Supporting Information

Metal-free [3 + 3] benzannulation of 1-indanylidene-malononitrile with Morita–Baylis–Hillman carbonates: direct access to functionalized fluorene and fluorenone derivatives

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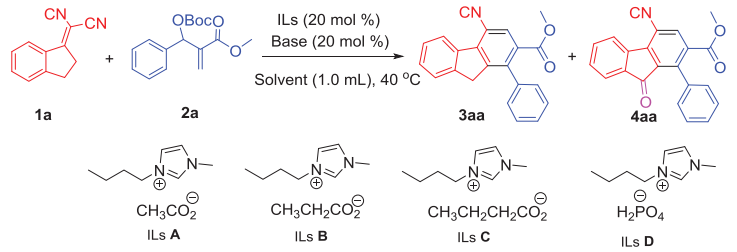
1. General experimental information

Reactions were monitored by TLC and visualized with ultraviolet light. All reagents were obtained from commercial supplier without further purification. Column chromatography was performed using silica gel (200–300 mesh) eluting with ethyl acetate and petroleum ether. NMR spectra were recorded with tetramethylsilane as the internal standard. 1H NMR and 13C NMR spectra of DMSO solutions were recorded either at 400 and 100 MHz or at 300 and 75 MHz (Bruker Avance), respectively and resonances (δ) are given in parts per million relatives to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. High resolution mass spectra were obtained with the Q-TOF-Premier mass spectrometer. The X-ray crystal-structure determinations of **3ba** were obtained on a Bruker APEX DUO system. All melting points are uncorrected.

2. Optimization of the reaction conditions

Table S1. Optimization of the Reaction Conditions[a]



Entry	Base	ILs	Solvent	Time (h)	Yield (%)[b] **3aa/4aa**
1	DABCO	**A**	CH_3CN	48	51 /trace
2	DMAP	**A**	CH_3CN	96	trace/ trace
3	DBU	**A**	CH_3CN	96	16/ trace
4	Et_3N	**A**	CH_3CN	96	11/ trac
5	PPh_3	**A**	CH_3CN	96	-/ -
6	-	**A**	CH_3CN	96	-/ -
7	DABCO	**-**	CH_3CN	168	18/ trace
8	DABCO	**A**	Toluene	48	10/ trace
9	DABCO	**A**	$CHCl_3$	48	17/ trace
10	DABCO	**A**	THF	48	24/ trace
11	DABCO	**A**	DMF	2	63/ trace
12	DABCO	**A**	DMSO	48	18 / trace
13[c]	DABCO	**A**	DMF	2	28 / trace
14[d]	DABCO	**A**	DMF	2	40 / trace
15[e]	DABCO	**A**	DMF	7	48 / trace
16[f]	DABCO	**A**	DMF	0.5	50/ trace

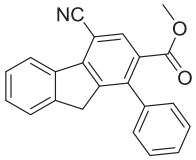
[a] Reaction conditions: **1a** (0.10) mmol, **2a** (0.10 mmol), ILs (20 mol %), catalyst (20 mol %), solvent (1.0 mL), 40 °C, air, sealed tube. [b] Yield of isolated **3aa** after purification by silica gel column chromatography. [c] the mole ratios to 1.5:1.0 (**1a**/**2a**); [d] the mole ratios to 1.0:1.5 (**1a**/**2a**); [e] 10 mol % of DABCO and 10 mol % ILs **A** were used;[f] 40 mol % of DABCO and 40 mol % ILs **A** were used;

3. General experimental procedures for synthesis of compounds 3

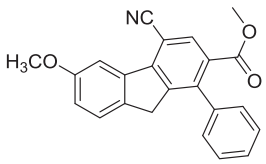
A mixture of DABCO (0.02 mmol, 20 mol %), ILs **D** (0.02 mmol, 20 mol %), 1-indanylidenemalononitrile **1** (0.10 mmol, 1.0 equiv.) and MBH carbonates **2** (0.10 mmol, 1.0 equiv.) and DMF (1.0 mL) were added to a sealed reaction tube equipped with a stir bar. The tube was then sealed and the resulting mixture was stirred at 60 °C for the time indicated in Scheme 2. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE:EtOAc = 30:1) to afford pure products **3**.

4. General experimental procedures for synthesis of compounds 4

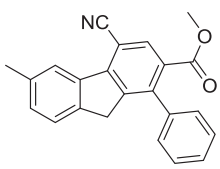
A mixture of catalyst DABCO (0.02 mmol, 20 mol%), ILs **D** (0.02 mmol, 20 mol %), 1-indanylidenemalononitrile **1** (0.10 mmol, 1.0 equiv.) and MBH carbonates **2** (0.10 mmol, 1.0 equiv.) and DMF (1.0 mL) were added to a reaction tube equipped with a stir bar. The resulting mixture was stirred at 60 °C under oxygen condition for the time indicated in Scheme 2. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE:EtOAc = 20:1) to afford pure products **4**.



Methyl 4-cyano-1-phenyl-9H-fluorene-2-carboxylate (3aa). White solid, 23.7 mg, 73% yield, m.p. 235.7-235.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.6 Hz, 1H), 8.23 (s, 1H), 7.47 – 7.34 (m, 6H), 7.20 (d, *J* = 7.7 Hz, 2H), 3.61 (d, *J* = 13.2 Hz, 5H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 145.6, 144.9, 144.8, 144.0, 138.4, 138.1, 134.2, 129.5, 128.6, 128.3, 127.9, 127.6 (2C), 127.6, 125.0, 123.0, 117.6, 103.2, 52.2, 36.9 ppm. IR (KBr) υ: 707, 768, 807, 906, 980, 1030, 1173, 1197, 1262, 1314, 1377, 1455, 1494, 1734, 2952cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{15}NO_2Na$ $(M+Na)^+$ 348.0995, found 348.0991.

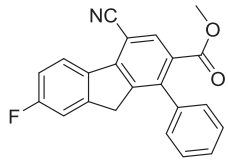


Methyl 4-cyano-6-methoxy-1-phenyl-9H-fluorene-2-carboxylate (3ba). Yellow solid, 24.5 mg, 69% yield, m.p.167.4-168.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.94 (d, *J* = 2.1 Hz, 1H), 7.38 (dd, *J* = 6.6, 4.5 Hz, 3H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.18 (dd, *J* = 7.6, 1.7 Hz, 2H), 6.96 – 6.89 (m, 1H), 3.84 (s, 3H), 3.58 (s, 3H), 3.53 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 159.5, 145.9, 145.7, 144.0, 139.3, 138.4, 137.3, 134.1, 128.6, 128.3, 127.9, 127.8, 125.6, 117.7, 117.4, 106.6, 103.1, 55.6, 52.3, 36.3 ppm. IR (KBr) υ: 703, 801, 859, 1035, 1117, 1221, 1292, 1433, 1731, 2227, 2851, 2923 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{18}NO_3$ $(M+H)^+$ 356.1281, found 356.1276.

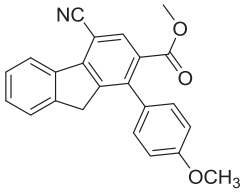


Methyl 4-cyano-6-methyl-1-phenyl-9H-fluorene-2-carboxylate (3ca). White solid, 24.1 mg, 71% yield, m.p. 266.4-266.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (d, *J* = 5.6 Hz, 2H), 7.53 – 7.41 (m, 3H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 5.6 Hz, 3H), 3.64 (d, *J* = 10.8 Hz, 5H), 2.48 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.4, 145.7, 145.2, 144.0, 142.1, 138.4,

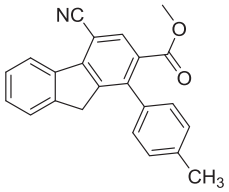
138.3, 137.4, 134.2, 130.6, 128.4, 128.3, 127.8, 127.7, 124.6, 123.3, 117.7, 103.0, 77.4, 77.0, 76.6, 52.2, 36.5, 21.6 ppm. IR (KBr) υ: 709, 789, 818, 997, 1110, 1164, 1203, 1212, 1292, 1429, 1730, 2227, 2845, 2923 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{17}NO_2Na$ $(M+Na)^+$ 362.1151, found 362.1138.



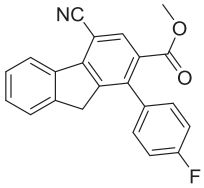
Methyl 4-cyano-7-fluoro-1-phenyl-9H-fluorene-2-carboxylate (3da). White solid, 26.8 mg, 78% yield, m.p. 240.8-241.0 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.52 – 8.42 (m, 1H), 8.29 (s, 1H), 7.54 – 7.42 (m, 3H), 7.28 – 7.15 (m, 4H), 3.67 (d, *J* = 7.8 Hz, 5H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.3, 163.6 (d, *J* = 250.4 Hz), 147.4 (d, *J* = 9.3 Hz), 144.8, 144.6 (d, *J* = 1.9 Hz), 144.0, 138.2, 134.3, 134.2, 128.4, 128.3, 128.0, 127.6, 124.5 (d, *J* = 9.4 Hz). 117.5, 115.2 (d, *J* = 23.1 Hz), 112.3 (d, *J* = 23.1 Hz). 102.9, 52.3, 36.9 ppm. IR (KBr) υ: 712， 794， 871， 1022， 1095， 1133， 1209， 1231， 1293， 1334， 1388， 1433， 1482， 1590， 1716， 2230， 1847， 2924 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{15}FNO_2$ $(M+H)^+$ 344.1081, found 344.1082.



