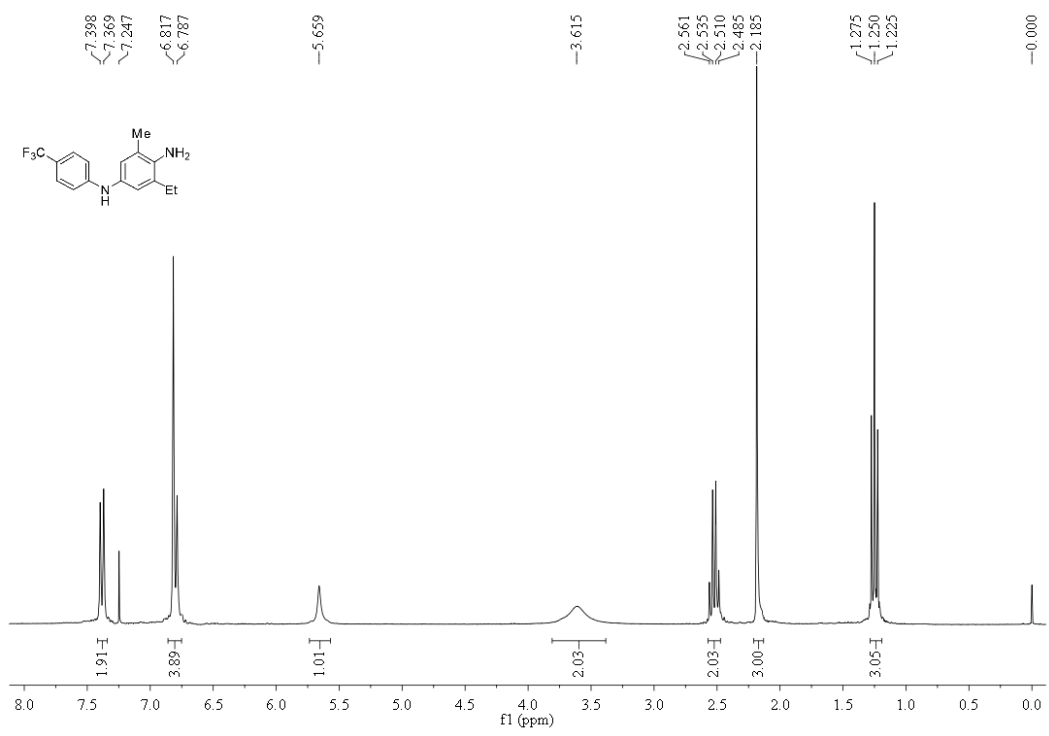
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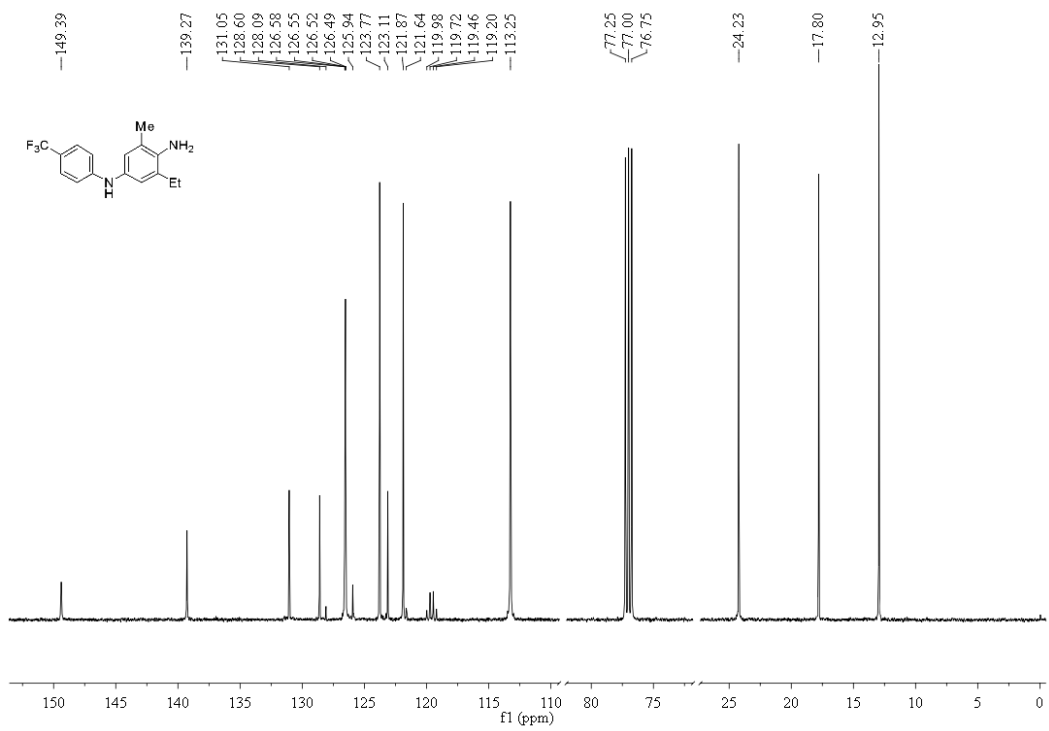
9d ^{13}C NMR, 126 MHz, CDCl_3



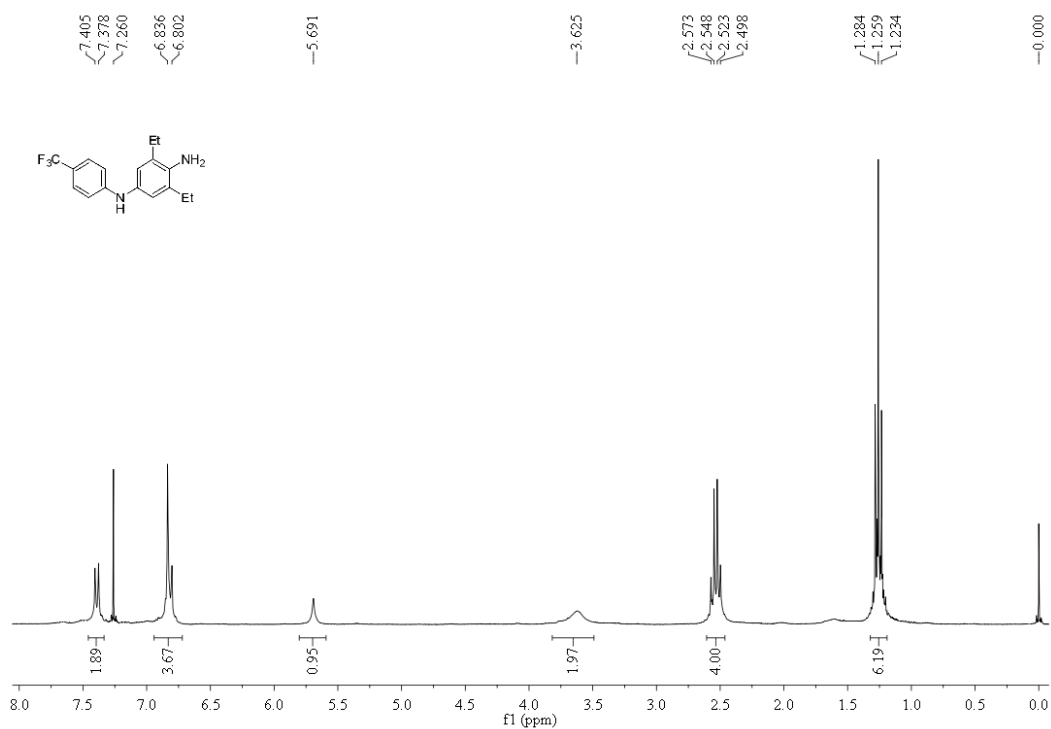
9e ^1H NMR, 300 MHz, CDCl_3



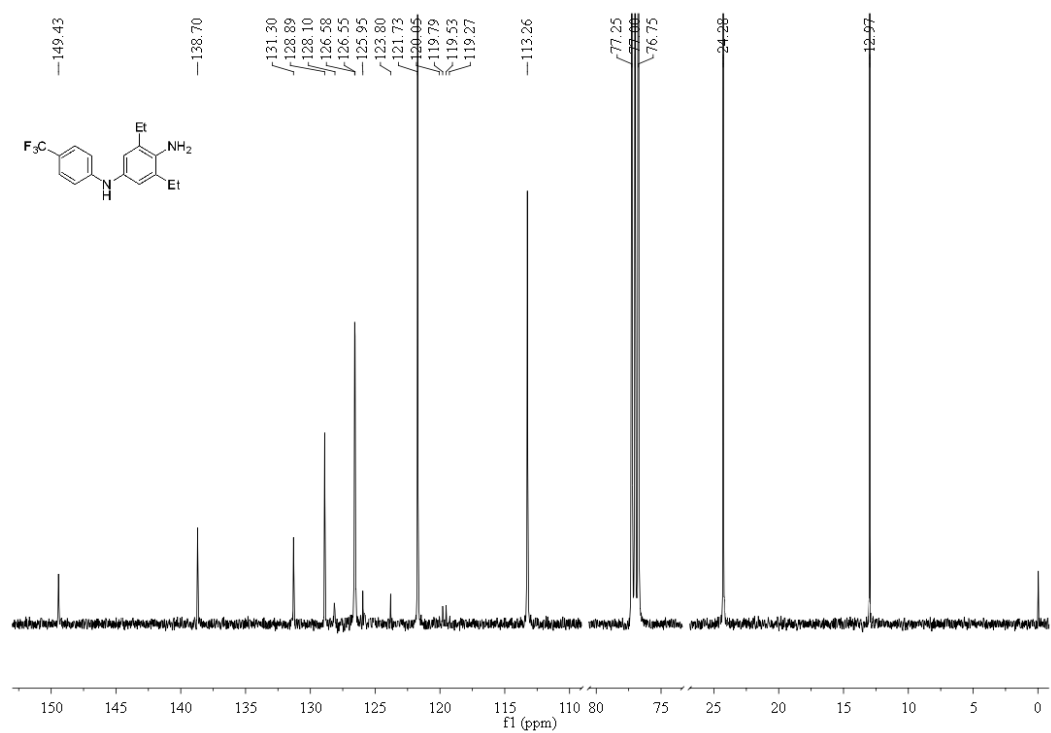
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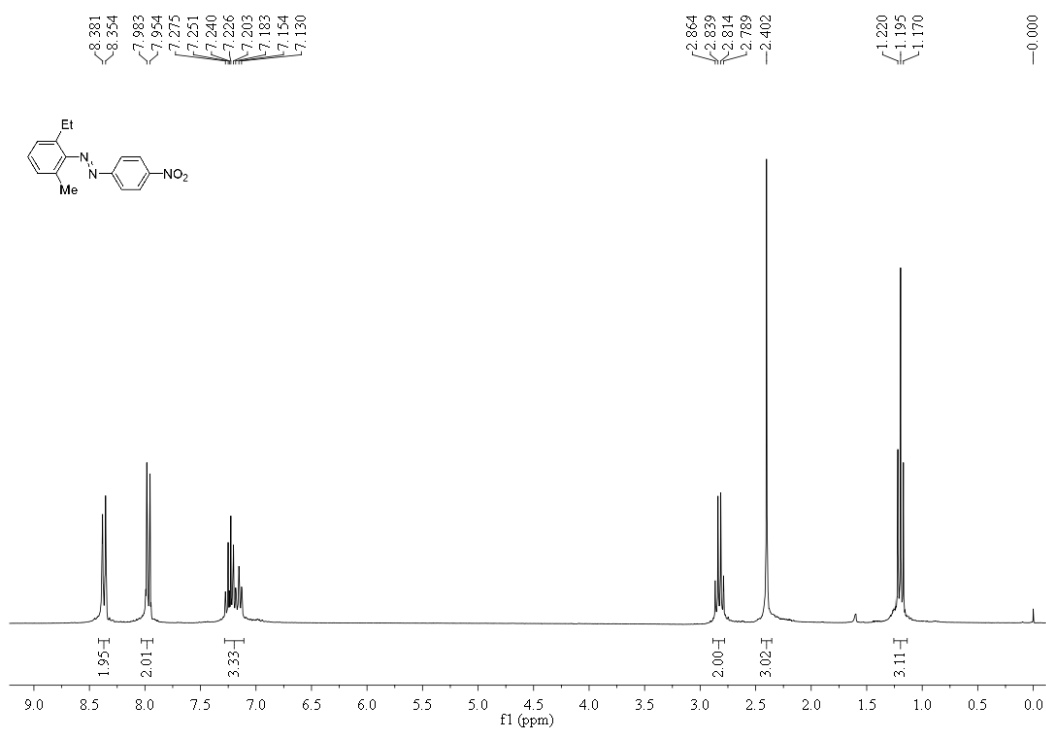
9f ^1H NMR, 300 MHz, CDCl_3



