Supporting Information

Palladium catalyzed dual C-H functionalization of indoles with cyclic diaryliodoniums, an approach to ring fused carbazole derivatives

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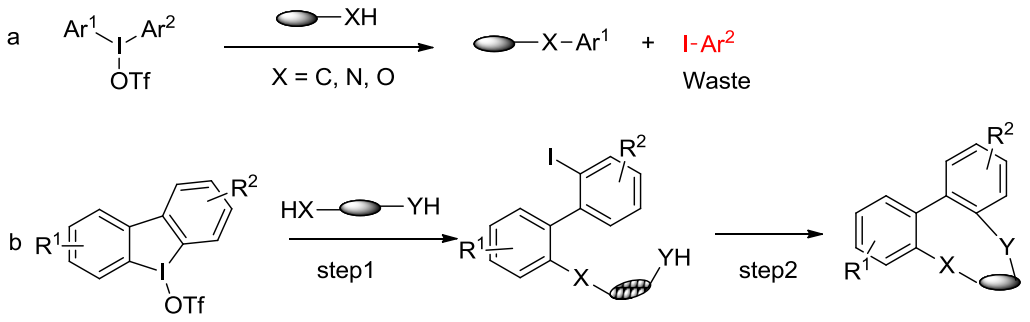
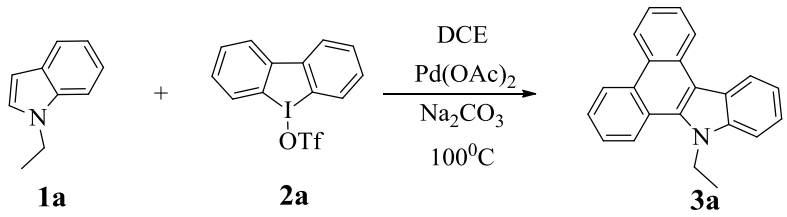


Scheme S1. Arylation with linear and cyclic diaryl iodoniums

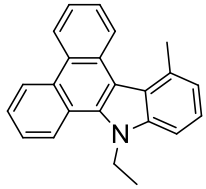
General information

All reaction under standard conditions were carried out under air and monitored by thin-layer chromatography. All the reagents, catalysts, and solvents purchased from the vendors were used without further purification unless stated otherwise. All products were purified through silica gel (200-300 mesh) column chromatography with petroleum ether (60-90℃), dichloromethane as eluent. ^{1}H and ^{13}C spectra were recorded in $CDCl_3$ on Bruker Avance 400 spectrometer. Chemical shifts are given in ppm (δ) referenced to $CDCl_3$ with 7.26 for ^{1}H and 77.16 for ^{13}C, and to DMSO-d_6 with 2.50 for ^{1}H and 39.5 for ^{13}C. Signals are abbreviated as follows: s, singlet; dd, doublet of doublets; d, doublet; t, triplet; q, quartet; m, multiplet. High resolution mass spectra were recorded in LTQ Orbitrap XL spectrometer (Thermo Fisher)

General procedure to synthesize dibenzocarbazoles from indoles and cyclic diaryliodoniums: The synthesis of **3a** was exemplified herein.

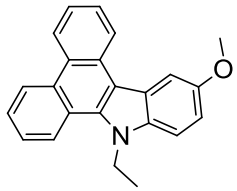


9-Ethyl-9H-dibenzo[a,c]carbazole (3a): To a stirred solution of **1a** (30 mg, 206.6 umol) in DCE was added **2a** (106.6 mg, 248 umol), $Pd(OAc)_2$ (4.64 mg, 20.6 umol) and Na_2CO_3(43.8 mg, 413.2 umol). The reaction proceeded at 100℃ for 17h before the mixture which was diluted with dichloromethane was filtered with celite. The filtrate was then concentrated by rotary evaporation and the crude product was purified by column chromatography on silica gel (PE/DCM=15/1) to afford **3a** (41 mg, 67% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 – 8.85 (m, 2H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.67 (d, *J* = 8.0 Hz, 1H), 8.53 (m, 1H), 7.78 (t, *J* = 8.0 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.61 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 4.82 (q, *J* = 7.2 Hz, 2H), 1.71 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 133.7, 131.0, 130.1, 127.3, 126.9, 126.5, 125.6, 124.2, 123.8, 123.7, 123.7, 123.6, 123.6, 123.50, 122.6, 122.0, 120.5, 113.7, 109.5, 40.9, 15.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{22}H_{18}N$, 296.1439; found, 296.1426. IR (KBr) υ: 1606, 1515, 1438, 1340, 1224, 1155, 737. MP: 143.5-144.6℃.



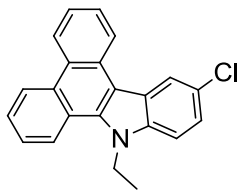
3b

9-Ethyl-13-methyl-9H-dibenzo[a,c]carbazole (3b): Obtained from **1b** and **2a** as a yellow solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 – 8.84 (m, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.67 (d, *J* = 7.2 Hz, 1H), 8.51 (m, 1H), 7.75 – 7.63 (m, 3H), 7.57 (ddd, *J* = 8.4, 7.2, 1.3 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.23 (d, *J* = 7.2 Hz, 1H), 4.84 (q, *J* = 7.2 Hz, 2H), 3.09 (s, 3H), 1.76 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1, 134.4, 131.7, 131.3, 129.2, 127.4, 127.2, 126.6, 126.0, 125.6, 124.2, 124.2, 123.7, 123.6, 123.6, 123.5, 123.3, 122.68, 115.3, 107.1, 41.4, 25.2, 15.4.HRMS (ESI) m/z: $[M]^+$ calcd for $C_{23}H_{19}N$, 309.1517; found, 309.1507. IR (KBr) υ: 3760, 3612, 3345, 2879, 1332, 1150, 952, 755. MP: 156.4-157.8℃.



3c

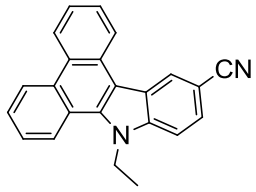
9-Ethyl-12-methoxy-9H-dibenzo[a,c]carbazole (3c): Obtained from **1c** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (m, 1H), 8.78 (t, *J* = 8.4 Hz, 2H), 8.51 (m, 1H), 8.08 (d, *J* = 2.4 Hz, 1H), 7.78 – 7.73 (m, 1H), 7.73 – 7.65 (m, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.17 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.82 (q, *J* = 7.2 Hz, 2H), 4.05 (s, 3H), 1.70 (t, *J* = 7.2 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 135.6, 134.4, 131.1, 130.3, 127.5, 126.9, 126.6, 125.7, 124.4, 124.0, 123.9, 123.6, 123.4, 122.7, 113.5, 113.3, 110.2, 105.2, 56.5, 41.3, 15.5. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{23}H_{19}NO$, 325.1467; found, 325.1458. IR (KBr) υ: 3477, 2924, 1606, 1473, 1245, 1033, 728. MP: 140.0-141.7℃.



3d

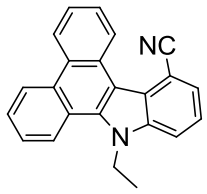
12-Chloro-9-ethyl-9H-dibenzo[a,c]carbazole (3d): Obtained from **1d** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{11}H NMR (400 MHz, $CDCl_3$) δ 8.94 – 8.82 (m, 1H), 8.77 (m, 2H), 8.59 (d, *J* = 2.0 Hz, 1H), 8.56 – 8.50 (m, 1H), 7.77 (t, *J* = 7.2Hz, 1H), 7.74 – 7.67 (m, 2H), 7.60 (t, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.46 (dd, *J* = 8.8, 2.0 Hz, 1H), 4.86 (q, *J* = 7.2 Hz, 2H), 1.72 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5, 134.5, 131.3, 129.7, 127.6, 127.0, 126.7, 126.1, 126.0, 124.6, 124.3, 124.0, 123.9, 123.6, 123.4, 122.6, 121.5, 113.1, 110.4, 41.2,

15.3.HRMS (ESI) m/z: $[M]^+$ calcd for $C_{22}H_{16}ClN$, 329.0971; found, 329.0963. IR (KBr) υ: 1606, 1515, 1464, 1427, 1300, 749. MP: 169.4-170.7℃.



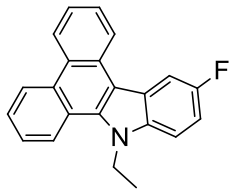
3e

9-Ethyl-9H-dibenzo[a,c]carbazole-12-carbonitrile (3e): Obtained from **1e** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (s, 2H), 8.75 (d, *J* = 8.0 Hz, 1H), 8.69 (d, *J* = 8.0 Hz, 1H), 8.47 (s, 1H), 7.81 – 7.66 (m, 4H), 7.62 (m, 2H), 4.82 (q, *J* = 6.8Hz, 2H), 1.71 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6, 131.6, 129.2, 128.0, 127.4, 127.1, 127.0, 126.7, 124.7, 124.5, 123.8, 123.6, 123.5, 123.1, 122.7, 120.9, 110.2, 103.4, 100.1, 41.4, 15.3. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{23}H_{16}N_2$, 320.1313; found, 320.1306. IR (KBr) υ: 2370, 2217, 1607, 1471, 1422, 755. MP: 223.1-224.6℃.



3f

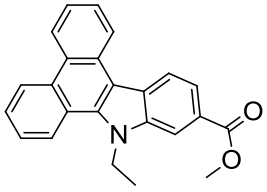
9-Ethyl-9H-dibenzo[a,c]carbazole-13-carbonitrile (3f): Obtained from **1f** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (d, *J* = 7.6 Hz, 1H), 8.87 (m, 1H), 8.75 (d, *J* = 8.4 Hz, 1H), 8.51 (m, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.85 – 7.79 (m, 2H), 7.78 – 7.69 (m, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.58 – 7.49 (t, *J* = 8.0 Hz, 1H), 4.90 (q, *J* = 7.2 Hz, 2H), 1.78 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.5, 135.9, 133.3, 132.1, 129.2, 128.3, 127.2, 127.0, 126.9, 126.8, 126.8, 124.6, 124.4, 123.3, 123.1, 123.0, 121.5, 114.3, 100.0, 99.3, 41.5, 29.7, 15.3. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{23}H_{16}N_2$, 320.1313; found, 320.1306. IR (KBr) υ: 2362, 1607, 1444, 752. MP: 220.0-221.3℃.



3g

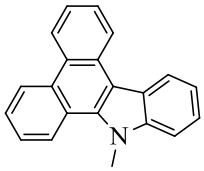
9-Ethyl-12-fluoro-9H-dibenzo[a,c]carbazole (3g): Obtained from **1g** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 – 8.85 (m, 1H), 8.77 (d, *J* = 8.0 Hz, 1H), 8.72 (d, *J* = 8.0 Hz, 1H), 8.57 – 8.48 (m, 1H), 8.27 (dd, *J* = 10.4, 2.4 Hz, 1H), 7.78 – 7.73 (t, *J* = 8.0 Hz, 1H), 7.73 – 7.69 (m, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.55 (q, *J* = 4.0 Hz, 1H), 4.86 (q, *J* = 7.2 Hz, 2H), 1.72 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3 (d, *J* = 234.9 Hz), 136.7, 134.9, 131.3, 129.9, 127.6, 126.9, 126.7, 126.1, 124.4, 124.0, 123.8, 123.7, 123.6, 123.3, 122.7,

111.8 (d, J = 25.6 Hz), 110.0 (d, J = 9.6 Hz), 107.4 (d, J = 24.6 Hz), 41.3, 15.4. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{22}H_{16}FN$, 313.1267; found, 313.1254. IR (KBr) υ: 2923, 2856, 1612, 1468, 1139, 737. MP: 146.4-147-6℃.



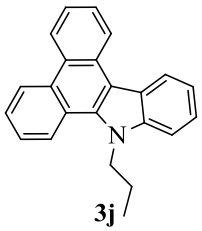
3h

Methyl 9-ethyl-9H-dibenzo[a,c]carbazole-11-carboxylate (3h): Obtained from **1h** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 – 8.79 (m, 2H), 8.75 (d, J = 8.0 Hz, 1H), 8.60 (d, J = 8.4 Hz, 1H), 8.53 (m, 1H), 8.35 (s, 1H), 8.06 (d, J = 7.2 Hz, 1H), 7.73 (m, 2H), 7.59 (t, J = 7.2 Hz, 1H), 4.90 (q, J = 7.2 Hz, 2H), 4.03 (s, 3H), 1.73 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 139.5, 136.0, 131.7, 129.8, 127.7, 127.2, 127.1, 126.8, 126.5, 125.1, 124.4, 124.2, 123.7, 123.6, 123.4, 123.1, 121.5, 111.5, 52.3, 41.2, 15.5. HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{24}H_{20}NO_2$, 354.1494, ; found, 354.1484. IR (KBr) υ: 1701, 1606, 1449, 1240, 738. MP: 206.2-207.3℃.



3i

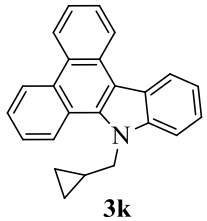
9-Methyl-9H-dibenzo[a,c]carbazole (3i):[1] Obtained from **1i** and **2a** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 – 8.82 (m, 2H), 8.77 (d, J = 8.4 Hz, 1H), 8.69 – 8.65 (m, 1H), 8.62 (d, J = 8.0 Hz, 1H), 7.76 (t, J = 7.2 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.59 (m, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 7.2 Hz, 1H), 4.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 134.8, 131.1, 130.1, 127.4, 127.1, 126.3, 125.7, 124.3, 124.1, 123.9, 123.8, 123.7, 123.6, 123.0, 122.0, 120.5, 113.6, 109.7, 34.7. IR (KBr) υ: 1604, 1511, 1463, 742. MP: 132.9-134.1℃.



3j

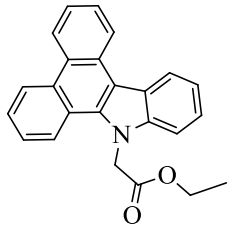
9-Propyl-9H-dibenzo[a,c]carbazole (3j): Obtained from **1j** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 – 8.86 (m, 2H), 8.79 (d, J = 8.4 Hz, 1H), 8.65 (d, J = 8.0 Hz, 1H), 8.52 (m, 1H), 7.76 (t, J = 7.2 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.65 (d, J = 8.4 Hz, 1H), 7.59 (t, J = 7.2 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), 7.42 (t, J = 7.2 Hz, 1H), 4.79 – 4.74 (t, J = 8.0 Hz, 1H), 2.17 (m, 2H), 1.14 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8, 133.9, 131.2, 130.2, 127.5, 127.1, 126.6, 125.7, 124.4, 123.9, 123.8, 123.8, 123.7, 123.6, 122.7, 122.1, 120.5,

113.9, 109.9, 48.0, 23.6, 11.5. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{23}H_{19}N$, 309.1517; found, 309.1506. IR (KBr) υ: 2957, 1604, 1465, 1352, 1097, 1030, 731. MP: 111.1-112.5℃.



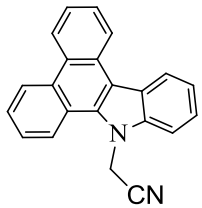
3k

9-(Cyclopropylmethyl)-9H-dibenzo[a,c]carbazole (3k): Obtained from **1k** and **2a** as a white solid following a procedure for the synthesis of **3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 – 8.86 (m, 2H), 8.81 (t, *J* = 8.4 Hz, 2H), 8.64 (d, *J* = 8.0 Hz, 1H), 7.73 (m, 3H), 7.65 – 7.56 (m, 2H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 4.87 (d, *J* = 5.2 Hz, 2H), 1.63 – 1.43 (m, 1H), 0.68 – 0.58 (m, 2H), 0.52 (t, *J* = 5.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 134.2, 131.1, 130.0, 127.4, 127.0, 126.4, 126.0, 125.6, 125.2, 124.2, 123.7, 123.7, 123.6, 123.5, 123.1, 121.9, 120.4, 113.9, 110.1, 48.9, 11.4, 3.6. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{24}H_{19}N$, 321.1517; found, 321.1509. IR (KBr) υ: 1467, 1345, 1016, 742. MP: 132.6-133.9℃.



3l

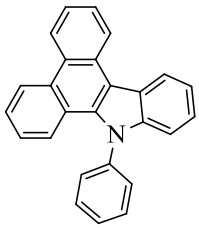
Methyl 2-(9H-dibenzo[a,c]carbazol-9-yl)acetate (3l): Obtained from **1l** and **2a** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (t, *J* = 8.4 Hz, 2H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.63 (d, *J* = 8.0 Hz, 1H), 8.32 – 8.27 (m, 1H), 7.77 (t, *J* = 7.2 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.53 – 7.51 (m, 2H), 7.45 (m, 1H), 5.47 (s, 1H), 4.32 (q, *J* = 7.2 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3, 141.4, 134.5, 131.2, 129.9, 127.6, 127.4, 126.6, 126.0, 124.5, 124.4, 124.2, 124.2, 123.9, 123.6, 123.5, 122.2, 122.3, 121.3, 114.61, 109.5, 62.1, 49.1, 14.3. HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{244}H_{20}NO_2$, 354.1494; found, 354.1486. IR (KBr) υ: 1737, 1459, 1370, 1207, 731. MP: 172.2-173.4℃.



3m

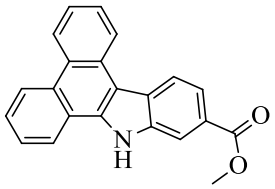
2-(9H-dibenzo[a,c]carbazol-9-yl)acetonitrile (3m): Obtained from **1m** and **2a** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.05 (d, *J* = 8.0 Hz, 1H), 8.94 (t, *J* = 8.4 Hz, 2H), 8.74 (q, *J* = 8.0 Hz, 2H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.77 (m, 3H), 7.67 (t, *J* = 7.2 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 6.25 (s, 2H). ^{13}C NMR (101

MHz, DMSO-d_6) δ 140.1, 132.9, 130.3, 128.6, 128.0, 127.3, 126.9, 126.6, 124.8, 124.7, 124.5, 123.9, 123.6, 123.2, 122.7, 122.3, 121.9, 116.9, 114.2, 110.5, 35.5. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{22}H_{14}N_2$, 306.1157; found, 306.1148. IR (KBr) υ: 2363, 1466, 1369, 738. MP: 216.3-217.5℃.



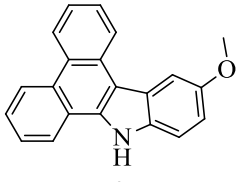
3n

9-Phenyl-9H-dibenzo[a,c]carbazole (3n):[2] Obtained from **1n** and **2a** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, *J* = 8.0 Hz, 1H), 8.81 (dd, *J* = 8.0, 3.2 Hz, 2H), 8.66 (d, *J* = 7.6 Hz, 1H), 7.80 (t, *J* = 7.2 Hz, 1H), 7.70 – 7.60 (m, 4H), 7.55 (m, 3H), 7.50 – 7.35 (m, 4H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 140.5, 134.8, 134.7, 131.1, 131.0, 130.4, 130.1, 129.3, 129.3, 129.1, 127.5, 127.5, 126.1, 125.9, 124.2, 124.1, 124.0, 123.7, 123.4, 121.8, 121.2, 117.9, 114.4, 114.2, 111.1. IR (KBr) υ: 3157, 2357, 1088, 828, 757. MP: 192.1-194.2℃.



3o

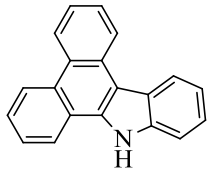
Methyl 9H-dibenzo[a,c]carbazole-11-carboxylate (3o): Obtained from methyl indole-6- carboxylate and **2a** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, DMSO-*d6*) δ 12.73 (s, 1H), 8.93 (dd, J = 12.0, 8.4 Hz, 2H), 8.83 (d, J = 8.0 Hz, 1H), 8.68 (d, J = 8.4 Hz, 1H), 8.59 (d, J = 8.0 Hz, 1H), 8.32 (s, 1H), 7.93 (d, J = 8.4 Hz, 1H), 7.86 – 7.73 (m, 3H), 7.63 (t, J = 7.6 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.9, 137.8, 136.6, 129.9, 129.2, 127.9, 127.4, 127.3, 127.0, 126.4, 124.3, 124.2, 124.1, 123.5, 122.6, 122.2, 121.2, 120.6, 113.2, 111.1, 52.1. HRMS (ESI) m/z: $[M-H]^-$ calcd for $C_{22}H_{14}NO_2$, 324.1025; found, 324.1032. IR (KBr) υ: 3353, 2923, 2853, 2360, 1697, 1618, 1456, 1292, 1218, 757. MP: 223.2-224.8℃.



3p

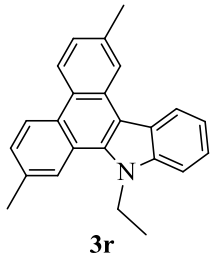
12-Methoxy-9H-dibenzo[a,c]carbazole (3p):[2] Obtained from 5-methoxy-indole and **2a** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.25 (s, 1H), 8.88 (t, *J* = 8.0 Hz, 2H), 8.77 (d, *J* = 7.6 Hz, 1H), 8.55 (d, *J* = 6.8 Hz, 1H), 7.99 (d, *J* = 2.4 Hz, 1H), 7.77 (q, *J* = 8.0 Hz, 2H), 7.70 (t, *J* = 6.8 Hz, 1H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H),

7.10 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 154.1, 134.7, 133.5, 129.7, 129.2, 127.6, 126.9, 126.4, 126.1, 124.0, 123.9, 123.4, 123.3, 122.8, 122.2, 122.1, 113.2, 112.4, 111.1, 103.9, 55.8. IR (KBr) υ: 3343, 2923, 2362, 1612, 1447, 1308, 1218, 806, 753. MP: 158.6-159.8℃.



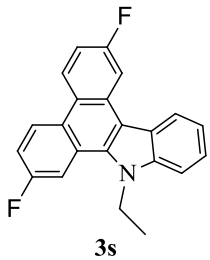
3q

9H-dibenzo[a,c]carbazole (3q): Obtained from 1-H-indole and **2a** as a yellow solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.40 (s, 1H), 8.91 (t, *J* = 8.4 Hz, 2H), 8.81 (d, *J* = 7.6 Hz, 1H), 8.58 (t, *J* = 8.4 Hz, 2H), 7.78 (t, *J* = 7.6 Hz, 2H), 7.75 – 7.69 (m, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 7.2 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 138.5, 138.4, 134.9, 134.1, 129.6, 129.3, 127.6, 127.0, 126.5, 126.2, 123.9, 123.6, 123.5, 123.4, 122.6, 122.2, 121.3, 120.0, 111.8, 111.2, 40.2. IR (KBr) υ: 3417, 2922, 2364, 1457, 745. MP: 170.6-171.9℃.



3r

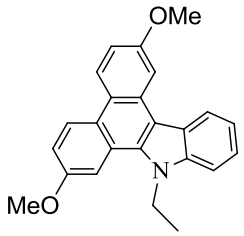
9-Ethyl-2,7-dimethyl-9H-dibenzo[a,c]carbazole (3r): Obtained from **1a** and **2b** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, J = 8.4 Hz, 1H), 8.66 (d, J = 7.2 Hz, 2H), 8.62 (d, J = 8.4 Hz, 1H), 8.31 (s, 1H), 7.63 (d, J = 8.4 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.41 (q, J = 7.6 Hz, 2H), 4.86 (q, J = 7.2 Hz, 2H), 2.69 (s, 3H), 2.65 (s, 3H), 1.74 (t, J = 7.2 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 140.3, 136.7, 135.6, 133.9, 129.9, 129.0, 127.2, 125.4, 125.0, 124.0, 123.9, 123.7, 123.5, 123.5, 123.3, 122.6, 122.1, 120.3, 113.6, 109.5, 41.1, 22.2, 22.1, 15.4. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{24}H_{21}N$, 323.1674; found, 323.1668. IR (KBr) υ: 2879, 1332, 1150, 755. MP: 157.2-158.9℃.



3s

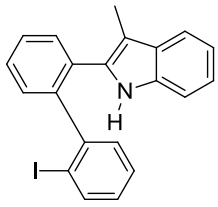
9-Ethyl-2,7-difluoro-9H-dibenzo[a,c]carbazole (3s): Obtained from **1a** and **2c** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, J = 9.2, 6.0 Hz, 1H), 8.57 (dd, J = 9.2, 6.0 Hz, 1H), 8.49 (d, J = 8.0 Hz, 1H), 8.39 (dd, J = 10.8, 2.8 Hz, 1H), 8.08 (dd, J = 10.8, 2.8 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.53 (t, J = 7.2 Hz, 1H), 7.46 – 7.40 (m, 1H), 7.40 – 7.35

(m, 1H), 7.30 – 7.23 (m, 1H), 4.76 (q, J = 7.2 Hz, 2H), 1.69 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ162.9 (d, *J* = 87.8 Hz), 160.50 (d, *J* = 85.8 Hz), 140.2, 130.9, 127.4, 127.3, 126.3 (d, *J* = 8.0 Hz), 125.5 (d, *J* = 9.0 Hz), 124.6, 124.0 (d, *J* = 8.0 Hz), 123.2 (d, *J* = 2.0 Hz), 121.8, 121.0, 114.4 (d, *J* = 23.2 Hz), 112.5 (d, *J* = 23.2 Hz), 109.7, 108.6 (d, *J* = 22.2 Hz), 108.0 (d, *J* = 24.2 Hz), 40.8, 15.4. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{22}H_{15}F_2N$, 331.1173; found, 331.1161. IR (KBr) υ: 2970, 1618, 1465, 1185, 734. MP: 162.7-164.1℃.



3t

9-Ethyl-2,7-dimethoxy-9H-dibenzo[a,c]carbazole (3t): Obtained from **1a** and **2d** as a white solid following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 9.2 Hz, 1H), 8.58 (m, 2H), 8.25 (d, *J* = 2.4 Hz, 1H), 7.97 (d, *J* = 2.4 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.31 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.20 (dd, *J* = 9.2, 2.4 Hz, 1H), 4.88 (q, *J* = 7.2 Hz, 2H), 4.10 (s, 3H), 4.03 (s, 3H), 1.77 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 157.6, 140.4, 130.4, 129.0, 125.4, 124.6, 123.9, 123.8, 123.6, 121.8, 121.5, 120.6, 114.5, 113.2, 112.6, 109.6, 105.6, 105.5, 55.7, 55.6, 41.1, 15.6. HRMS (ESI) m/z: $[M]^+$ calcd for $C_{24}H_{21}NO_2$, 355.1572; found, 355.1562. IR (KBr) υ: 2924, 2857, 1613, 1464, 1397, 1226, 816, 734. MP: 148.1-149.5℃.

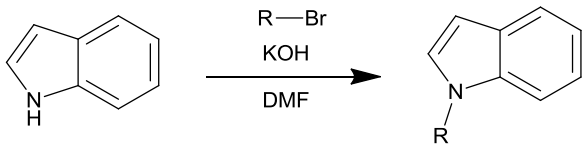


4

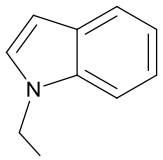
2-(2'-Iodo-[1,1'-biphenyl]-2-yl)-3-methyl-1H-indole (4): Obtained from 3-methy-1-H-lindole and **2a** as a yellow oil following a procedure for the synthesis of **3a.** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 1H), 7.57 – 7.53 (m, 3H), 7.52 – 7.48 (m, 2H), 7.30 (s, 1H), 7.22 – 7.16 (m, 3H), 7.16 – 7.10 (m, 2H), 2.15 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 141.1, 135.8, 133.8, 131.7, 131.4, 130.8, 129.3, 129.2, 129.0, 128.5, 128.4, 127.4, 127.4, 127.1, 121.9, 119.2, 118.9, 110.6, 109.67, 9.3. IR (KBr) υ: 2879, 1382, 1150, 752, 731. HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{21}H_{17}IN$, 410.0406; found, 410.0397.

General procedure for the preparation of *N*-substituted indole

These *N*-substituted indoles were synthesized according to Zhang's work [4]. The synthesis of 1a was examplified herein.

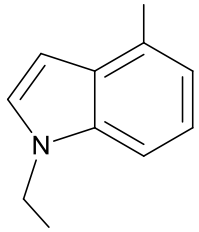


1



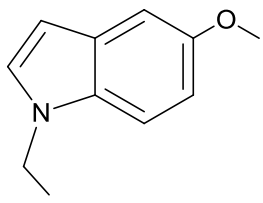
1a

1-Ethyl-indole (1a): To a stirred solution of indole (1g, 8.54mmol) and KOH (1.44g, 25.61mmol) in DMF(8mL) was injected ethyl bromide(1.27mL, 17.07mmol) at room temperature. The mixture was stirred for 3h before the mixture was extracted with EtOAc. The combined organic layers were washed with H_2O and brine, dried over anhydrous Na_2SO_4, concentrated by rotary evaporation. The crude product was purified by column chromatography on a silica gel (PE) to afford **1a** (1.15g, 100% yield) as a yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.36 (m, 1H), 7.95 (m, 3H), 7.59 (d, *J* = 3.2 Hz, 1H), 7.26 (d, *J* = 3.2 Hz, 1H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.90 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.6, 128.7, 126.8, 121.2, 120.8, 119.1, 109.2, 100.8, 40.4, 15.0.



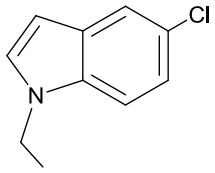
1b

1-Ethyl-4-methyl-indole (1b): Obtained from 4-methyl-indole and ethyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.0 Hz, 1H), 7.05 – 6.99 (m, 1H), 6.98 (d, *J* = 3.2 Hz, 1H), 6.81 (d, *J* = 6.8 Hz, 1H), 6.40 (d, *J* = 3.2, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 2.46 (s, 3H), 1.33 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.5, 130.5, 128.6, 126.4, 121.6, 119.5, 107.0, 99.6, 41.15, 18.9, 15.6.



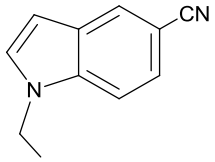
1c

1-Ethyl-5-methoxy-indole (1c): Obtained from 5-methoxy-indole and ethyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.8 Hz, 1H), 7.31 (d, *J* = 2.4 Hz, 1H), 7.23 (d, *J* = 3.2 Hz, 1H), 7.10 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.62 (dd, *J* = 2.8, 0.4 Hz, 1H), 4.22 (q, *J* = 7.2 Hz, 2H), 4.02 (s, 3H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 131.1, 129.0, 127.5, 111.7, 110.0, 102.6, 100.5, 55. 8, 41.0, 15.4.



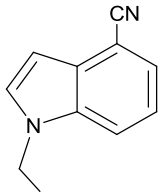
1d

5-Chloro-1-ethyl-indole (1d): Obtained from 5-chloro-indole and ethyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 1.6 Hz, 1H), 7.20 – 7.12 (m, 1H), 7.10 – 7.02 (m, 2H), 6.34 (d, *J* = 3.2 Hz, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.3, 129.8, 128.4, 125.1, 121.8, 120.4, 110.4, 100.9, 41.3, 15.5.



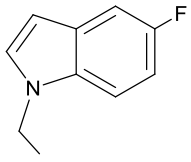
1e

5-Cynao-1-ethyl-indole (1e): Obtained from 5-cynao-indole and ethyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.32 – 7.23 (m, 2H), 7.13 (d, *J* = 3.2 Hz, 1H), 6.46 (d, *J* = 2.8 Hz, 1H), 4.08 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 129.4, 128.3, 126.5, 124.2, 120.9, 110.1, 102.3, 102.2, 41.3, 15.6.



1f

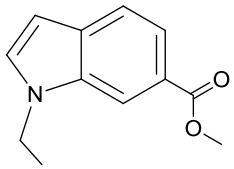
4-Cynao-1-ethyl-indole (1f): Obtained from 4-cynao-indole and ethyl bromide as a white solid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.4 Hz, 1H), 7.29 (d, *J* = 6.8 Hz, 1H), 7.14 (d, *J* = 3.2 Hz, 1H), 7.10 – 7.04 (t, *J* =8.0 Hz, 1H), 6.54 (d, *J* = 2.4 Hz, 1H), 4.04 (q, *J* = 7.2 Hz, 2H), 1.32 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.3, 129.7, 124.6, 120.9, 118.8, 114.1, 102.9, 100.0, 99.9, 41.2, 15.4.



1g

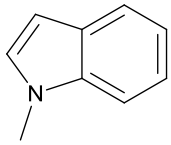
5-Fluro-1-ethyl-indole (1g): Obtained from 5-fluro-indole and ethyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (m, 2H), 7.02 (d, J = 2.8 Hz, 1H), 6.85 (t, J = 8.0 Hz, 1H), 6.33 (s, 1H), 6.33 (s, 1H), 4.01 (q, J = 7.2 Hz, 2H), 1.33 (t, J = 7.2

Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ157.9 (d, *J* = 233.5 Hz), 132.5, 128.6, 109.9 (d, *J* = 10.1 Hz) 109.7 (d, *J* = 27.3 Hz), 105.8 (d, *J* = 23.2 Hz), 101.1, 41.3, 15.5.



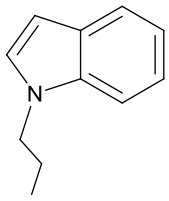
1h

Methyl 1-ethyl-indole-6-carboxylate (1h): Obtained from methyl indole-6-carboxylate and ethyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.68 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.08 (d, *J* = 3.2 Hz, 1H), 6.37 (d, *J* = 3.2 Hz, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.80 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 135.0, 132.3, 130.3, 123.0, 120.4, 120.3, 111.7, 101.5, 51.8, 41.0, 15.5.



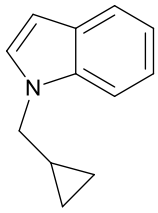
1i

1-Methyl-indole (1i): Obtained from indole and methyl iodide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (m, 1H), 8.18 – 8.08 (m, 2H), 8.02 – 7.91 (m, 1H), 7.56 (d, *J* = 3.2 Hz, 1H), 7.40 (d, *J* = 3.2 Hz, 1H), 4.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 128.5, 128.4, 121.2, 120.6, 119.1, 109.1, 100.6, 31.7.



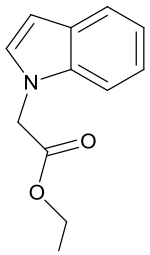
1j

1-Propyl-indole (1j): Obtained from indole and propyl bromide as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.16 (m, 2H), 6.55 (d, *J* = 2.4 Hz, 1H), 4.12 (t, *J* = 7.2 Hz, 2H), 2.01 – 1.80 (m, 2H), 0.98 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.1, 128.7, 128.0, 121.4, 121.0, 119.3, 109.5, 100.9, 48.2, 23.7, 11.7.



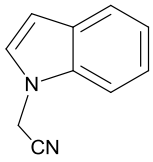
1k

1-(Cyclopropylmethyl)-indole (1k): Obtained from indole and (bromomethyl)cyclopropane as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.32 (m, 1H), 7.27 (m, 2H), 6.66 (s, 1H), 3.95 (d, *J* = 5.6 Hz, 2H), 1.38 – 1.20 (m, 1H), 0.67 (d, *J* = 7.2 Hz, 2H), 0.41 (d, *J* = 4.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.1, 128.6, 127.4, 121.3, 120.9, 119.2, 109.4, 100.9, 50.4, 11.2, 4.0.



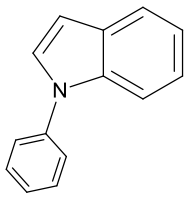
1l

Ethyl 2-(1H-indol-1-yl)-acetate (1l): Obtained from indole and methyl 2-bromoacetate as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.14 – 7.07 (m, 2H), 7.02 (m, 1H), 6.95 (d, *J* = 3.2 Hz, 1H), 6.45 (d, *J* = 3.2 Hz, 1H), 4.67 (s, 2H), 4.07 (q, *J* = 7.2 Hz, 2H), 1.12 (t, *J* = 7.2 Hz,3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 136.6, 128.6, 122.1, 121.2, 119.9, 109.0, 102.5, 61.7, 47.9, 14.2.



1m

2-(1H-indol-1-yl)-acetonitrile (1m): Obtained from indole and 2-bromoacetonitrile as a yellow liquid following a procedure for the synthesis of **1a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.16 (m, 2H), 7.07 (m, 1H), 6.84 (d, *J* = 3.2 Hz, 1H), 6.44 (d, *J* = 3.2 Hz, 1H), 4.62 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.7, 128.9, 127.2, 122.9, 121.5, 120.8, 114.6, 108.9, 104.0, 34.0.