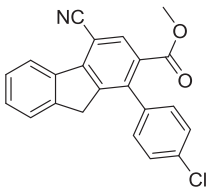
Methyl 4-cyano-1-(4-methoxyphenyl)-9H-fluorene-2-carboxylate (3ab). White solid, 30.6 mg, 86% yield, m.p. 177.2-178.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.6 Hz, 1H), 8.25 (s, 1H), 7.46 (ddt, *J* = 8.1, 7.2, 3.9 Hz, 3H), 7.21 (d, *J* = 8.6 Hz, 2H), 7.02 (t, *J* = 5.6 Hz, 2H), 3.89 (s, 3H), 3.71 (d, *J* = 10.3 Hz, 5H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 159.3, 145.5, 145.2, 144.9, 143.8, 138.3, 134.1, 130.5, 129.4, 129.0, 128.9, 127.6, 125.0, 123.0, 117.7, 113.8, 103.0, 55.2, 52.3, 37.0 ppm. IR (KBr) υ: 753, 911, 968, 1134, 1164, 1203, 1232, 1283, 1433, 1565, 1293, 1736, 2231, 2849, 2918 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{18}NO_3$ $(M+H)^+$ 356.1281, found 356.1285.



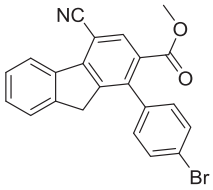
Methyl 4-cyano-1-p-tolyl-9H-fluorene-2-carboxylate (3ac). White solid, 23.1 mg, 68% yield, m.p. 258.1-258.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.6 Hz, 1H), 8.28 (s, 1H), 7.54 – 7.42 (m, 3H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 3.70 (d, *J* = 5.3 Hz, 5H), 2.45 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.5, 144.6, 144.0, 143.9, 143.2, 137.2, 136.7, 134.3, 133.1, 128.5, 128.1, 127.7, 126.6, 126.6, 124.0, 122.0, 116.7, 102.1, 51.3, 36.0, 20.4 ppm. IR (KBr) υ: 745, 778, 998, 1126, 1202, 1291, 1432, 1453, 1733, 2228, 2949 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{17}NO_2Na$ $(M+Na)^+$ 362.1151, found 362.1142.



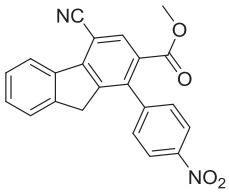
Methyl 4-cyano-1-(4-fluorophenyl)-9H-fluorene-2-carboxylate (3ad). White solid, 23.7 mg, 69% yield, m.p. 282.7-283.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.1 Hz, 1H), 8.29 (s, 1H), 7.54 – 7.41 (m, 3H), 7.28 – 7.14 (m, 4H), 3.69 (d, *J* = 8.7 Hz, 5H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.2, 162.4 (d, *J* = 247.5 Hz), 145.8, 145.0, 144.8, 143.1, 138.0, 134.3, 134.2 (d, *J* = 3.6 Hz), 129.6, 129.4 (d, *J* = 8.1 Hz). 128.4, 127.6, 125.0, 123.0, 117.5, 115.5 (d, *J* = 21.7 Hz), 103.4, 52.3, 36.9 ppm. IR (KBr) υ: 751, 778, 860, 1007, 1132, 1169, 1120, 1129, 1435, 1456, 1523, 1614, 1730, 2228, 2921, 2950 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{14}FNO_2Na$ $(M+Na)^+$ 366.0901, found 366.0897.



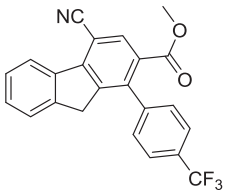
Methyl 1-(4-chlorophenyl)-4-cyano-9H-fluorene-2-carboxylate (3ae). White solid, 63% yield (22.7 mg), m.p.283.8-284.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.6 Hz, 1H), 8.32 (s, 1H), 7.54 – 7.44 (m, 5H), 7.21 (d, *J* = 8.2 Hz, 2H), 3.71 (s, 3H), 3.67 (s, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.0, 145.9, 144.9, 144.8, 142.9, 137.9, 136.8, 134.4, 134.0, 129.7, 129.1, 128.6, 128.1, 127.7, 125.0, 123.0, 117.4, 103.5, 52.4, 36.8 ppm. IR (KBr) υ: 787, 857, 969, 1046, 1090, 1140, 1438, 1514, 1722, 2225, 2850, 2930 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{15}ClNO_2$ $(M+H)^+$ 360.0786, found 360.0784.



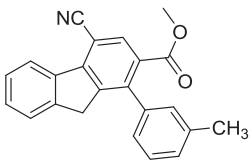
Methyl 1-(4-bromophenyl)-4-cyano-9H-fluorene-2-carboxylate (3af). White solid, 29.9 mg, 74% yield, m.p. 264.1-264.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.5 Hz, 1H), 8.31 (s, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.55 – 7.42 (m, 3H), 7.15 (d, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.66 (s, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.0, 145.9, 144.8 (2C), 142.9, 138.0, 137.3, 134.4, 131.6, 129.7, 129.4, 128.1, 127.7, 125.0, 123.1, 122.2, 117.5, 103.6, 52.4, 36.9 ppm. IR (KBr) υ: 745, 780, 854, 901, 1001, 1022, 1131, 1205, 1291, 1429, 1494, 1733, 2228, 2954 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{15}BrNO_2$ $(M+H)^+$ 404.0281, found 404.0286.



Methyl 4-cyano-1-(4-nitrophenyl)-9H-fluorene-2-carboxylate (3ag). White solid, 19.3 mg, 52% yield, m.p. 240.1-241.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 7.5 Hz, 1H), 8.38 (t, 3H), 7.56 – 7.43 (m, 5H), 3.73 (s, 3H), 3.63 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.4, 147.4, 146.4, 145.6, 144.6, 144.4, 142.0, 137.7, 134.7, 130.0, 128.8, 127.9, 127.3, 125.1, 123.7, 123.2, 117.2, 104.2, 52.5, 36.7. IR (KBr) υ: 751, 857, 910, 978, 1205, 1229, 1273, 1353, 1435, 1520, 1559, 1606, 1712, 2232, 2916, 2954, 3086 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{15}N_2O_4$ $(M+H)^+$ 371.1026, found 371.1021.

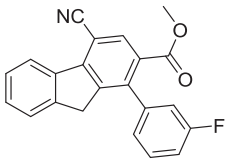


Methyl 4-cyano-1-(4-(trifluoromethyl)phenyl)-9H-fluorene-2-carboxylate (3ah). White solid, 23.2 mg, 59% yield, m.p. 209.1-210.3 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.52 (d, *J* = 7.5 Hz, 1H), 8.37 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.57 – 7.46 (m, 3H), 7.40 (d, *J* = 8.0 Hz, 2H), 3.71 (s, 3H), 3.64 (s, 2H) ppm. IR (KBr) υ: 745, 779, 859, 1007, 1067, 1129, 1161, 1202, 1295, 1330, 1437, 1741, 2230, 2924, 2959 cm^{-1}. HRMS (ESI) m/z calcd for $C_{23}H_{14}F_3NO_2Na$ $(M+Na)^+$ 416.0869, found 416.0869.

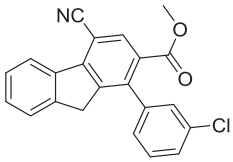


Methyl 4-cyano-1-m-tolyl-9H-fluorene-2-carboxylate (3ai). White solid, 22.1 mg, 65% yield, m.p. 230.0-230.6 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.4 Hz, 1H), 8.27 (s, 1H), 7.54 – 7.41 (m, 3H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 9.3 Hz, 2H), 3.69 (d, *J* = 7.1 Hz, 5H), 2.42 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 145.6, 144.9, 144.8, 144.2, 138.3, 138.1, 138.1, 137.9, 134.1, 129.4, 128.7, 128.6, 128.2, 127.5, 124.9, 124.8, 123.0, 117.6, 103.1, 52.2, 36.9, 21.5 ppm. IR (KBr) υ: 740, 772, 797, 857,

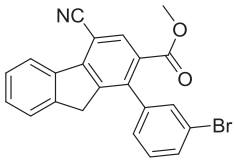
1024, 1102, 1124, 1186, 1208, 1262, 1293, 1435, 1731, 2223, 2854, 2924, 2955 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{17}NO_2Na$ $(M+Na)^+$ 362.1151, found 362.1151.



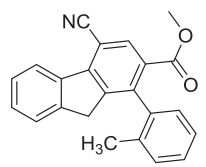
Methyl 4-cyano-1-(3-fluorophenyl)-9H-fluorene-2-carboxylate (3aj). White solid, 21.3 mg, 62% yield, m.p. 212.2-212.8 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.51 (d, *J* = 6.9 Hz, 1H), 8.32 (s, 1H), 7.56 – 7.41 (m, 4H), 7.20 – 7.11 (m, 1H), 7.06 – 6.94 (m, 2H), 3.69 (d, *J* = 4.9 Hz, 5H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.0, 162.6 (d, *J* = 246.7 Hz), 145.9, 145.0, 144.7, 142.6 (d, *J* = 1.6 Hz), 140.5 (d, *J* = 8.0 Hz), 138.0, 134.3, 130.0, (d, *J* = 8.5 Hz), 129.7, 128.2, 127.7, 125.0, 123.5 (d, *J* = 3.0 Hz), 123.1, 117.4, 114.9 (d, *J* = 21.8 Hz), 114.9 (d, *J* = 21.0 Hz), 103.7, 52.3, 36.7 ppm. IR (KBr) υ: 747, 777, 801, 865, 1017, 1097, 1156, 1210, 1262, 1297, 1438, 1585, 1730, 2225, 2852, 2921, 2967 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{14}FNO_2Na$ $(M+Na)^+$ 366.0901, found 366.0898.