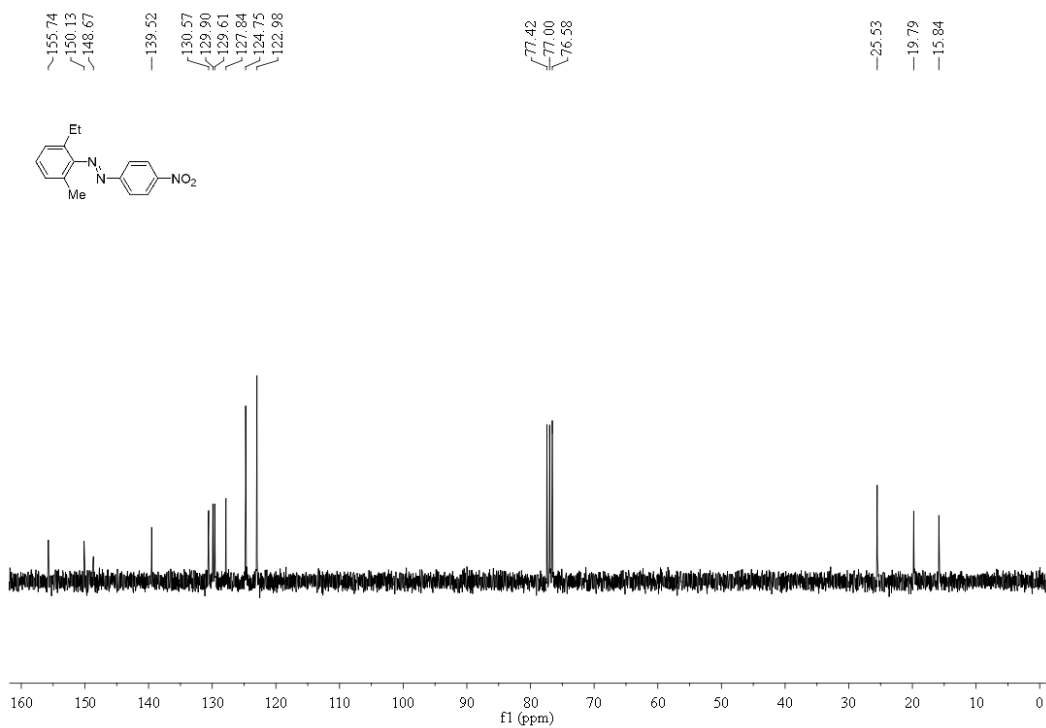
9f ^{13}C NMR, 126 MHz, CDCl_3



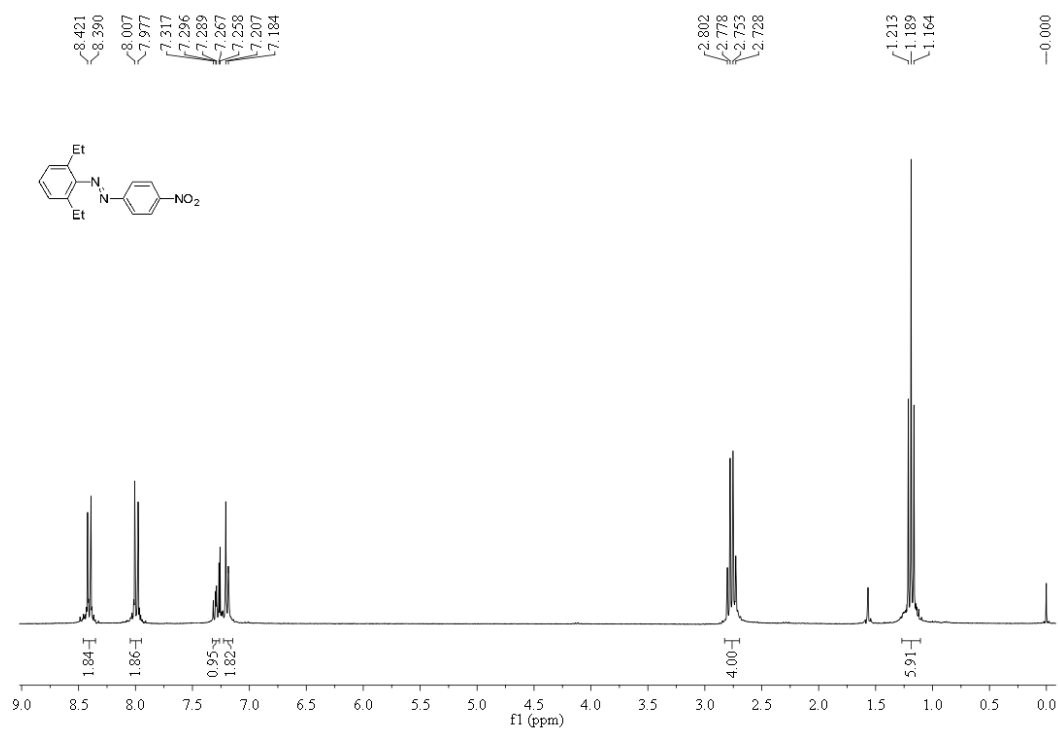
11b ¹H NMR, 300 MHz, CDCl₃



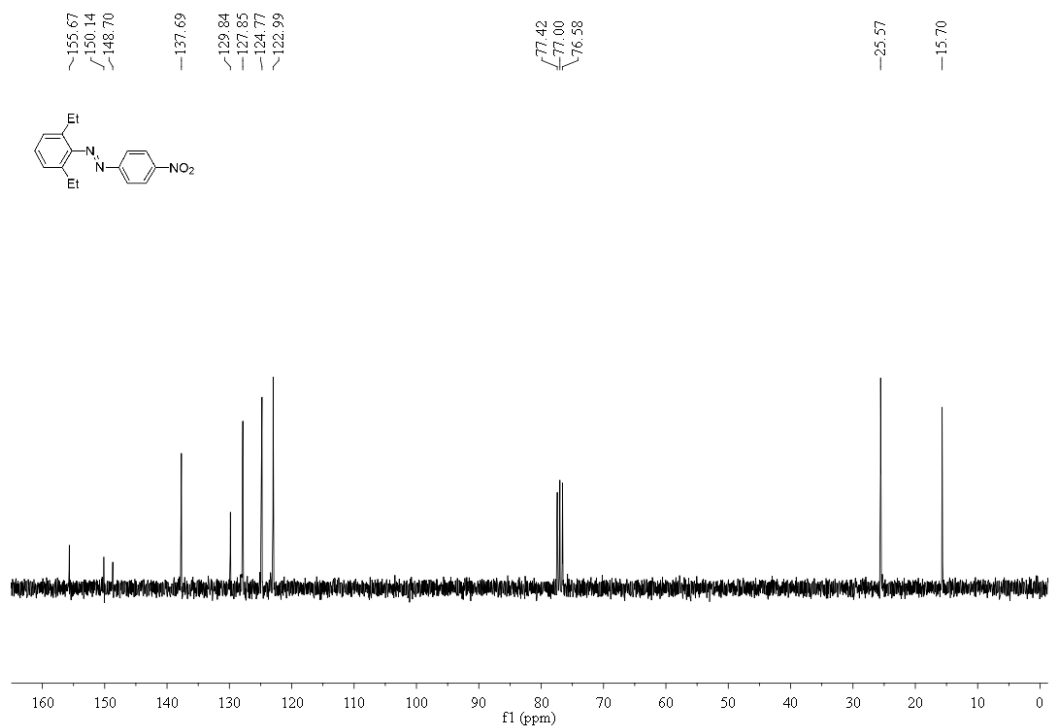
11b ¹³C NMR, 75 MHz, CDCl₃



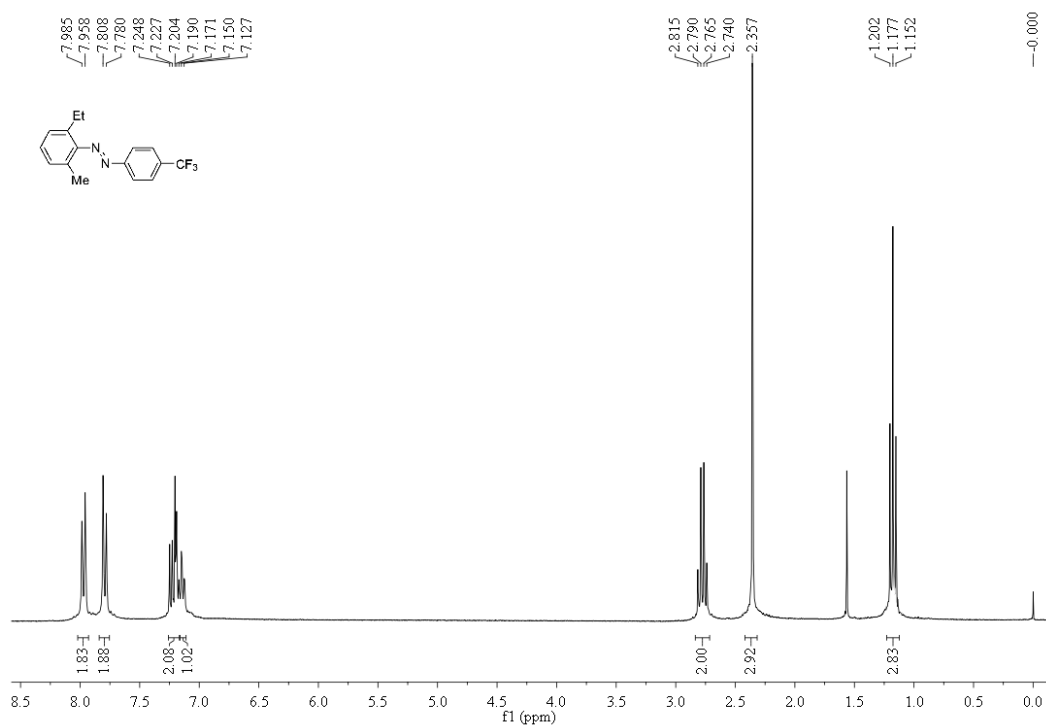
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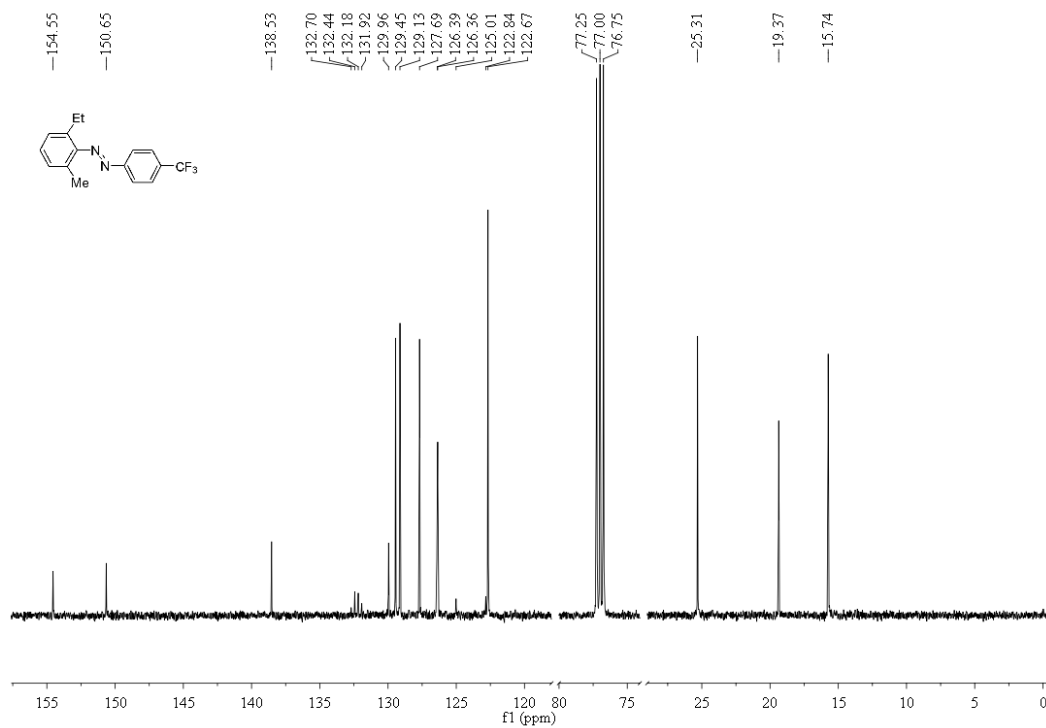
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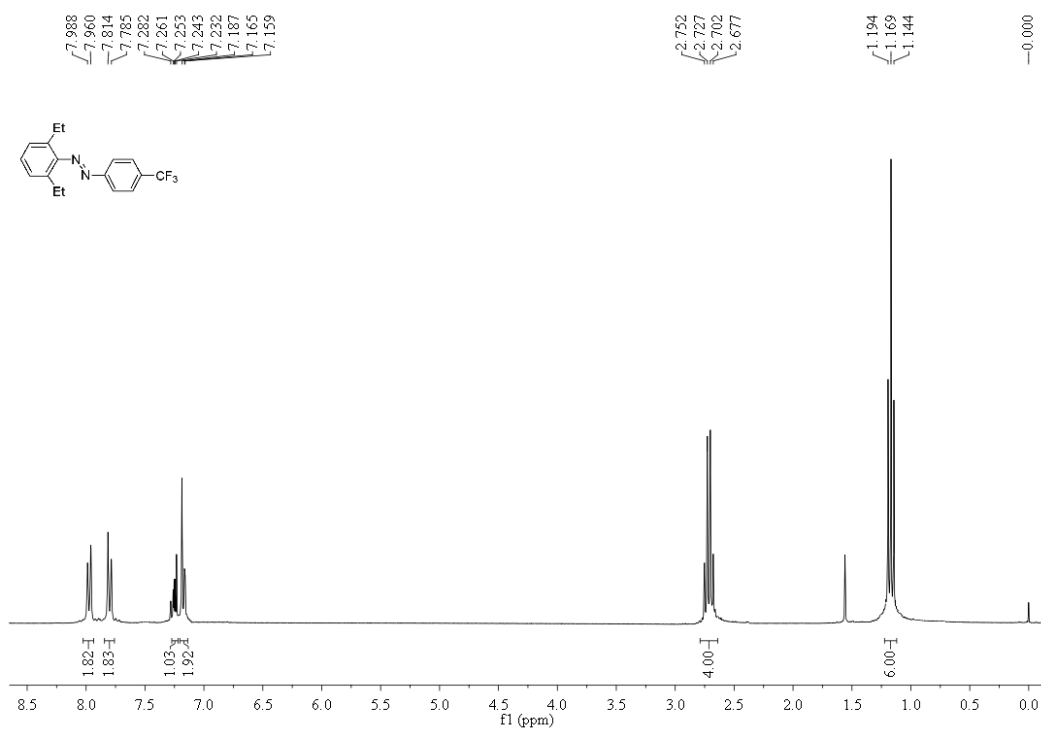
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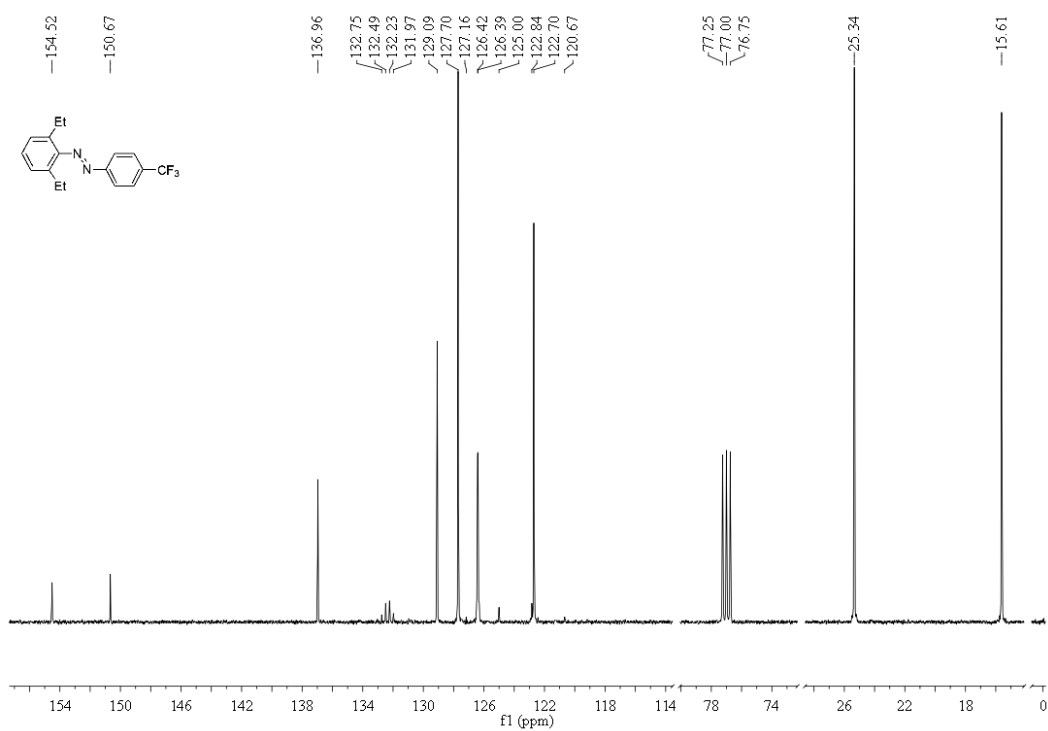
11e ^{13}C NMR, 126 MHz, CDCl_3



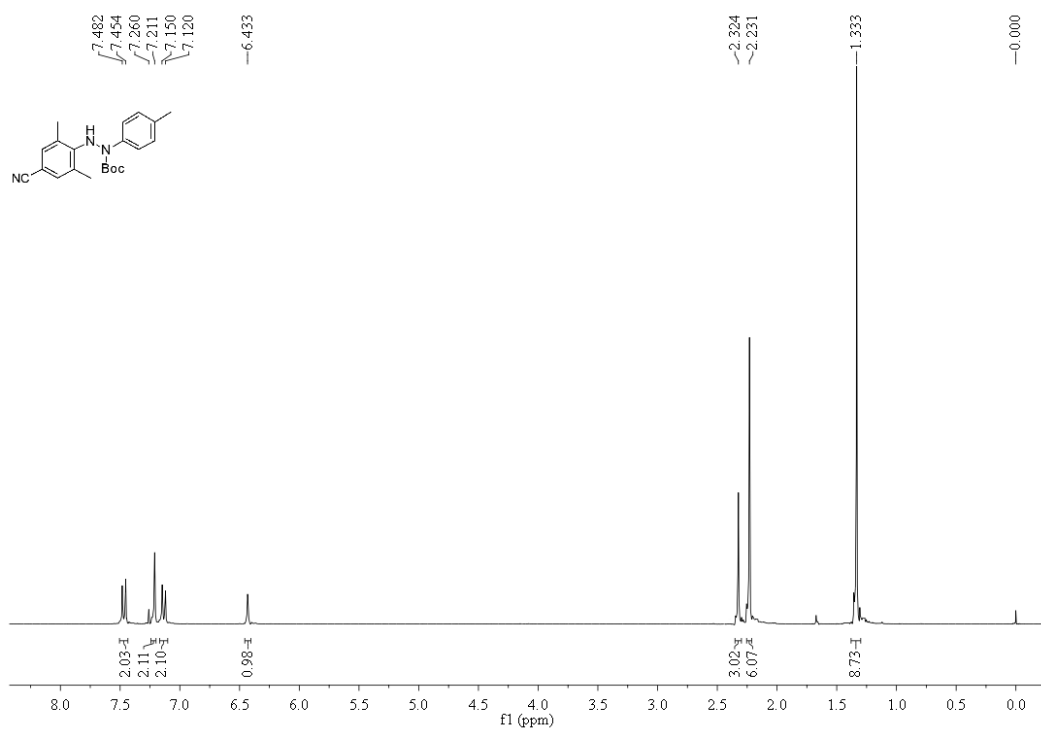
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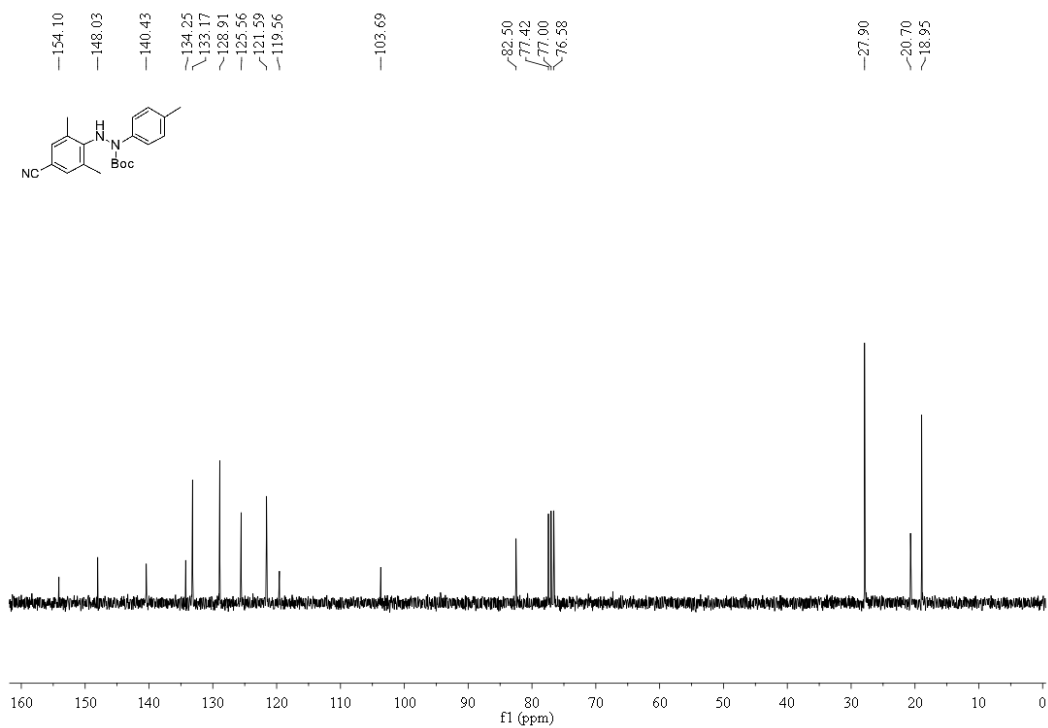
11f ^{13}C NMR, 126 MHz, CDCl_3



