Supporting Information

One-pot Total Synthesis of Streptindole, Arsindoline B and Their Congeners Through Tandem Decarboxylative Deaminative Dual-Coupling Reaction of Amino Acids with Indoles

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1. General

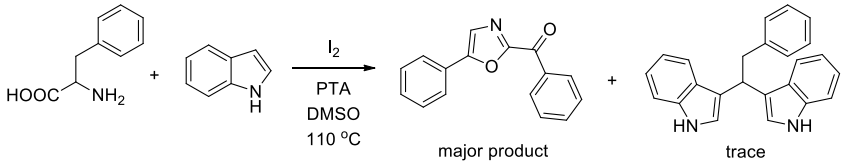
All substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). IR spectra were recorded on a Perkin-Elmer PE-983 infrared spectrometer as KBr pellets with absorption in cm^{-1}.^{1}H spectra were recorded in $CDCl_3$ or DMSO-d_6 or CD_3COCD_3 on 400/600 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet q = quadruple), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$ or DMSO-d_6 or CD_3COCD_3 on 100/150 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source. The X-ray crystal-structure determinations of **3b** and **3g** were obtained on a Bruker SMART APEX CCD system. Melting points were determined using XT-4 apparatus and not corrected. Optical rotation were measured with polarimeter: Atopol IV (an average value of 10 times parallel tests).

2. General procedure for the synthesis of 3 and 4 (3a and 4a as an example)

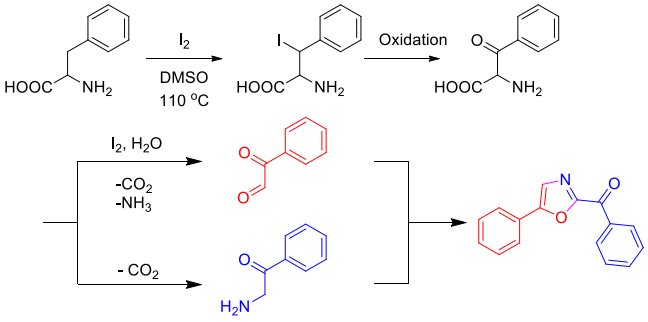
A mixture of 2-amino-2-phenylacetic acid **1a** (0.5 mmol), 1H-indole **2a** (1.0 mmol), alloxan monohydrate (1.0 mmol), phosphotungstic acid 44-hydrate (0.125 mmol) in DMF (1.0 mL) was stirred at 110 °C for 6 hours. Then added 50 mL water and 30 mL saturated brine solution to the mixture, extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $NaHCO_3$ solution, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc=5/1) to afford the product **3a** as yellow solid.

A mixture of 3-acetoxy-2-aminopropanoic acid hydrochloride **1'a** (0.5 mmol), 1H-indole **2a** (1.0 mmol), alloxan monohydrate (1.0 mmol), phosphotungstic acid 44-hydrate (0.125 mmol) in DMF (1.0 mL) was stirred at 110 °C for 6 hours. Then added 50 mL water and 30 mL saturated brine solution to the mixture, extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $NaHCO_3$ solution, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc=2/1) to afford the product **4a** as yellow oil.

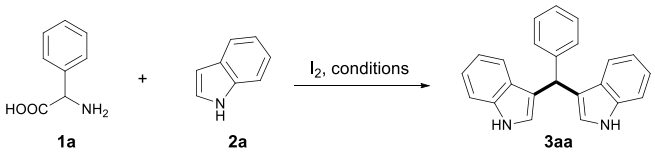
3. The side reaction of benzyl group amino acid in present of I_2 (phenylalanine as an example)



Probable Reaction Pathway:



4. Optimization details

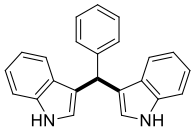


entry	solvent	Additive[a]	Acid	temp (℃)	Time	Yield[j] (%)
1	DMSO	AM	—	100	6h	22
2	DMA	AM	–	100	6h	15
3	DMF	AM	–	100	6h	40
4	CH_3CN	AM	–	reflux	6h	11
5	*t*-BuOH	AM	–	reflux	6h	trace
6	dioxane	AM	–	reflux	6h	trace
7	H_2O	AM	–	reflux	6h	0
8	DMF	AM	–	80	6h	trace
9	DMF	AM	–	90	6h	27
10	DMF	AM	–	110	6h	44
11	DMF	AM	–	120	6h	43
12	DMF	AM	–	110	4h	49
13	DMF	AM	TFA (0.25 eq.)	110	4h	75
14	DMF	AM	CF_3SO_3H (0.25 eq.)	110	4h	73
15	DMF	AM	$MeSO_3H$ (0.25 eq.)	110	4h	62
16	DMF	AM	HI (0.25 eq.)	110	4h	67
14	DMF	AM	$CuSO_4$ $5H_2O$ (0.25 eq.)	110	4h	52
17	DMF	AM	$Cu(OAc)_2$ $2H_2O$ (0.25 eq.)	110	4h	27
18	DMF	AM	$CuBr_2$ (0.25 eq.)	110	4h	15
19	DMF	AM	$CuCl_2$ (0.25 eq.)	110	4h	79
20	DMF	AM	$ZnCl_2$ (0.25 eq.)	110	4h	80
21	DMF	AM	$AlCl_3$ (0.25 eq.)	110	4h	78
22	DMF	AM	$FeCl_3$ (0.25 eq.)	110	4h	74
23	DMF	AM	Ti(*i*-PrO)$_4$ (0.25 eq.)	110	4h	0
24[b]	DMF	AM0.2	PTA (0.25 eq.)	110	4h	23
25[c]	DMF	AM0.4	PTA (0.25 eq.)	110	4h	37
27[d]	DMF	AM2.0	PTA (0.25 eq.)	110	6h	80
28	DMF	AM	PTA (0.25 eq.)	110	4h	86
29	DMF	AM	PTA (1.0 eq.)	110	4h	trace
30	DMF	AM	PTA (0.5 eq.)	110	4h	37

31[e]	DMF	I_2	PTA (1.0 eq.)	110	4h	84
32[f]	DMSO	I_2	PTA (1.0 eq.)	110	4h	87
33[g]	DMSO	I_2	PTA (1.0 eq.)	110	4h	37
34[h]	DMSO	I_2	PTA (1.0 eq.)	110	4h	0
35[i]	DMSO	I_2	PTA (1.0 eq.)	110	4h	trace
36	DMSO	NaClO	PTA (1.0 eq.)	110	4h	0
37	DMF	NaClO	PTA (1.0 eq.)	110	4h	0
38	DMF	IBX	PTA (1.0 eq.)	110	4h	0

AM = Alloxan Monohydrate; PTA = phosphotungstic acid 44-hydrate; [a]Reaction conditions: **1a** (0.5 mmol), **2a** (1.0 mmol), Addictive (1.0 mmol. If no otherwise specified), solvent (1.0 mL). [b]AM (0.2 eq.). [c]AM (0.4 eq.). [d]AM (2.0 eq.). [e]I_2 (1.0 eq.). [f] I_2 (0.2 eq.). [g]I_2 (0.2 eq.). for aliphatic amino acid. [h]I_2 (0.2 eq.). for amino acid hydrochloride. [i]I_2 (0.2 eq.). for aromatic amino acids. [j]isolated yields.

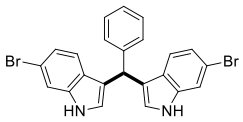
5. Characterization data for compound 3, 4 and 6



3a

3,3'-(phenylmethylene)bis(1H-indole) (**3a**)

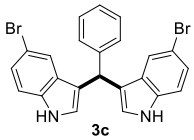
yellow solid; mp = 86-87 ℃ ^{1}H NMR (600 MHz, dmso-d_6) δ 10.84 (br, 2H), 7.37 (m, 4H), 7.31 – 7.24 (m, 4H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.04 (t, *J* = 7.2 Hz, 2H), 6.90 – 6.82 (m, 4H), 5.85 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) IR (KBr): 1620.79, 1490.42, 1454.28, 1416.13, 1337.45, 1216.99, 1091.94, 1009.68. HRMS (ESI): m/z [M+Na]+ calcd for C23H18N2Na : 345.1362； found: 345.1365.



3b

3,3'-(phenylmethylene)bis(6-bromo-1H-indole)

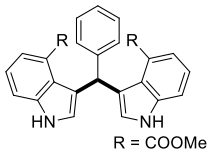
Red solid; mp = 140-142 ℃ ^{1}H NMR (600 MHz, dmso-d_6) δ 11.03 (br, 1H), 7.57 (s, 2H), 7.34 (m, 2H), 7.27 (m, 2H), 7.19 (m, , 3H), 7.01 (d, *J* = 7.8 Hz, 2H), 6.87 (s, 2H), 5.83 (s, 1H). ^{13}C NMR (100 MHz, dmso-d_6) δ 144.34, 137.50, 137.34, 128.25, 126.05, 125.60, 124.68, 124.52, 121.18, 120.84, 118.16, 114.10, 113.86. IR (KBr):1687.23, 1610.42, 1451.65, 1404.27, 1332.34, 1284.79, 1221.54, 1133.97, 1094.93, 1047.51. HRMS (ESI): m/z [M+Na]+ calcd for C23H16Br2N2Na :500.9572；found: 500.9573.



3c

3,3'-(phenylmethylene)bis(5-bromo-1H-indole)

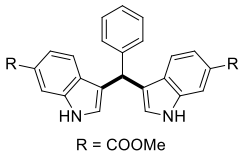
yellow solid; mp = 230-232 ℃；^{1}H NMR (600 MHz, dmso-d_6) δ 11.09 (br, 2H), 7.43 (s, 2H), 7.34 (d, *J* = 8.4 Hz, 4H), 7.29 (m, 2H), 7.24 – 7.11 (m, 3H), 6.89 (s, 2H), 5.86 (s, 1H). ^{13}C NMR (100 MHz, dmso-d_6) δ 144.32, 135.31, 128.42, 128.26, 126.11, 125.30, 123.53, 121.26, 117.70, 113.65, 111.00. IR (KBr):1598.14, 1558.08, 1455.91, 1416.74, 1333.07, 1216.33, 1098.23. HRMS (ESI): m/z [M+Na]+ calcd for C23H16Br2N2Na : 500.9572； found: 500.9581



3d

dimethyl 3,3'-(phenylmethylene)bis(1H-indole-4-carboxylate)

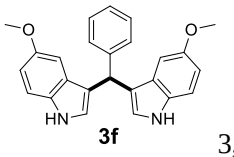
White solid; mp = 251-253 ℃；^{1}H NMR (600 MHz, dmso-d_6) δ 11.12 (br, 2H), 7.59 (d, *J* = 7.8Hz, 2H), 7.23 (m, 4H), 7.16 (m, 1H), 7.12 (m, 2H), 6.99 (d, *J* = 7.2 Hz, 2H), 6.39 (s, 1H), 6.32 (s, 2H), 3.38 (s, 6H). ^{13}C NMR (100 MHz, dmso-d_6) δ 168.56, 145.57, 137.90, 129.02, 127.62, 127.24, 125.53, 124.85, 122.84, 120.73, 119.88, 119.02, 115.33, 51.47, 40.98. IR (KBr): 2948.80, 1704.03, 1613.51, 1495.85, 1433.76, 1344.88, 1280.51, 1243.23, 1198.55, 1143.32, 1036.28. HRMS (ESI): m/z [M+Na]+ calcd for C27H22N2NaO4 : 461.1472； found: 461.1475.



3e

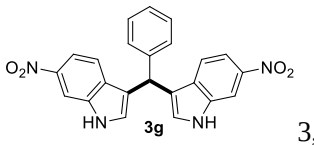
dimethyl 3,3'-(phenylmethylene)bis(1H-indole-6-carboxylate)

White solid; mp = 258-261 ℃；^{1}H NMR (600 MHz, dmso-d_6) δ 11.31 (br, 2H), 8.05 (s, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 4H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 2H), 5.93 (s, 1H), 3.83 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.28, 144.29, 135.87, 129.98, 128.80 – 128.39 (m), 127.67, 122.07, 119.03, 118.85, 118.46, 113.64, 51.7, IR (KBr): 1696.87, 1623.33, 1567.29, 1500.36, 1438.20, 1410.83, 1359.07, 1303.66, 1273.72, 1222.66, 1088.27. HRMS (ESI): m/z [M+Na]+ calcd for C27H22N2NaO4 : 461.1472；found: 461.1475.



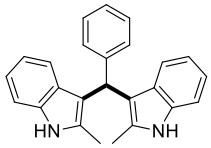
3f 3,3'-(phenylmethylene)bis(5-methoxy-1H-indole)

Pale red solid; mp = 215-216 ℃；^{1}H NMR (600 MHz, dmso-d_6) δ 10.74 (s, 2H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.36 – 7.26 (m, 4H), 7.19 (t, *J* = 7.2 Hz, 1H), 6.91 (s, 2H), 6.84 (s, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 5.84 (s, 1H), 3.62 (s, 6H). ^{13}C NMR (150 MHz, dmso-d_6) δ 152.81, 145.11, 131.95, 128.45, 128.11, 127.17, 125.84, 124.44, 117.85, 112.16, 110.70, 101.58, 55.30, 39.83. IR (KBr): 2937.48, 2829.91, 1622.11, 1584.33, 1485.20, 1450.00, 1331.96, 1291.41, 1258.69, 1208.51, 1171.40, 1127.40, 1095.04, 1024.07. HRMS (ESI): m/z [M+Na]+ calcd for C25H22N2NaO2 : 405.1573；found: 405.1578.



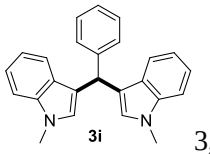
3g 3,3'-(phenylmethylene)bis(6-nitro-1H-indole)

Yellow solid; mp = 268-270 ℃；^{1}H NMR (400 MHz, dmso-d_6) δ 11.69 (br, 2H), 8.33 (s, 2H), 7.78 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.35 (s, 2H), 7.31 (s, 4H), 7.21 (s, 1H), 6.02 (s, 1H). ^{13}C NMR (100 MHz, dmso-d_6)) δ 141.93, 134.99, 131.04, 130.7, 128.48, 128.21, 119.17, 118.93, 113.67, 109.36, 108.51. IR (KBr): 1737.65, 1619.40, 1587.25, 1501.51, 1456.64, 1416.07, 1373.16, 1333.60, 1105.12, 1057.28. HRMS (ESI): m/z [M+Na]+ calcd for C23H16N4NaO4 : 435.1064；found: 435.1070.



3h 3,3'-(phenylmethylene)bis(2-methyl-1H-indole)

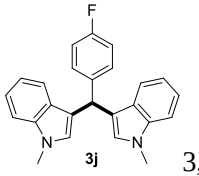
Yellow solid; mp = 257-258 ℃；^{1}H NMR (600 MHz, dmso-d_6) δ 10.75 (s, 2H), 7.27 – 7.22 (m, 2H), 7.22 (m, 1H), 7.20 (m, 4H), 6.88 (t, *J* = 7.8 Hz, 2H), 6.80 (d, *J* = 7.8 Hz, 2H), 6.67 (t, *J* = 7.2 Hz, 2H), 5.92 (s, 1H), 2.06 (s, 6H). ^{13}C NMR (100 MHz, dmso-d_6) δ 143.93, 134.79, 131.75, 128.40, 128.01, 127.56, 125.41, 119.25, 118.23, 117.65, 111.92, 110.00, 38.38, 11.63. IR (KBr): 2919.23, 1598.01, 1488.07, 1460.10, 1426.35, 1340.51, 1298.34, 1220.93, 1133.17, 1011.65. HRMS (ESI): m/z [M+Na]+ calcd for C25H22N2Na : 373.1675；found: 373.1676.



3i 3,3'-(phenylmethylene)bis(1-methyl-1H-indole)

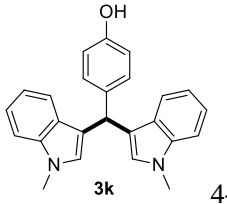
Pale yellow solid; mp = 200-201 ℃；^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.8 Hz, 2H), 7.36 (m, 2H), 7.33 – 7.27 (m, 4H), 7.22 (m, 3H), 7.01 (t, *J* = 7.2 Hz, 2H), 6.54 (s, 2H), 5.90 (s, 1H), 3.69 (s, 6H). ^{13}C NMR (100 MHz, dmso-d_6) δ 144.38, 137.32, 128.64, 128.23, 128.16, 127.37, 125.97, 121.35,

119.98, 118.57, 118.16, 109.02, 40.01, 32.66. IR (KBr): 2933.88, 1615.96, 1549.16, 1474.03, 1424.27, 1368.49, 1328.04, 1227.01, 1200.36, 1152.02, 1119.60, 1055.18, 1010.97. HRMS (ESI): m/z [M+Na]+ calcd for C25H22N2Na : 373.1675；found: 373.1677.



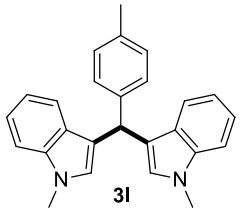
3,3'-((4-fluorophenyl)methylene)bis(1-methyl-1H-indole)

Pale yellow solid; mp = 202-204 ℃；^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.8 Hz, 2H), 7.28 (m, 4H), 7.20 (m, 3H), 6.97 (m, 4H), 6.50 (s, 2H), 5.86 (s, 1H), 3.66 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.27 (*d*, *J* = 242 Hz), 140.06, 137.34, 129.96 (*d*, *J* = 7.4 Hz), 128.17, 127.22, 121.47, 119.90, 118.66, 118.01, 114.88 (*d*, *J* = 21 Hz), 109.09, 39.28, 32.65. IR (KBr): 2935.40, 2845.35, 1894.64, 1599.08, 1550.48, 1501.82, 1472.47, 1424.37, 1368.57, 1328.47, 1218.25, 1153.02, 1119.65, 1091.86, 1056.89, 1010.97. HRMS (ESI): m/z [M+Na]+ calcd for C25H21FN2Na : 391.1581；found: 391.1581.



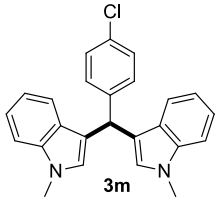
4-(bis(1-methyl-1H-indol-3-yl)methyl)phenol

Red solid; mp = 248-249 ℃；^{1}H NMR (400 MHz, dmso-d_6) δ 9.21 (s, 1H), 7.34 (m, 4H), 7.14 (m, 4H), 6.92 (m, 2H), 6.78 (s, 2H), 6.70 (m, 2H), 5.74 (s, 1H), 3.67 (s, 6H). ^{13}C NMR (100 MHz, dmso-d_6) δ 155.40, 136.98, 135.00, 129.13, 127.77, 126.95, 121.00, 119.35, 118.26, 117.99, 114.88, 109.54, 32.21. IR (KBr): 3457.56, 3107.37, 3050.25, 2933.36, 1669.94, 1604.61, 1545.20, 1508.17, 1474.58, 1370.26, 1330.18, 1289.21, 1254.72, 1231.94, 1196.96, 1159.19, 1129.67, 1053.64, 1011.37. HRMS (ESI): m/z [M+Na]+ calcd for C25H22N2NaO : 389.1624；found: 389.1623.



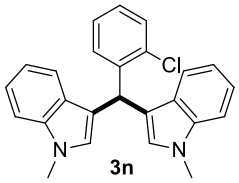
3,3'-(p-tolylmethylene)bis(1-methyl-1H-indole)

Red solid; mp = 202-203 ℃；^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.8 Hz, 2H), 7.26 (m, 2H), 7.22 (m, 2H), 7.19 – 7.15 (m, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 6.97 (t, *J* = 7.2 Hz, 2H), 6.51 (s, 2H), 5.84 (s, 1H), 3.62 (s, 6H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.35, 137.29, 135.29, 128.83, 128.45, 128.13, 127.38, 121.29, 119.99, 118.51, 118.34, 108.97, 39.58, 32.59, 21.08. IR (KBr): 2915.01, 2825.11, 1909.76, 1614.31, 1550.34, 1507.85, 1472.65, 1422.66, 1370.30, 1328.83, 1224.78, 1151.72, 1118.45, 1057.13, 1011.48. HRMS (ESI): m/z [M+Na]+ calcd for C26H24N2Na : 387.1832；found: 387.1831.



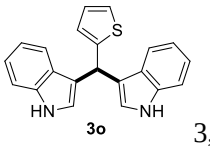
3,3'-((4-chlorophenyl)methylene)bis(1-methyl-1H-indole)

Red solid; mp = 209-212 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.8 Hz, 2H), 7.31 – 7.23 (m, 4H), 7.20 (m, 4H), 6.99 (m, 2H), 6.49 (s, 2H), 5.84 (s, 1H), 3.64 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.94 137.32, 131.57 129.98 (s), 128.27, 128.20, 127.17, 121.50, 119.85, 118.70, 117.62, 109.11, 39.43, 32.64. IR (KBr): 2930.46, 2862.45, 2818.70, 1902.16, 1614.17, 1586.11, 1547.31, 1480.63, 1329.67, 1253.08, 1224.12, 1200.90, 1152.55, 1127.68, 1085.48, 1058.98, 1011.98. HRMS (ESI): m/z [M+Na]+ calcd for C25H21ClN2Na : 407.1285; found: 407.1287.



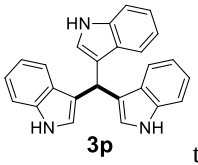
3,3'-((2-chlorophenyl)methylene)bis(1-methyl-1H-indole)

White solid; mp = 264-265 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (m, 3H), 7.28 (m, 2H), 7.228 (m, 4H), 7.138 (m, 2H) 6.50 (s, 2H), 6.34 (s, 1H), 3.66 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.69, 137.40, 133.83, 130.30, 129.43, 128.38, 127.35, 126.56, 121.47, 119.92, 118.68, 116.83, 109.06, 36.45, 32.68. IR (KBr): 2929.96, 2821.48, 1922.60, 1613.35, 1548.40, 1475.43, 1424.53, 1371.06, 1331.02, 1245.64, 1222.74, 1202.59, 1156.04, 1127.08, 1035.23, 1010.70. HRMS (ESI): m/z [M+Na]+ calcd for C25H21ClN2Na : 407.1285; found: 407.1287.



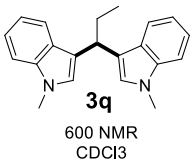
3,3'-(thiophen-2-ylmethylene)bis(1H-indole)

Pale red solid; mp = 171-174 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 2H), 7.47 (d, *J* = 7.8 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.21 – 7.14 (m, 3H), 7.04 (M, 2H), 6.92 (M, 2H), 6.83 (s, 2H), 6.17 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.60, 136.55, 126.73, 126.39, 125.11, 123.58, 123.14, 122.00, 119.74, 119.70, 119.35, 111.08, 77.32, 77.00, 76.68, 35.30. IR (KBr): 1619.36, 1456.24, 1418.50, 1336.37, 1217.33, 1091.23, 1009.90. HRMS (ESI): m/z [M+Na]+ calcd for C21H16N2S : 351.0926; found: 351.0929.



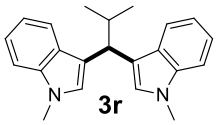
tri(1H-indol-3-yl)methane

Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.73 (br, 3H), 7.41 (d, *J* = 6.8 Hz, 3H), 7.35 (d, *J* = 6.8 Hz, 3H), 7.02 (m, 3H), 6.95 (s, 3H), 6.86 (m, 3H), 6.07 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.54, 126.73, 123.16, 120.57, 119.25, 118.24, 117.89, 111.33. IR (KBr): 3258.22, 3052.04, 2922.32, 2588.32, 1618.05, 1485.57, 1455.06, 1338.65, 1240.95, 1216.52, 1225.91, 1093.99, 1022.28, 1003.19. MS: m/z [M]+ calcd for C29H19N3 : 361.16; found: 361.36.



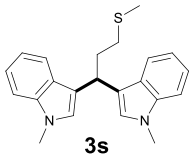
3,3'-(propane-1,1-diyl)bis(1-methyl-1H-indole)

White solid; mp = 88-90 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (m, 2H), 7.42 – 7.36 (m, 2H), 7.33 (s, 2H), 7.18 (m, 2H), 6.97 (s, 2H), 4.52 (m, 1H), 3.78 (s, 6H), 2.37 (m, 2H), 1.21 – 1.06 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.14, 127.52, 126.13, 121.14, 119.68, 118.88, 118.29, 109.01, 35.68, 32.48, 29.16, 13.17. IR (KBr): 2957.08, 2924.95, 2866.10, 1915.48, 1879.76, 1761.55, 1612.09, 1585.35, 1549.25, 1476.09, 1423.20, 1371.17, 1327.82, 1250.41, 1228.94, 1195.25, 1156.49, 1132.64, 1085.11, 1052.96, 1011.39. HRMS (ESI): m/z [M+Na]+ calcd for C21H22N2Na : 325.1675; found: 325.1672.



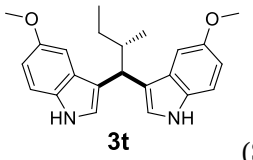
3r 3,3'-(2-methylpropane-1,1-diyl)bis(1-methyl-1H-indole)

White solid; mp = 102-103 ℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.8 Hz, 2H), 7.24 – 7.18 (m, 2H), 7.15 (t, *J* = 8.4 Hz, 2H), 7.03 (t, *J* = 6.6 Hz, 2H), 6.92 (s, 2H), 4.21 (d, *J* = 9.0 Hz, 1H), 3.67 (m, 6H), 2.69 – 2.51 (m, 1H), 0.97 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.83, 127.93, 128.07, 127.78, 126.37, 121.06, 119.96, 119.7, 118.30, 108.94, 40.94, 33.24, 32.62, 21.90. IR (KBr): 2956.41, 2867.47, 1612.97, 1541.31, 1472.37, 1423.39, 1371.34, 1327.24, 1228.66, 1157.33, 1127.79, 1055.32, 1011.63. HRMS (ESI): m/z [M+Na]+ calcd for C22H24N2Na : 339.1832; found: 339.1832.



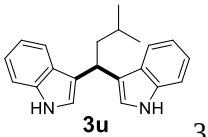
3s 3,3'-(3-(methylthio)propane-1,1-diyl)bis(1-methyl-1H-indole)

Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.8 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.03 (t, *J* = 7.2 Hz, 2H), 6.85 (s, 2H), 4.65 (s, 1H), 3.66 (s, 6H), 2.55 (t, *J* = 7.2 Hz, 2H), 2.47 (t, *J* = 7.2 Hz, 2H), 2.07 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.13, 127.25, 126.20, 121.28, 119.56, 118.46, 118.02, 109.06, 35.30, 32.81, 32.75, 32.52, 15.46. IR (KBr): 2921.08, 1613.80, 1546.10, 1471.08, 1423.00, 1371.83, 1326.62, 1237.90, 1153.88, 1125.06, 1064.22, 1012.40. HRMS (ESI): m/z [M+Na]+ calcd for C22H24N2NaS : 371.1552; found: 371.1553.



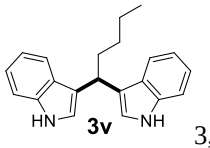
3t (S)-3,3'-(2-methylbutane-1,1-diyl)bis(5-methoxy-1H-indole)

Red oil; $[a]_D$ +1.83 (c 10mg/ml, MeOH). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.06 (m, 4H), 6.89 (s, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 4.23 (d, *J* = 7.8 Hz, 1H), 3.77 (m, 6H), 2.31 (m, 1H), 1.64 – 1.55 (m, 1H), 1.17 – 1.08 (m, 1H), 0.95 (d, *J* = 6.6 Hz, 3H), 0.90 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.41, 131.53, 131.40, 128.18, 127.98, 122.78, 122.56, 119.19, 118.64, 111.60, 111.16, 102.02, 55.90, 39.35, 39.14, 27.89, 17.68, 11.97. IR (KBr): 2958.22, 2872.27, 2830.29, 1623.79, 1580.76, 1482.81, 1454.38, 1376.77, 1347.05, 1291.58, 1248.39, 1209.91, 1171.95, 1095.93, 1027.95. MS: m/z [M]+ calcd for C23H26N2O2 : 362.20; found: 362.37.



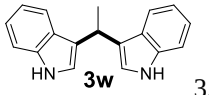
3u 3,3'-(3-methylbutane-1,1-diyl)bis(1H-indole)

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.43 (s, 2H), 7.09 (s, 1H), 7.08 (s, 1H), 7.02 (m, 2H), 6.65 (d, *J* = 2.0 Hz, 2H), 4.53 (t, *J* = 7.6 Hz, 1H), 2.02 (t, *J* = 7.2 Hz, 2H), 1.65 – 1.49 (m, 1H), 0.93 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.34, 126.88, 121.50, 121.46, 120.09, 119.40, 118.82, 111.14, 77.32, 77.00, 76.68, 45.11, 31.46, 25.80, 22.77. IR (KBr): 2953.91, 2865.73, 1618.06, 1456.93, 1419.00, 1338.93, 1220.38, 1094.36, 1010.92. HRMS (ESI): m/z [M+Na]+ calcd for C21H22N2Na : 325.1675；found: 325.1675.



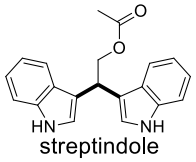
3v 3,3'-(pentane-1,1-diyl)bis(1H-indole)

Red oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.8 Hz, 2H), 7.50 (s, 2H), 7.15 (d, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 7.8 Hz, 2H), 7.01 (t, *J* = 7.2 Hz, 2H), 6.75 (s, 2H), 4.41 (t, *J* = 7.2 Hz, 1H), 2.16 (d, *J* = 6.6 Hz, 2H), 1.35 (s, 4H), 0.84 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.43, 127.05, 121.57, 121.42, 120.34, 119.55, 118.88, 111.08, 35.57, 33.86, 30.47, 22.77, 14.08. IR (KBr): 2954.67, 2926.62, 2857.79, 1617.55, 1521.63, 1486.14, 1455.68, 1418.68, 1337.90, 1219.63, 1151.37, 1093.40, 1010.27. MS: m/z [M]+ calcd for C21H22N2 : 302.18；found: 302.34.



3w 3,3'-(ethane-1,1-diyl)bis(1H-indole) (vibrindole A)

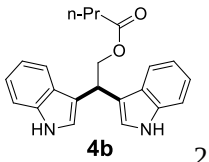
White solid; mp = 153-155℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (br, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.22 (t, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 7.2 Hz, 2H), 6.86 (s, 2H), 4.71 (d, *J* = 6.6 Hz, 1H), 1.84 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.56, 126.83, 121.69, 121.53, 121.19, 119.66, 118.94, 111.05, 28.11, 21.69. IR (KBr): 2958.13, 2866.18, 2836.91, 1624.23, 1548.86, 1484.13, 1454.83, 1421.09, 1337.75, 1291.37, 1220.61, 1124.66, 1095.80, 1013.70. HRMS (ESI): m/z [M+Na]+ calcd for C18H16N2Na : 283.1206；found: 283.1209.



streptindole

4a 2,2-di(1H-indol-3-yl)ethyl acetate

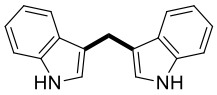
Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (br, 2H), 7.57 (d, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.11 (t, *J* = 7.8 Hz, 2H), 7.01 (t, *J* = 7.2 Hz, 2H), 6.70 (s, 2H), 4.88 (t, *J* = 7.2 Hz, 1H), 4.67 (d, *J* = 6.6 Hz, 2H), 1.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.41, 136.34, 126.90, 122.14, 121.93, 119.40, 116.07, 111.16, 67.42, 33.45, 21.03. IR (KBr): 2924.62, 2853.71, 1721.32, 1631.42, 1457.13, 1422.17, 1384.17, 1263.84, 1097.32, 1038.64. HRMS (ESI): m/z [M+Na]+ calcd for C20H18N2NaO : 341.1260；found: 341.1261.



4b 2,2-di(1H-indol-3-yl)ethyl butyrate

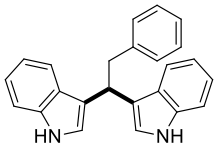
Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (br, 2H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.22 (m, 2H), 7.13 (m, 2H), 7.03 (m, 2H), 6.76 (s, 2H), 4.90 (t, *J* = 7.2 Hz, 1H), 4.70 (d, *J* = 7.2 Hz, 2H), 2.17 (t, *J* = 7.2 Hz, 2H), 1.51 (m, 2H), 0.79 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.00, 136.35, 126.93,

122.15, 121.89, 119.42, 119.22, 116.11, 111.12, 77.32, 77.00, 76.68, 67.12, 36.17, 33.50, 18.28, 13.50. IR (KBr): 2962.23, 2928.69, 2872.81, 1714.79, 1456.92, 1421.18, 1385.17, 1341.43, 1266.21, 1184.96, 1096.08, 1008.02. HRMS (ESI): m/z [M+Na]+ calcd for C22H22N2NaO2 : 369.1573；found: 369.1577.



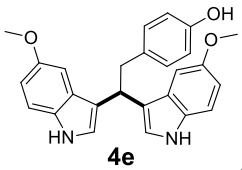
4c di(1H-indol-3-yl)methane

Yellow oil; ^{1}H NMR (600 MHz, dmso-d_6) δ 10.83 (br, 2H), 7.63 (d, J = 7.8 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 7.22 (s, 2H), 7.12 (m, 2H), 7.01 (m, 2H), 4.24 (s, 2H). ^{13}C NMR (150 MHz, dmso-d_6) δ 136.54, 136.38, 127.34, 122.87, 122.71, 120.91, 118.83, 118.20, 114.37, 114.33, 111.45, 21.10. IR (KBr): 2921.85, 1620.61, 1488.27, 1455.74, 1422.61, 1341.12, 1221.66, 1091.03, 1006.56. HRMS (ESI): m/z [M+Na]+ calcd for C17H14N2Na : 269.1049；found: 269.1047.



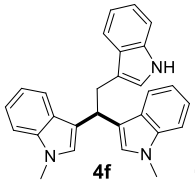
4d 3,3'-(2-phenylethane-1,1-diyl)bis(1H-indole)

White solid; mp = 76-78℃; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, J = 7.8 Hz, 2H), 7.15 – 7.08 (m, 10H), 7.05 (m, 3H), 6.61 (m, 2H), 4.76 (t, J = 7.8 Hz, 1H), 3.50 (d, J = 7.2 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.17, 136.26, 128.85, 127.89, 126.68, 125.63, 121.99, 121.54, 119.46, 118.91, 118.88, 111.11, 41.57, 36.02. IR (KBr):3416, 3054, 1631, 1492, 1455, 1417, 1340, 1244, 1094, 1011. MS: m/z [M]+ calcd for C24H20N2 :336.16；found: 336.22.