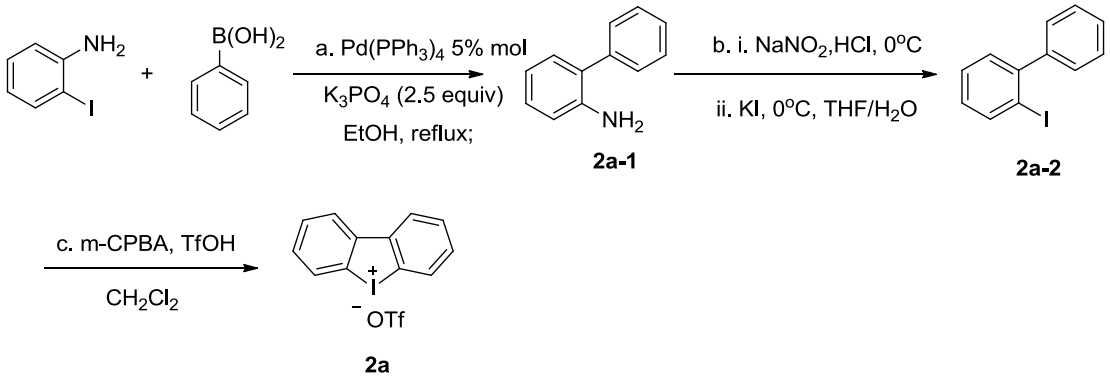


1n

1-Phenyl-indole (1n) [5]**:** To a stirred solution of indole (300 mg, 2.56 mmol) in DMF (5 mL) was added iodobenzene (627 mg, 3.07 mmol), cesium carbonate (1.67 g, 5.12 mmol), $Cu(OAc)_2$ (46 mg, 256 umol). The reaction proceeded at a 120℃ for 12h under argon atmosphere. The mixture was extract with EtOAc and the combined organic layers were washed with H_2O and brine, dried over anhydrous Na_2SO_4, concentrated by rotary evaporation. The crude product was purified by column chromatography on a silica gel (PE) to afford **1n** (100mg, 21% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.6 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 4.8 Hz, 4H), 7.44 – 7.36 (m, 2H), 7.31 – 7.17 (m, 2H), 6.74 (d, *J* = 3.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 136.0, 129.7, 129.5, 128.1, 126.6, 124.5, 122.5, 121.3, 120.5, 110.6, 103.7.

General procedure for the preparation of cyclic diaryliodoniums

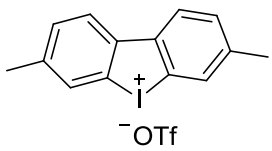
These diphenyleneiodoniums were synthesized according to our previous work [6]. The synthesis of diphenyleniodonium triflate (**2a**) was exemplified herein.



[1,1'-biphenyl]-2-amine (2a-1): To a stirred solution of 2-iodoaniline (1.0 g, 4.57 mmol) in EtOH (10 mL) was added phenylboronic acid (0.68 g, 5.48 mmol), K_3PO_4 (2.91g, 13.7 mmol) and $Pd(PPh_3)_4$ (52.76 mg, 45.66 μmol). The reaction proceeded at a reflux for 12h under argon atmosphere before EtOH was removed by rotary evaporation. The residue was extracted with EtOAc, and the combined organic layers were washed with H_2O and brine, dried over anhydrous Na_2SO_4, concentrated by rotary evaporation. The crude product was purified by column chromatography on a silica gel (PE/EtOAc = 20/1) to afford **2a-1** (750 mg, 97% yield) as a yellow liquid.

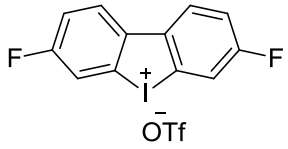
2-Iodo-1,1'-biphenyl (2a-2): To a stirred solution of **2a-1** (750 mg, 4.43 mmol) in THF (10 mL) was added 4 M aqueous HCl (11.1 mL), and the solution was cooled with an ice bath. $NaNO_2$ (458.2 mg, 6.65 mmol) dissolved in H_2O (5 mL) was added dropwise. KI (2.21 g, 13.3 mmol) dissolved in H_2O (5 mL) was added after 20 min. The reaction mixture was stirred for 10 min with the ice bath, then slowly warmed up to rt and stirred for 1 h. The mixture was extracted with EtOAc, and the combined organic layers were washed with H_2O and brine. Then the organic layer was washed with 1M aqueous $Na_2S_2O_3$ until the color of the organic layer didn't change, dried over anhydrous Na_2SO_4, concentrated by rotary evaporation. The crude product was purified by column chromatography on silica gel (PE) to afford **2a-2** (1.1 g, 85% yield) as a colorless liquid.

Dibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (**2a**): To a stirred solution of **2a-2** (1.1 g, 3.93 mmol) in anhydrous CH_2Cl_2 (10 mL) was added *m*-CPBA (1.02 g, 5.89 mmol), TfOH (1.04 mL, 11.78 mmol). The solution was stirred for 1h at rt. CH_2Cl_2 was removed by rotary evaporation before Et_2O (15 mL) was added, and the mixture was stirred for 20 min, and filtered. The collected solid was washed with Et_2O three times, dried in vacuo to afford **2a** (1.68 g, 100% yield) as a white solid. ^{1}H NMR (400 Hz, DMSO-d_6) δ: 8.40 (d, J = 6.8 Hz, 2H), 8.17 (d, J = 7.6 Hz, 2H), 7.88 – 7.75 (m, 2H), 7.74 – 7.58 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ = 141.7, 131.1, 130.7, 130.5, 126.9, 121.5.



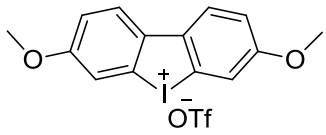
2b

3,7-Dimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (2b): Brown solid (680 mg, 89% yield); ^{1}H NMR (400 Hz, DMSO-d_6) δ: 8.22 (t, J = 6.4, 2H), 7.90 (s, 2H), 7.59 (s, 2H), 2.45 (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ: 141.0, 139.1, 131.6, 130.1, 126.2, 121.3, 119.1, 21.1



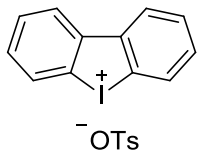
2c

3,7-Difluorodibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (**2c**): White solid (650 mg, 84% yield); ^{1}H NMR (400 Hz, DMSO-d_6) δ: 8.39 (s, 2H), 7.91 (s, 2H), 7.71 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ: 161.85 (d, J = 252.1 Hz), 137.3, 128.3, 122.3, 119.0, 118.8 (d, J = 22.8 Hz), 117.5 (d, J = 27.0 Hz).



2d

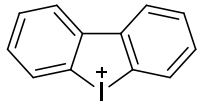
3,7-Dimethoxydibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (**2d**): Yellow solid (550 mg, 75 % yield); ^{1}H NMR (400 Hz, DMSO-d_6) δ: 8.23 (d, J = 8.8 Hz, 2H), 7.70 (d, J = 2.4 Hz, 2H), 7.39 (dd, J = 8.8, 2.4 Hz, 2H), 3.89 (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ : 159.8, 134.2, 126.8, 121.9, 117.8, 114.7, 56.0.



2e

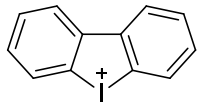
Dibenzo[b,d]iodol-5-ium 4-methylbenzenesulfonate (**2e**): To a stirred solution of **2a-2** (300 mg, 1.07 mmol) in anhydrous CH_2Cl_2 (10 mL) was added *m*-CPBA (277.1 mg, 1.61 mmol), TsOH (553.3 mg, 3.21 mmol). The solution was stirred for 1h at rt. CH_2Cl_2 was removed by rotary evaporation before Et_2O (15 mL) was added, and the mixture was stirred for 20 min, and filtered. The collected solid was washed with Et_2O three times, dried in vacuo to afford **2e** (335 mg, 97% yield) as a white solid. ^{1}H NMR (400 MHz, DMSO-*d6*) δ8.47 (d, J = 7.6 Hz, 2H), 8.25 (d, J = 8.0 Hz, 2H), 7.85 (t, J = 7.6 Hz,

2H), 7.70 (t, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 145.4, 141.8, 137.8, 131.0, 130.7, 128.1, 126.9, 125.49, 121.6, 20.8.



2f

Dibenzo[b,d]iodol-5-ium chloride (**2f**): To a stirred solution of **2a-2** (300 mg, 1.07 mmol) in anhydrous CH_2Cl_2 (10 mL) was added *m*-CPBA (277.1 mg, 1.61 mmol), TfOH (0.28 mL, 3.21 mmol). The solution was stirred for 1h at rt before CH_2Cl_2 was removed by rotary evaporation. To the residue mixture dissolved in formic acid was added brine, and the mixture was stirred for 20 min, and filtered. The collected solid was washed with H_2O and Et_2O three times, dried in vacuo to afford **2f** (336.1 mg, 100% yield) as a white solid. ^{1}H NMR (400 Hz, DMSO-d_6) δ: 8.40 (d, *J* = 6.8 Hz, 2H), 8.17 (d, *J* = 7.6 Hz, 2H), 7.88 – 7.75 (m, 2H), 7.74 – 7.58 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ = 141.7, 131.1, 130.7, 130.5, 126.9, 121.5.



2g

Dibenzo[b,d]iodol-5-ium trifluoroacetate (**2g**): To a stirred solution of **2a-2** (300 mg, 1.07 mmol) in anhydrous CH_2Cl_2 (10 mL) was added *m*-CPBA (277.1 mg, 1.61 mmol), TFA (0.284 mL, 3.21 mmol). The solution was stirred for 1h at rt. CH_2Cl_2 was removed by rotary evaporation before Et_2O (15 mL) was added, and the mixture was stirred for 20 min, and filtered. The collected solid was washed with Et_2O three times, dried in vacuo to afford **2g** (3.23 g, 92% yield) as a white solid. ^{1}H NMR (400 Hz, DMSO-d_6) δ: 8.40 (d, *J* = 6.8 Hz, 2H), 8.17 (d, *J* = 7.6 Hz, 2H), 7.88 – 7.75 (m, 2H), 7.74 – 7.58 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ = 141.7, 131.1, 130.7, 130.5, 126.9, 121.5.

Reference:

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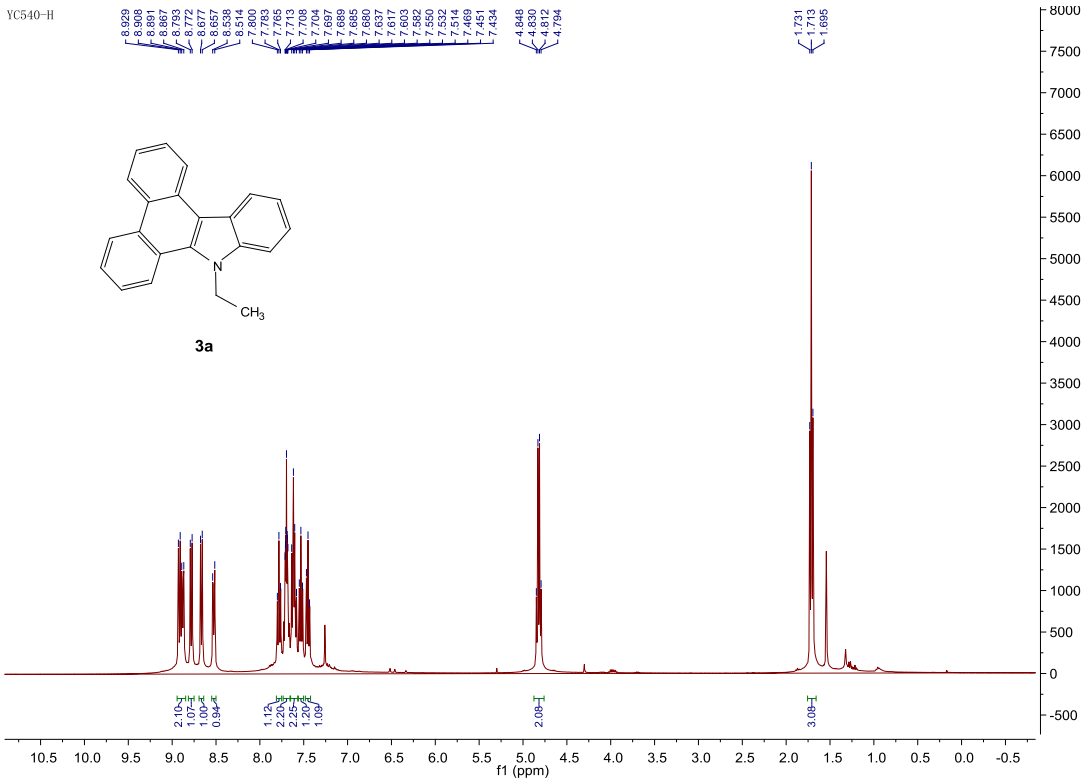
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7.765
7.713
7.708
7.704
7.697
7.689
7.685
7.680
7.637
7.617
7.603
7.582
7.550
7.532
7.514
7.469
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4.830
4.812
4.794
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1.713
1.695
N
CH3
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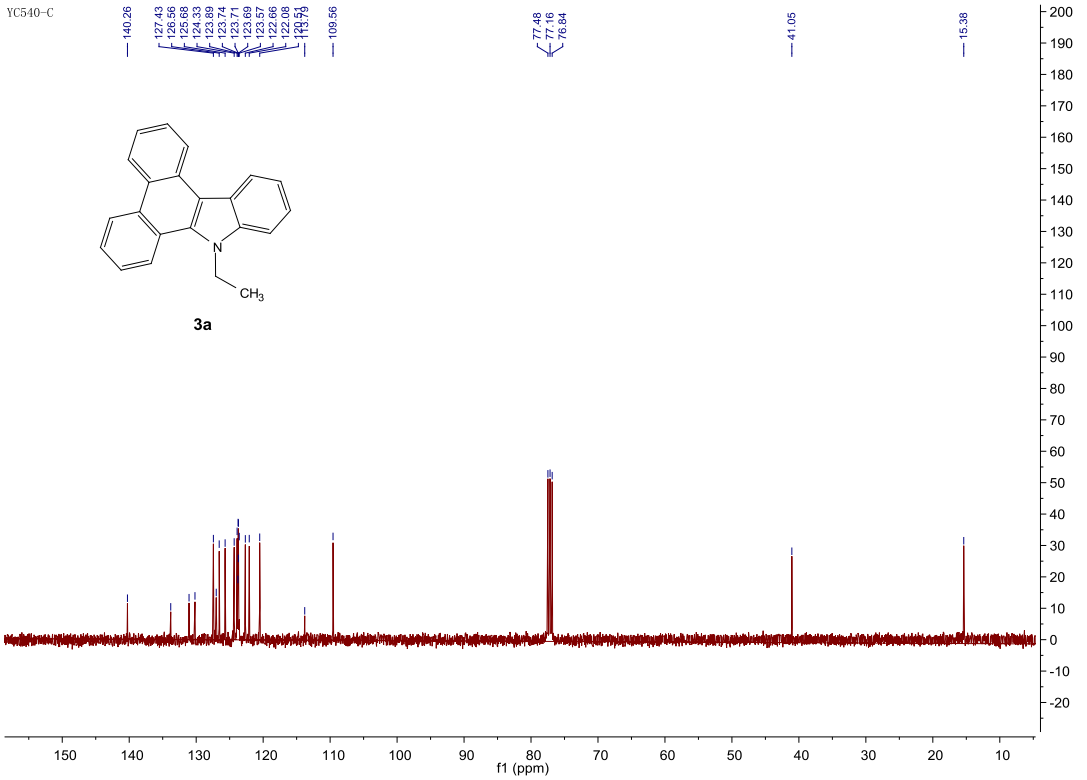
3.08
f1 (ppm)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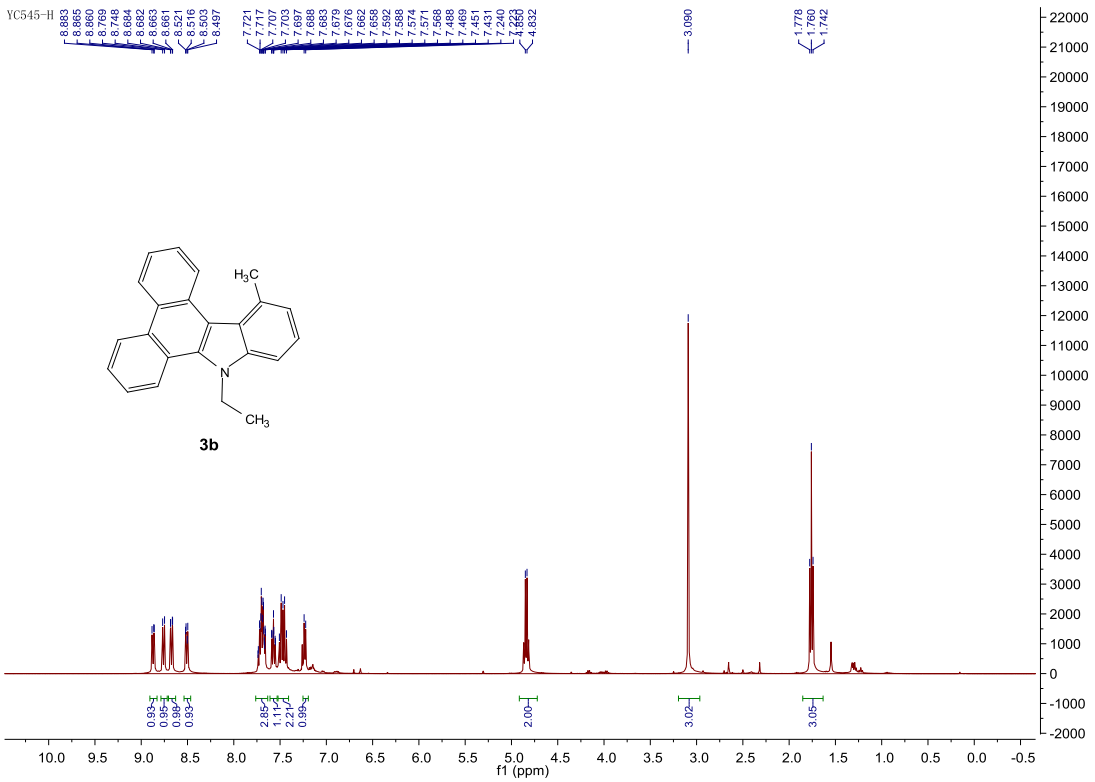
CH3
3a
f1 (ppm)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7.688
7.685
7.679
7.676
7.662
7.658
7.592
7.588
7.574
7.571
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7.488
7.469
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N
CH3
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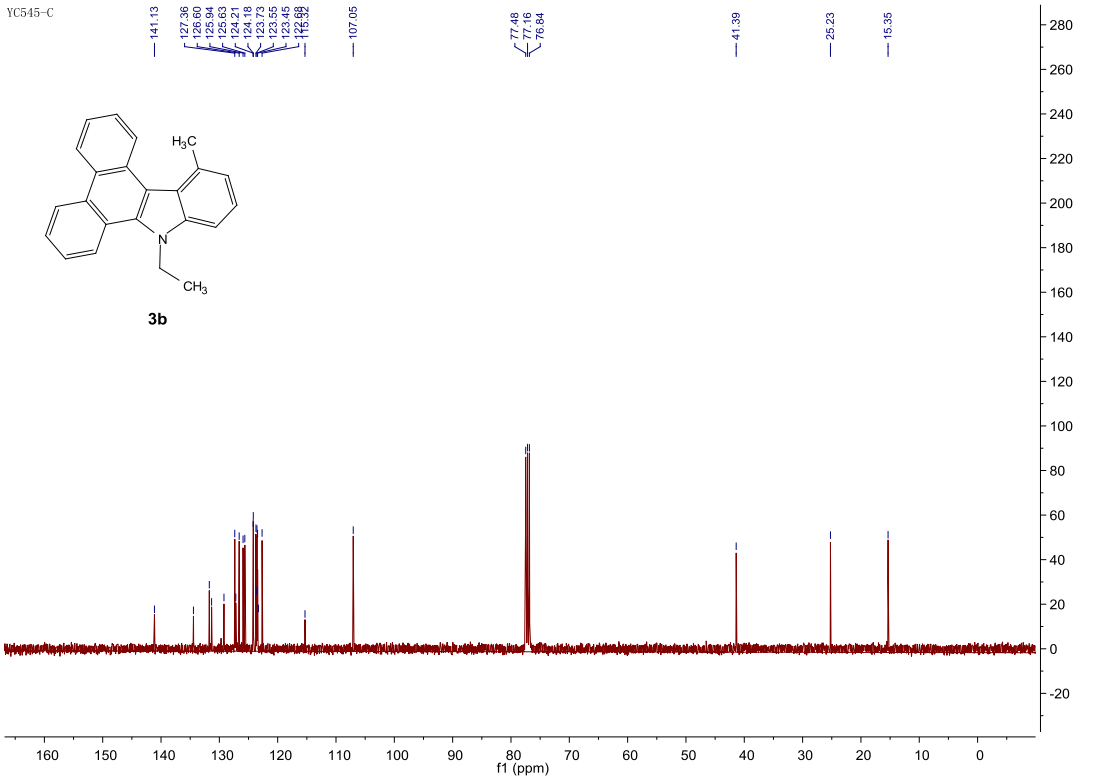
f1 (ppm)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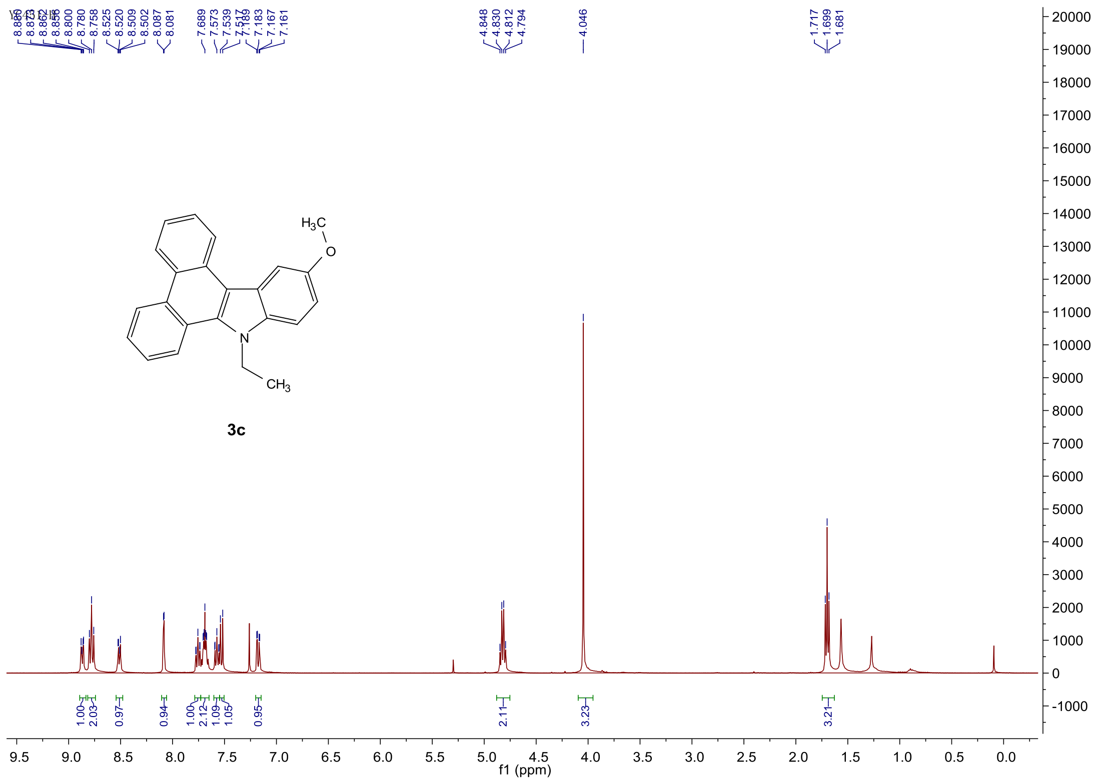
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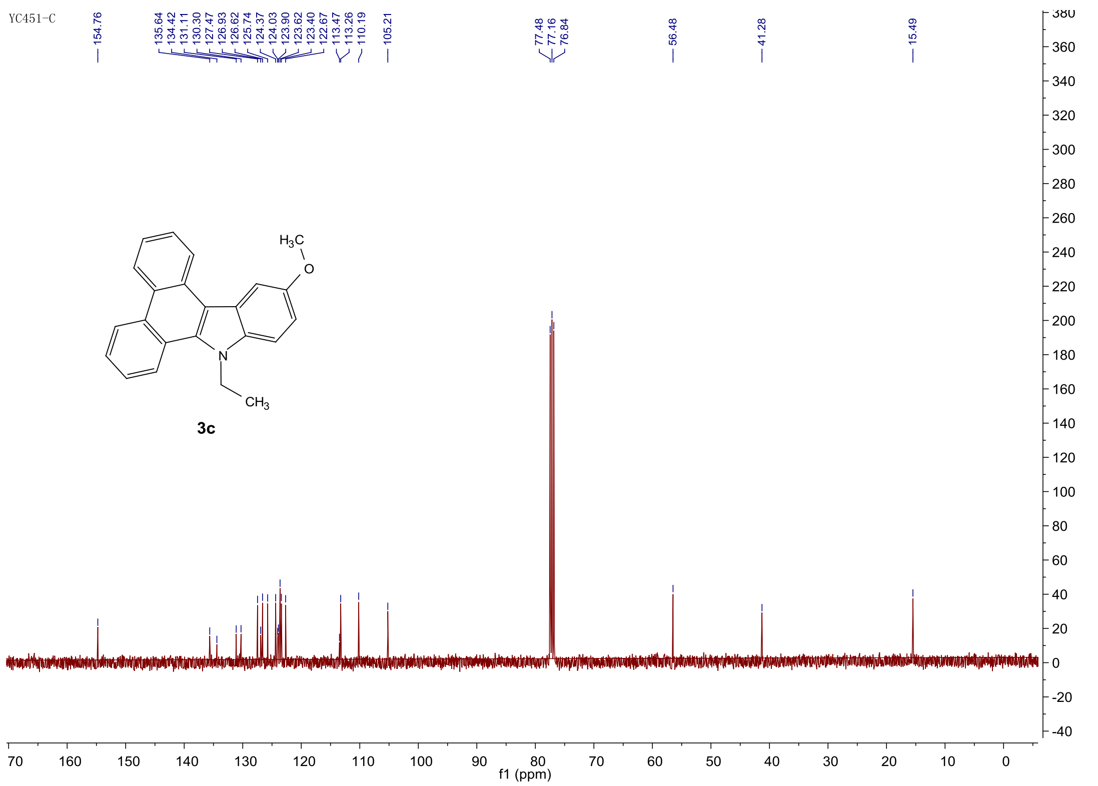
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CH3
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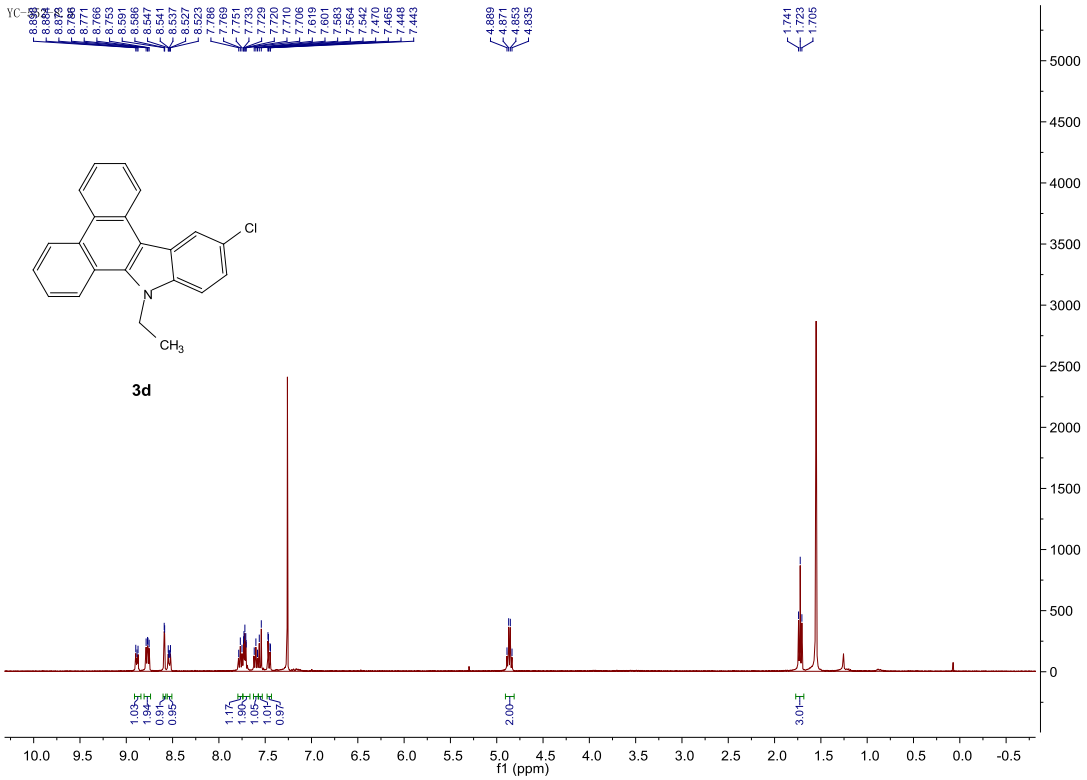
f1 (ppm)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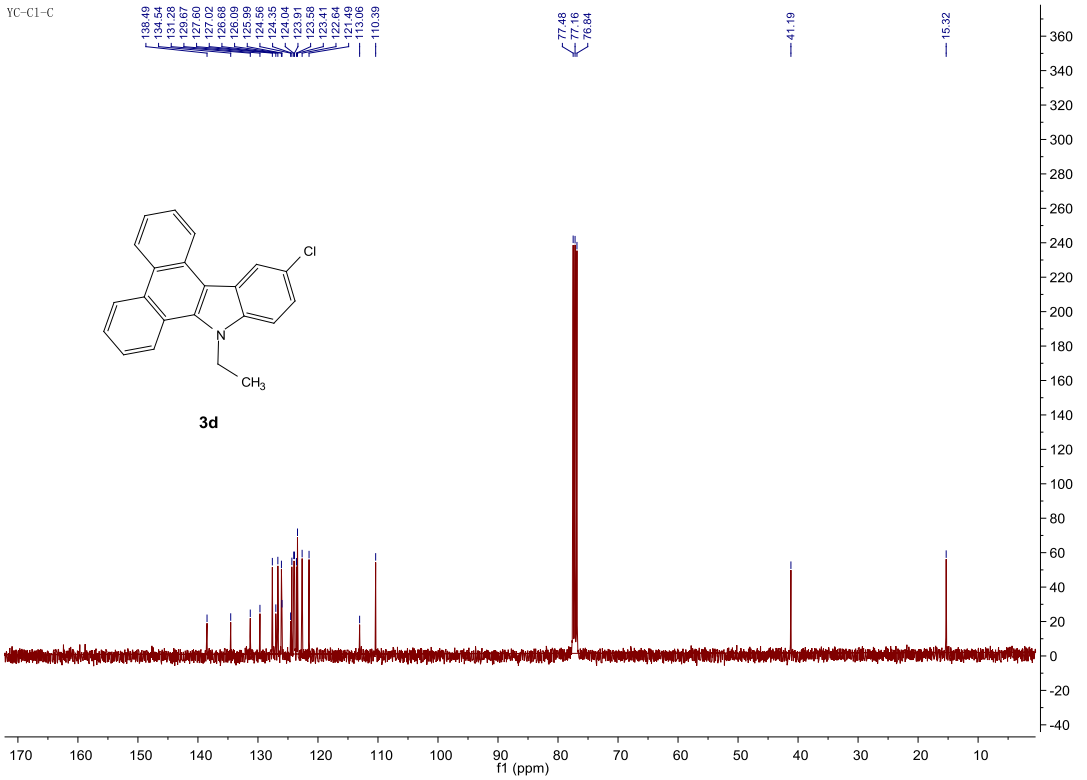
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CH3
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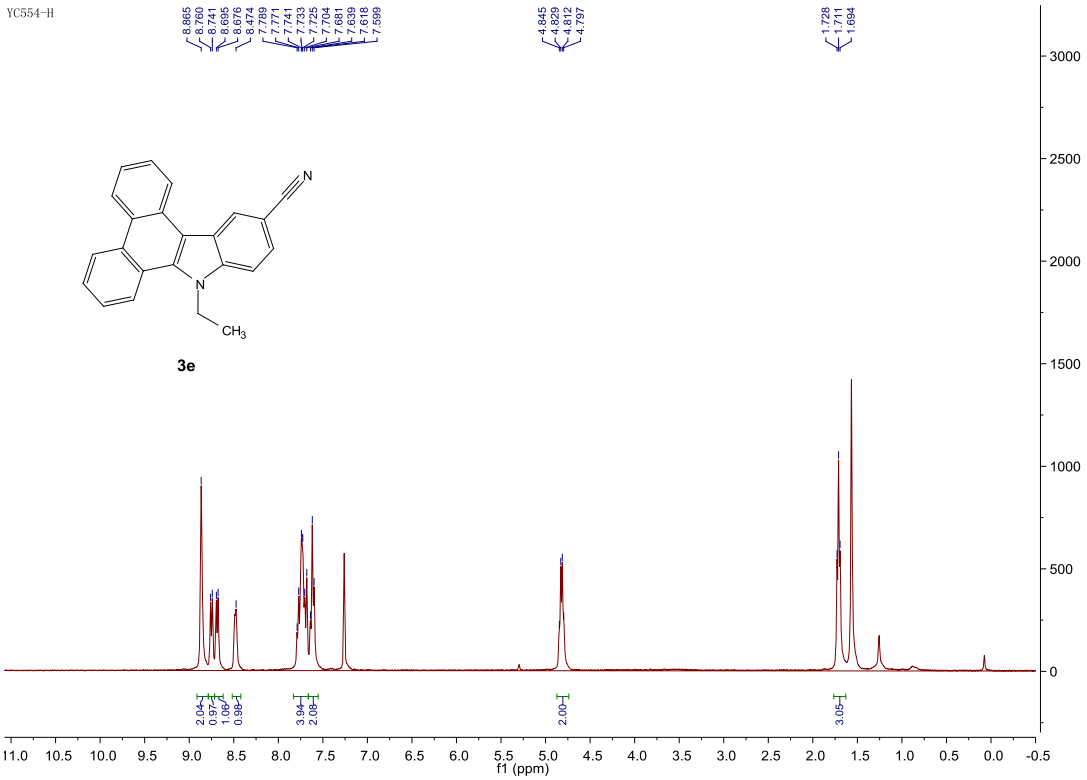
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4.797
1.728
1.711
1.694
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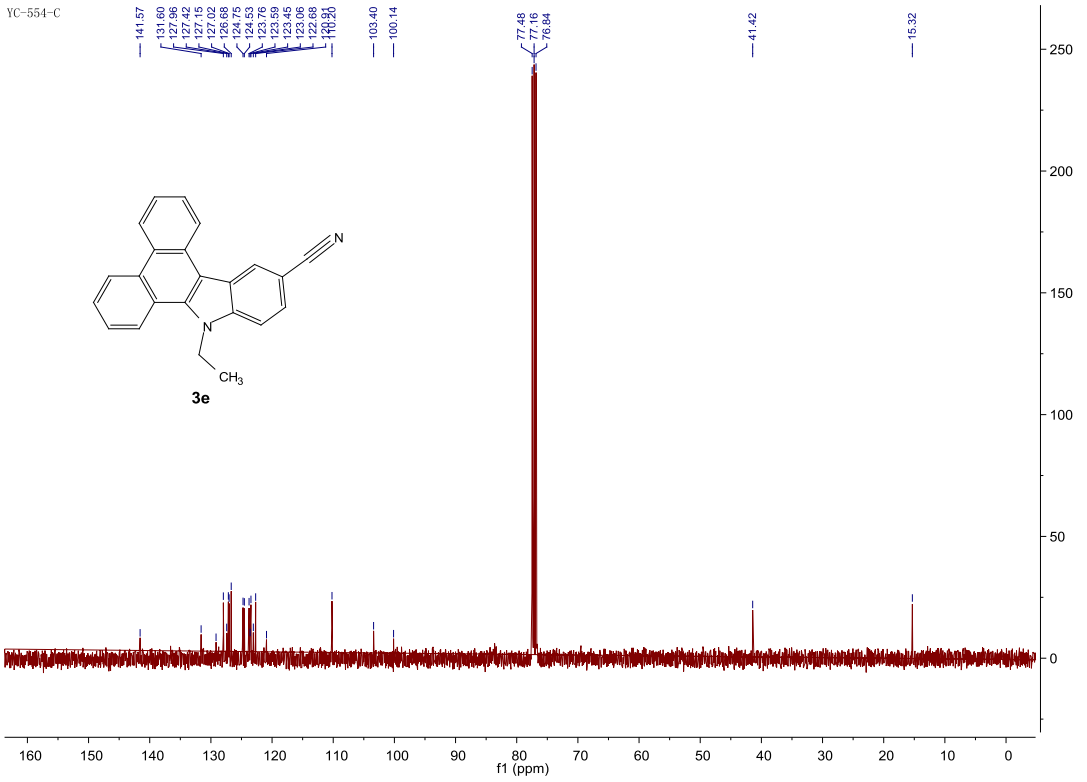
f1 (ppm)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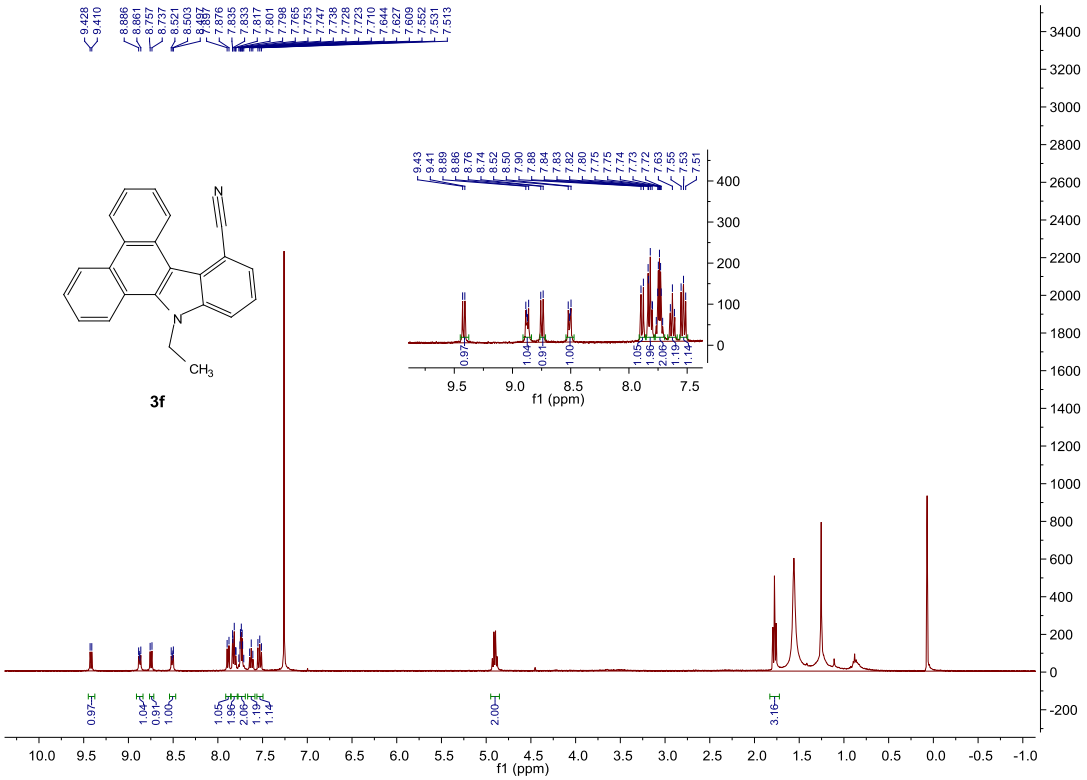
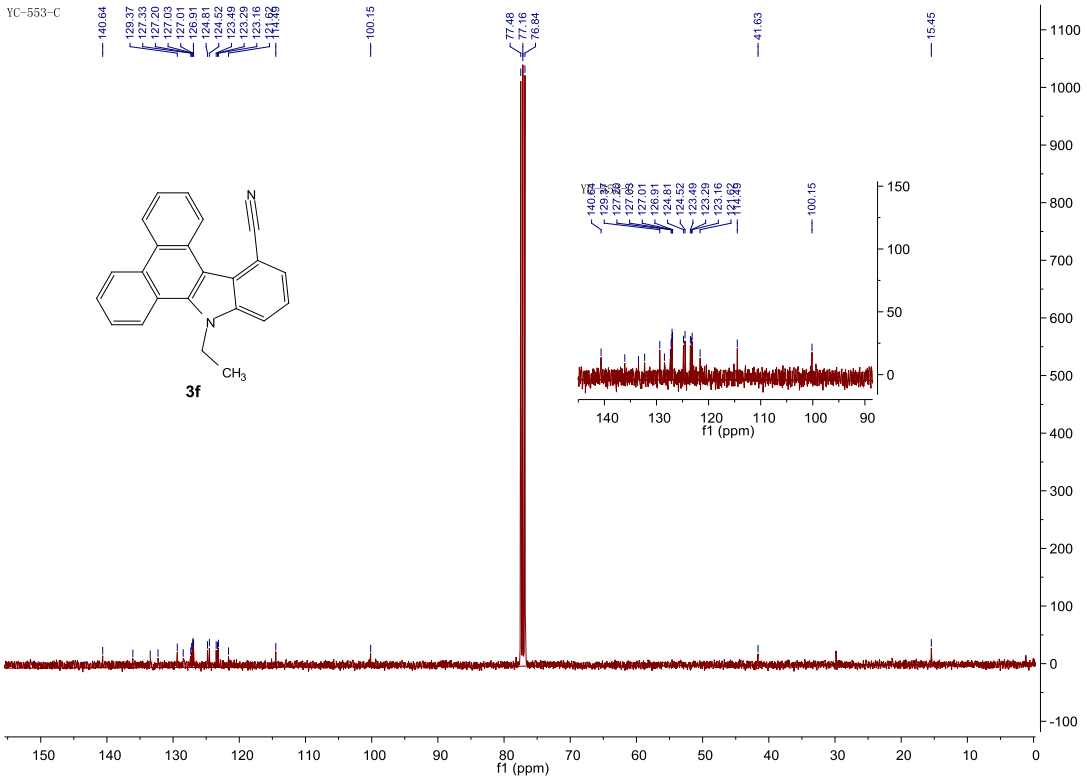
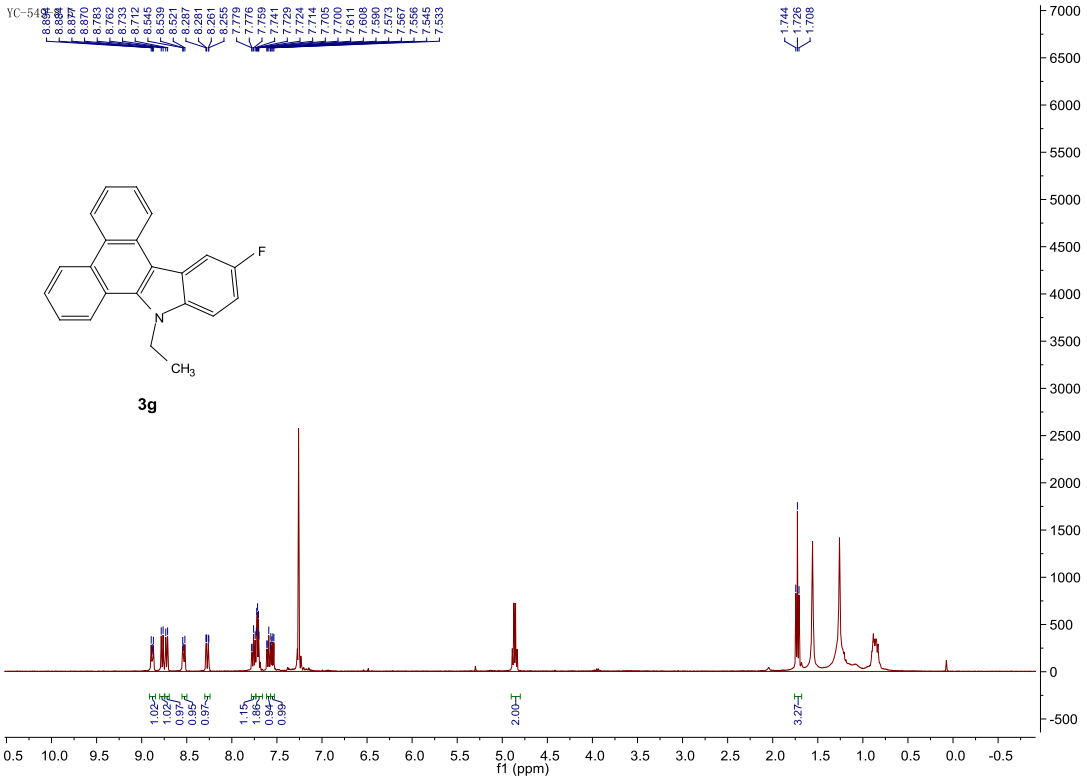
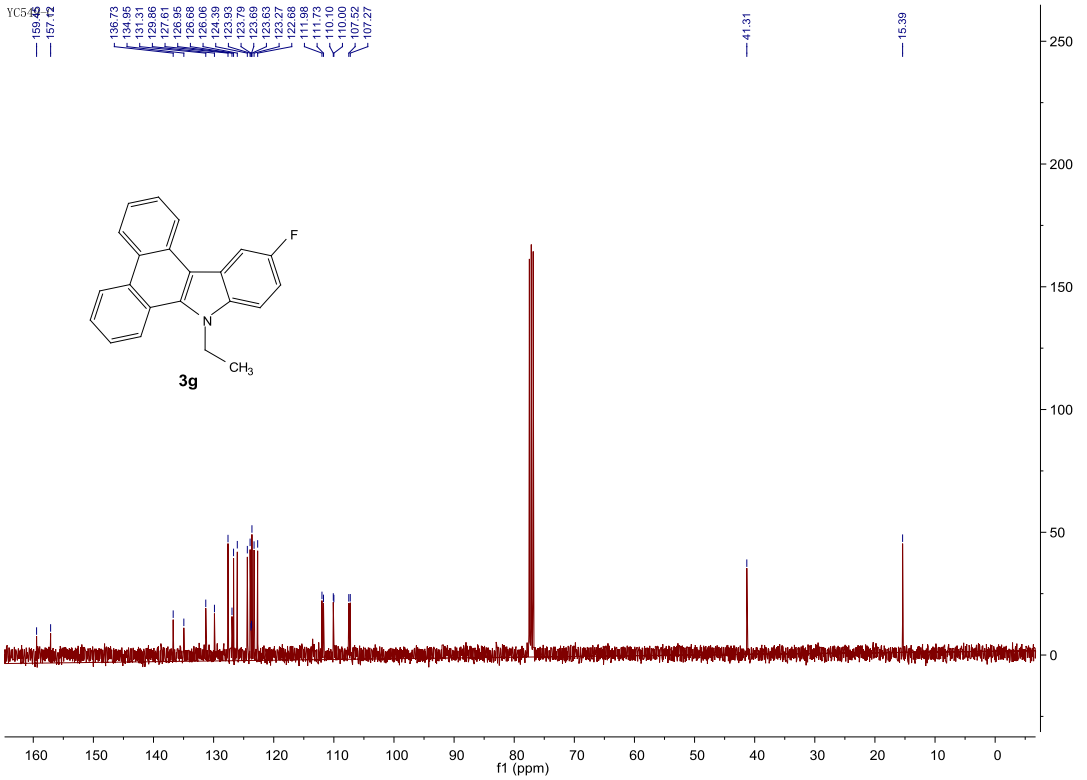
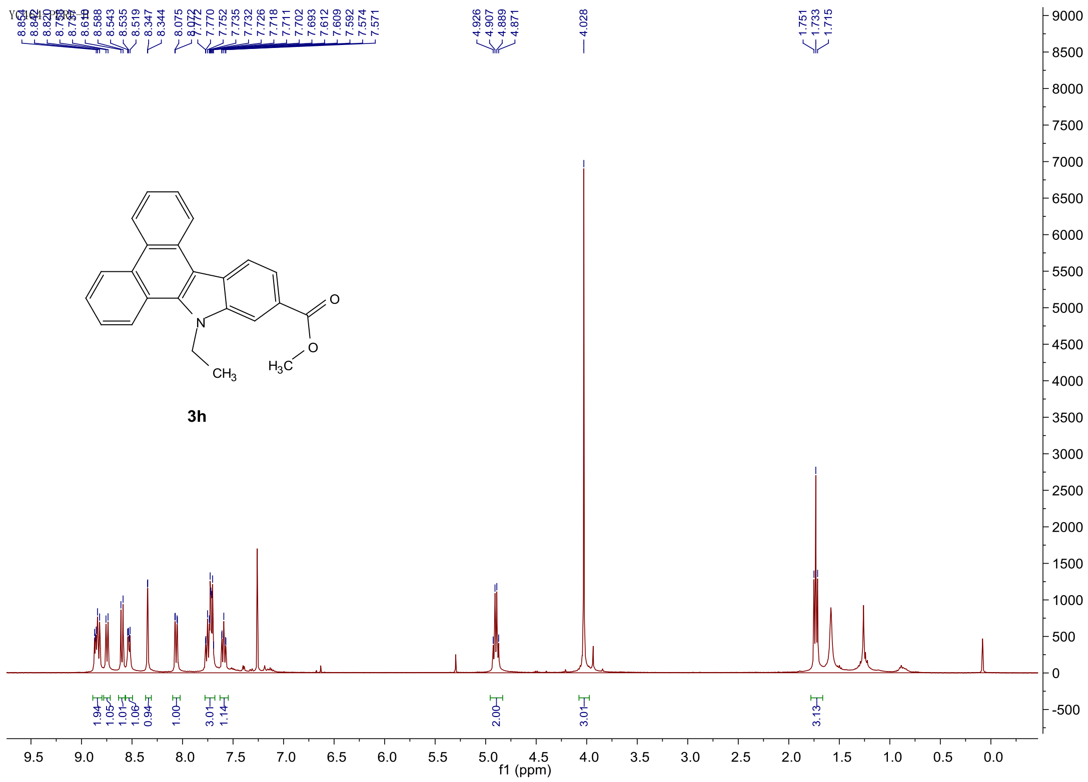
122.68
103.40
100.14
77.48
77.16
76.84
41.42
15.32
N
N
CH3
3e
f1 (ppm)