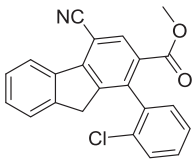
Methyl 1-(3-chlorophenyl)-4-cyano-9H-fluorene-2-carboxylate (3ak). White solid, 20.1 mg, 56% yield, m.p. 235.3-236.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.3 Hz, 1H), 8.32 (s, 1H), 7.55 – 7.41 (m, 5H), 7.28 (s, 1H), 7.19 – 7.12 (m, 1H), 3.69 (d, *J* = 11.4 Hz, 5H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.9, 146.0, 144.8 (2C), 142.5, 140.2, 137.9, 134.4, 134.3, 129.7, 129.6, 128.1 (2C), 127.8, 127.7, 126.0, 125.0, 123.1, 117.4, 103.7, 52.4, 36.8 ppm. IR (KBr) υ: 742, 774, 894, 1091, 1128, 1201, 1297, 1429, 1563, 1735, 2228, 2927, 2952 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{14}ClNO_2Na$ $(M+Na)^+$ 382.0605, found 382.0623.



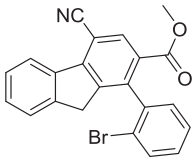
Methyl 1-(3-bromophenyl)-4-cyano-9H-fluorene-2-carboxylate (3al). White solid, 24.3 mg, 60% yield, m.p. 240.0-240.7 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.2 Hz, 1H), 8.33 (s, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.42 (m, 4H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 3.70 (d, *J* = 9.3 Hz, 5H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.9, 146.0, 144.8 (2C), 142.4, 140.4, 137.9, 134.4, 131.0, 130.6, 129.9, 129.8, 128.1, 127.7, 126.5, 125.0, 123.1, 122.4, 117.4, 103.7, 52.4, 36.8 ppm. IR (KBr) υ: 740, 775, 798, 896, 998, 1098, 1128, 1199, 1258, 1290, 1431, 1452, 1559, 1734, 2225, 2848, 2924, 2952 cm^{-1}. H RMS (ESI) calcd for $C_{22}H_{14}BrNO_2Na$ $(M+Na)^+$ 426.0100, found 426.0090.



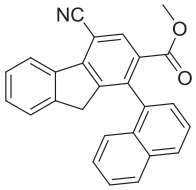
Methyl 4-cyano-1-o-tolyl-9H-fluorene-2-carboxylate (3am). White solid, 17.3 mg, 51% yield, m.p. 237.1-237.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 7.9 Hz, 1H), 8.39 (s, 1H), 7.55 – 7.42 (m, 3H), 7.39 – 7.27 (m, 3H), 7.06 (d, *J* = 7.4 Hz, 1H), 3.69 (s, 3H), 3.55 (dd, *J* = 66.2, 22.8 Hz, 2H), 2.03 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.7, 145.9, 145.0, 144.9, 144.2, 138.2, 138.0, 134.7, 134.4, 129.9, 129.6, 128.1, 128.0, 127.6, 127.1, 125.8, 125.0, 123.0, 117.6, 103.3, 52.3, 36.7, 19.6 ppm. IR (KBr) υ: 735, 744, 773, 900, 997, 1130, 1195, 1206, 1260, 1295, 1433, 1476, 1730, 2225, 2924, 2947 cm^{-1}. HRMS (ESI) m/z calcd for $C_{23}H_{17}NO_2Na$ $(M+Na)^+$ 362.1151, found 362.1154.



Methyl 1-(2-chlorophenyl)-4-cyano-9H-fluorene-2-carboxylate (3an). White solid, 18.4 mg, 51% yield, m.p. 226.8-228.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 7.5 Hz, 1H), 8.44 (s, 1H), 7.56 – 7.45 (m, 4H), 7.44 – 7.38 (m, 2H), 7.24 – 7.19 (m, 1H), 3.72 (s, 3H), 3.63 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 146.2, 145.2, 144.9, 141.5, 138.1, 137.5, 134.5, 132.1, 129.7, 129.4, 129.4, 129.1, 127.9, 127.6, 126.8, 125.1, 123.1, 117.5, 103.9, 52.3, 36.5 ppm. IR (KBr) υ:736, 744, 770, 792, 902, 996, 1065, 1186, 1260, 1295, 1434, 1450, 1592, 1726, 2228, 2846, 2923, 2959 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{14}ClNO_2Na$ $(M+Na)^+$ 382.0605, found 382.0610.

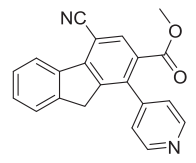


Methyl 1-(2-bromophenyl)-4-cyano-9H-fluorene-2-carboxylate (3ao). White solid, 24.7 mg, 61% yield, m.p. 244.3-245.2 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (d, *J* = 7.4 Hz, 1H), 8.44 (s, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.42 (m, 4H), 7.38 – 7.30 (m, 1H), 7.23 – 7.18 (m, 1H), 3.73 (s, 3H), 3.61 (d, *J* = 2.5 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.2, 146.3, 145.0, 144.9, 143.1, 139.5, 138.1, 134.6, 132.6, 129.7, 129.4, 129.0, 127.7, 127.6, 127.4, 125.1, 123.1, 121.9, 117.5, 103.9, 52.4, 36.6 ppm. IR (KBr) υ: 727, 740, 772, 789, 902, 1026, 1132, 1212, 1286, 1296, 1335, 1380, 1562, 1646, 1719, 2223, 2854, 2921, 2952 cm^{-1}. HRMS (ESI) m/z calcd for $C_{22}H_{15}BrNO_2^+$ $(M+H)^+$ 404.0281, found 404.0284.

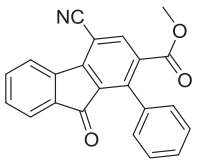


Methyl 4-cyano-1-(naphthalen-1-yl)-9H-fluorene-2-carboxylate (3ap). White solid, 19.5 mg, 52% yield, m.p. 239.7-240.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 7.8 Hz, 1H), 8.47 (s, 1H), 7.96 (d, *J* = 8.2 Hz, 2H), 7.61 – 7.56 (m, 1H), 7.54 – 7.47 (m, 2H), 7.45 – 7.39 (m, 2H), 7.37 – 7.28 (m, 3H), 3.61 (d, *J* = 22.9 Hz, 1H), 3.50 (s, 3H), 3.40 (d, *J* = 22.9 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 146.0, 145.9, 144.9, 142.8, 138.1, 136.2, 134.5, 133.4, 131.0, 129.6, 129.3, 128.5, 128.3, 127.6, 126.5, 126.0, 125.3, 125.1, 125.0, 124.7, 123.1, 117.6, 103.7, 52.1, 36.6 ppm. IR (KBr) υ: 653, 744, 775, 803, 902, 1002, 1191, 1208, 1260, 1295, 1402, 1434, 1570, 1587, 1732, 2227, 2851, 2923, 2948 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{17}NO_2Na$ $(M+Na)^+$ 398.1151, found 398.1164.

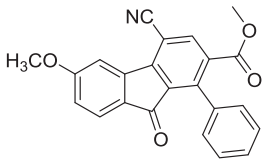
Methyl 4-cyano-1-(pyridin-4-yl)-9H-fluorene-2-carboxylate (3aq).



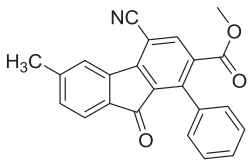
Yellow solid, 11.1 mg, 34% yield, m.p. 139.1-141.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.3 Hz, 1H), 8.45 8.45 (d, J = 7.5 Hz, 1H), 8.27 (s, 1H), 7.74-7.79 (m, 1H), 7.50 – 7.34 (m, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 3.70 (s, 2H), 3.62 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.10, 156.98, 149.56, 146.40, 145.05, 144.73, 142.47, 137.93, 136.29, 134.43, 129.74, 128.23, 127.66, 125.04, 123.41, 123.14, 122.75, 117.54, 104.01, 52.39, 36.43 ppm. IR (KBr) υ: 747, 778, 904, 999, 1133, 1201, 1296, 1428, 1587, 1732, 2228, 2856, 2930 cm^{-1}. HRMS (ESI) calcd for C_{21} H_{15} N_2 O_2 $(M+H)^+$ 327.1128, found 327.1124.



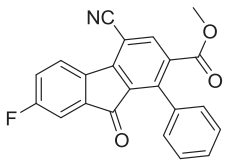
Methyl 4-cyano-9-oxo-1-phenyl-9H-fluorene-2-carboxylate (4aa). Yellow solid, 18.7 mg, 55% yield, m.p. 244.8-254.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.7 Hz, 1H), 8.20 (s, 1H), 7.68 – 7.62 (m, 2H), 7.50 – 7.44 (m, 4H), 7.26 – 7.21 (m, 2H), 3.61 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.3, 165.7, 149.1, 145.6, 139.7, 138.6, 135.5, 134.6, 134.3, 133.8, 131.9, 131.7, 128.5, 127.9, 127.7, 124.7, 123.1, 116.4, 104.3, 52.5 ppm. IR (KBr) υ: 636, 698, 746, 789, 904, 978, 1134, 1199, 1226, 1270, 1355, 1431, 1559, 1604, 1721, 2230, 1952, 3074 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.



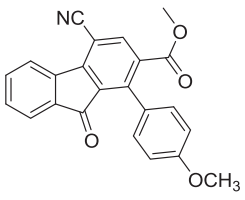
Methyl 4-cyano-6-methoxy-9-oxo-1-phenyl-9H-fluorene-2-carboxylate (4ba). Yellow solid, 21.4 mg, 58% yield, m.p. 171.4-173.1°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.75 (d, *J* = 2.1 Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 1H), 7.39 – 7.34 (m, 3H), 7.19 – 7.14 (m, 2H), 6.83 (dd, *J* = 8.3, 2.2 Hz, 1H), 3.88 (s, 3H), 3.52 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.9, 165.9, 165.8, 148.2, 145.0, 142.3, 138.0, 134.6, 134.1, 133.0, 128.5, 128.0, 127.7, 127.3, 126.7, 116.7, 116.5, 108.8, 104.1, 56.0, 52.5 ppm. IR (KBr) υ: 701, 800, 861, 1039, 1115, 1221, 1292, 1368, 1433, 1591, 1710, 2224, 2851, 2923, 2955 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{15}NO_4Na$ $(M+Na)^+$ 392.0893, found 392.0883.