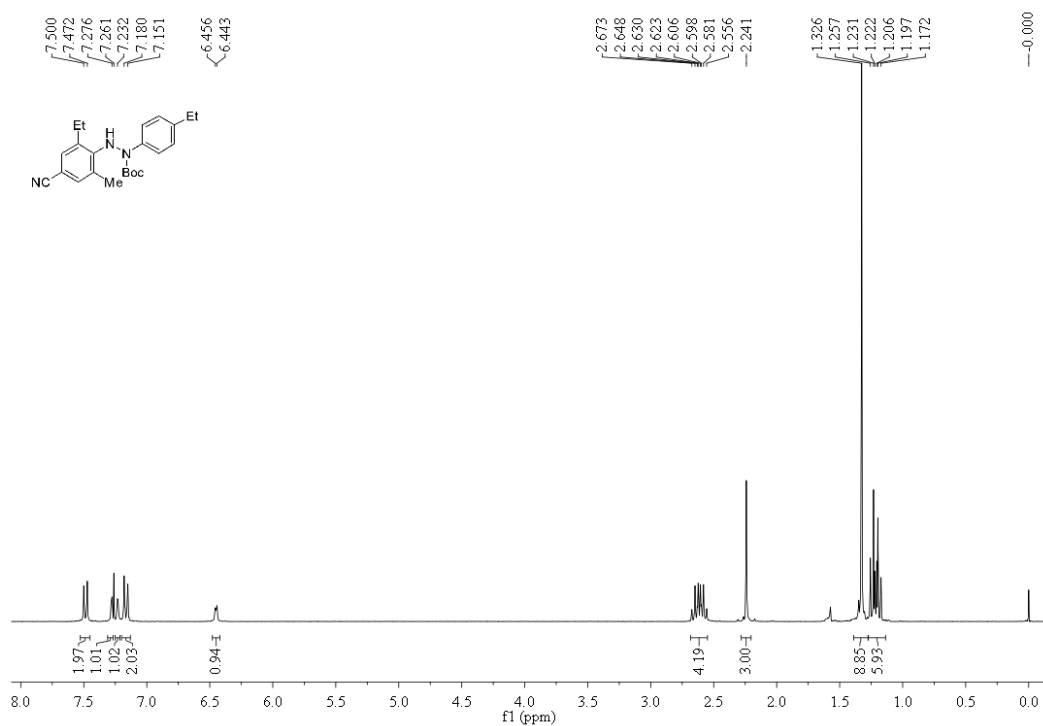
14a ^1H NMR, 300 MHz, CDCl_3



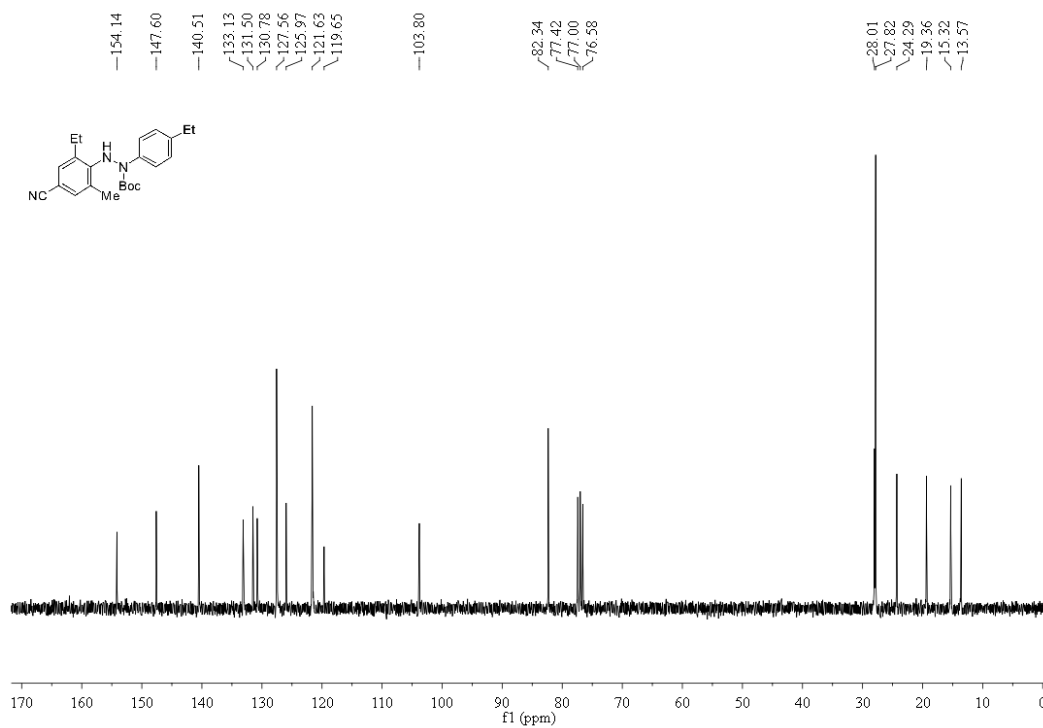
14a ^{13}C NMR, 75 MHz, CDCl_3



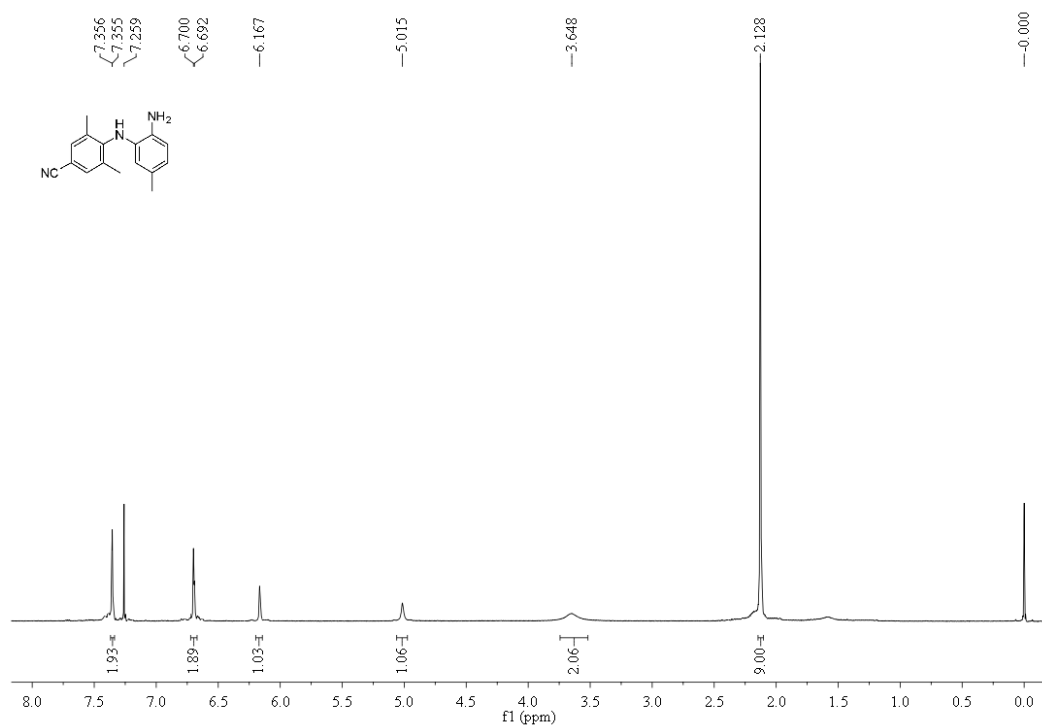
14b ^1H NMR, 300 MHz, CDCl_3



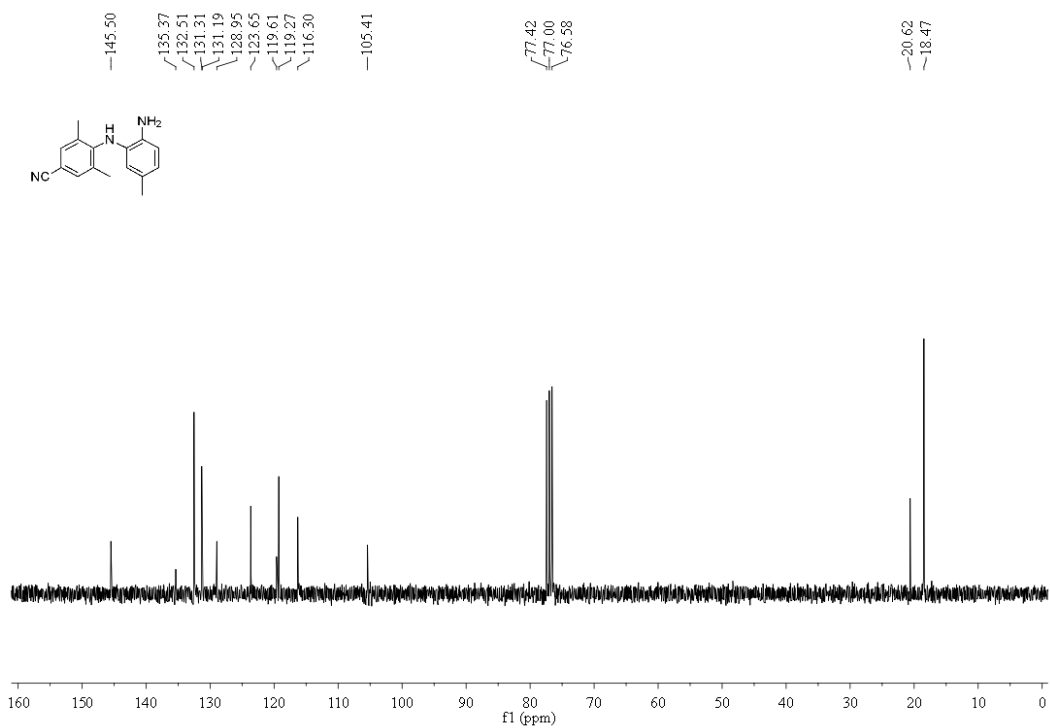
14b ^{13}C NMR, 75 MHz, CDCl_3



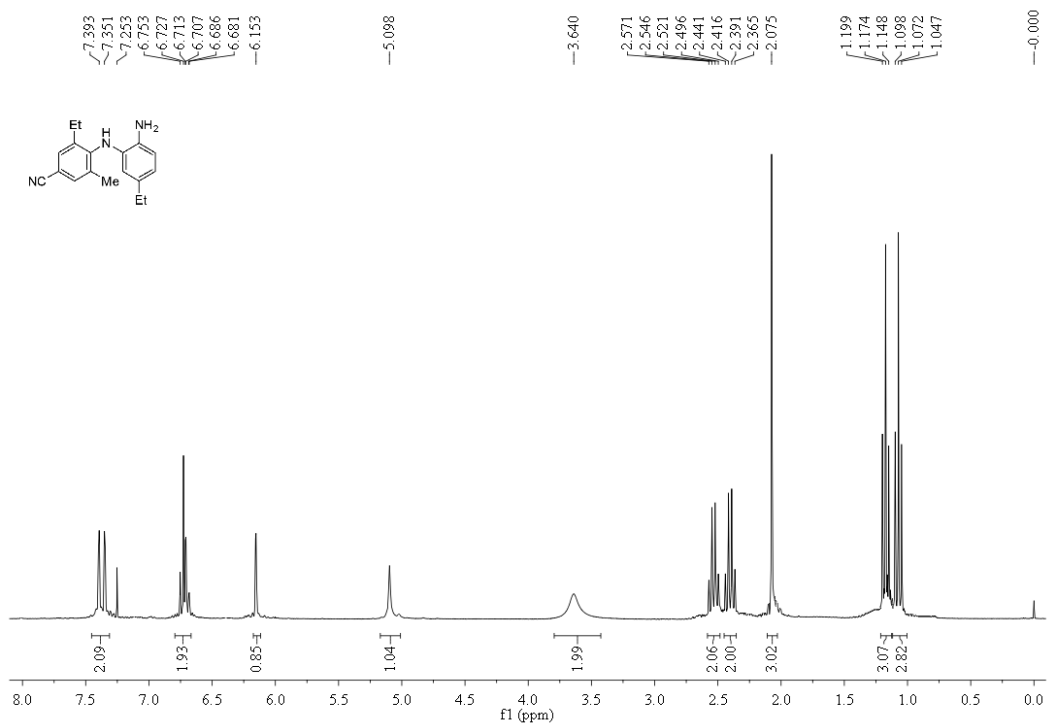
15a ^1H NMR, 300 MHz, CDCl_3



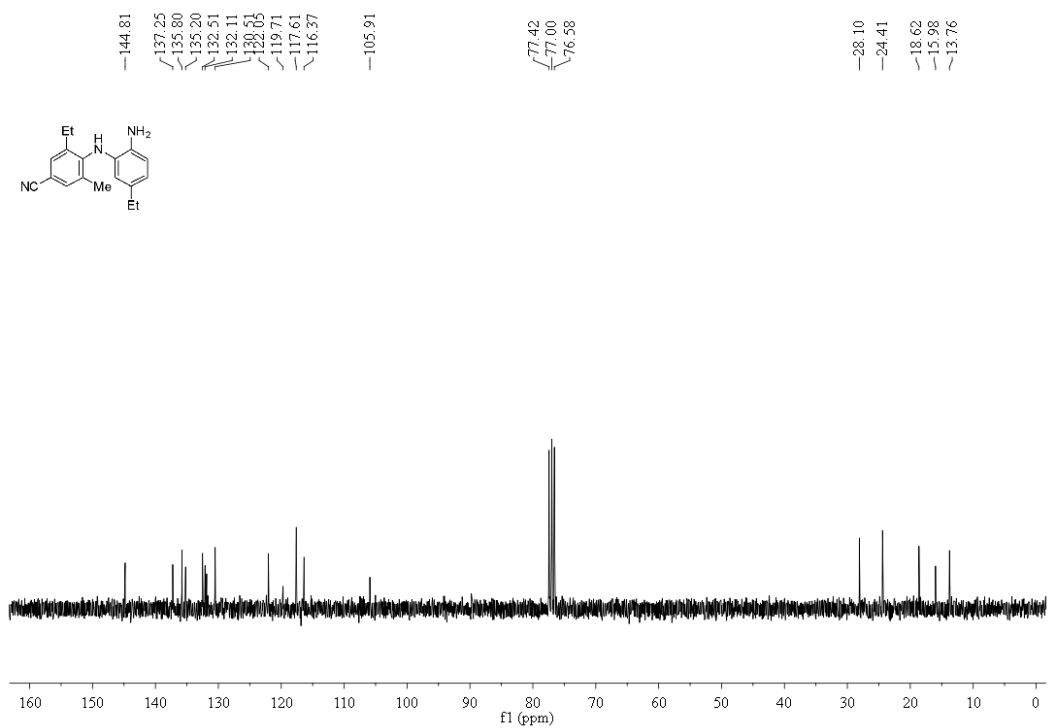
15a ^{13}C NMR, 75 MHz, CDCl_3



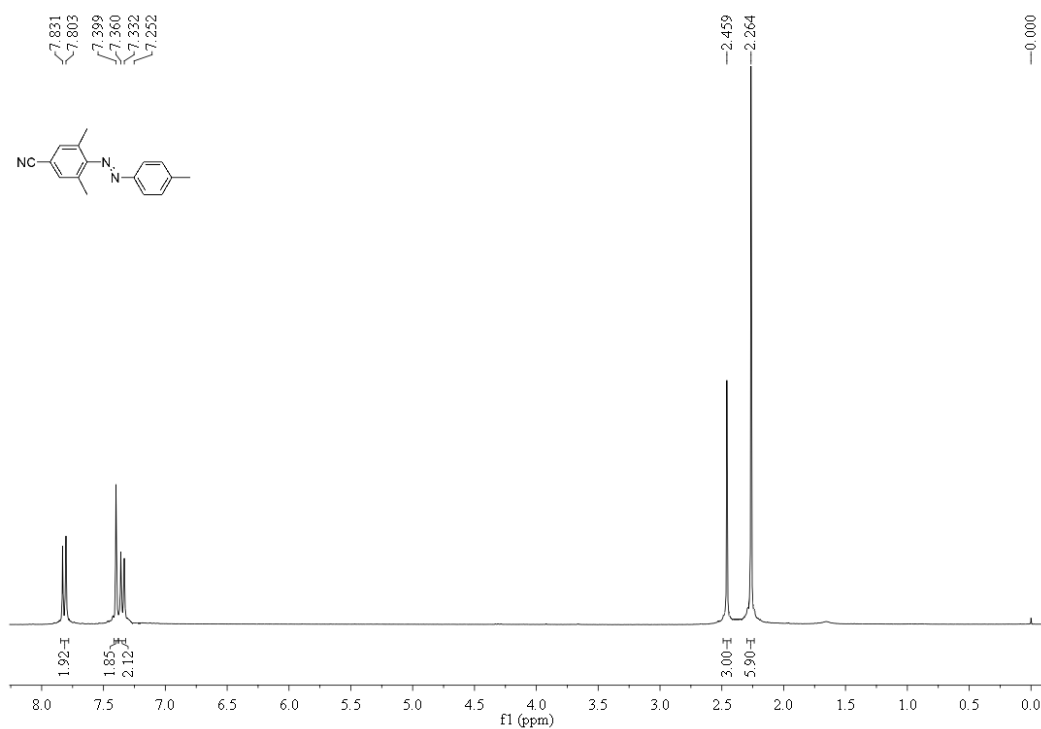
15b ^1H NMR, 300 MHz, CDCl_3



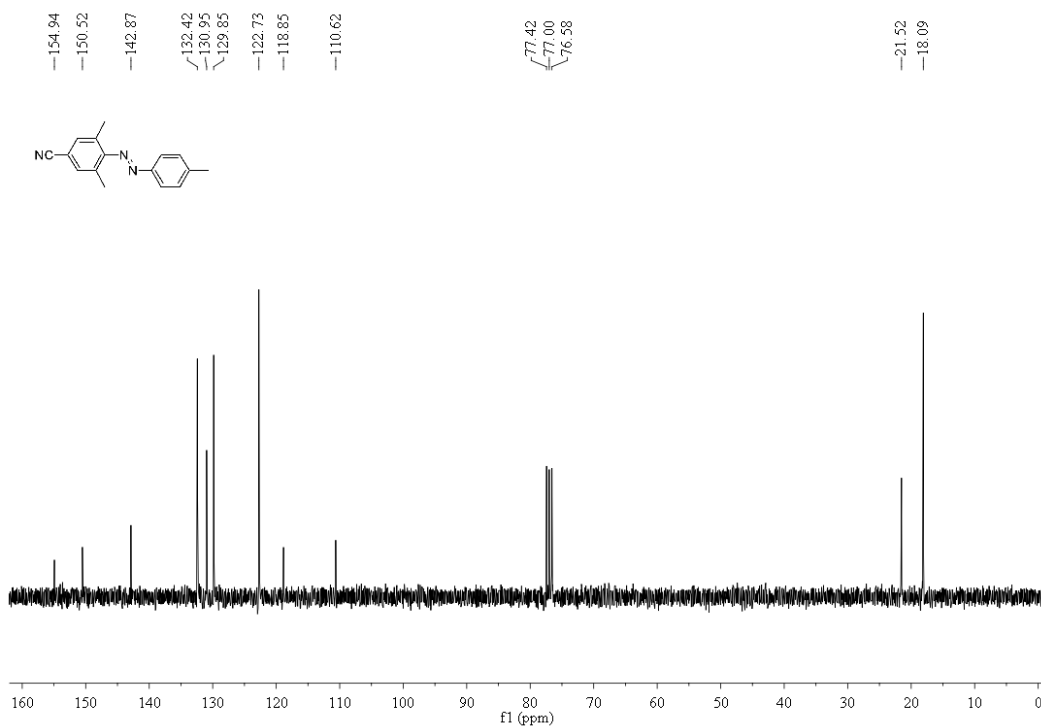
15b ^{13}C NMR, 75 MHz, CDCl_3



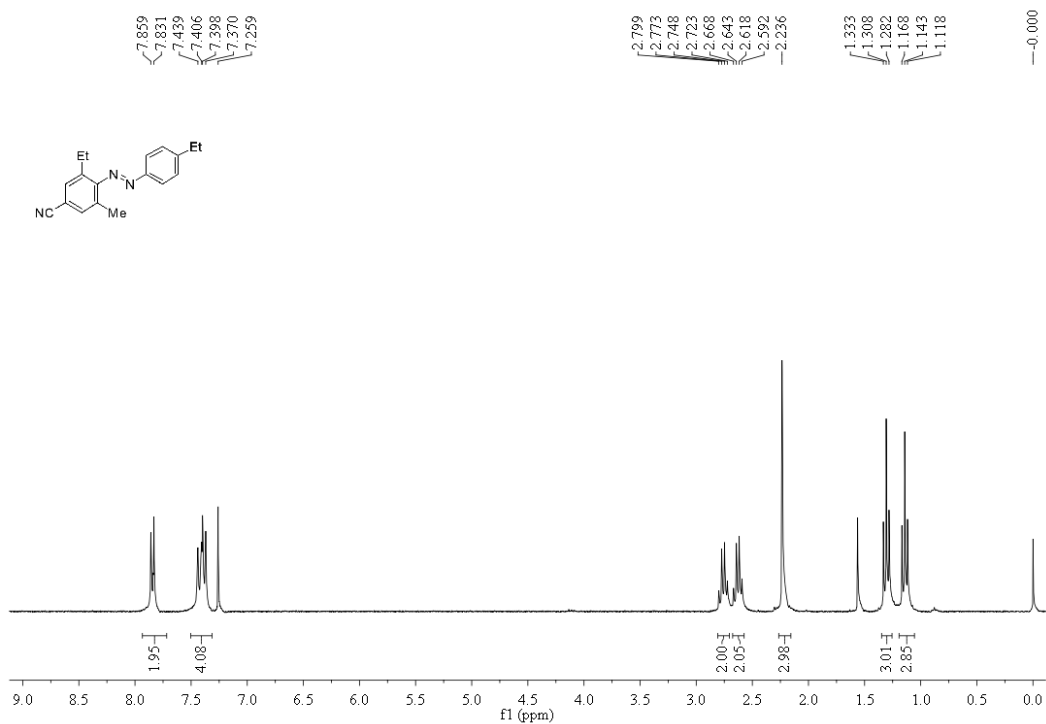
16a ^1H NMR, 300 MHz, CDCl_3



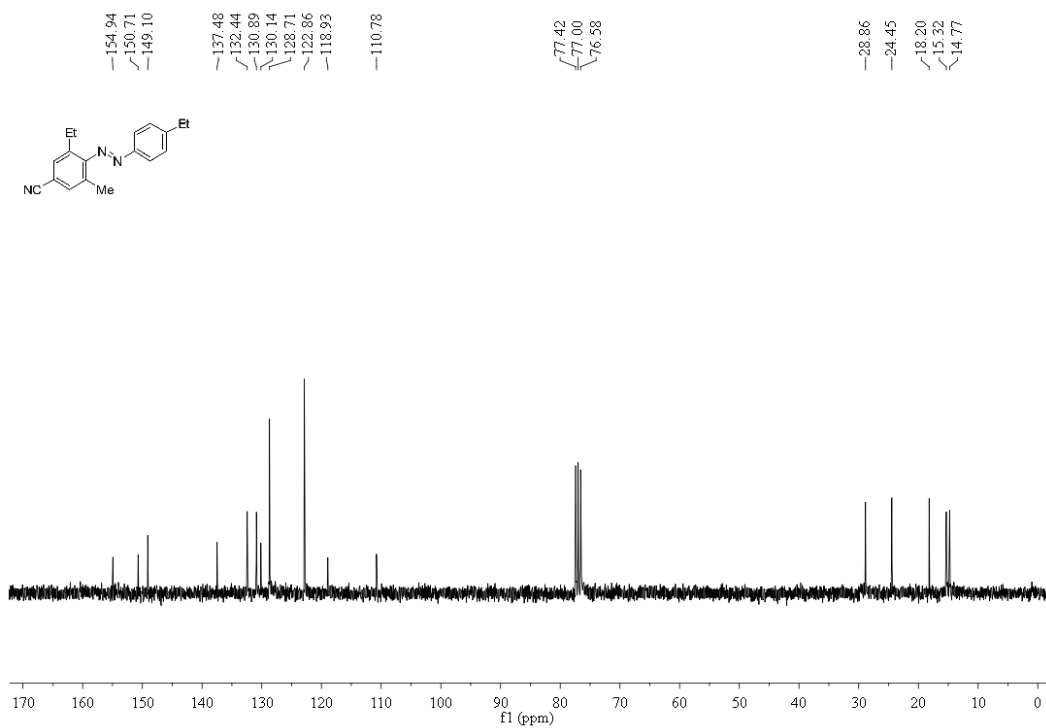
16a ^{13}C NMR, 75 MHz, CDCl_3



16b ^1H NMR, 300 MHz, CDCl_3



16b ^{13}C NMR, 75 MHz, CDCl_3



4. Details of LC-MS

Liquid chromatography/electrospray/time-of-flight mass spectrometry in positive ionization electrospray mode was used to analyze the components of intercrossing experiments with methanol and aqueous 0.2% formic acid as mobile phases A and B. The LC conditions were as follows: 45% A at the initial time, then a linear gradient progressing from 45% A to 70% A in 2 min, after which a gradient increased A to 98% in 4 min, followed by a stop time of 6 min and a post time of 0.5 min 45% A. The flow rate was 0.3 mL/min, and 5 μ L of sample was injected. The LC system was connected to a time-of-flight mass spectrometer equipped with an electrospray interface under the following operating parameters: capillary 3.50 KV, cone 25.00 V, extractor 3.00 V, source temperature 100 $^{\circ}$ C, desolvation temperature 350 $^{\circ}$ C, cone gas flow 45 L/h, desolvation gas flow 653 L/h, multiplier 650 V. The mass axis was calibrated using the mixture provided by the manufacturer over the range of 50-3200 at m/z . A second orthogonal sprayer with a reference solution was used as a continuous calibration using the reference masses 121.0509 and 922.0098 at m/z . Spectra were acquired over the range of 100-800 at m/z at a scan rate of 0.3 scan/s.

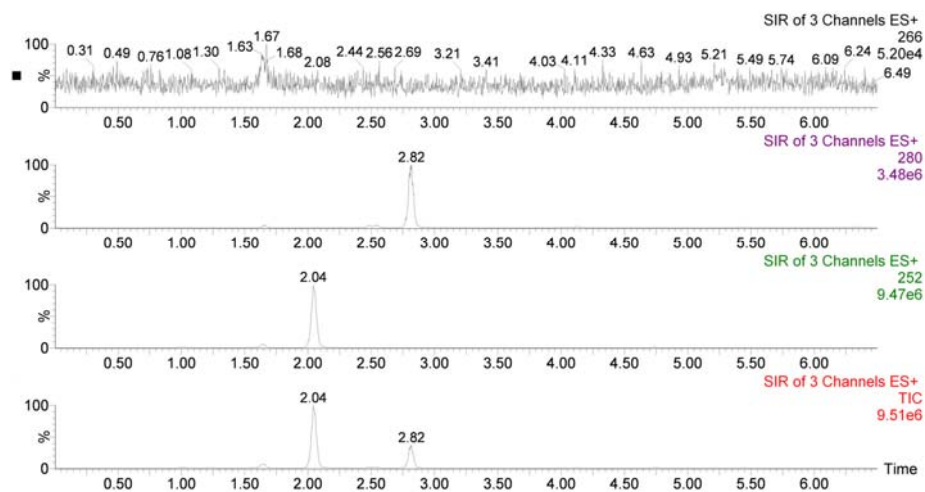


Figure S1. LC-MS for intercrossing experiment of **14a** and **14b**

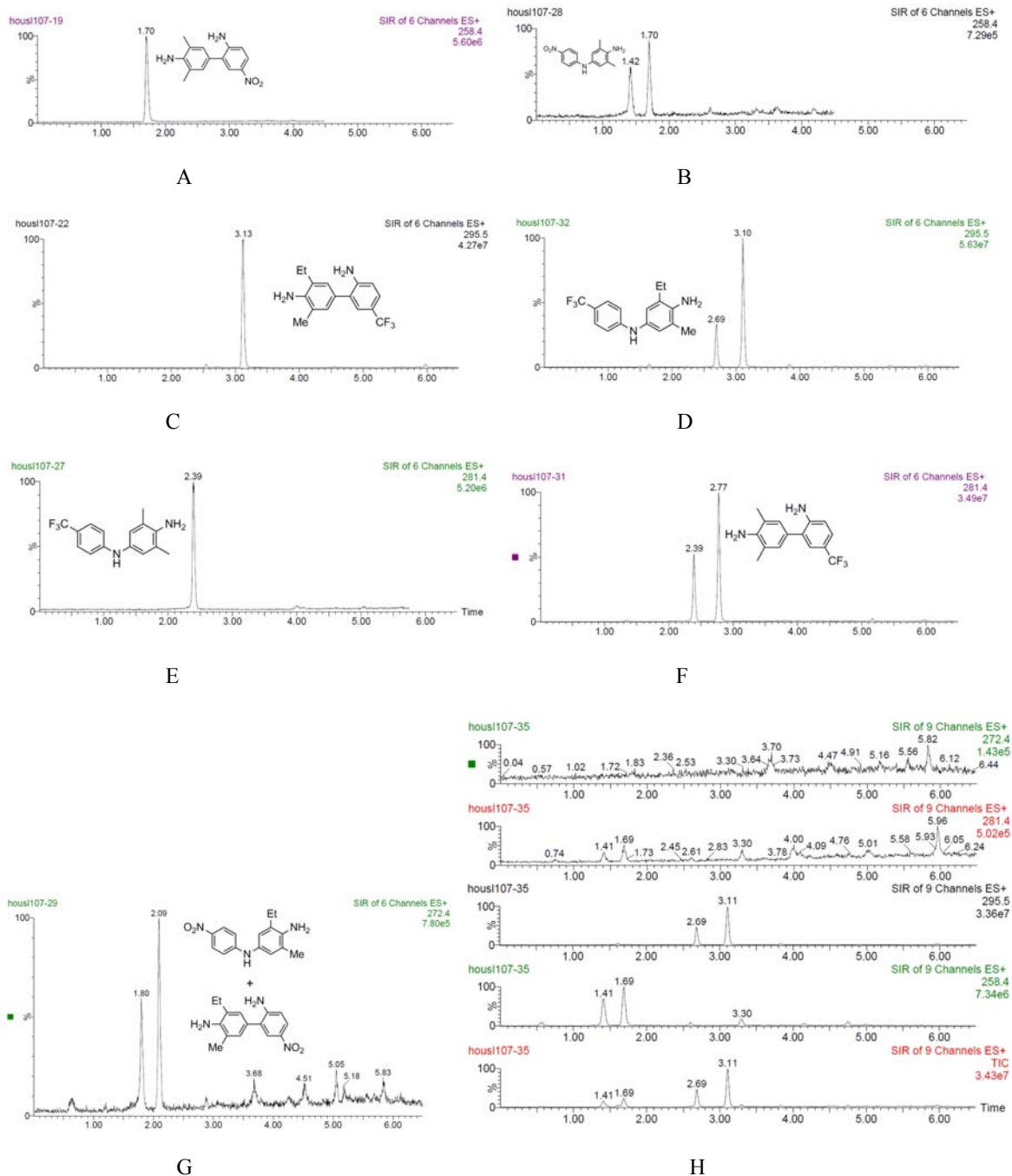


Figure S2. LC-MS for the intercrossing experiment of **7a** and **7e**

A. LC-MS of sample **8a**, B. LC-MS of mixed sample of **8a** and **9a**

C. LC-MS of sample **8e**, D. LC-MS of mixed sample of **8e** and **9e**

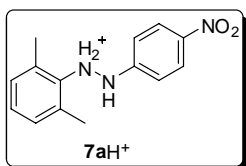
E. LC-MS of sample **9b (9ea)**, F. LC-MS of mixed sample of **8b (8ae)** and **9b (9ea)**

G. LC-MS of mixture of **8d (8ea)** and **9d (9ae)**, H. LC-MS for the intercrossing experiment of **7a** and **7e**

5. Details of Calculations

All of the DFT calculations were performed with the Gaussian 09 program package.¹ DFT calculations using the B3LYP/6-311++G(d,p) level were used to locate all the stationary points involved.² Frequency calculations at the same level were performed to confirm each stationary point to be either an intermediate or a transition structure. The free energies in solution were computed by a self-consistent reaction field (SCRF) using the CPCM method in ethanol at the same level.³

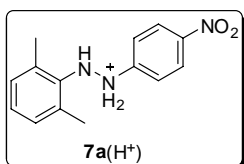
6. Coordinates of All Stationary Points



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.528791	1.447861	0.052352
2	6	0	3.191300	1.276466	-0.314008
3	6	0	2.706255	-0.036277	-0.292763
4	6	0	3.460123	-1.161594	0.059325
5	6	0	4.789907	-0.929687	0.417363
6	6	0	5.315792	0.359342	0.416226
7	1	0	4.950264	2.445812	0.048841
8	1	0	5.412652	-1.770444	0.698370
9	1	0	6.349998	0.516647	0.698808
10	7	0	1.281445	-0.250386	-0.653223
11	1	0	0.969804	0.494954	-1.291464
12	7	0	0.426858	-0.330866	0.516229

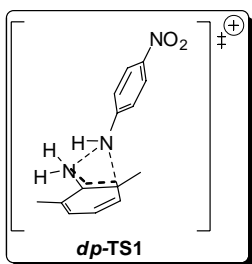
13	1	0	0.813850	0.267409	1.238756
14	6	0	-0.959867	-0.194793	0.309445
15	6	0	-1.730381	0.265157	1.389788
16	6	0	-1.578402	-0.565028	-0.890948
17	6	0	-3.104758	0.353148	1.270483
18	1	0	-1.250113	0.550973	2.317857
19	6	0	-2.957938	-0.466856	-1.013659
20	1	0	-1.014461	-0.941000	-1.734569
21	6	0	-3.707271	-0.011348	0.065466
22	1	0	-3.707813	0.708285	2.093880
23	1	0	-3.447060	-0.747510	-1.935417
24	1	0	1.195353	-1.136557	-1.161176
25	7	0	-5.161137	0.090199	-0.066310
26	8	0	-5.671509	-0.230839	-1.137149
27	8	0	-5.803978	0.492058	0.900891
28	6	0	2.341843	2.455166	-0.725008
29	1	0	2.015027	2.378426	-1.767786
30	1	0	1.452589	2.568696	-0.098739
31	1	0	2.916364	3.376522	-0.639296
32	6	0	2.885618	-2.556138	0.044289
33	1	0	1.995511	-2.637318	0.673165
34	1	0	2.614366	-2.869579	-0.970266
35	1	0	3.621333	-3.270205	0.412123



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.627787	1.359396	-0.184811
2	6	0	3.246665	1.275708	-0.376373
3	6	0	2.640841	0.008826	-0.249600
4	6	0	3.385627	-1.149165	0.043469
5	6	0	4.760580	-1.009915	0.247622