4e 4-(2,2-bis(5-methoxy-1H-indol-3-yl)ethyl)phenol

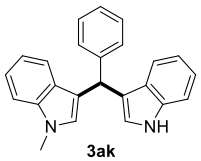
Yellow oil; ^{1}H NMR (600 MHz, dmso-d_6) δ 10.54 (br, 2H), 9.03 (s, 1H), 7.17 (m, 4H), 6.97 (m, 4H), 6.65 (m, 2H), 6.54 (d, J = 7.8 Hz, 2H), 4.56 (t, J = 7.8 Hz, 1H), 3.67 (s, 6H), 3.35 (d, J = 7.8 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.60, 153.46, 133.47, 131.78, 130.12, 127.43, 122.79, 119.15, 114.80, 111.64, 111.55, 101.99, 55.90, 40.71, 36.53. IR (KBr): 3413.36, 2933.77, 2831.05, 1619.97, 1582.11, 1513.25, 1482.86, 1446.52, 1350.50, 1290.68, 1211.98, 1170.18, 1097.02, 1058.26, 1025.49. HRMS (ESI): m/z [M+Na]+ calcd for C26H24N2O3Na: 435.1679；found: 435.1687.



4f 3,3'-(2-(1H-indol-3-yl)ethane-1,1-diyl)bis(1-methyl-1H-indole)

^{1}H NMR (600 MHz, acetone-d_6) δ 9.75 (br, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.63 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 7.8 Hz, 1H), 7.28 (d, J = 8.4 Hz, 2H), 7.10 (m, 3H), 7.09 – 7.04 (m, 2H), 7.01 (m, 1H), 6.94 (m, 2H), 6.90 (s, 1H), 5.00 (t, J = 7.2 Hz, 1H), 3.85 – 3.55 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.23, 135.88, 127.88, 127.50, 126.62, 122.14, 121.60, 121.22, 121.21, 119.76, 119.03, 118.88,

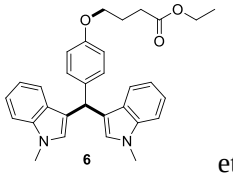
118.77, 118.45, 115.37, 110.91, 109.06, 34.27, 32.60, 31.92. IR (KBr):3050.19, 2927.13, 1616.00, 1547.46, 1475.55, 1421.04, 1372.09, 1328.48, 1244.95, 1154.10, 1125.57, 1012.44. HRMS (ESI): m/z [M+Na]+ calcd for C28H25N2Na: 426.1941；found: 426.1952.



3ak

3-((1H-indol-3-yl)(phenyl)methyl)-1-methyl-1H-indole

Red oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (br, 1H), 7.36 (m, 2H), 7.31 (m, 2H), 7.27 – 7.08 (m, 7H), 6.96 (m, 2H), 6.51 (s, 1H), 6.45 (s, 1H), 5.85 (s, 1H), 3.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.15, 137.24, 136.36, 128.55, 128.08, 127.31, 126.81, 125.96, 123.50, 121.64, 121.34, 119.89, 119.66, 119.25, 119.00, 118.57, 117.90, 110.99, 109.05, 40.00, 32.19 . IR (KBr): 2929.97, 1609.63, 1546.59, 1455.04, 1418.74, 1369.65, 1330.07, 1221.13, 1153.63, 1123.54, 1091.74, 1048.21, 1010.29. HRMS (ESI): m/z [M+Na]+ calcd for C24H20N2Na: 359.1519；found: 359.1518.



6

ethyl 4-(4-(bis(1-methyl-1H-indol-3-yl)methyl)phenoxy)butanoate

Red oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.8 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.22 (m, 2H), 7.19 (t, *J* = 7.2 Hz, 2H), 6.98 (t, *J* = 7.2 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 6.51 (s, 2H), 5.82 (s, 1H), 4.13 (m, 2H), 3.96 (t, *J* = 6.6 Hz, 2H), 3.66 (s, 6H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.083 (m, 2H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.16, 157.02, 137.32, 136.64, 129.44, 128.07, 127.35, 121.28, 119.96, 118.48, 114.00, 108.94, 100.76, 39.15, 32.50, 30.80, 24.67, 14.16. IR (KBr): 2933.26, 1731.78, 1609.57, 1507.87, 1470.47, 1422.45, 1371.27, 1327.34, 1244.44, 1175.10, 1121.39, 1046.63. HRMS (ESI): m/z [M+Na]+ calcd for C31H32N2NaO: 503.2305；found: 503.2308.

4. 3,3'-(phenylmethylene)bis(1-methyl-1H-indole)

X-ray structure determination was obtained via slow evaporation of compound 3i in $CHCl_3$/MeOH (10:1) at room temperature.

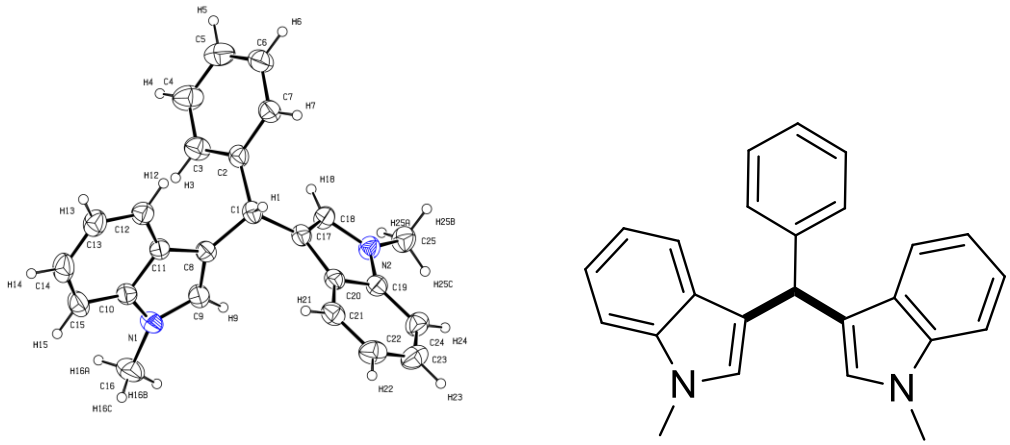
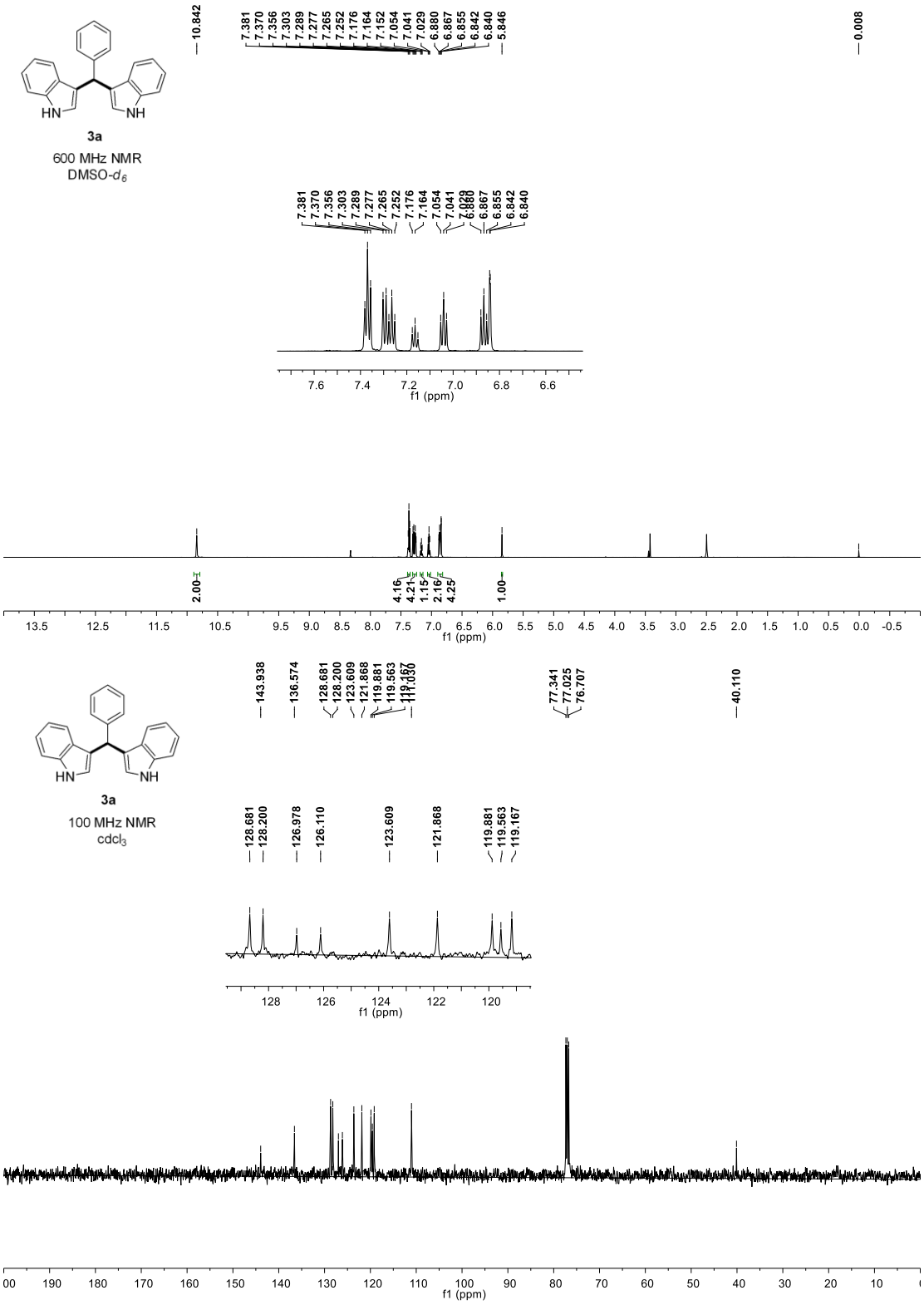


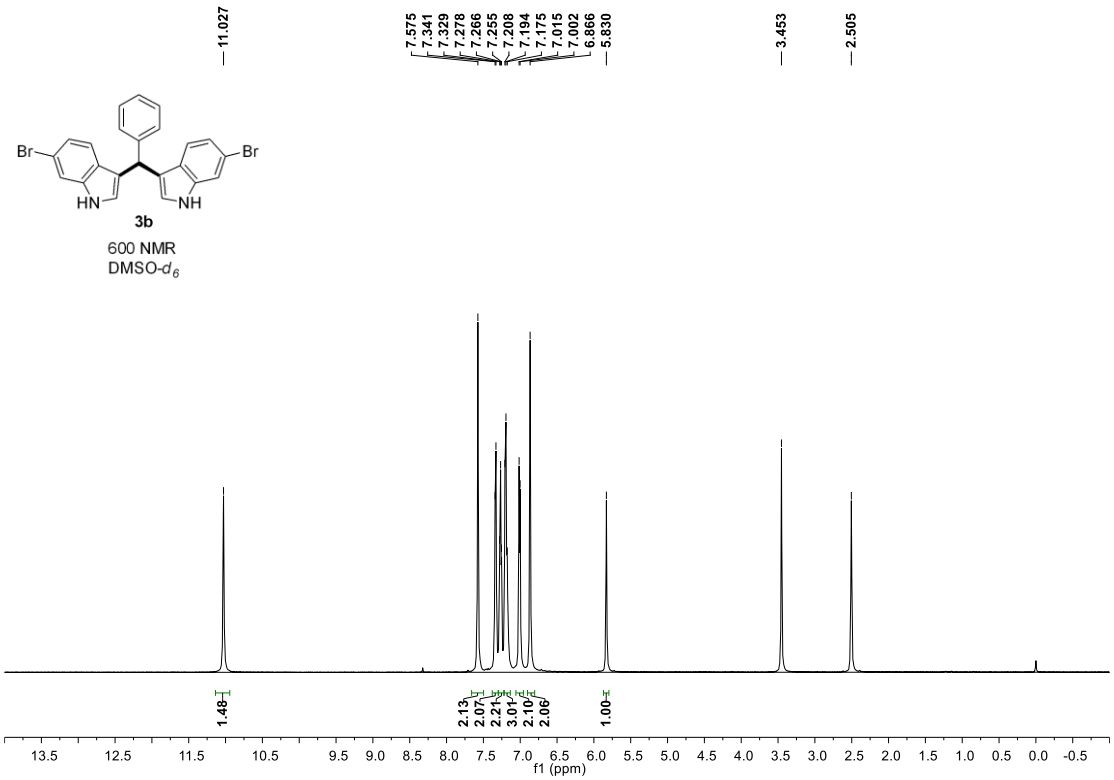
Figure S1 X-ray crystal structure of **3i**; ellipsoids depicted at the 30% probability level.

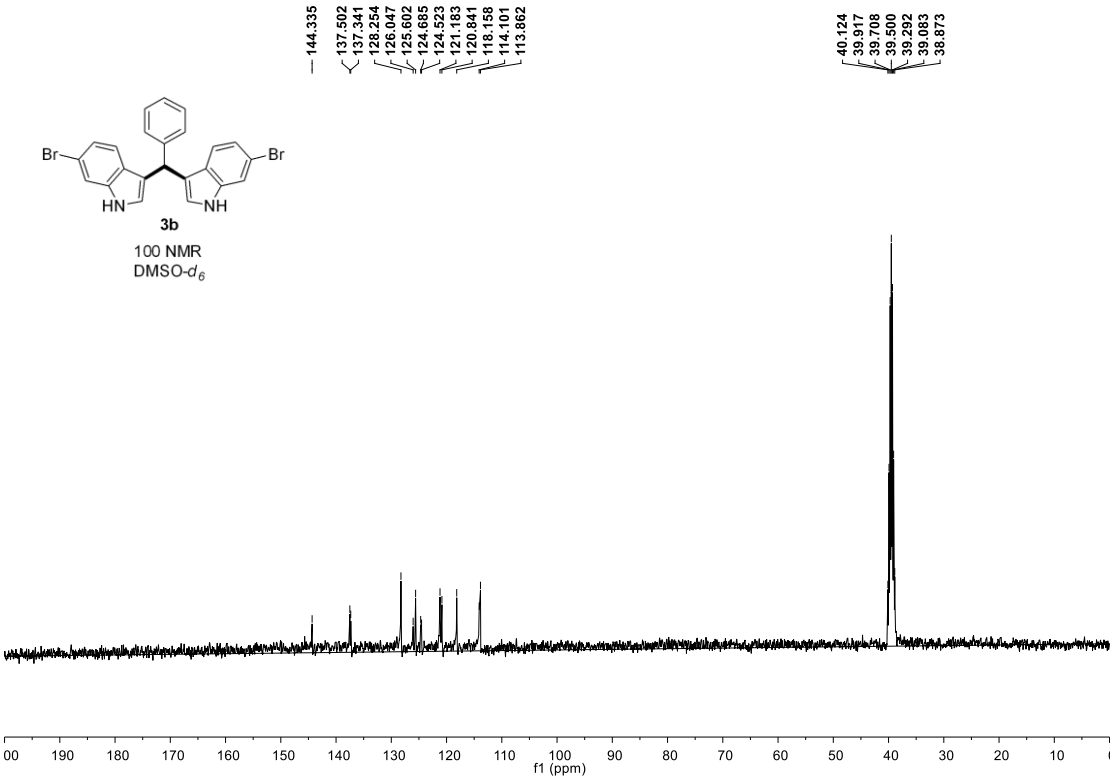
Table S1. Crystal data and structure refinement for compound **3i** (**CCDC: 1030461**)

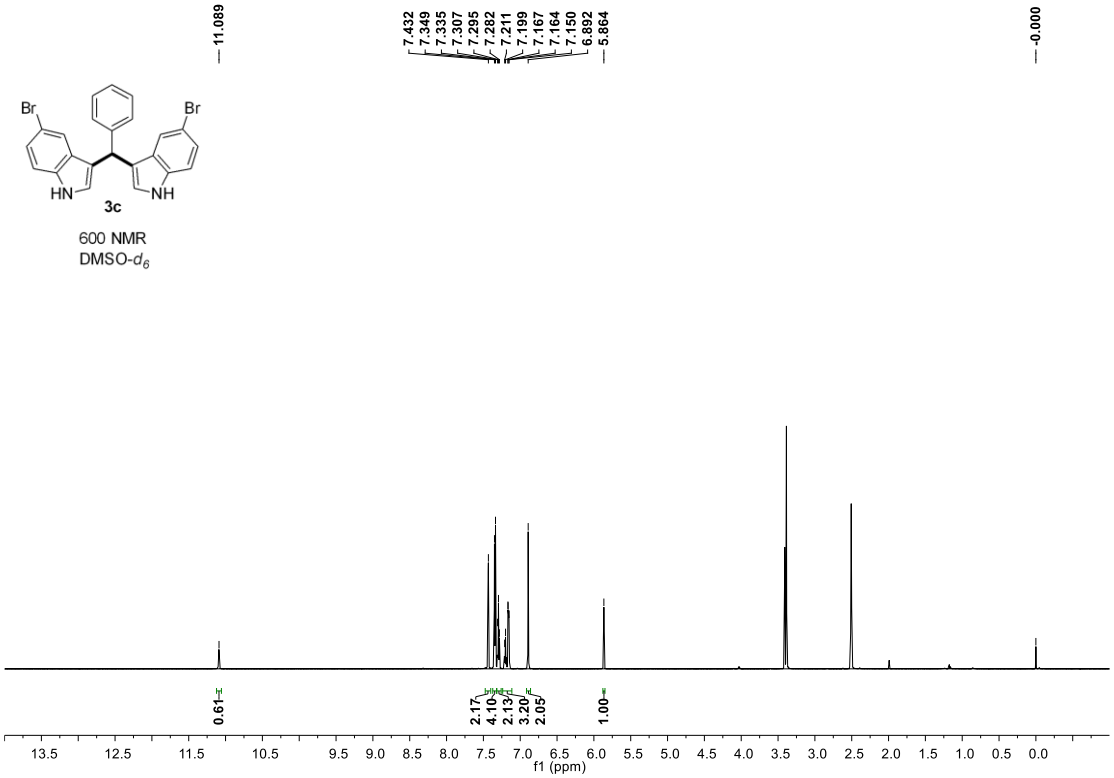
Empirical formula	$C_{25}H_{22}N_2$		Absorption coefficient	0.070 mm^{-1}
Formula weight	350.45		F(000)	744
Temperature	298(2)		Crystal size	0.15 x 0.12 x 0.10 mm^3
Wavelength	0.71073		Reflections collected	12169
Crystal system	Monoclinic		Independent reflections	3388 [R(int) = 0.0446]
Space group	P 21/c		Max. and min. transmission	0.992 and 0.993
Unit cell dimensions	a = 9.4408(17) Å	α= 90.00(4) °	Refinement method	Full-matrix least-squares on F^2
	b = 25.506(5) Å	β= 95.641(4) °	Goodness-of-fit on F^2	1.014
	c = 8.0660(15) Å	γ = 90.00(4) °	Final R indices [I>2sigma(I)]	R1 =0.0476, wR2 = 0.1148
Volume	558.7(2) $Å^3$		R indices (all data)	R1 = 0.0871, wR2 = 0.1367
Z	4		Largest diff. peak and hole	0.180 and -0.162e.$^{-3}$
Density (calculated)	1.204 Mg/m^3			

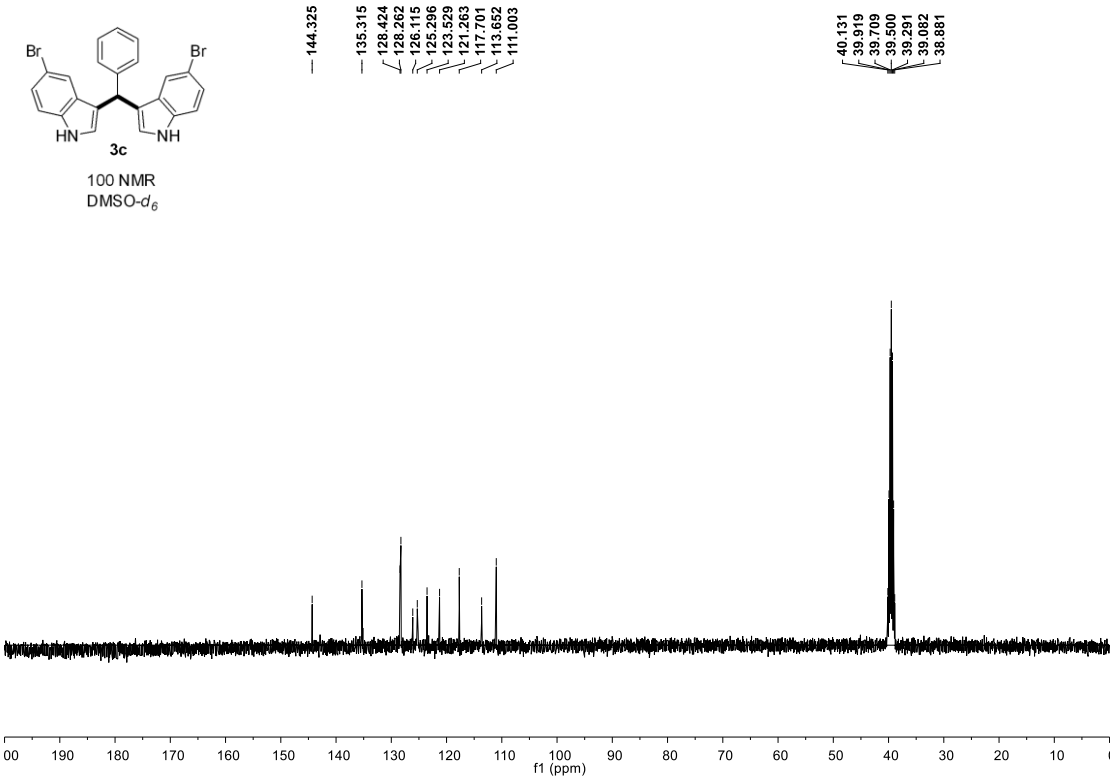
5. Copies of ^{1}H NMR , ^{13}C NMR and HRMS/MS Spectra

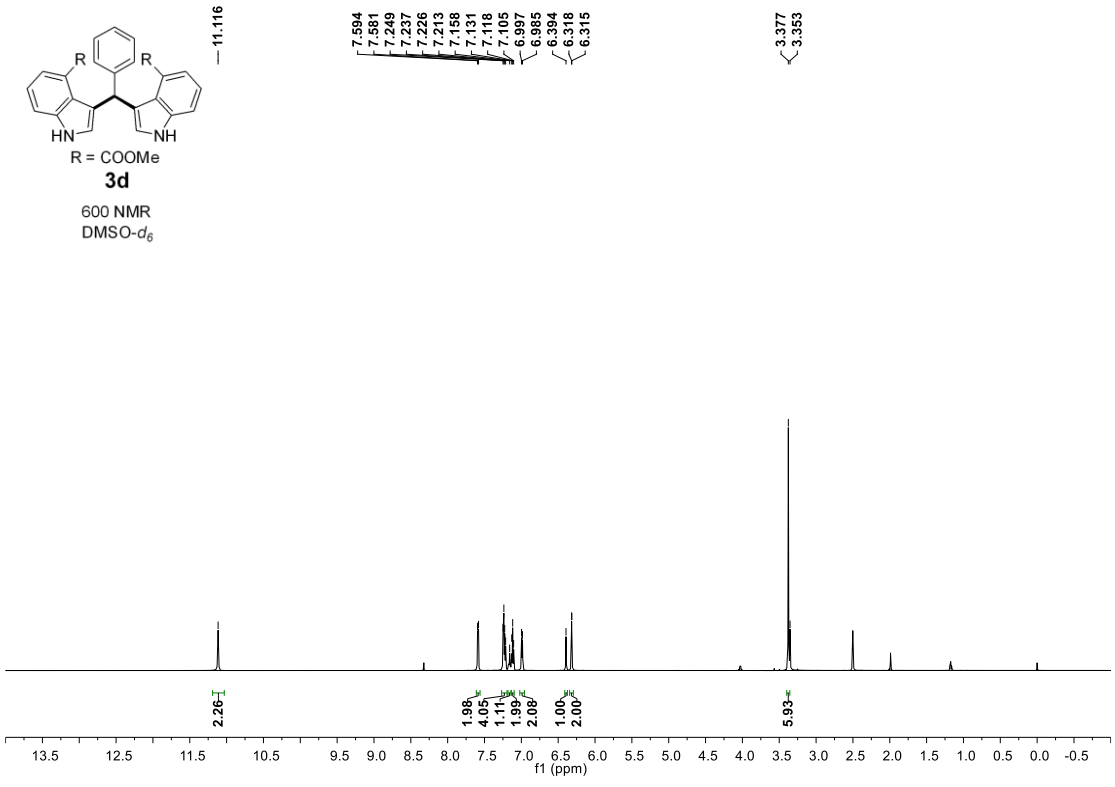


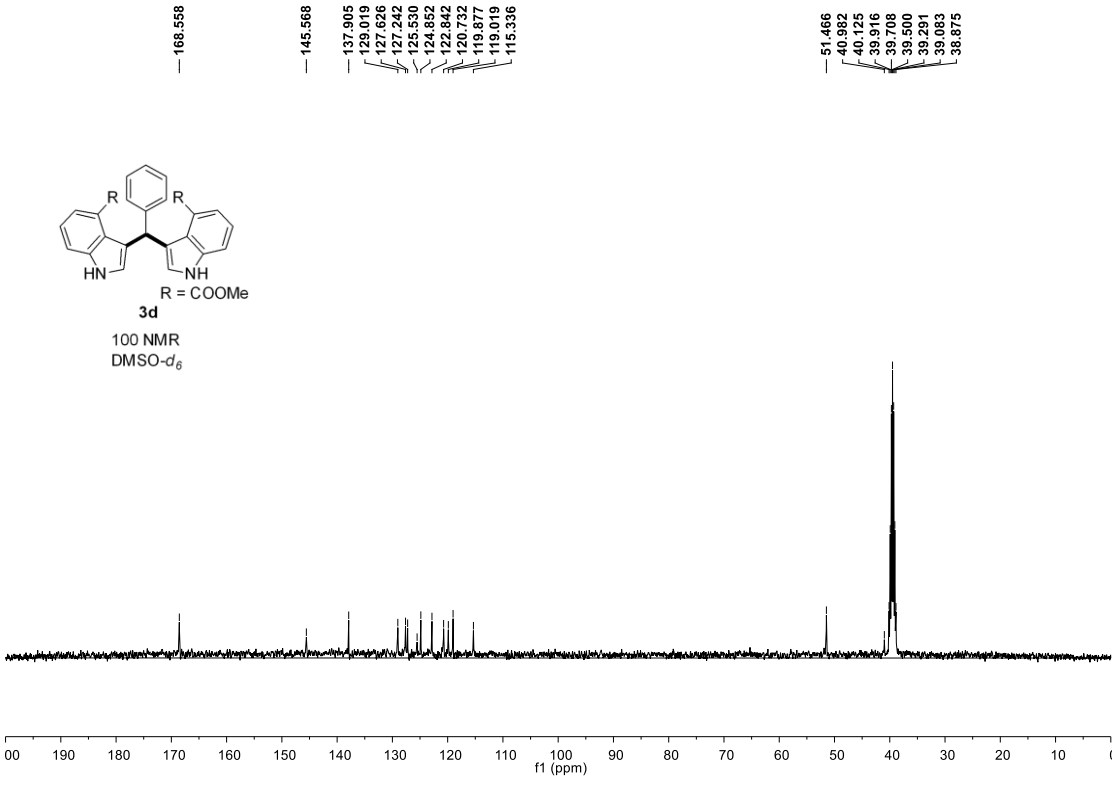

11.027
7.575
7.341
7.329
7.278
7.266
7.255
7.208
7.194
7.175
7.015
7.002
6.866
5.830
3.453
2.505
Br
Br
HN
NH
3b
600 NMR
DMSO-d6
1.48
2.13
2.07
2.21
3.01
2.10
2.06
1.00
f1 (ppm)

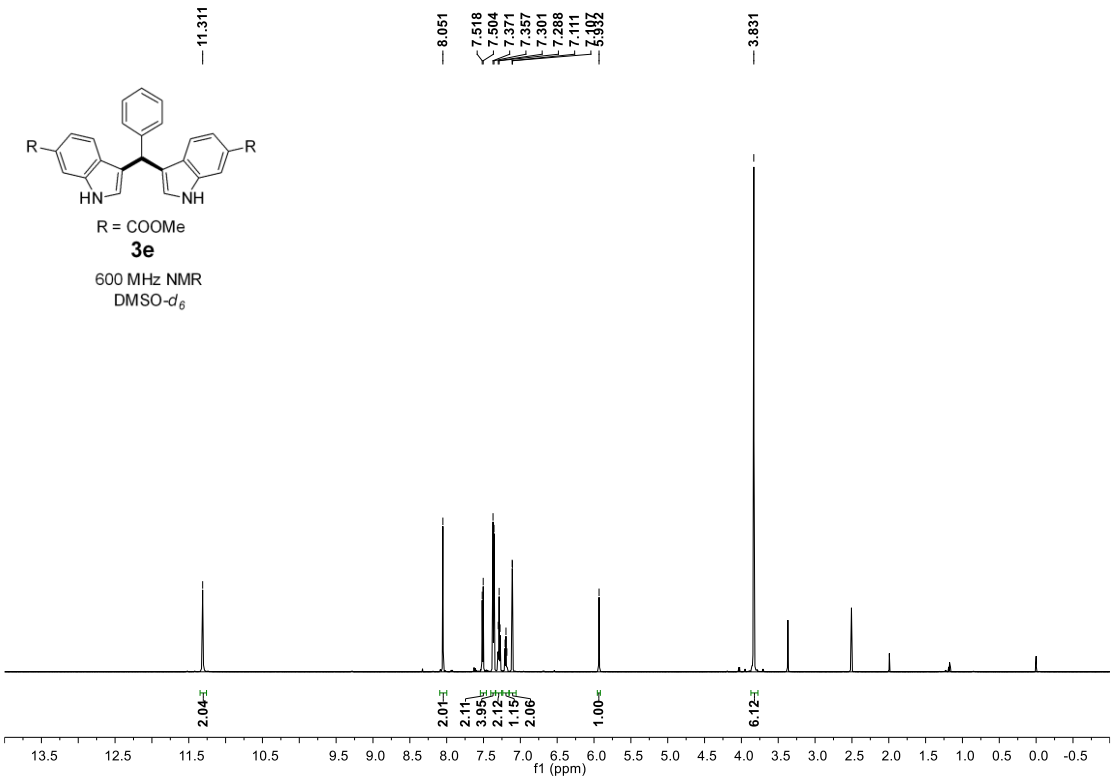

144.335
137.502
137.341
128.254
126.047
125.602
124.685
124.523
121.183
120.841
118.158
114.101
113.862
40.124
39.917
39.708
39.500
39.292
39.083
38.873
Br
Br
HN
NH
3b
100 NMR
DMSO-d6
f1 (ppm)

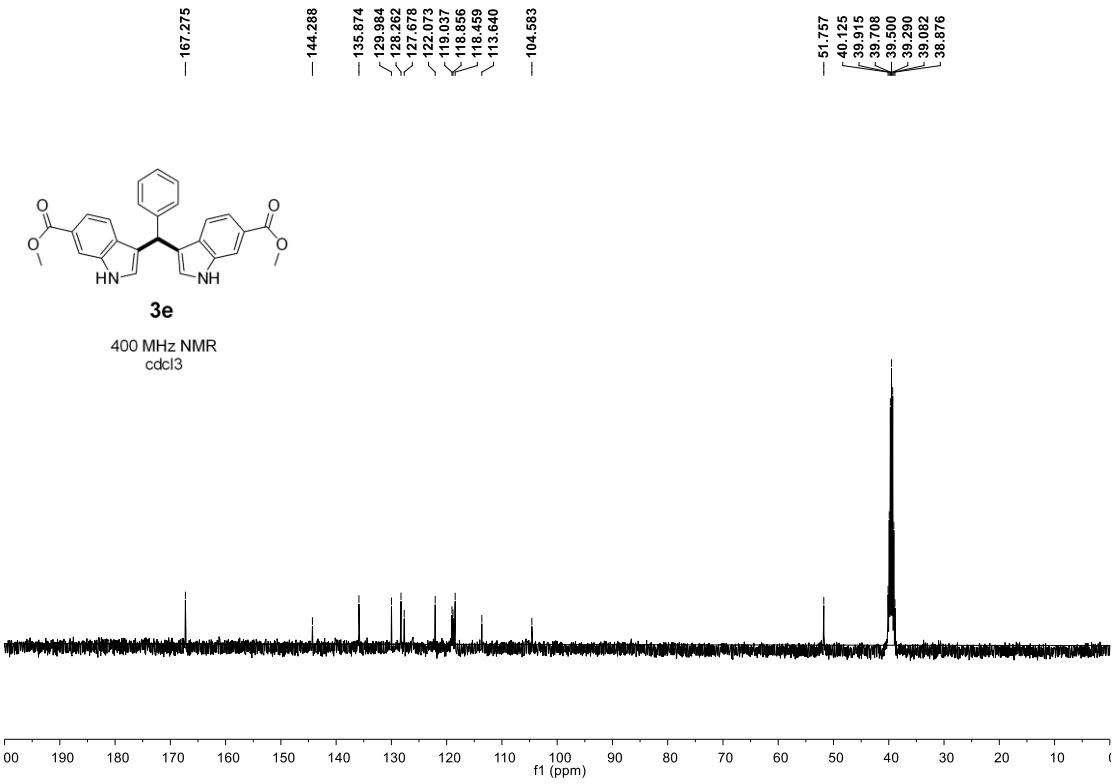

11.089
7.432
7.349
7.335
7.307
7.295
7.282
7.211
7.199
7.167
7.164
7.150
6.892
5.864
-0.000
Br
Br
HN
NH
3c
600 NMR
DMSO-d_6
0.61
2.17
4.10
2.13
3.20
2.05
1.00
f1 (ppm)