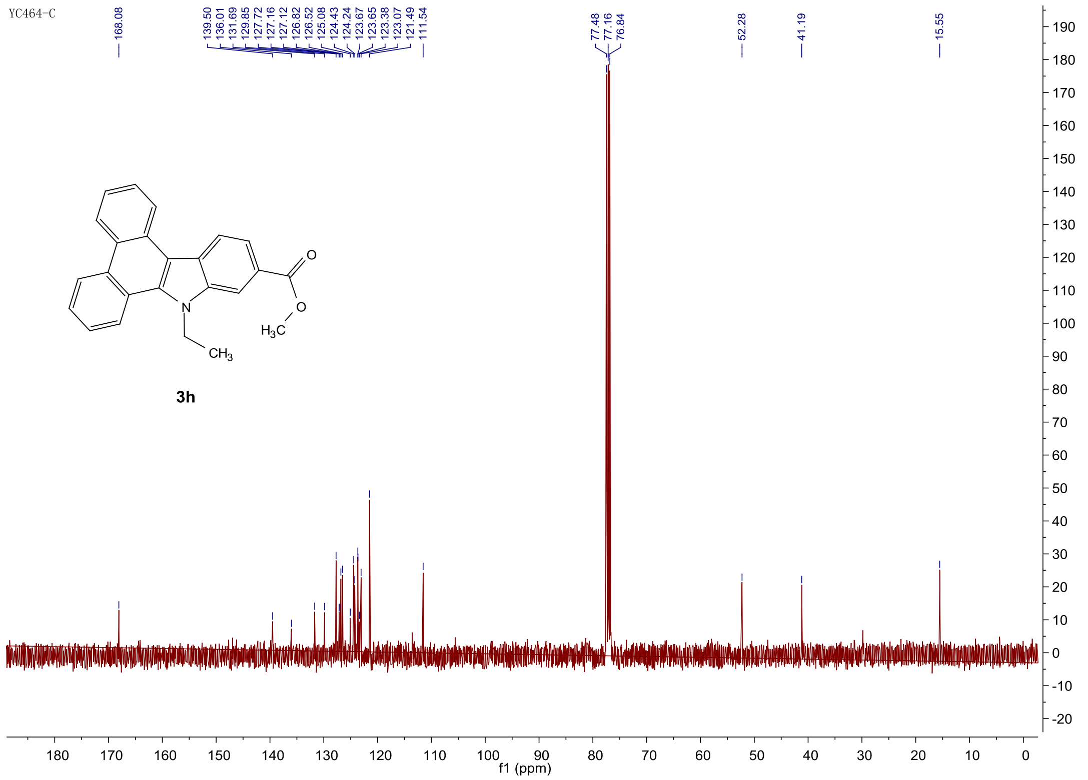

9.428
9.410
8.886
8.861
8.757
8.737
8.521
8.503
7.876
7.835
7.833
7.817
7.801
7.708
7.765
7.753
7.747
7.738
7.728
7.723
7.710
7.644
7.627
7.609
7.552
7.531
7.513
N
N
CH3
3f
f1 (ppm)
0.97
1.04
0.91
1.00
1.05
1.96
2.06
1.19
1.14
2.00
3.16

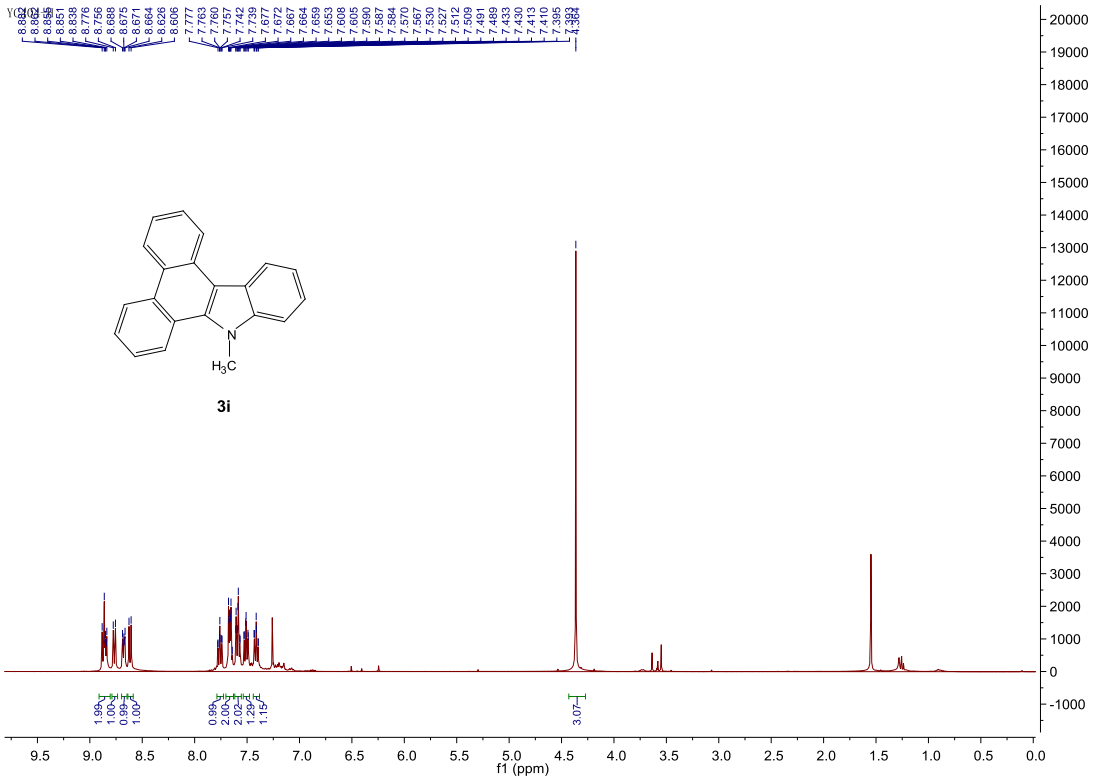

YC-553-C
140.64
129.37
127.33
127.20
127.03
127.01
126.91
124.81
124.52
123.49
123.29
123.16
100.15
77.48
77.16
76.84
41.63
15.45
N
N
CH3
3f
f1 (ppm)

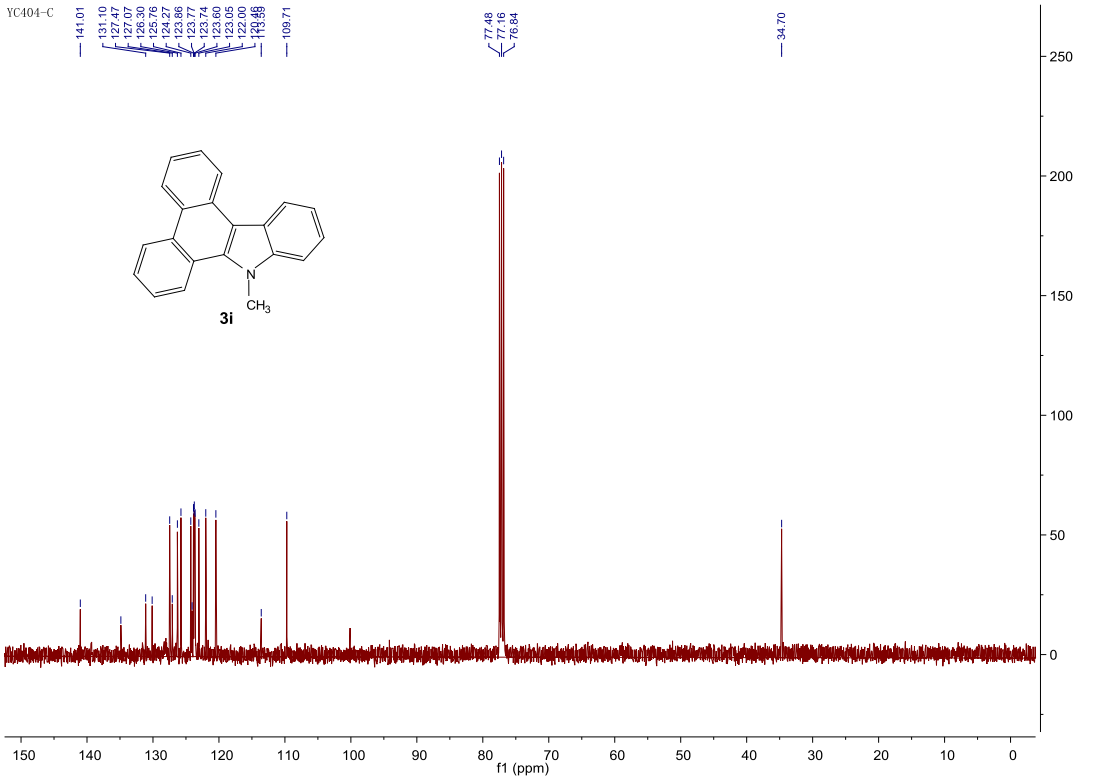

F
N
CH3
3g
f1 (ppm)

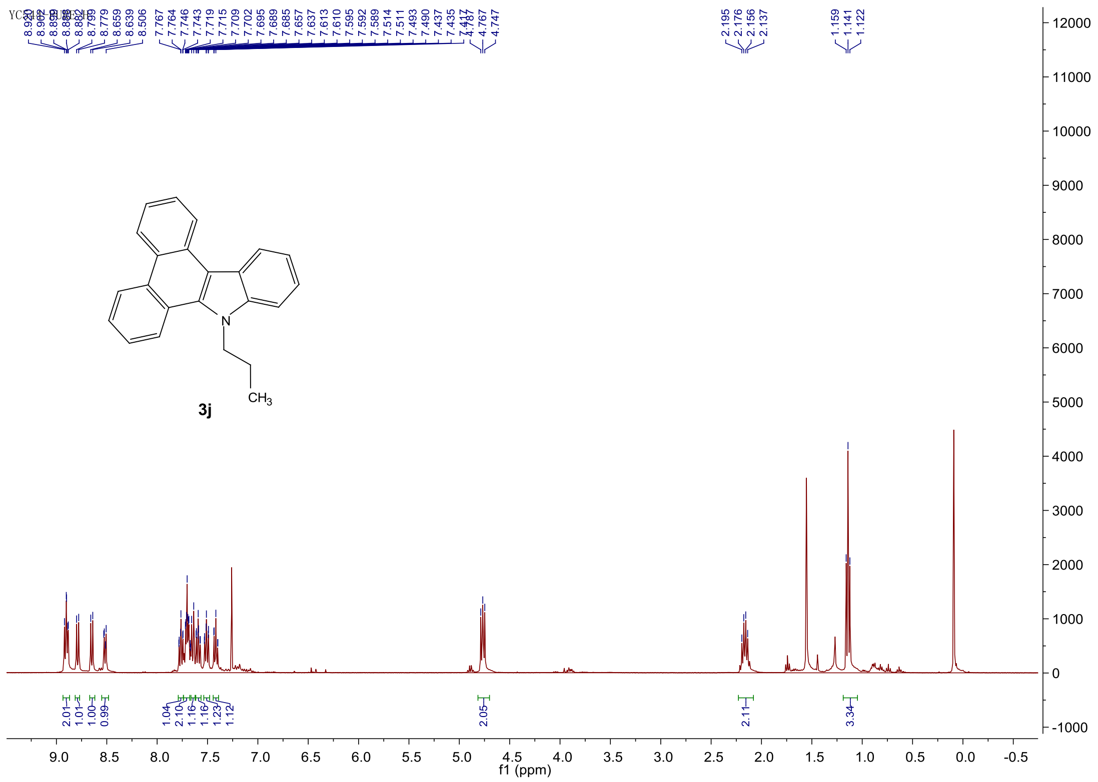

F
N
CH3
3g
f1 (ppm)

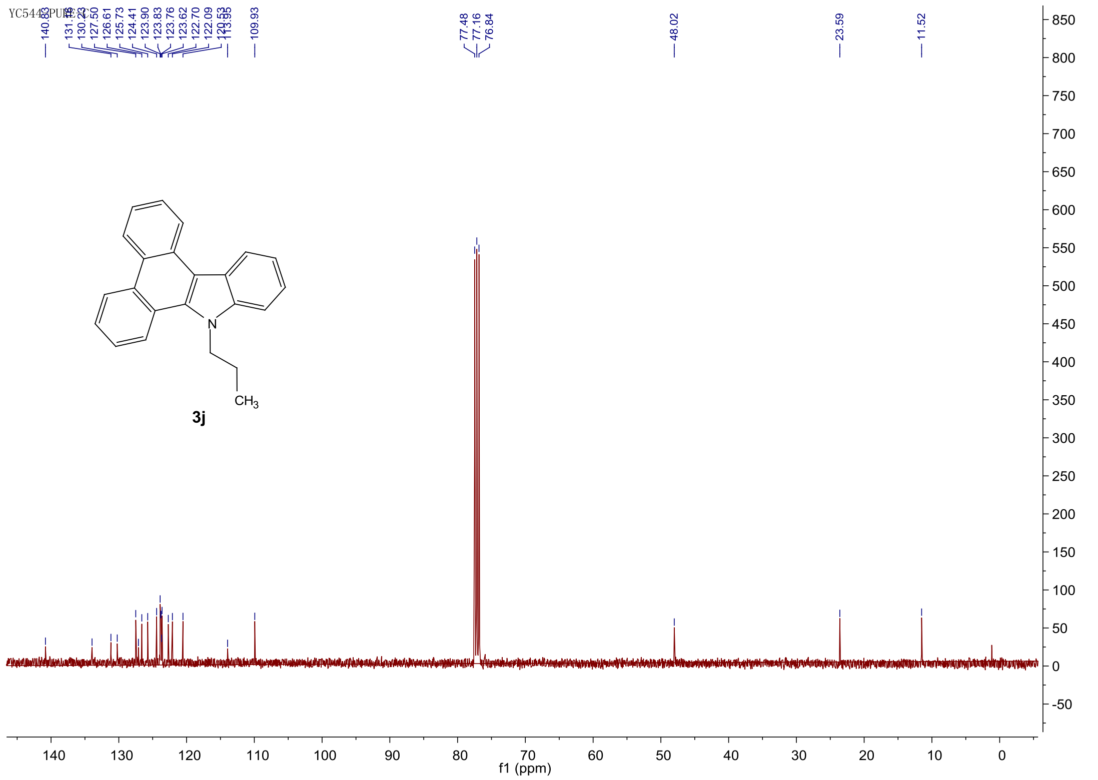

8.854
8.842
8.820
8.758
8.737
8.616
8.610
8.588
8.543
8.535
8.519
8.347
8.344
8.075
8.072
7.772
7.770
7.752
7.735
7.732
7.726
7.718
7.711
7.702
7.693
7.612
7.609
7.592
7.574
7.571
4.926
4.907
4.889
4.871
4.028
1.751
1.733
1.715
CH3
H3C
O
N
3h
1.94
1.05
1.01
1.06
0.94
1.00
3.01
1.14
2.00
3.01
3.13
f1 (ppm)

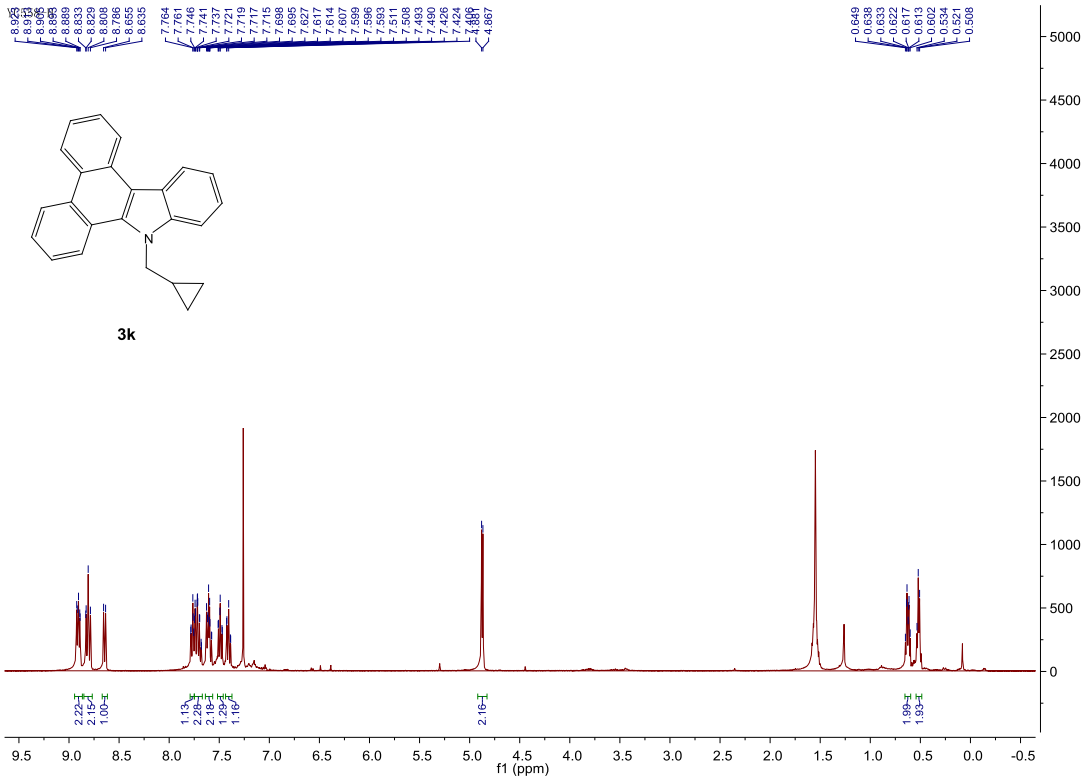

YC464-C
168.08
139.50
136.01
131.69
129.85
127.72
127.16
127.12
126.82
126.52
125.08
124.43
124.24
123.67
123.65
123.38
123.07
121.49
111.54
77.48
77.16
76.84
52.28
41.19
15.55
CH3
H3C
O
N
3h
f1 (ppm)

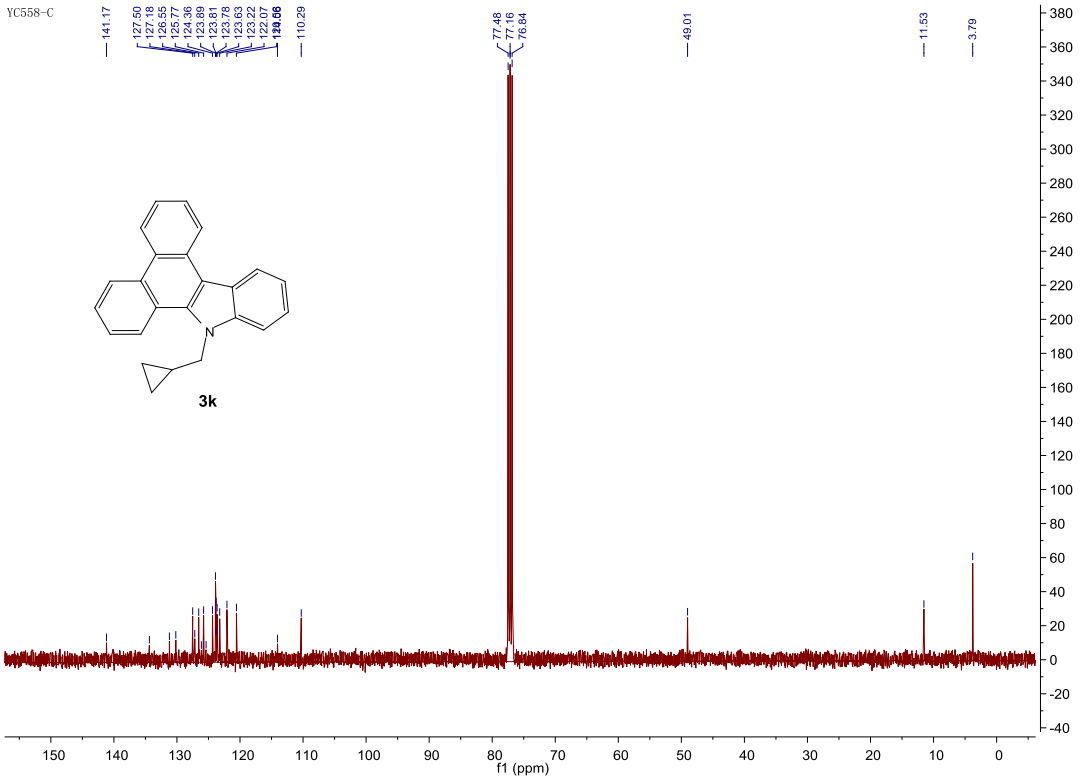

8.882
8.862
8.851
8.838
8.776
8.756
8.688
8.675
8.671
8.664
8.626
8.606
7.777
7.763
7.760
7.757
7.742
7.739
7.677
7.672
7.667
7.664
7.659
7.653
7.608
7.605
7.590
7.587
7.584
7.570
7.567
7.530
7.527
7.512
7.509
7.491
7.489
7.453
7.430
7.413
7.410
7.395
7.393
7.384
N
H3C
3i
1.99
1.00
0.99
1.00
0.99
2.05
2.02
1.29
1.15
3.07
f1 (ppm)