Methyl 4-cyano-6-methyl-9-oxo-1-phenyl-9H-fluorene-2-carboxylate (4ca). Yellow solid, 20.8 mg, 59% yield, m.p. 296.7-296.9 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (s, 1H), 8.10 (s, 1H), 7.54 – 7.41 (m, 4H), 7.28 – 7.21 (m, 3H), 3.61 (s, 3H), 2.50 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.9, 165.7, 149.0, 147.0, 145.3, 140.0, 138.4, 134.6, 133.6, 132.3 (2C), 132.0, 128.4, 127.8, 127.7, 124.6, 123.7, 116.5, 104.0, 52.5, 22.3 ppm. IR (KBr) υ: 703, 712, 804, 911, 1110, 1199, 1229, 1213, 1353, 1431, 1557, 1591, 1713, 2236, 2854, 2923, 2952 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{15}NO_3Na$ $(M+Na)^+$ 376.0944, found 376.0933.

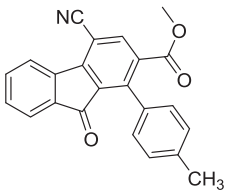


Methyl 4-cyano-7-fluoro-9-oxo-1-phenyl-9H-fluorene-2-carboxylate (4da). Yellow solid, 19.7 mg, 55% yield, m.p. 248.9-250.1 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 – 8.27 (m, 1H), 8.21 (s, 1H), 7.47 (d, *J* = 3.7 Hz, 3H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 4.1 Hz, 2H), 3.61 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.0, 165.6, 164.9 (d, *J* = 254.3 Hz), 148.6, 145.8, 138.9, 136.8 (d, *J* = 7.8 Hz), 135.5 (d, *J* = 3.0 Hz), 134.3, 133.5, 132.0, 128.7, 127.8, 127.8, 124.9 (d, *J* = 8.5 Hz), 121.9 (d, *J* = 23.4 Hz), 116.3, 112.3 (d, *J* = 23.8 Hz), 104.1, 52.5 ppm. IR (KBr) υ: IR (KBr) υ: 736, 796, 876, 980, 1035, 1065, 1131, 1201, 1260, 1381, 1394, 1450, 1475, 1592, 1729, 2226, 2846, 2927 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{12}FNO_3Na$ $(M+Na)^+$ 380.0693, found 380.0692.

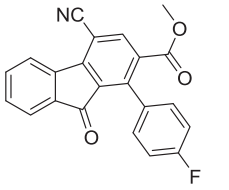


Methyl 4-cyano-1-(4-methoxyphenyl)-9-oxo-9H-fluorene-2-carboxylate (4ab). Yellow solid, 22.2 mg, 60% yield, m.p. 234.1-234.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.7 Hz, 1H),

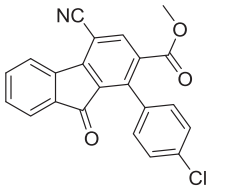
8.13 (s, 1H), 7.68 – 7.60 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.19 (d, *J* = 8.6 Hz, 2H), 6.98 (d, *J* = 8.7 Hz, 2H), 3.88 (s, 3H), 3.65 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.5, 166.1, 159.9, 149.1, 145.3, 139.7, 138.4, 135.4, 134.2, 134.2, 131.7, 131.6, 129.5, 126.3, 124.6, 123.0, 116.5, 113.2, 103.9, 55.1, 52.6 ppm. IR (KBr) υ: 657, 757, 772, 785, 835, 911, 969, 1026, 1037, 1128, 1227, 1244, 1270, 1288, 1433, 1520, 1561, 1611, 1722, 1738, 2230, 2834, 2950 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{15}NO_4Na$ $(M+Na)^+$ 392.0893, found 392.0897.



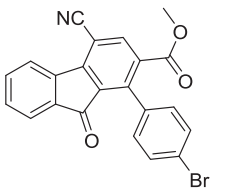
Methyl 4-cyano-9-oxo-1-p-tolyl-9H-fluorene-2-carboxylate (4ac). Yellow solid, 19.8 mg, 56% yield, m.p. 260.8-261.7 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.8 Hz, 1H), 8.18 (s, 1H), 7.65 (t, *J* = 6.6 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 3.65 (s, 3H), 2.45 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.4, 165.8, 149.1, 145.8, 139.7, 138.5, 138.4, 135.4, 134.3, 133.9, 131.8, 131.7, 131.4, 128.5, 127.8, 124.7, 123.0, 116.5, 104.1, 52.5, 21.5 ppm. IR (KBr) υ: 540, 631, 703, 789, 846, 980, 1021, 1052, 1184, 1251, 1416, 1442, 1600, 1674, 2190, 2984, 3221 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 376.0944, found 376.0935.



Methyl 4-cyano-1-(4-fluorophenyl)-9-oxo-9H-fluorene-2-carboxylate (4ad). Yellow solid, 18.6 mg, 52% yield, m.p. 289.7-290.6 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.5 Hz, 1H), 8.21 (s, 1H), 7.66 (t, *J* = 7.4 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.25 – 7.09 (m, 4H), 3.65 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.3, 165.5, 162.8 (d, *J* = 248.1 Hz), 149.2, 144.5, 139.6, 138.8, 135.6, 134.2, 133.6, 131.9, 131.8, 130.3 (d, *J* = 3.5 Hz), 129.8 (d, *J* = 8.3 Hz), 124.7, 123.1, 116.3, 115.0 (d, *J* = 21.8 Hz). 104.5, 52.6 ppm. IR (KBr) υ: 666, 705, 796, 813, 891, 980, 1208, 1236, 1268, 1351, 1431, 1476, 1561, 1708, 1728, 2233, 2949 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{12}FNO_3Na$ $(M+Na)^+$ 380.0693, found 380.0695.

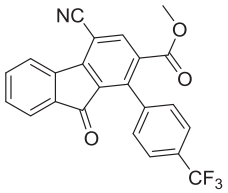


Methyl 1-(4-chlorophenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (4ae). Yellow solid, 19.1 mg, 51% yield, m.p. 270.5-271.4 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.5 Hz, 1H), 8.23 (s, 1H), 7.66 (t, *J* = 7.7 Hz, 2H), 7.52 – 7.40 (m, 3H), 7.17 (d, *J* = 8.4 Hz, 2H), 3.66 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.2, 165.3, 149.2, 144.3, 139.6, 138.9, 138.9, 135.6, 134.6, 134.1, 133.3, 132.9, 131.9, 129.3, 128.1, 124.8, 123.1, 116.3, 104.6, 52.6 ppm. IR (KBr) υ: 757, 820, 833, 979, 1091, 1204, 1229, 1281, 1328, 1352, 1432, 1500, 1556, 1602, 1715, 2347, 2952 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{12}ClNO_3Na$ $(M+Na)^+$ 396.0398, found 396.0379.

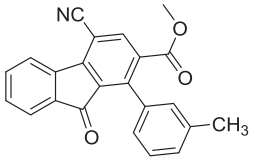


Methyl 1-(4-bromophenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (4af). Yellow solid, 19.2 mg, 46% yield, m.p. 242.4-243.2 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.5 Hz, 1H), 8.24 (s, 1H), 7.69 – 7.56 (m, 4H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 8.3 Hz, 2H), 3.67 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.2, 165.3, 149.2, 144.3, 139.6, 138.9, 135.6, 134.1, 133.4, 133.2, 131.9, 131.8, 131.0, 129.6, 124.8, 123.1, 122.9, 116.3, 104.6, 52.6 ppm. IR (KBr) υ: 643, 678, 737, 756, 789, 842, 910, 976, 1016, 1068, 1136, 1208, 1229,

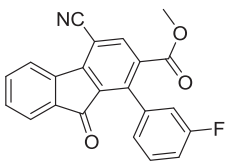
1274, 1354, 1389, 1431, 1471, 1556, 1602, 1715, 2230, 2948 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.



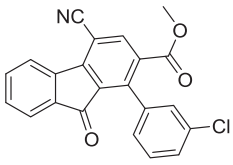
Methyl 4-cyano-9-oxo-1-(4-(trifluoromethyl)phenyl)-9H-fluorene-2-carboxylate (4ag). Yellow solid, 18.3 mg, 45% yield, m.p. 231.0-232.0 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 8.37 – 8.28 (m, 2H), 7.74 – 7.62 (m, 4H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 3.65 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.2, 165.0, 149.3, 144.0, 139.6, 139.2, 138.5 (2C), 135.7, 134.1, 132.8, 132.0 (2C), 130.7, 130.2, 128.3, 124.8 (2C), 124.7, 124.6, 123.2, 116.2, 105.0, 52.6 ppm. IR (KBr) υ: 540, 692, 748, 779, 857, 1006, 1128, 1168, 1206, 1297, 1433, 1457, 1522, 1567, 1608, 1732, 2230, 2923, 2952 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{12}F_3NO_3Na$ $(M+Na)^+$ 430.0661, found 430.0646.



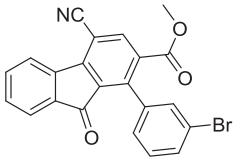
Methyl 4-cyano-9-oxo-1-m-tolyl-9H-fluorene-2-carboxylate (4ah). Yellow solid, 19.1 mg, 54% yield, m.p. 230.1-231.0 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.8 Hz, 1H), 8.18 (s, 1H), 7.69 – 7.61 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.26 (m, 2H), 7.04 (d, *J* = 6.9 Hz, 2H), 3.62 (s, 3H), 2.41 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.3, 165.8, 149.1, 145.7, 139.7, 138.5, 137.3, 135.4, 134.4, 134.2, 133.8, 131.8, 131.7, 129.3, 128.4, 127.6, 125.0, 124.7, 123.0, 116.5, 104.1, 52.5, 21.5 ppm. IR (KBr) υ: 666, 696, 751, 796, 980, 1019, 1201, 1223, 1263, 1431, 1600, 1719, 2224, 2921, 2955 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{15}NO_3Na$ $(M+Na)^+$ 376.0944, found 376.0942.