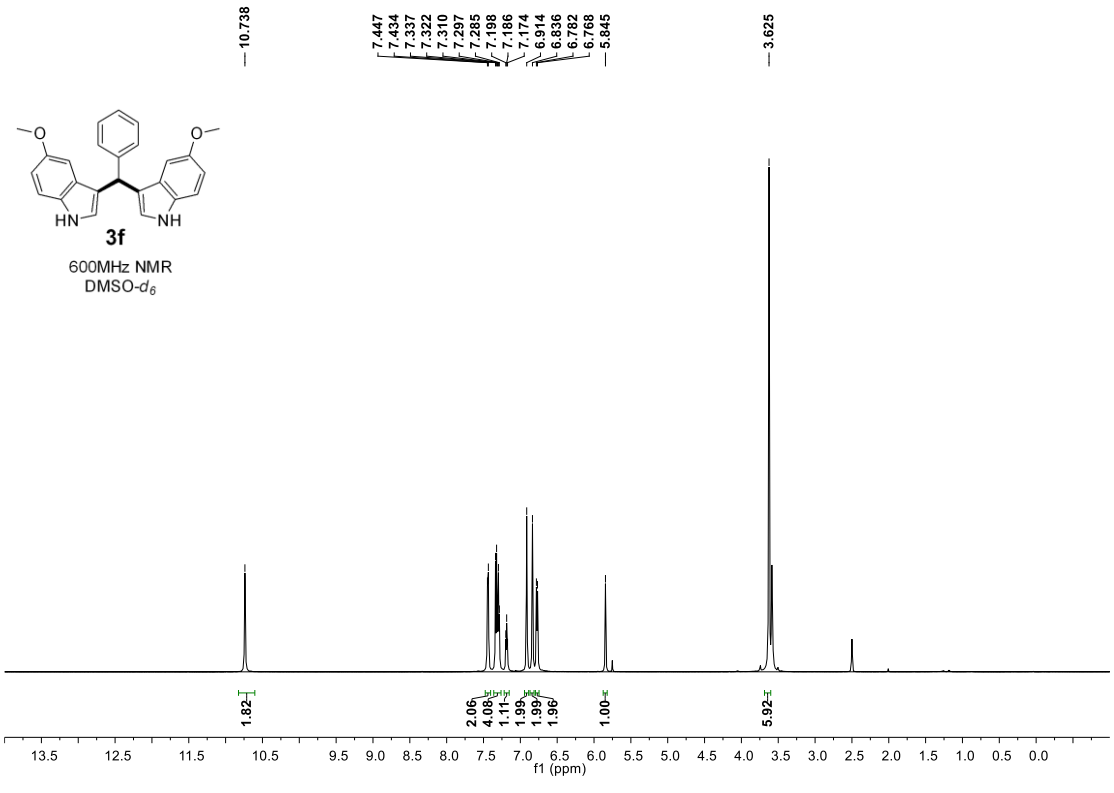

144.325
135.315
128.424
128.262
126.115
125.296
123.529
121.263
117.701
113.652
111.003
40.131
39.919
39.709
39.500
39.291
39.082
38.881
Br
Br
HN
NH
3c
100 NMR
DMSO-d_6
f1 (ppm)


11.116
7.594
7.581
7.249
7.237
7.226
7.213
7.158
7.131
7.118
7.105
6.997
6.985
6.394
6.318
6.315
3.377
3.353
R = COOMe
3d
600 NMR
DMSO-d_6
2.26
1.98
4.05
1.11
1.99
2.08
1.00
2.00
5.93
f1 (ppm)


168.558
145.568
137.905
129.019
127.626
127.242
125.530
124.852
122.842
120.732
119.877
119.019
115.336
51.466
40.982
40.125
39.916
39.708
39.500
39.291
39.083
38.875
R = COOMe
3d
100 NMR
DMSO-d_6
f1 (ppm)

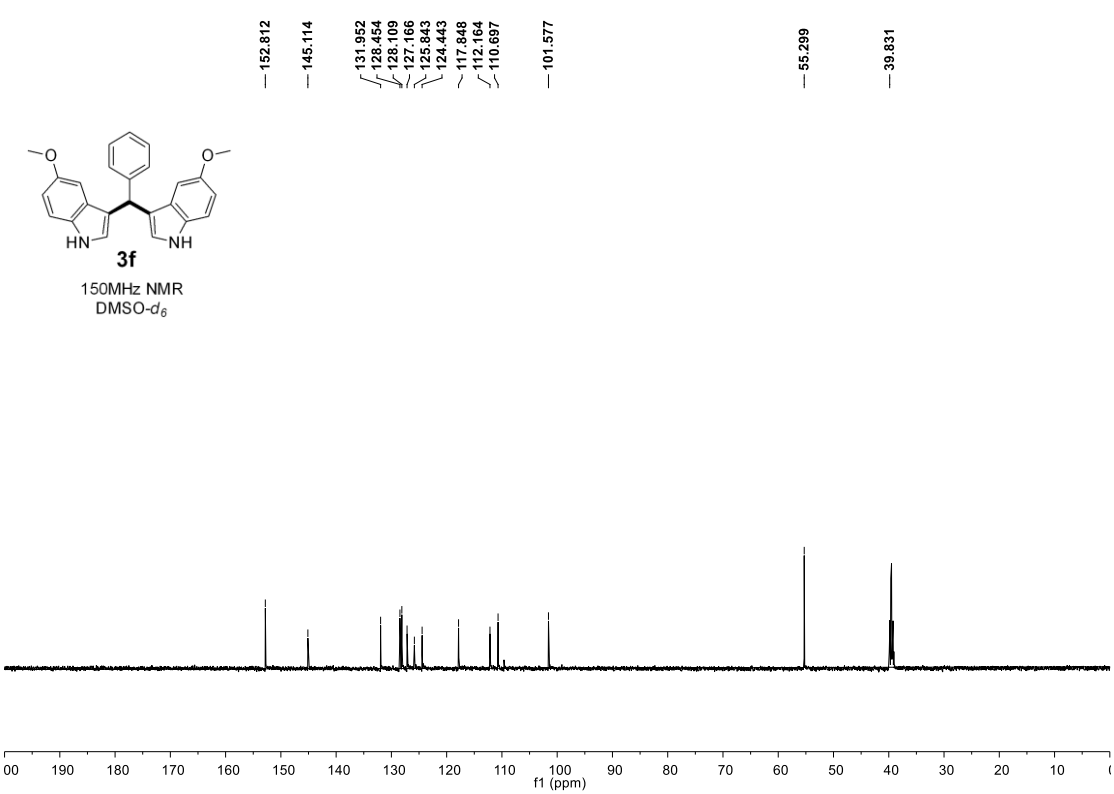

11.311
8.051
7.518
7.504
7.371
7.357
7.301
7.288
7.111
3.831
R
R
HN
NH
R = COOMe
3e
600 MHz NMR
DMSO-d6
2.04
2.01
2.11
3.95
2.12
1.15
2.06
1.00
6.12
f1 (ppm)


167.275
144.288
135.874
129.984
128.262
127.678
122.073
119.037
118.856
118.459
113.640
104.583
51.757
40.125
39.915
39.708
39.500
39.290
39.082
38.876
O
O
O
O
HN
NH
3e
400 MHz NMR
cdcl3
f1 (ppm)



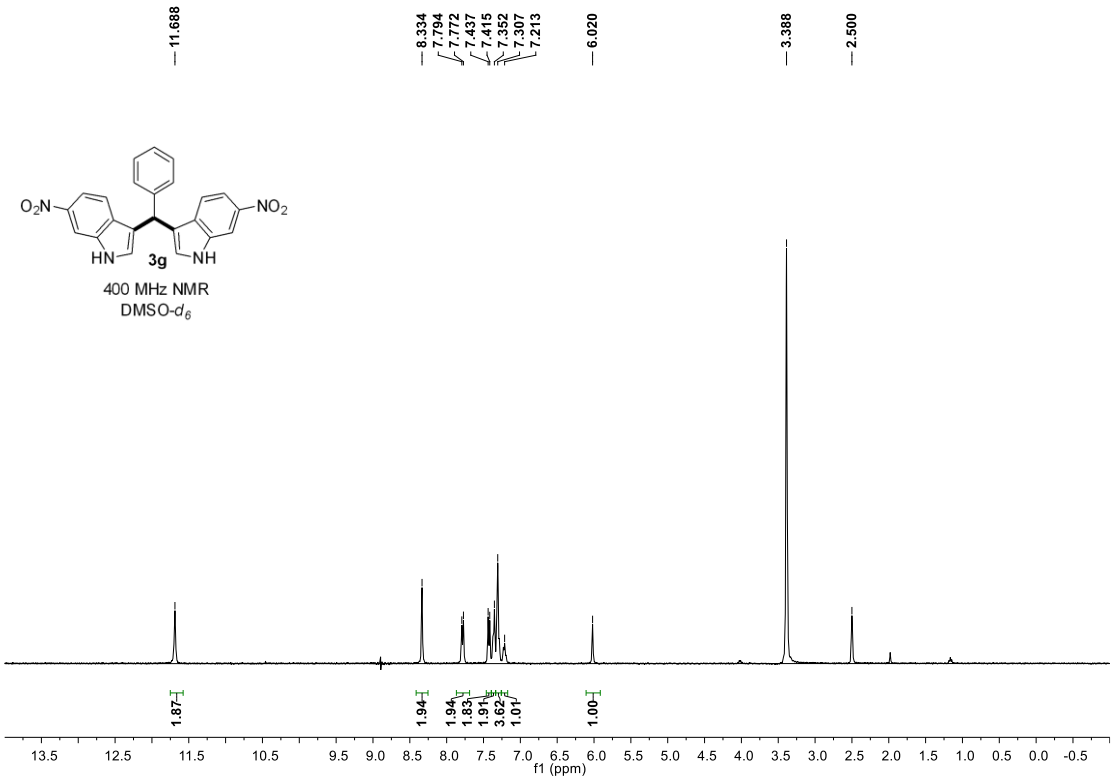
3f

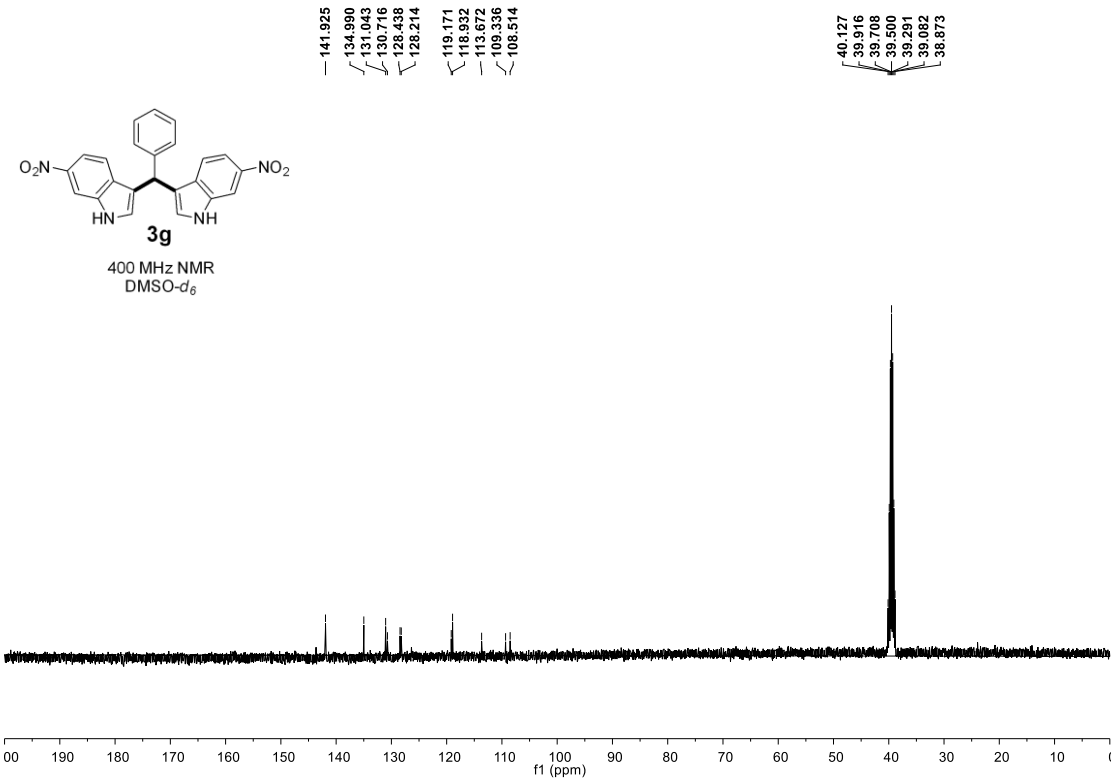
600MHz NMR
DMSO-d_6

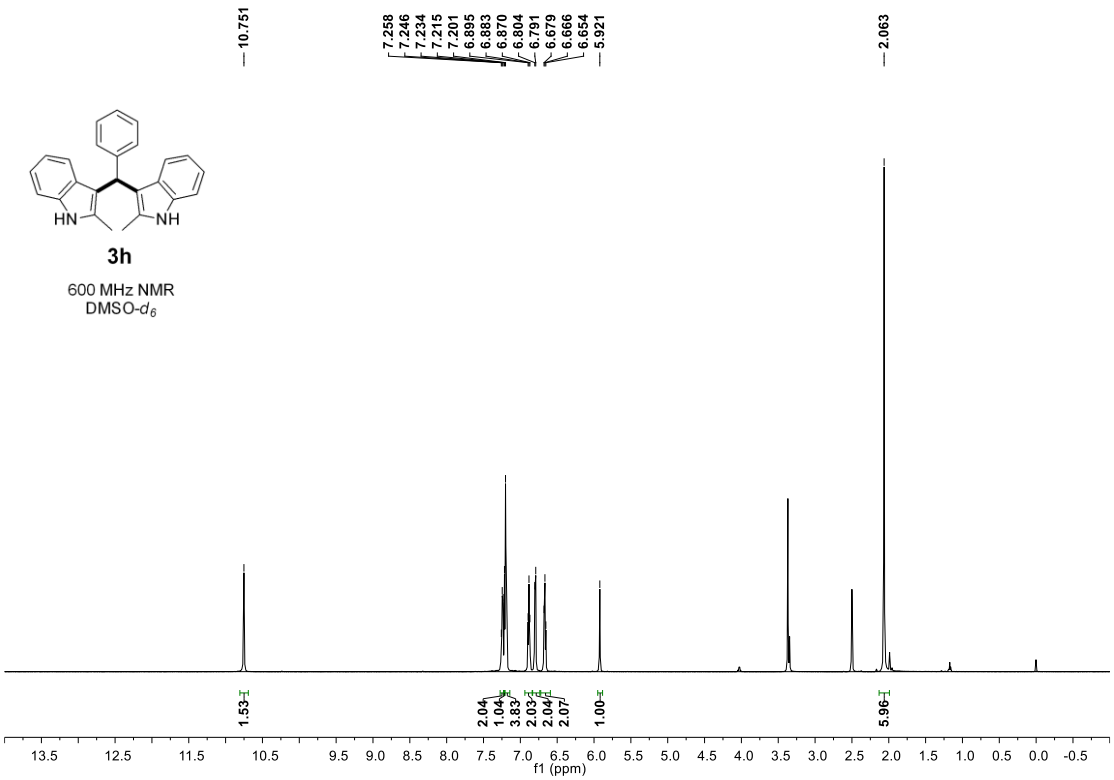


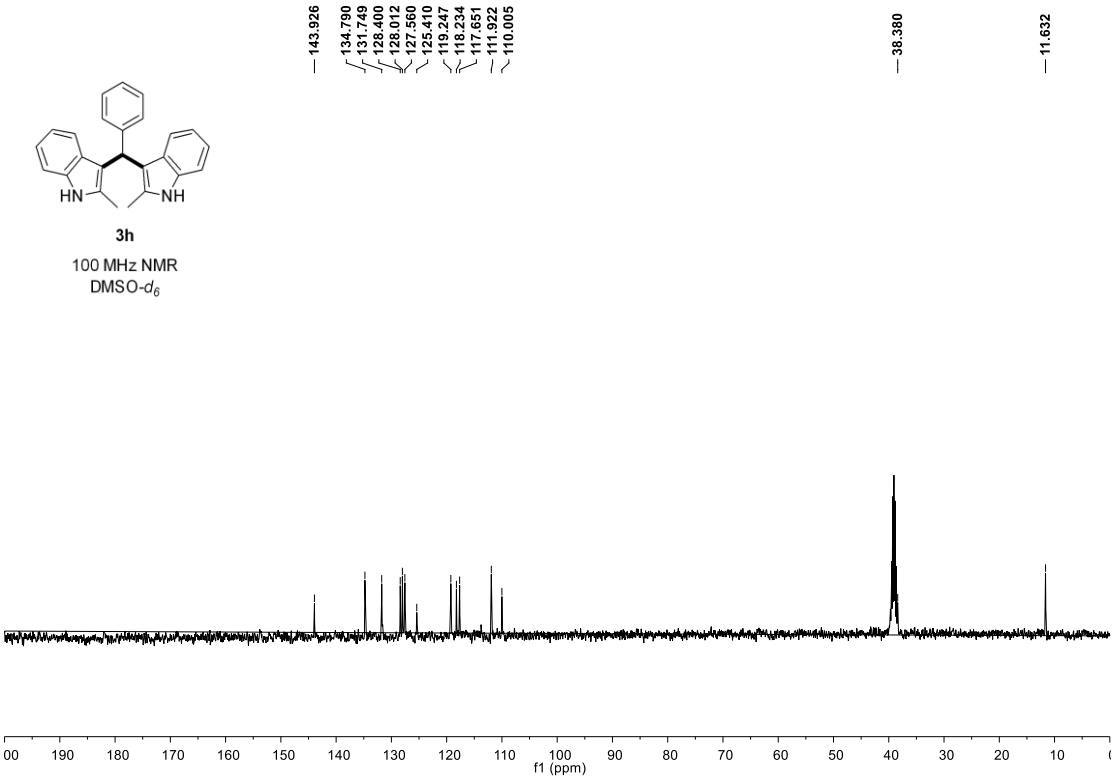
3f

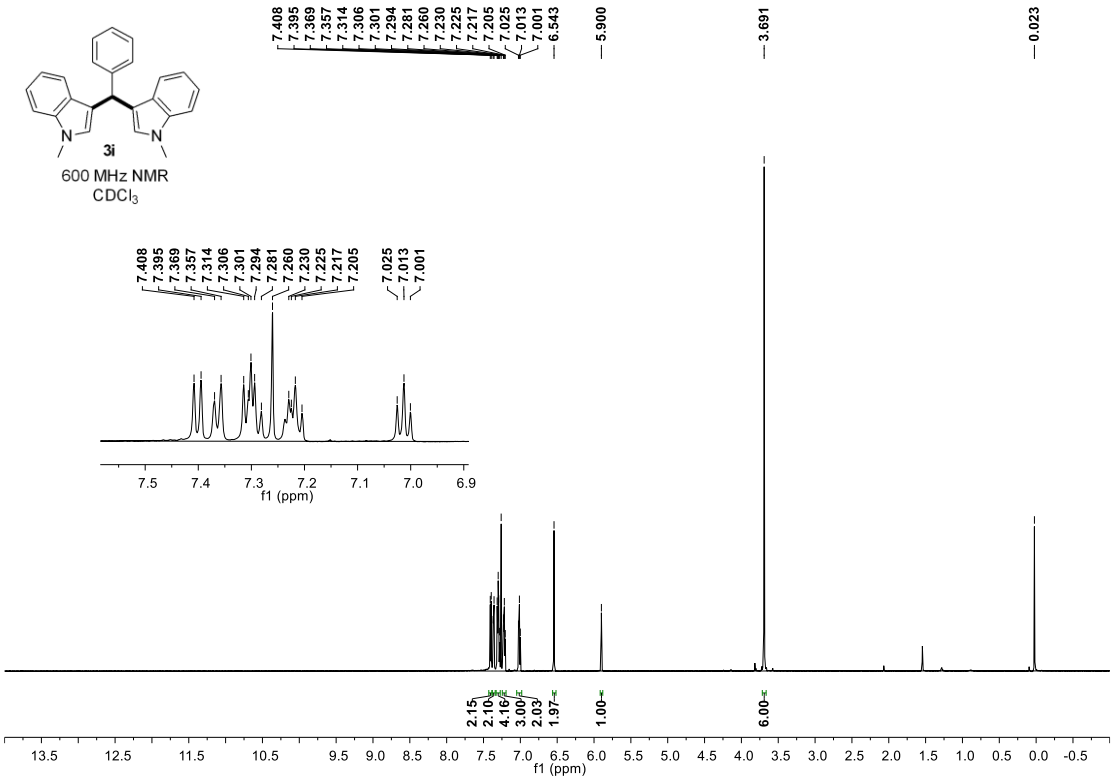
150MHz NMR
DMSO-d_6

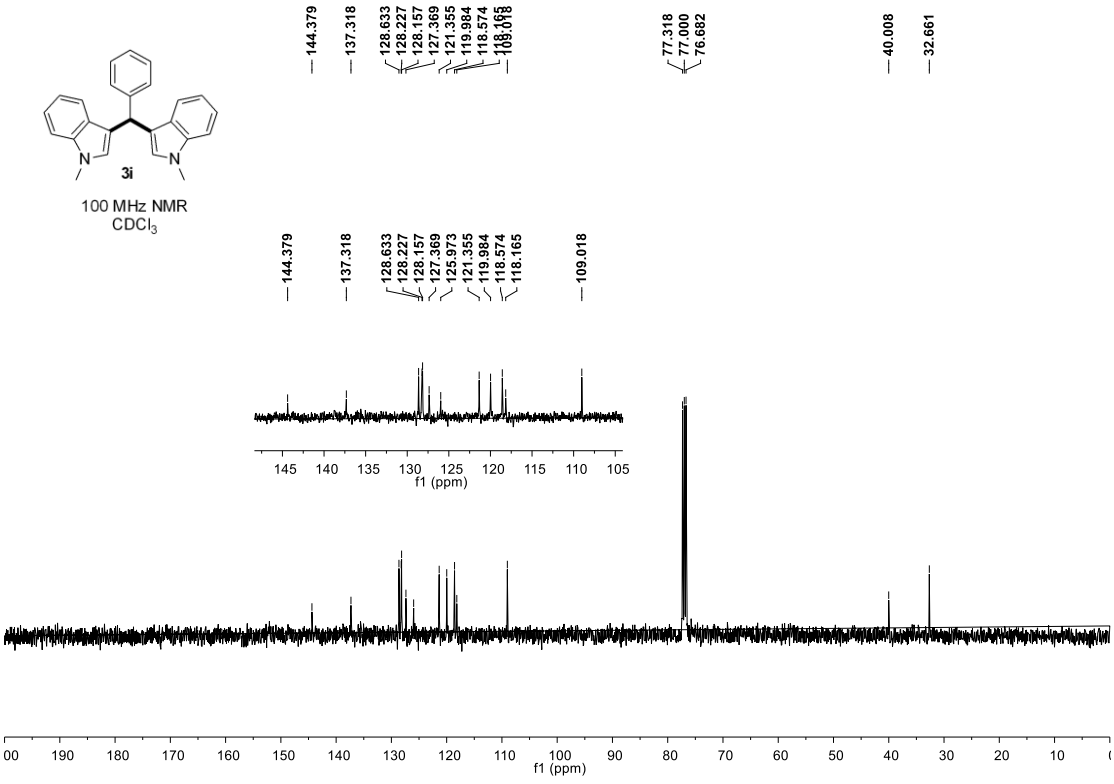

11.688
8.334
7.794
7.772
7.437
7.415
7.352
7.307
7.213
6.020
3.388
2.500
O2N
NO2
HN
NH
3g
400 MHz NMR
DMSO-d6
1.87
1.94
1.94
1.83
1.91
3.62
1.01
1.00
f1 (ppm)


141.925
134.990
131.043
130.716
128.438
128.214
119.171
118.932
113.672
109.336
108.514
40.127
39.916
39.708
39.500
39.291
39.082
38.873
O2N
NO2
HN
NH
3g
400 MHz NMR
DMSO-d6
f1 (ppm)


10.751
7.258
7.246
7.234
7.215
7.201
6.895
6.883
6.870
6.804
6.791
6.679
6.666
6.654
5.921
2.063
HN
NH
3h
600 MHz NMR
DMSO-d6
1.53
2.04
1.04
3.83
2.03
2.04
2.07
1.00
5.96
f1 (ppm)


143.926
134.790
131.749
128.400
128.012
127.560
125.410
119.247
118.234
117.651
111.922
110.005
38.380
11.632
HN
NH
3h
100 MHz NMR
DMSO-d6
f1 (ppm)


7.408
7.395
7.369
7.357
7.314
7.306
7.301
7.294
7.281
7.260
7.230
7.225
7.217
7.205
7.025
7.013
7.001
6.543
5.900
3.691
0.023
3i
600 MHz NMR
CDCl3
f1 (ppm)
2.15
2.10
4.16
3.00
2.03
1.97
1.00
6.00


144.379
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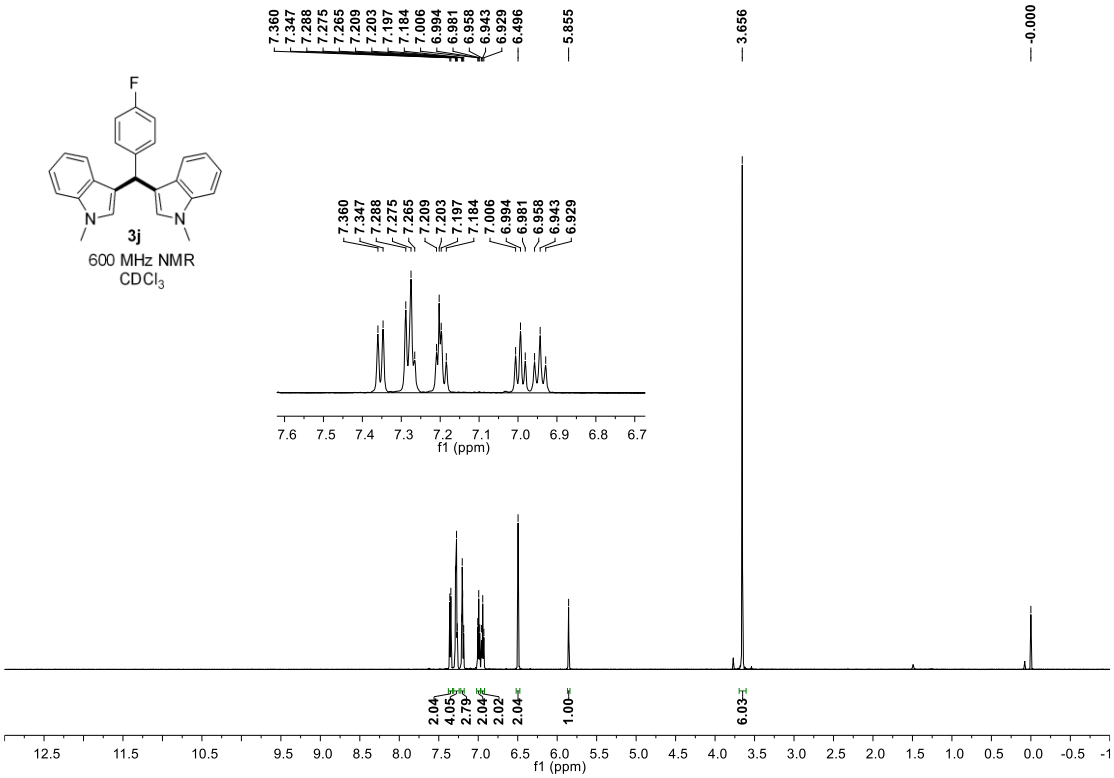
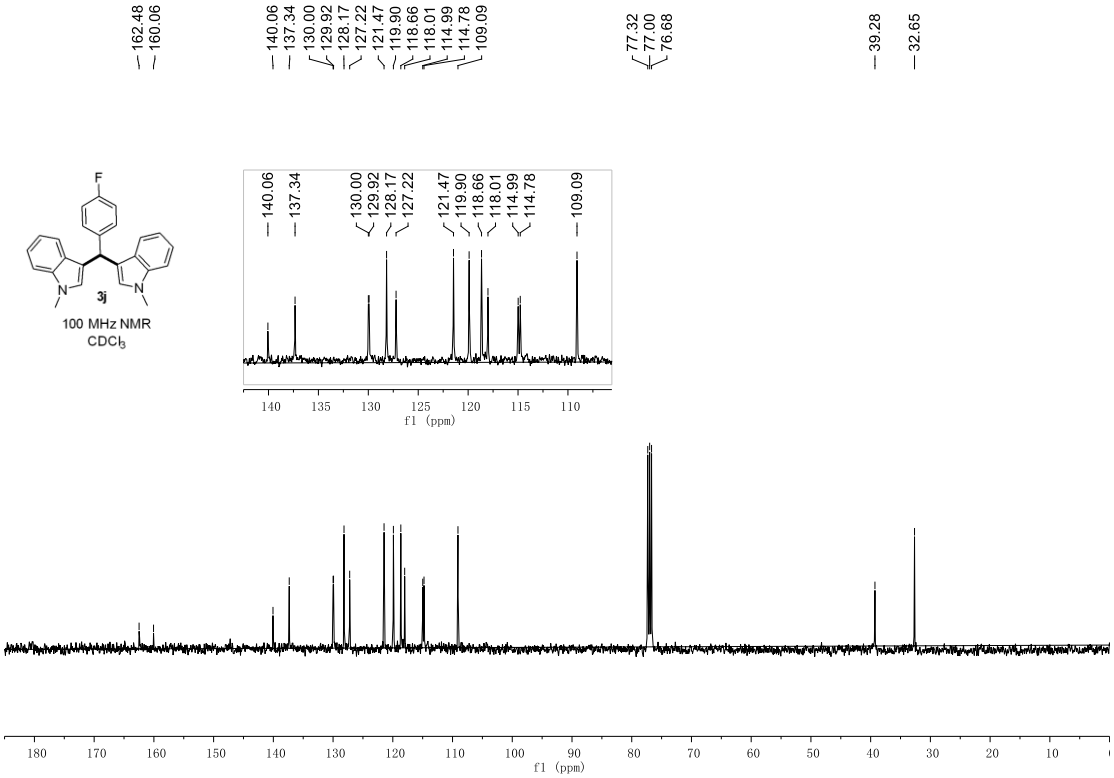
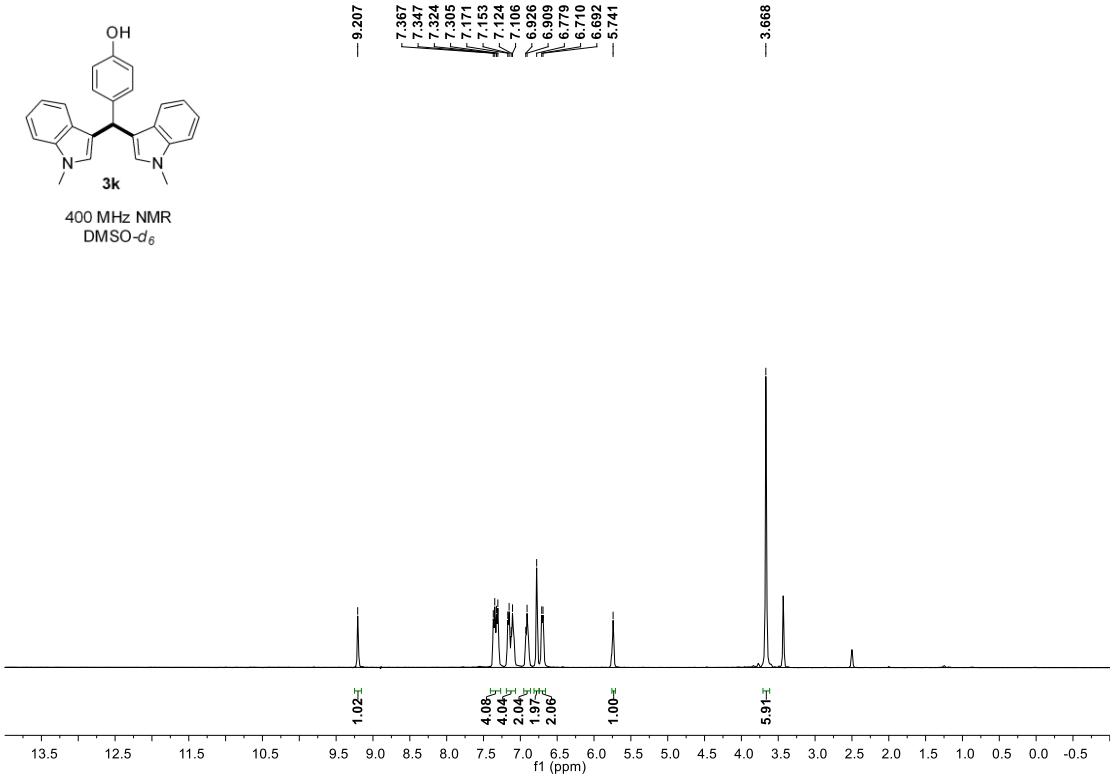
128.633
128.227
128.157
127.369
121.355
119.984
118.574
109.018
77.318
77.000
76.682
40.008
32.661
3i
100 MHz NMR
CDCl3
f1 (ppm)


7.360
7.347
7.288
7.275
7.265
7.209
7.203
7.197
7.184
7.006
6.994
6.981
6.958
6.943
6.929
6.496
5.855
3.656
-0.000
F
N
N
3j
600 MHz NMR
CDCl3
f1 (ppm)
2.04
4.05
2.79
2.04
2.02
2.04
1.00
6.03


162.48
160.06
140.06
137.34
130.00
129.92
128.17
127.22
121.47
119.90
118.66
118.01
114.99
114.78
109.09
77.32
77.00
76.68
39.28
32.65
F
N
N
3j
100 MHz NMR
CDCl3
f1 (ppm)