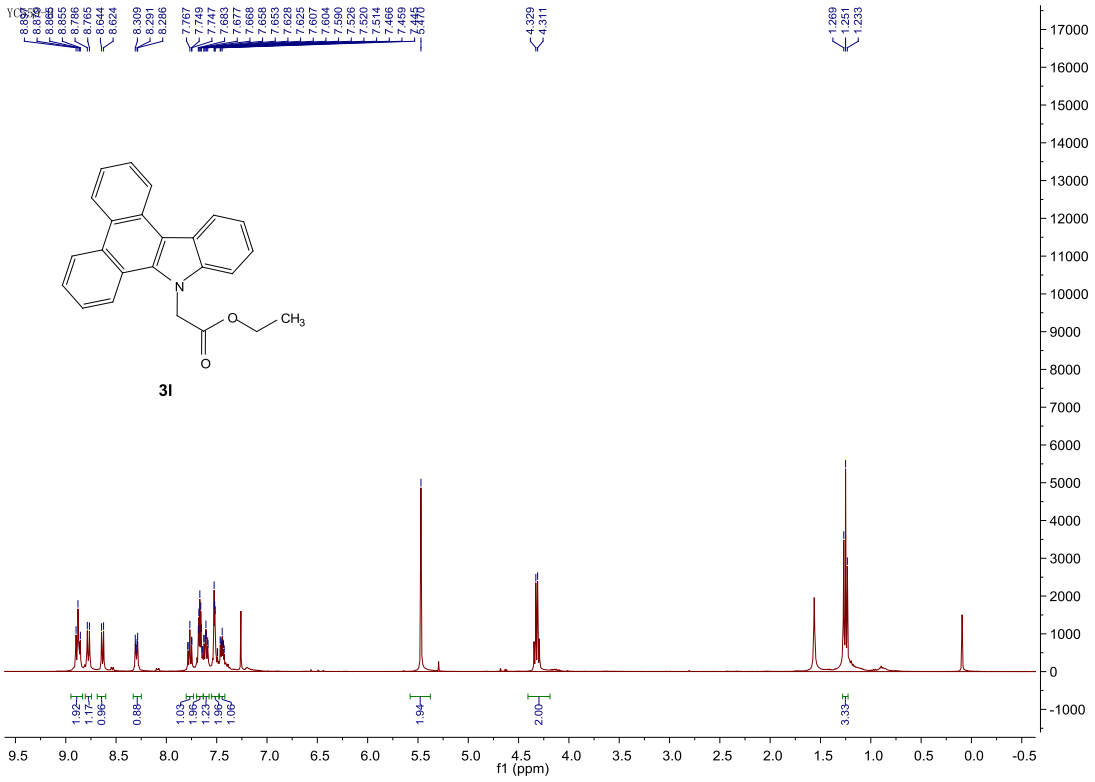

YC404-C
141.01
131.10
127.47
127.07
126.30
125.76
124.27
123.86
123.77
123.74
123.60
123.05
122.00
120.66
120.59
109.71
77.48
77.16
76.84
34.70
N
CH3
3i
f1 (ppm)

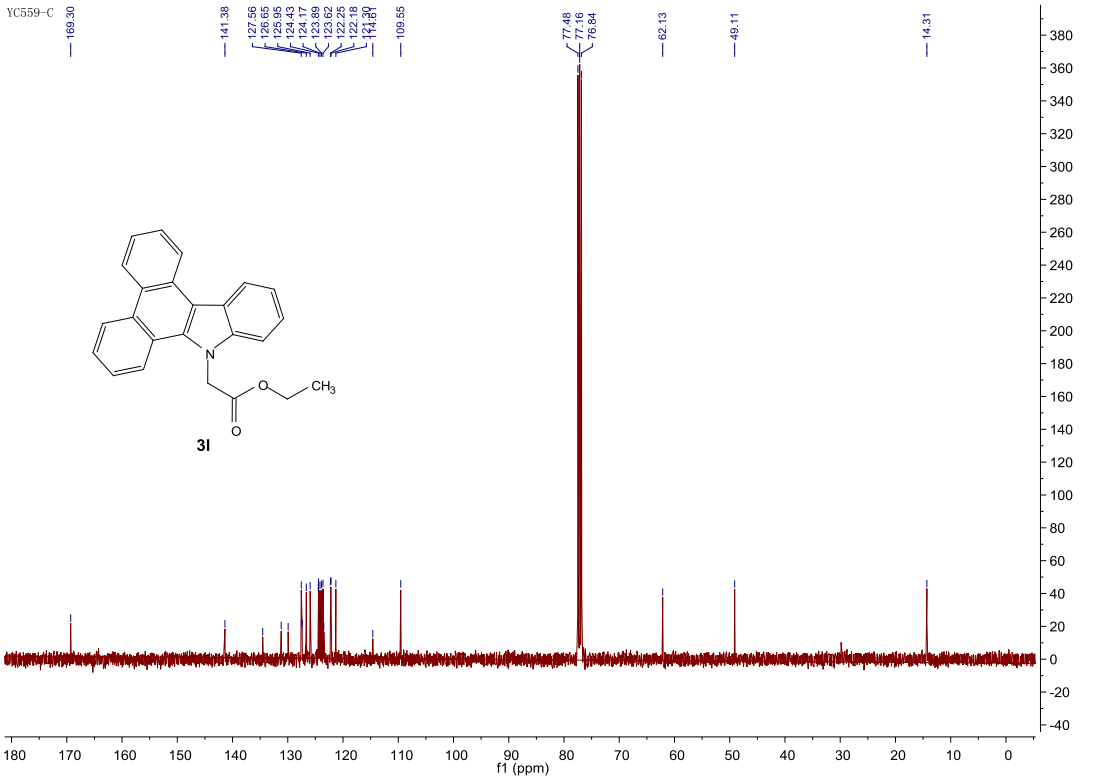

8.920
8.902
8.799
8.779
8.659
8.639
8.506
7.767
7.764
7.746
7.743
7.719
7.715
7.709
7.702
7.695
7.689
7.685
7.657
7.637
7.613
7.610
7.595
7.592
7.589
7.514
7.511
7.493
7.490
7.437
7.435
4.787
4.767
4.747
2.195
2.176
2.156
2.137
1.159
1.141
1.122
N
CH_3
3j
2.01
1.01
1.00
0.99
1.04
2.10
1.16
1.16
1.23
1.12
2.05
2.11
3.34
f1 (ppm)

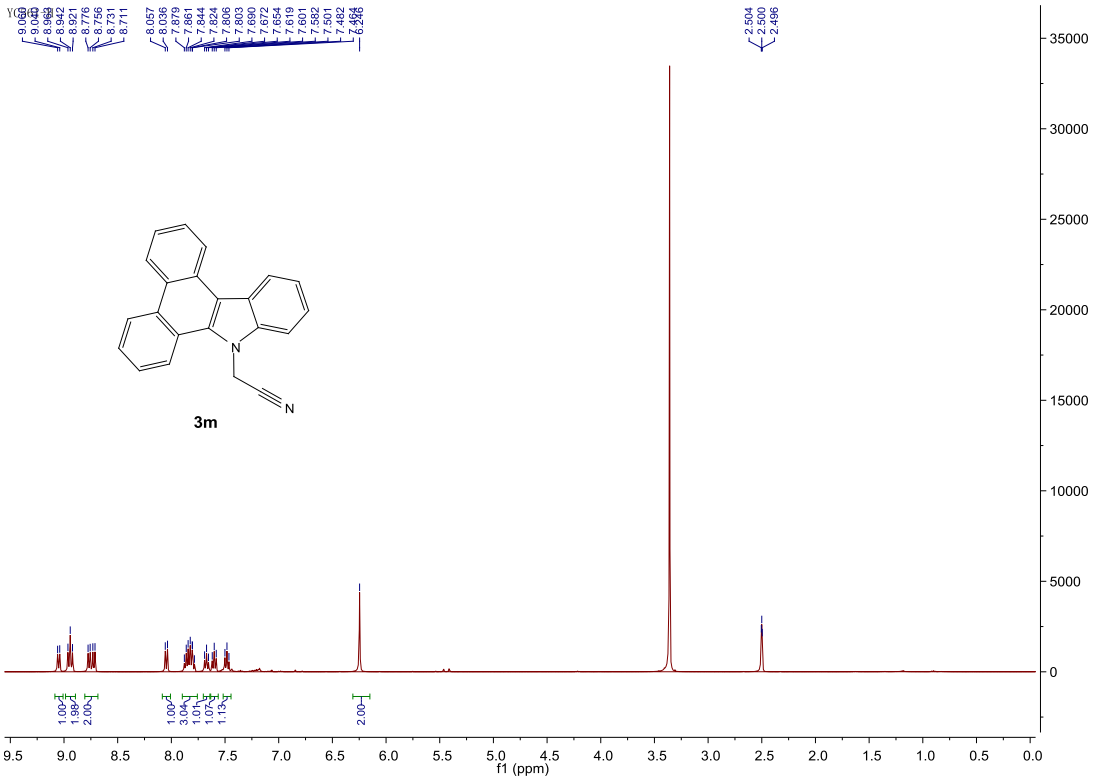

140.83
131.34
130.23
127.50
126.61
125.73
124.41
123.90
123.83
123.76
123.62
122.70
122.09
109.93
77.48
77.16
76.84
48.02
23.59
11.52
N
CH_3
3j
f1 (ppm)

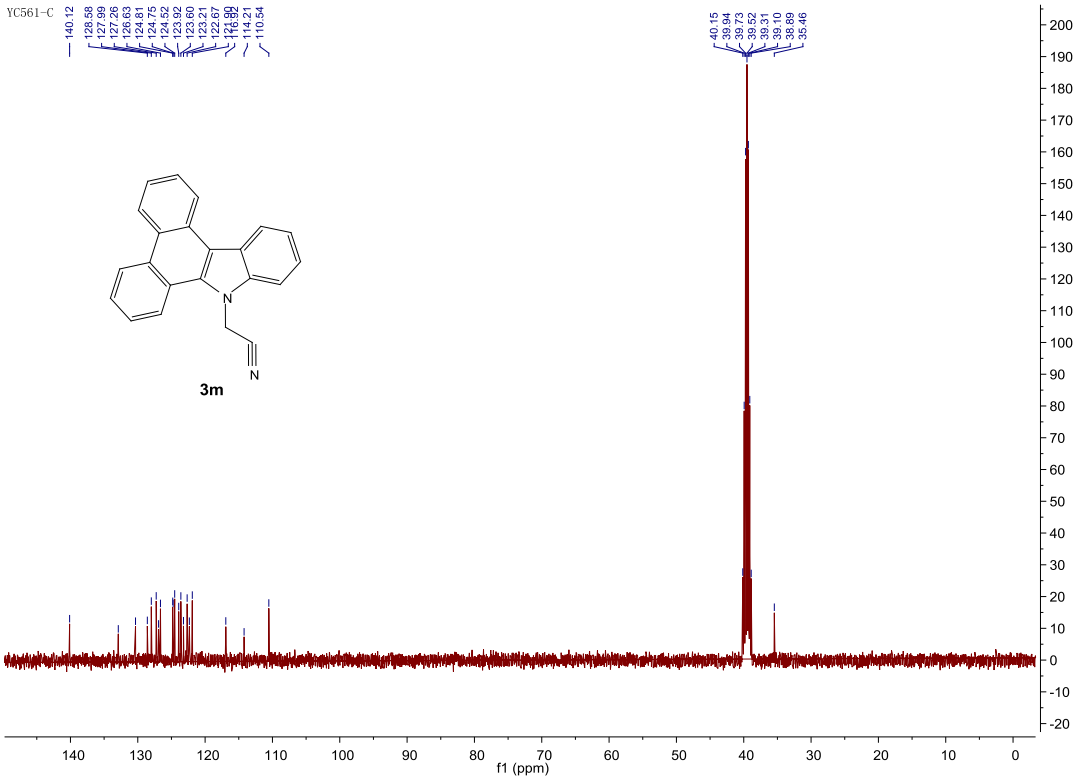

3k
f1 (ppm)

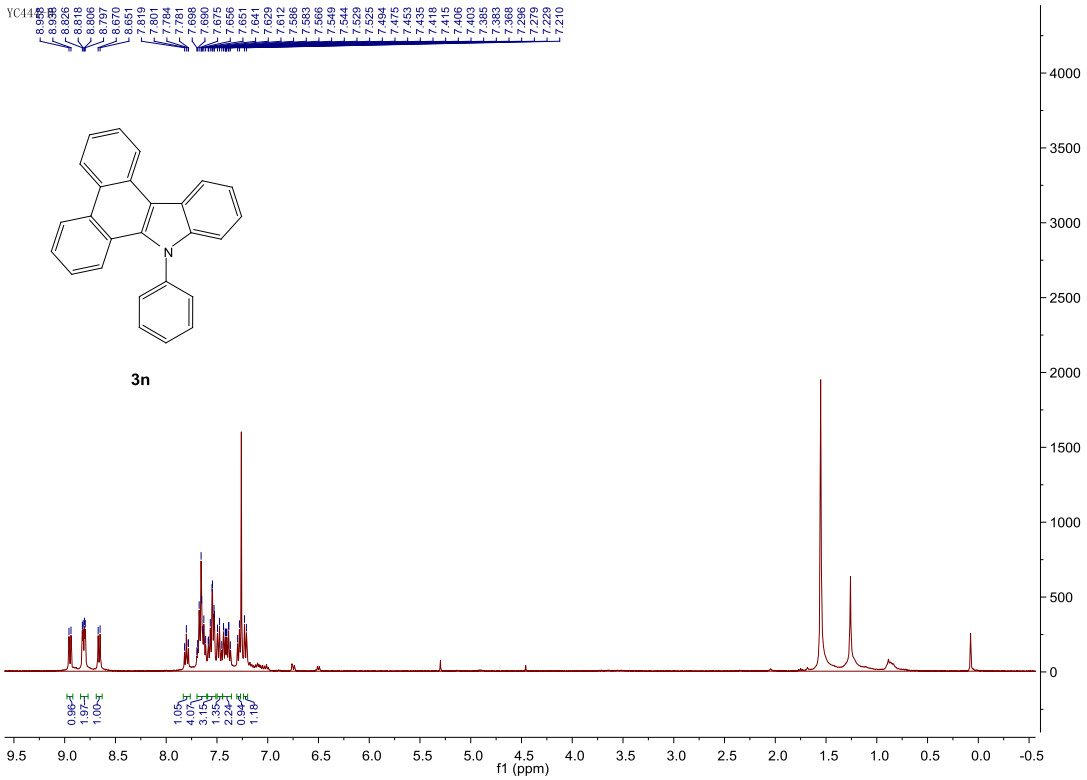

YC558-C
3k
f1 (ppm)

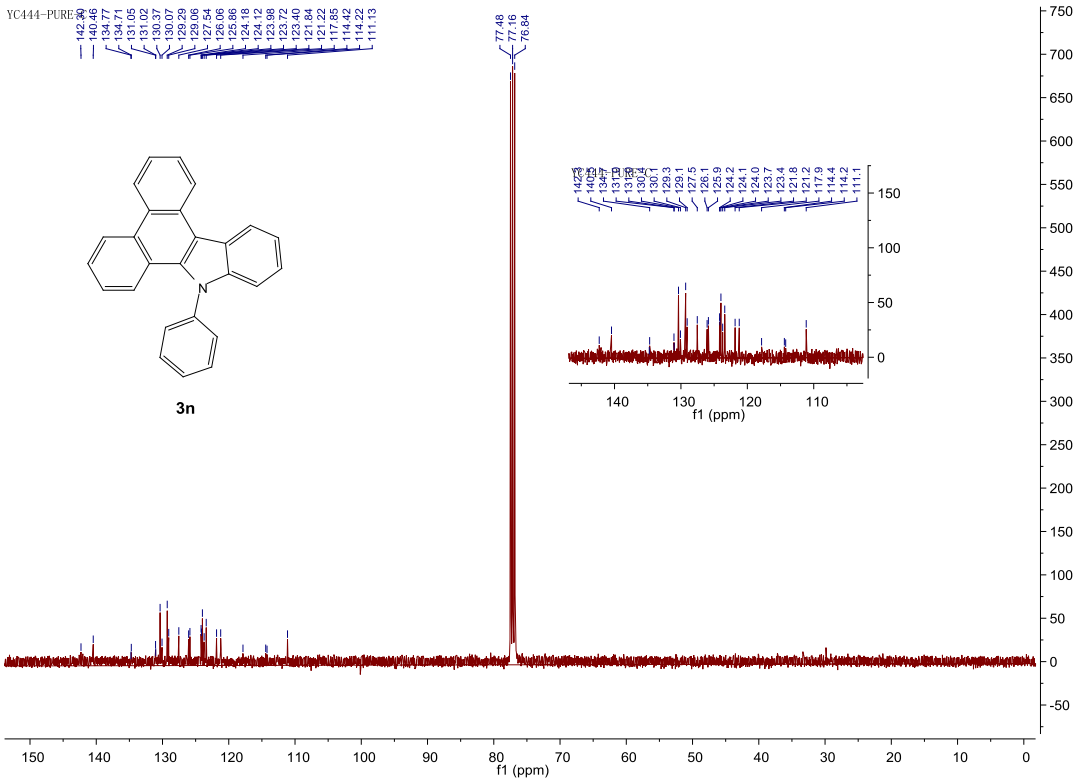

8.855
8.786
8.765
8.644
8.624
8.309
8.291
8.286
7.767
7.749
7.747
7.683
7.677
7.668
7.658
7.653
7.628
7.625
7.607
7.604
7.590
7.586
7.520
7.514
7.466
7.459
4.329
4.311
1.269
1.251
1.233
N
O
CH3
O
3l
1.92
1.17
0.96
0.88
1.03
1.96
1.23
1.96
1.06
1.94
2.00
3.33
f1 (ppm)

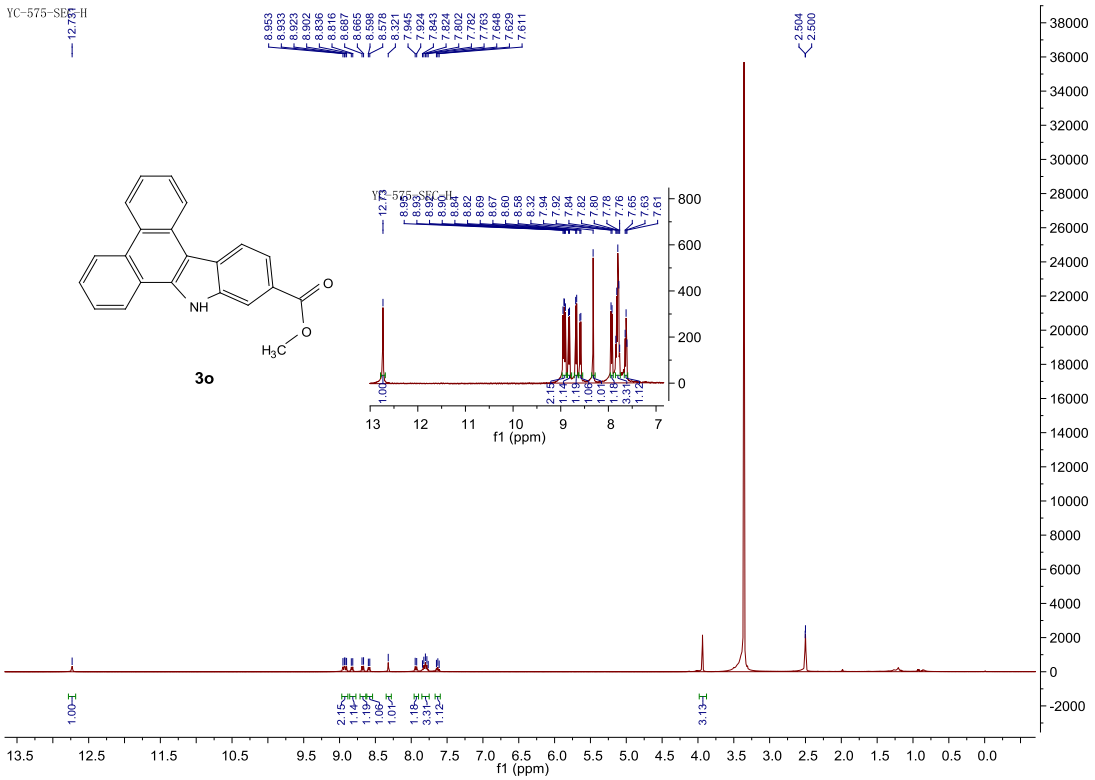

YC559-C
169.30
141.38
127.56
126.65
125.95
124.43
124.17
123.89
123.62
122.25
122.18
121.80
109.55
77.48
77.16
76.84
62.13
49.11
14.31
N
O
CH3
O
3l
f1 (ppm)

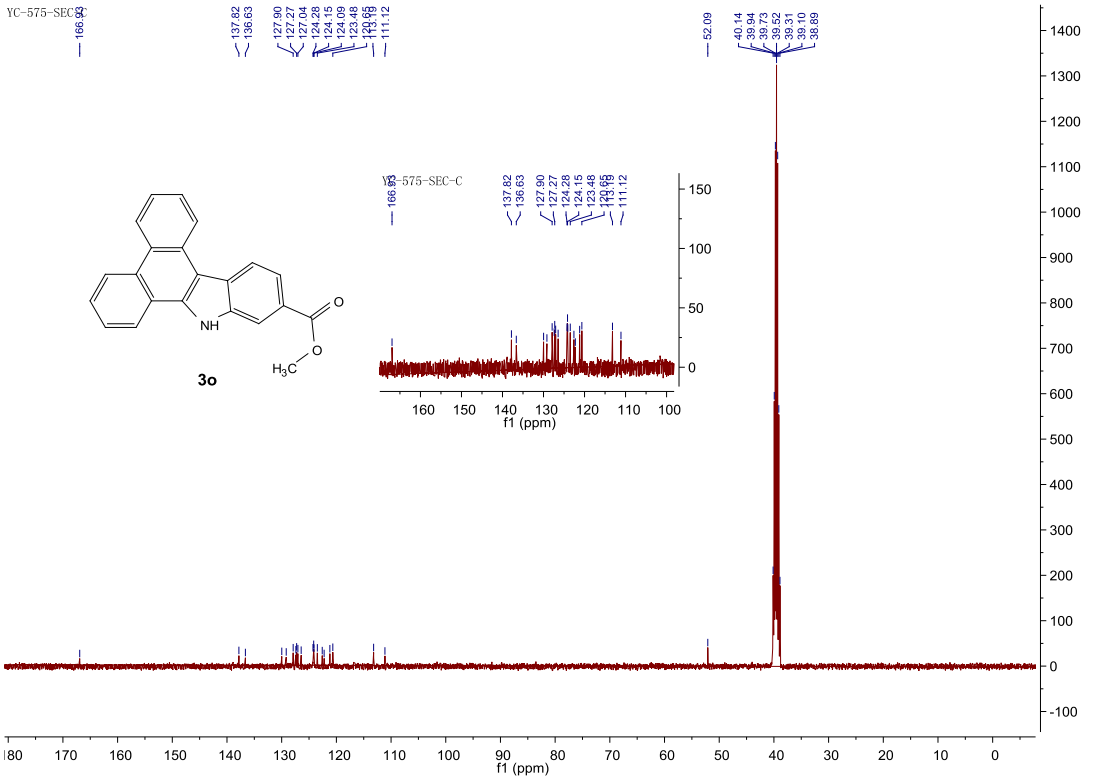

3m
f1 (ppm)

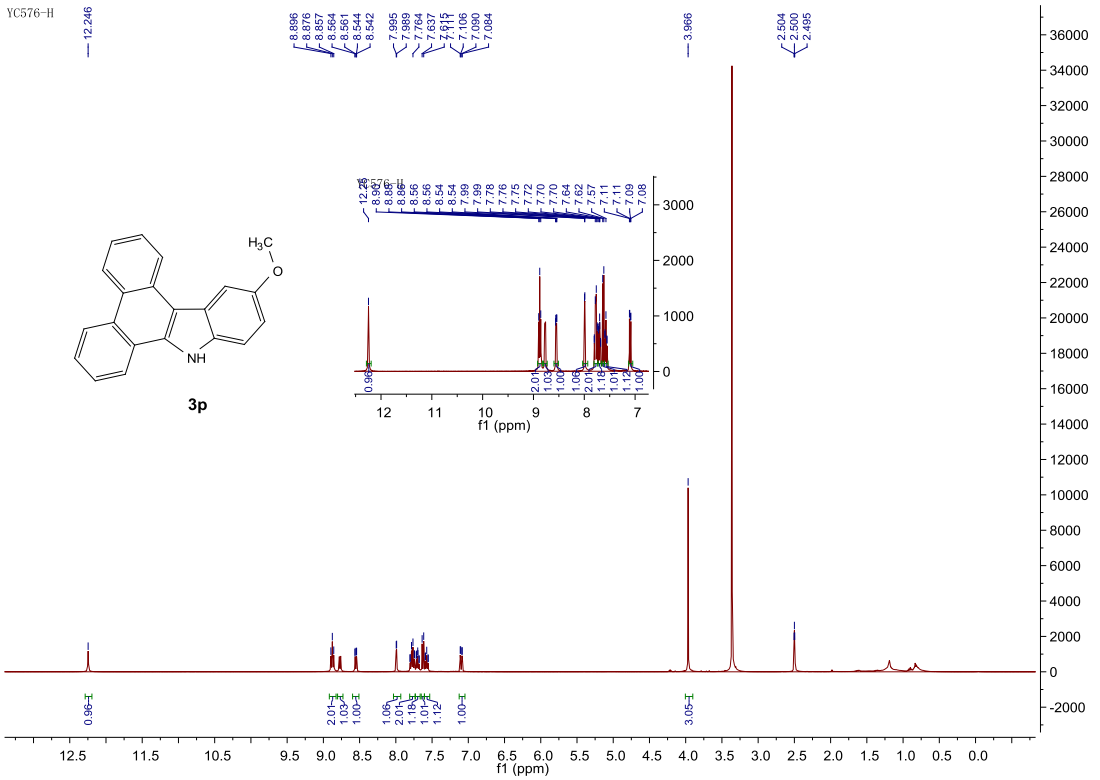

YC561-C
3m
f1 (ppm)

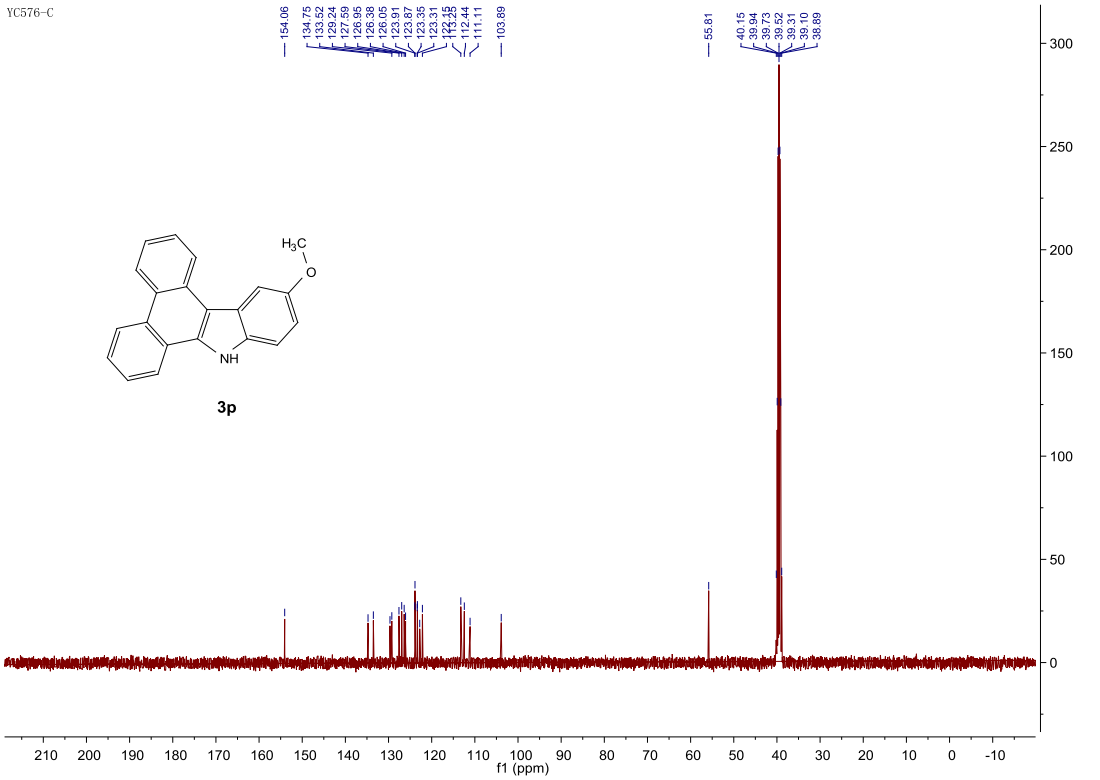

3n
f1 (ppm)

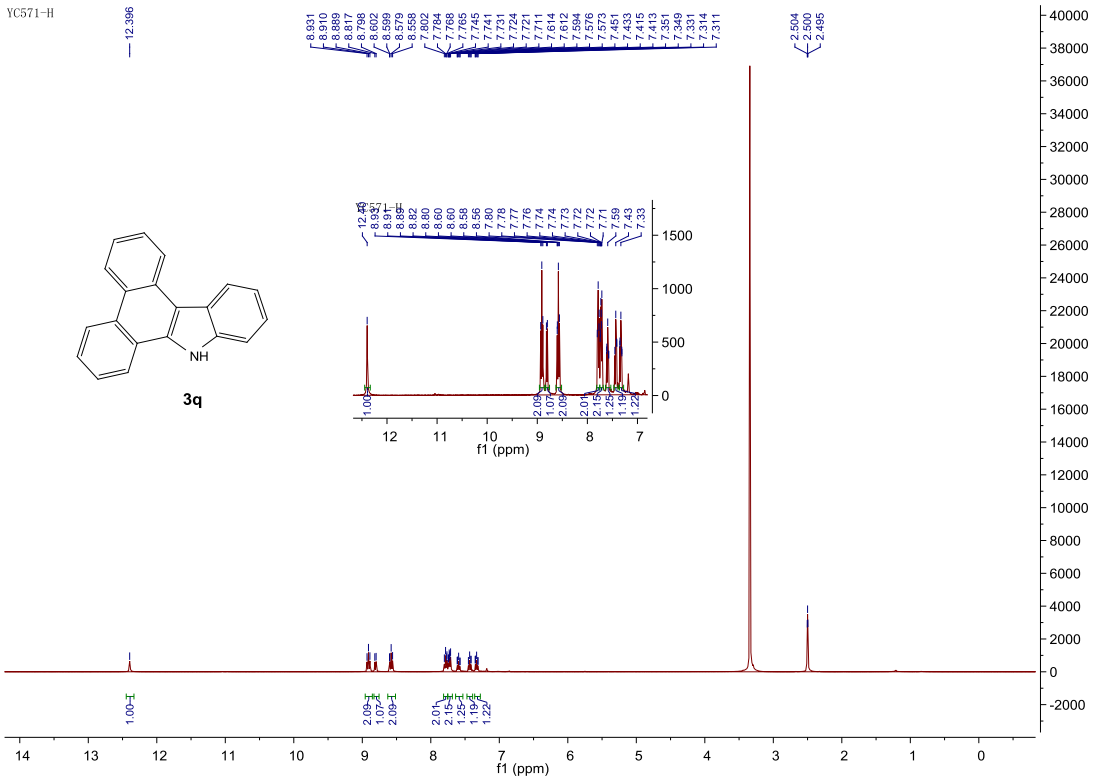

3n
f1 (ppm)
f1 (ppm)

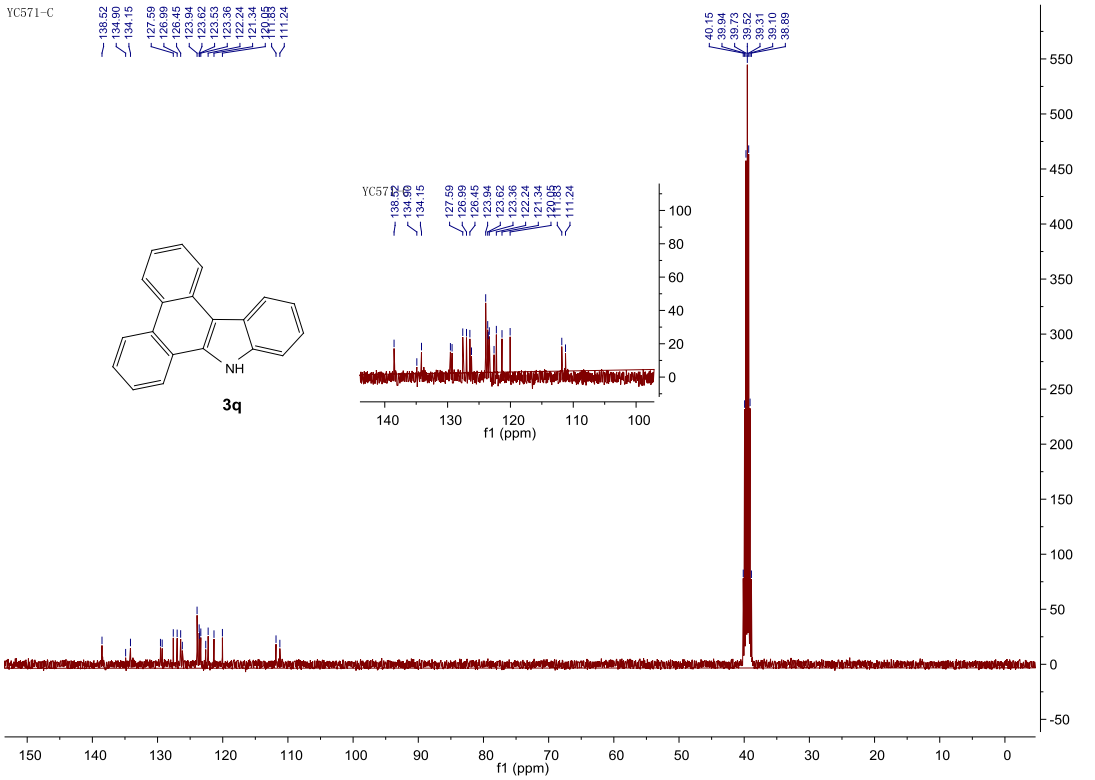

YC-575-SEC-H
12.751
8.963
8.933
8.923
8.902
8.836
8.816
8.687
8.665
8.598
8.578
8.321
8.045
7.924
7.843
7.824
7.802
7.782
7.763
7.648
7.629
7.611
2.504
2.500
NH
O
O
H3C
3o
1.00
2.15
1.14
1.15
1.09
1.01
1.18
3.31
1.12
3.13
f1 (ppm)

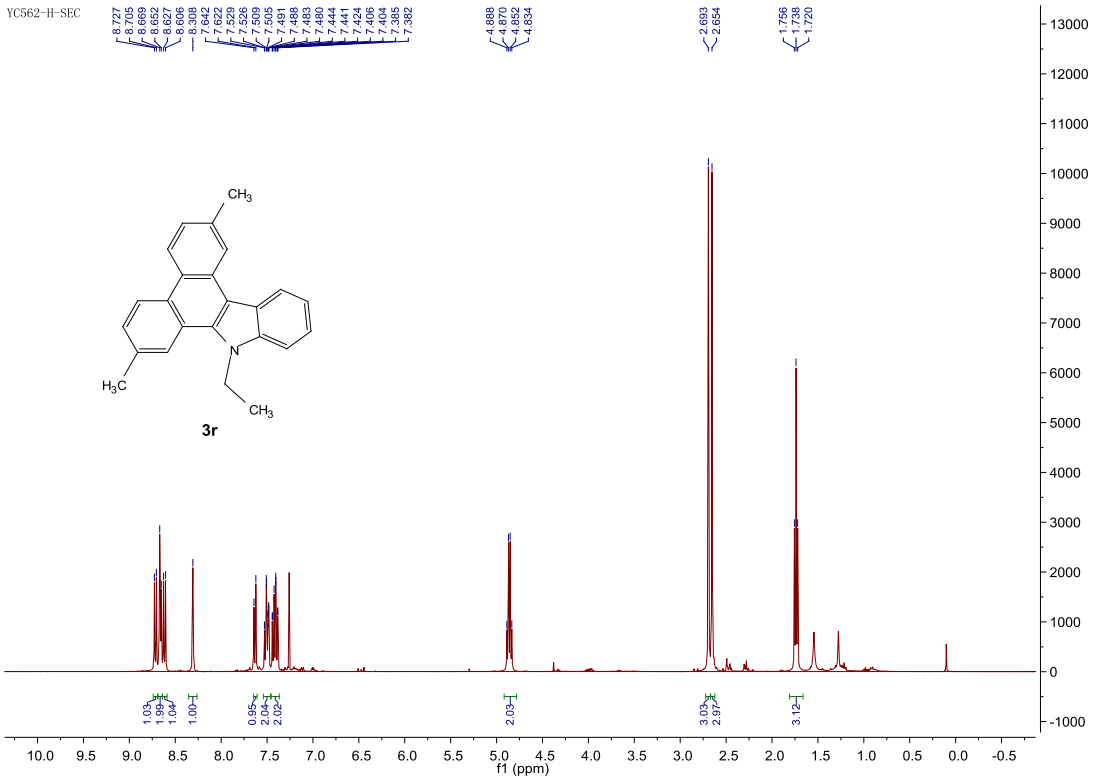

YC-575-SEC-C
166.93
137.82
136.63
127.90
127.27
127.04
124.28
124.15
124.09
123.48
120.15
119.16
111.12
52.09
40.14
39.94
39.73
39.52
39.31
39.10
38.89
NH
O
O
H3C
3o
f1 (ppm)