6	6	0	5.378001	0.231680	0.136632
7	1	0	5.115561	2.322214	-0.285742
8	1	0	5.350946	-1.890102	0.476132
9	1	0	6.447608	0.319567	0.288572
10	7	0	1.229785	-0.136841	-0.504664
11	1	0	0.836780	0.701442	-0.923908
12	7	0	0.443511	-0.334854	0.738760
13	1	0	0.729040	0.322246	1.476683
14	6	0	-1.008169	-0.229949	0.500288
15	6	0	-1.698160	0.826243	1.081080
16	6	0	-1.623323	-1.176117	-0.312586
17	6	0	-3.064672	0.939127	0.848690
18	1	0	-1.193816	1.549511	1.709768
19	6	0	-2.987567	-1.061880	-0.546406
20	1	0	-1.061358	-1.984947	-0.759839
21	6	0	-3.680604	-0.007007	0.039090
22	1	0	-3.637364	1.743881	1.286039
23	1	0	-3.505058	-1.777293	-1.168781
24	7	0	-5.134823	0.111929	-0.210721

25	8	0	-5.660092	-0.724535	-0.934029
26	8	0	-5.731502	1.040139	0.319531
27	6	0	2.459464	2.512852	-0.743720
28	1	0	2.008910	2.430651	-1.738806
29	1	0	1.656184	2.726387	-0.032483
30	1	0	3.116200	3.382647	-0.760673
31	6	0	2.742446	-2.511679	0.125392
32	1	0	2.309172	-2.704985	1.114816
33	1	0	1.955755	-2.629487	-0.622880
34	1	0	3.485576	-3.293007	-0.037640
35	1	0	0.675816	-1.273915	1.078474

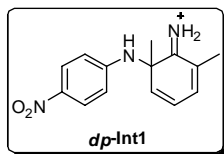


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-3.421215	0.518133	-1.657806
2	7	0	-0.623734	0.302857	-0.991213
3	6	0	-2.439361	1.215953	0.432673
4	6	0	-3.107150	0.219276	-0.398156
5	1	0	-3.865371	-0.155487	-2.264934
6	1	0	-3.205044	1.418904	-2.059177

7	1	0	-1.028084	-0.610981	-1.211303
8	6	0	-2.153308	0.874550	1.764017
9	1	0	-1.691126	1.617457	2.402022
10	6	0	-3.407392	-1.091454	0.125934
11	6	0	0.669209	0.122878	-0.669615
12	6	0	1.285877	-1.165791	-0.602503
13	1	0	0.682377	-2.049016	-0.775599
14	6	0	1.470347	1.277830	-0.410377
15	1	0	1.002596	2.252746	-0.452429
16	6	0	2.633763	-1.287971	-0.341128
17	1	0	3.115060	-2.254692	-0.303602
18	6	0	2.813262	1.153836	-0.133032
19	1	0	3.432220	2.019100	0.055716
20	6	0	3.377333	-0.127207	-0.106713
21	6	0	-2.463577	-0.373210	2.259366
22	1	0	-2.240045	-0.618955	3.290350
23	6	0	-3.084474	-1.346452	1.435743
24	1	0	-3.309485	-2.320644	1.853432
25	6	0	-2.300509	2.627831	-0.044847
26	1	0	-1.753280	2.681451	-0.988721
27	1	0	-3.285262	3.081809	-0.205912
28	1	0	-1.771742	3.229812	0.693135
29	6	0	-4.079572	-2.118303	-0.743065
30	1	0	-5.068683	-1.781360	-1.071314
31	1	0	-3.492793	-2.343384	-1.640019
32	1	0	-4.212894	-3.049670	-0.193998
33	7	0	4.814799	-0.258226	0.182384
34	8	0	5.450073	0.766137	0.412424

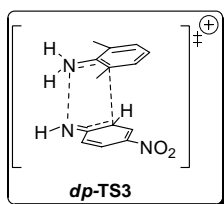
35 8 0 5.301918 -1.384518 0.178703



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.125468	-0.126589	-0.018305
2	6	0	-2.986271	1.241922	-0.274717
3	6	0	-1.725123	1.798924	-0.310472
4	6	0	-0.578638	1.004216	-0.089480
5	6	0	-0.742352	-0.371021	0.164304
6	6	0	-2.008135	-0.931483	0.200757
7	1	0	-3.862663	1.852407	-0.440511
8	1	0	-1.611177	2.858271	-0.509024
9	1	0	0.111167	-1.012236	0.337630
10	1	0	-2.133385	-1.986785	0.398163
11	7	0	0.666112	1.602814	-0.167813
12	6	0	1.915128	0.999058	0.279298
13	6	0	2.401335	-0.057049	-0.711974
14	6	0	1.895938	0.506392	1.702322
15	6	0	3.156893	-1.192772	-0.273230
16	6	0	2.554966	-0.605668	2.065073
17	1	0	1.405430	1.149962	2.423031
18	6	0	3.207574	-1.424834	1.074482

19	1	0	2.603146	-0.910475	3.102690
20	1	0	3.746362	-2.299687	1.422245
21	7	0	2.160274	0.163974	-1.978099
22	1	0	0.664548	2.612683	-0.195702
23	1	0	2.516802	-0.439146	-2.707989
24	1	0	1.564315	0.937360	-2.254151
25	6	0	3.008602	2.123145	0.240922
26	1	0	3.050449	2.555381	-0.760994
27	1	0	2.743638	2.896490	0.962498
28	1	0	3.986278	1.718341	0.497652
29	6	0	3.783456	-2.118732	-1.280742
30	1	0	3.027448	-2.595499	-1.913527
31	1	0	4.481177	-1.586086	-1.934388
32	1	0	4.336069	-2.909876	-0.775418
33	7	0	-4.450678	-0.715950	0.021937
34	8	0	-5.424289	0.014825	-0.174537
35	8	0	-4.551584	-1.923577	0.250310

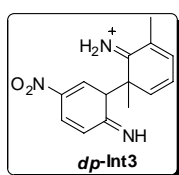


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.851849	2.370503	-0.934447

2	7	0	2.362138	1.369323	1.091764
3	6	0	0.972450	-0.593656	0.916307
4	6	0	-0.130042	0.212691	-0.780098
5	6	0	2.189298	0.154681	0.593654
6	6	0	-0.191478	1.676193	-0.597800
7	6	0	-1.360573	-0.526579	-0.698854
8	6	0	0.967662	-1.989770	0.539338
9	1	0	0.611596	-0.140210	-1.484586
10	1	0	1.748849	1.759504	1.792174
11	1	0	3.159506	1.933370	0.832503
12	1	0	0.696461	3.366577	-0.757639
13	1	0	0.146146	-2.603733	0.887382
14	1	0	-1.386416	-1.570012	-0.978460
15	6	0	3.166545	-0.385400	-0.314248
16	6	0	3.017952	-1.689053	-0.704184
17	6	0	1.939426	-2.510581	-0.252405
18	1	0	1.909510	-3.551720	-0.547996
19	1	0	3.758794	-2.124274	-1.365207
20	6	0	-1.424595	2.244167	-0.062446
21	1	0	-1.438297	3.301196	0.176611
22	6	0	-2.535543	1.490091	0.082400
23	1	0	-3.464079	1.907892	0.444283
24	6	0	-2.486394	0.095244	-0.267949
25	6	0	4.335246	0.455261	-0.750801
26	1	0	4.005031	1.379552	-1.235128
27	1	0	4.973644	0.729283	0.096205
28	1	0	4.951337	-0.093842	-1.461882
29	6	0	0.160765	-0.214694	2.135216