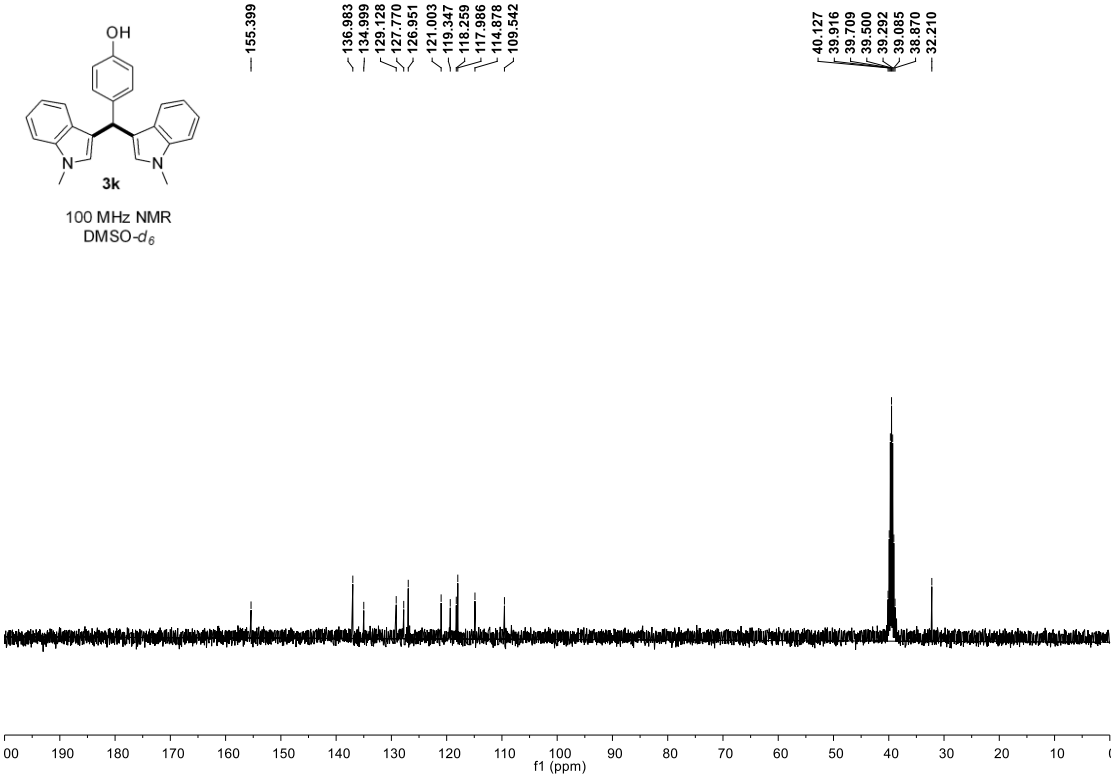
3k

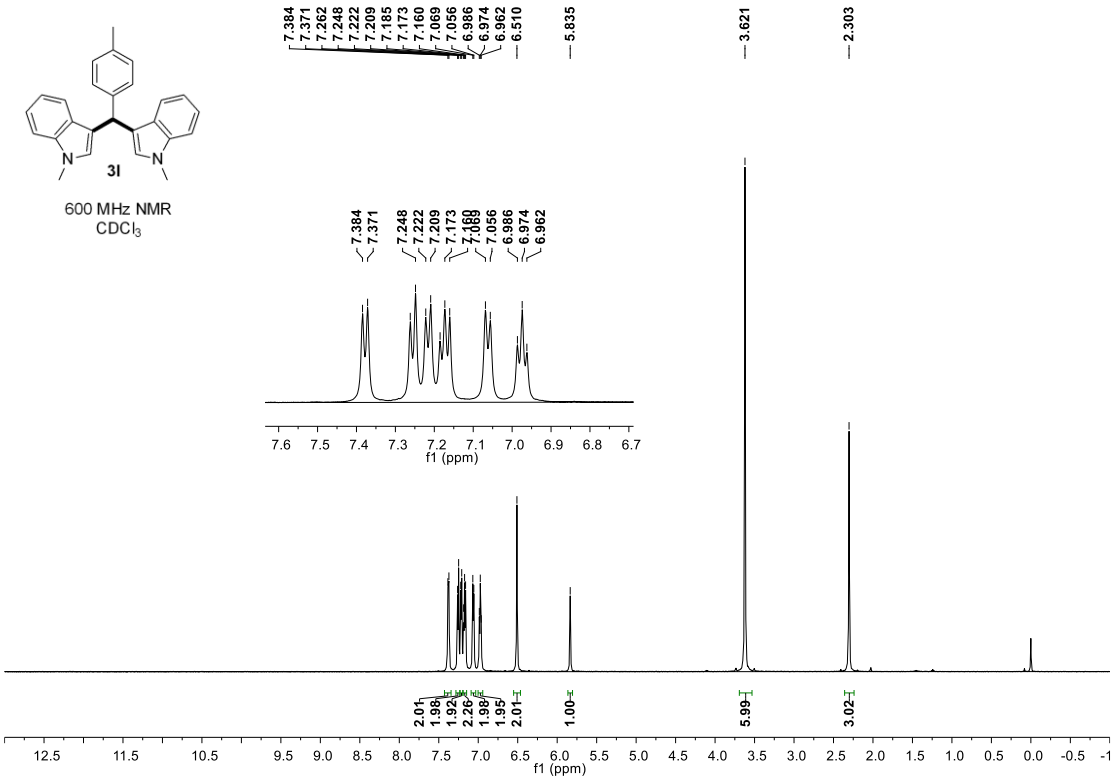
400 MHz NMR
DMSO-d_6

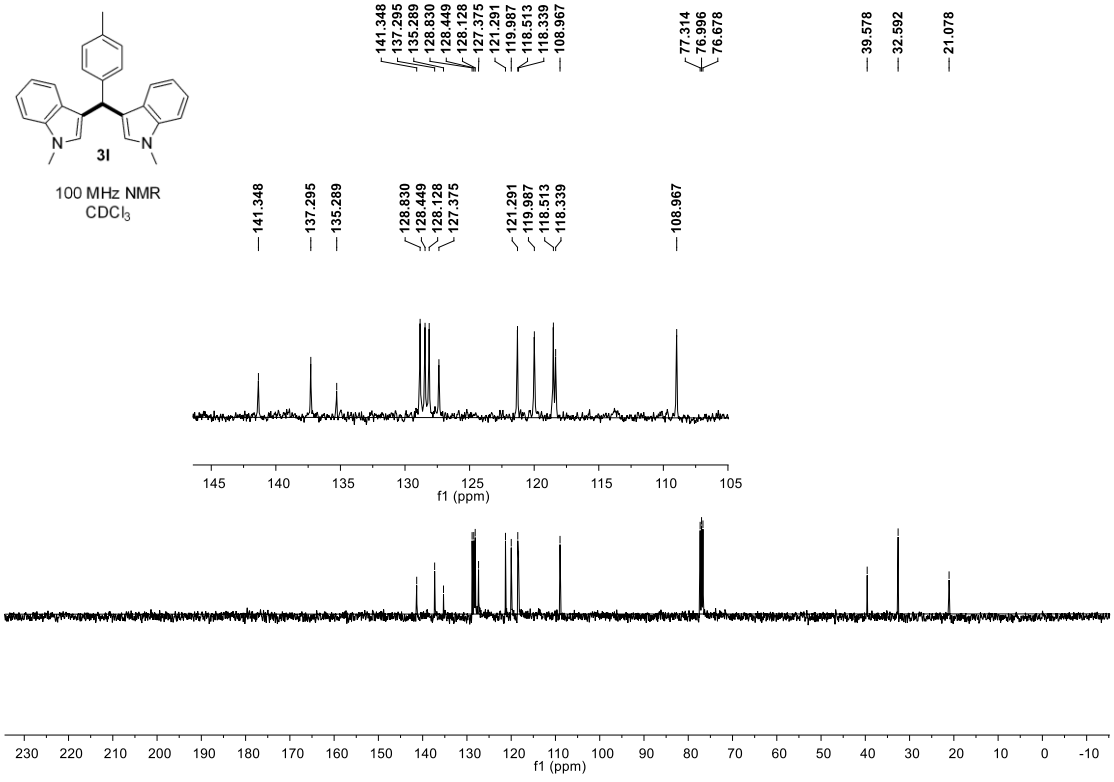


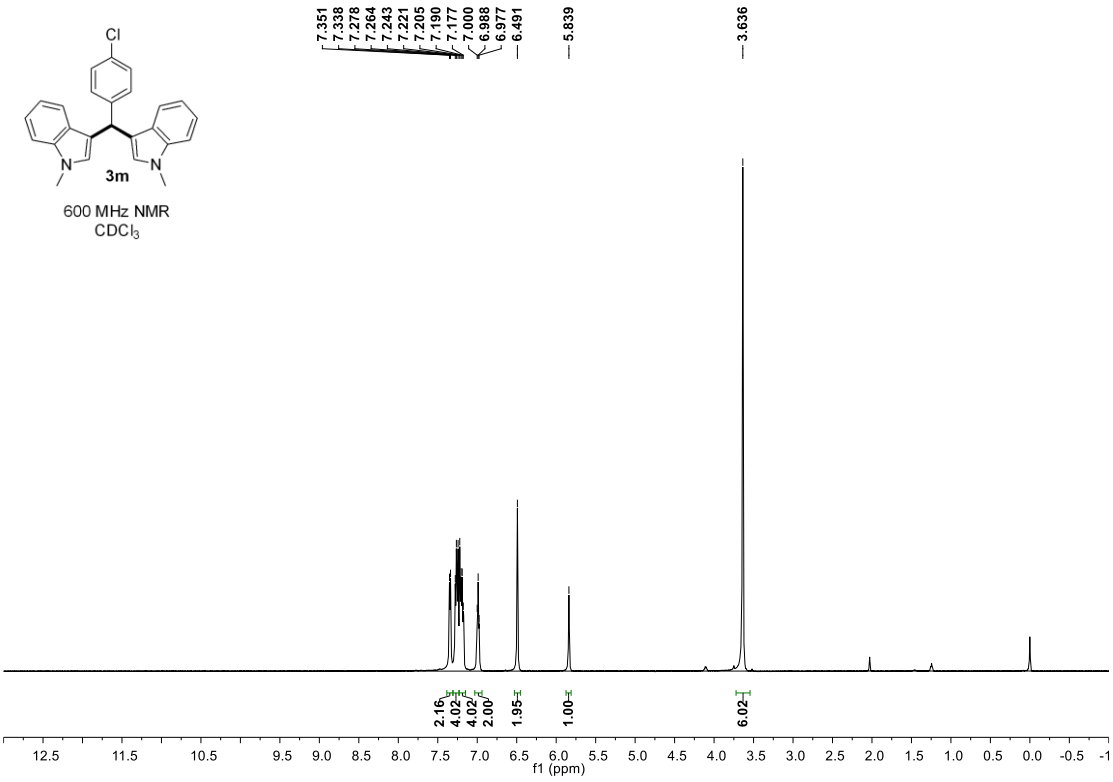
3k

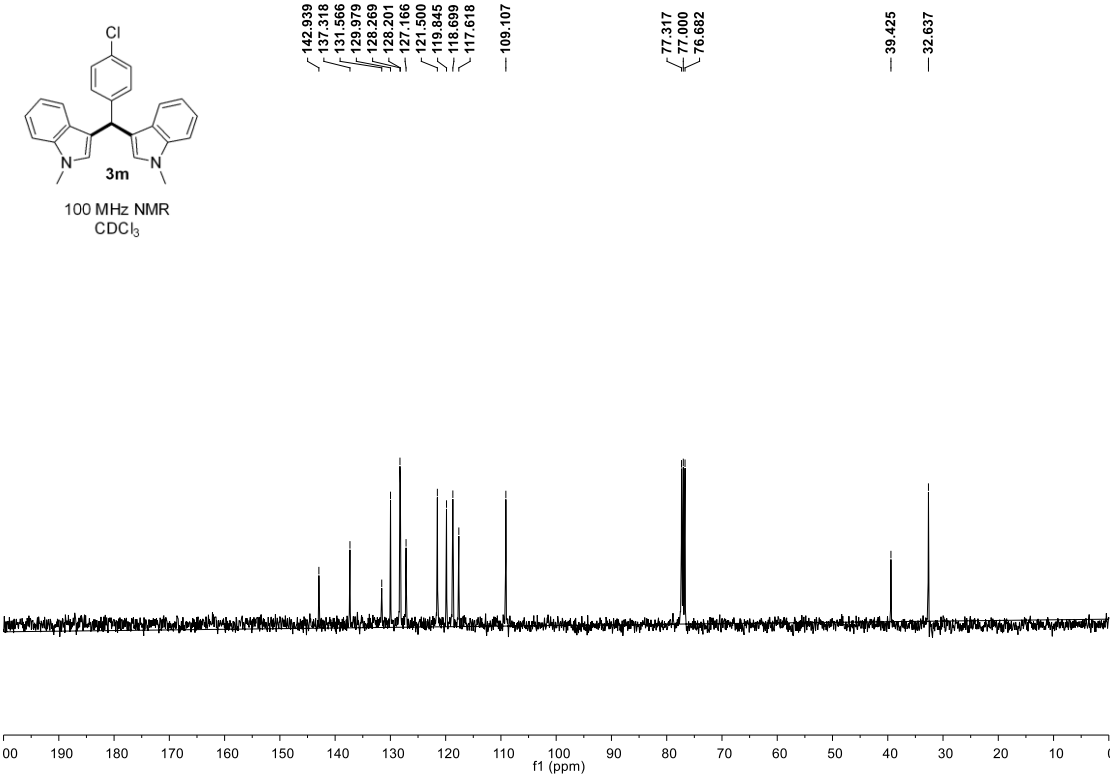
100 MHz NMR
DMSO-d_6

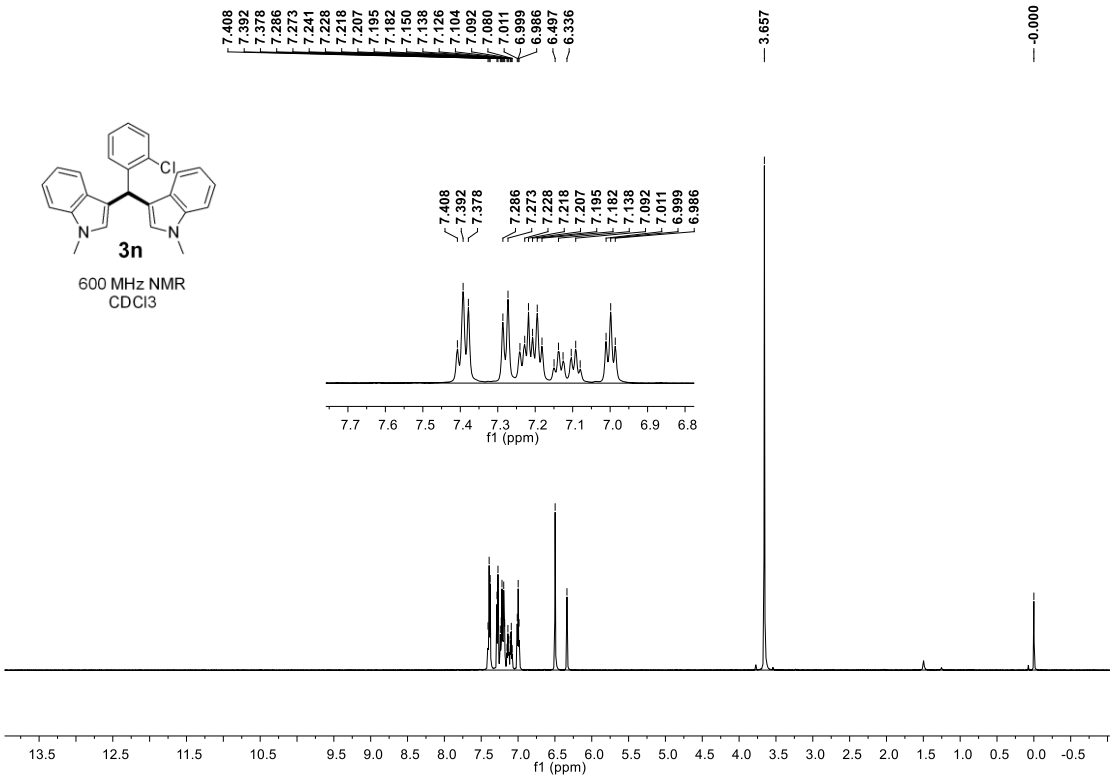


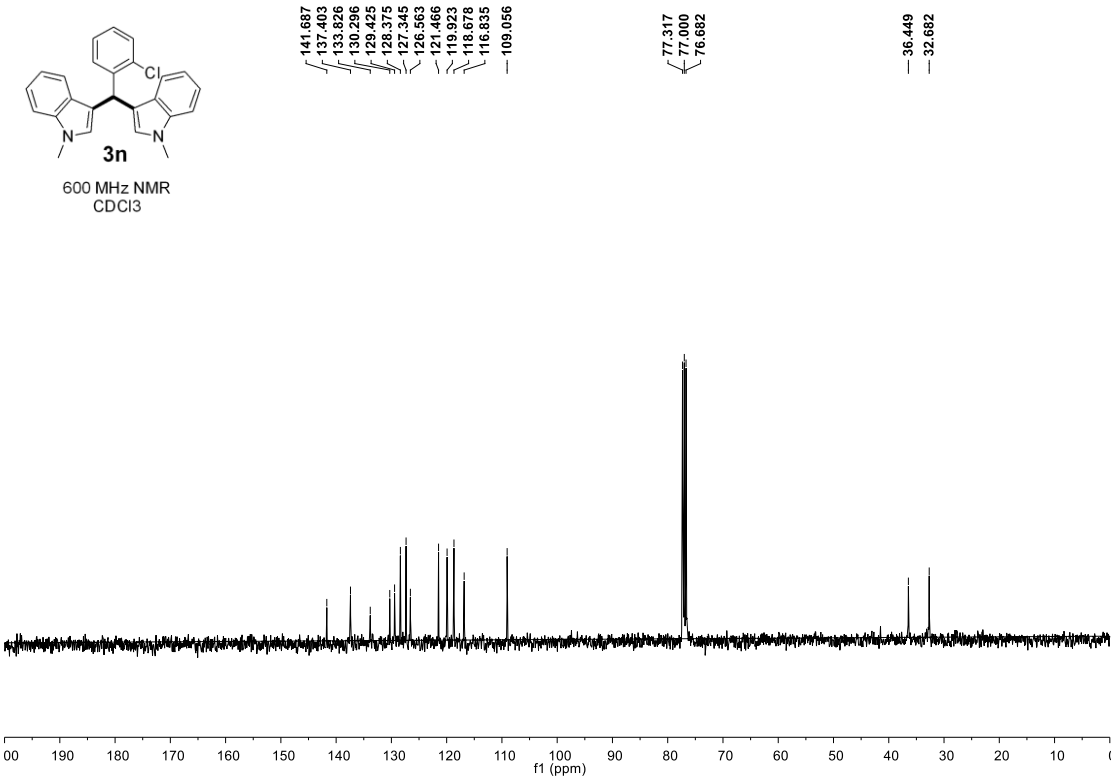

3l
600 MHz NMR
CDCl3
7.384
7.371
7.262
7.248
7.222
7.209
7.185
7.173
7.160
7.069
7.056
6.986
6.974
6.962
6.510
5.835
3.621
2.303
f1 (ppm)

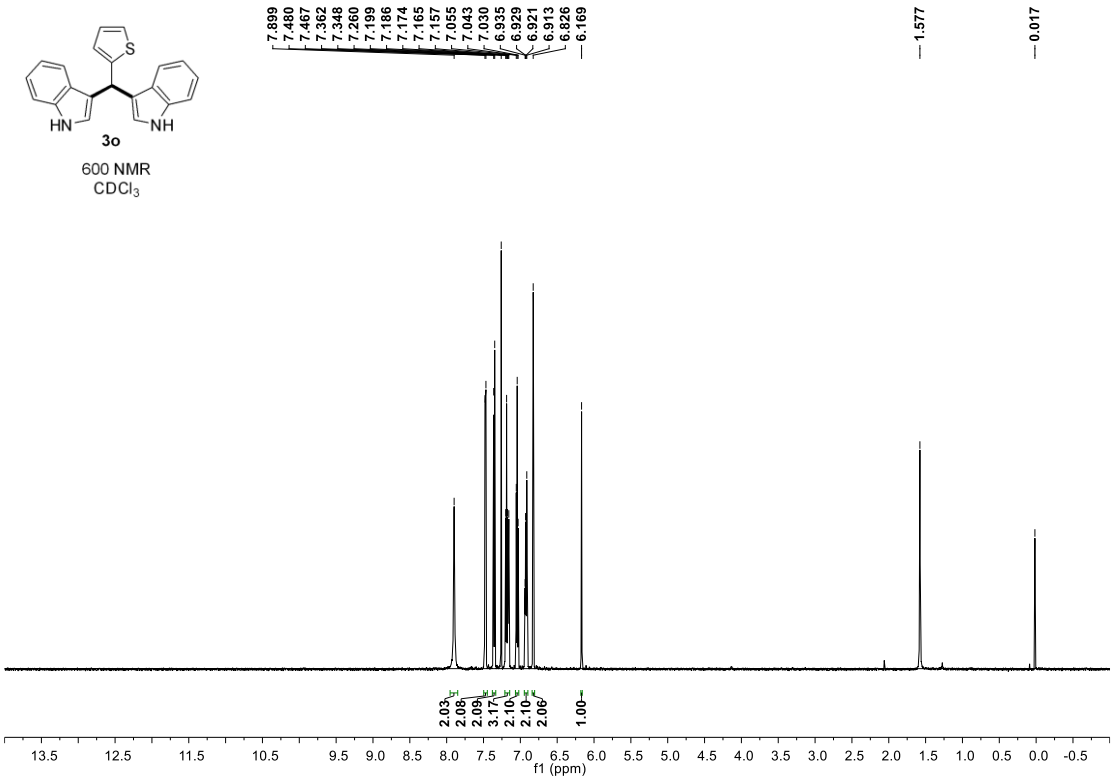

3l
100 MHz NMR
CDCl3
141.348
137.295
135.289
128.830
128.449
128.128
127.375
121.291
119.987
118.513
118.339
108.967
77.314
76.996
76.678
39.578
32.592
21.078
f1 (ppm)

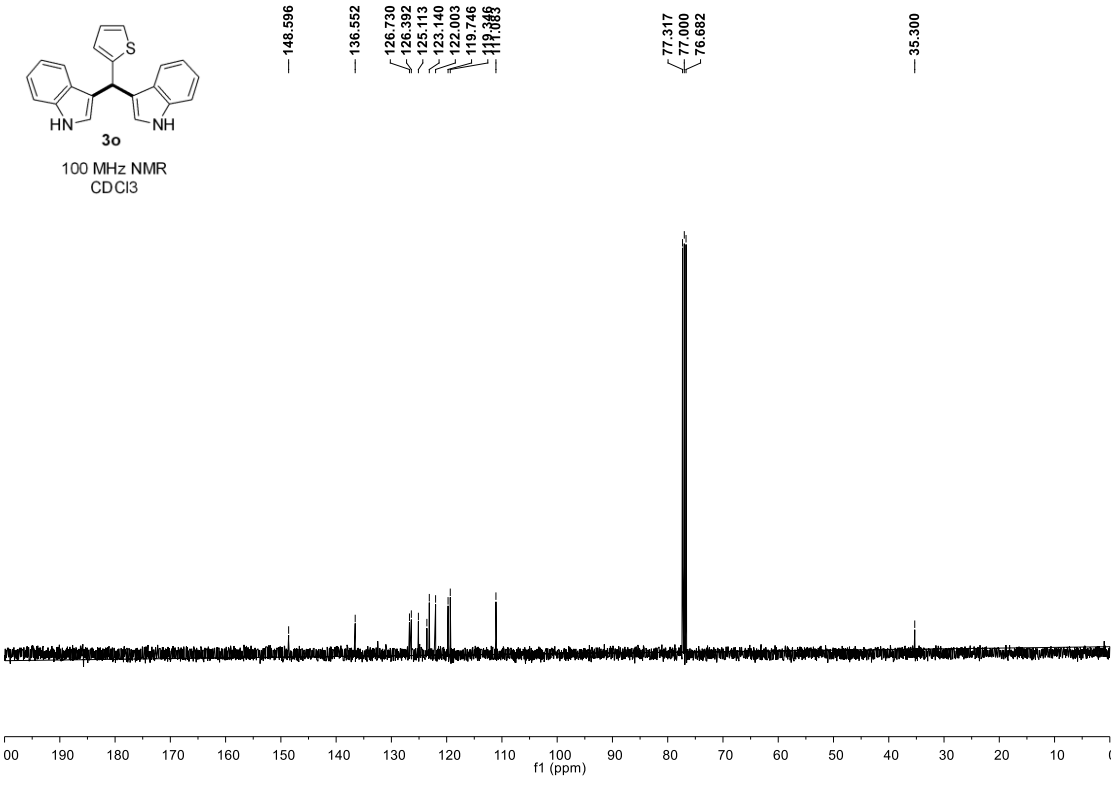

Cl
N
N
3m
600 MHz NMR
CDCl3
7.351
7.338
7.278
7.264
7.243
7.221
7.205
7.190
7.177
7.000
6.988
6.977
6.491
5.839
3.636
2.16
4.02
4.02
2.00
1.95
1.00
6.02
f1 (ppm)

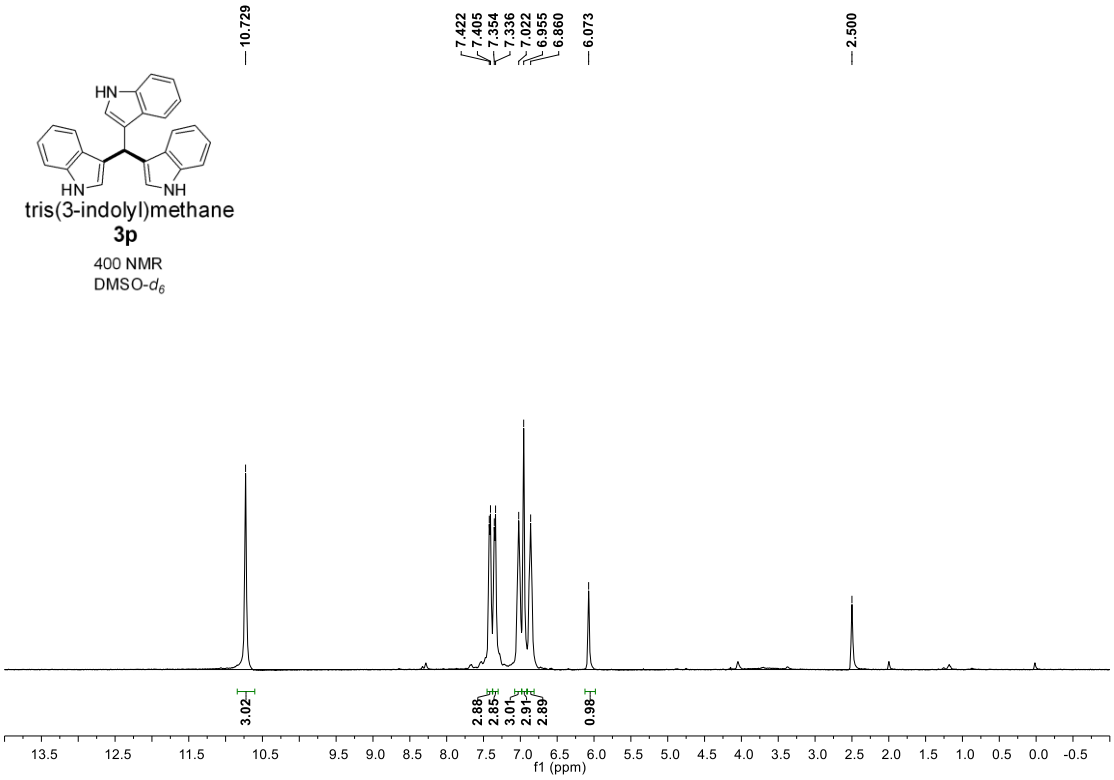

Cl
N
N
3m
100 MHz NMR
CDCl3
142.939
137.318
131.566
129.979
128.269
128.201
127.166
121.500
119.845
118.699
117.618
109.107
77.317
77.000
76.682
39.425
32.637
f1 (ppm)

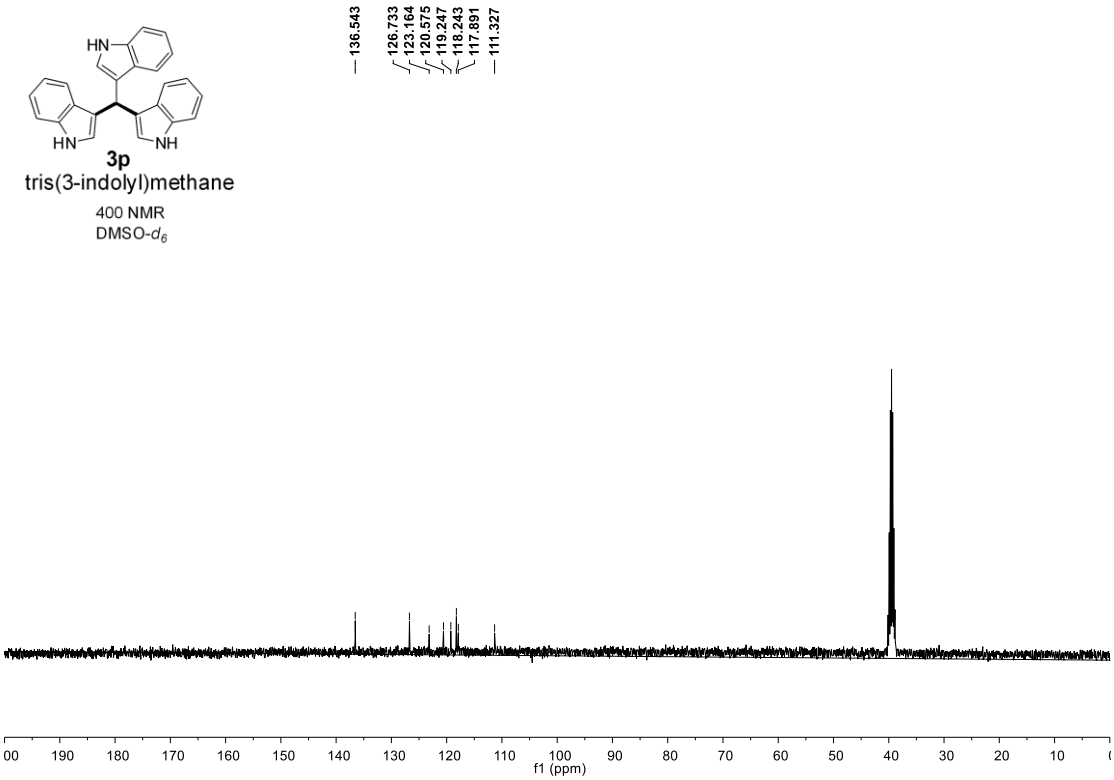

7.408
7.392
7.378
7.286
7.273
7.241
7.228
7.218
7.207
7.195
7.182
7.150
7.138
7.126
7.104
7.092
7.080
7.011
6.999
6.986
6.497
6.336
3.657
-0.000
Cl
N
N
3n
600 MHz NMR
CDCl3
f1 (ppm)

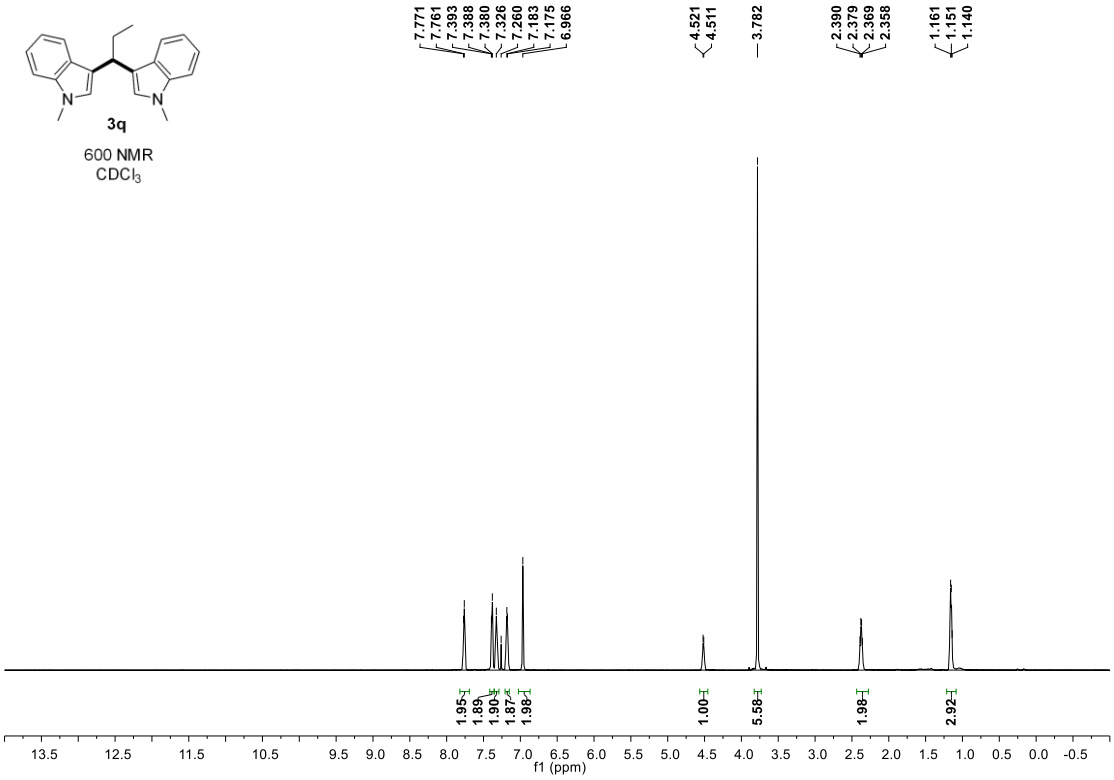

141.687
137.403
133.826
130.296
129.425
128.375
127.345
126.563
121.466
119.923
118.678
116.835
109.056
77.317
77.000
76.682
36.449
32.682
Cl
N
N
3n
600 MHz NMR
CDCl3
f1 (ppm)