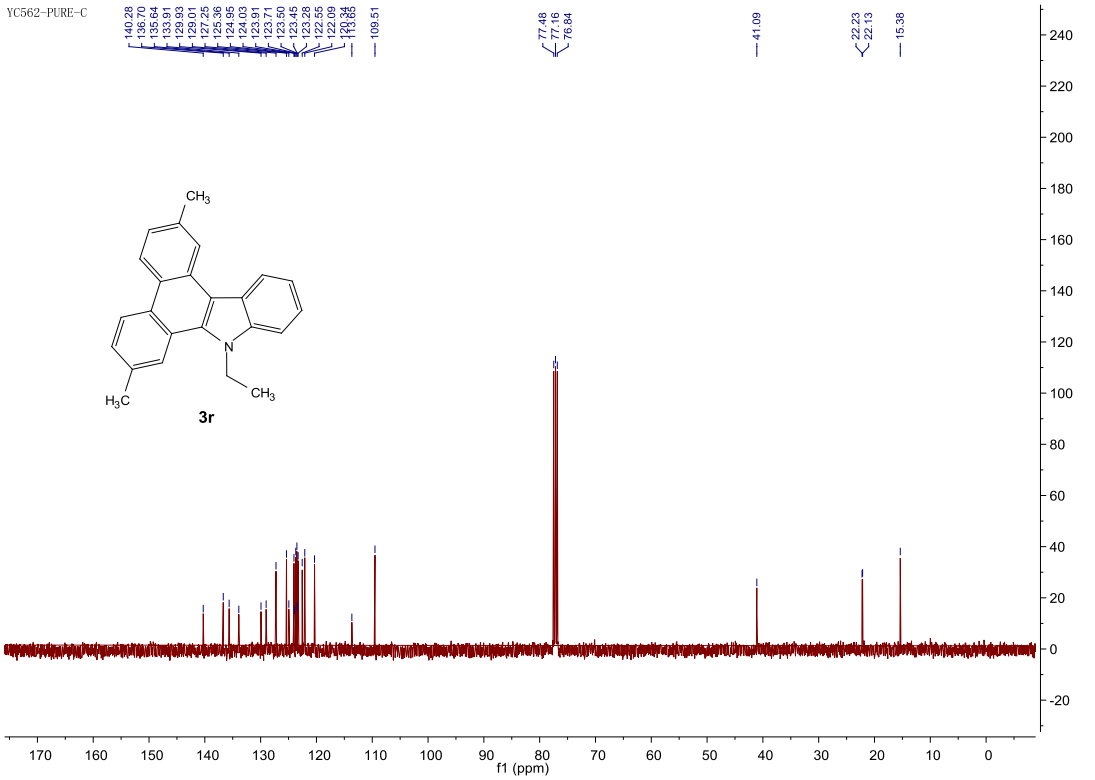

YC576-H
12.246
8.896
8.876
8.857
8.564
8.561
8.544
8.542
7.995
7.989
7.764
7.637
7.615
7.611
7.106
7.090
7.084
3.966
2.504
2.500
2.495
H3C
O
NH
3p
f1 (ppm)

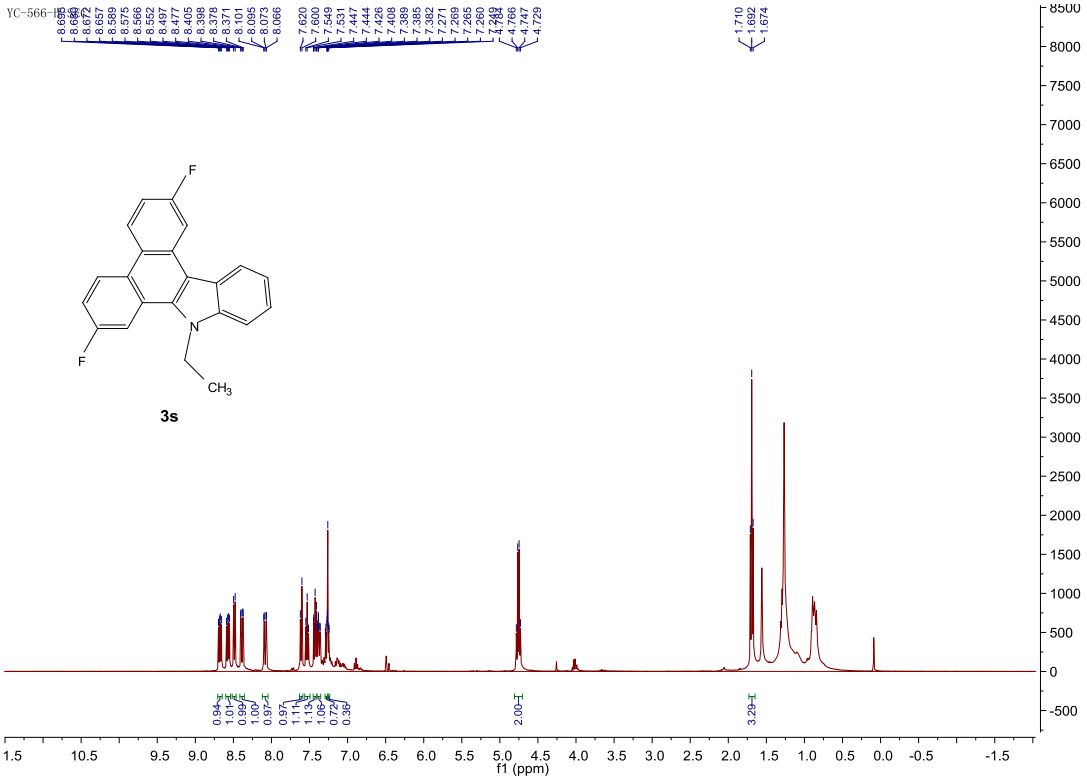

YC576-C
154.06
134.75
133.52
129.24
127.59
126.95
126.38
126.05
123.91
123.87
123.35
123.31
122.15
113.25
112.44
111.11
103.89
55.81
40.15
39.94
39.73
39.52
39.31
39.10
38.89
H3C
O
NH
3p
f1 (ppm)

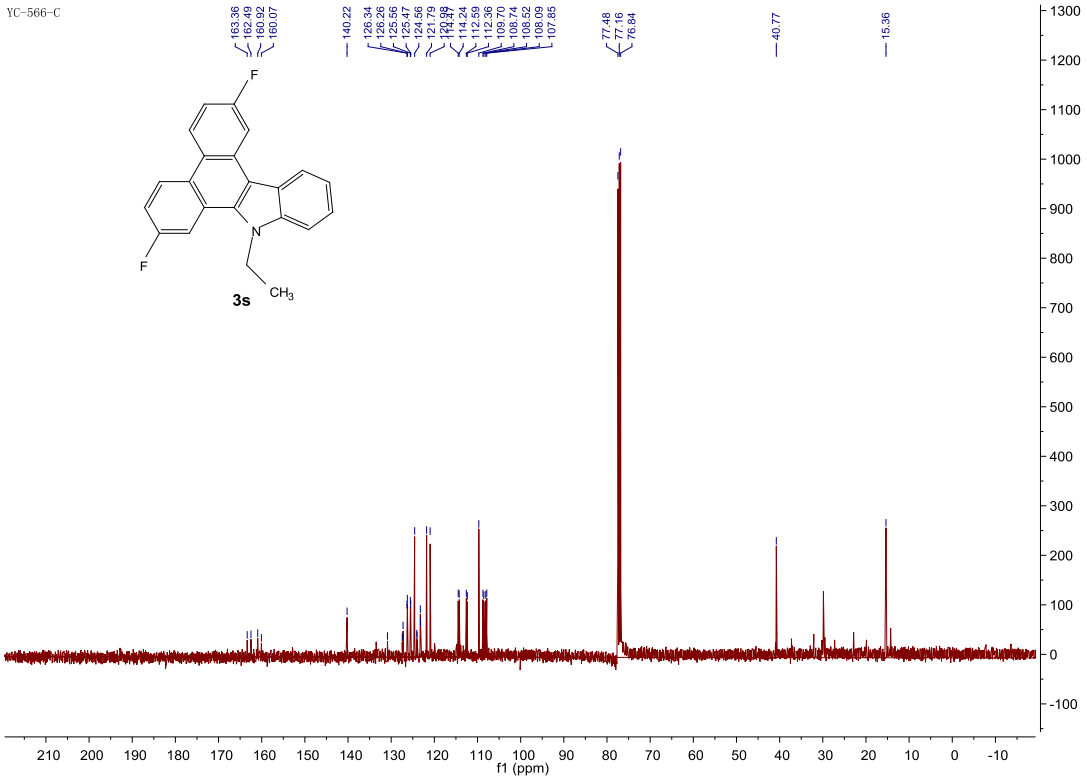

YC571-H
12.396
8.931
8.910
8.889
8.817
8.798
8.602
8.599
8.579
8.558
7.802
7.784
7.768
7.765
7.745
7.741
7.731
7.724
7.721
7.711
7.614
7.612
7.594
7.575
7.573
7.451
7.433
7.415
7.413
7.351
7.349
7.331
7.314
7.311
2.504
2.500
2.495
NH
3q
f1 (ppm)

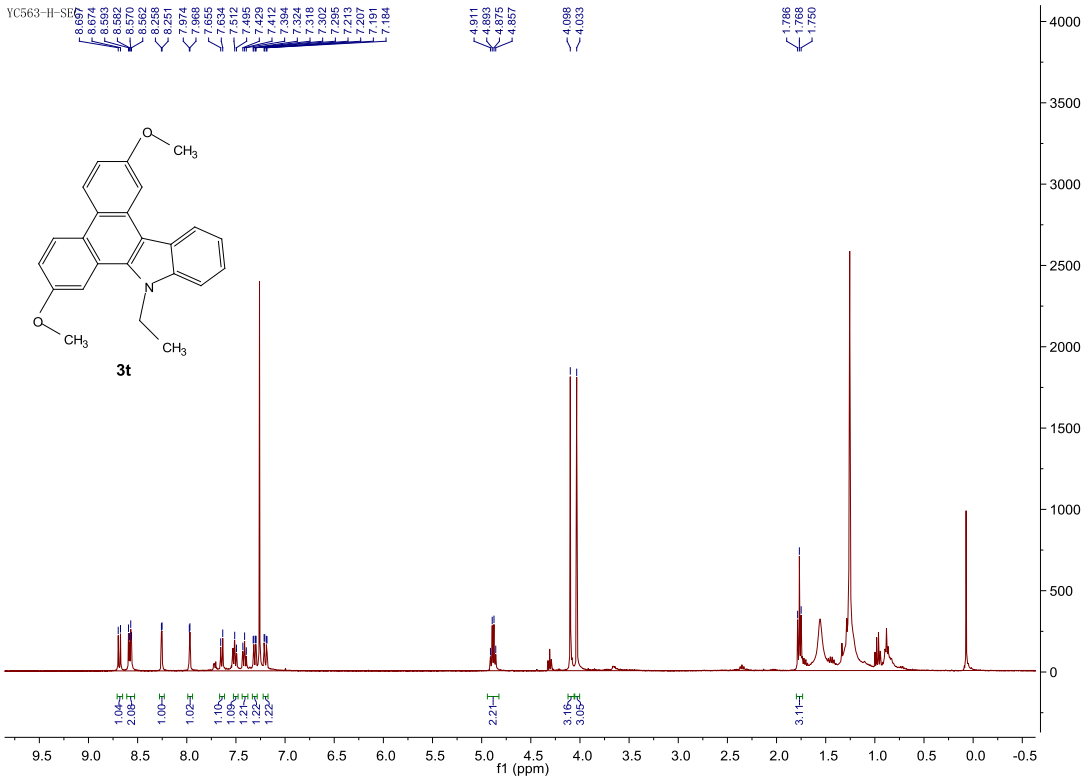

YC571-C
136.52
134.90
134.15
127.59
126.99
126.45
123.94
123.62
123.53
123.36
122.24
121.34
111.83
111.24
40.15
39.94
39.73
39.52
39.31
39.10
38.89
NH
3q
f1 (ppm)

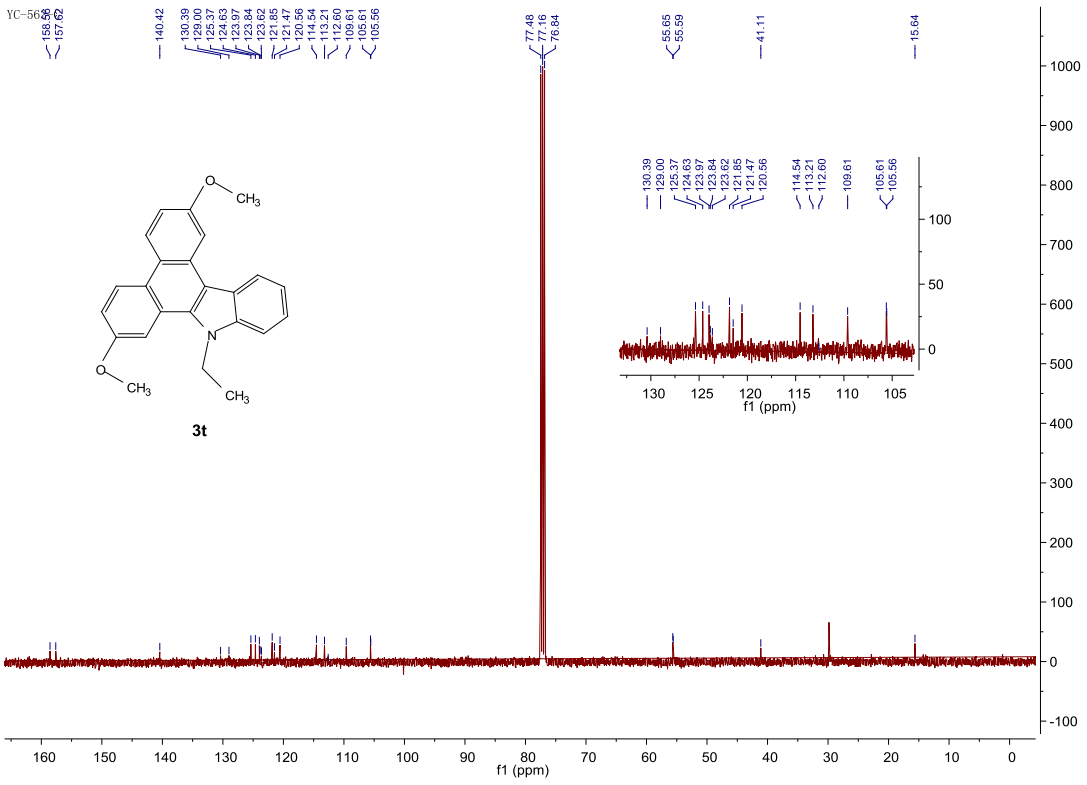

YC562-H-SEC
8.727
8.705
8.693
8.652
8.627
8.606
8.308
7.642
7.622
7.529
7.526
7.509
7.505
7.491
7.488
7.483
7.480
7.444
7.441
7.424
7.406
7.404
7.385
7.382
4.888
4.870
4.852
4.834
2.693
2.654
1.756
1.738
1.720
CH3
N
H3C
CH3
3r
1.03
1.99
1.04
1.00
0.95
2.04
2.02
2.03
3.03
2.97
3.12
f1 (ppm)

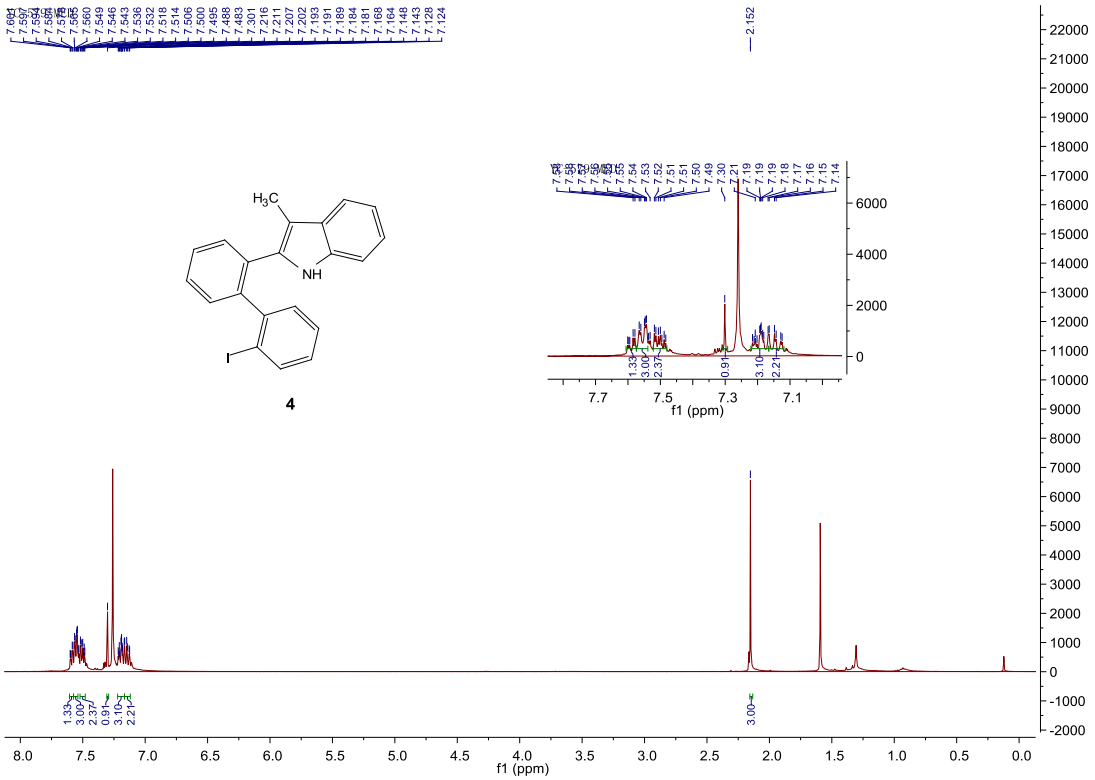

YC562-PURE-C
140.28
136.70
135.64
133.91
129.93
129.01
127.25
125.36
124.95
124.03
123.91
123.71
123.50
123.45
123.28
122.55
122.09
120.34
113.85
109.51
77.48
77.16
76.84
41.09
22.23
22.13
15.38
CH3
N
H3C
CH3
3r
f1 (ppm)

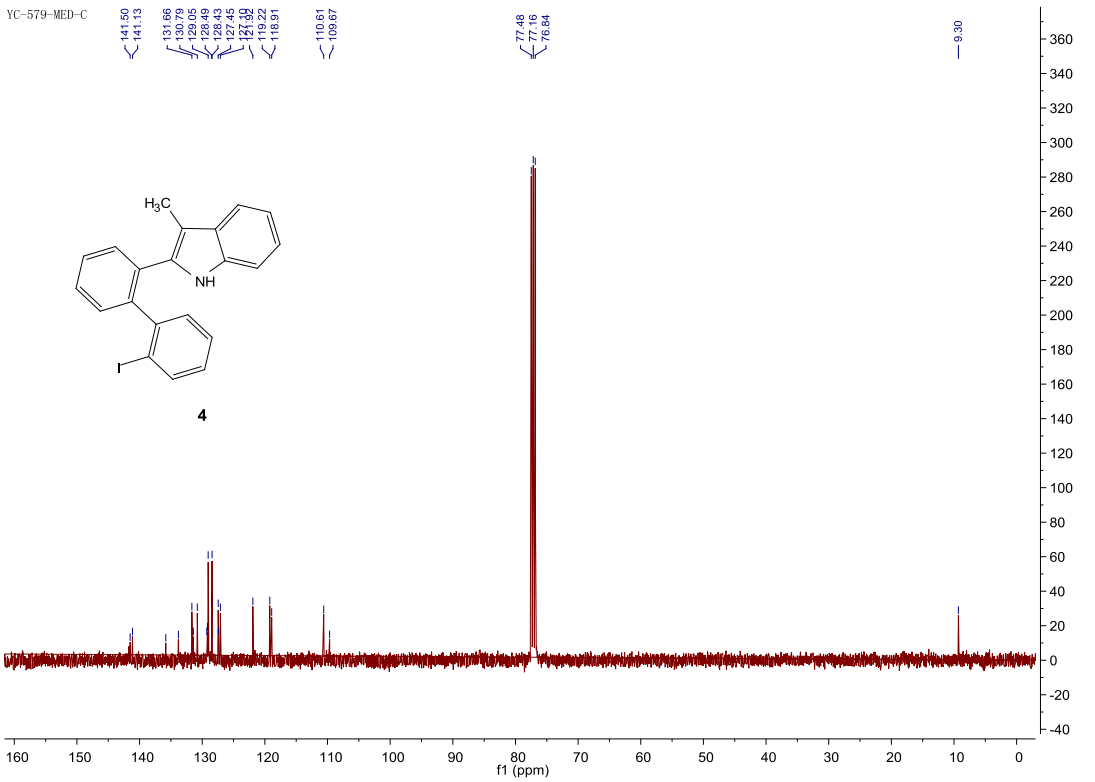

F
F
N
CH3
3s
f1 (ppm)

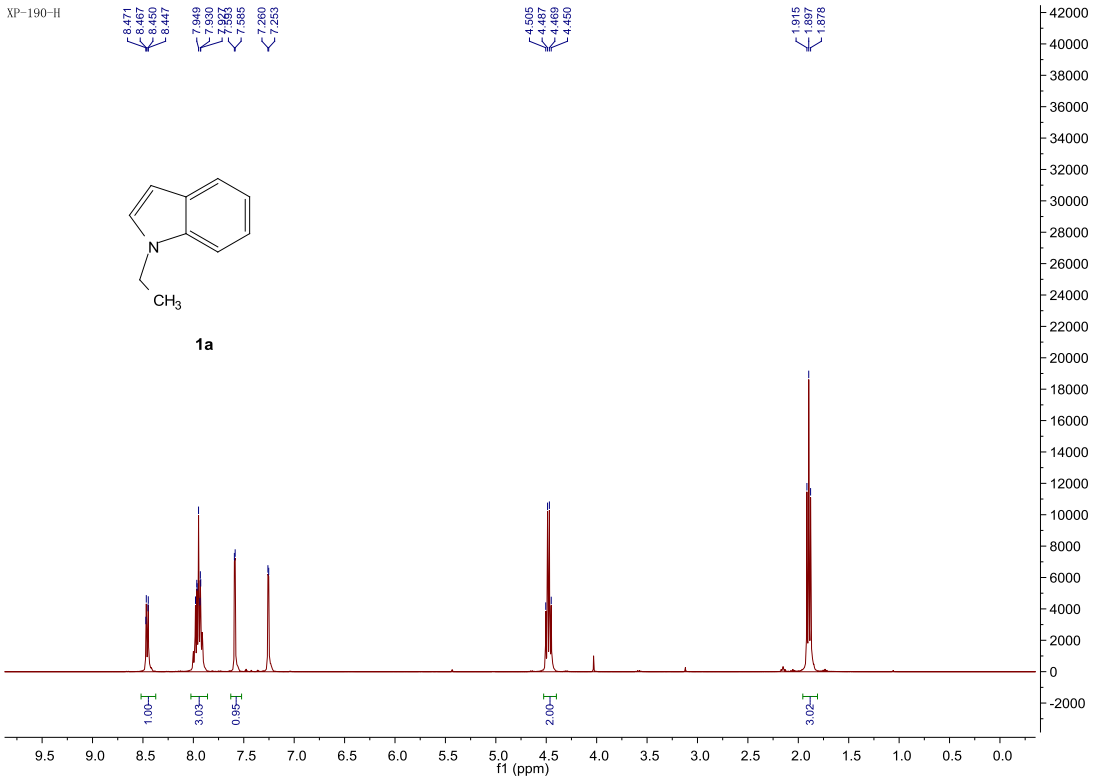

YC-566-C
F
F
N
CH3
3s
f1 (ppm)

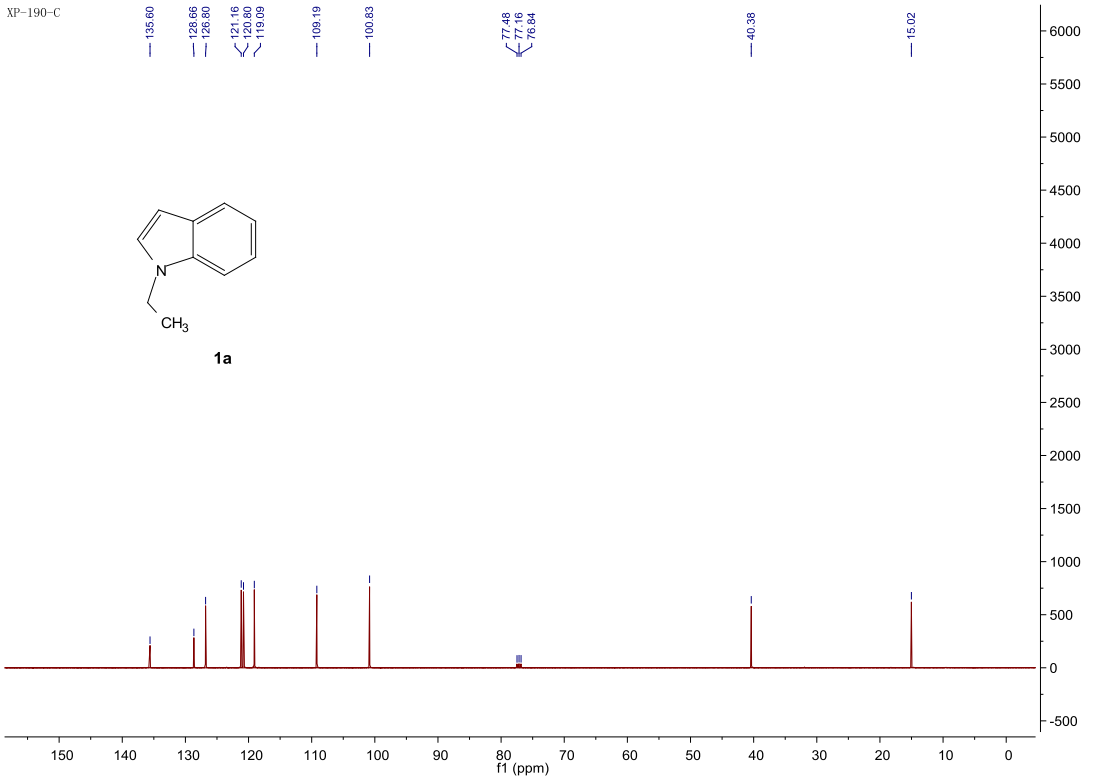

YC563-H-SE
8.697
8.674
8.593
8.582
8.570
8.562
8.558
8.251
7.974
7.968
7.655
7.634
7.512
7.495
7.429
7.412
7.394
7.324
7.318
7.302
7.295
7.213
7.207
7.191
7.184
4.911
4.893
4.875
4.857
4.098
4.033
1.786
1.768
1.750
O
CH3
N
CH3
O
CH3
CH3
3t
1.04
2.08
1.00
1.02
1.10
1.09
1.21
1.22
1.22
2.21
3.16
3.05
3.11
f1 (ppm)

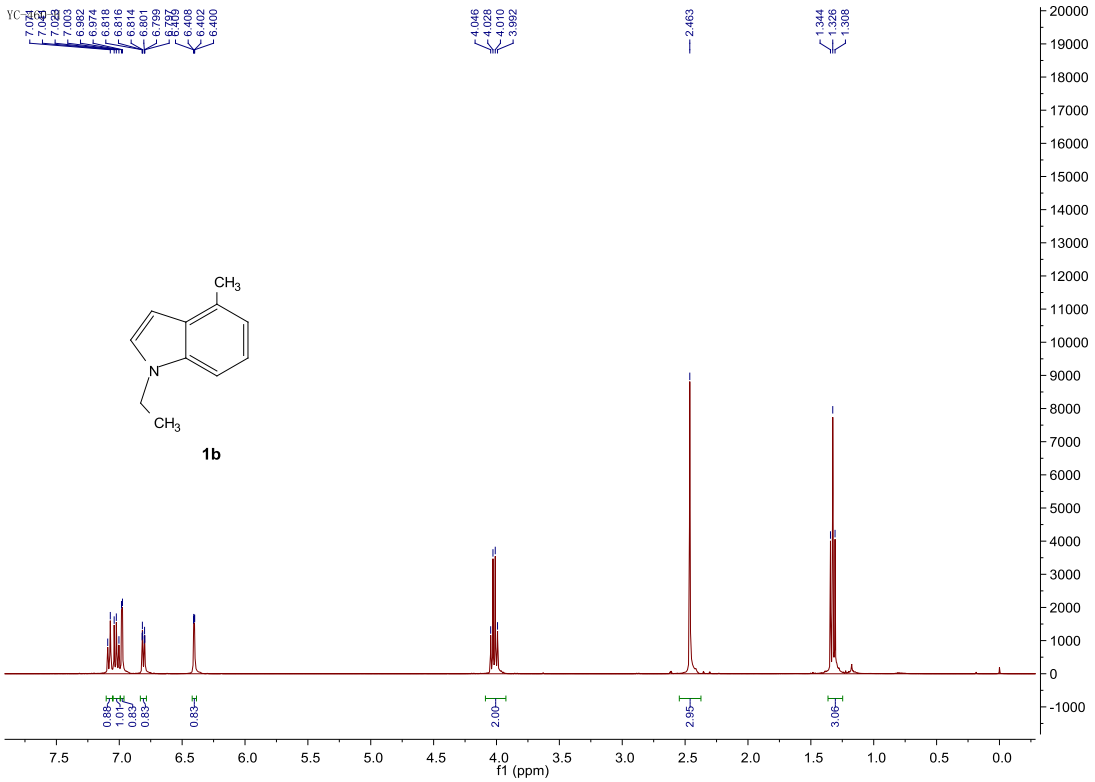

YC-563
158.36
157.62
140.42
130.39
129.00
125.37
124.63
123.97
123.84
123.62
121.85
121.47
120.56
114.54
113.21
112.60
109.61
105.61
105.56
77.48
77.16
76.84
55.65
55.59
41.11
15.64
O
CH3
N
CH3
O
CH3
CH3
3t
f1 (ppm)

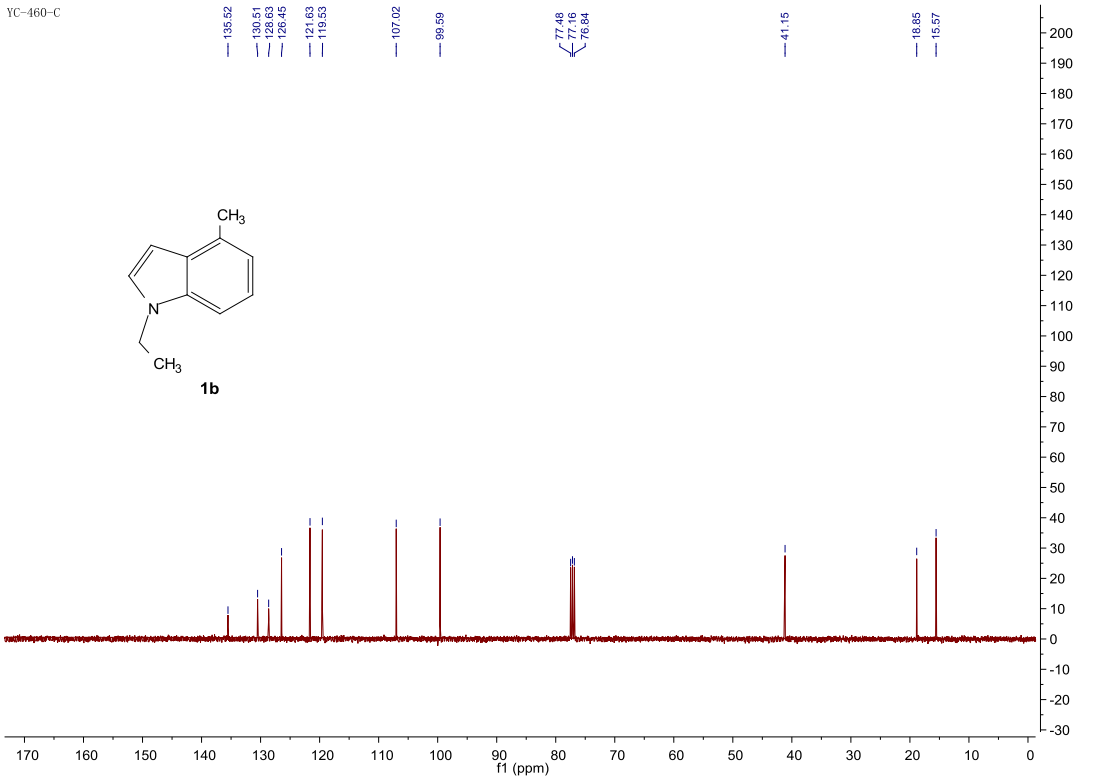

H3C
NH
I
4
f1 (ppm)

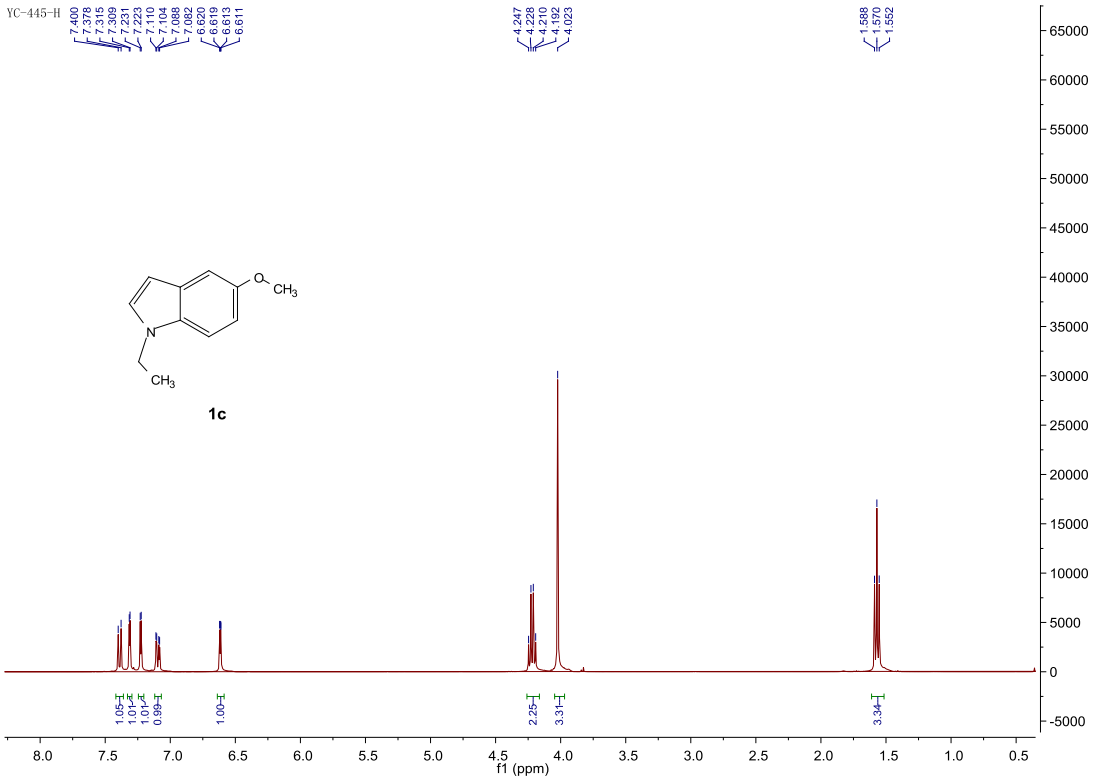

YC-579-MED-C
H3C
NH
I
4
f1 (ppm)