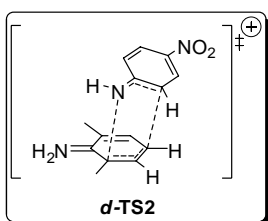
30	1	0	0.695018	-0.540295	3.033339
31	1	0	-0.035204	0.853128	2.229151
32	1	0	-0.800710	-0.728541	2.123634
33	7	0	-3.736926	-0.686449	-0.192020
34	8	0	-4.762288	-0.081513	0.101394
35	8	0	-3.687077	-1.888873	-0.422674



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.300030	0.415973	-0.797882
2	6	0	-0.277336	1.686924	0.053016
3	6	0	-1.515657	-0.436894	-0.564973
4	6	0	-1.581355	2.239352	0.437280
5	6	0	-2.617602	0.104552	-0.025957
6	1	0	-1.546526	-1.453446	-0.930796
7	6	0	-2.693012	1.481643	0.427585
8	1	0	-1.606845	3.252201	0.822930
9	1	0	-3.641977	1.862711	0.777170
10	7	0	0.852924	2.181327	0.376260
11	1	0	0.752947	3.060152	0.887642
12	6	0	1.093340	-0.308842	-0.846383
13	6	0	1.668854	-0.587300	0.528706

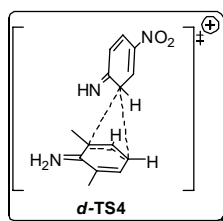
14	6	0	2.040006	0.465361	-1.720374
15	6	0	3.069128	-0.448720	0.793346
16	6	0	3.345317	0.599671	-1.427334
17	1	0	1.640688	0.817807	-2.665045
18	6	0	3.852247	0.111321	-0.180406
19	1	0	4.022728	1.086807	-2.116824
20	1	0	4.914204	0.216417	0.014439
21	7	0	0.873803	-1.083278	1.454323
22	1	0	1.227688	-1.362179	2.359799
23	1	0	-0.121503	-1.196677	1.317188
24	1	0	-0.459554	0.780251	-1.828681
25	7	0	-3.830766	-0.732576	0.090731
26	8	0	-4.829236	-0.208024	0.571134
27	8	0	-3.779792	-1.895801	-0.290162
28	6	0	3.634923	-0.887665	2.117971
29	1	0	3.208141	-0.314943	2.948016
30	1	0	3.444287	-1.948953	2.308308
31	1	0	4.713672	-0.737216	2.135832
32	6	0	0.977680	-1.710930	-1.552916
33	1	0	0.393536	-2.408822	-0.952350
34	1	0	0.508415	-1.593488	-2.530353
35	1	0	1.971584	-2.135007	-1.694322



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.646491	-1.257457	0.608055
2	6	0	-0.603540	-0.955332	-1.267926
3	7	0	-0.983924	-0.267449	2.016371
4	6	0	-2.819293	-1.016577	-0.265754
5	6	0	-1.744815	-1.665690	-0.801894
6	6	0	-2.820072	0.435969	-0.284015
7	7	0	-3.869760	1.091367	0.198146
8	6	0	-1.730614	1.177139	-0.883620
9	6	0	-0.664681	0.473404	-1.363416
10	6	0	0.161732	-0.135955	1.413402
11	6	0	0.991443	1.060188	1.450397
12	6	0	1.968937	-1.231396	0.086693
13	6	0	2.711868	-0.094666	0.225334
14	6	0	2.227954	1.074363	0.895025
15	1	0	0.123466	-1.481508	-1.871504
16	1	0	-1.732680	-2.748739	-0.827197
17	1	0	-4.647138	0.608739	0.624529
18	1	0	-3.907981	2.100045	0.203409
19	1	0	0.162471	1.000600	-1.823088
20	1	0	0.610500	1.932989	1.967688
21	1	0	0.178771	-2.217184	0.769236
22	1	0	2.379709	-2.100800	-0.407400
23	1	0	2.861286	1.948451	0.948058
24	6	0	-4.000215	-1.758020	0.289879

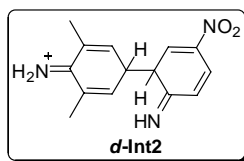
25	1	0	-4.150828	-1.526240	1.349328
26	1	0	-4.922828	-1.504981	-0.242671
27	1	0	-3.848777	-2.833187	0.204108
28	6	0	-1.795923	2.676478	-0.965589
29	1	0	-2.675538	3.012090	-1.524476
30	1	0	-1.839390	3.131921	0.029779
31	1	0	-0.912817	3.067048	-1.469612
32	7	0	4.078291	-0.072020	-0.320321
33	8	0	4.471598	-1.050510	-0.947021
34	8	0	4.753785	0.932524	-0.117448
35	1	0	-1.229170	0.596677	2.506751



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.897394	0.681717	0.515237
2	6	0	-2.296056	0.445844	1.740775
3	6	0	-1.694129	-0.788924	2.031621
4	6	0	-1.720072	-1.826287	1.082100
5	6	0	-2.316865	-1.650035	-0.155592
6	6	0	-2.912488	-0.374822	-0.463326
7	1	0	-2.283487	1.236524	2.481074

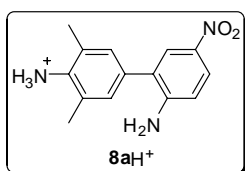
8	1	0	-1.279061	-2.786235	1.324087
9	6	0	0.554451	0.506648	-0.089217
10	6	0	1.563938	-0.429133	-0.028574
11	6	0	0.859804	1.921100	-0.258970
12	6	0	2.887495	0.001708	-0.092533
13	1	0	1.371894	-1.485147	0.085156
14	6	0	2.264580	2.303906	-0.312887
15	6	0	3.248689	1.359524	-0.230836
16	1	0	2.517725	3.351021	-0.431788
17	1	0	4.300810	1.601119	-0.270955
18	7	0	-3.489026	-0.173510	-1.668367
19	1	0	-3.922776	0.714356	-1.900671
20	7	0	-0.157973	2.746433	-0.361417
21	1	0	0.141855	3.737030	-0.465038
22	1	0	-1.234030	-0.952902	2.997810
23	1	0	-0.482869	0.234469	-0.020142
24	1	0	-3.544276	-0.916890	-2.357477
25	6	0	-2.369524	-2.766330	-1.175260
26	1	0	-3.407657	-3.045442	-1.401505
27	1	0	-1.874345	-2.482767	-2.113931
28	1	0	-1.867538	-3.657411	-0.791611
29	6	0	-3.465299	2.036816	0.165738
30	1	0	-2.781554	2.547910	-0.525111
31	1	0	-4.465932	1.968351	-0.278523
32	1	0	-3.549236	2.654294	1.063436
33	7	0	3.956296	-1.000332	-0.003540
34	8	0	3.585695	-2.220526	0.133900
35	8	0	5.158381	-0.561575	-0.075298



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.033763	-0.608553	-0.588264
2	6	0	-1.866366	-1.109945	-1.043277
3	6	0	-0.590362	-0.352807	-1.058651
4	6	0	-0.674975	0.997283	-0.444164
5	6	0	-1.814298	1.531481	0.040058
6	6	0	-3.029044	0.729951	-0.025216
7	1	0	-1.845725	-2.109082	-1.463608
8	1	0	0.236623	1.584538	-0.414031
9	6	0	0.622061	-1.212838	-0.503444
10	6	0	1.919009	-0.588527	-0.917593
11	6	0	0.481652	-1.458734	1.000037
12	6	0	2.779642	-0.117992	-0.006289
13	1	0	2.142350	-0.515742	-1.974464
14	6	0	1.434554	-0.791436	1.893002
15	6	0	2.533329	-0.172188	1.425839
16	1	0	1.247809	-0.848329	2.959722
17	1	0	3.251351	0.285322	2.091551
18	7	0	-4.153603	1.236901	0.436206
19	1	0	-5.021611	0.719819	0.409260

20	7	0	-0.460513	-2.233006	1.387825
21	1	0	-0.483586	-2.302387	2.407376
22	1	0	-0.348745	-0.198471	-2.125217
23	1	0	0.545680	-2.179096	-1.012285
24	1	0	-4.195493	2.165405	0.833039
25	7	0	4.042613	0.492151	-0.468388
26	8	0	4.807900	0.919069	0.390138
27	8	0	4.264409	0.543867	-1.672513
28	6	0	-1.865911	2.914725	0.632833
29	1	0	-2.547059	3.565663	0.075141
30	1	0	-2.196273	2.893232	1.676131
31	1	0	-0.877690	3.372151	0.607862
32	6	0	-4.317838	-1.393523	-0.632233
33	1	0	-4.721861	-1.558044	0.371924
34	1	0	-5.082828	-0.882240	-1.225166
35	1	0	-4.147025	-2.369932	-1.083583

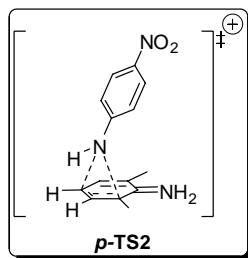


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.899323	0.705065	0.801659
2	6	0	-1.537648	0.991383	0.685906
3	6	0	-0.682938	0.199515	-0.089120

4	6	0	-1.212126	-0.905918	-0.762752
5	6	0	-2.566074	-1.236643	-0.681170
6	6	0	-3.372545	-0.406529	0.100319
7	1	0	-1.139410	1.838170	1.232355
8	1	0	-0.561430	-1.522386	-1.371506
9	6	0	0.775479	0.497285	-0.173674
10	6	0	1.690777	-0.474210	0.203039
11	6	0	1.257654	1.752719	-0.651671
12	6	0	3.064685	-0.229600	0.138178
13	1	0	1.342383	-1.430972	0.566949
14	6	0	2.655028	1.975081	-0.701950
15	6	0	3.549401	1.003829	-0.313185
16	1	0	3.020561	2.929030	-1.063628
17	1	0	4.614395	1.183169	-0.358018
18	7	0	-4.815525	-0.739753	0.210031
19	1	0	-5.012731	-1.371799	0.993876
20	1	0	-5.388266	0.096903	0.349295
21	7	0	0.408668	2.737274	-1.050464
22	1	0	0.776682	3.546736	-1.525101
23	1	0	-5.163452	-1.197110	-0.636969
24	1	0	-0.570400	2.544300	-1.189639
25	6	0	-3.795243	1.563172	1.661372
26	1	0	-4.607650	2.017436	1.083712
27	1	0	-4.243144	0.993692	2.481360
28	1	0	-3.223401	2.378790	2.102265
29	6	0	-3.111472	-2.438282	-1.413314
30	1	0	-3.556692	-3.165627	-0.727909
31	1	0	-3.872882	-2.159988	-2.150316

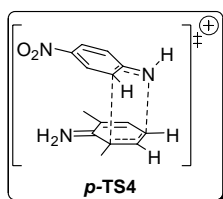
32	1	0	-2.312867	-2.943490	-1.955101
33	7	0	3.989314	-1.257969	0.545839
34	8	0	5.201364	-1.021307	0.486431
35	8	0	3.539534	-2.340559	0.939658



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.574990	-0.043105	-0.041587
2	6	0	2.745532	1.082632	0.040191
3	6	0	1.392501	0.892216	0.197608
4	6	0	0.838869	-0.431124	0.273248
5	6	0	1.736534	-1.550635	0.182163
6	6	0	3.088836	-1.356003	0.028279
7	1	0	3.174309	2.072547	-0.019870
8	1	0	0.715187	1.733688	0.264731
9	1	0	1.331065	-2.554031	0.238001
10	1	0	3.775152	-2.187739	-0.040896
11	7	0	-0.478251	-0.545122	0.422786
12	6	0	-3.387920	-1.082606	-0.208453
13	6	0	-3.239862	0.277037	-0.686569

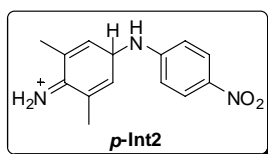
14	6	0	-3.214172	-1.313946	1.138641
15	6	0	-2.957104	1.363028	0.224689
16	6	0	-2.853297	-0.274321	2.009408
17	1	0	-3.323273	-2.320705	1.524362
18	6	0	-2.772727	1.055289	1.549596
19	1	0	-2.694182	-0.486703	3.059595
20	1	0	-2.540699	1.845676	2.253336
21	7	0	-3.424132	0.538625	-1.983054
22	1	0	-3.332690	1.472952	-2.353510
23	1	0	-3.631526	-0.191641	-2.648071
24	1	0	-0.739126	-1.533845	0.439140
25	7	0	5.022434	0.160543	-0.209283
26	8	0	5.739080	-0.833987	-0.273525
27	8	0	5.436379	1.314194	-0.275830
28	6	0	-2.854503	2.770492	-0.286988
29	1	0	-2.046474	2.873516	-1.020253
30	1	0	-3.782086	3.095987	-0.770525
31	1	0	-2.648030	3.458357	0.532152
32	6	0	-3.754817	-2.183912	-1.161314
33	1	0	-4.722891	-1.995206	-1.638560
34	1	0	-3.011290	-2.298507	-1.957367
35	1	0	-3.824620	-3.134588	-0.634032



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.433336	-0.334194	2.597061
2	6	0	-3.309384	0.357412	0.383162
3	6	0	-0.002131	0.964186	1.210816
4	6	0	-1.223127	1.343843	-0.409871
5	6	0	2.014529	-0.107712	0.433230
6	7	0	0.024364	0.052814	-2.032958
7	6	0	1.339291	1.041645	0.696575
8	6	0	-0.991423	0.105280	-1.186730
9	6	0	-0.441409	-0.334911	1.773123
10	6	0	-2.491048	1.434904	0.265572
11	6	0	0.299578	-1.522053	1.351006
12	6	0	-2.972825	-0.878117	-0.253179
13	6	0	1.495040	-1.414827	0.726795
14	6	0	-1.852223	-1.036691	-1.024169
15	1	0	0.588251	0.862049	-2.248741
16	1	0	0.224514	-0.784901	-2.562393
17	1	0	-3.649299	-1.717752	-0.139978
18	1	0	-4.240226	0.429805	0.930884
19	1	0	-2.743456	2.377426	0.735805
20	1	0	1.802428	1.999882	0.510524
21	1	0	-0.357282	1.832820	1.750432
22	1	0	2.077069	-2.284717	0.458121
23	1	0	-0.100465	-2.494498	1.614161
24	1	0	-1.662189	-1.286959	2.892487

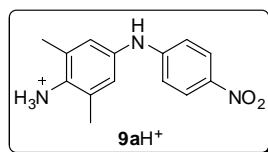
25	7	0	3.385335	-0.010640	-0.118302
26	8	0	3.811418	1.096543	-0.421438
27	8	0	4.017013	-1.053054	-0.241812
28	6	0	-0.673840	2.649473	-0.959541
29	1	0	0.385472	2.617565	-1.212723
30	1	0	-1.228788	2.916298	-1.863239
31	1	0	-0.814753	3.450123	-0.232844
32	6	0	-1.565960	-2.313958	-1.766902
33	1	0	-1.632142	-2.167816	-2.850444
34	1	0	-0.569271	-2.705368	-1.542066
35	1	0	-2.292267	-3.078574	-1.493921



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.133774	1.347786	0.163402
2	6	0	-1.827939	1.052955	0.020933
3	6	0	-1.317155	-0.305508	-0.344326
4	6	0	-2.374967	-1.356949	-0.414856
5	6	0	-3.691083	-1.102063	-0.296443
6	6	0	-4.101544	0.271207	-0.018121
7	1	0	-1.080402	1.826318	0.159968
8	1	0	-2.029419	-2.367016	-0.604825

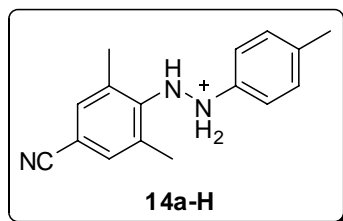
9	7	0	-5.380991	0.542212	0.090411
10	1	0	-6.088458	-0.172259	-0.019065
11	1	0	-5.712759	1.476619	0.290277
12	7	0	-0.212092	-0.739741	0.502586
13	6	0	1.116578	-0.462931	0.303532
14	6	0	2.034292	-0.801924	1.328447
15	6	0	1.616627	0.116934	-0.883399
16	6	0	3.384805	-0.582810	1.171668
17	1	0	1.665155	-1.244475	2.246358
18	6	0	2.973206	0.334768	-1.040241
19	1	0	0.953919	0.402695	-1.688590
20	6	0	3.858217	-0.013596	-0.017714
21	1	0	4.079156	-0.845141	1.957491
22	1	0	3.351763	0.777774	-1.950751
23	1	0	-0.936761	-0.228602	-1.375105
24	1	0	-0.473371	-1.033734	1.433442
25	7	0	5.273784	0.220512	-0.185325
26	8	0	5.669934	0.726965	-1.240213
27	8	0	6.037305	-0.095318	0.733068
28	6	0	-4.737046	-2.176604	-0.429613
29	1	0	-5.346503	-2.259969	0.475411
30	1	0	-5.405890	-1.980530	-1.273631
31	1	0	-4.263669	-3.142259	-0.601001
32	6	0	-3.619253	2.729125	0.513507
33	1	0	-4.260966	3.138952	-0.272765
34	1	0	-4.186253	2.730245	1.449538
35	1	0	-2.774139	3.404991	0.636030



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.726546	-0.936530	0.349731
2	6	0	-2.456996	-1.484846	0.185344
3	6	0	-1.380011	-0.708692	-0.260966
4	6	0	-1.586639	0.640462	-0.569603
5	6	0	-2.838629	1.232034	-0.407285
6	6	0	-3.876599	0.423188	0.061860
7	1	0	-2.299943	-2.531805	0.417599
8	1	0	-0.779332	1.237436	-0.970858
9	7	0	-5.217101	1.033846	0.246452
10	1	0	-5.153617	2.020753	0.510248
11	1	0	-5.741394	0.566503	0.991037
12	7	0	-0.138608	-1.337516	-0.443740
13	1	0	-0.185184	-2.319939	-0.675644
14	6	0	1.132970	-0.834799	-0.261067
15	6	0	2.223083	-1.601924	-0.733345
16	6	0	1.398871	0.377721	0.410233
17	6	0	3.521457	-1.172761	-0.556238
18	1	0	2.033023	-2.537354	-1.246822
19	6	0	2.700349	0.809938	0.584611
20	1	0	0.591559	0.966552	0.820639

21	6	0	3.760356	0.041326	0.097633
22	1	0	4.350735	-1.760291	-0.924288
23	1	0	2.902692	1.733031	1.109528
24	1	0	-5.793844	0.986349	-0.600798
25	6	0	-4.873733	-1.788283	0.836186
26	1	0	-5.274647	-1.429256	1.790632
27	1	0	-5.695905	-1.813614	0.115082
28	1	0	-4.543289	-2.814030	0.994537
29	6	0	-3.045321	2.686966	-0.751259
30	1	0	-3.825509	2.820943	-1.506246
31	1	0	-3.322806	3.277649	0.128773
32	1	0	-2.126478	3.117184	-1.147804
33	7	0	5.119887	0.500464	0.280865
34	8	0	5.306762	1.588949	0.833390
35	8	0	6.043117	-0.214006	-0.121599

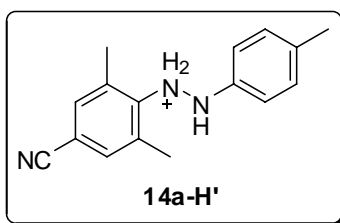


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.214911	-1.083347	0.713022
2	6	0	2.854674	-0.881386	0.935213
3	6	0	2.262042	0.260817	0.415743