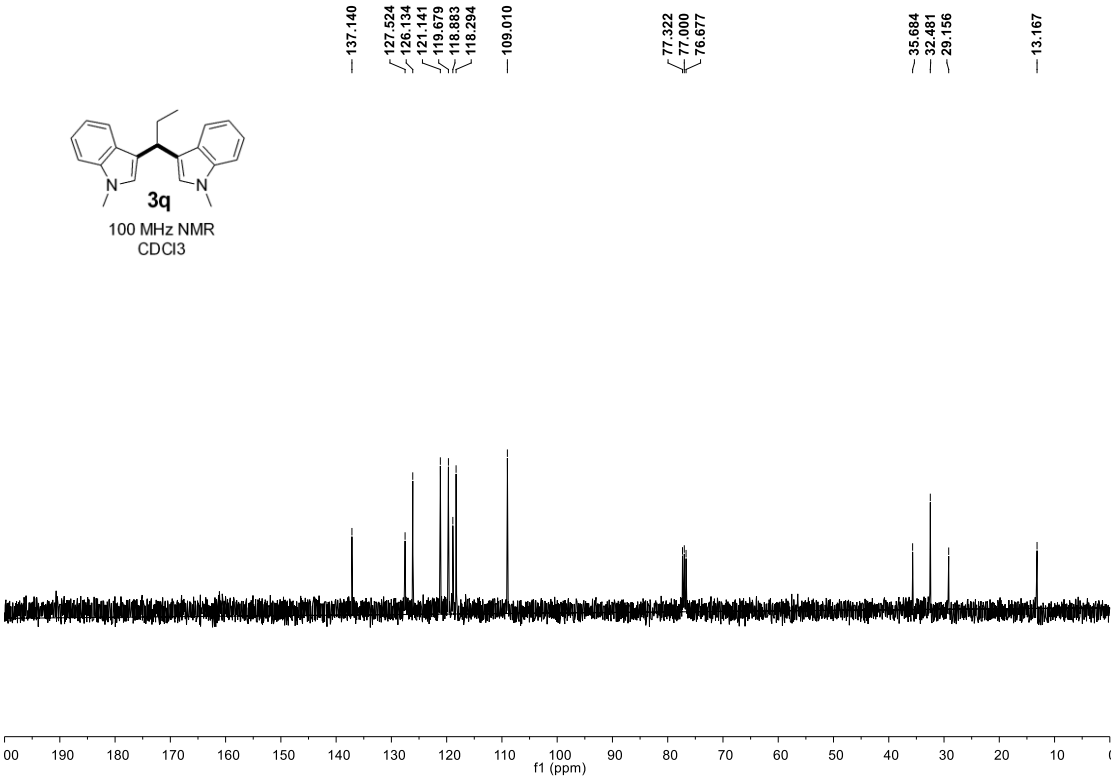

7.899
7.480
7.467
7.362
7.348
7.260
7.199
7.186
7.174
7.165
7.157
7.055
7.043
7.030
6.935
6.929
6.921
6.913
6.826
6.169
1.577
0.017
HN
NH
S
3o
600 NMR
CDCl3
2.03
2.08
2.09
3.17
2.10
2.10
2.06
1.00
f1 (ppm)

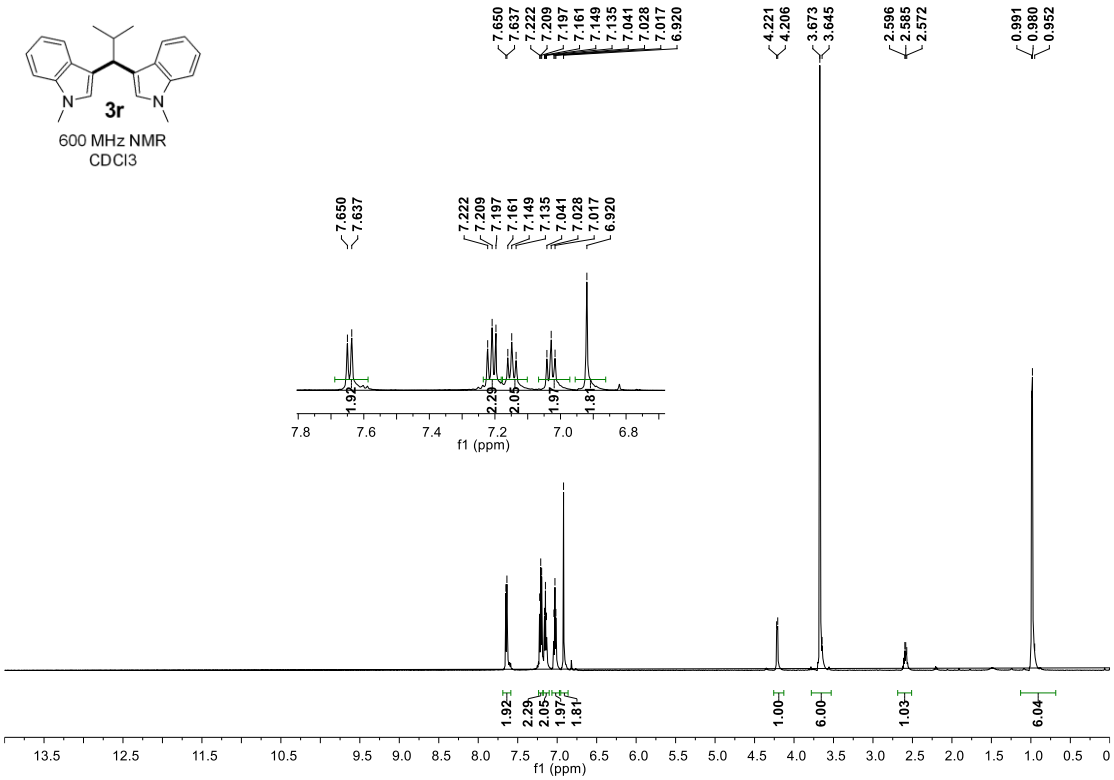

148.596
136.552
126.730
126.392
125.113
123.140
122.003
119.746
111.083
77.317
77.000
76.682
35.300
HN
NH
S
3o
100 MHz NMR
CDCl3
f1 (ppm)

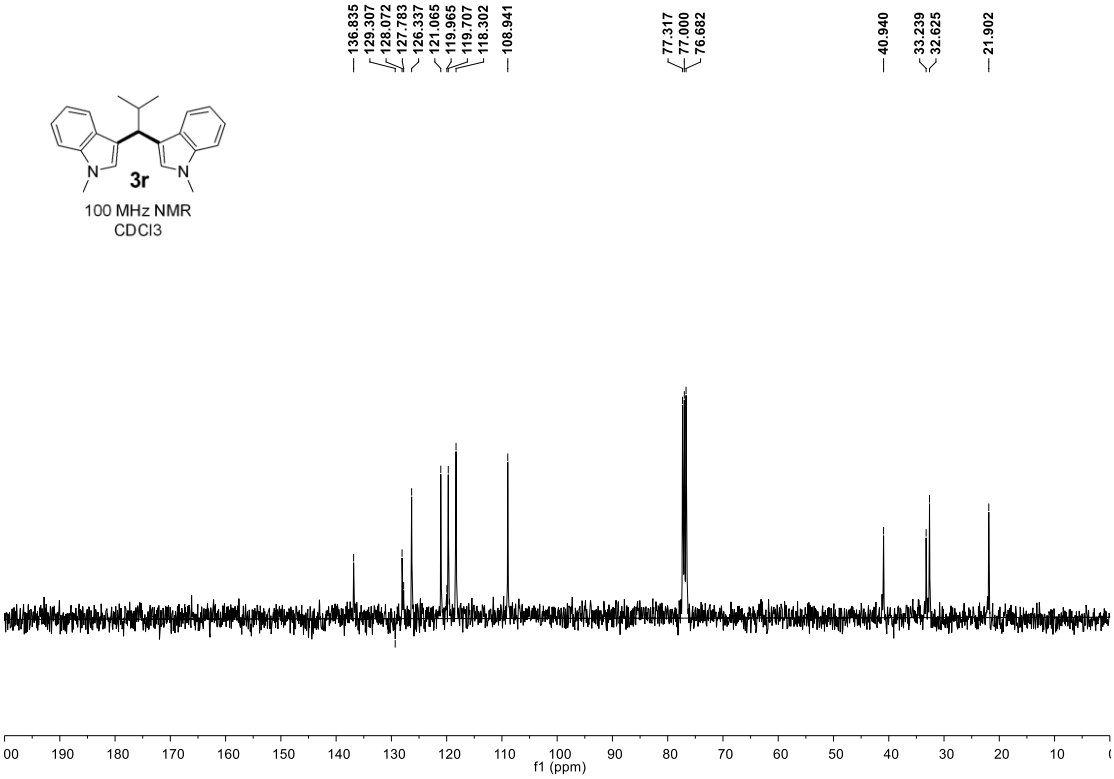

10.729
7.422
7.405
7.354
7.336
7.022
6.955
6.860
6.073
2.500
HN
HN
NH
tris(3-indolyl)methane
3p
400 NMR
DMSO-d6
3.02
2.88
2.85
3.01
2.91
2.89
0.98
f1 (ppm)

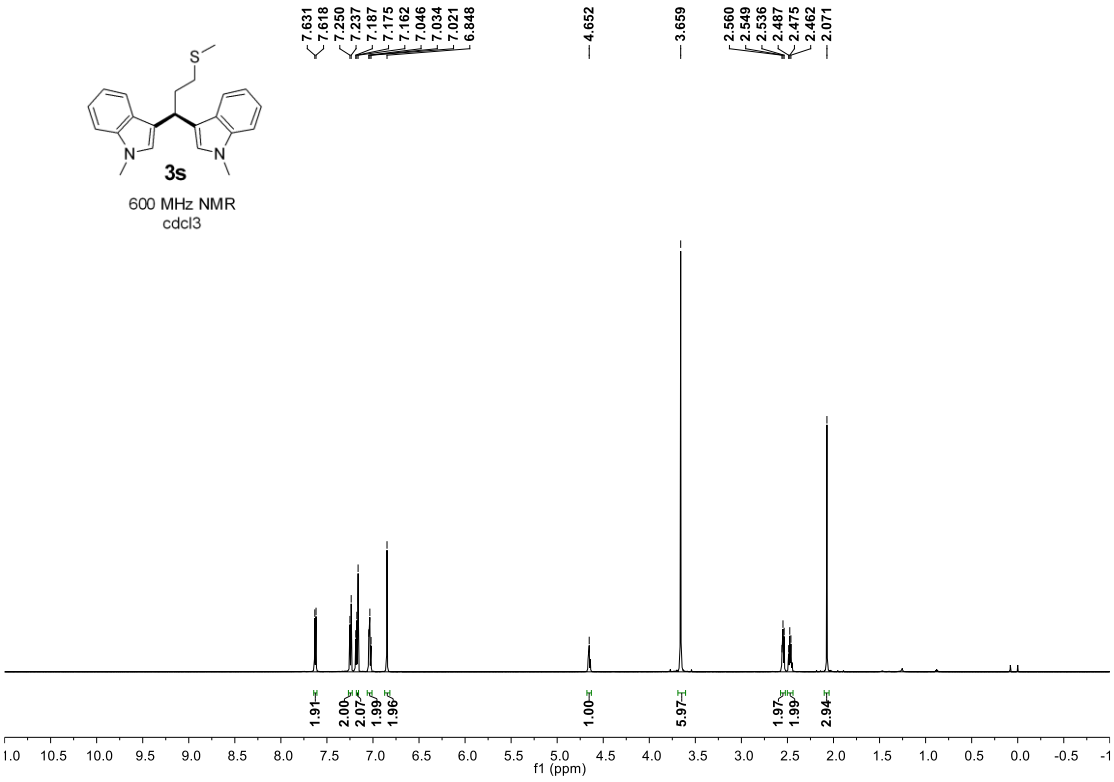

136.543
126.733
123.164
120.575
119.247
118.243
117.891
111.327
HN
HN
NH
3p
tris(3-indolyl)methane
400 NMR
DMSO-d6
f1 (ppm)

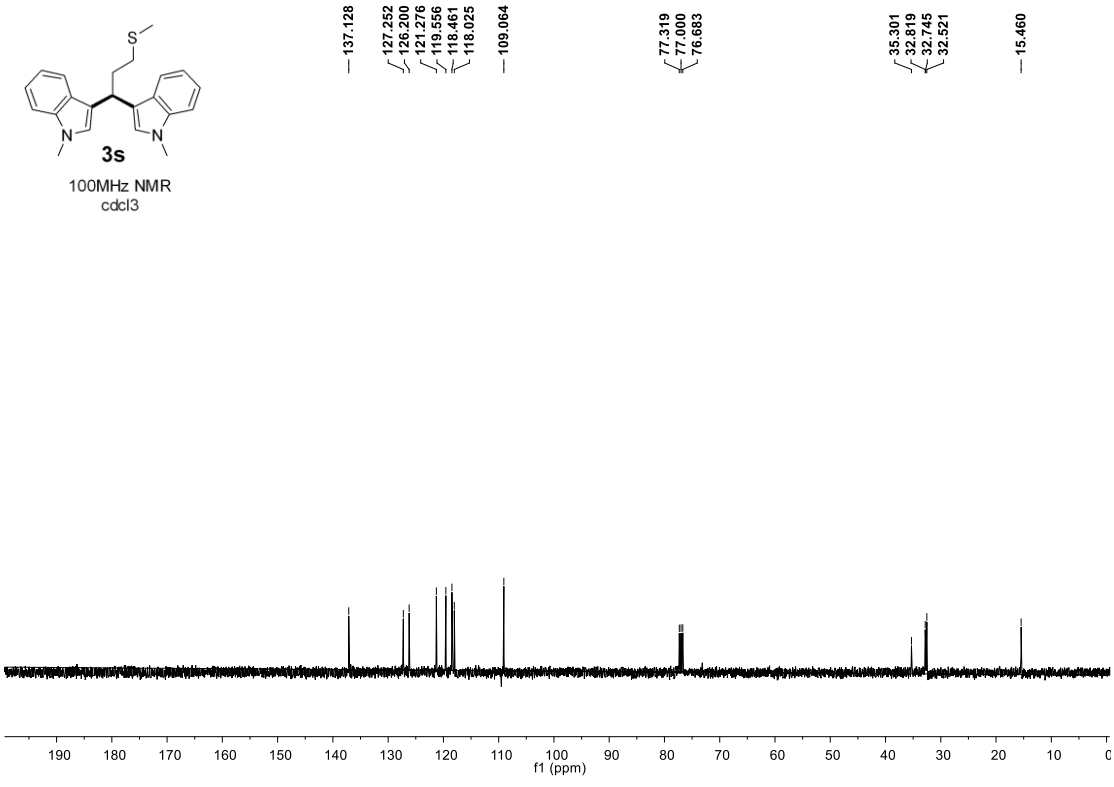

3q
600 NMR
CDCl3
7.771
7.761
7.393
7.388
7.380
7.326
7.260
7.183
7.175
6.966
4.521
4.511
3.782
2.390
2.379
2.369
2.358
1.161
1.151
1.140
1.95
1.89
1.90
1.87
1.98
1.00
5.58
1.98
2.92
f1 (ppm)

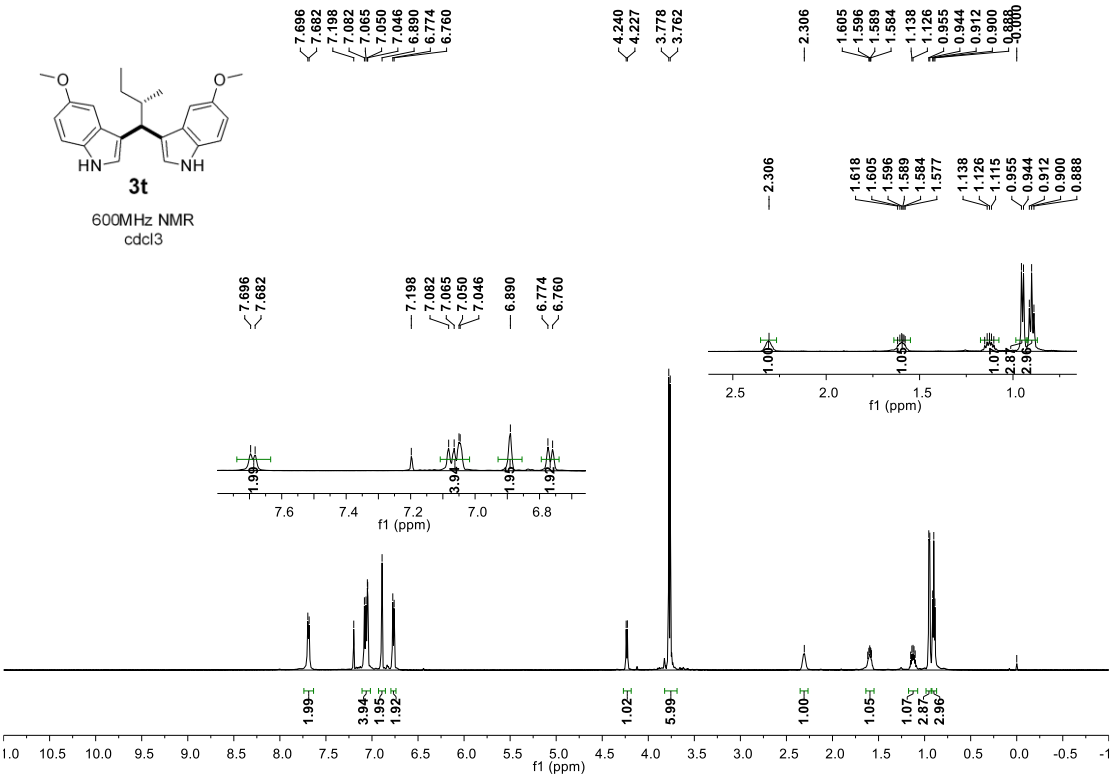

137.140
127.524
126.134
121.141
119.679
118.883
118.294
109.010
77.322
77.000
76.677
35.684
32.481
29.156
13.167
3q
100 MHz NMR
CDCl3
f1 (ppm)

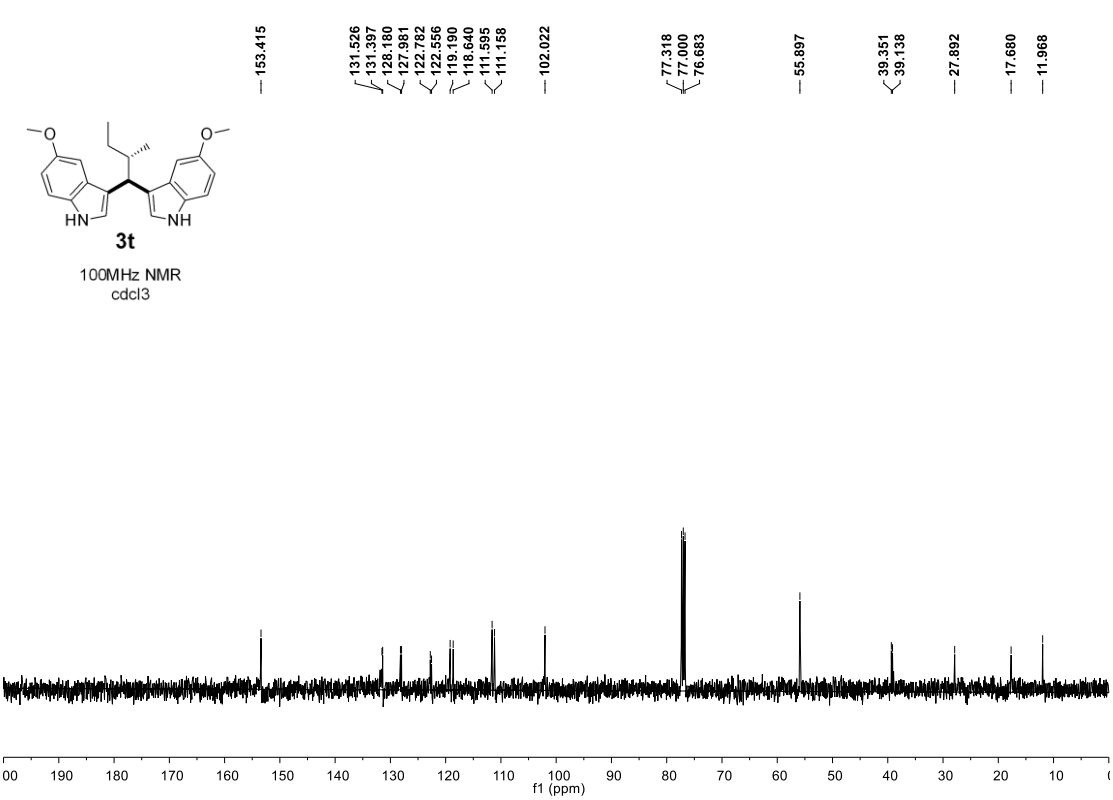

3r
600 MHz NMR
CDCl3
7.650
7.637
7.222
7.209
7.197
7.161
7.149
7.135
7.041
7.028
7.017
6.920
4.221
4.206
3.673
3.645
2.596
2.585
2.572
0.991
0.980
0.952
1.92
2.29
2.05
1.97
1.81
1.00
6.00
1.03
6.04
f1 (ppm)

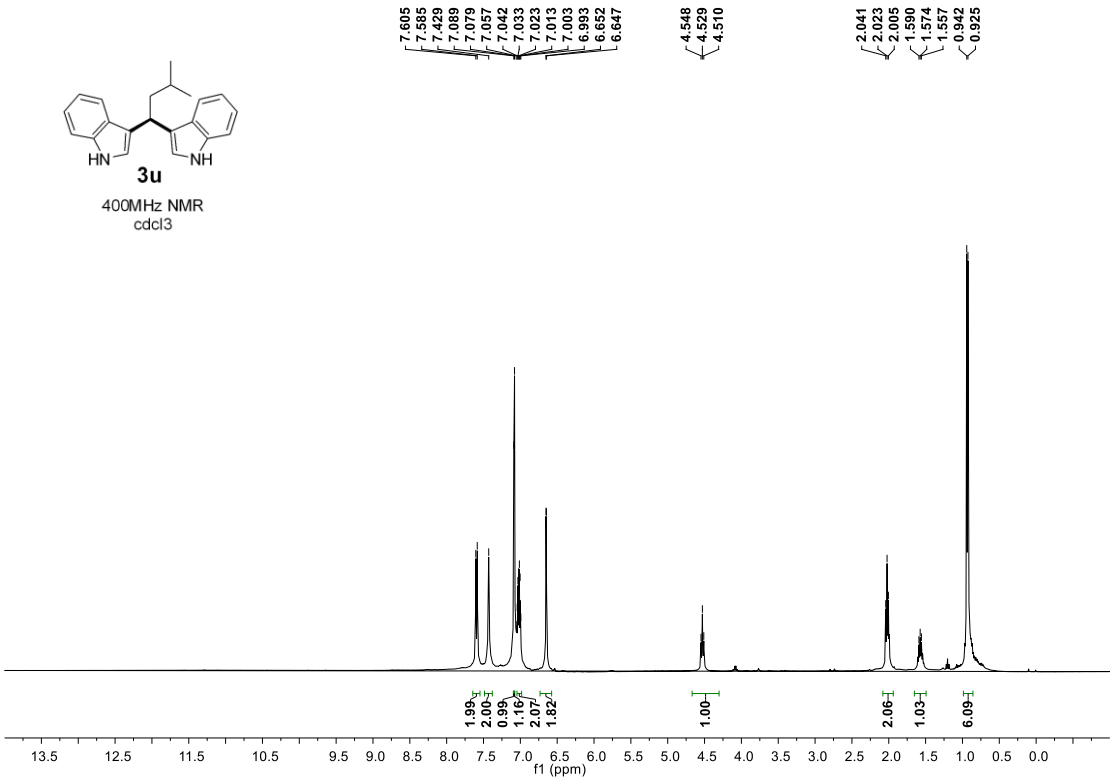

3r
100 MHz NMR
CDCl3
136.835
129.307
128.072
127.783
126.337
121.065
119.965
119.707
118.302
108.941
77.317
77.000
76.682
40.940
33.239
32.625
21.902
f1 (ppm)

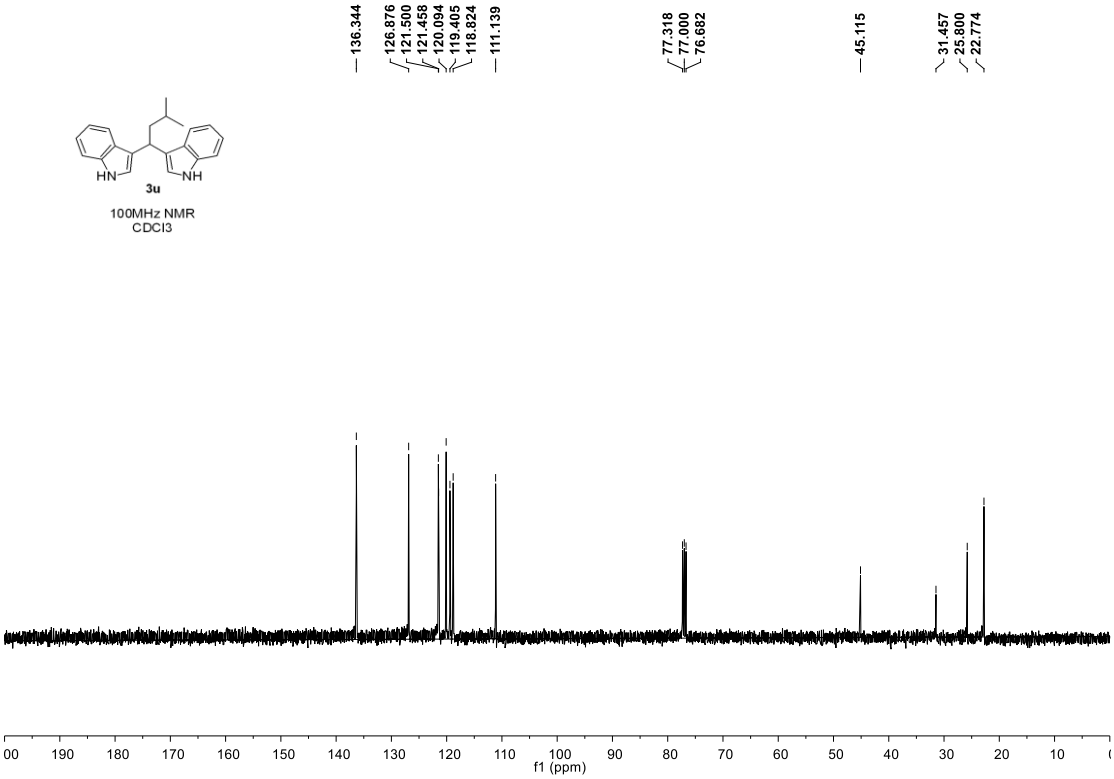

7.631
7.618
7.250
7.237
7.187
7.175
7.162
7.046
7.034
7.021
6.848
4.652
3.659
2.560
2.549
2.536
2.487
2.475
2.462
2.071
3s
600 MHz NMR
cdcl3
1.91
2.00
2.07
1.99
1.96
1.00
5.97
1.97
1.99
2.94
f1 (ppm)

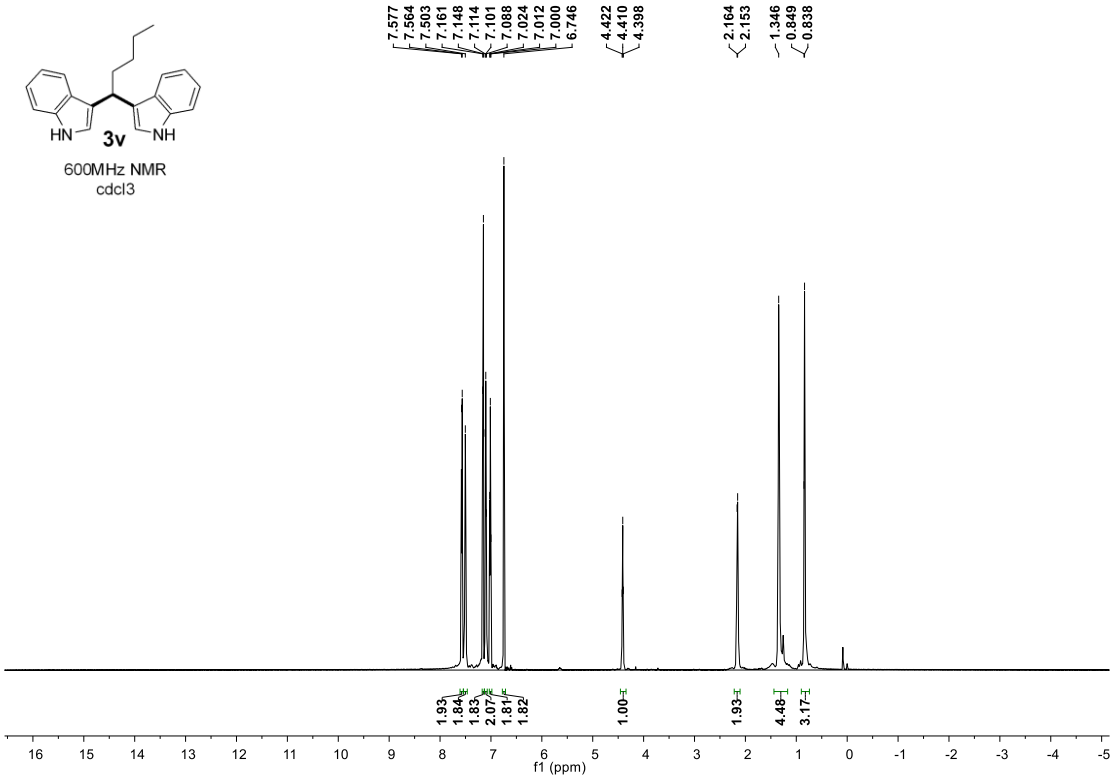

137.128
127.252
126.200
121.276
119.556
118.461
118.025
109.064
77.319
77.000
76.683
35.301
32.819
32.745
32.521
15.460
3s
100MHz NMR
cdcl3
f1 (ppm)

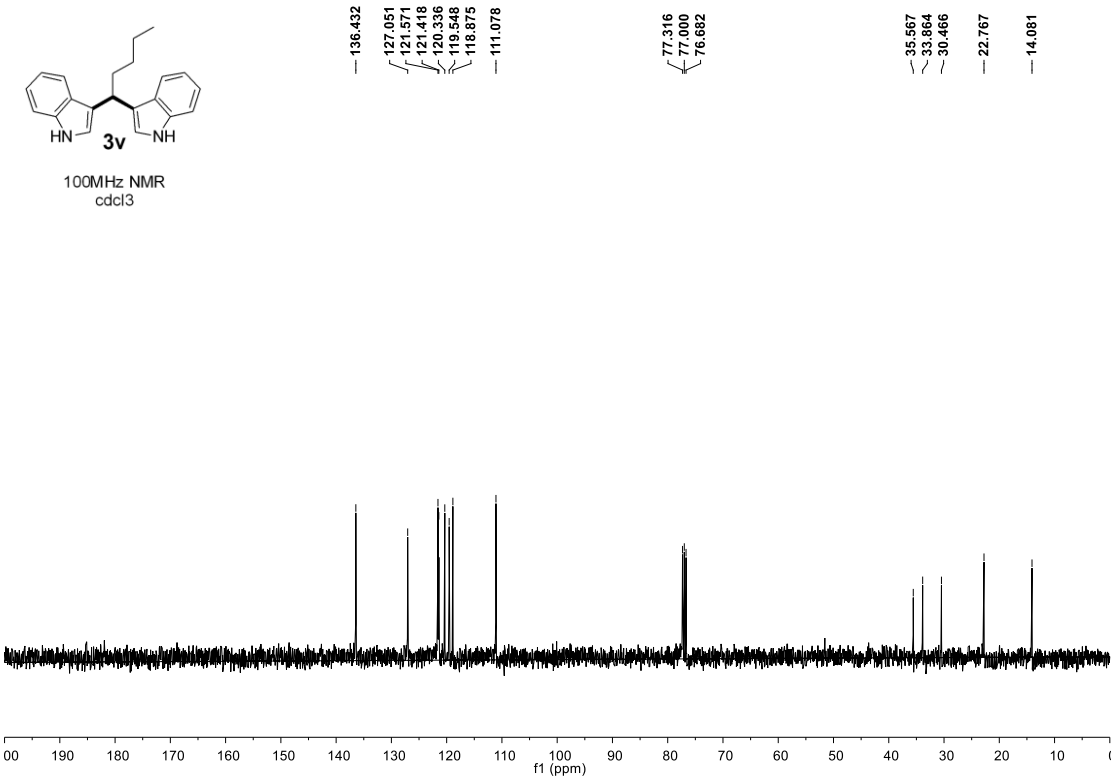

3t
600MHz NMR
cdcl3
f1 (ppm)

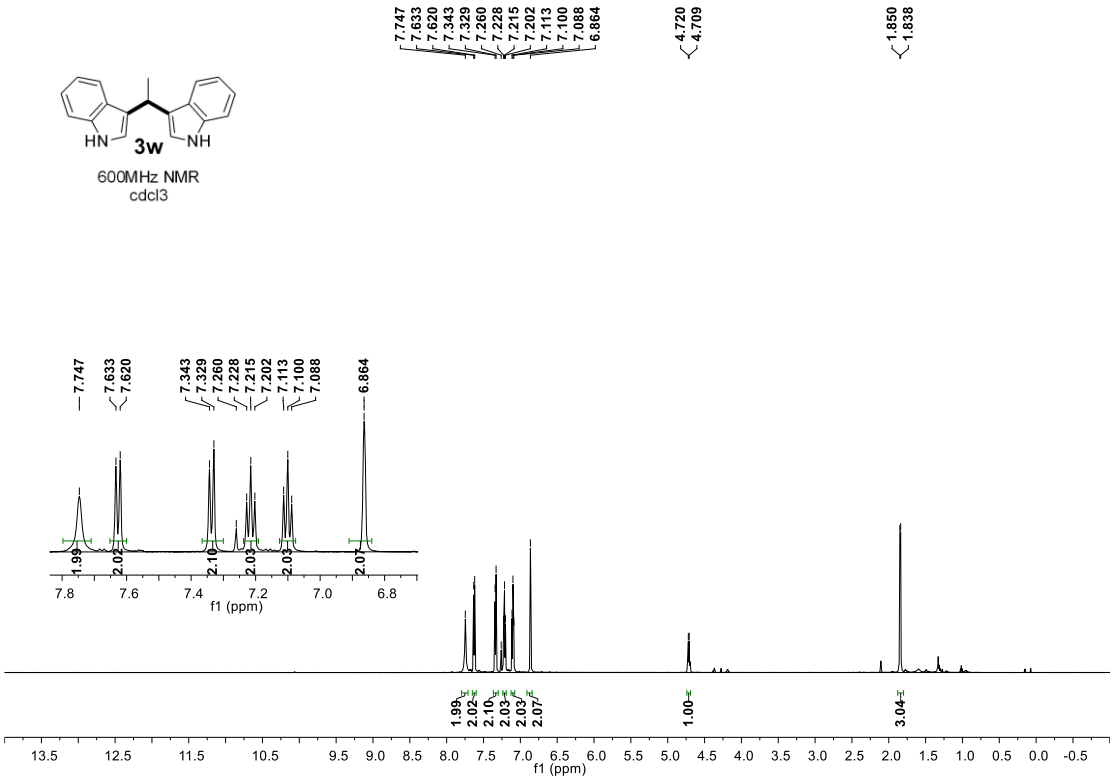

3t
100MHz NMR
cdcl3
f1 (ppm)