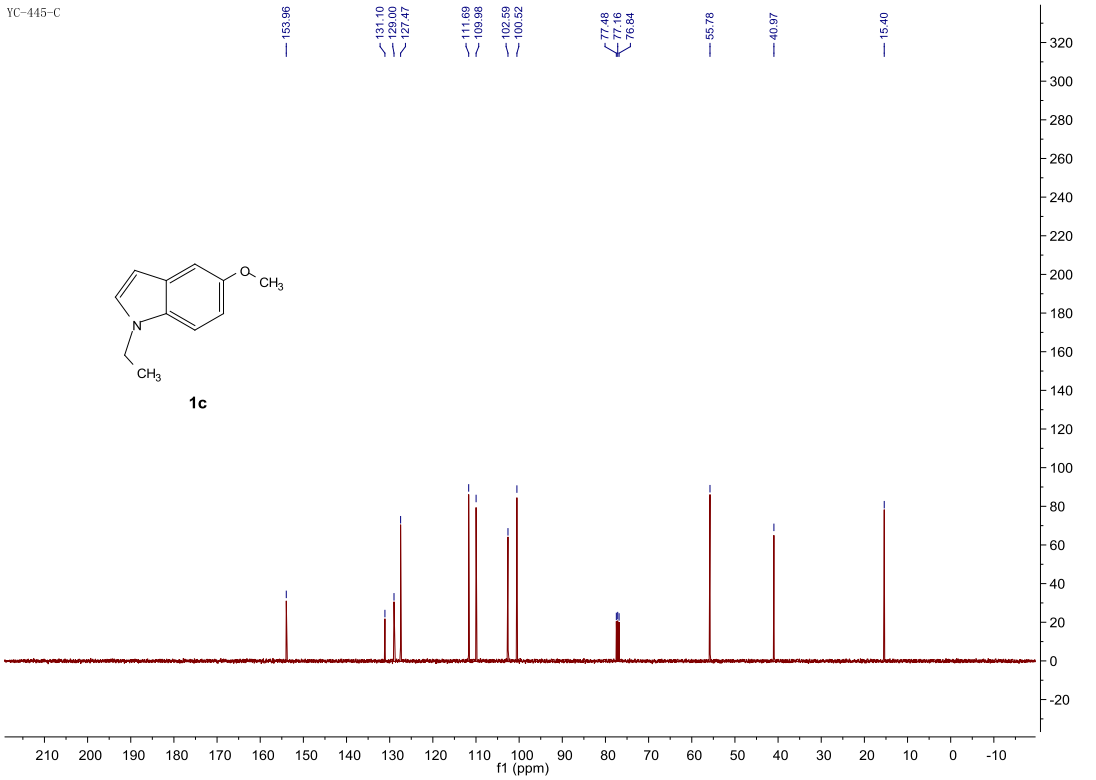

XP-190-H
8.471
8.467
8.450
8.447
7.949
7.930
7.927
7.593
7.585
7.260
7.253
4.505
4.487
4.469
4.450
1.915
1.897
1.878
N
CH3
1a
1.00
3.03
0.95
2.00
3.02
f1 (ppm)

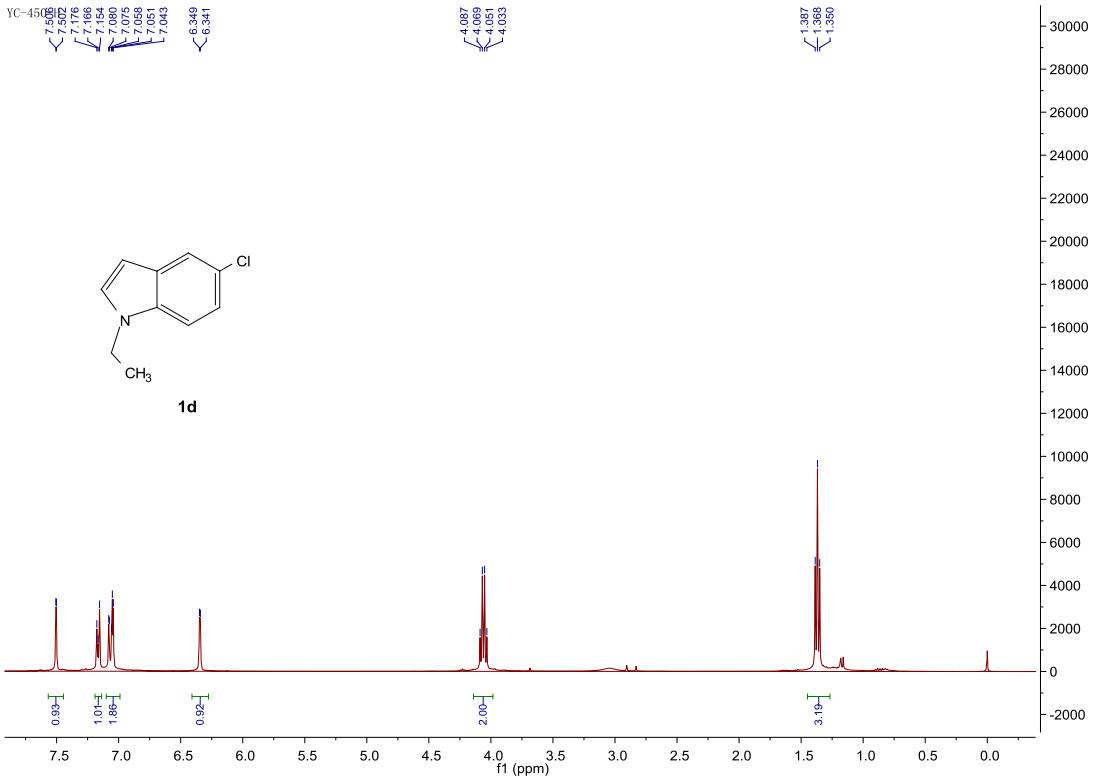

XP-190-C
135.60
128.66
126.80
121.16
120.80
119.09
109.19
100.83
77.48
77.16
76.84
40.38
15.02
N
CH3
1a
f1 (ppm)

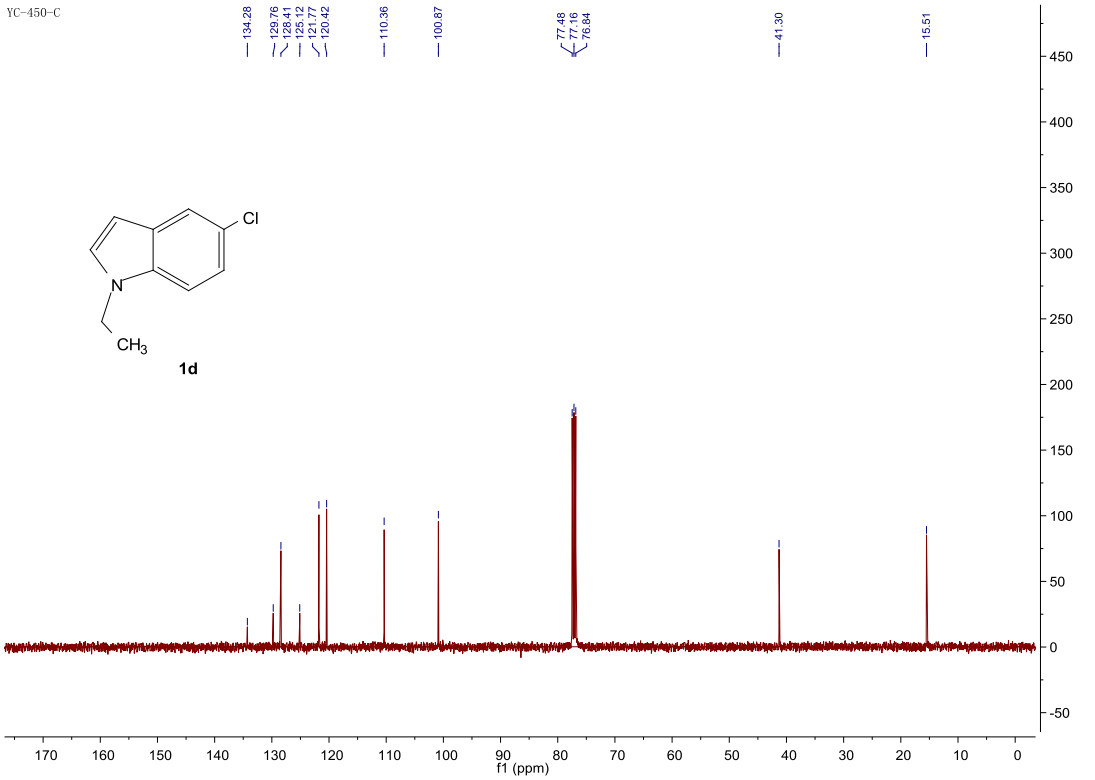

7.024
7.006
7.003
6.982
6.974
6.818
6.816
6.814
6.801
6.799
6.408
6.402
6.400
4.046
4.028
4.010
3.992
2.463
1.344
1.326
1.308
CH3
N
CH3
1b
0.88
1.01
0.83
0.83
0.83
2.00
2.95
3.06
f1 (ppm)

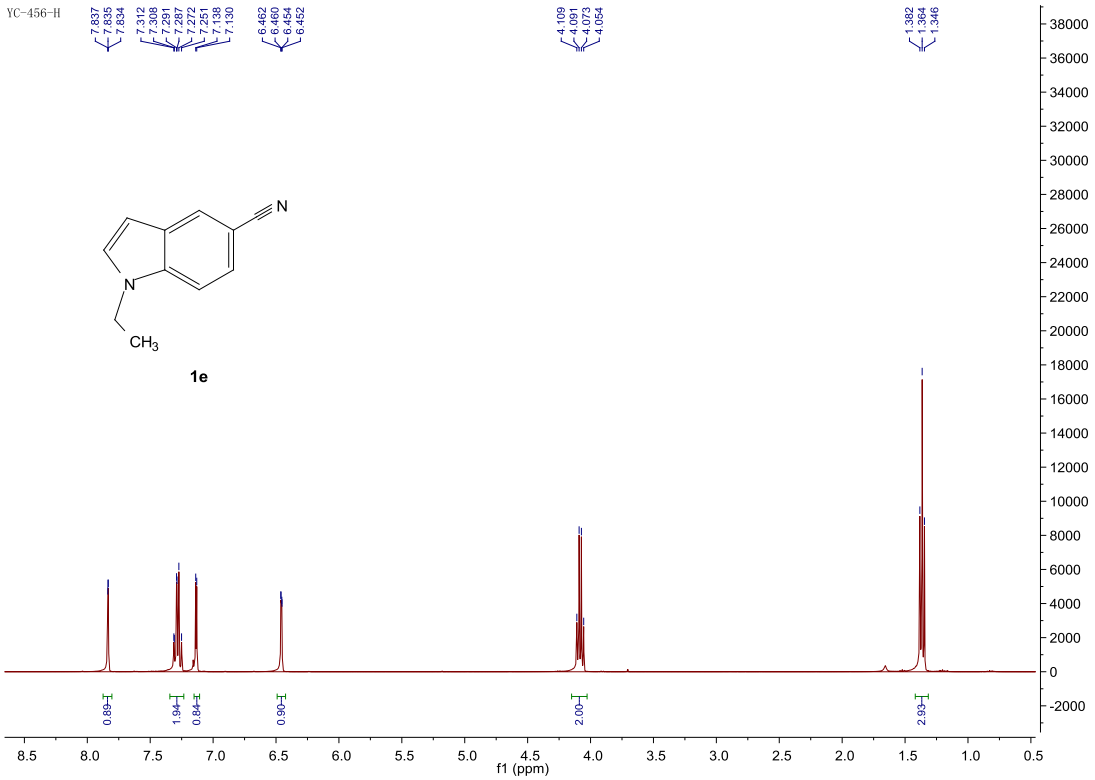

YC-460-C
135.52
130.51
128.63
126.45
121.63
119.53
107.02
99.59
77.48
77.16
76.84
41.15
18.85
15.57
CH3
N
CH3
1b
f1 (ppm)

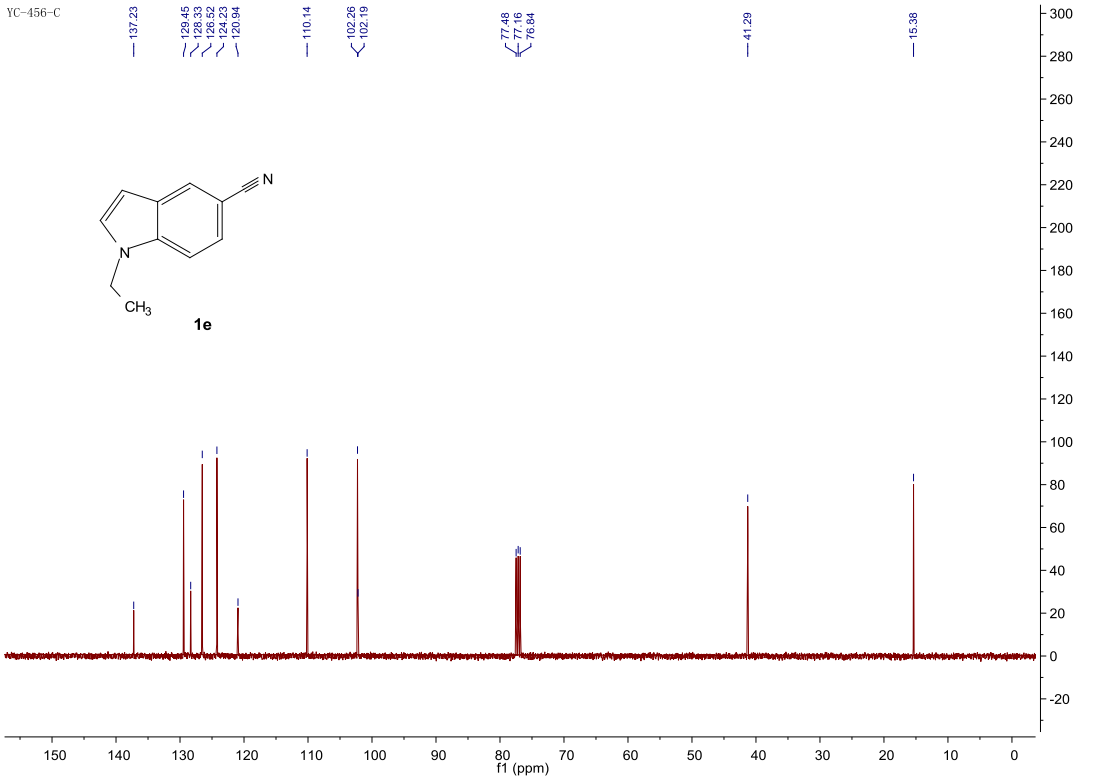

YC-445-H
7.400
7.378
7.315
7.309
7.231
7.223
7.110
7.104
7.088
7.082
6.620
6.619
6.613
6.611
4.247
4.228
4.210
4.192
4.023
1.588
1.570
1.552
O
CH3
N
CH3
1c
1.05
1.01
1.01
0.99
1.00
2.25
3.31
3.34
f1 (ppm)

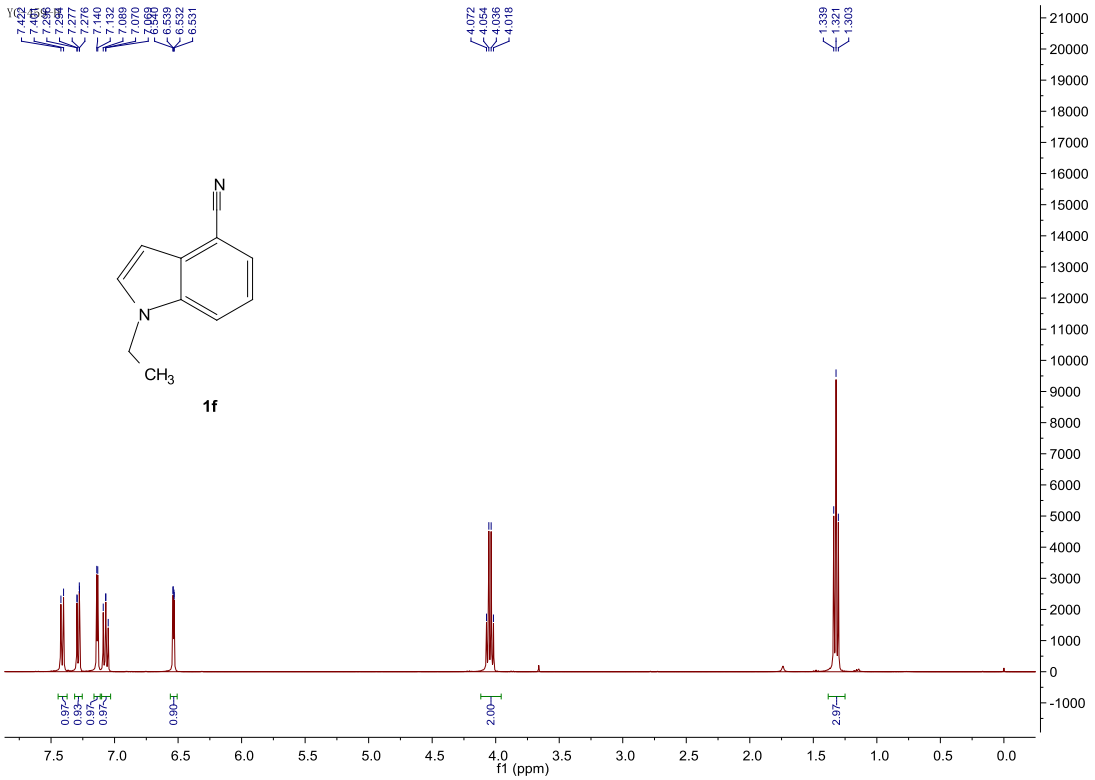

YC-445-C
153.96
131.10
129.00
127.47
111.69
109.98
102.59
100.52
77.48
77.16
76.84
55.78
40.97
15.40
O
CH3
N
CH3
1c
f1 (ppm)

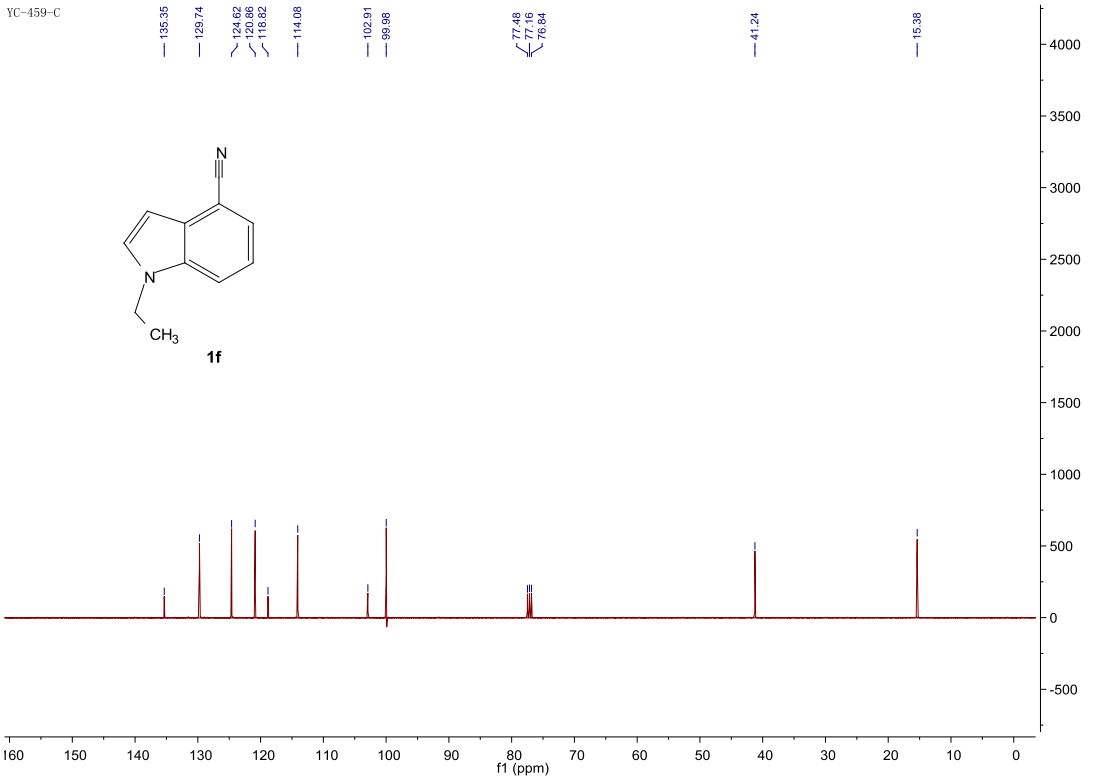

YC-450
7.506
7.502
7.176
7.166
7.154
7.080
7.075
7.058
7.051
7.043
6.349
6.341
4.087
4.069
4.051
4.033
1.387
1.368
1.350
Cl
N
CH3
1d
0.93
1.01
1.86
0.92
2.00
3.19
f1 (ppm)

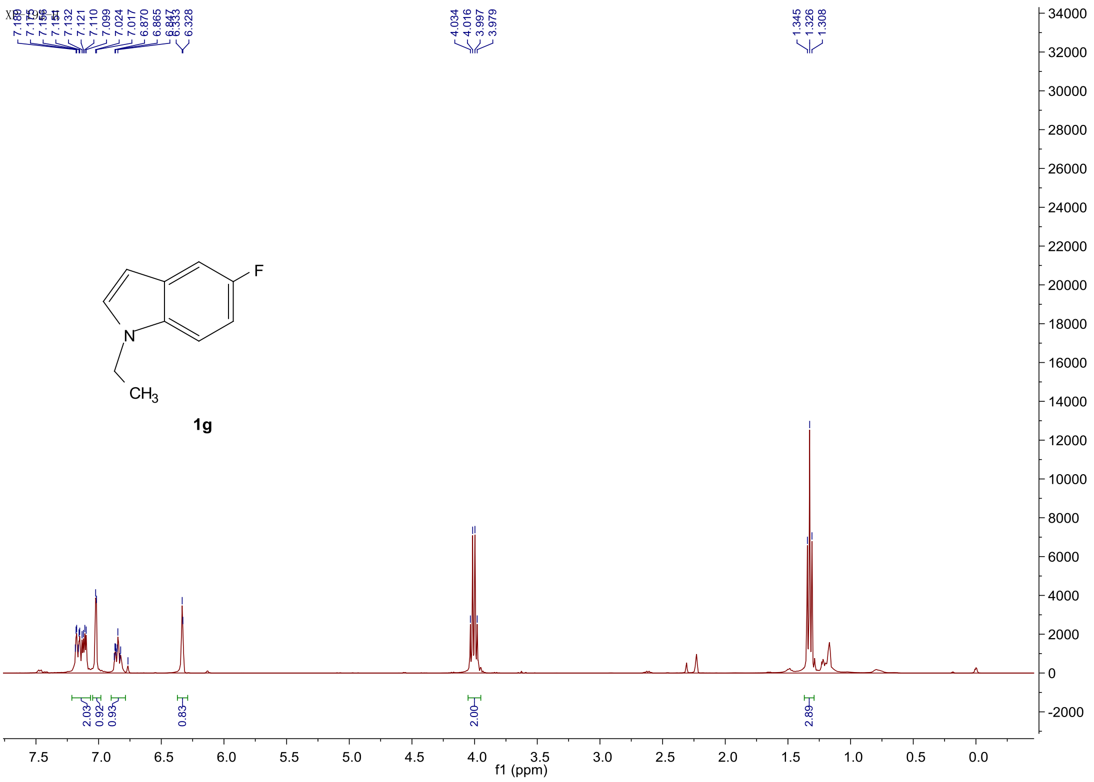

YC-450-C
134.28
129.76
128.41
125.12
121.77
120.42
110.36
100.87
77.48
77.16
76.84
41.30
15.51
Cl
N
CH3
1d
f1 (ppm)

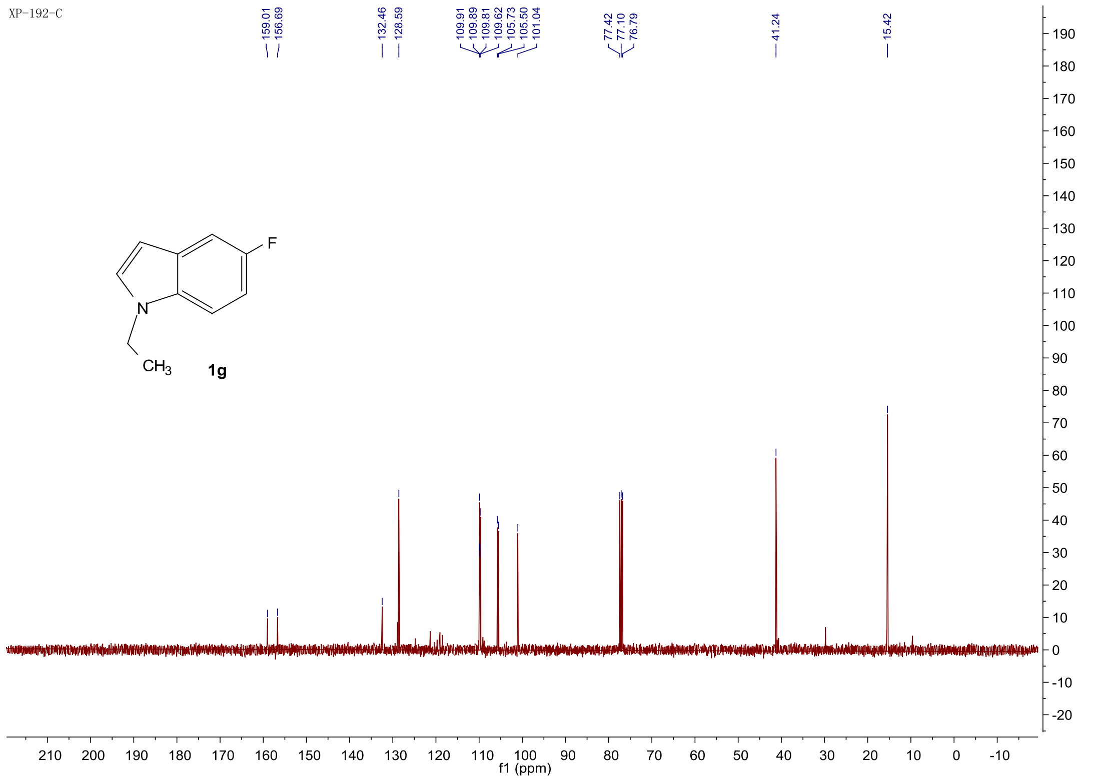

YC-456-H
7.837
7.835
7.834
7.312
7.308
7.291
7.287
7.272
7.251
7.138
7.130
6.462
6.460
6.454
6.452
4.109
4.091
4.073
4.054
1.382
1.364
1.346
N
N
CH3
1e
0.89
1.94
0.84
0.90
2.00
2.83
f1 (ppm)

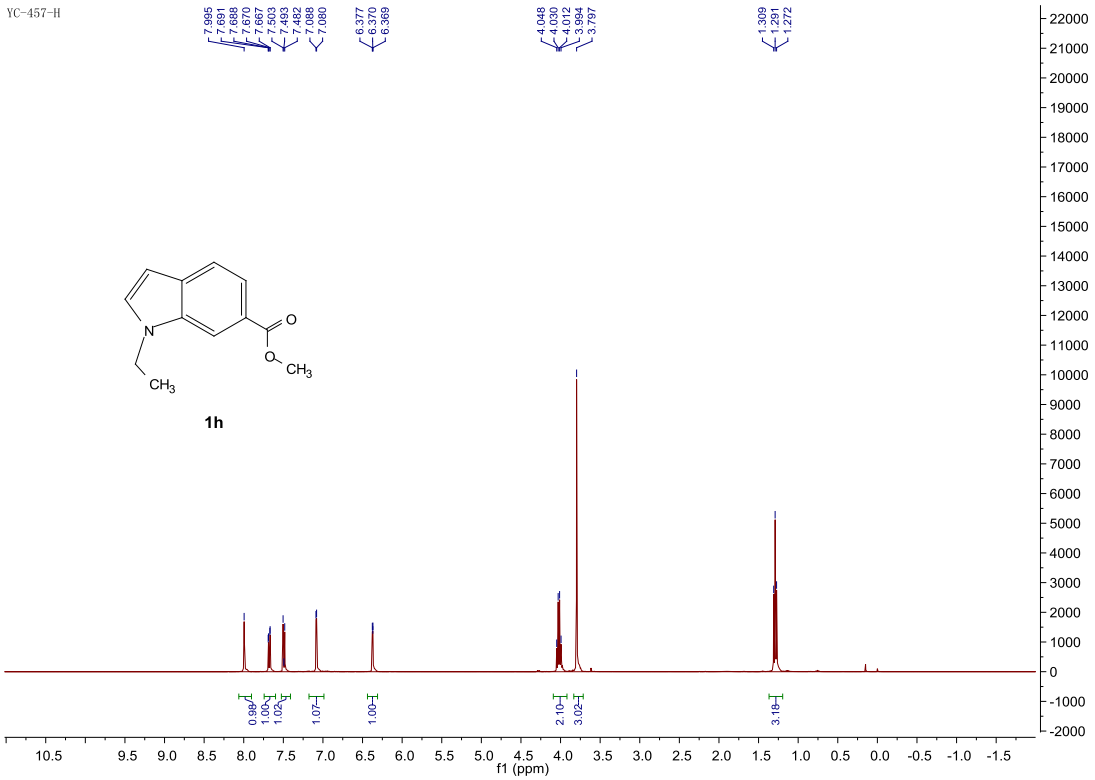

YC-456-C
137.23
129.45
128.33
126.52
124.23
120.94
110.14
102.26
102.19
77.48
77.16
76.84
41.29
15.38
N
N
CH3
1e
f1 (ppm)


7.422
7.461
7.296
7.294
7.277
7.276
7.140
7.132
7.089
7.070
6.539
6.532
6.531
4.072
4.054
4.036
4.018
1.339
1.321
1.303
N
N
CH3
1f
0.97
0.93
0.97
0.97
0.90
2.00
2.97
f1 (ppm)

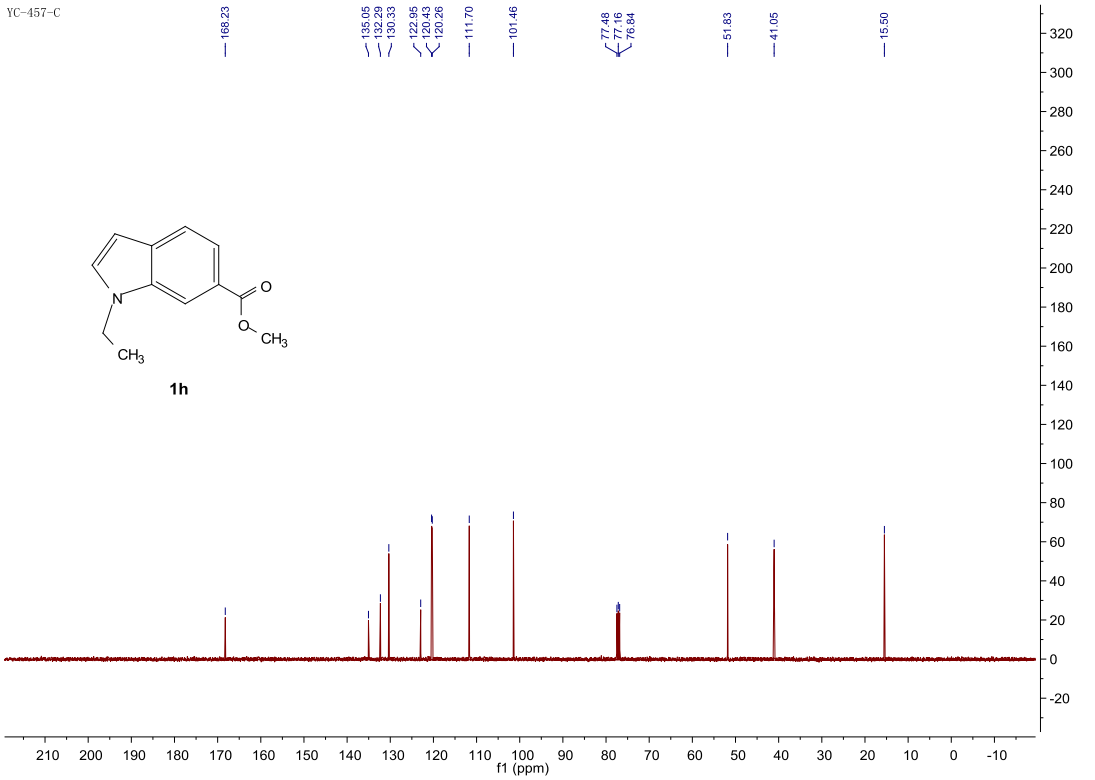

YC-459-C
135.35
129.74
124.62
120.86
118.82
114.08
102.91
99.98
77.48
77.16
76.84
41.24
15.38
N
N
CH3
1f
f1 (ppm)


7.180
7.175
7.156
7.151
7.132
7.121
7.110
7.099
7.024
7.017
6.870
6.865
6.847
6.333
6.328
4.034
4.016
3.997
3.979
1.345
1.326
1.308
F
N
CH3
1g
2.03
0.92
0.93
0.83
2.00
2.89
f1 (ppm)

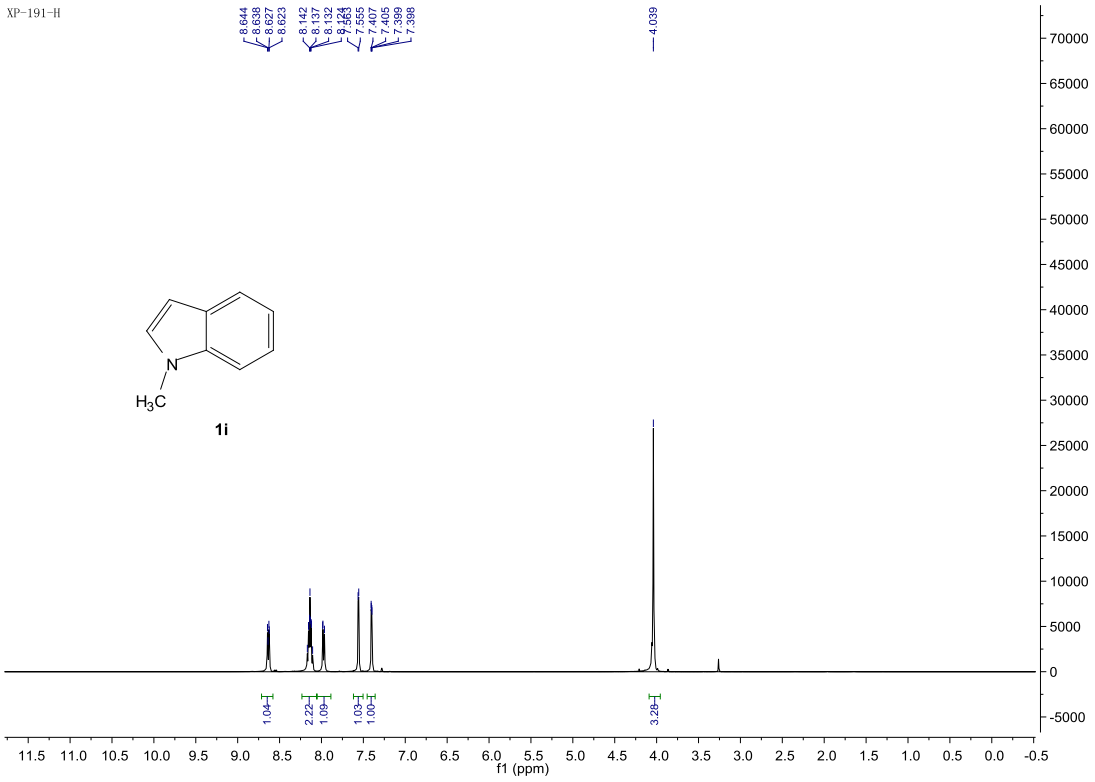

XP-192-C
159.01
156.69
132.46
128.59
109.91
109.89
109.81
109.62
105.73
105.50
101.04
77.42
77.10
76.79
41.24
15.42
F
N
CH3
1g
f1 (ppm)


YC-457-H
7.995
7.691
7.688
7.670
7.667
7.503
7.493
7.482
7.088
7.080
6.377
6.370
6.369
4.048
4.030
4.012
3.994
3.797
1.309
1.291
1.272
O
N
O
CH3
CH3
0.99
1.00
1.02
1.07
1.00
2.10
3.02
3.18
f1 (ppm)