4	6	0	2.978031	1.196324	-0.322605
5	6	0	4.333426	0.974444	-0.532427
6	6	0	4.973707	-0.163115	-0.018438
7	1	0	4.688047	-1.970185	1.117850
8	1	0	2.278438	-1.602356	1.504099
9	1	0	2.494557	2.077421	-0.726554
10	1	0	4.902706	1.698427	-1.103908
11	7	0	0.818275	0.469513	0.629346
12	1	0	0.507568	-0.061382	1.452838
13	7	0	0.018428	0.127900	-0.566209
14	1	0	0.408868	-0.748913	-0.897943
15	6	0	-1.390903	0.034806	-0.314790
16	6	0	-2.026063	-1.223571	-0.381448
17	6	0	-2.111343	1.224925	-0.093784
18	6	0	-3.405564	-1.271525	-0.199113
19	6	0	-3.486787	1.135478	0.106336
20	6	0	-4.132712	-0.103733	0.057619
21	1	0	-3.918592	-2.223679	-0.246954
22	1	0	-4.062208	2.036385	0.278606
23	1	0	0.637505	1.456974	0.832667
24	6	0	-1.263886	-2.497005	-0.662436
25	1	0	-0.777231	-2.472740	-1.642833
26	1	0	-0.494180	-2.690553	0.090379
27	1	0	-1.942709	-3.349349	-0.661525
28	6	0	-1.440542	2.575651	-0.093988
29	1	0	-1.011457	2.820658	0.884910
30	1	0	-0.648068	2.624080	-0.844176
31	1	0	-2.164087	3.360430	-0.314871

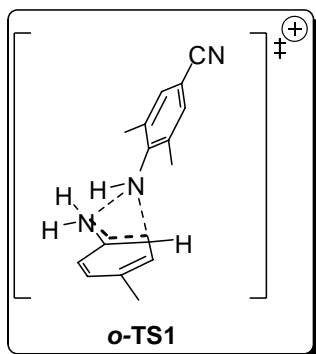
32	6	0	6.450259	-0.371828	-0.234826
33	1	0	6.735746	-0.134591	-1.262188
34	1	0	7.029738	0.283652	0.423253
35	1	0	6.742360	-1.401102	-0.022350
36	6	0	-5.547480	-0.177296	0.255602
37	7	0	-6.690649	-0.237556	0.416951



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.272327	-1.173348	-0.476289
2	6	0	-2.893002	-1.103744	-0.660655
3	6	0	-2.222699	0.096579	-0.420815
4	6	0	-2.934527	1.218416	0.013190
5	6	0	-4.306081	1.127641	0.218185
6	6	0	-5.000455	-0.065489	-0.029555
7	1	0	-4.785802	-2.107023	-0.676900
8	1	0	-2.346811	-1.978376	-0.997356
9	1	0	-2.419693	2.158743	0.173415
10	1	0	-4.849362	2.002625	0.558209
11	7	0	-0.806147	0.225025	-0.654031
12	1	0	-0.465596	-0.506683	-1.273617

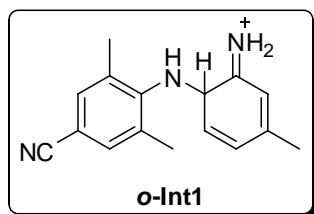
13	7	0	-0.026233	0.050114	0.604996
14	1	0	-0.327270	-0.791076	1.113711
15	6	0	1.430919	0.021020	0.374924
16	6	0	2.067706	-1.226572	0.370613
17	6	0	2.081842	1.243413	0.163190
18	6	0	3.440213	-1.231416	0.124932
19	6	0	3.452971	1.192760	-0.079988
20	6	0	4.124521	-0.034064	-0.103760
21	1	0	3.977170	-2.170774	0.114631
22	1	0	3.999513	2.111462	-0.248769
23	6	0	1.341473	-2.522099	0.641627
24	1	0	0.883310	-2.529432	1.635868
25	1	0	0.560522	-2.724429	-0.095895
26	1	0	2.040747	-3.356156	0.606278
27	6	0	1.359907	2.565677	0.208299
28	1	0	0.567771	2.612549	-0.541614
29	1	0	0.908155	2.743762	1.190517
30	1	0	2.056192	3.382145	0.023195
31	6	0	-6.494769	-0.138010	0.158937
32	1	0	-6.796293	0.323108	1.102640
33	1	0	-7.012044	0.398199	-0.643313
34	1	0	-6.847263	-1.170556	0.151175
35	1	0	-0.271175	0.848787	1.197306
36	6	0	5.534097	-0.063805	-0.356494
37	7	0	6.670838	-0.087799	-0.560611



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.105005	1.487076	1.885512
2	7	0	-0.100174	0.566427	0.520761
3	6	0	2.648105	1.090336	-0.425659
4	6	0	2.811557	0.805484	0.958636
5	1	0	2.218186	1.306413	2.872311
6	1	0	1.413475	2.167838	1.608686
7	1	0	1.981642	1.886770	-0.726976
8	1	0	0.418646	-0.207782	0.937188
9	6	0	3.379714	0.384413	-1.368857
10	1	0	3.253505	0.623292	-2.418680
11	6	0	3.718691	-0.219285	1.344114
12	1	0	3.845432	-0.451790	2.395153
13	6	0	-1.350272	0.234186	0.298551
14	6	0	-1.902461	-1.081632	0.624370
15	6	0	-2.207298	1.250136	-0.309940
16	6	0	-3.222971	-1.334716	0.332611
17	1	0	-3.657570	-2.299600	0.559393

18	6	0	-3.522462	0.937079	-0.577055
19	1	0	-4.176867	1.670160	-1.030360
20	6	0	-4.026893	-0.339625	-0.262968
21	6	0	4.279857	-0.619943	-0.995005
22	6	0	4.430023	-0.901524	0.385469
23	1	0	5.122763	-1.677226	0.693024
24	6	0	-1.042478	-2.125018	1.267006
25	1	0	-0.173659	-2.364104	0.645054
26	1	0	-0.664844	-1.783211	2.236334
27	1	0	-1.605173	-3.043363	1.428426
28	6	0	-1.650567	2.598121	-0.633992
29	1	0	-1.271392	3.086119	0.268223
30	1	0	-0.802445	2.510585	-1.318648
31	1	0	-2.410349	3.233301	-1.088087
32	6	0	5.070290	-1.388824	-2.013617
33	1	0	6.141148	-1.347703	-1.791427
34	1	0	4.786989	-2.447238	-2.004648
35	1	0	4.910464	-1.002735	-3.020856
36	6	0	-5.392167	-0.637007	-0.552712
37	7	0	-6.498253	-0.878190	-0.787676

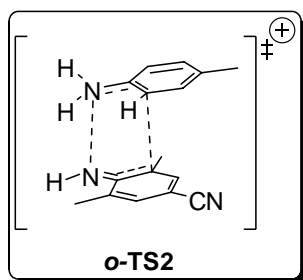


Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.284191	0.445246	-0.258391
2	6	0	3.105573	-0.525303	0.734827
3	6	0	1.876818	-1.153483	0.902187
4	6	0	0.804264	-0.806369	0.045214
5	6	0	0.984162	0.142419	-0.986182
6	6	0	2.222259	0.766690	-1.110874
7	1	0	3.928891	-0.779781	1.391003
8	1	0	2.370446	1.496070	-1.897903
9	7	0	-0.427151	-1.490559	0.204806
10	6	0	-1.694482	-0.795580	0.456432
11	6	0	-2.710969	-0.960664	-0.650728
12	6	0	-1.634529	0.580268	1.047912
13	6	0	-3.783004	-0.029341	-0.733765
14	6	0	-2.631474	1.473548	0.878900
15	1	0	-0.800423	0.782926	1.709200
16	6	0	-3.729299	1.118119	-0.000581
17	1	0	-4.590597	-0.206102	-1.433172
18	1	0	-4.539947	1.831664	-0.107490
19	7	0	-2.605392	-2.000719	-1.434078
20	1	0	-0.328851	-2.272686	0.834876
21	1	0	-3.303286	-2.222151	-2.132777
22	1	0	-2.198877	-1.369337	1.259565
23	1	0	-1.779553	-2.587469	-1.367115
24	6	0	1.709469	-2.185218	1.992252
25	1	0	0.888620	-1.929931	2.669773
26	1	0	1.506828	-3.182093	1.585211

27	1	0	2.619029	-2.260296	2.588074
28	6	0	-0.096645	0.459054	-1.988528
29	1	0	-0.481327	-0.452528	-2.452236
30	1	0	-0.940575	0.992064	-1.541366
31	1	0	0.297769	1.096179	-2.780507
32	6	0	-2.653863	2.819277	1.552282
33	1	0	-2.711094	3.621822	0.811385
34	1	0	-3.531313	2.911018	2.199199
35	1	0	-1.761398	2.972255	2.159298
36	6	0	4.546501	1.093860	-0.409493
37	7	0	5.569948	1.620314	-0.531272

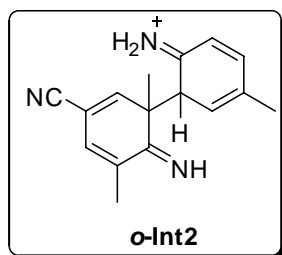


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.844868	-2.375187	1.077488
2	7	0	1.044063	-2.515198	-1.020593
3	6	0	0.889418	-0.112536	-0.828239
4	6	0	-0.354709	-0.050717	0.898653
5	6	0	1.607431	-1.363844	-0.674067
6	6	0	-1.229318	-1.233052	0.616627

7	6	0	-0.948061	1.254974	0.678134
8	6	0	1.660349	1.105620	-0.740136
9	1	0	0.056434	-0.117114	-1.522893
10	1	0	0.180453	-2.552636	-1.540478
11	1	0	1.528339	-3.392385	-0.884093
12	1	0	-1.496260	-3.119700	0.823504
13	1	0	1.171635	2.031828	-1.016818
14	1	0	-0.419371	2.128137	1.038122
15	6	0	2.918828	-1.339673	-0.120346
16	1	0	3.420149	-2.274974	0.097511
17	6	0	3.550771	-0.144756	0.059140
18	6	0	2.945298	1.116626	-0.287464
19	1	0	4.562091	-0.141467	0.451765
20	6	0	-2.461625	-1.030233	-0.176041
21	6	0	-2.874608	0.231692	-0.441783
22	1	0	-3.792132	0.402415	-0.991649
23	6	0	-2.137732	1.385691	0.032738
24	6	0	0.584260	-0.141719	2.075429
25	1	0	0.007722	0.062246	2.984034
26	1	0	1.022893	-1.130191	2.171892
27	1	0	1.367899	0.614760	2.011216
28	6	0	-3.269855	-2.224156	-0.600087
29	1	0	-2.676949	-2.934025	-1.184760
30	1	0	-3.660797	-2.764361	0.268488
31	1	0	-4.119388	-1.913107	-1.207344
32	6	0	3.753046	2.378251	-0.155718
33	1	0	4.071727	2.527093	0.880611
34	1	0	4.660012	2.324044	-0.765373

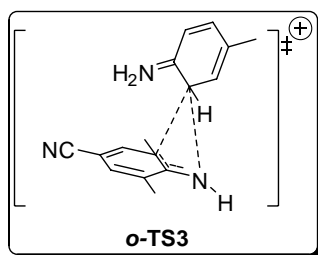
35	1	0	3.179556	3.251574	-0.467767
36	6	0	-2.693913	2.686984	-0.178395
37	7	0	-3.156552	3.730808	-0.356414



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.318587	-0.040270	0.765210
2	6	0	0.523327	1.218325	-0.094588
3	6	0	1.478171	-1.002609	0.694470
4	6	0	1.912521	1.645377	-0.381432
5	6	0	2.692756	-0.598069	0.268808
6	1	0	1.337188	-1.999836	1.096633
7	6	0	2.920086	0.761746	-0.219841
8	1	0	3.935237	1.040215	-0.476535
9	7	0	-0.526090	1.833741	-0.481048
10	1	0	-0.308686	2.696490	-0.979936
11	6	0	-1.037083	-0.759123	0.384549
12	6	0	-1.196553	-1.040900	-1.089901
13	6	0	-2.271717	-0.197733	1.024107
14	6	0	-2.479173	-0.950635	-1.691021

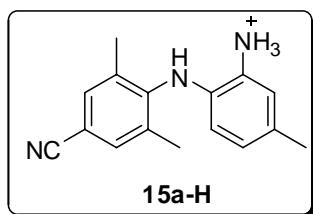
15	6	0	-3.473480	-0.126433	0.413702
16	1	0	-2.191095	0.069645	2.068607
17	6	0	-3.553300	-0.525306	-0.968571
18	1	0	-2.584082	-1.213189	-2.736859
19	1	0	-4.517538	-0.470979	-1.464010
20	7	0	-0.169815	-1.437708	-1.813025
21	1	0	-0.289811	-1.684849	-2.787048
22	1	0	0.763099	-1.532926	-1.432837
23	1	0	-0.962896	-1.768724	0.829152
24	6	0	0.304305	0.438746	2.254343
25	1	0	-0.429084	1.233836	2.389753
26	1	0	0.077820	-0.389972	2.927819
27	1	0	1.286589	0.833694	2.516182
28	6	0	2.146959	3.021754	-0.936181
29	1	0	3.213803	3.216420	-1.044721
30	1	0	1.684681	3.137961	-1.922015
31	1	0	1.720482	3.788795	-0.282608
32	6	0	-4.717811	0.362578	1.106885
33	1	0	-5.132832	1.232985	0.590048
34	1	0	-5.490552	-0.411726	1.110833
35	1	0	-4.509178	0.644198	2.139455
36	6	0	3.806692	-1.497475	0.317216
37	7	0	4.717494	-2.207730	0.347153



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.161850	-1.333459	-1.007436
2	6	0	2.542980	-0.099600	-1.477836
3	6	0	2.858928	0.939962	-0.577602
4	6	0	2.082483	-1.547316	0.451614
5	7	0	1.693977	-2.715538	0.853716
6	6	0	2.804115	0.765360	0.827333
7	1	0	3.068713	1.594983	1.470340
8	6	0	2.430705	-0.439200	1.366965
9	1	0	2.606215	0.085168	-2.542143
10	1	0	1.666030	-2.776672	1.873479
11	6	0	-2.026607	-0.224873	-0.019675
12	1	0	-1.065557	-0.719494	-0.088017
13	6	0	-2.094274	1.105994	0.462077
14	6	0	-3.181258	-0.887801	-0.395486
15	1	0	-3.108792	-1.905932	-0.761282
16	6	0	-4.443695	-0.277352	-0.306159
17	6	0	-4.502110	1.045801	0.182322
18	1	0	-5.464969	1.538811	0.261937

19	6	0	-3.365596	1.728953	0.560054
20	1	0	-3.431539	2.746233	0.928794
21	7	0	-0.970462	1.775260	0.820814
22	1	0	-1.016314	2.712859	1.189161
23	1	0	-0.059567	1.352186	0.748159
24	6	0	-5.696924	-1.000444	-0.709481
25	1	0	-6.395193	-1.073577	0.130963
26	1	0	-6.219931	-0.462436	-1.507300
27	1	0	-5.481193	-2.009391	-1.063031
28	6	0	2.385426	-0.648256	2.846578
29	1	0	1.381851	-0.933386	3.178616
30	1	0	3.067807	-1.449131	3.149743
31	1	0	2.671647	0.260462	3.373914
32	6	0	1.835252	-2.454602	-1.934552
33	1	0	2.514607	-3.296096	-1.768720
34	1	0	0.827308	-2.832570	-1.744244
35	1	0	1.910743	-2.135295	-2.973151
36	6	0	3.261630	2.205200	-1.096226
37	7	0	3.592299	3.230716	-1.516266

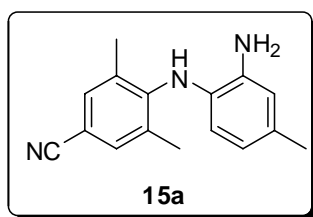


Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	2.502338	-1.158079	-0.646613
2	6	0	1.177964	-0.728228	-0.744995
3	6	0	0.865894	0.586325	-0.318054
4	6	0	1.887040	1.476640	0.103092
5	6	0	3.196007	1.019100	0.157037
6	6	0	3.509746	-0.302544	-0.192262
7	1	0	2.756378	-2.161412	-0.965924
8	1	0	3.981564	1.685748	0.490933
9	7	0	-0.452185	1.071205	-0.339032
10	6	0	-1.633331	0.400899	0.001450
11	6	0	-1.733090	-0.479569	1.086904
12	6	0	-2.806672	0.655843	-0.726832
13	6	0	-2.928361	-1.117611	1.399878
14	6	0	-4.022096	0.052937	-0.414347
15	1	0	-2.742395	1.335223	-1.569627
16	6	0	-4.066894	-0.857915	0.652493
17	1	0	-2.973099	-1.803539	2.238479
18	1	0	-4.994985	-1.356732	0.904600
19	7	0	-0.573874	-0.693006	1.980284
20	1	0	-0.807523	-1.360573	2.719993
21	1	0	-0.574600	2.027463	-0.639294
22	1	0	0.254743	-1.056649	1.491221
23	1	0	-0.286918	0.176386	2.442736
24	6	0	0.162312	-1.638538	-1.398541
25	1	0	-0.503283	-2.137838	-0.688428
26	1	0	-0.471441	-1.080124	-2.090554

27	1	0	0.677285	-2.418509	-1.959932
28	6	0	1.559994	2.894853	0.495337
29	1	0	1.198852	3.477517	-0.359671
30	1	0	0.780559	2.928376	1.261858
31	1	0	2.444908	3.399909	0.882424
32	6	0	-5.265345	0.357796	-1.210835
33	1	0	-5.040479	0.967735	-2.086593
34	1	0	-5.749547	-0.562692	-1.546859
35	1	0	-5.991313	0.900113	-0.597411
36	6	0	4.857268	-0.765715	-0.106281
37	7	0	5.949580	-1.140709	-0.034472

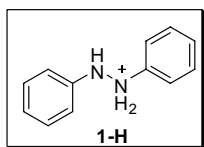


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.484846	-1.271994	-0.443167
2	6	0	1.163051	-0.850240	-0.543748
3	6	0	0.869183	0.524111	-0.326267
4	6	0	1.927224	1.447133	-0.080678
5	6	0	3.231797	0.986254	-0.007541
6	6	0	3.526574	-0.376219	-0.169880

7	1	0	2.714837	-2.317730	-0.610085
8	1	0	4.033507	1.687572	0.191258
9	7	0	-0.422338	1.027576	-0.396698
10	6	0	-1.644075	0.401663	0.005141
11	6	0	-1.797830	-0.166249	1.285940
12	6	0	-2.730330	0.441772	-0.875105
13	6	0	-3.049859	-0.717180	1.608768
14	6	0	-3.982294	-0.073668	-0.542396
15	1	0	-2.570600	0.887230	-1.851885
16	6	0	-4.115069	-0.668998	0.719578
17	1	0	-3.183854	-1.172042	2.585211
18	1	0	-5.066402	-1.101301	1.013404
19	7	0	-0.783320	-0.121910	2.245537
20	1	0	-0.885015	-0.790632	2.996753
21	1	0	-0.484326	2.032591	-0.460092
22	6	0	0.113993	-1.856681	-0.955921
23	1	0	-0.555578	-2.131208	-0.136941
24	1	0	-0.511008	-1.466643	-1.762419
25	1	0	0.597689	-2.768203	-1.310560
26	6	0	1.637023	2.915104	0.111759
27	1	0	1.199601	3.367946	-0.785865
28	1	0	0.937101	3.083379	0.936977
29	1	0	2.554157	3.460869	0.334277
30	6	0	-5.148305	0.007680	-1.499183
31	1	0	-4.815172	0.252794	-2.509884
32	1	0	-5.695044	-0.938342	-1.543239
33	1	0	-5.862708	0.779053	-1.191273