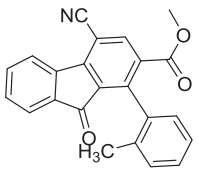
Methyl 4-cyano-1-(3-fluorophenyl)-9-oxo-9H-fluorene-2-carboxylate (4ai). Yellow solid, 18.2 mg, 51% yield, m.p. 289.8-290.0 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.4 Hz, 1H), 8.25 (s, 1H), 7.66 (t, *J* = 7.4 Hz, 2H), 7.52 – 7.38 (m, 2H), 7.17 (t, *J* = 7.5 Hz, 1H), 6.98 (t, *J* = 9.5 Hz, 2H), 3.66 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.1, 165.2, 162.2 (d, *J* = 246.3 Hz), 149.2, 143.9 (d, *J* = 2.2 Hz), 139.6, 139.0, 136.7 (d, *J* = 8.3 Hz), 135.6, 134.2, 133.2, 131.9 (2C), 129.4 (d, *J* = 8.3 Hz), 124.8, 123.6 (d, *J* = 3.1 Hz), 123.2, 116.3, 115.4 (d, *J* = 20.3 Hz), 115.3 (d, *J* = 22.5 Hz), 104.8, 52.6 ppm. IR (KBr) υ: 757, 796, 915, 978, 1134, 1210, 1229, 1273, 1357, 1433, 1565, 1600, 1721, 2230, 2955 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.



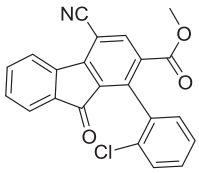
Methyl 1-(3-chlorophenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (4aj). Yellow solid, 18.3 mg, 49% yield, m.p. 282.4-283.3 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.6 Hz, 1H), 8.26 (s, 1H), 7.67 (t, *J* = 7.2 Hz, 2H), 7.52 – 7.36 (m, 3H), 7.23 (s, 1H), 7.12 (d, *J* = 7.4 Hz, 1H), 3.66 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.1, 165.2, 149.3, 143.8, 139.6, 139.0, 136.3, 135.6, 134.2, 133.8, 133.1, 132.0, 131.9, 129.0, 128.6, 128.0, 126.1, 124.8, 123.2, 116.3, 104.8, 52.7 ppm. IR (KBr) υ: 753, 796, 909, 978, 1077, 1136, 1206, 1225, 1270, 1431, 1556, 1591, 1602, 1717, 2230, 2955 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.



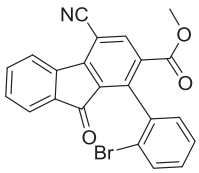
Methyl 1-(3-bromophenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (4ak). Yellow solid, 20.1 mg, 48% yield, m.p. 294.9-295.8 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.8 Hz, 1H), 8.26 (s, 1H), 7.71 – 7.56 (m, 3H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.41 – 7.30 (m, 2H), 7.17 (d, *J* = 7.6 Hz, 1H), 3.67 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.1, 165.1, 149.3, 143.7 (2C), 139.59, 139.01, 136.55, 135.61, 134.16, 133.07, 131.93, 131.48, 130.74, 129.23, 126.61, 124.83, 123.17, 121.79, 116.25, 104.80, 52.66 ppm. IR (KBr) υ: 753, 796, 906, 978, 1208, 1225, 1275, 1353, 1431, 1556, 1591, 1719, 2224, 2955 cm^{-1}. HRMS (ESI) m/z calcd for $C_{22}H_{12}BrNO_3Na$ $(M+Na)^+$ 439.9893, found 439.9889.



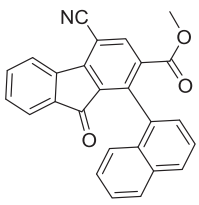
Methyl 4-cyano-9-oxo-1-o-tolyl-9H-fluorene-2-carboxylate (4al). Yellow solid, 14.1 mg, 40% yield, m.p. 234.5-235.1 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 – 8.26 (m, 2H), 7.71 – 7.61 (m, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.23 (m, 3H), 6.96 (d, *J* = 7.4 Hz, 1H), 3.63 (s, 3H), 2.05 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.3, 165.1, 149.3, 145.6, 139.9, 139.1, 135.5, 135.1, 134.8, 134.3, 133.2, 132.3, 131.8, 129.4, 128.5, 126.9, 125.4, 124.7, 123.2, 116.5, 104.4, 52.5, 19.9 ppm. IR (KBr) υ: 701, 961, 794, 948, 985, 1013, 1052, 1104, 1242, 1407, 1442, 1608, 1665, 2193, 2993, 3169, 3354 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.



Methyl 1-(2-chlorophenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (4am). Yellow solid, 18.3 mg, 49% yield, m.p. 246.7-247.8 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.34 (d, *J* = 7.5 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 2H), 7.52 – 7.33 (m, 4H), 7.17 – 7.12 (m, 1H), 3.70 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.0, 164.4, 149.5, 142.6, 139.8, 139.6, 135.6, 134.3, 134.2, 132.5, 132.2, 132.0, 131.9, 129.7, 128.9 (2C), 126.3, 124.8, 123.2, 116.3, 105.0, 52.7 ppm. IR (KBr) υ: 677, 727, 742, 751, 785, 911, 969, 1065, 1136, 1203, 1283, 1435, 1559, 1589, 1734, 2230, 2851, 2921, 2950 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{12}ClNO_3Na$ $(M+Na)^+$ 396.0398, found 396.0390.



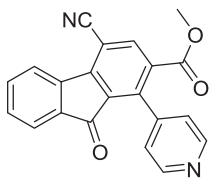
Methyl 1-(2-bromophenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (4an). Yellow solid, 19.2 mg, 46% yield, m.p. 230.0-230.7 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.34 (d, *J* = 7.6 Hz, 1H), 7.71 – 7.62 (m, 3H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.44 – 7.32 (m, 2H), 7.18 – 7.11 (m, 1H), 3.70 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.9, 164.2, 149.5, 144.1, 139.8, 139.6, 136.2, 135.5, 134.2, 133.9, 132.3, 132.0, 131.9, 129.7, 128.8, 126.9, 124.8, 123.2, 121.7, 116.3, 105.0, 52.6 ppm. IR (KBr) υ: 657, 757, 848, 909, 978, 1158, 1227, 1273, 1355, 1433, 1517, 1561, 1600, 1717, 2227, 2848, 2921, 2952 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.



Methyl 4-cyano-1-(naphthalen-1-yl)-9-oxo-9H-fluorene-2-carboxylate (4ao). Yellow solid, 14.4 mg, 37% yield, m.p. 247.8-248.3 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.44 – 8.32 (m, 2H), 7.95 (t, *J* = 9.0 Hz, 2H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.59 – 7.52 (m, 2H), 7.50 – 7.42 (m, 2H), 7.34 – 7.24 (m, 3H), 3.42

(s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.9, 164.9, 149.4, 144.3, 139.8, 139.2, 135.4, 134.3, 133.9, 133.2, 133.0, 132.9, 131.8, 131.5, 128.7, 128.6, 126.3, 125.8, 125.1, 124.9, 124.8, 124.4, 123.2, 116.5, 104.7, 52.4 ppm. IR (KBr) υ: 536, 705, 766, 789, 928, 1015, 1049, 1189, 1243, 1405, 1602, 1635, 1661, 2184, 2978, 3184 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{13}NO_3Na$ $(M+Na)^+$ 362.0788, found 362.0791.

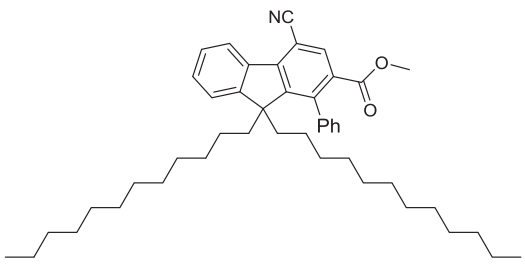
Methyl 4-cyano-1-(pyridin-4-yl)- 9-oxo-9H -fluorene-2-carboxylate (4ap).



Yellow solid, 9.2 mg, 27% yield, m.p. 151.9-153.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 3.0 Hz, 1H), 8.25-8.27 (m, 2H), 7.76 (t, *J* = 7.3 Hz, 1H), 7.57-7.61 (m, 2H), 7.36 – 7.43 (m, 2H), 7.31 – 7.34 (m, 1H), 3.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.35, 164.97, 153.57, 149.37, 149.06, 139.88, 139.45, 135.69, 135.61, 134.28, 132.70, 132.27, 131.95, 124.86, 124.08, 123.28, 123.19, 116.35, 105.12, 52.68 ppm. IR (KBr) υ: 750, 786, 915, 976, 1144, 1206, 1228, 1290, 1429, 1563, 1589, 1725, 2238, 2857, 2924, 2955 cm^{-1}. HRMS (ESI) calcd for C_{21} H_{13} N_2 O_3 $(M+H)^+$ 341.0921, found 341.0908.

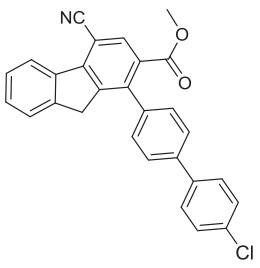
4. Procedure for the synthesis of compounds 5 and 6

Procedure for the synthesis of compounds 5: Under nitrogen atmosphere, to a dried tube (10 mL), compound **3aa** (60.6 mg, 0.15 mmol), *t*-BuOK (3.0 equiv.), 1-bromododecane (2.2 equiv.) were successively added, followed by adding THF (1.0 mL). The resulting mixture was stirred at 30 °C for 1.5 h till almost full consumption of **3aa** (monitored by TLC), and then the reaction mixture was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate) to afford the corresponding product **5**.