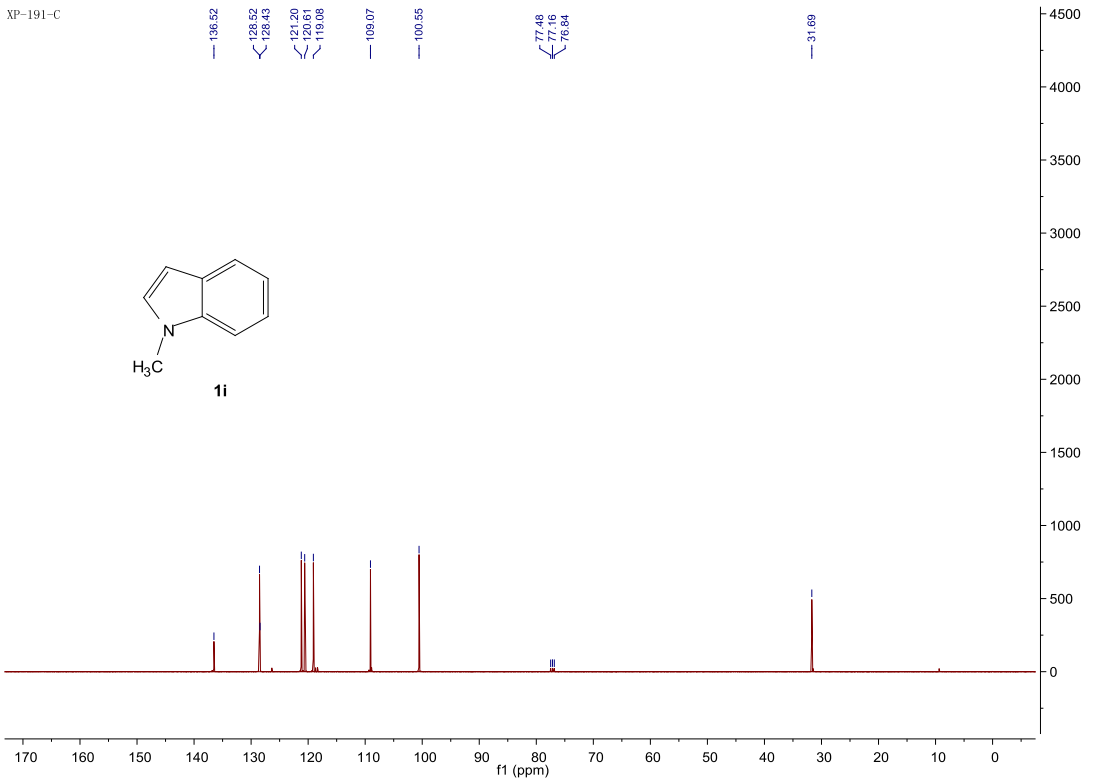
1h


YC-457-C
168.23
135.05
132.29
130.33
122.95
120.43
120.26
111.70
101.46
77.48
77.16
76.84
51.83
41.05
15.50
O
N
O
CH3
CH3
f1 (ppm)

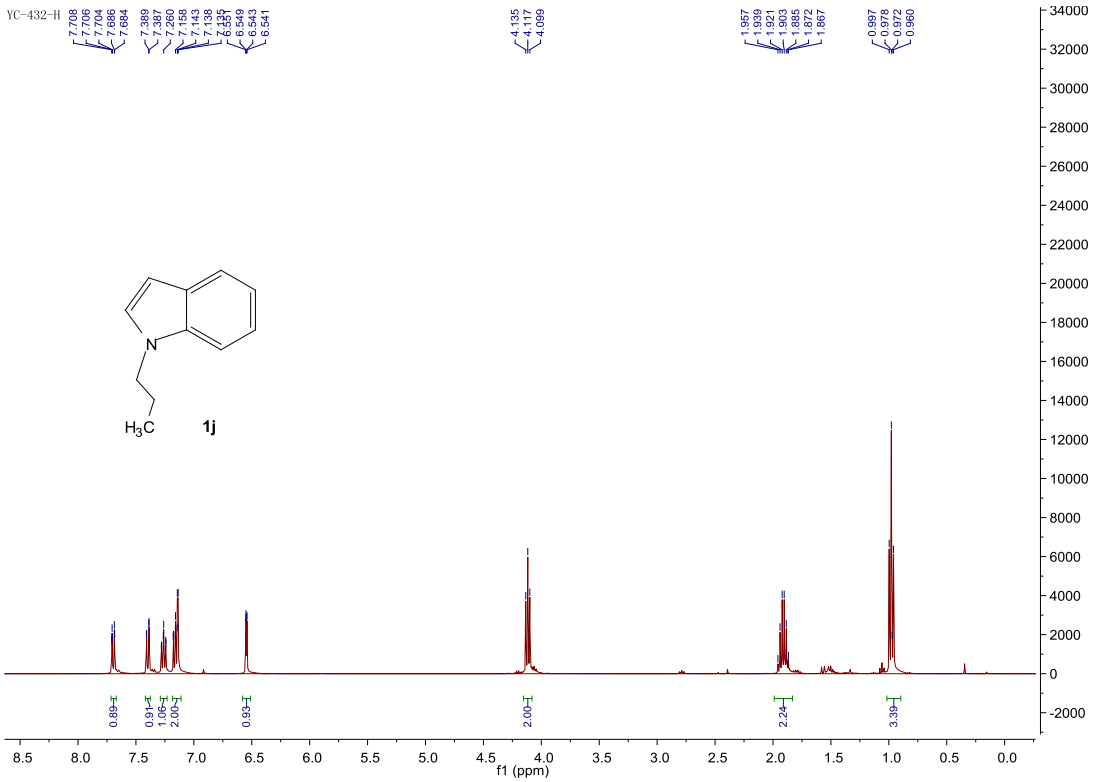
1h

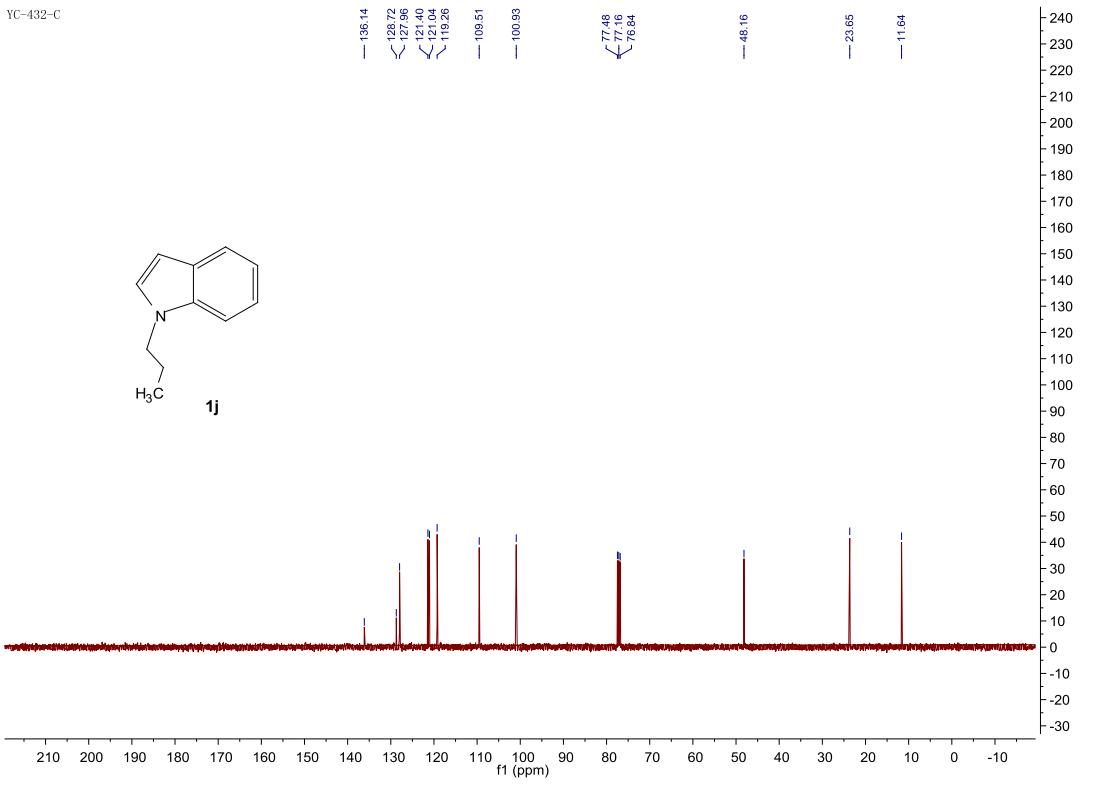

XP-191-H
8.644
8.638
8.627
8.623
8.142
8.137
8.132
7.555
7.407
7.405
7.399
7.398
4.039
1.04
2.22
1.09
1.03
1.00
3.28
f1 (ppm)

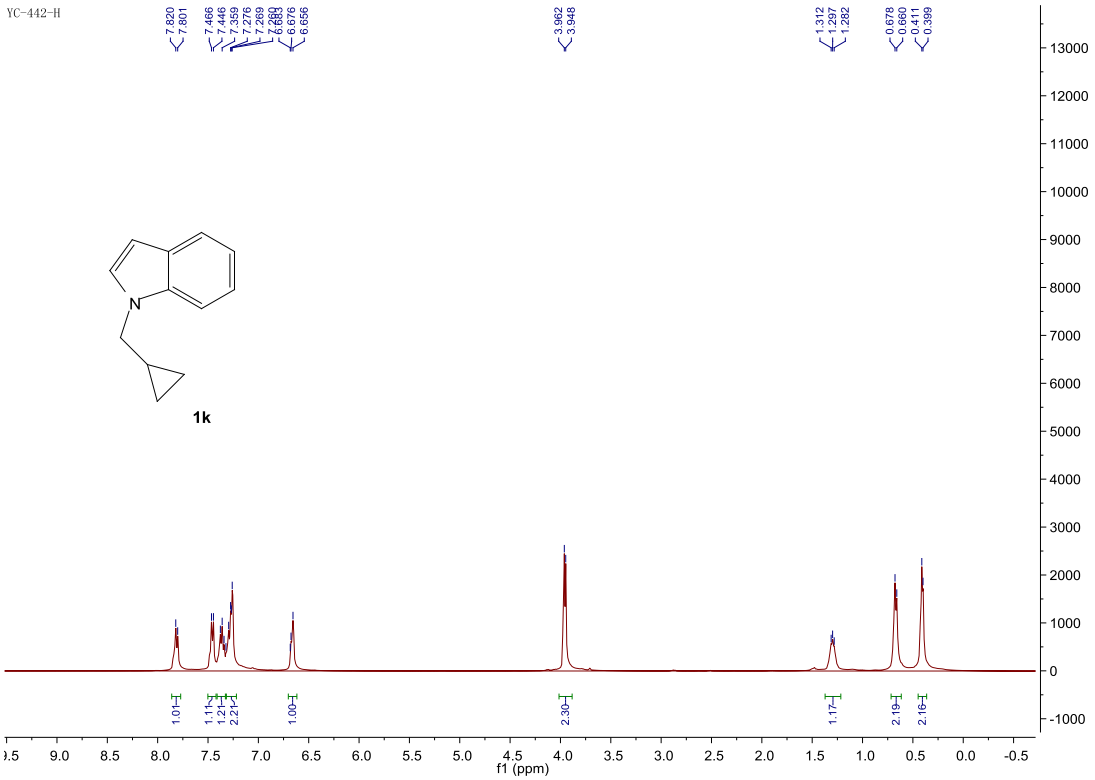
1i

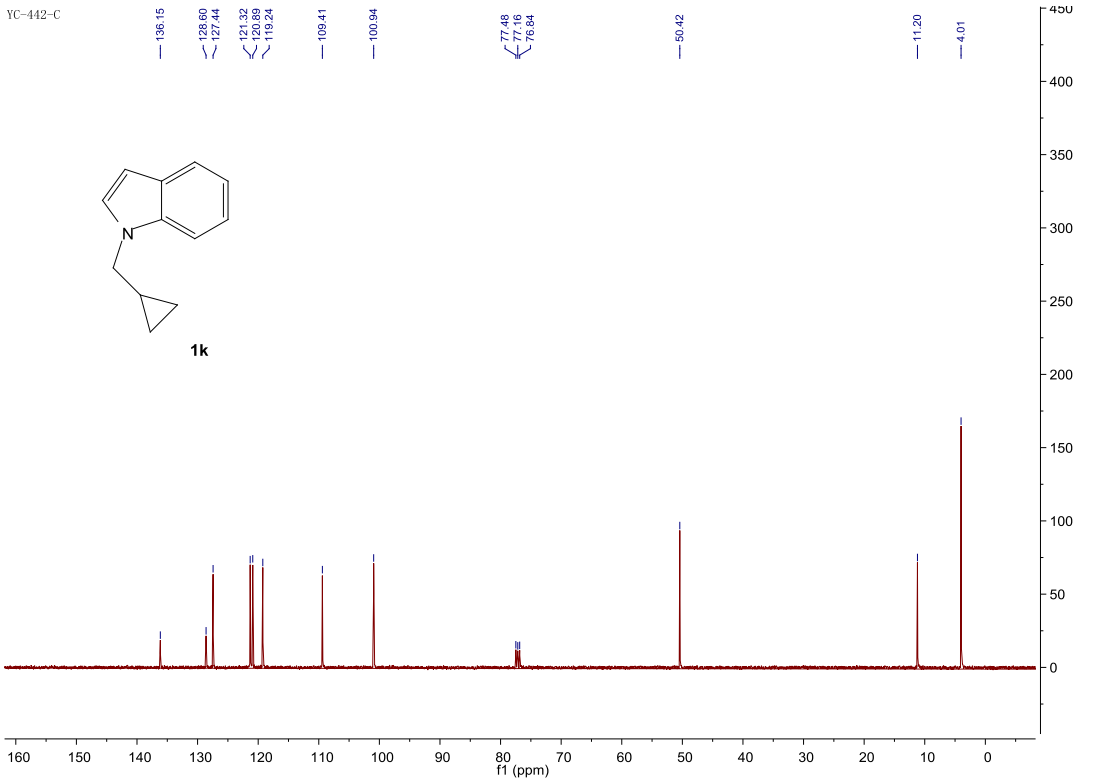

XP-191-C
136.52
128.52
128.43
121.20
120.61
119.08
109.07
100.55
77.48
77.16
76.84
31.69
f1 (ppm)

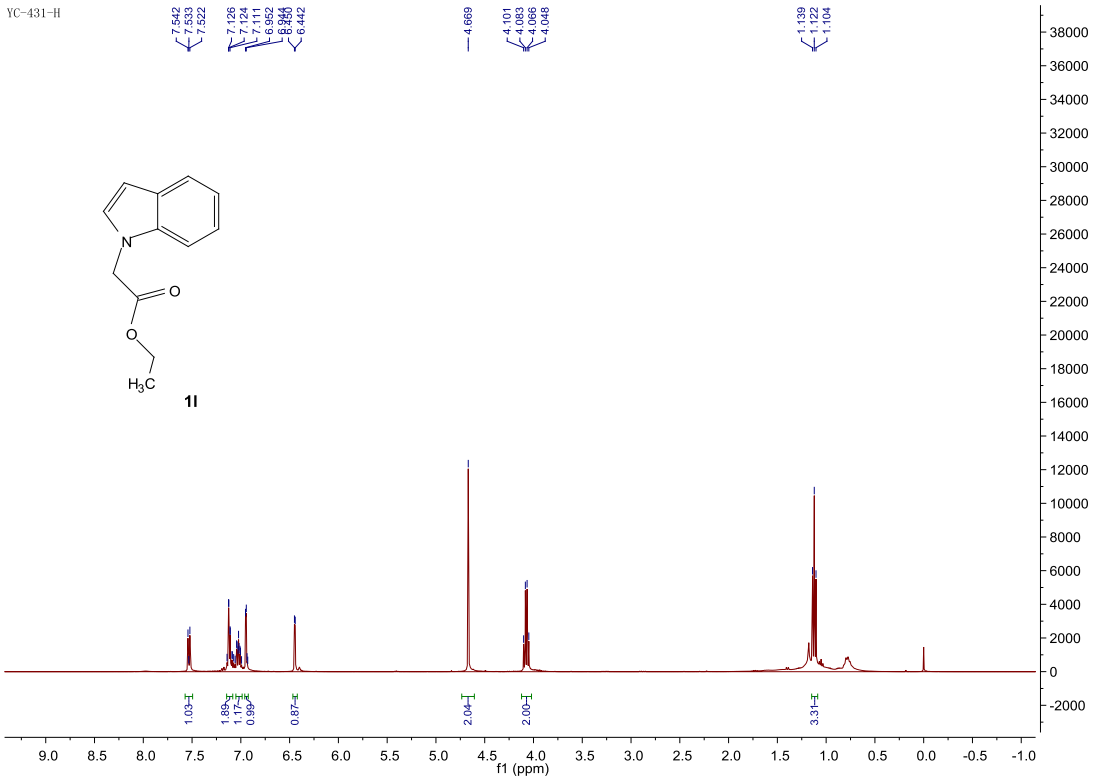
1i


YC-432-H
7.708
7.706
7.704
7.686
7.684
7.389
7.387
7.360
7.158
7.143
7.138
6.551
6.543
6.541
4.135
4.117
4.099
1.957
1.939
1.921
1.903
1.885
1.872
1.867
0.997
0.978
0.972
0.960
0.89
0.91
1.06
2.00
0.93
2.00
2.24
3.39
f1 (ppm)
1j

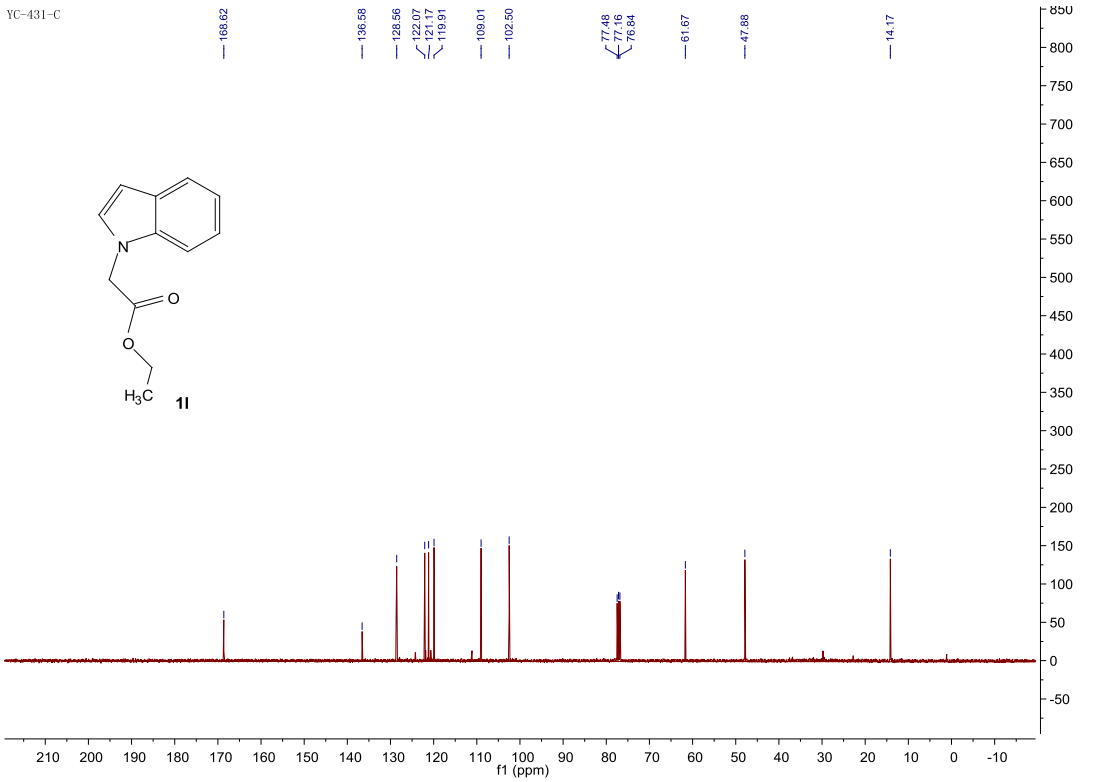

YC-432-C
136.14
128.72
127.96
121.40
121.04
119.26
109.51
100.93
77.48
77.16
76.84
48.16
23.65
11.64
f1 (ppm)
1j


YC-442-H
7.820
7.801
7.466
7.446
7.359
7.276
7.269
6.676
6.656
3.962
3.948
1.312
1.297
1.282
0.678
0.660
0.411
0.399
1k
1.01
1.11
1.21
2.21
1.00
2.30
1.17
2.19
2.16
f1 (ppm)

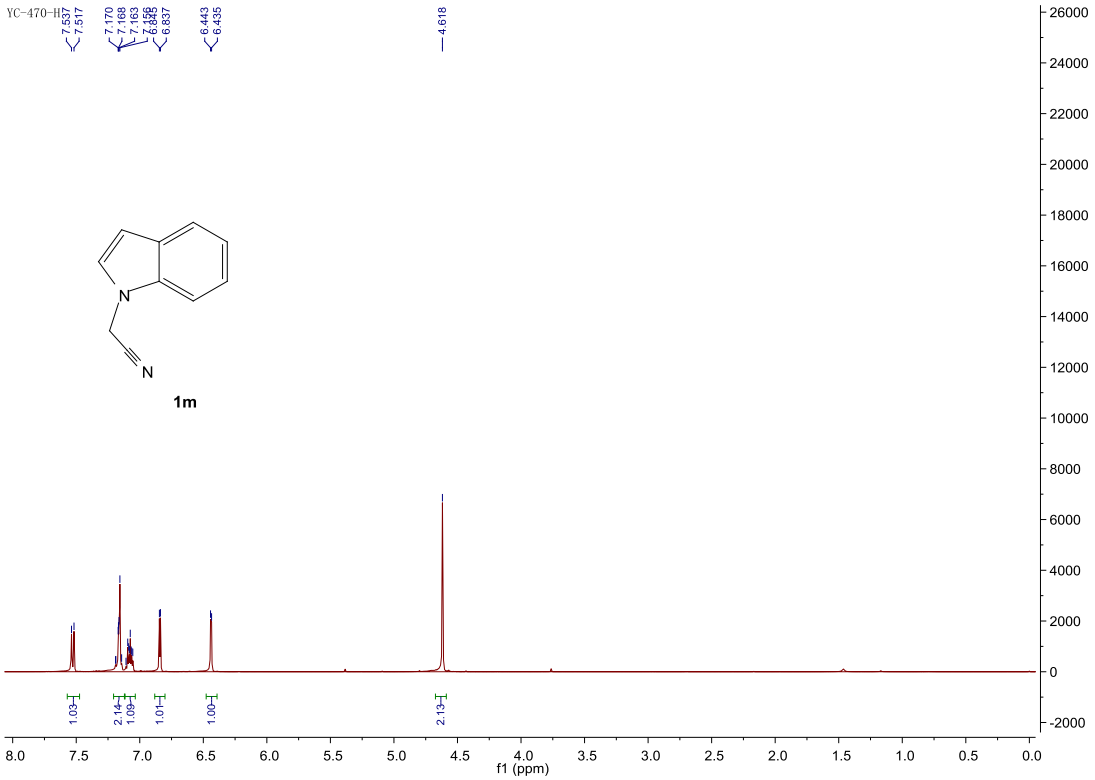

YC-442-C
136.15
128.60
127.44
121.32
120.89
119.24
109.41
100.94
77.48
77.16
76.84
50.42
11.20
4.01
1k
f1 (ppm)

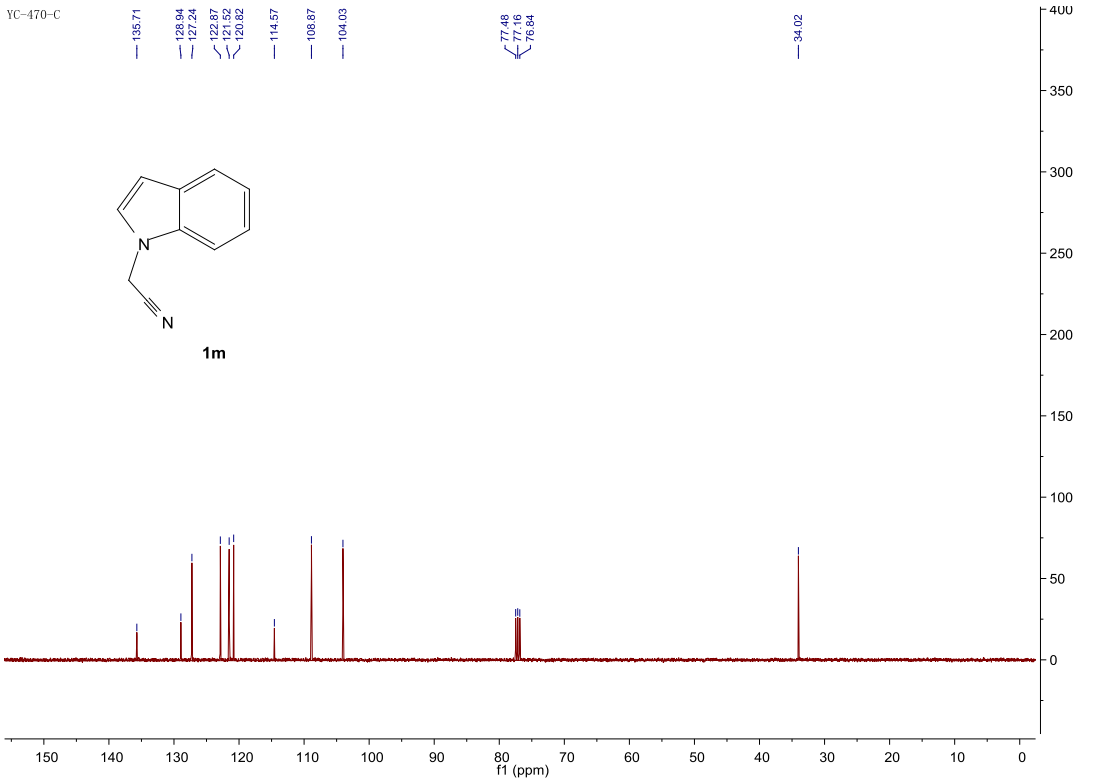

YC-431-H
7.542
7.533
7.522
7.126
7.124
7.111
6.952
6.442
4.669
4.101
4.083
4.066
4.048
1.139
1.122
1.104
1.03
1.89
1.17
0.99
0.87
2.04
2.00
3.31
f1 (ppm)

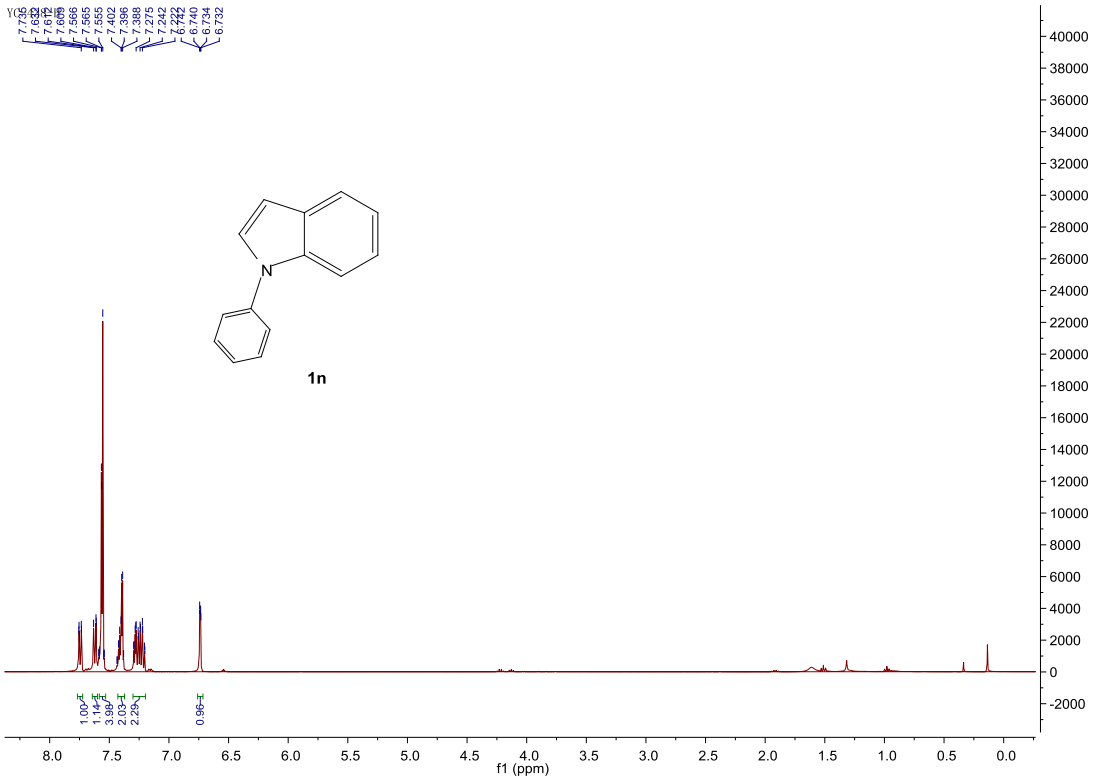
1l

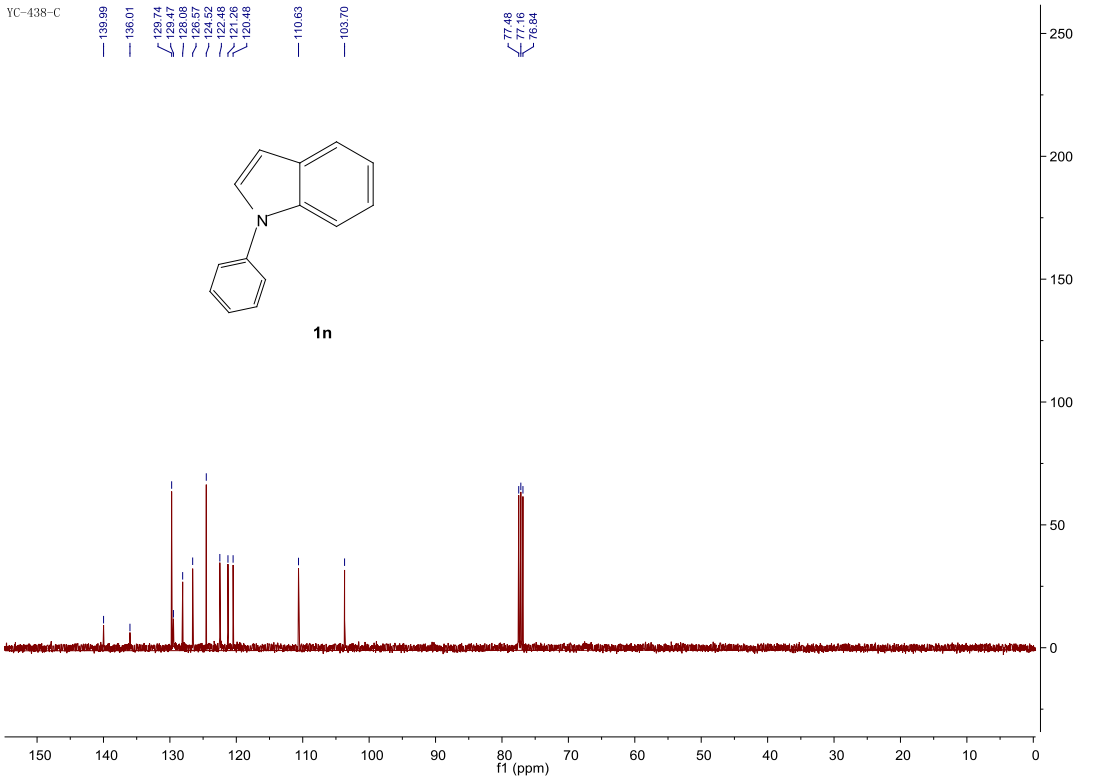

YC-431-C
168.62
136.58
128.56
122.07
121.17
119.91
109.01
102.50
77.48
77.16
76.84
61.67
47.88
14.17
f1 (ppm)

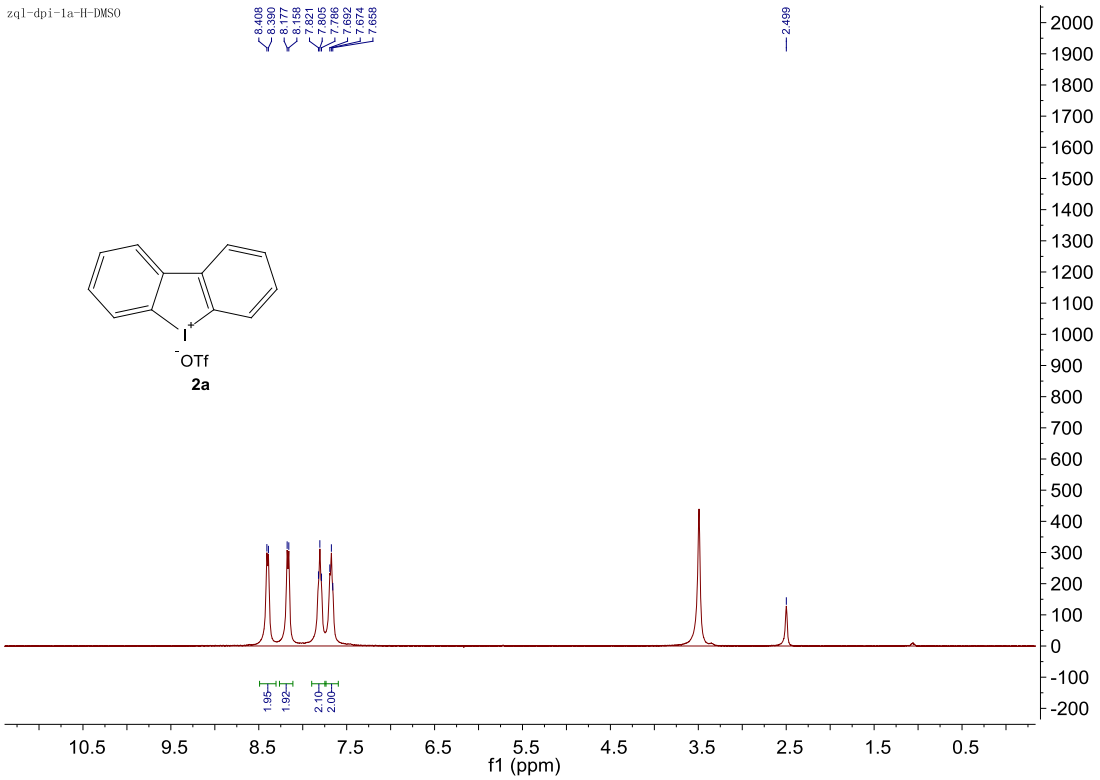
1l

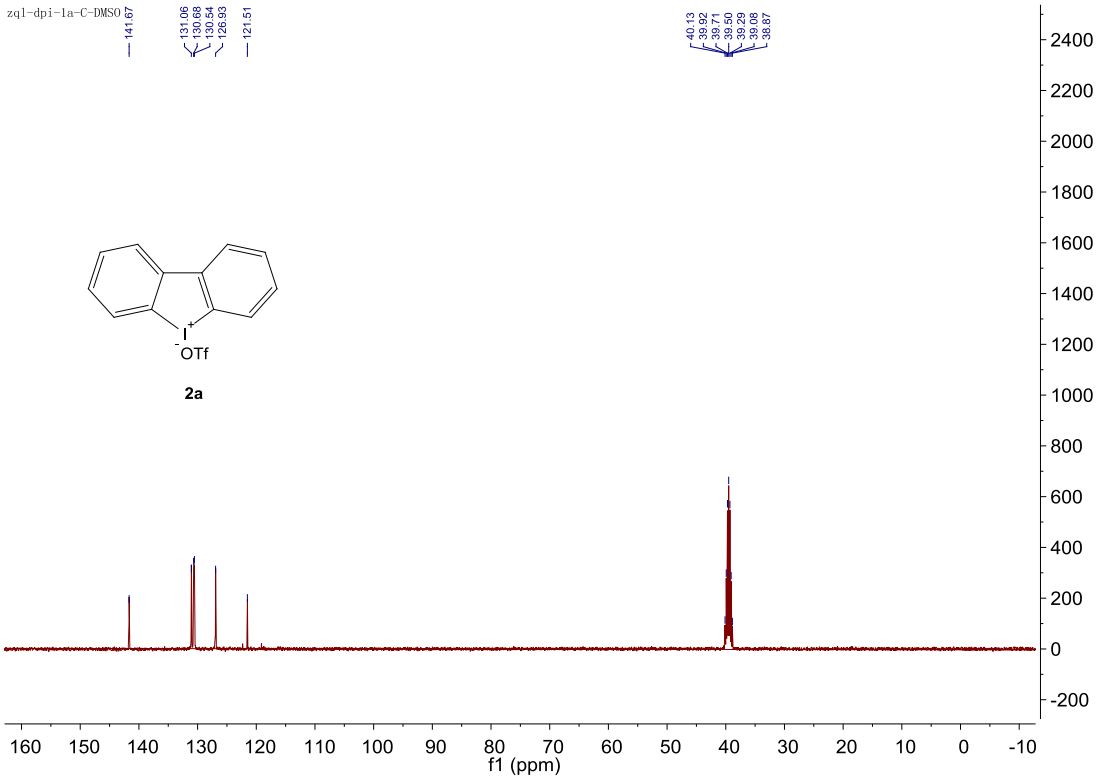

YC-470-H
7.537
7.517
7.170
7.168
7.163
6.837
6.443
6.435
4.618
1m
1.03
2.14
1.09
1.01
1.00
2.13
f1 (ppm)