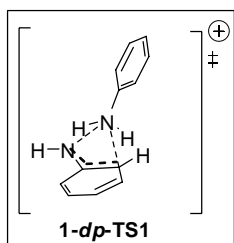
34	1	0	0.165058	-0.100561	1.898872
35	6	0	4.869269	-0.839974	-0.076832
36	7	0	5.962311	-1.217073	0.000117



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.950177	-1.141663	0.224566
2	6	0	2.586961	-1.164257	0.517342
3	6	0	1.853328	-0.001096	0.328724
4	6	0	2.420349	1.176590	-0.144265
5	6	0	3.782016	1.182606	-0.431559
6	6	0	4.543852	0.027030	-0.247943
7	1	0	4.541466	-2.037187	0.368738
8	1	0	4.246366	2.090159	-0.796684
9	1	0	5.603385	0.039760	-0.473451
10	7	0	0.406985	-0.021764	0.619567
11	1	0	0.176735	-0.834014	1.207900
12	7	0	-0.413683	0.007909	-0.611426
13	1	0	-0.133808	-0.822101	-1.130784
14	6	0	-1.823534	-0.011633	-0.316475

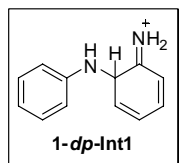
15	6	0	-2.577769	-1.172064	-0.502616
16	6	0	-2.434202	1.170359	0.111486
17	6	0	-3.951331	-1.144667	-0.266222
18	1	0	-2.097889	-2.086132	-0.834785
19	6	0	-3.801243	1.180525	0.374147
20	1	0	-1.848572	2.076605	0.219165
21	6	0	-4.561964	0.026233	0.180580
22	1	0	-4.539038	-2.041415	-0.422293
23	1	0	-4.275321	2.095246	0.709332
24	1	0	0.147234	0.809970	1.157599
25	1	0	-5.628234	0.041993	0.372765
26	1	0	1.817416	2.064789	-0.287767
27	1	0	2.117293	-2.068467	0.886689



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.727068	1.966268	-0.771404
2	7	0	0.582683	0.571571	-0.096239

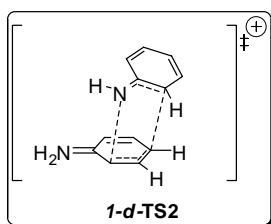
3	6	0	-2.096052	0.433284	1.049620
4	6	0	-2.343711	0.862372	-0.282352
5	1	0	-1.911226	2.298969	-1.705670
6	1	0	-1.077401	2.489310	-0.205415
7	1	0	0.054065	0.082417	-0.823350
8	6	0	-2.723162	-0.708127	1.537819
9	1	0	-2.536858	-1.019469	2.558837
10	6	0	-3.221100	0.104126	-1.099526
11	6	0	1.837998	0.178988	-0.092269
12	6	0	2.374338	-0.810607	-1.001417
13	1	0	1.709121	-1.263810	-1.727623
14	6	0	2.724915	0.780690	0.877550
15	1	0	2.308141	1.518920	1.551219
16	6	0	3.699059	-1.159097	-0.934105
17	1	0	4.109916	-1.898325	-1.609683
18	6	0	4.047204	0.415776	0.925043
19	1	0	4.718149	0.862025	1.647661
20	6	0	4.534041	-0.549689	0.024211
21	6	0	-3.587287	-1.442830	0.729752
22	1	0	-4.075784	-2.329111	1.115734
23	6	0	-3.830404	-1.025330	-0.591397
24	1	0	-4.503283	-1.596454	-1.220238
25	1	0	-1.450518	1.023967	1.685108
26	1	0	-3.407742	0.422871	-2.118729
27	1	0	5.579088	-0.833518	0.068076



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.561852	-0.827220	-0.736844
2	6	0	-3.693087	0.123677	0.278247
3	6	0	-2.571104	0.732941	0.828061
4	6	0	-1.286341	0.400927	0.369210
5	6	0	-1.154626	-0.552177	-0.648678
6	6	0	-2.288207	-1.158402	-1.192069
7	1	0	-4.676223	0.391345	0.648795
8	1	0	-2.683972	1.469173	1.617155
9	1	0	-0.179964	-0.828014	-1.032876
10	1	0	-2.165464	-1.894206	-1.978747
11	7	0	-0.175420	1.077385	0.912936
12	6	0	1.161215	0.524565	0.844996
13	6	0	1.880057	0.872290	-0.445190
14	6	0	1.355746	-0.898876	1.293280
15	6	0	2.960584	0.055213	-0.881138
16	6	0	2.350368	-1.654267	0.795041

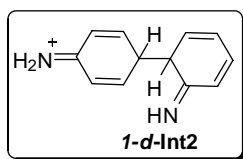
17	1	0	0.722713	-1.239631	2.103649
18	6	0	3.173580	-1.149382	-0.276608
19	1	0	2.540954	-2.649086	1.176570
20	1	0	3.979126	-1.776726	-0.641379
21	7	0	1.506147	1.956141	-1.070954
22	1	0	-0.371518	1.557813	1.779261
23	1	0	1.986605	2.297779	-1.893548
24	1	0	0.694470	2.462896	-0.730171
25	1	0	-4.438134	-1.301345	-1.162248
26	1	0	1.762664	1.092089	1.579920
27	1	0	3.555675	0.367499	-1.730098



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.312682	0.812599	0.807314
2	6	0	0.268132	1.495292	-0.613947
3	7	0	0.029374	-0.872065	1.808533
4	6	0	2.323149	0.898761	0.531756

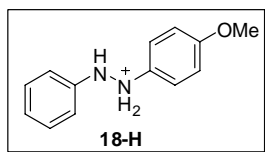
5	6	0	1.301022	1.777387	0.328614
6	6	0	2.434203	-0.278883	-0.277896
7	7	0	3.452759	-1.123550	-0.099082
8	6	0	1.470713	-0.509006	-1.306220
9	6	0	0.430731	0.358733	-1.474310
10	6	0	-0.921036	-0.596350	0.971167
11	6	0	-1.643164	-1.581286	0.173332
12	6	0	-2.527271	1.120926	0.126003
13	6	0	-3.223774	0.135000	-0.512639
14	6	0	-2.756017	-1.225584	-0.515079
15	1	0	-0.372107	2.303578	-0.938592
16	1	0	1.243972	2.683603	0.919386
17	1	0	4.141271	-0.971992	0.623082
18	1	0	3.552518	-1.953508	-0.664749
19	1	0	-0.292222	0.188423	-2.262355
20	1	0	-1.293441	-2.607507	0.190595
21	1	0	-0.947499	1.498393	1.558414
22	1	0	-2.885618	2.142916	0.124648
23	1	0	-3.317151	-1.969592	-1.068033
24	1	0	0.219687	-1.877872	1.811998
25	1	0	1.579348	-1.376711	-1.945852
26	1	0	3.083534	1.095004	1.278311
27	1	0	-4.151265	0.369030	-1.021580



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.202175	0.384396	0.956644
2	6	0	-0.238572	-0.255599	1.134287
3	7	0	0.634114	2.205745	-0.514221
4	6	0	-2.486393	0.714664	0.669206
5	6	0	-1.308061	0.760912	1.319171
6	6	0	-2.733379	-0.317577	-0.302772
7	7	0	-3.879010	-0.356399	-0.950316
8	6	0	-1.722060	-1.312085	-0.566096
9	6	0	-0.553696	-1.278967	0.100366
10	6	0	1.301855	1.118477	-0.381938
11	6	0	2.148418	0.525057	-1.418184
12	6	0	2.260706	-0.661044	1.179036
13	6	0	3.088282	-1.058207	0.202350
14	6	0	2.997348	-0.484164	-1.134546
15	1	0	-0.170089	-0.793013	2.096545
16	1	0	-1.127589	1.543854	2.046295
17	1	0	-4.604854	0.327904	-0.782564

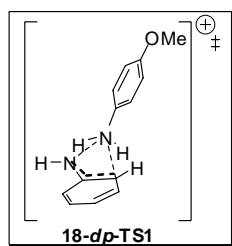
18	1	0	-4.073945	-1.070791	-1.639250
19	1	0	0.199237	-2.033372	-0.098348
20	1	0	2.103962	0.958397	-2.412072
21	1	0	1.280329	1.133181	1.750412
22	1	0	2.319222	-1.095896	2.171451
23	1	0	3.644428	-0.879991	-1.909621
24	1	0	0.748026	2.591610	-1.454168
25	1	0	-1.925078	-2.077905	-1.305430
26	1	0	-3.257742	1.452769	0.853350
27	1	0	3.838631	-1.817334	0.390017



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.074346	-0.959551	0.374186
2	6	0	1.703436	-0.995891	0.621443
3	6	0	0.943616	0.144434	0.413923
4	6	0	1.511745	1.330812	-0.048691
5	6	0	2.871777	1.367542	-0.294795
6	6	0	3.663614	0.224529	-0.084973
7	1	0	3.661388	-1.850342	0.544744
8	1	0	3.344948	2.274669	-0.648566

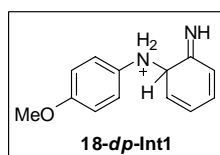
9	7	0	-0.504532	0.094331	0.663235
10	1	0	-0.729941	-0.713511	1.259046
11	7	0	-1.299102	0.079781	-0.589389
12	1	0	-0.957451	-0.731888	-1.100515
13	6	0	-2.711970	-0.022402	-0.327547
14	6	0	-3.387443	-1.233615	-0.494902
15	6	0	-3.406574	1.130062	0.050445
16	6	0	-4.765286	-1.287051	-0.290537
17	1	0	-2.842897	-2.124492	-0.788371
18	6	0	-4.777959	1.061163	0.280161
19	1	0	-2.881607	2.074349	0.143516
20	6	0	-5.459351	-0.144346	0.104745
21	1	0	-5.291655	-2.223394	-0.432530
22	1	0	-5.317234	1.953403	0.575021
23	1	0	-0.803278	0.926913	1.178811
24	1	0	0.902405	2.210746	-0.215257
25	1	0	1.248179	-1.912463	0.978723
26	1	0	-6.529189	-0.190574	0.270520
27	8	0	4.980784	0.368327	-0.352235
28	6	0	5.856578	-0.750516	-0.156778
29	1	0	6.847626	-0.396289	-0.430001
30	1	0	5.855328	-1.068547	0.888753
31	1	0	5.573370	-1.584992	-0.803008



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-2.603508	2.059324	-0.297200
2	7	0	-0.421900	0.257493	-0.680220
3	6	0	-2.668323	0.099731	1.033071
4	1	0	-1.829313	0.476702	1.600458
5	1	0	-3.088024	2.581003	-1.030924
6	6	0	-3.244763	0.957502	0.007693
7	6	0	0.918263	0.089911	-0.525817
8	6	0	-3.256571	-1.114326	1.340282
9	1	0	-2.832656	-1.744143	2.112171
10	6	0	1.651870	0.948869	0.328614
11	1	0	1.140612	1.760021	0.833127
12	6	0	1.600495	-0.968949	-1.181387
13	1	0	1.051273	-1.631740	-1.839745
14	6	0	-4.457094	0.506344	-0.652215
15	1	0	-4.895265	1.139958	-1.414894
16	6	0	-5.011782	-0.696721	-0.323200
17	1	0	-5.912202	-1.038797	-0.818330
18	6	0	-4.412429	-1.514863	0.670827
19	6	0	3.006275	0.768113	0.520063
20	1	0	3.543161	1.442485	1.171980
21	6	0	3.670907	-0.290229	-0.132149
22	6	0	2.946458	-1.154842	-0.983569
23	1	0	3.476831	-1.959551	-1.477035

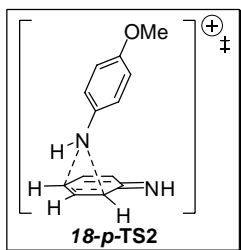
24	1	0	-0.890009	-0.280824	-1.397988
25	1	0	-4.875812	-2.461450	0.922234
26	8	0	4.979769	-0.554930	-0.010745
27	6	0	5.800540	0.270541	0.833954
28	1	0	5.455435	0.224920	1.868916
29	1	0	6.801283	-0.146634	0.759770
30	1	0	5.801873	1.303157	0.478901
31	1	0	-0.870557	1.150123	-0.457747



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.849694	-0.075615	-0.407947
2	6	0	2.576654	0.127291	0.949585
3	6	0	1.326689	-0.217773	1.460802
4	6	0	0.363711	-0.758801	0.622640
5	6	0	0.624961	-0.974868	-0.730074
6	6	0	1.865562	-0.630947	-1.240754
7	1	0	3.317965	0.544182	1.616056
8	1	0	2.094071	-0.792930	-2.286643
9	7	0	-0.954347	-1.119306	1.180593
10	6	0	-2.112487	-0.152440	0.938148
11	6	0	-2.880450	-0.666094	-0.284910

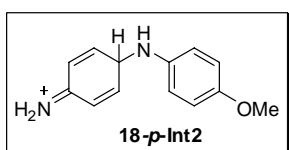
12	6	0	-1.734951	1.297280	0.904513
13	6	0	-3.642239	0.326949	-1.029854
14	6	0	-2.395927	2.131175	0.090821
15	1	0	-1.011289	1.658495	1.624247
16	6	0	-3.396867	1.642365	-0.853075
17	1	0	-4.334664	-0.023832	-1.786308
18	1	0	-3.925869	2.371792	-1.455705
19	7	0	-2.776118	-1.917275	-0.526172
20	1	0	-0.858934	-1.300143	2.181035
21	1	0	-3.342008	-2.223605	-1.316635
22	1	0	-2.784002	-0.297255	1.795117
23	1	0	1.121591	-0.061751	2.513958
24	1	0	-0.123838	-1.412385	-1.377794
25	1	0	-1.304539	-1.996931	0.738977
26	1	0	-2.197481	3.195448	0.123803
27	8	0	4.027763	0.223086	-1.006179
28	6	0	5.082495	0.788116	-0.217545
29	1	0	5.911608	0.940775	-0.904504
30	1	0	4.780432	1.747120	0.211264
31	1	0	5.387029	0.102582	0.577514



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.594747	0.263477	0.027525
2	6	0	2.996431	-1.012020	0.058912
3	6	0	1.630503	-1.133619	-0.097702
4	6	0	0.817690	0.009409	-0.292247
5	6	0	1.431024	1.290074	-0.316998
6	6	0	2.789982	1.409869	-0.161765
7	1	0	3.592729	-1.901525	0.205212
8	1	0	1.171538	-2.114959	-0.073362
9	1	0	0.820306	2.173618	-0.460922
10	1	0	3.268432	2.381011	-0.180077
11	7	0	-0.521482	-0.118867	-0.465185
12	6	0	-3.586299	1.220237	0.216377
13	6	0	-3.622335	0.075315	1.115550
14	6	0	-3.528607	1.039515	-1.141965
15	6	0	-3.537472	-1.247820	0.517597
16	6	0	-3.467165	-0.265053	-1.682773
17	1	0	-3.521297	1.893473	-1.808005
18	6	0	-3.482091	-1.399916	-0.845413
19	1	0	-3.552029	-2.099866	1.186016
20	1	0	-3.439929	-2.388580	-1.285345
21	7	0	-3.745595	0.161046	2.411240
22	1	0	-3.634386	2.214106	0.646968
23	1	0	-3.803250	1.140227	2.703575
24	1	0	-1.114259	0.691522	-0.556734
25	1	0	-3.427732	-0.394167	-2.757385

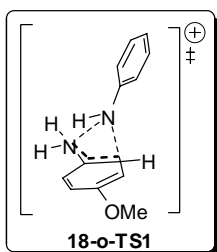
26	1	0	-0.969028	-1.019693	-0.396664
27	8	0	4.909503	0.491337	0.168564
28	6	0	5.807948	-0.614030	0.364062
29	1	0	6.797056	-0.171074	0.444855
30	1	0	5.564967	-1.149361	1.284317
31	1	0	5.774261	-1.293309	-0.490294



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.215853	-1.075407	-0.897168
2	6	0	-1.946904	-0.806826	-0.543596
3	6	0	-1.589257	0.145961	0.556619
4	6	0	-2.767607	0.850487	1.148704
5	6	0	-4.034975	0.563982	0.810597
6	6	0	-4.306677	-0.421770	-0.212207
7	1	0	-1.122628	-1.285821	-1.060044
8	1	0	-2.551358	1.604090	1.896868
9	7	0	-5.548020	-0.706338	-0.529610
10	1	0	-6.328568	-0.255849	-0.068710
11	1	0	-5.770304	-1.384353	-1.247564
12	7	0	-0.548193	1.107913	0.183881
13	6	0	0.797663	0.695501	0.037334

14	6	0	1.603830	1.328870	-0.924502
15	6	0	1.389691	-0.265004	0.860602
16	6	0	2.950101	1.021798	-1.043867
17	1	0	1.168125	2.075025	-1.581106
18	6	0	2.745284	-0.586448	0.737132
19	1	0	0.814923	-0.777327	1.622716
20	6	0	3.536233	0.057591	-0.214169
21	1	0	3.562245	1.518714	-1.787442
22	1	0	3.160985	-1.337623	1.394697
23	1	0	-1.192188	-0.466174	1.381767
24	1	0	-0.849889	1.701556	-0.579652
25	1	0	-3.445843	-1.764526	-1.701120
26	1	0	-4.871301	1.069957	1.277691
27	8	0	4.869588	-0.182585	-0.415074
28	6	0	5.513868	-1.152237	0.411012
29	1	0	6.552472	-1.176842	0.086835
30	1	0	5.468944	-0.866720	1.466475
31	1	0	5.068780	-2.143440	0.280329

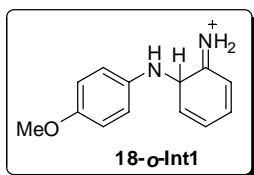


Standard orientation:

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

1	7	0	-0.395123	2.302200	-0.185109
2	7	0	1.578505	0.414504	-0.086706
3	6	0	-1.321509	0.414596	0.988787
4	6	0	-1.392176	1.401341	-0.038663
5	1	0	-0.422753	2.963459	-0.948818
6	1	0	0.516912	2.082337	0.213884
7	1	0	1.064776	0.044068	-0.891009
8	6	0	-2.332850	-0.506119	1.136152
9	1	0	-2.291141	-1.256414	1.915790
10	6	0	-2.533886	1.425228	-0.883145
11	6	0	2.832841	-0.002305	-0.107676
12	6	0	3.373454	-0.864254	-1.131097
13	1	0	2.722864	-1.185025	-1.936868
14	6	0	3.706531	0.421944	0.958358
15	1	0	3.294428	1.068998	1.722905
16	6	0	4.685118	-1.269872	-1.074095
17	1	0	5.090178	-1.920768	-1.838931
18	6	0	5.017268	0.009027	0.990304
19	1	0	5.672850	0.328120	1.790878
20	6	0	5.510818	-0.836425	-0.019422
21	6	0	-3.456228	-0.477814	0.286722
22	6	0	-3.548015	0.508245	-0.723034
23	1	0	-4.405095	0.547671	-1.380598
24	1	0	-0.474302	0.413124	1.660482
25	1	0	-2.599610	2.171916	-1.665903
26	1	0	6.544170	-1.160553	0.014343
27	8	0	-4.390164	-1.414330	0.515203