Methyl 4-cyano-9,9-didodecyl-1-phenyl-9H-fluorene-2-carboxylate (5). White solid, 20.8 mg, 21% yield, m.p. 222.4-225.1 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (dd, *J* = 6.2, 2.3 Hz, 1H), 8.17 (s, 1H), 7.47 – 7.41 (m, 5H), 7.28 (dd, *J* = 6.1, 2.4 Hz, 1H), 7.20 (dd, *J* = 7.6, 1.5 Hz, 2H), 3.57 (s, 3H), 1.67 – 1.60 (m, 4H), 1.29 – 0.98 (m, 38H), 0.87 (t, *J* = 6.9 Hz, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 153.2, 148.4, 146.1, 143.5, 137.0, 136.9, 133.7, 130.8, 130.2, 128.3, 128.1, 127.6, 127.5, 122.7, 121.9, 117.9, 103.5, 57.5, 52.2, 39.3, 31.9, 29.6, 29.5, 29.3, 29.2, 23.4, 22.7, 14.1. HRMS (ESI) calcd for $C_{46}H_{63}NO_2Na$ $(M+Na)^+$ 684.4751, found 684.4764 .

Procedure for the synthesis of compounds 6: Under nitrogen atmosphere, to a dried tube (10 mL), compound **3af** (60.6 mg, 0.15 mmol), 4-chlorophenylboronic acid (1.5 equiv.), Cs_2CO_3 (2.0 equiv.), $Pd(OAc)_2$ (0.05 equiv.) and butyl di-1-adamantylphosphine (0.06 equiv.) were successively added, followed by adding DME (2.0 mL). The resulting mixture was stirred at 80 °C for 40 h till almost full consumption of **3af** (monitored by TLC), and then the reaction mixture was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate) to afford the corresponding product **6**.



Methyl 1-(2--(4-chlorophenyl)-phenyl)-4-cyano-9-oxo-9H-fluorene-2-carboxylate (6). Yellow solid, 30.1 mg, 46% yield, m.p. 94.6-97.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 7.6 Hz, 1H), 8.33 (s, 1H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.51 (t, *J* = 8.3 Hz, 2H), 7.48 – 7.42 (m, 3H), 7.35 (d, *J* = 8.2 Hz, 2H), 3.74 (s, 2H), 3.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 145.9, 145.0, 144.9, 143.7, 139.4, 138.9, 138.2, 137.8, 134.4, 133.7, 129.7, 129.0, 128.5, 128.4, 128.3, 127.7, 126.9, 125.0, 123.1, 117.6, 103.5, 52.4, 37.0. HRMS (ESI) calcd for $C_{28}H_{18}ClNO_2Na$ $(M+Na)^+$ 458.0924, found 458.0935.

5. Studying the reaction mechanism

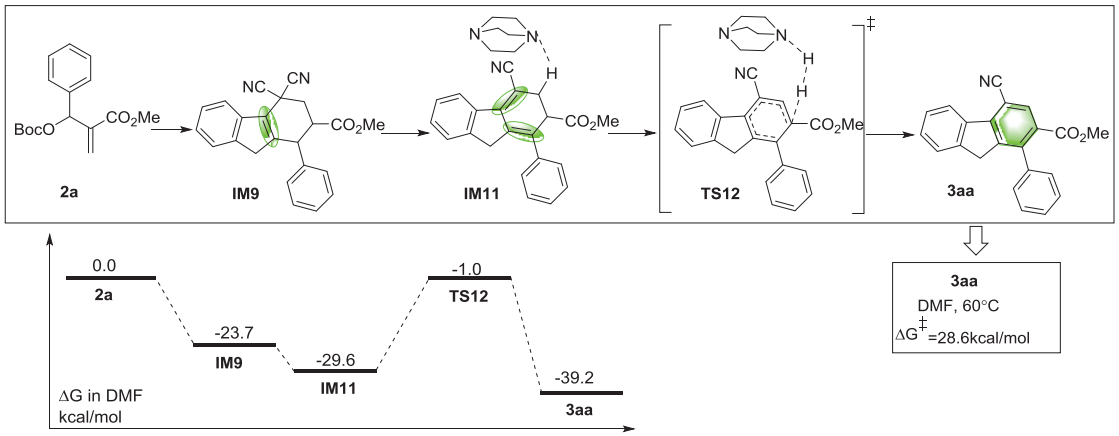


Figure s1. Proposed process for the benzannulation of **2a** and DFT calculation study

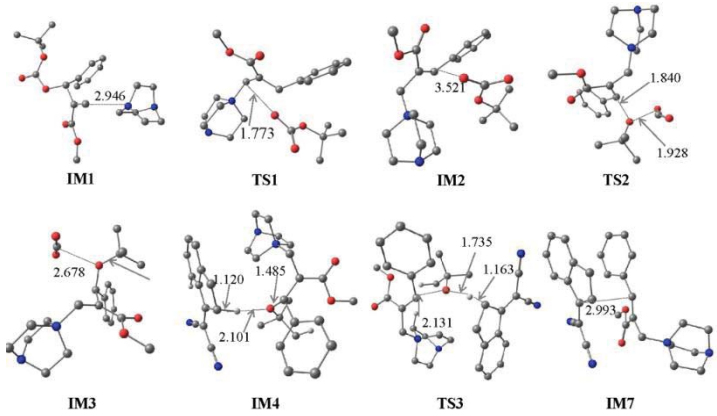


Figure S2. Optimized structures of the key stationary points for stage I at the m062x+D3/def2-TZVPP (smd, solvent = DMF)//BP86+D3(BJ)/def2-SVP(smd, solvent = DMF) level. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue).

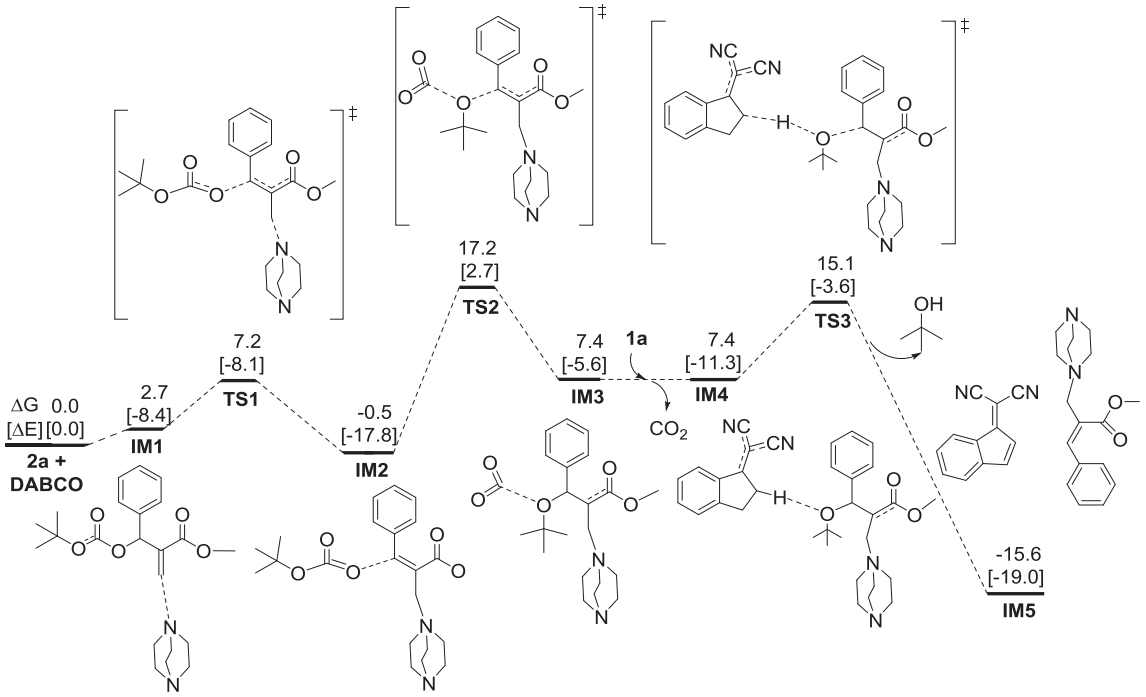


Figure S3. Gibbs free energy profile (in kcal/mol) for the stage I of the target reaction at the m062x + D3/def2-TZVPP (smd, solvent = DMF)//BP86+D3(BJ)/def2-SVP(smd, solvent = DMF) level. The optimized geometries are detailed in the Figure S1.

Stage I: formation of the intermediate IM5. As shown by the reaction course in Figure S1 and S2, the reaction initiates from the DABCO addition to the terminal unsaturated CH_2 species of MBH carbonates (**2a**) forming the slightly less stable intermediate **IM1**. After crossing a small barrier of 2.7 kcal/mol (**IM1→TS1**), the C-N bond formation is achieved leading to the intermediate **IM2** with exoergic by 0.5 kcal/mol with respect to the initial reactants. The following CO_2 and new ^{tBu}O-C bond formation step can be readily completed via a barrier of 17.7 kcal/mol (**IM2→TS2**), providing the weak intermediate **IM3**. With the addition of the substrate 1-indanylidenemalononitrile **(1a)**, the CO_2 can be easily released generating the comparable intermediate **IM4**. The barrier for the following C-H bond activation and H-O^{tBu} bond formation step is predicted to be 7.7 kcal/mol (**IM4→TS3**), which is quite low for experimental realization at mild conditions. With H-O^{t}Bu liberate, the thermodynamically more stable **IM5** is formed with exoergic by 23.0 kcal/mol relative to **IM4**.