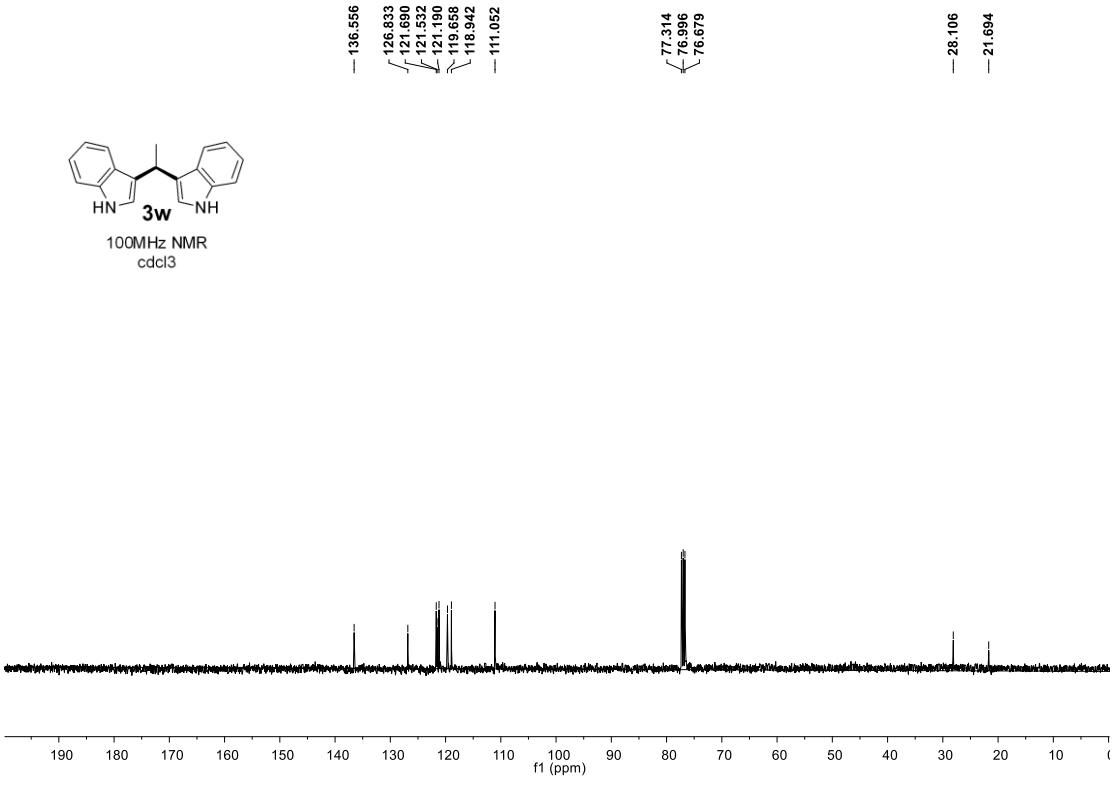

7.605
7.585
7.429
7.089
7.079
7.057
7.042
7.033
7.023
7.013
7.003
6.993
6.652
6.647
4.548
4.529
4.510
2.041
2.023
2.005
1.590
1.574
1.557
0.942
0.925
HN
NH
3u
400MHz NMR
cdcl3
1.99
2.00
0.99
1.16
2.07
1.82
1.00
2.06
1.03
6.09
f1 (ppm)


136.344
126.876
121.500
121.458
120.094
119.405
118.824
111.139
77.318
77.000
76.682
45.115
31.457
25.800
22.774
HN
NH
3u
100MHz NMR
CDCl3
f1 (ppm)


7.577
7.564
7.503
7.161
7.148
7.114
7.101
7.088
7.024
7.012
7.000
6.746
4.422
4.410
4.398
2.164
2.153
1.346
0.849
0.838
HN
NH
3v
600MHz NMR
cdcl3
1.93
1.84
1.83
2.07
1.81
1.82
1.00
1.93
4.48
3.17
f1 (ppm)


136.432
127.051
121.571
121.418
120.336
119.548
118.875
111.078
77.316
77.000
76.682
35.567
33.864
30.466
22.767
14.081
HN
NH
3v
100MHz NMR
cdcl3
f1 (ppm)

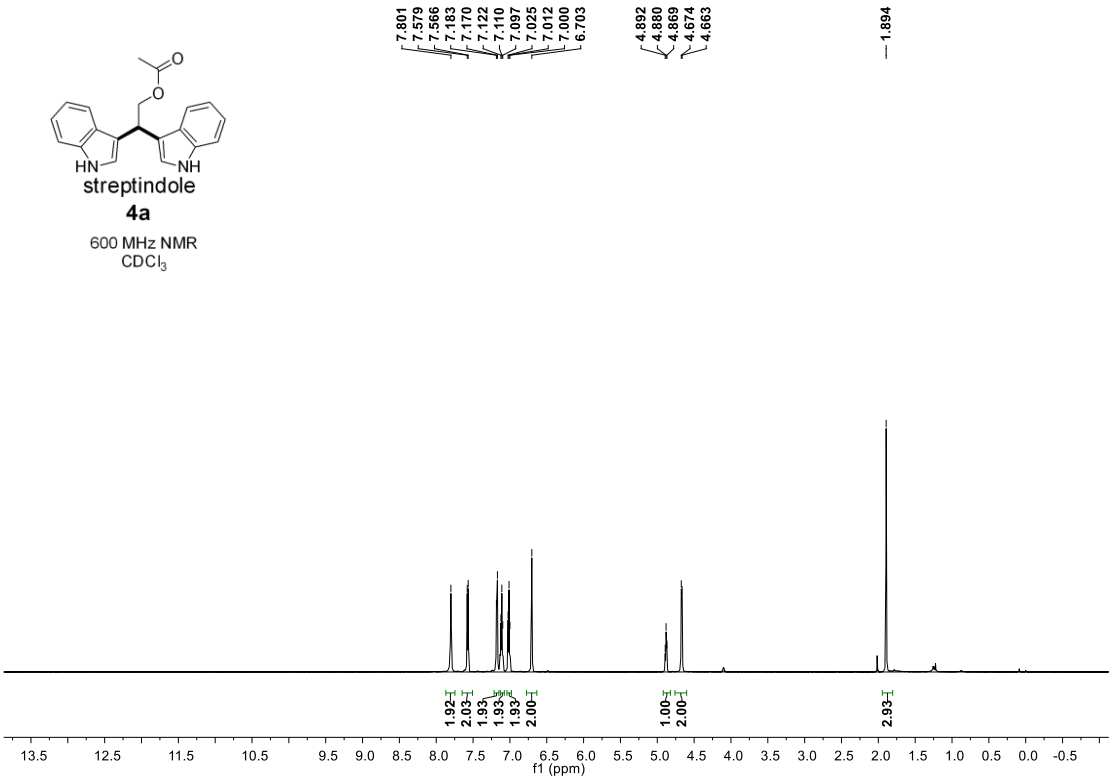

7.747
7.633
7.620
7.343
7.329
7.260
7.228
7.215
7.202
7.113
7.100
7.088
6.864
4.720
4.709
1.850
1.838
HN
NH
3w
600MHz NMR
cdcl3
1.99
2.02
2.10
2.03
2.03
2.07
1.00
3.04
f1 (ppm)


136.556
126.833
121.690
121.532
121.190
119.658
118.942
111.052
77.314
76.996
76.679
28.106
21.694
HN
NH
3w
100MHz NMR
cdcl3
f1 (ppm)

streptindole

4a

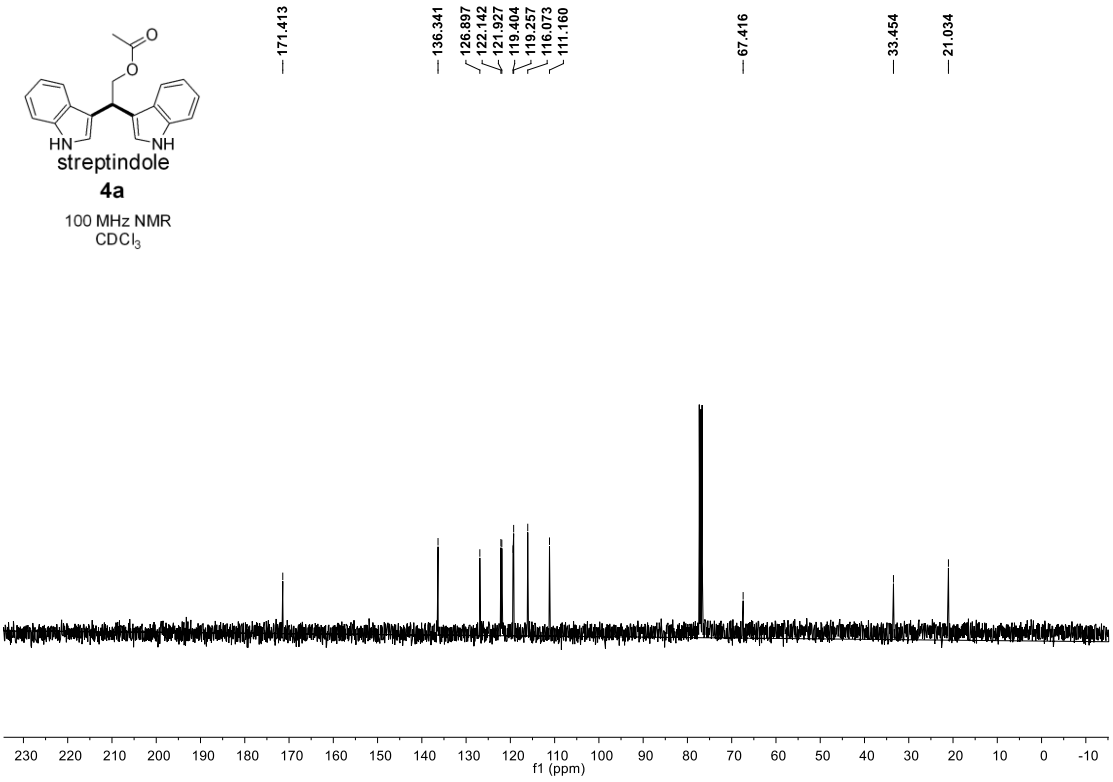
600 MHz NMR
$CDCl_3$



streptindole

4a

100 MHz NMR
$CDCl_3$

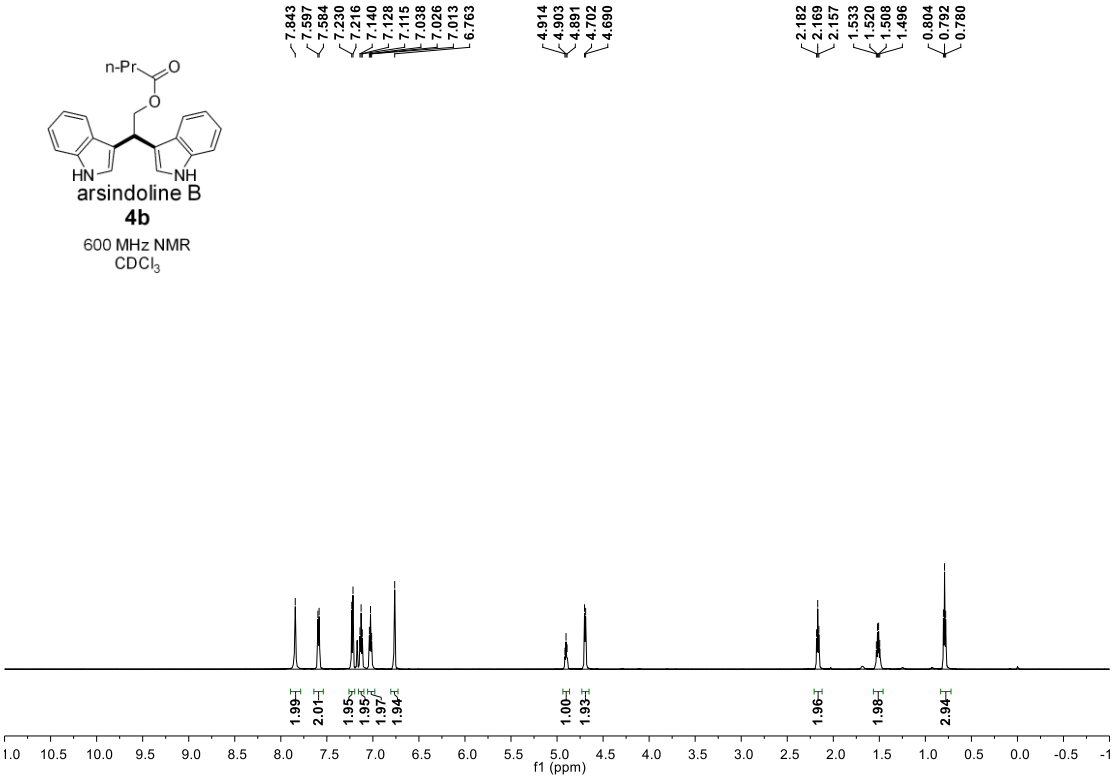


arsindoline B

4b

600 MHz NMR

$CDCl_3$

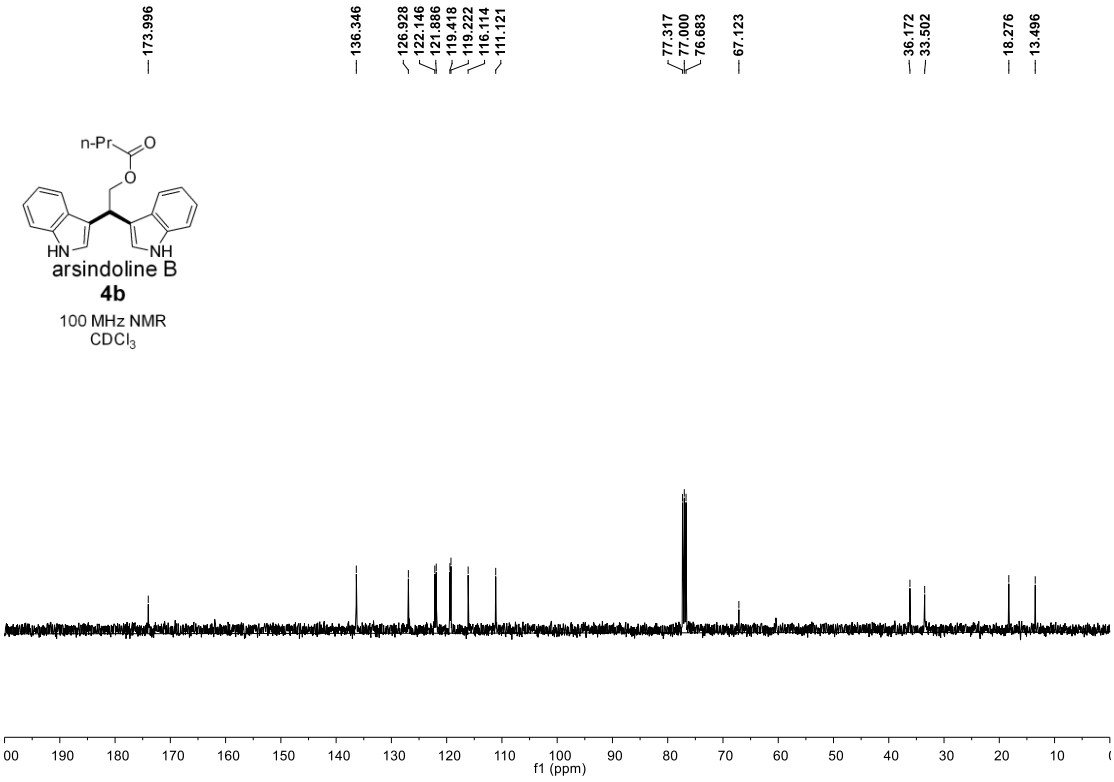


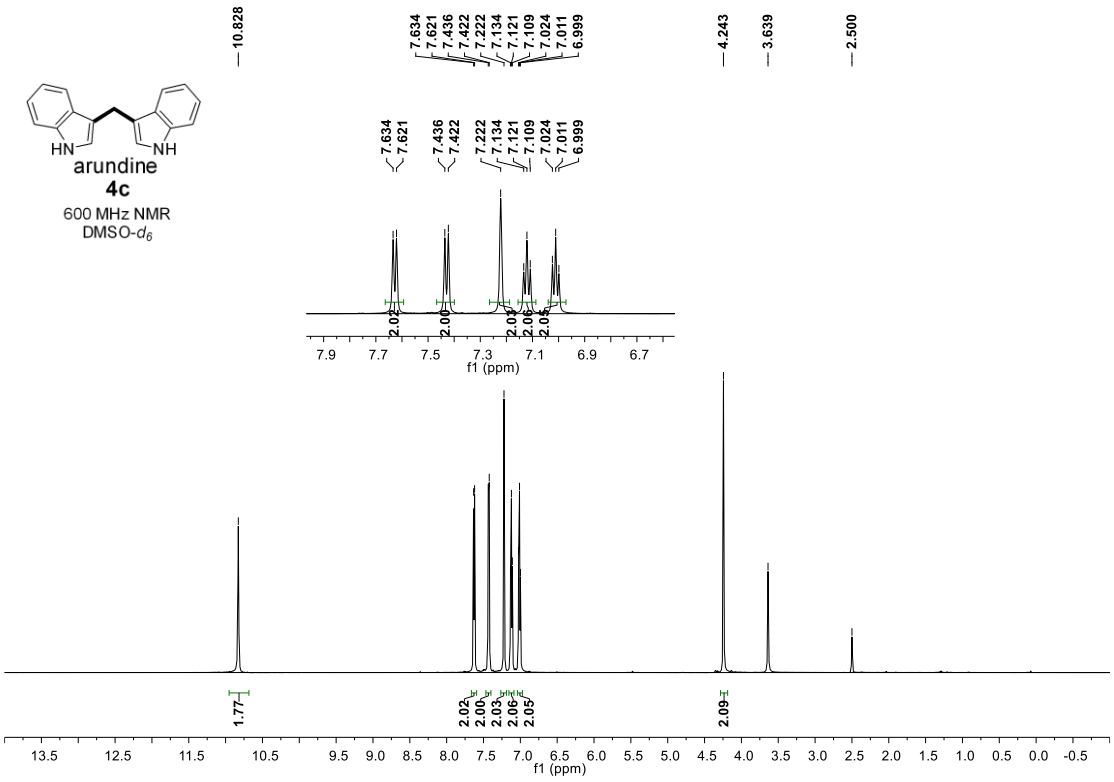
arsindoline B

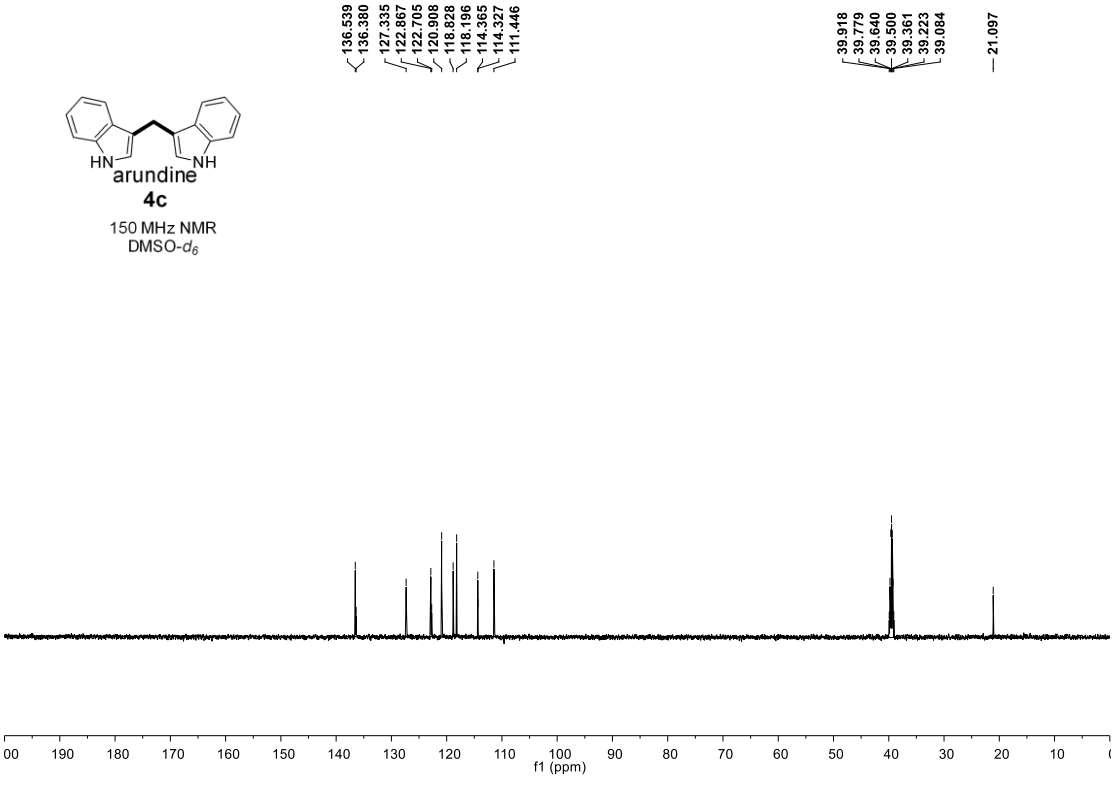
4b

100 MHz NMR

$CDCl_3$




10.828
7.634
7.621
7.436
7.422
7.222
7.134
7.121
7.109
7.024
7.011
6.999
4.243
3.639
2.500
HN
NH
arundine
4c
600 MHz NMR
DMSO-d_6
1.77
2.02
2.00
2.03
2.06
2.05
2.09
f1 (ppm)


136.539
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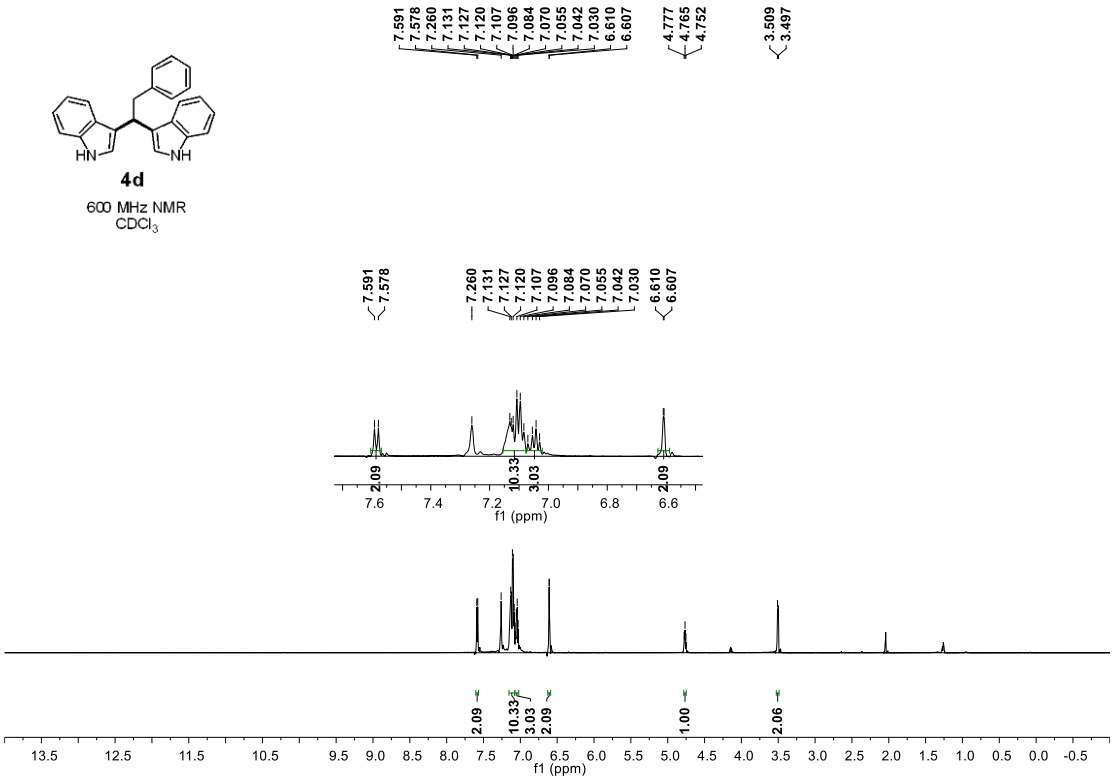
127.335
122.867
122.705
120.908
118.828
118.196
114.365
114.327
111.446
39.918
39.779
39.640
39.500
39.361
39.223
39.084
21.097
HN
NH
arundine
4c
150 MHz NMR
DMSO-d_6
f1 (ppm)