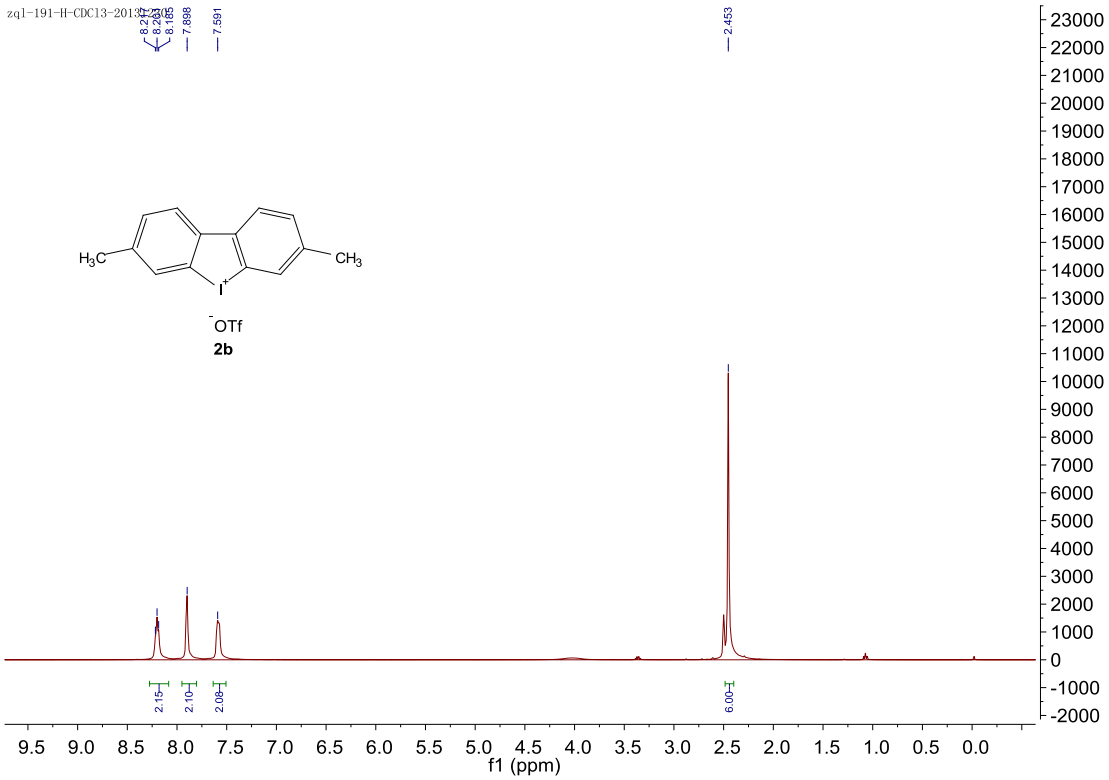

YC-470-C
135.71
128.94
127.24
122.87
121.82
120.02
114.57
108.87
104.03
77.48
77.16
76.84
34.02
1m
f1 (ppm)

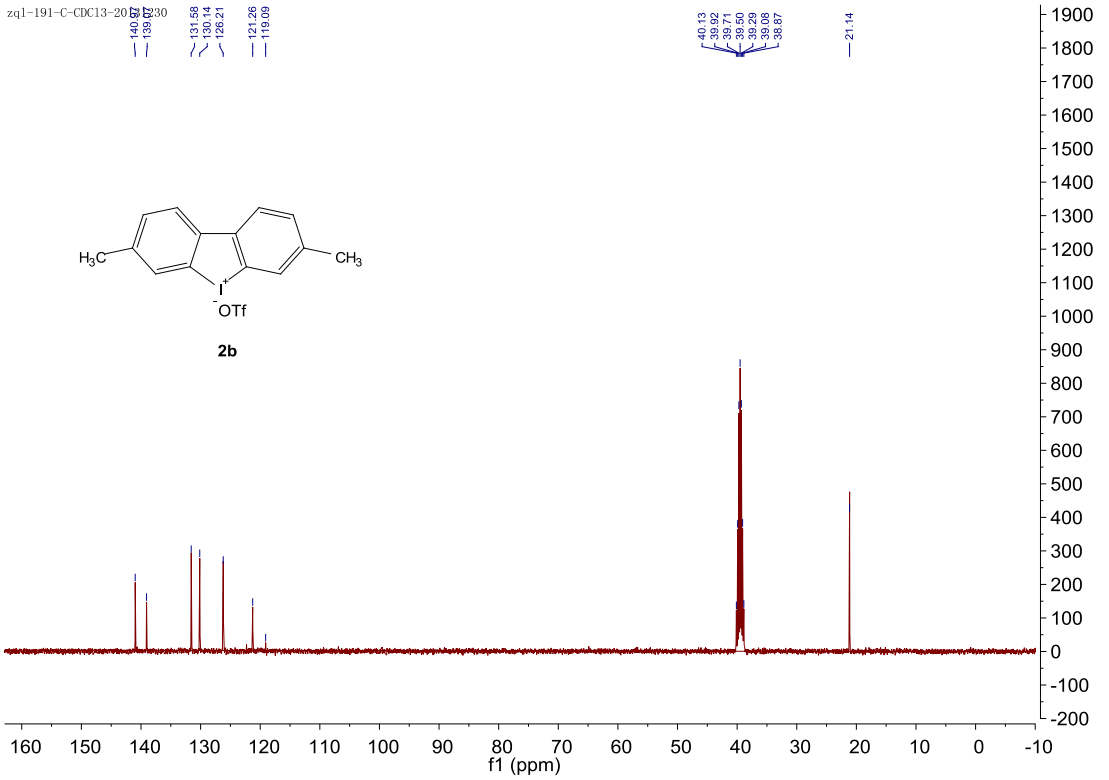

7.735
7.632
7.612
7.566
7.555
7.402
7.396
7.388
7.275
7.242
6.740
6.734
6.732
1n
1.00
1.14
3.98
2.03
2.29
0.96
f1 (ppm)

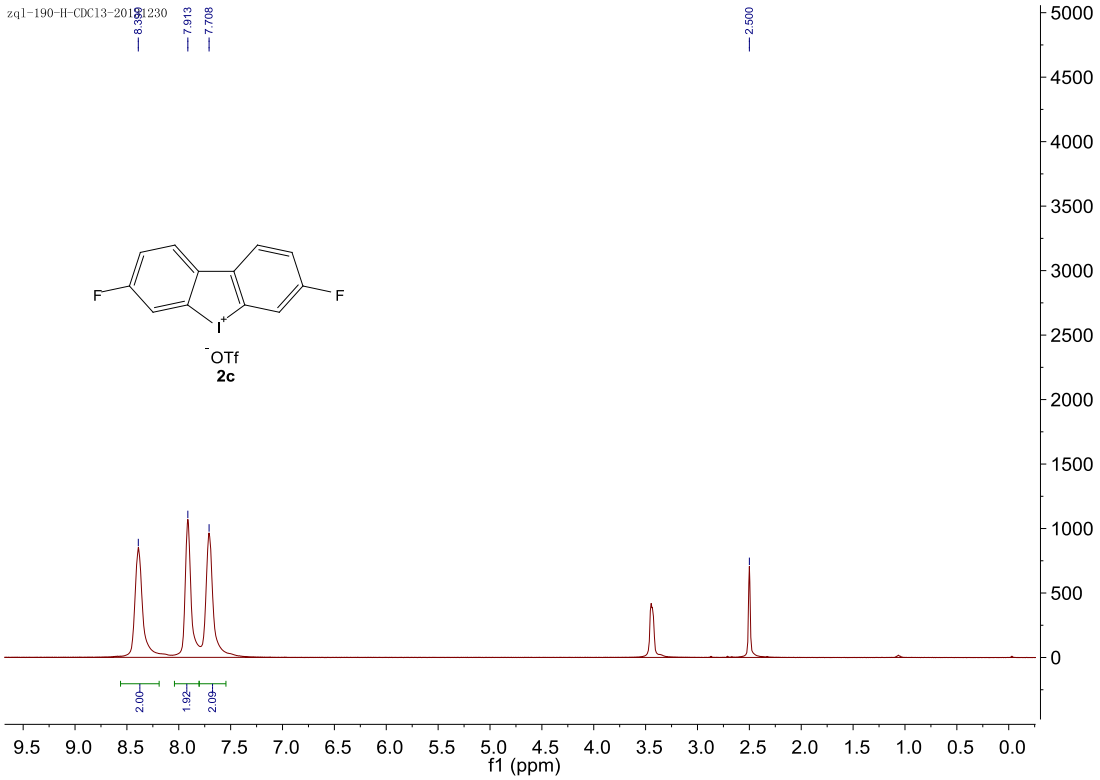

YC-438-C
139.99
136.01
129.74
129.47
128.06
126.57
124.52
122.48
121.26
120.48
110.63
103.70
77.48
77.16
76.84
1n
f1 (ppm)

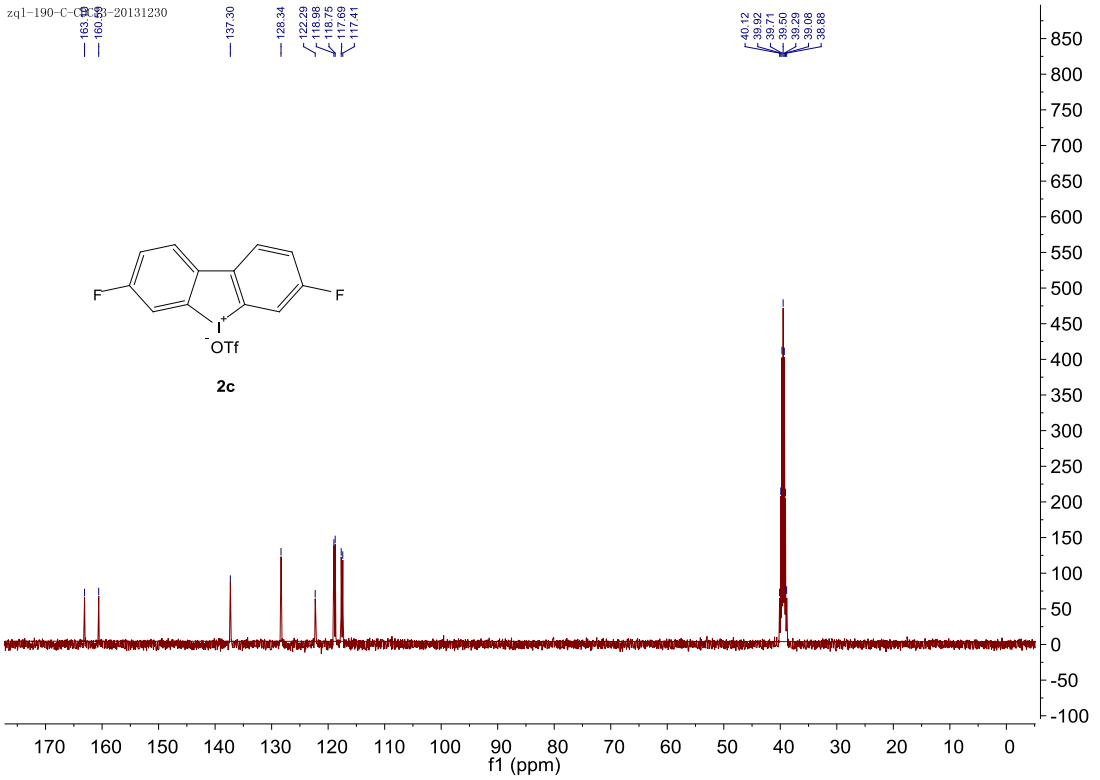

zql-dpi-1a-H-DMSO
8.408
8.390
8.177
8.158
7.821
7.805
7.786
7.692
7.674
7.658
2.499
OTf
2a
1.95
1.92
2.10
2.00
f1 (ppm)

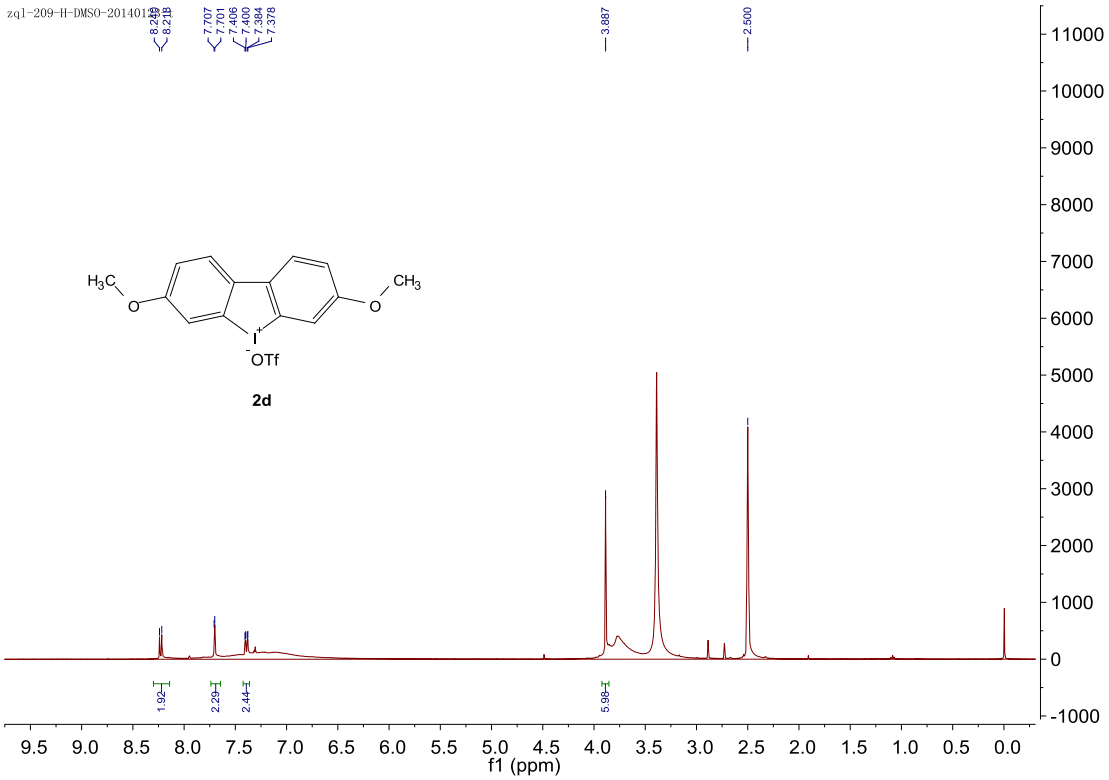

zql-dpi-1a-C-DMSO
141.67
131.06
130.68
130.54
126.93
121.51
40.13
39.92
39.71
39.50
39.29
39.08
38.87
OTf
2a
f1 (ppm)

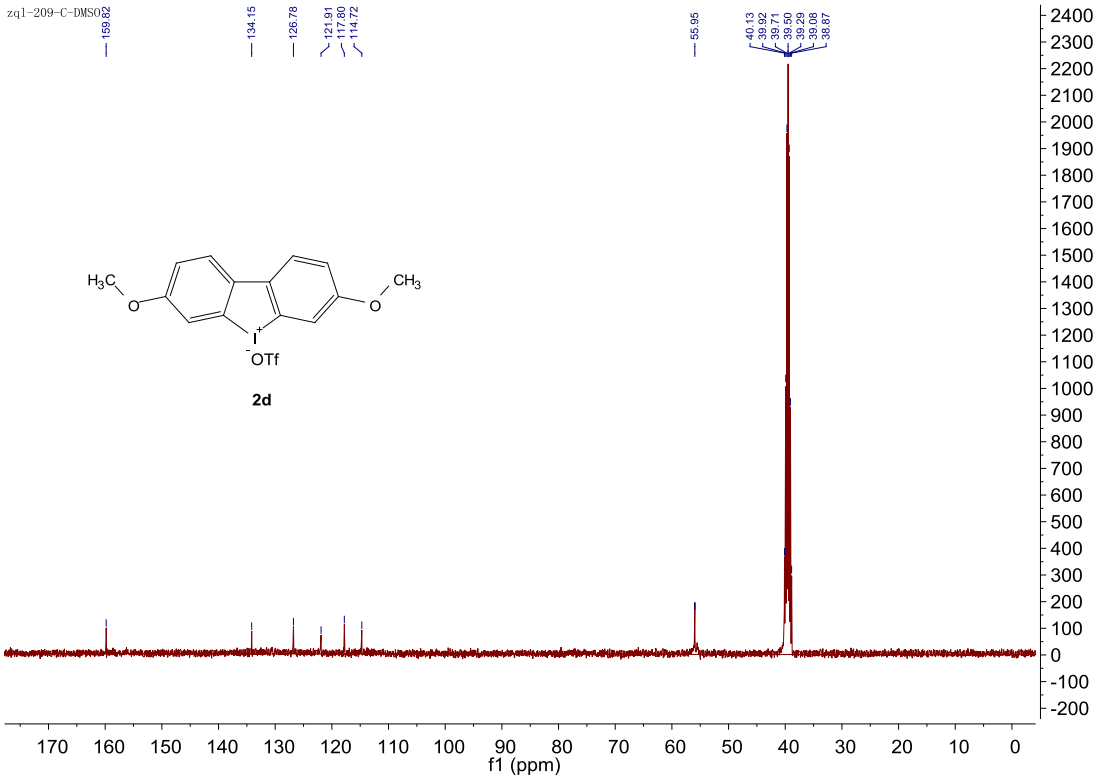

zq1-191-H-CDCl3-20130
8.247
8.243
8.185
7.898
7.591
2.453
H3C
CH3
I+
OTf
2b
2.15
2.10
2.08
6.00
f1 (ppm)

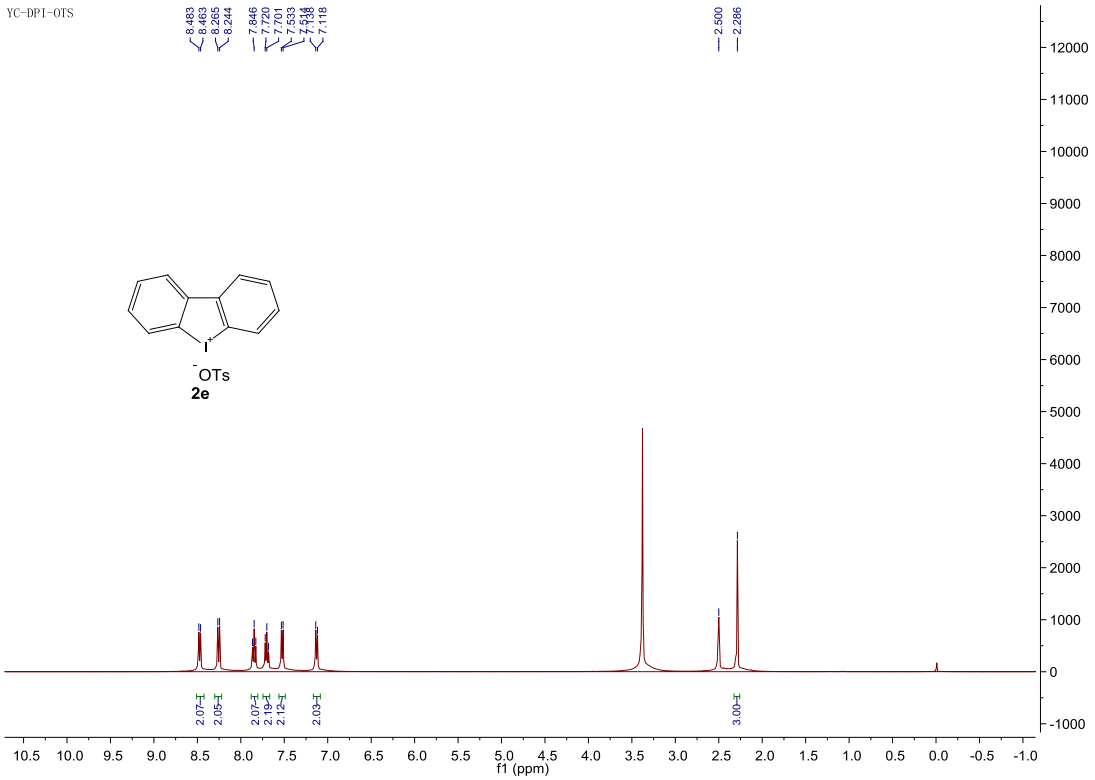

zq1-191-C-CDCl3-20130
140.97
139.77
131.58
130.14
126.21
121.26
119.09
40.13
39.92
39.71
39.50
39.29
39.08
38.87
21.14
H3C
CH3
I+
OTf
2b
f1 (ppm)

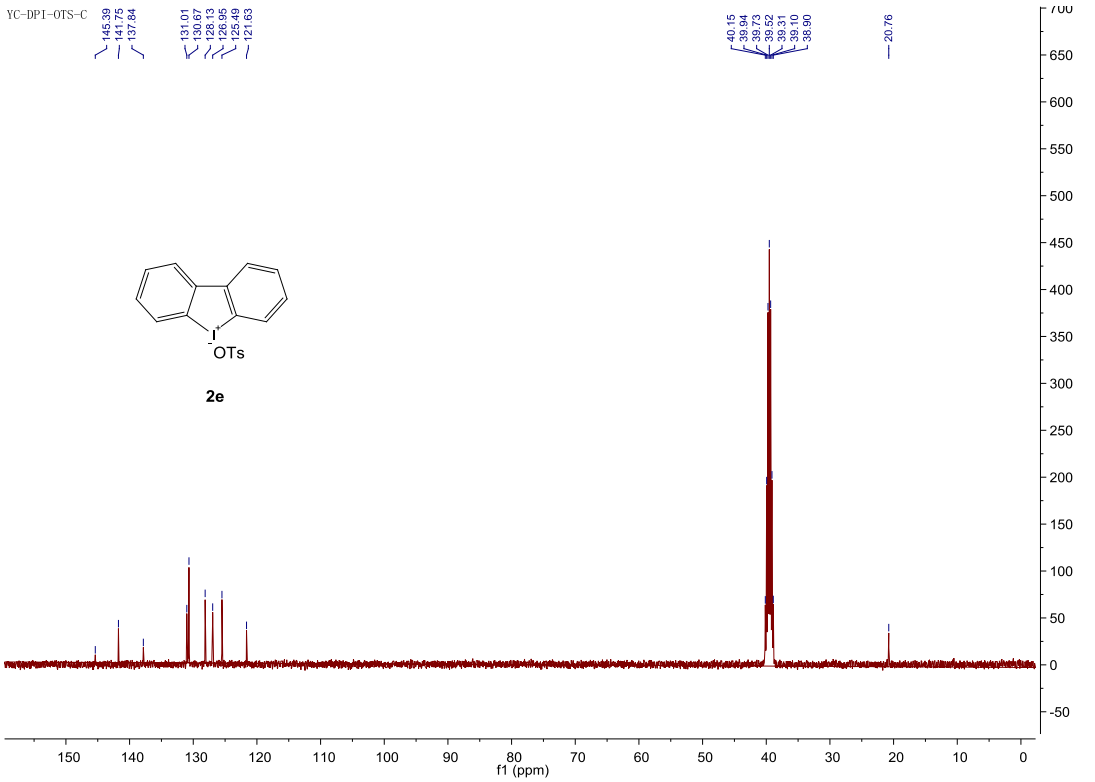

zq1-190-H-CDCl3-20131230
8.399
7.913
7.708
2.500
F
F
I+
OTf
2c
2.00
1.92
2.09
f1 (ppm)

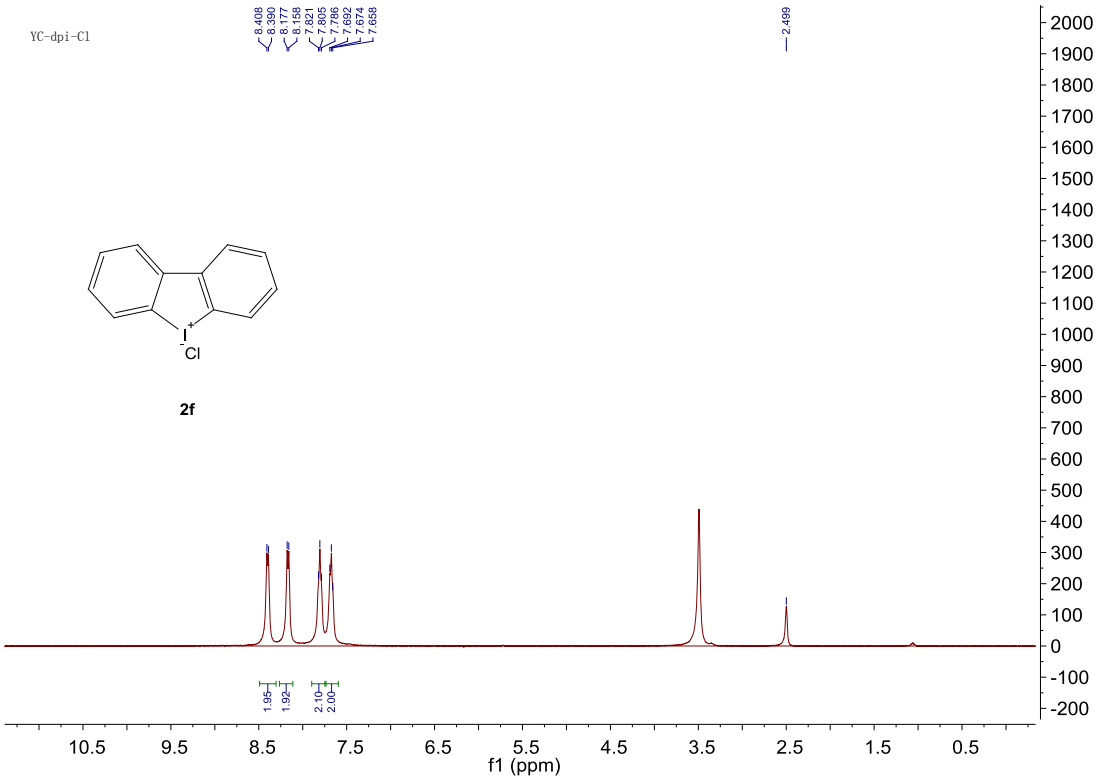

zq1-190-C-CDCl3-20131230
163.19
160.83
137.30
128.34
122.29
118.98
118.75
117.69
117.41
40.12
39.92
39.71
39.50
39.29
39.08
38.88
F
F
I+
OTf
2c
f1 (ppm)

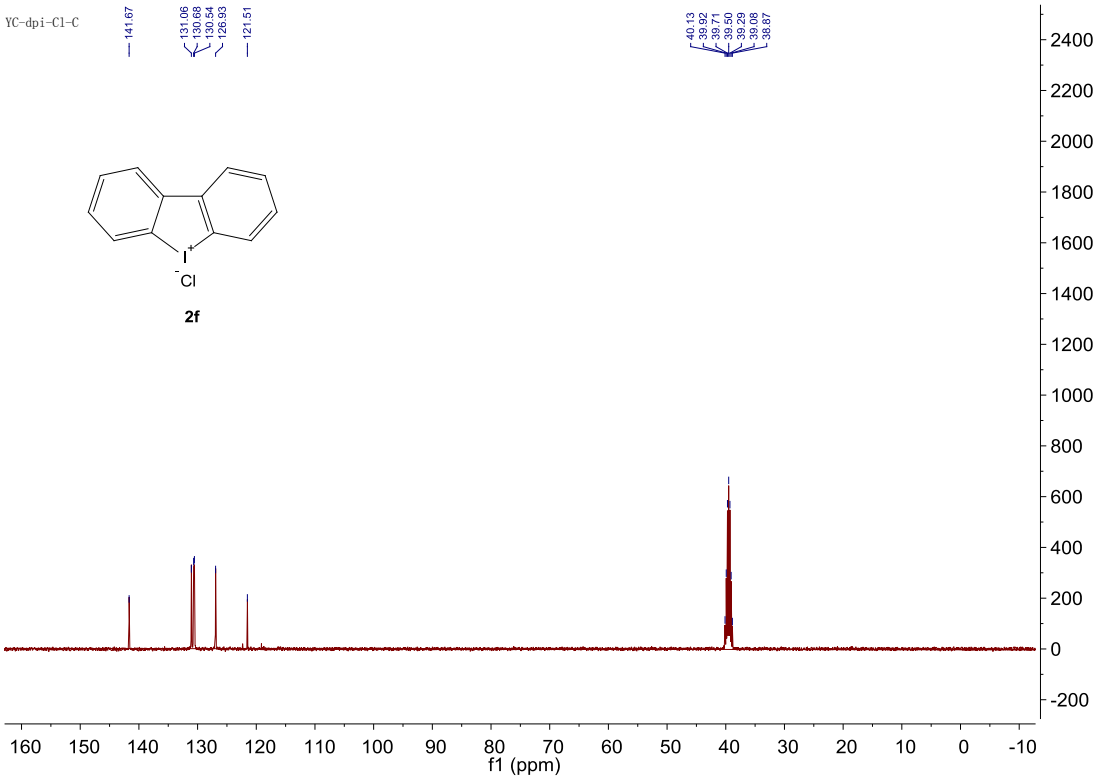

zq1-209-H-DMSO-20140123
8.218
7.707
7.701
7.406
7.400
7.384
7.378
3.887
2.500
H3C
O
CH3
O
I+
-OTf
2d
1.92
2.29
2.44
5.98
f1 (ppm)

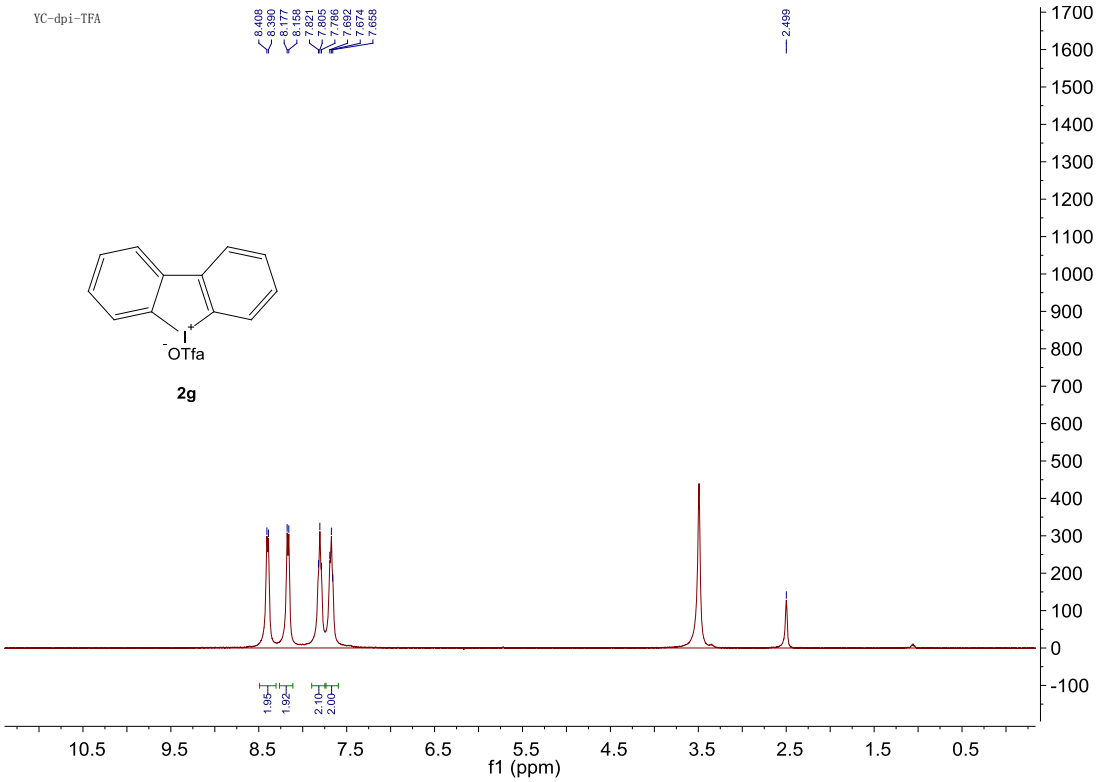

zq1-209-C-DMSO
159.82
134.15
126.78
121.91
117.80
114.72
55.95
40.13
39.92
39.71
39.50
39.28
39.08
38.87
H3C
O
CH3
O
I+
-OTf
2d
f1 (ppm)

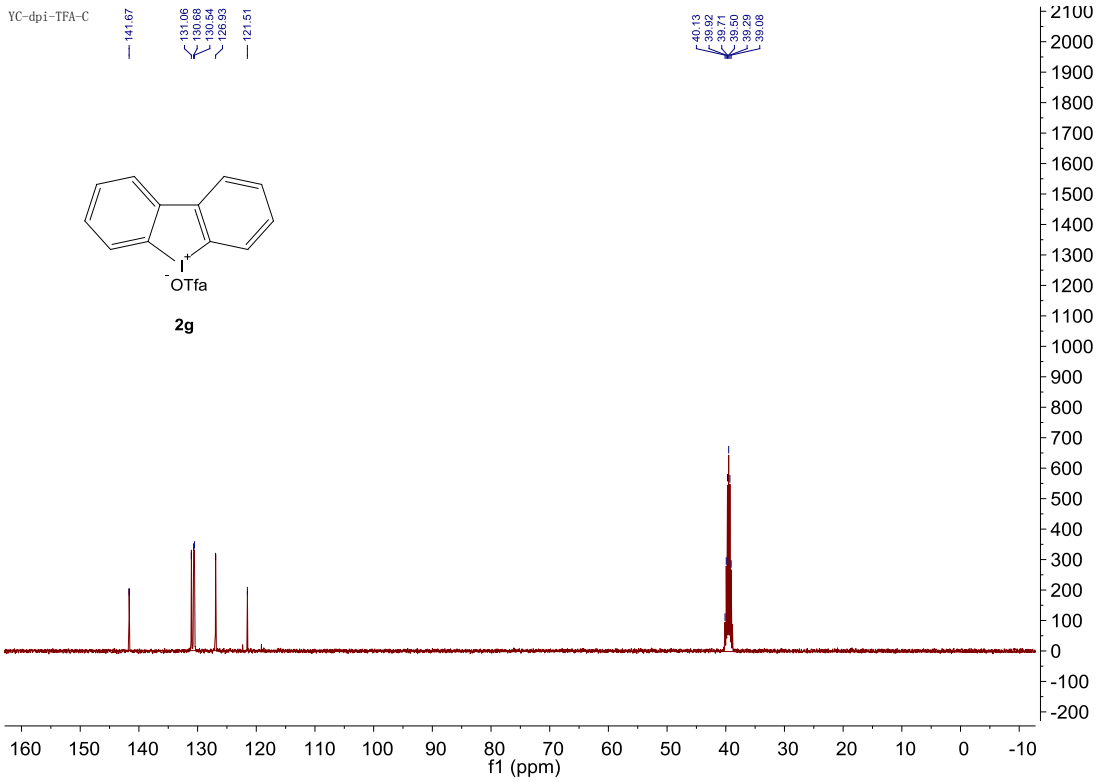

YC-DPI-OTS
8.483
8.463
8.265
8.244
7.846
7.720
7.701
7.533
7.514
7.138
7.118
2.500
2.286
OTs
2e
2.07
2.05
2.07
2.19
2.12
2.03
3.00
f1 (ppm)


YC-DPI-OTS-C
145.39
141.75
137.84
131.01
130.67
128.13
126.95
125.49
121.63
40.15
39.94
39.73
39.52
39.31
39.10
38.90
20.76
OTs
2e
f1 (ppm)


YC-dpi-Cl
8.408
8.390
8.177
8.158
7.821
7.805
7.786
7.692
7.674
7.658
2.499
Cl
2f
1.95
1.92
2.10
2.00
f1 (ppm)


YC-dpi-Cl-C
141.67
131.06
130.68
130.54
126.93
121.51
40.13
39.92
39.71
39.50
39.29
39.08
38.87
Cl
2f
f1 (ppm)


YC-dpi-TFA
8.408
8.390
8.177
8.158
7.821
7.805
7.786
7.692
7.674
7.658
2.499
OTfa
2g
1.95
1.92
2.10
2.00
f1 (ppm)


YC-dpi-TFA-C
141.67
131.06
130.68
130.54
126.93
121.51
40.13
39.92
39.71
39.50
39.29
39.08
OTfa
2g
f1 (ppm)