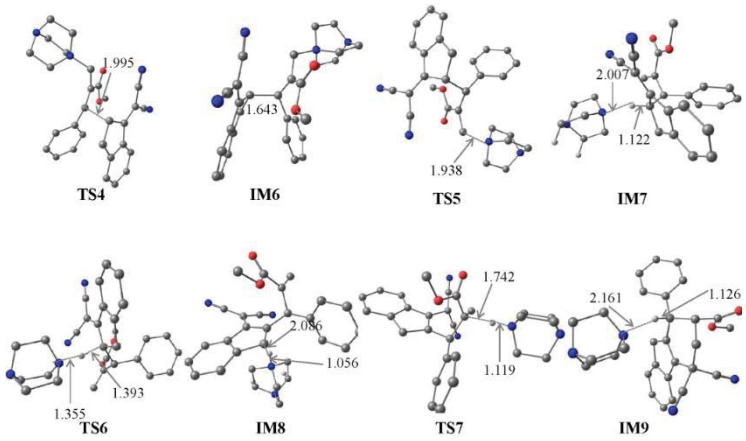


Figure S4. Optimized structures of the key stationary points for stage II at the m062x+D3/def2-TZVPP (smd, solvent = DMF)//BP86+D3(BJ)/def2-SVP(smd, solvent = DMF)

level. The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue).

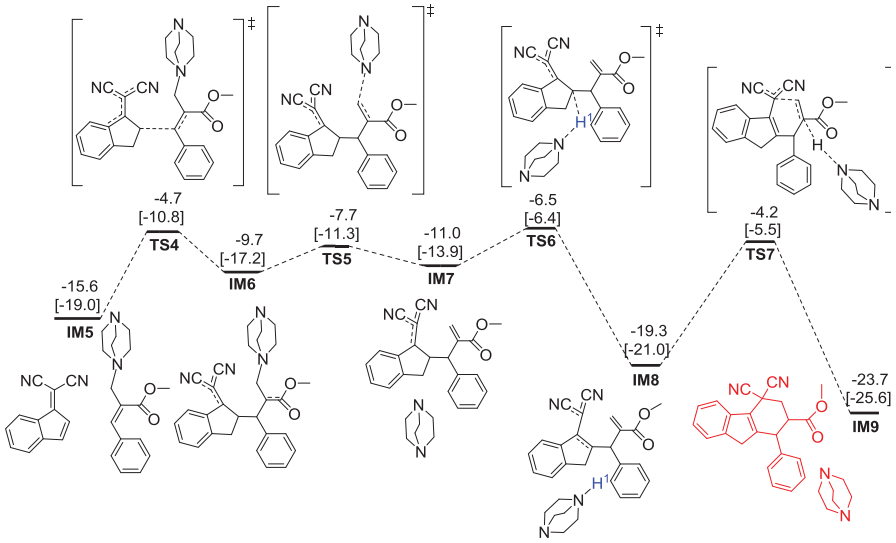
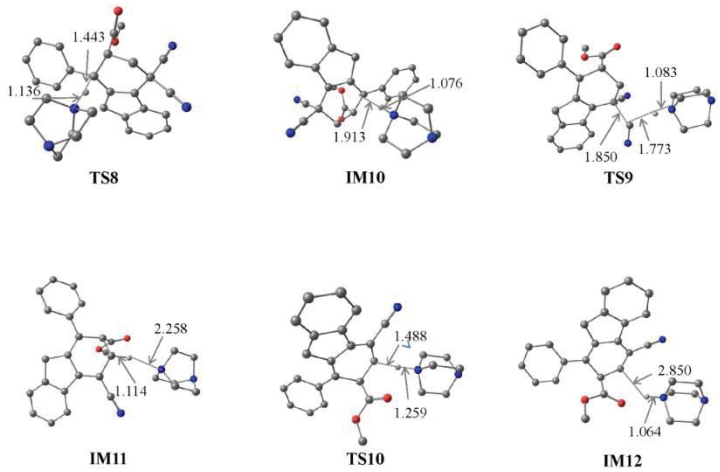


Figure S5. Gibbs free energy profile (in kcal/mol) for the stage II of the target reaction at the m062x + D3/def2-TZVPP (smd, solvent = DMF)//BP86+D3(BJ)/def2-SVP(smd, solvent = DMF) level. The optimized geometries are detailed in the Figure S3 of SI.

Stage II: generation of the experimentally observed six-membered-ring species IM11. Figure S4 shows the free energy profile for stage II, while the optimized structures are given in Figure S3 of SI. As shown by the reaction course, after crossing a barrier of 10.9 kcal/mol (**IM5→TS4**), the C-C coupling intermediate **IM6** is formed. Subsequently, DABCO can be easily liberated from the terminal CH_2 via a very small barrier of 2.0 kcal mol-1 (**TS5**), giving the slightly more stable intermediate **IM7**. The DABCO then can abstract the H-atom of substrate **2a** via the transition state **TS6** with the barrier of 4.5 kcal/mol, providing the thermodynamically more stable intermediate **IM8** with exoergic by 19.3 kcal/mol. After overcoming a barrier of 15.1 kcal/mol, the terminal CH_2 will attack the C^{CN2} center and form the six-membered-ring species **IM9**, which is 23.7 kcal/mol more stable than the initial reactants. It is worthy of mentioning that structure **IM9** has been successfully observed in experiment and confirmed by ESI-HRMS (**IM9** was observed in the reaction of **1a** and **2a** under the standard conditions after 10 minutes HRMS (ESI) calcd for $C_{22}H_{17}NNaO_2$ (**IM9**+Na)$^+$ 377.1260, found 377.1243), which suggest the herein reasonable reaction pathway.



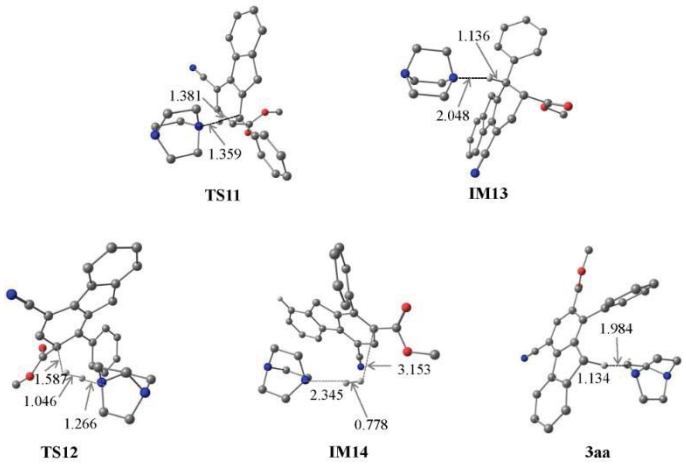


Figure S5. Optimized structures of the key stationary points for stage III at the m062x+D3/def2-TZVPP (smd, solvent = DMF)//BP86+D3(BJ)/def2-SVP(smd, solvent = DMF) level.The key bond distances are given in Å. All of the hydrogen atoms are omitted for clarity (color code, C: black, O: red, H: white, N: blue).

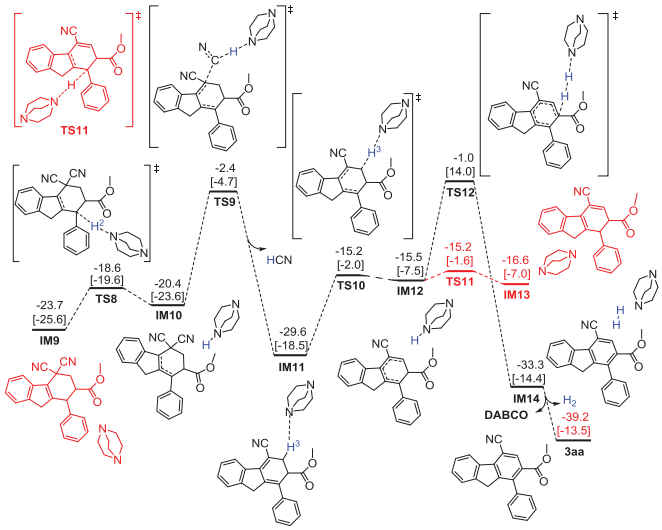


Figure S7. Gibbs free energy profile (in kcal/mol) for the stage II of the target reaction at the m062x + D3/def2-TZVPP (smd, solvent = DMF)//BP86+D3(BJ)/def2-SVP(smd, solvent = DMF) level. The optimized geometries are detailed in the Figure S3 of SI.

Stage III: formation of the experimentally detected aromatic complex 3aa.

Subsequent to the formation of the six-membered-ring intermediate **IM9**, the HCN could be released successfully via the following stepwise mechanism (see Figure S6). By overcoming a barrier (**TS8**), the H^2-atom is first transferred to DABCO moiety, giving the **IM10** intermediate. The DABCO-H^2 moiety then slightly adjusts its position and transfer the activated H-atom to the C^{CN} center via the **TS9** transition state, liberating HCN and generating the **IM11** intermediate. The barriers for the two steps are 5.1, and 18.0 kcal/mol, respectively. The process is also exoergic respect to **IM9**. Therefore, the HCN liberation is kinetically and thermodynamically favorable.

The H^3-atom can be further transferred to the DABCO moiety by crossing a barrier of 14.4 kcal/mol (**IM11→TS10**) providing the less stable intermediate **IM12**, fllowed by reversible H-transfer step via very small barrier (**IM12→TS11**) to generate the weak complex **IM13**, which agree well with the experimentally detected intermediate. Nonetheless, because of the favorable aromatic driving force, the

thermodynamically less stable **IM13** will easily transfer back to **IM12**, followed by the C-H bond activation and H-H molecule formation step via a barrier of 14.5 kcal/mol (**IM12→TS12**) leading to the aromatic complex **IM14**. If measured from the more stable **IM11**, the barrier is predicted to be 28.6 kcal/mol, which is also the highest barrier during the whole catalysis. Therefore, the aromatic H_2 release step should be the rate-determining step for the target reaction. With H_2 and DABCO release, the final aromatic product **3aa** is formed with highly exoergic by 39.2 kcal/mol, implying a thermodynamically favorable process.

Table S2 : Coordinates of the calculated structures at the BP86+D3(BJ)/def2-SVP(smd, solvent= N,N-DiMethylFormamide) level. The reaction energies at the M06-2X+D3/def2-TZVPP(smd, solvent= N,N-DiMethylFormamide)//BP86+D3(BJ)/def2-SVP (smd, solvent= N,N-DiMethylFormamide) level.