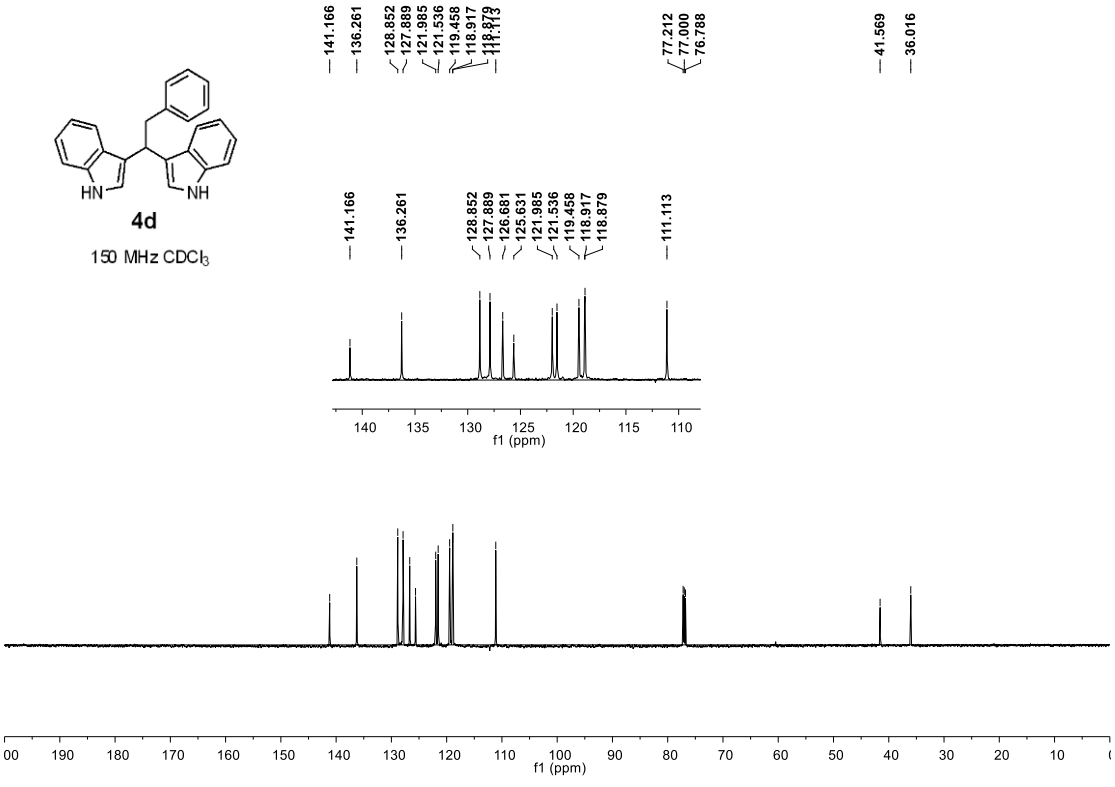
4d

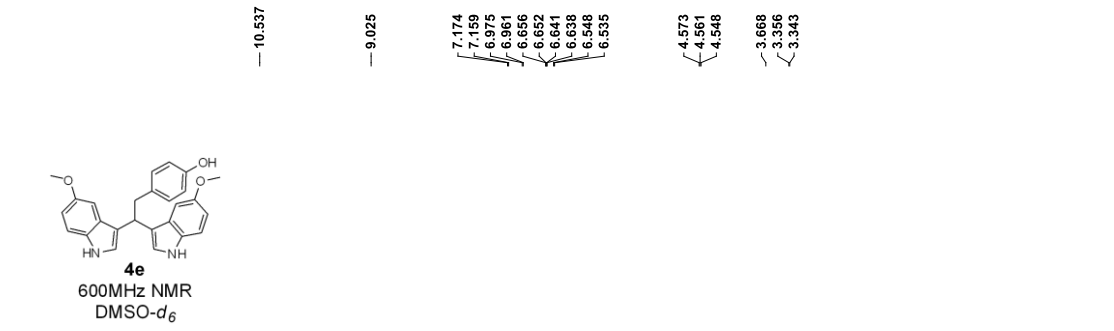
600 MHz NMR
$CDCl_3$



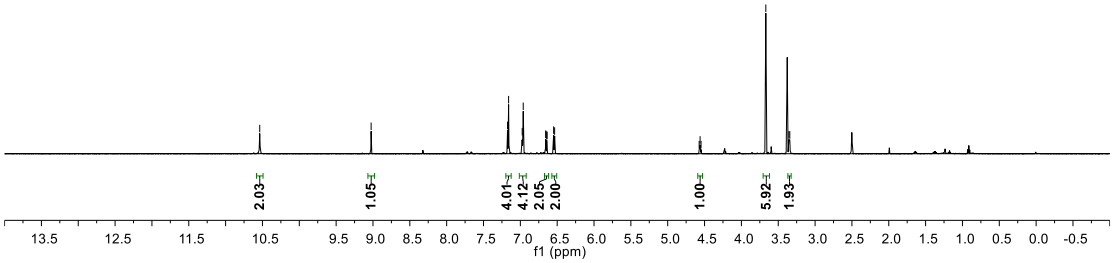
4d

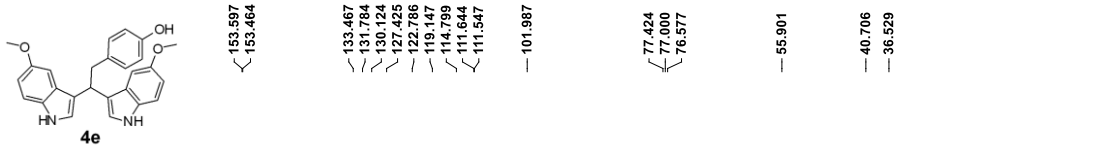
150 MHz $CDCl_3$



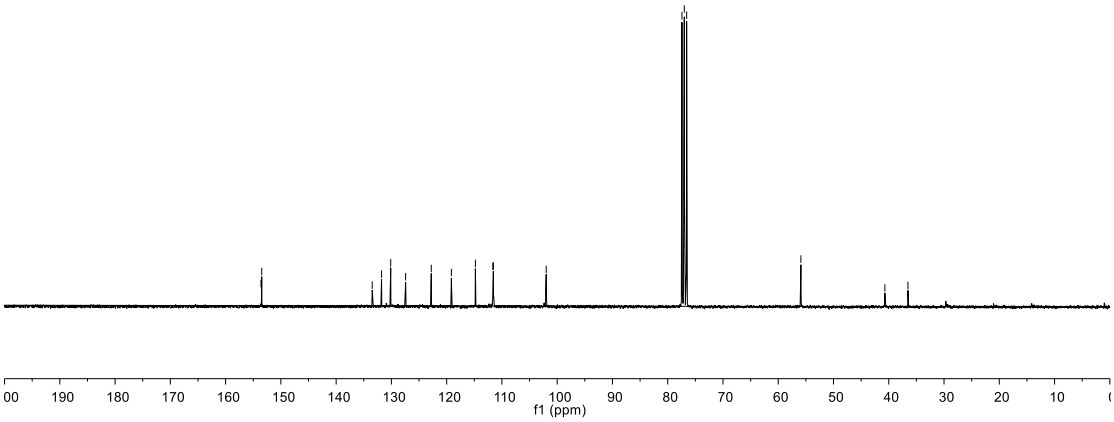


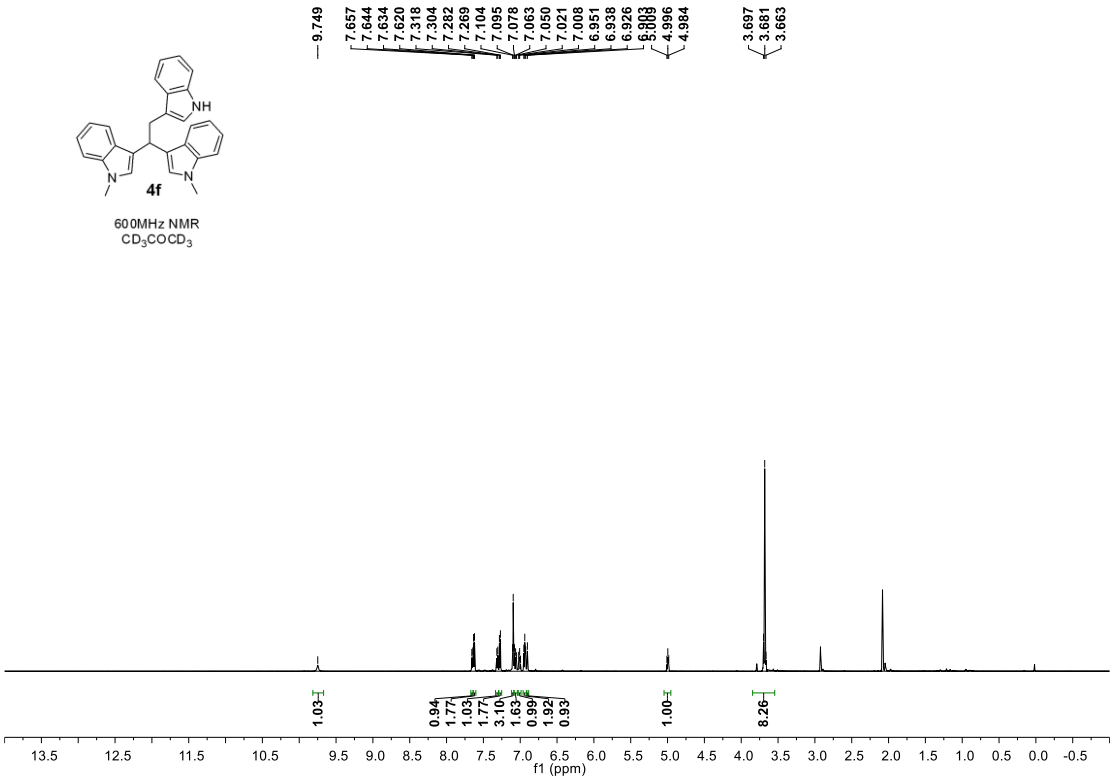
4e
600MHz NMR
DMSO-d_6

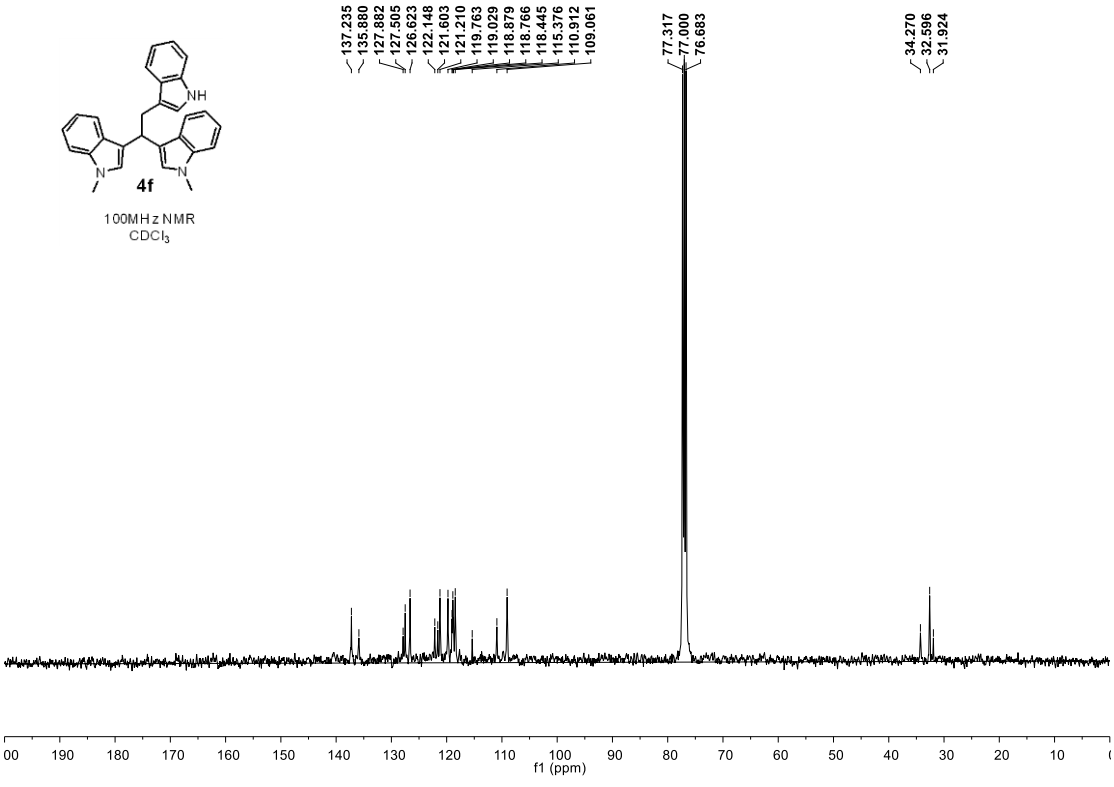




4e
75MHz NMR
CDCl3

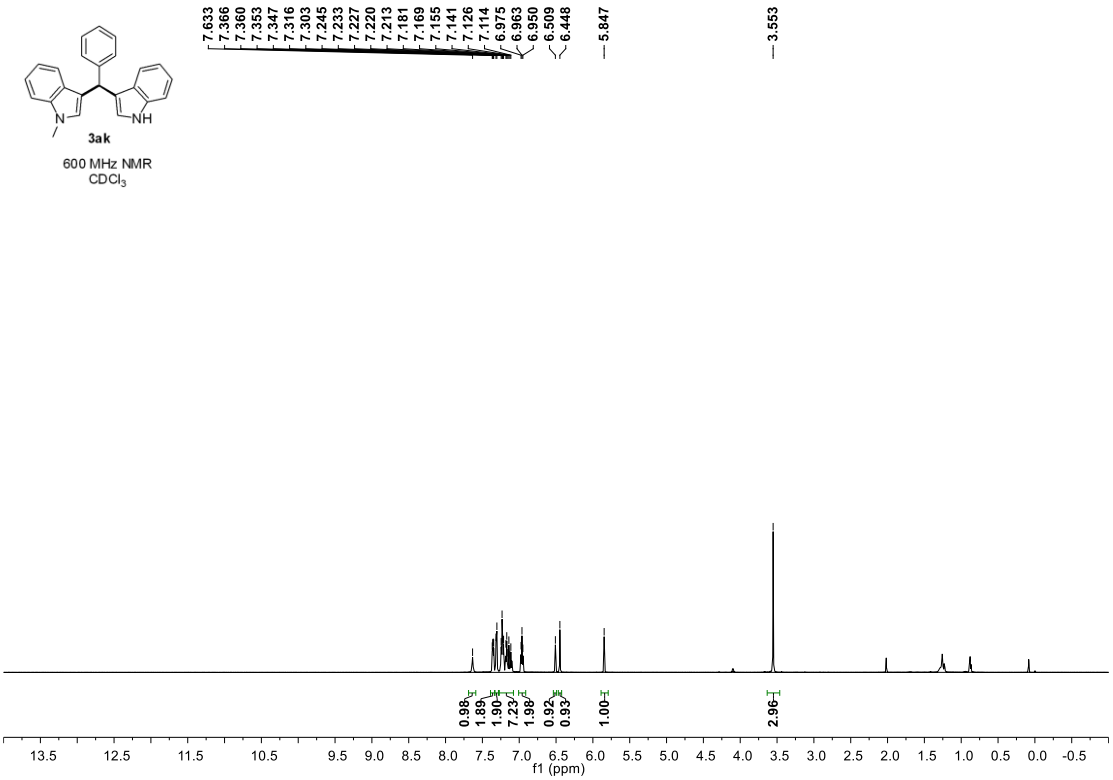



9.749
7.657
7.644
7.634
7.620
7.318
7.304
7.282
7.269
7.104
7.095
7.078
7.063
7.050
7.021
7.008
6.951
6.938
6.926
6.903
5.009
4.996
4.984
3.697
3.681
3.663
4f
600MHz NMR
CD3COCD3
1.03
0.94
1.77
1.03
1.77
3.10
1.63
0.99
1.92
0.93
1.00
8.26
f1 (ppm)


137.235
135.880
127.882
127.505
126.623
122.148
121.603
121.210
119.763
119.029
118.879
118.766
118.445
115.376
110.912
109.061
77.317
77.000
76.683
34.270
32.596
31.924
4f
100MHz NMR
CDCl3
f1 (ppm)

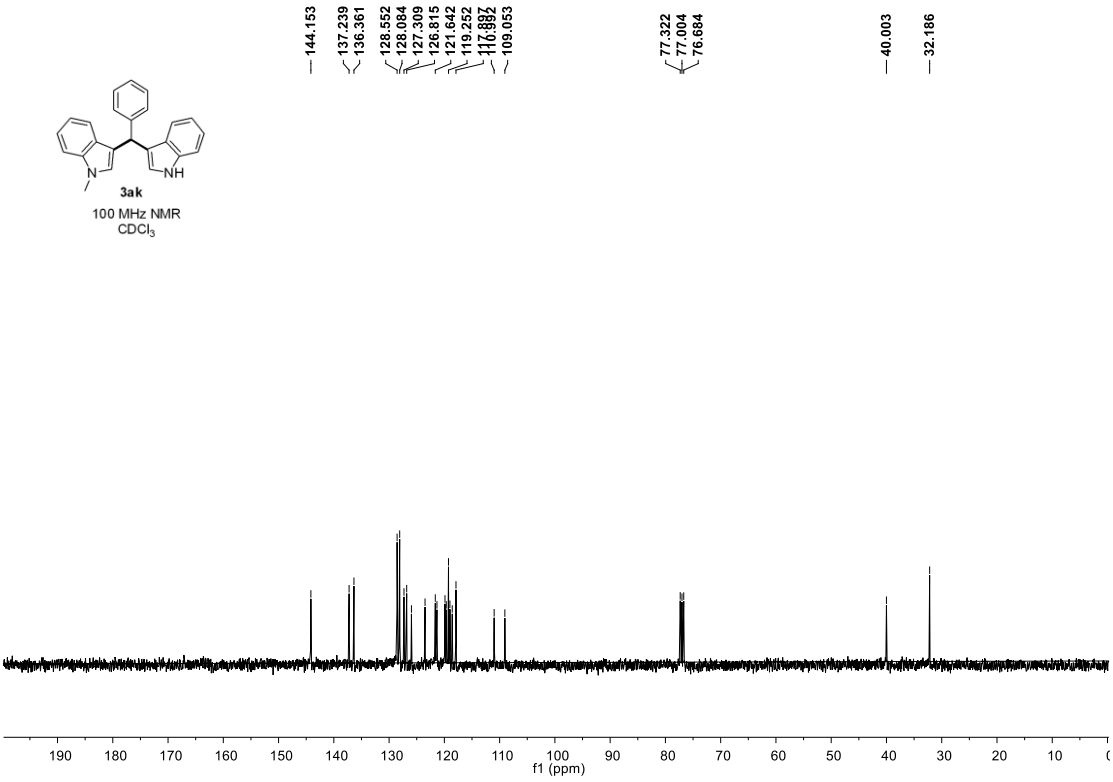
3ak

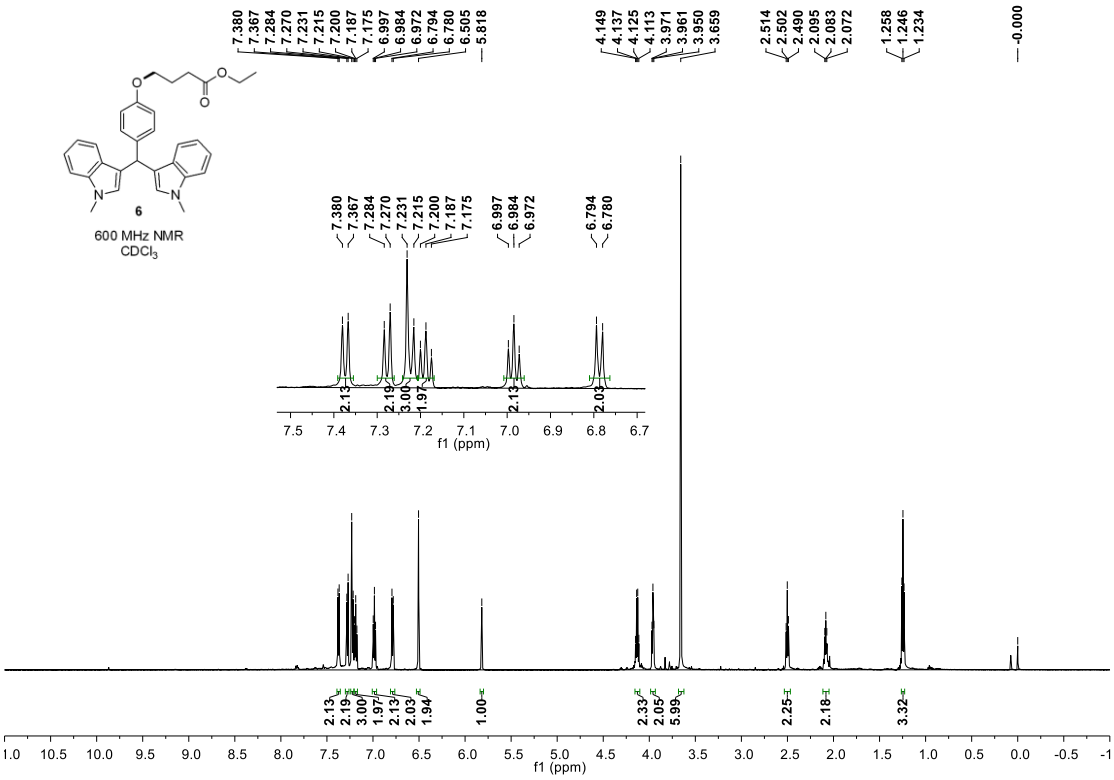
600 MHz NMR
$CDCl_3$

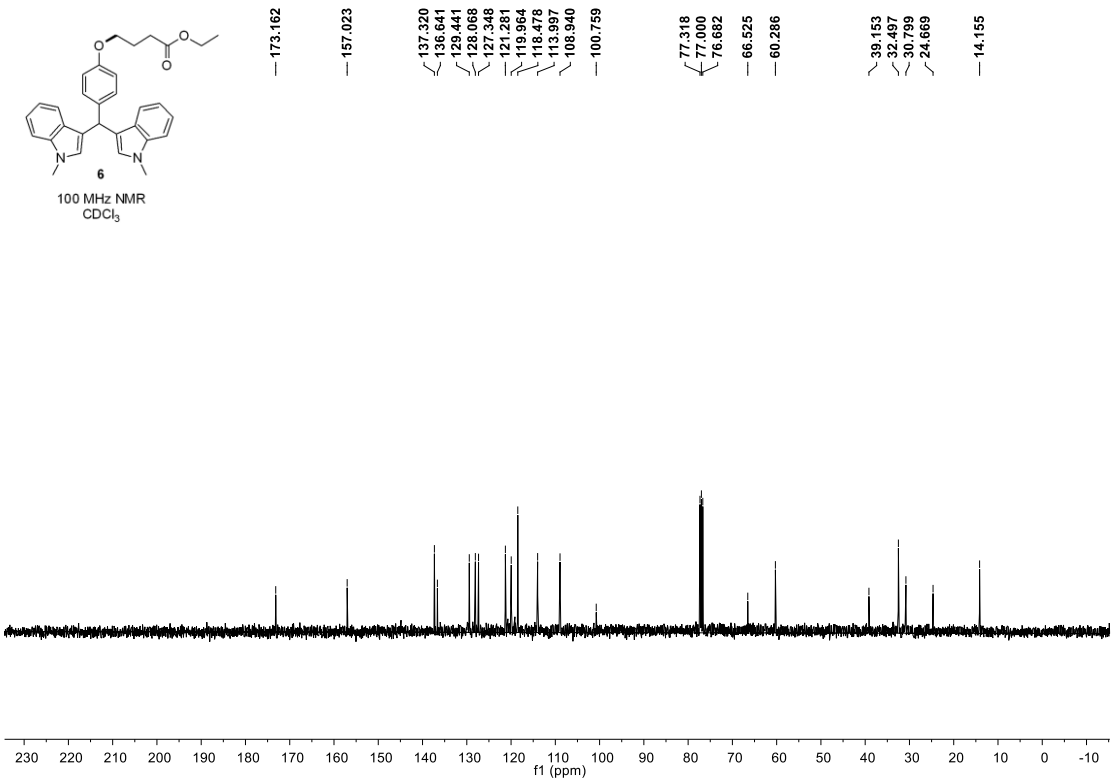


3ak

100 MHz NMR
$CDCl_3$




7.380
7.367
7.284
7.270
7.231
7.215
7.200
7.187
7.175
6.997
6.984
6.972
6.794
6.780
6.505
5.818
4.149
4.137
4.125
4.113
3.971
3.961
3.950
3.659
2.514
2.502
2.490
2.095
2.083
2.072
1.258
1.246
1.234
-0.000
6
600 MHz NMR
CDCl3
2.13
2.19
3.00
1.97
2.13
2.03
1.94
1.00
2.33
2.05
5.99
2.25
2.18
3.32
f1 (ppm)


173.162
157.023
137.320
136.641
129.441
128.068
127.348
121.281
119.964
118.478
113.997
108.940
100.759
77.318
77.000
76.682
66.525
60.286
39.153
32.497
30.799
24.669
14.155
6
100 MHz NMR
CDCl3
f1 (ppm)

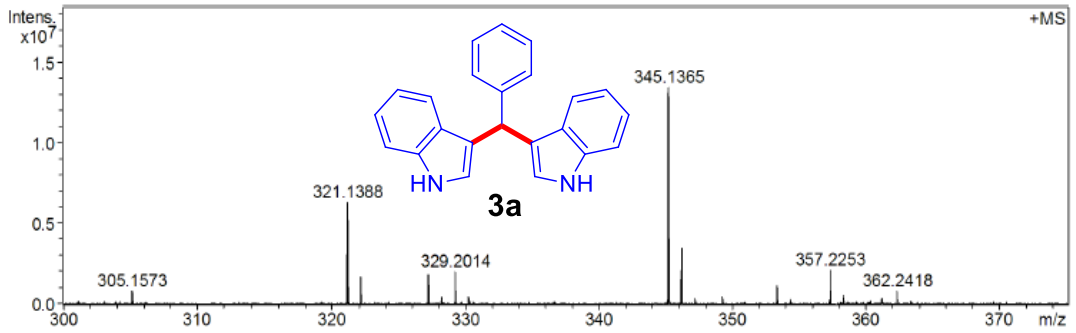
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc520_000002.d	Acquisition Date	2014-7-2 17:03:20
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	1310972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
345.1365	1	C 23 H 18 N 2 Na	345.1362	-0.8	-0.7	15.5	ok	even	3.81	0.0054	0.0003	0.0024	0.0003	0.8427

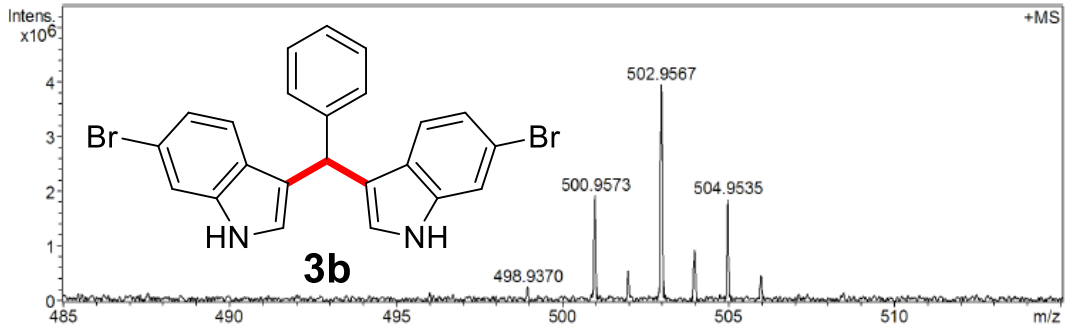
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc513_000002.d	Acquisition Date	2014-7-2 17:04:27
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
500.9573	1	C 23 H 16 Br 2 N 2 Na	500.9572	-0.2	-0.7	15.5	ok	even	18.27	0.0170	0.0011	0.0059	0.0018	0.8427

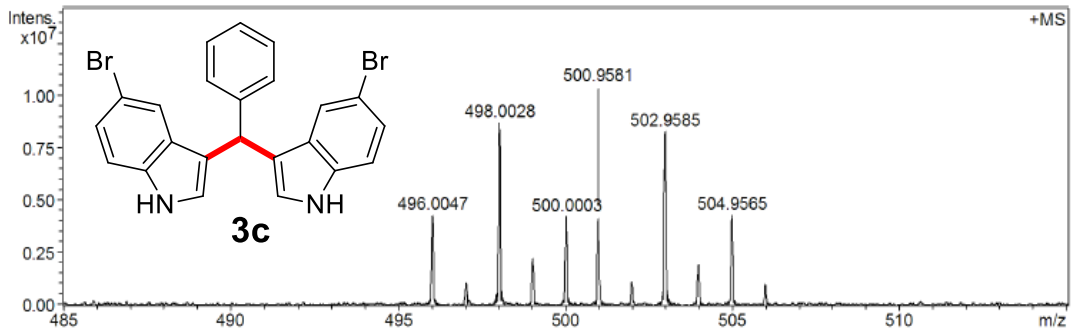
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc518_000002.d	Acquisition Date	2014-7-2 17:05:12
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
500.9581	1	C 23 H 16 Br 2 N 2 Na	500.9572	-1.6	-5.2	15.5	ok	even	9.75	0.0103	0.0028	0.0045	0.0012	0.8427

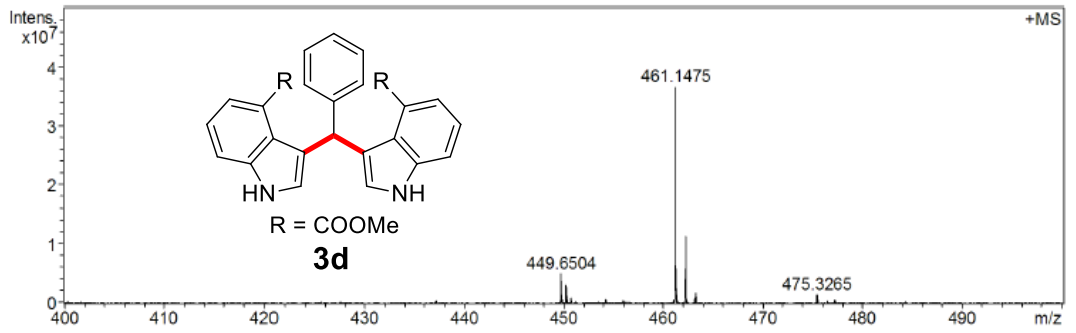
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc534_000002.d	Acquisition Date	2014-7-2 17:07:41
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
461.1475	1	C 27 H 22 N 2 Na O 4	461.1472	-0.7	-0.7	17.5	ok	even	5.19	0.0074	0.0004	0.0031	0.0001	0.8427

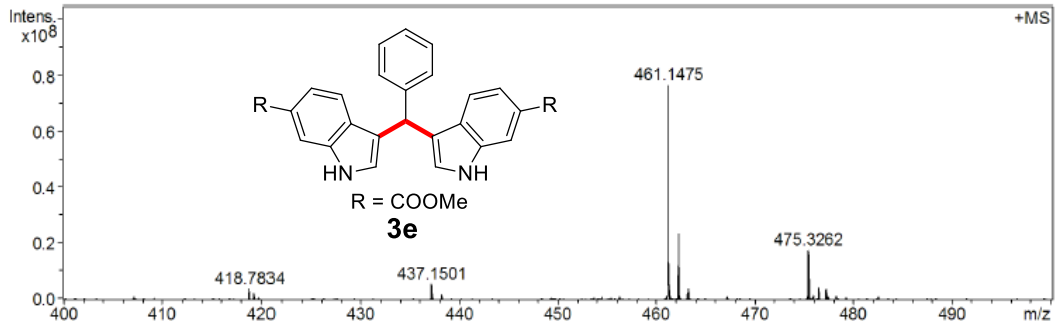
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc535_000002.d	Acquisition Date	2014-7-2 17:08:27
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
461.1475	1	C 27 H 22 N 2 Na O 4	461.1472	-0.7	-0.6	17.5	ok	even	3.20	0.0047	0.0003	0.0017	0.0003	0.8427

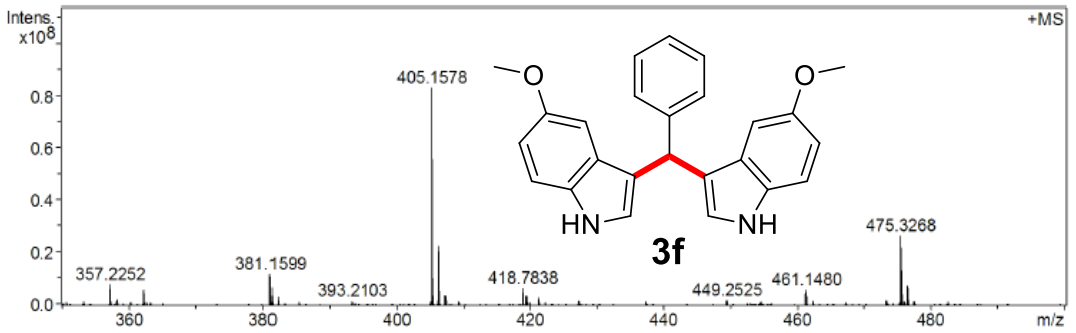
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc564_000002.d	Acquisition Date	2014-7-2 17:09:15
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
405.1578	1	C 25 H 22 N 2 Na O 2	405.1573	-1.1	-1.0	15.5	ok	even	2.45	0.0034	0.0004	0.0016	0.0001	0.8427

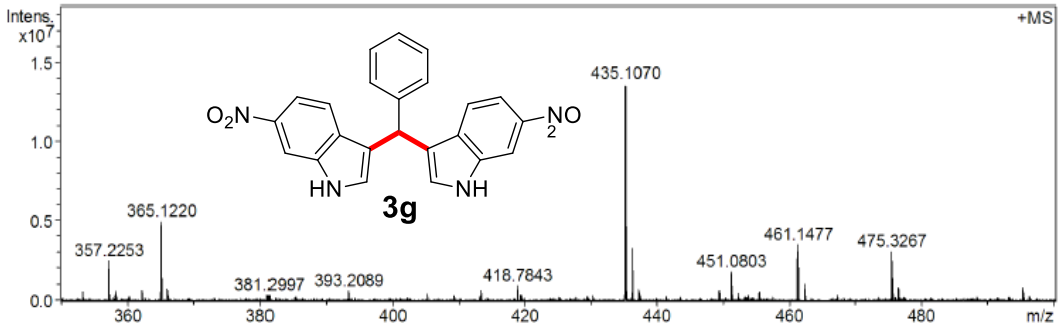
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc533_000002.d	Acquisition Date	2014-7-2 17:10:09
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2810972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
435.1070	1	C 23 H 16 N 4 Na O 4	435.1064	-1.5	-1.6	17.5	ok	even	12.84	0.0169	0.0007	0.0098	0.0003	0.8427

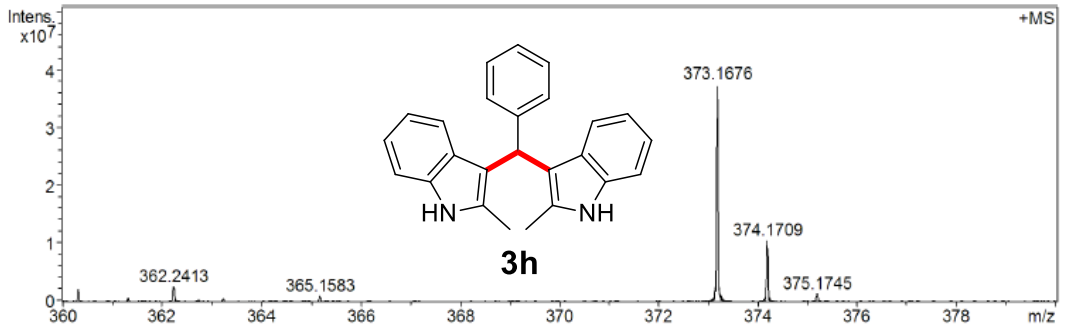
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc519_000002.d	Acquisition Date	2014-7-2 17:11:05
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
373.1676	1	C 25 H 22 N 2 Na	373.1675	-0.2	-0.2	15.5	ok	even	1.79	0.0025	0.0001	0.0011	0.0000	0.8427

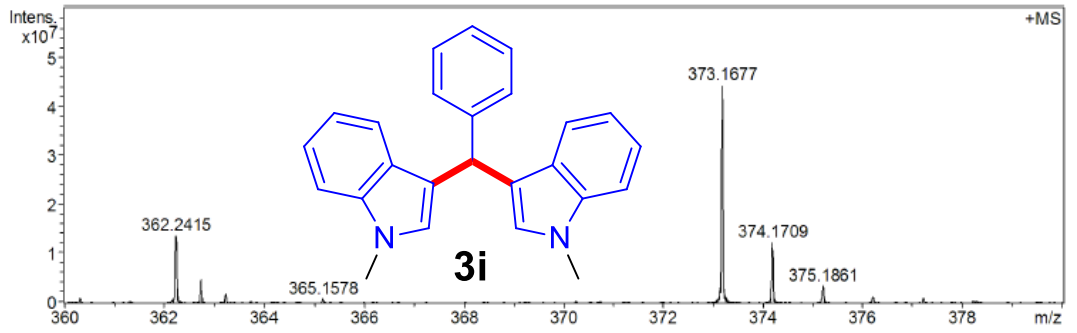
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc508_000002.d	Acquisition Date	2014-7-2 17:11:55
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010172
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
373.1677	1	C 25 H 22 N 2 Na	373.1675	-0.4	-2.2	15.5	ok	even	24.10	0.0385	0.0029	0.0255	0.0001	0.8427

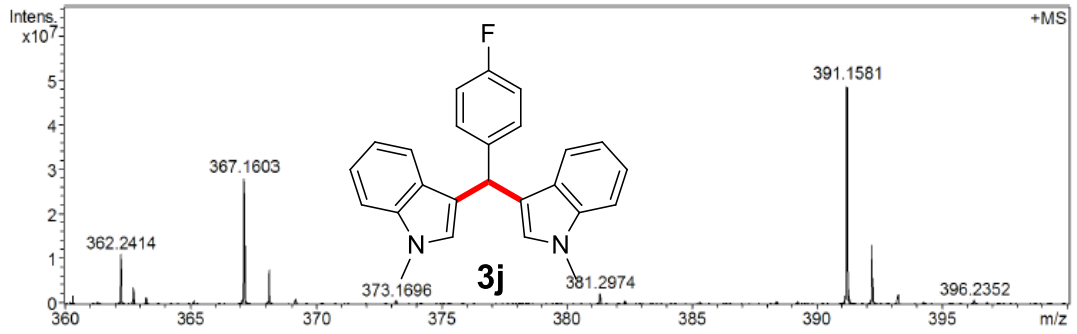
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc522_000002.d	Acquisition Date	2014-7-2 17:12:46
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	1M 972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	ej¥ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
391.1581	1	C 25 H 21 F N 2 Na	391.1581	0.1	0.1	15.5	ok	even	4.40	0.0074	0.0001	0.0034	0.0001	0.8427

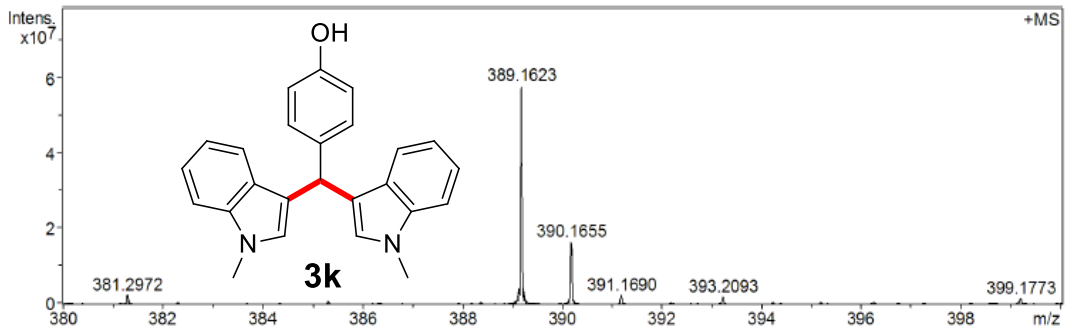
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc523_000002.d	Acquisition Date	2014-7-2 17:13:57
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2M 1072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
389.1623	1	C 25 H 22 N 2 Na O	389.1624	0.3	0.4	15.5	ok	even	4.55	0.0071	0.0002	0.0031	0.0001	0.8427

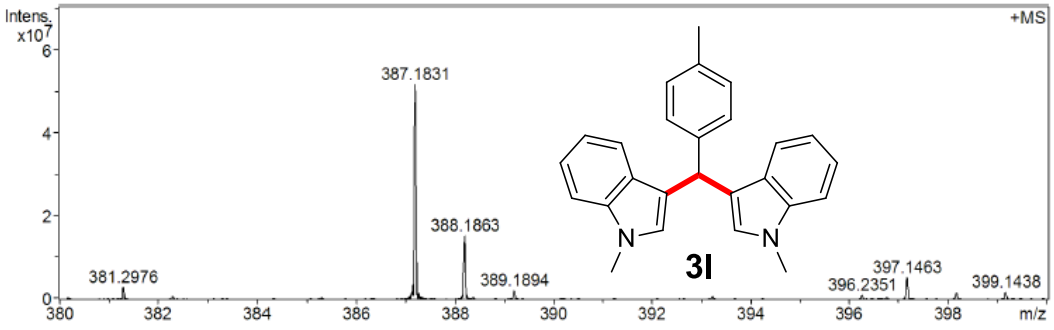
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc525_000002.d	Acquisition Date	2014-7-2 17:15:08
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	ej¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
387.1831	1	C 26 H 24 N 2 Na	387.1832	0.2	0.3	15.5	ok	even	3.95	0.0052	0.0001	0.0025	0.0001	0.8427

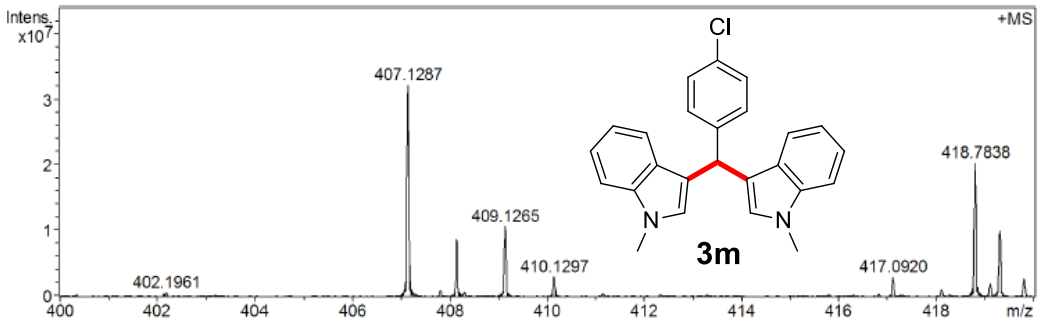
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc526_000002.d	Acquisition Date	2014-7-2 17:16:24
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	1M 972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
407.1287	1	C 25 H 21 Cl N 2 Na	407.1285	-0.4	-0.8	15.5	ok	even	12.34	0.0158	0.0004	0.0050	0.0004	0.8427