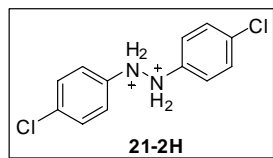
28	6	0	-5.580514	-1.451088	-0.290655
29	1	0	-5.331193	-1.630953	-1.338491
30	1	0	-6.164924	-2.281533	0.096616
31	1	0	-6.144635	-0.521758	-0.188405



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.716469	-1.498233	0.886151
2	6	0	4.069603	-0.872061	-0.311714
3	6	0	3.167959	-0.045206	-0.971787
4	6	0	1.885965	0.173780	-0.442495
5	6	0	1.531798	-0.453976	0.758348
6	6	0	2.445009	-1.282762	1.411823
7	1	0	5.053480	-1.030388	-0.738942
8	1	0	3.452288	0.436144	-1.901744
9	1	0	0.552856	-0.305461	1.197736
10	1	0	2.151494	-1.760400	2.339788
11	7	0	1.019048	1.060986	-1.112272
12	6	0	-0.414466	1.031593	-0.899740
13	6	0	-0.840689	1.843574	0.303229

14	6	0	-1.108578	-0.292240	-1.038431
15	6	0	-2.076145	1.535260	0.933584
16	6	0	-2.253222	-0.560865	-0.369022
17	1	0	-0.726689	-0.975636	-1.786433
18	6	0	-2.742187	0.391042	0.605893
19	1	0	-3.666209	0.180565	1.128696
20	7	0	-0.080723	2.840747	0.673118
21	1	0	1.281048	1.243889	-2.070322
22	1	0	-0.349220	3.476822	1.412940
23	1	0	0.814734	2.973141	0.212709
24	1	0	4.420790	-2.143305	1.397521
25	1	0	-0.849859	1.639256	-1.716161
26	1	0	-2.449814	2.181814	1.717350
27	8	0	-2.902851	-1.723265	-0.637518
28	6	0	-4.050197	-2.100642	0.138545
29	1	0	-4.339040	-3.079765	-0.236103
30	1	0	-3.803090	-2.177763	1.200223
31	1	0	-4.876140	-1.400517	-0.009334

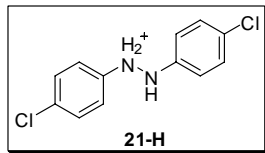


Standard orientation:

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

1	6	0	4.251065	1.185256	-0.046705
2	6	0	2.927694	1.351510	-0.366391
3	6	0	2.121570	0.213353	-0.665374
4	6	0	2.687527	-1.094730	-0.611370
5	6	0	4.012041	-1.252092	-0.291762
6	6	0	4.794476	-0.114460	-0.009563
7	1	0	4.877239	2.038576	0.174964
8	1	0	4.458231	-2.236491	-0.256487
9	7	0	0.820726	0.371338	-0.969580
10	1	0	0.463385	1.291487	-1.200804
11	7	0	-0.820680	0.369804	0.969877
12	1	0	-0.462974	1.289661	1.201597
13	6	0	-2.121516	0.212359	0.665472
14	6	0	-2.927333	1.350892	0.367040
15	6	0	-2.687804	-1.095561	0.610762
16	6	0	-4.250738	1.185144	0.047267
17	1	0	-2.490924	2.341291	0.400770
18	6	0	-4.012368	-1.252404	0.291107
19	1	0	-2.070645	-1.957822	0.830799
20	6	0	-4.794494	-0.114421	0.009471
21	1	0	-4.876698	2.038734	-0.173971
22	1	0	-4.458832	-2.236662	0.255361
23	1	0	0.294457	-0.405253	-1.353895
24	1	0	2.070147	-1.956722	-0.831827
25	1	0	2.491570	2.342049	-0.399663
26	17	0	-6.454442	-0.316673	-0.390025
27	17	0	6.454362	-0.317368	0.389893

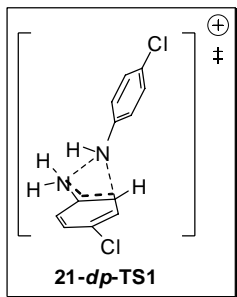
28 1 0 -0.294641 -0.407234 1.353603



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.947885	1.162310	0.415370
2	6	0	-2.574258	1.191152	0.641606
3	6	0	-1.838628	0.031398	0.443055
4	6	0	-2.421136	-1.155933	0.016018
5	6	0	-3.792171	-1.184202	-0.208821
6	6	0	-4.539407	-0.024560	-0.005973
7	1	0	-4.543679	2.051856	0.568254
8	1	0	-4.272097	-2.096872	-0.535092
9	7	0	-0.383056	0.065935	0.670083
10	1	0	-0.133886	0.883881	1.243466
11	7	0	0.379961	0.032960	-0.598766
12	1	0	0.077064	0.860948	-1.108324
13	6	0	1.801040	0.042883	-0.376885
14	6	0	2.555022	1.198390	-0.590161
15	6	0	2.428455	-1.147255	-0.000166
16	6	0	3.938513	1.165592	-0.437085
17	1	0	2.070628	2.123090	-0.882364
18	6	0	3.806127	-1.179109	0.184468

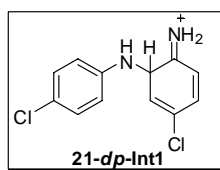
19	1	0	1.848241	-2.053396	0.131151
20	6	0	4.547153	-0.021483	-0.042349
21	1	0	4.529428	2.054660	-0.613412
22	1	0	4.298022	-2.096999	0.477838
23	1	0	-0.091838	-0.759580	1.202197
24	1	0	-1.824842	-2.045741	-0.142726
25	1	0	-2.100749	2.108271	0.970947
26	17	0	6.291879	-0.064704	0.167004
27	17	0	-6.269030	-0.064559	-0.287335



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.748742	2.787893	-0.020166
2	7	0	-0.476148	1.035356	0.001837
3	6	0	2.231676	0.662602	-1.046434
4	1	0	1.511856	0.865038	-1.826964
5	1	0	0.942624	2.892802	-0.618289
6	1	0	1.870168	3.461564	0.720752
7	6	0	2.459530	1.633708	-0.035786
8	6	0	-1.694973	0.557678	0.062877

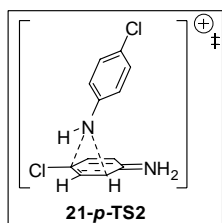
9	6	0	2.962982	-0.517797	-1.064147
10	1	0	2.792078	-1.249480	-1.842978
11	6	0	-2.534518	0.702503	-1.107008
12	1	0	-2.110711	1.188984	-1.976413
13	6	0	-2.253790	-0.095162	1.229259
14	1	0	-1.633042	-0.210710	2.110101
15	6	0	3.442529	1.373034	0.952376
16	1	0	3.625281	2.103008	1.732164
17	6	0	4.164369	0.198308	0.926507
18	1	0	4.914148	0.002474	1.682034
19	6	0	3.920035	-0.746587	-0.081870
20	6	0	-3.821241	0.240277	-1.108348
21	1	0	-4.457194	0.345220	-1.976818
22	6	0	-4.321074	-0.385831	0.053872
23	6	0	-3.540572	-0.554981	1.220610
24	1	0	-3.969402	-1.042896	2.085551
25	1	0	0.020861	0.880766	0.883583
26	17	0	4.847802	-2.233702	-0.101466
27	17	0	-5.936306	-0.966653	0.051121



Standard orientation:

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

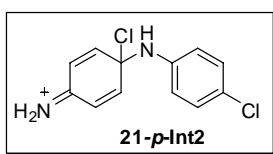
1	6	0	3.311265	0.372746	-0.169712
2	6	0	3.330606	-0.411043	0.981424
3	6	0	2.159022	-1.017624	1.414962
4	6	0	0.958711	-0.849714	0.707355
5	6	0	0.962297	-0.059716	-0.448022
6	6	0	2.136378	0.551862	-0.886310
7	1	0	4.248938	-0.546123	1.538367
8	1	0	2.124914	1.161263	-1.780703
9	7	0	-0.194227	-1.523229	1.156127
10	6	0	-1.522936	-1.106172	0.763874
11	6	0	-1.952339	-1.689436	-0.569183
12	6	0	-1.868638	0.350140	0.944320
13	6	0	-2.958827	-1.024046	-1.330046
14	6	0	-2.772903	0.934316	0.144752
15	1	0	-1.434173	0.854760	1.797243
16	6	0	-3.347687	0.230886	-0.979643
17	1	0	-3.359561	-1.497951	-2.217129
18	1	0	-4.091112	0.742864	-1.578396
19	7	0	-1.419852	-2.819927	-0.937056
20	1	0	-0.136574	-1.850042	2.110186
21	1	0	-1.713709	-3.307616	-1.774482
22	1	0	-2.218791	-1.616412	1.455393
23	1	0	-0.673298	-3.219963	-0.375269
24	1	0	2.176361	-1.628759	2.310547
25	1	0	0.062310	0.089825	-1.030966
26	17	0	4.798023	1.148110	-0.720966
27	17	0	-3.286049	2.588775	0.401500



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.990954	-0.034220	-0.024119
2	6	0	3.494555	0.044715	1.296823
3	6	0	2.144650	0.118388	1.487540
4	6	0	1.230888	0.114280	0.359134
5	6	0	1.794869	0.038164	-0.978736
6	6	0	3.144671	-0.036434	-1.160161
7	1	0	4.184676	0.044135	2.129342
8	1	0	1.716794	0.178147	2.480209
9	1	0	1.122276	0.040944	-1.828330
10	1	0	3.579402	-0.095451	-2.148650
11	7	0	-0.045558	0.173392	0.614132
12	6	0	-2.725626	1.059985	-1.296255
13	6	0	-2.986178	1.815108	-0.124411
14	6	0	-2.773654	-0.323978	-1.269647
15	6	0	-3.279304	1.119299	1.075101
16	6	0	-3.057993	-0.984722	-0.069759
17	1	0	-2.587022	-0.891172	-2.172615
18	6	0	-3.318247	-0.261515	1.099184
19	1	0	-3.480773	1.679415	1.980696

20	1	0	-3.544565	-0.782445	2.020562
21	7	0	-2.980616	3.171097	-0.157206
22	1	0	-3.128673	3.712814	0.679034
23	1	0	-2.504898	1.572791	-2.225178
24	1	0	-2.744409	3.671771	-0.998643
25	1	0	-0.599306	0.163176	-0.246778
26	17	0	-3.140819	-2.735909	-0.043786
27	17	0	5.682713	-0.129972	-0.264232



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.754065	-0.595824	-1.479359
2	6	0	1.556335	-0.331722	-0.921454
3	6	0	1.426838	-0.228711	0.527931
4	6	0	2.639542	-0.316558	1.337093
5	6	0	3.834535	-0.570982	0.772991
6	6	0	3.936222	-0.722042	-0.659046
7	1	0	0.672551	-0.282741	-1.539064
8	1	0	2.546994	-0.203422	2.410078
9	7	0	5.097794	-0.972567	-1.213048

10	1	0	5.940295	-1.069663	-0.658418
11	1	0	5.197420	-1.078854	-2.215577
12	7	0	0.271503	-0.405112	1.152843
13	6	0	-1.052918	-0.310613	0.659791
14	6	0	-2.019767	-1.142084	1.238674
15	6	0	-1.408506	0.622908	-0.320158
16	6	0	-3.336941	-1.068379	0.812226
17	1	0	-1.740203	-1.853269	2.006418
18	6	0	-2.729253	0.697993	-0.744042
19	1	0	-0.678506	1.321471	-0.705870
20	6	0	-3.678970	-0.152414	-0.182570
21	1	0	-4.088223	-1.715094	1.245071
22	1	0	-3.017680	1.424139	-1.492228
23	1	0	0.335608	-0.563625	2.154732
24	1	0	2.843121	-0.723052	-2.550750
25	1	0	4.728936	-0.652123	1.376903
26	17	0	-5.341371	-0.058262	-0.723789
27	17	0	1.702989	2.396529	0.378947

H₂O

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	8	0	0.000000	0.000000	0.117987

2	1	0	0.000000	0.762169	-0.471949
3	1	0	0.000000	-0.762169	-0.471949

H₃O⁺

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.082903	0.000000
2	1	0	-0.929873	-0.221339	0.000000
3	1	0	0.464936	-0.220943	0.805722
4	1	0	0.464936	-0.220943	-0.805722

7. Computed Energies

Table S3. Sum of electronic and zero-point energies (E , in Hartree), sum of electronic and thermal enthalpies (H , in Hartree), sum of electronic and thermal free energies (G , in Hartree) in solution. Relative energies (ΔE_{sol} , ΔH_{sol} and ΔG_{sol}) at 298 K are reported in kcal/mol.

Structure	E	H	G	ΔE_{sol}	ΔH_{sol}	ΔG_{sol}
Computed energies of diphenylene and <i>p</i> -semidine rearrangements						
7a-H	-857.490041	-857.471606	-857.537570	0.0	0.0	0.0
7a-H'	-857.483192	-857.465252	-857.529354	4.3	4.0	5.2
<i>dp</i>-TS1	-857.462077	-857.443360	-857.510420	17.5	17.7	17.0
<i>dp</i>-Int1	-857.517376	-857.499160	-857.562731	-17.2	-17.3	-15.8
<i>dp</i>-TS3	-857.453960	-857.435848	-857.499072	22.6	22.4	24.2
<i>dp</i>-Int3	-857.465790	-857.447534	-857.510915	15.2	15.1	16.7
<i>d</i>-TS2	-857.466188	-857.447690	-857.512506	15.0	15.0	15.7
<i>d</i>-TS4	-857.440761	-857.422793	-857.485175	30.9	30.6	32.9
<i>d</i>-int2	-857.484440	-857.465904	-857.531148	3.5	3.6	4.0
8a-H	-857.559057	-857.540212	-857.604940	-43.3	-43.1	-42.3
<i>p</i>-TS2	-857.456809	-857.437985	-857.504980	20.9	21.1	20.5
<i>p</i>-TS4	-857.458673	-857.440680	-857.503028	19.7	19.4	21.7
<i>p</i>-Int2	-857.525661	-857.507204	-857.572813	-22.4	-22.3	-22.1
9a-H	-857.548703	-857.530119	-857.595012	-36.8	-36.7	-36.0
Computed energies of <i>o</i> -semidine rearrangement						
14a-H	-784.497617	-784.478582	-784.544924	0.0	0.0	0.0
14 a-H'	-784.494988	-784.475825	-784.542405	1.6	1.7	1.6
<i>o</i>-TS1	-784.477228	-784.456976	-784.527316	12.8	13.6	11.0
<i>o</i>-Int1	-784.517021	-784.498044	-784.562382	-12.2	-12.2	-11.0
<i>o</i>-TS2	-784.466966	-784.447741	-784.512444	19.2	19.4	20.4
<i>o</i>-Int2	-784.476245	-784.457075	-784.521588	13.4	13.5	14.6

<i>o</i>-TS3	-784.470256	-784.449413	-784.522593	17.2	18.3	14.0
H₂O	-76.445088	-76.441308	-76.462738			
H₃O⁺	-76.816895	-76.813066	-76.836024			
15a	-784.128003	-784.108426	-784.175107	-1.4	-1.0	-2.2
15a-H	-784.544452	-784.524668	-784.591750	-29.4	-28.9	-29.4
Related energies of the formation of <i>p</i> -semidines 20 and 23 in the domino pathways C and E						
18H⁺	-688.856118	-688.841089	-688.899162	0.0	0.0	0.0
18-<i>dp</i>-TS1	-688.832497	-688.817077	-688.875539	14.8	15.1	14.8
18-<i>dp</i>-Int1	-688.854497	-688.839540	-688.896450	1.0	1.0	1.7
18-<i>p</i>-TS2	-688.828574	-688.812482	-688.872956	17.3	18.0	16.4
18-<i>p</i>-Int2	-688.875945	-688.860620	-688.918960	-12.4	-12.3	-12.4
18-<i>o</i>-TS1	-688.832791	-688.817160	-688.876581	14.6	15.0	14.2
18-<i>o</i>-Int1	-688.870789	-688.855396	-688.913388	-9.2	-9.0	-8.9
21H⁺	-1493.589061	-1493.574146	-1493.633402	0.0	0.0	0.0
21-<i>dp</i>-TS1	-1493.567802	-1493.552059	-1493.613015	13.3	13.9	12.8
21-<i>dp</i>-Int1	-1493.608075	-1493.593098	-1493.650546	-11.9	-11.9	-10.8
21-<i>p</i>-TS2	-1493.566474	-1493.550353	-1493.612269	14.2	14.9	13.3
21-<i>p</i>-Int2	-1493.620272	-1493.604606	-1493.663893	-19.6	-19.1	-19.1
21-<i>o</i>-TS1	-1493.567802	-1493.552059	-1493.613015	13.3	13.9	12.8
21-<i>o</i>-Int1	-1493.608075	-1493.593098	-1493.650546	-11.9	-11.9	-10.8

Fig. S1. Optimization process for the *exo*-H *o*-TS1 (A) to *endo*-H *o*-TS1 (B).

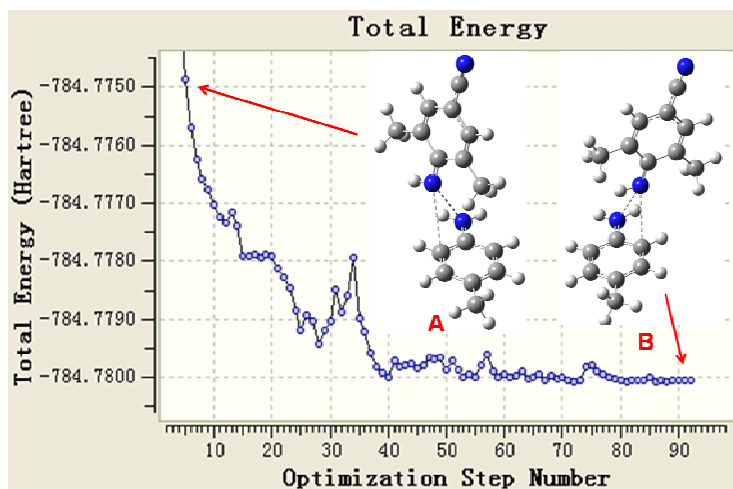
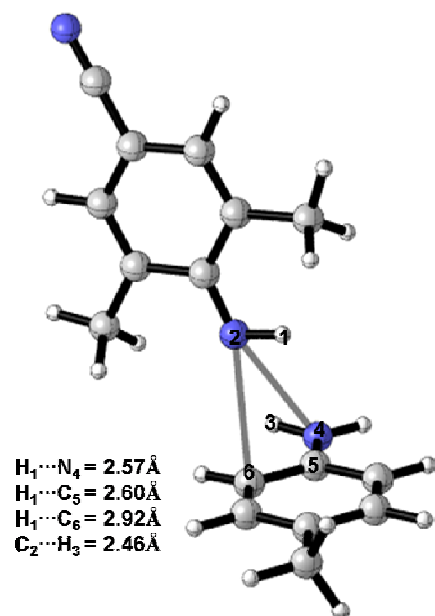


Fig. S2. Structure of the *endo*-H *o*-TS1.



8. References

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