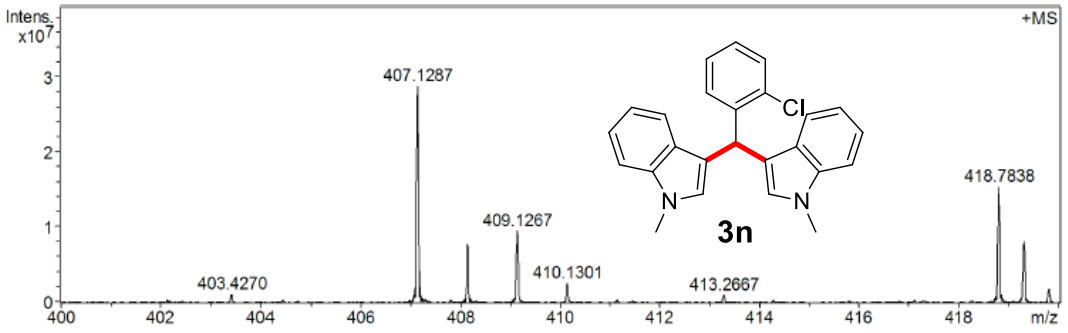
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc531_000002.d	Acquisition Date	2014-7-2 17:17:21
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
407.1287	1	C 25 H 21 Cl N 2 Na	407.1285	-0.3	-0.8	15.5	ok	even	11.76	0.0158	0.0005	0.0047	0.0006	0.8427

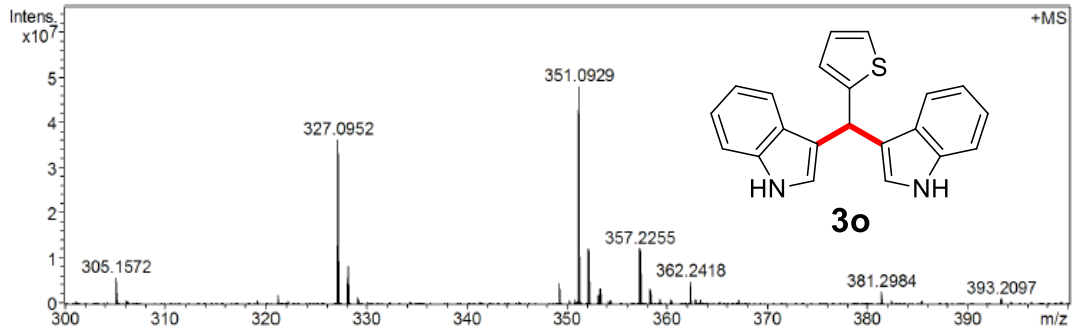
Mass Spectrum SmartFormula Report

Analysis Info

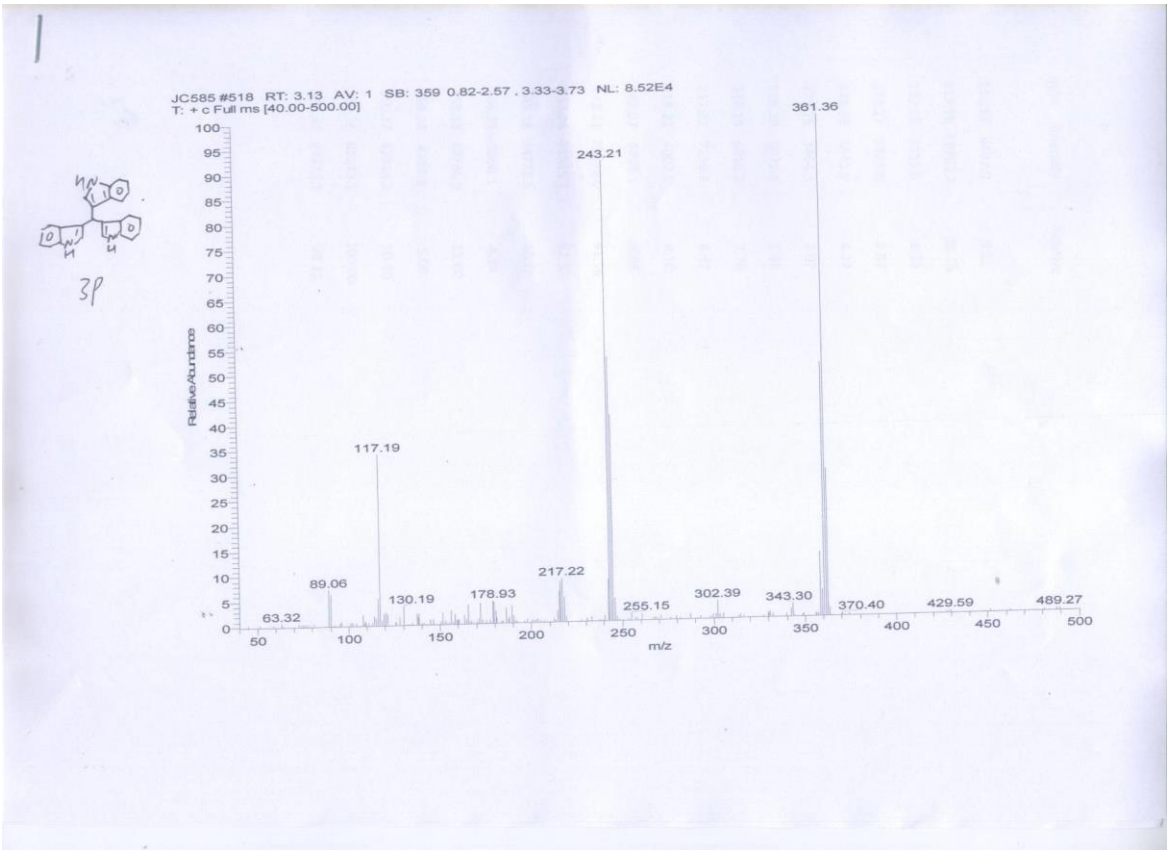
Analysis Name	H:\20140702-1\JC\jc524_000002.d	Acquisition Date	2014-7-2 17:05:57
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	201972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
351.0929	1	C 21 H 16 N 2 Na S	351.0926	-0.8	-0.6	14.5	ok	even	17.51	0.0307	0.0003	0.0141	0.0004	0.8427


JC585 #518 RT: 3.13 AV: 1 SB: 359 0.82-2.57 , 3.33-3.73 NL: 8.52E4
T: + c Full ms [40.00-500.00]
361.36
243.21
117.19
89.06
217.22
130.19
178.93
255.15
302.39
343.30
370.40
429.59
489.27
63.32
Relative Abundance
m/z
3p

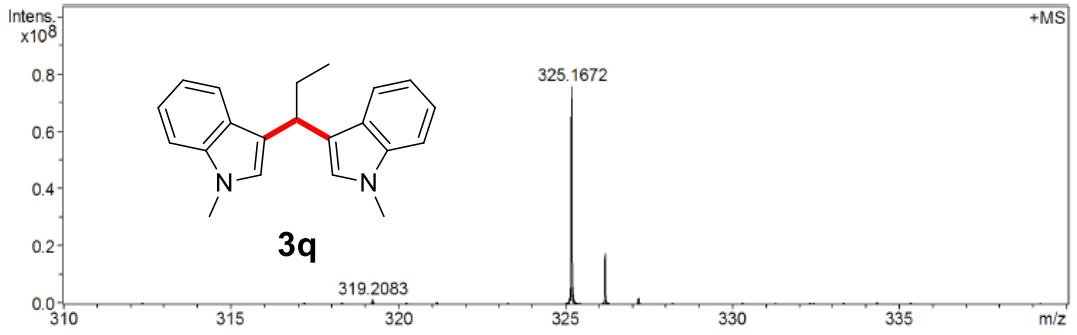
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc539_000002.d	Acquisition Date	2014-7-2 17:45:35
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	1310720
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
325.1672	1	C 21 H 22 N 2 Na	325.1675	1.0	1.0	11.5	ok	even	1.85	0.0034	0.0003	0.0016	0.0000	0.8427

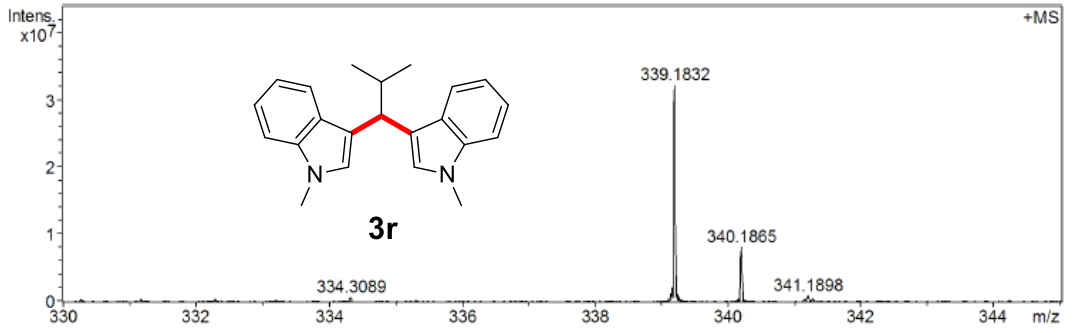
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc540_000002.d	Acquisition Date	2014-7-2 17:46:34
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
339.1832	1	C 22 H 24 N 2 Na	339.1832	-0.1	-0.1	11.5	ok	even	4.22	0.0062	0.0000	0.0027	0.0000	0.8427

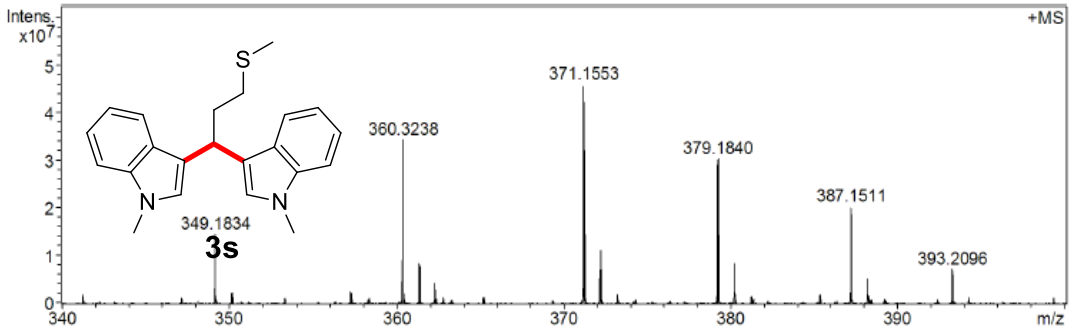
Mass Spectrum SmartFormula Report

Analysis Info

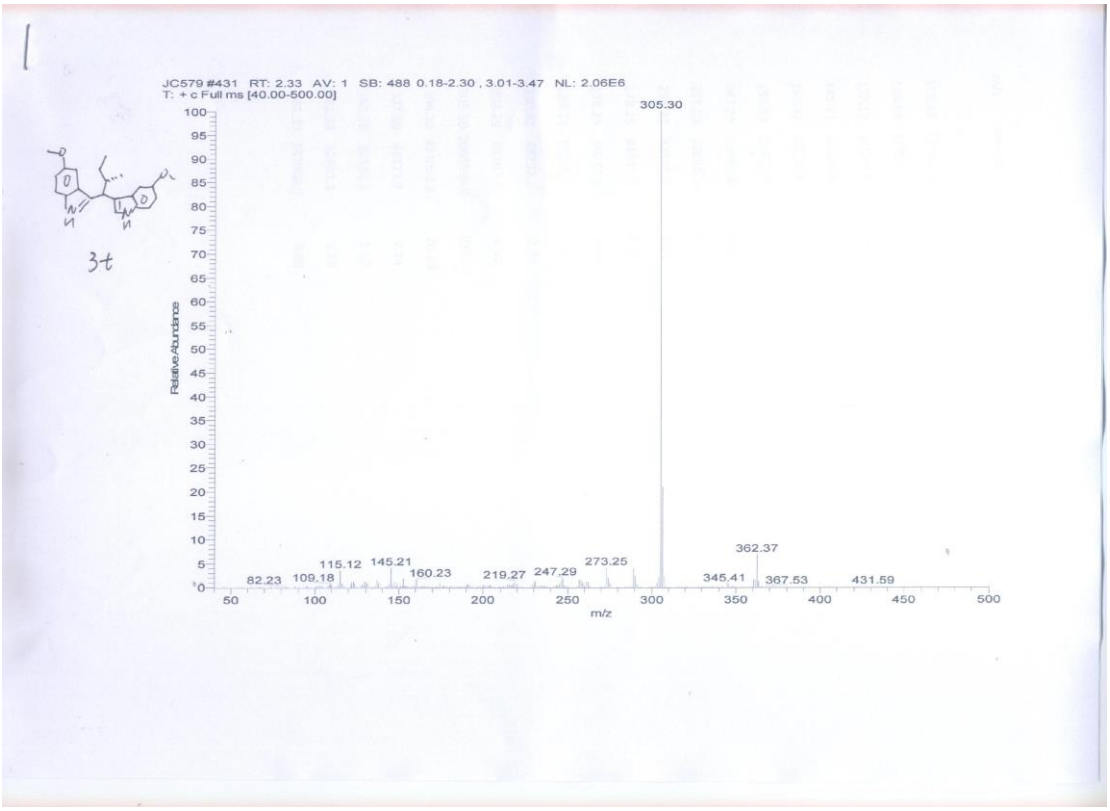
Analysis Name	H:\20140702-1\JC\jc541_000002.d	Acquisition Date	2014-7-2 17:47:25
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2810972
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
371.1553	1	C 22 H 24 N 2 Na S	371.1552	-0.1	-0.2	11.5	ok	even	17.03	0.0338	0.0003	0.0139	0.0010	0.8427


JC579 #431 RT: 2.33 AV: 1 SB: 488 0.18-2.30 , 3.01-3.47 NL: 2.06E6
T: + c Full ms [40.00-500.00]
3t
Relative Abundance
m/z
305.30
362.37
115.12
145.21
160.23
82.23
109.18
219.27
247.29
273.25
345.41
367.53
431.59

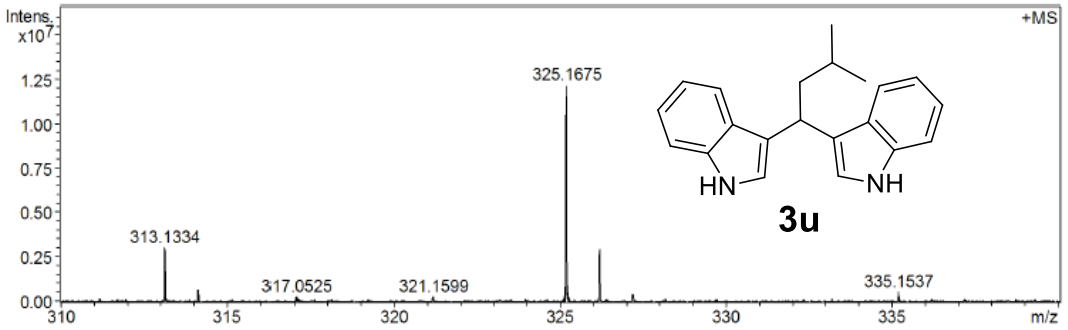
Mass Spectrum SmartFormula Report

Analysis Info

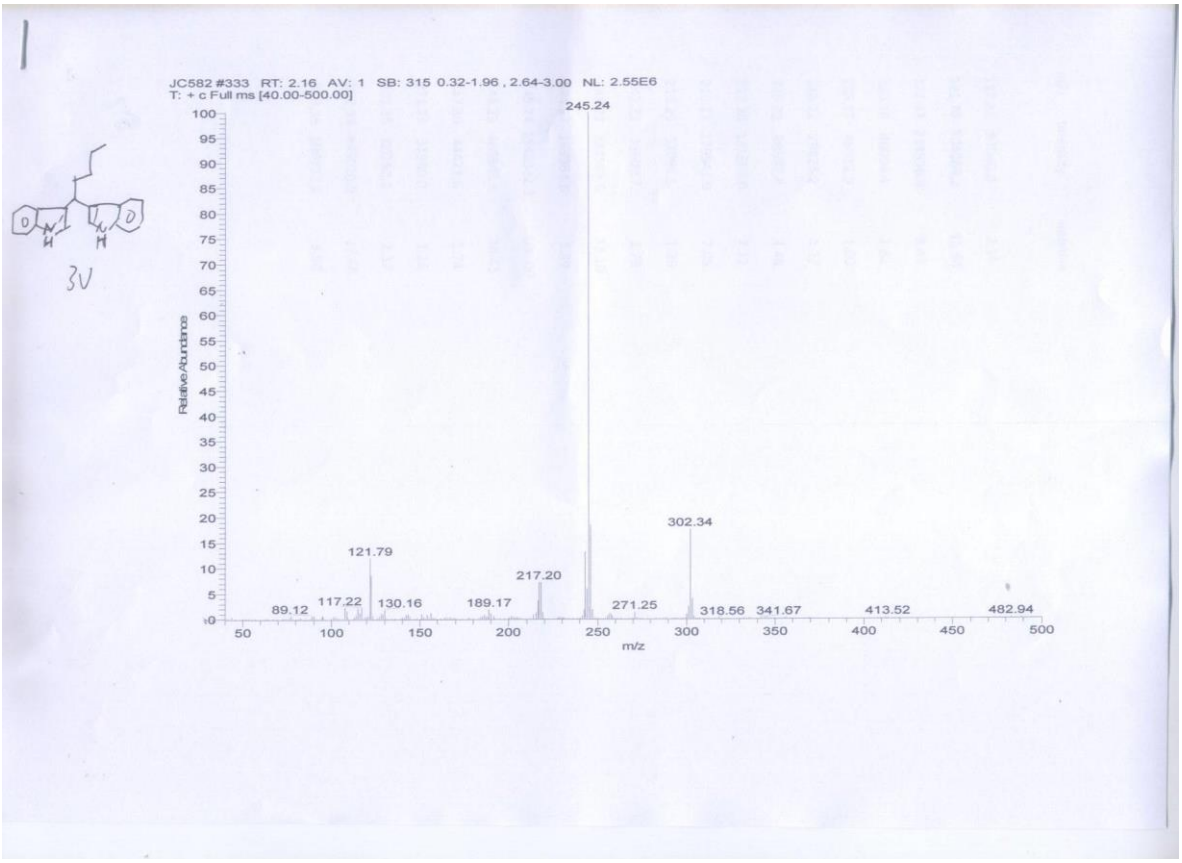
Analysis Name	H:\20140702-1\JC\jc550_000002.d	Acquisition Date	2014-7-2 17:51:30
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
325.1675	1	C 21 H 22 N 2 Na	325.1675	0.1	2.0	11.5	ok	even	9.15	0.0169	0.0036	0.0081	0.0000	0.8427


JC582 #333 RT: 2.16 AV: 1 SB: 315 0.32-1.96 , 2.64-3.00 NL: 2.55E6
T: + c Full ms [40.00-500.00]
245.24
302.34
121.79
217.20
89.12
117.22
130.16
189.17
271.25
318.56
341.67
413.52
482.94
Relative Abundance
m/z
3V

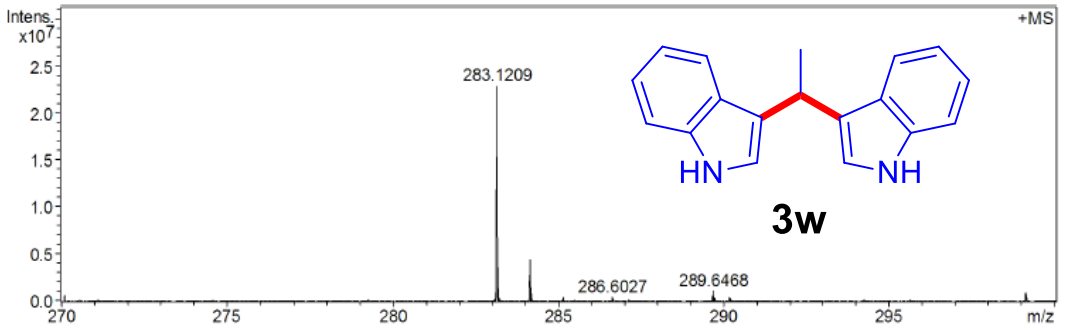
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc550-2_000002.d	Acquisition Date	2014-7-2 17:53:02
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	ej¥ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
283.1209	1	C 18 H 16 N 2 Na	283.1206	-1.3	-1.5	11.5	ok	even	4.50	0.0086	0.0004	0.0036	0.0002	0.8427

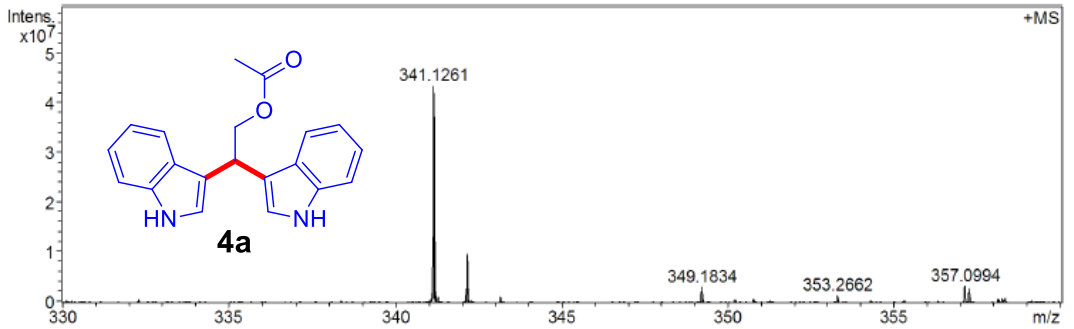
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc559_000002.d	Acquisition Date	2014-7-2 17:53:55
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
341.1261	1	C 20 H 18 N 2 Na O 2	341.1260	-0.2	-0.1	12.5	ok	even	2.33	0.0045	0.0001	0.0026	0.0000	0.8427

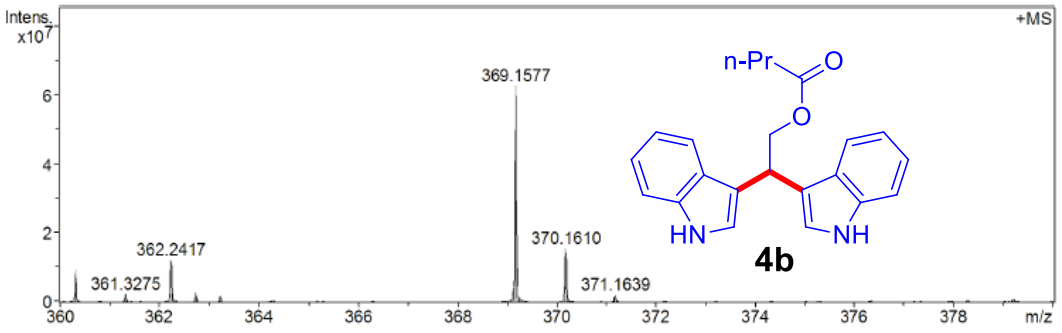
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc580_000002.d	Acquisition Date	2014-7-2 17:54:43
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010072
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
369.1577	1	C 22 H 22 N 2 Na O 2	369.1573	-0.9	-0.9	12.5	ok	even	0.82	0.0011	0.0003	0.0005	0.0000	0.8427

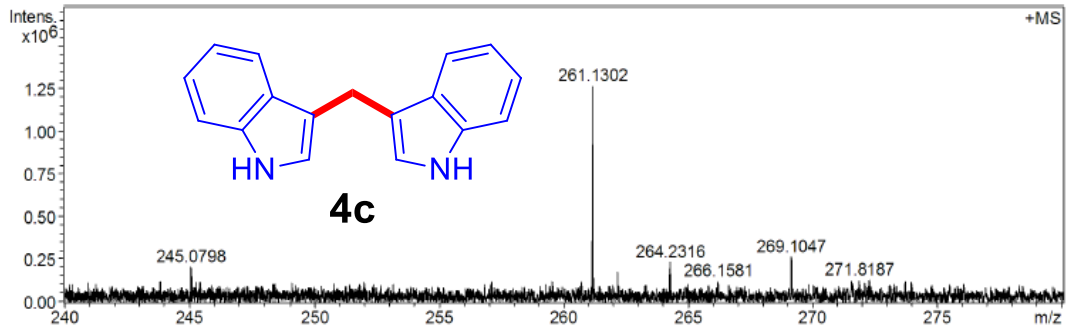
Mass Spectrum SmartFormula Report

Analysis Info

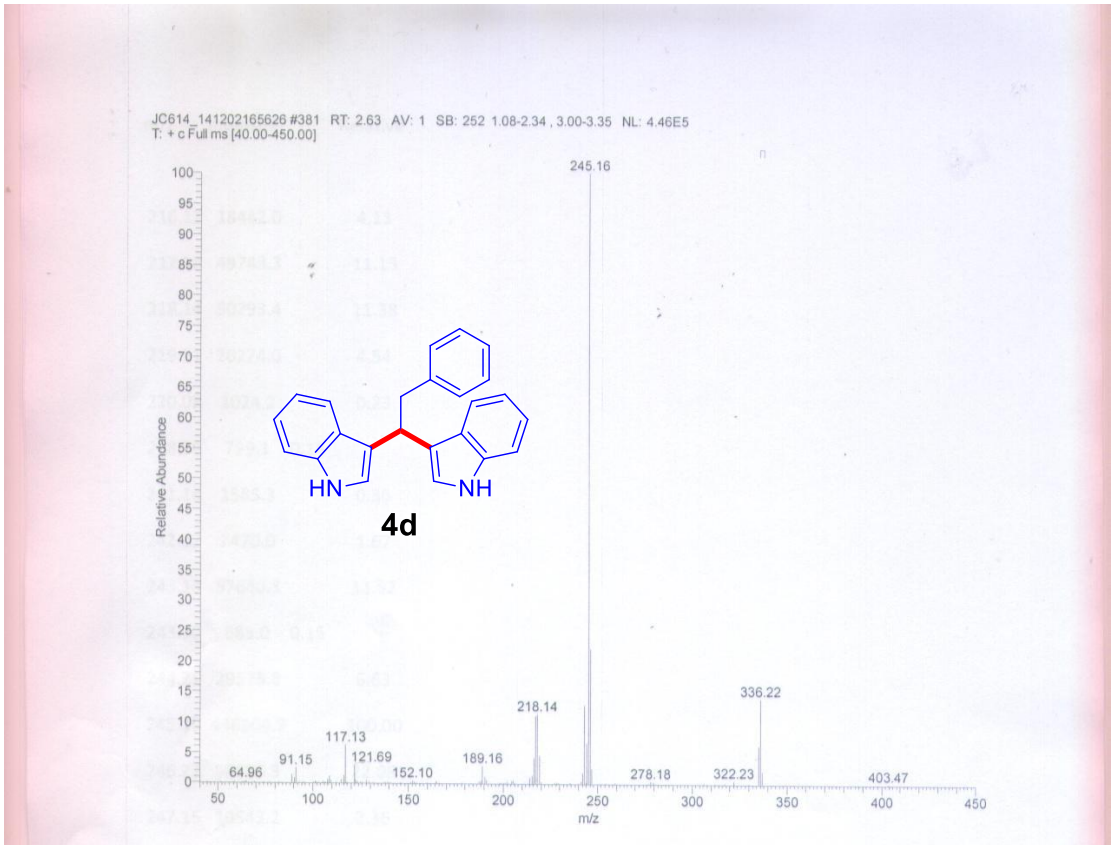
Analysis Name	H:\20140702-1\JC\jc551_000003.d	Acquisition Date	2014-7-2 17:48:59
Method	Student_LCms-140618		
Sample Name	Student_4-6	Operator	
Comment		Instrument	apex-Ultra

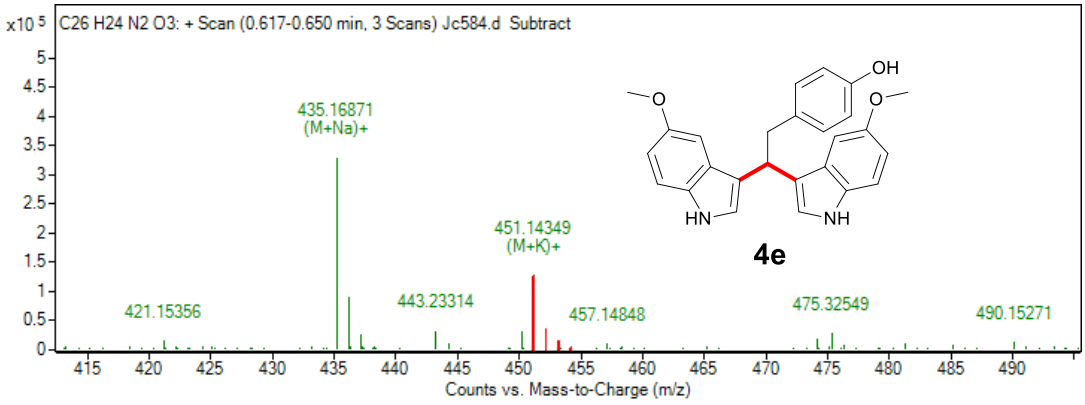
Acquisition Parameter

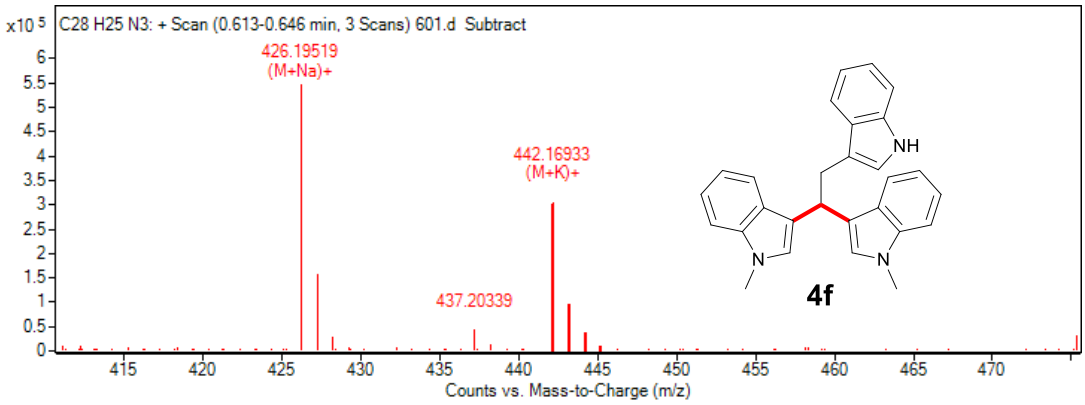
Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2010172
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
269.1047	1	C 17 H 14 N 2 Na	269.1049	0.6	0.6	11.5	ok	even	110.87	0.1920	0.0002	0.0910	0.0002	0.8427




x10 5
C26 H24 N2 O3: + Scan (0.617-0.650 min, 3 Scans) Jc584.d Subtract
435.16871
(M+Na)+
451.14349
(M+K)+
421.15356
443.23314
457.14848
475.32549
490.15271
OH
O
O
HN
NH
4e
Counts vs. Mass-to-Charge (m/z)


x10 5
C28 H25 N3: + Scan (0.613-0.646 min, 3 Scans) 601.d Subtract
426.19519
(M+Na)+
442.16933
(M+K)+
437.20339
NH
N
N
4f
Counts vs. Mass-to-Charge (m/z)

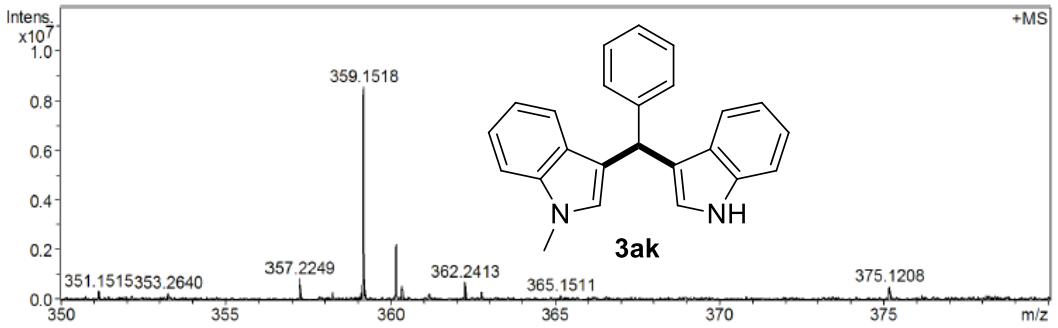
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc560_000003.d	Acquisition Date	2014-7-2 17:58:08
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2M
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
359.1518	1	C 24 H 20 N 2 Na	359.1519	0.2	0.3	15.5	ok	even	4.93	0.0086	0.0002	0.0040	0.0001	0.8427

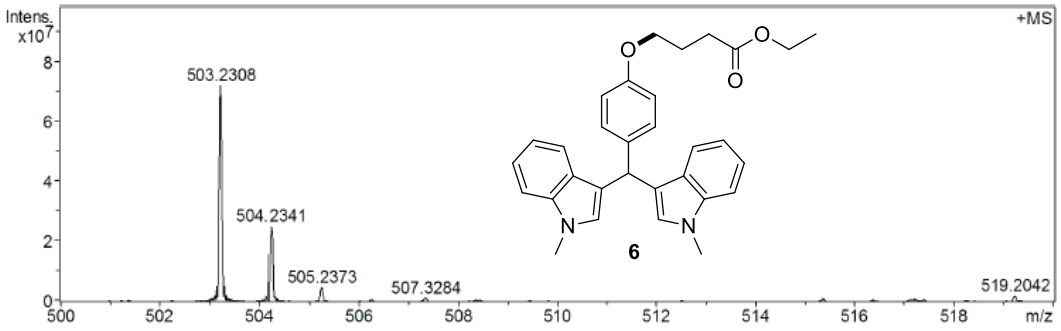
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	H:\20140702-1\JC\jc581_000002.d	Acquisition Date	2014-7-2 17:56:46
Method	Student_LCms-140618	Operator	
Sample Name	Student_4-6	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	2	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1200.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Jun 18 07:18:23
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	2[illegible]72
Ion Accumulation Time	0.1 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
503.2308														
	1	C 31 H 32 N 2 Na O 3	503.2305	-0.6	-0.5	16.5	ok	even	1.25	0.0020	0.0003	0.0009	0.0002	0.8427