1a

E= −571.2039949

G= −571.0809069

C	1.619824	-0.988222	0.000111
C	0.700757	0.102737	-0.000075
C	1.172165	1.439647	-0.000141
C	2.552638	1.665553	-0.000090
C	3.460572	0.581625	0.000037
C	3.001706	-0.746568	0.000137
H	0.477023	2.290212	-0.000281
H	2.935772	2.697601	-0.000184
H	4.543622	0.783196	0.000074
H	3.715608	-1.585096	0.000250
C	-0.654702	-0.425781	-0.000155
C	0.901509	-2.311572	0.000369
C	-0.598039	-1.936600	-0.000581
C	-1.859202	0.273184	0.000031
C	-1.957275	1.698278	0.000141
N	-2.056954	2.870390	0.000093
C	-3.099484	-0.440686	0.000028
N	-4.114640	-1.034883	0.000206
H	1.180655	-2.915697	0.889476
H	1.181644	-2.916849	-0.887618
H	-1.138827	-2.336259	0.884061
H	-1.137161	-2.335223	-0.886745

2a

E= −997.2382538

G= −996.9642658

C	0.270810	3.387768	0.872273
C	0.475046	2.042904	1.225409

C	0.351403	1.023696	0.260396
C	0.025518	1.365916	-1.065624
C	-0.187755	2.709624	-1.416996
C	-0.065750	3.725215	-0.451073
H	0.367070	4.174766	1.637313
H	0.729906	1.779138	2.265151
H	-0.059481	0.578929	-1.828691
H	-0.449320	2.965261	-2.456336
H	-0.233391	4.777933	-0.729193
C	0.558854	-0.421310	0.701158
H	-0.009857	-0.578387	1.638581
C	2.010592	-0.753886	0.993731
C	2.982414	-0.650312	-0.143727
O	2.701864	-0.247061	-1.263512
O	4.226084	-1.053849	0.208518
C	5.229925	-0.954406	-0.817134
H	5.338765	0.092509	-1.167128
H	6.172994	-1.299040	-0.355062
H	4.976290	-1.598021	-1.684500
C	2.399018	-1.090370	2.243381
O	0.089827	-1.371691	-0.290696
C	-1.240663	-1.478166	-0.538689
O	-1.639776	-2.155505	-1.467890
O	-1.962610	-0.788581	0.354889
C	-3.430241	-0.591699	0.185066
C	-3.683465	0.122373	-1.144953
C	-4.142640	-1.943471	0.277549
C	-3.782812	0.307354	1.370874
H	-3.118618	1.075818	-1.189744
H	-3.386880	-0.510049	-2.003339
H	-4.763595	0.354265	-1.239628
H	-3.876399	-2.461724	1.221839
H	-5.240110	-1.783028	0.272058
H	-3.876914	-2.595779	-0.575359
H	-4.865595	0.543946	1.355012
H	-3.550290	-0.195438	2.331673
H	-3.215558	1.259076	1.325589
H	1.663074	-1.155651	3.061647
H	3.453261	-1.298400	2.479815

DABCO

E= -345.1152273

G= −344. 9678213

C	-0.784194	-0.423353	-1.320853
C	0.783468	-0.423760	-1.321153
H	-1.188985	-1.434830	-1.538921
H	-1.188987	0.273232	-2.085906
H	1.187656	-1.435388	-1.539628
H	1.188319	0.272812	-2.086187
C	-0.783858	-0.932111	1.027303
H	-1.188427	-0.615529	2.012436
H	-1.188465	-1.942996	0.806309
C	0.783471	-0.932815	1.026952
H	1.188760	-0.616845	2.011987
H	1.187069	-1.944009	0.805524
C	0.784184	1.355606	0.293698
H	1.189086	1.669781	1.279471
H	1.188953	2.050060	-0.473357
C	-0.783065	1.356235	0.293754
H	-1.187635	1.671024	1.279468
H	-1.187329	2.050791	-0.473474
N	-1.284975	0.000700	0.000490
N	1.284968	-0.000260	0.000092

Co2

E= −188. 4562507

G= −188. 4657887

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.174938
O	0.000000	0.000000	-1.174938

Tbuoh

E= −233. 5158834

G= −233. 4146834

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C	0.007939	0.000000	0.018003
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H	1.997915	-0.898082	0.095287
H	1.656372	0.000078	-1.425419
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C	-0.678696	1.265189	-0.526284
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H	-0.620748	-1.320340	-1.633732

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H -0.620888 1.320237 -1.633761
H -1.754495 1.278223 -0.245523
H -0.202958 2.175742 -0.106268
O -0.050763 0.000013 1.460493
H -1.001540 -0.000002 1.693978

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G= -93.3604185
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H 0.000000 0.000000 -1.598409
N 0.000000 0.000000 0.661536

H2
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G= -1.1737446
H 0.000000 0.000000 0.384106
H 0.000000 0.000000 -0.384106

IM1
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G= -1341.927776
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C -0.572968 -1.656669 -0.350498
C -0.827923 -0.393508 0.218853
C -0.874226 -0.266479 1.621754
C -0.646262 -1.386865 2.439331
C -0.369343 -2.641979 1.866675
H -0.138227 -3.756403 0.007317
H -0.566038 -1.762927 -1.446957
H -1.068881 0.721140 2.062221
H -0.680999 -1.277515 3.535184
H -0.186287 -3.517153 2.510112
C -1.020870 0.801959 -0.705872
H -1.299933 0.413480 -1.704986
C 0.236052 1.638787 -0.884352
C 0.667974 2.538648 0.226336
O 0.170264 2.586862 1.344659
O 1.712895 3.330205 -0.137708

C	2.242965	4.175189	0.895887
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H	3.095494	4.713832	0.442770
H	1.481906	4.901956	1.247814
C	1.006306	1.478672	-1.988136
O	-2.080509	1.684574	-0.235429
C	-3.333364	1.189630	-0.091444
O	-4.178423	1.809130	0.529115
O	-3.471577	0.017129	-0.728780
C	-4.650935	-0.860302	-0.497043
C	-4.731095	-1.194520	0.994879
C	-5.914479	-0.174142	-1.021786
C	-4.307034	-2.102433	-1.319956
H	-3.782080	-1.652980	1.341309
H	-4.933780	-0.291217	1.601271
H	-5.550201	-1.921380	1.169321
H	-5.797430	0.096709	-2.091328
H	-6.774469	-0.869557	-0.936585
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H	-5.127174	-2.844485	-1.246698
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H	0.704378	0.789187	-2.793238
H	1.937367	2.043101	-2.119067
C	3.853366	-2.571133	-0.453929
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H	3.236945	-3.267883	0.153611
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H	6.203697	-1.444690	-0.934289
C	4.609502	0.080803	-1.236755
H	4.765146	1.156554	-1.009607
H	4.833685	-0.075050	-2.313170
C	2.866830	-0.012073	0.410639
H	3.052327	1.057874	0.636214
H	1.785867	-0.205456	0.559266
C	3.746365	-0.946171	1.308057
H	4.357376	-0.357701	2.025299
H	3.114727	-1.645824	1.895437
N	4.657107	-1.743639	0.464921

N	3.189708	-0.239298	-1.008170

TS1

E= −1342.366458

G= −1341.920616

C	-3.804850	2.099343	1.463729
C	-2.545193	1.478965	1.537496
C	-1.742302	1.324736	0.386328
C	-2.236640	1.792813	-0.849578
C	-3.499673	2.401663	-0.927766
C	-4.289033	2.561487	0.227025
H	-4.415083	2.209082	2.374722
H	-2.176747	1.101263	2.505461
H	-1.621069	1.667193	-1.748763
H	-3.873847	2.755104	-1.902483
H	-5.280054	3.038686	0.161256
C	-0.416755	0.630229	0.546739
H	-0.499631	-0.148154	1.324915
C	0.834066	1.330942	0.631632
C	1.094302	2.522712	-0.145488
O	0.341079	3.112616	-0.927445
O	2.382983	3.023645	0.076314
C	2.720101	4.188795	-0.673949
H	2.058594	5.046743	-0.426677
H	3.764749	4.439685	-0.405250
H	2.653433	4.007534	-1.768325
C	1.935740	0.714333	1.410375
O	-0.369469	-0.426969	-0.875446
C	-1.368176	-1.265376	-1.068084
O	-1.688919	-1.704227	-2.170922
O	-1.971398	-1.604684	0.111142
C	-3.274508	-2.291949	0.133749
C	-4.310832	-1.452914	-0.624819
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H	-4.046315	-1.367609	-1.695916
H	-5.310981	-1.926228	-0.544857
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H	-4.582449	-2.849121	1.787085

H	-2.829560	-2.890657	2.189021
H	-3.681859	-1.313089	2.042624
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H	2.698600	1.460112	1.693740
C	2.891710	-2.791725	-0.045830
C	2.070244	-1.735495	0.747483
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H	1.060856	-1.582399	0.326382
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C	4.126533	-0.531932	1.327377
H	4.635560	0.442233	1.198300
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C	4.903742	-1.705848	0.662237
H	5.901568	-1.355462	0.331057
H	5.054657	-2.531068	1.386522
N	4.171296	-2.230462	-0.498403
N	2.779571	-0.403005	0.661622

IM2

E= −1342.381922

G= −1341.932939

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C	-2.957560	0.723155	2.221955
C	-2.086746	1.074310	1.156490
C	-2.643156	1.263633	-0.134738
C	-4.024523	1.148583	-0.332280
C	-4.882521	0.843996	0.742967
H	-5.001813	0.363298	2.866320
H	-2.530789	0.532648	3.220412
H	-1.974111	1.466654	-0.978180
H	-4.439202	1.282990	-1.344167
H	-5.968600	0.759500	0.578042
C	-0.655184	1.132206	1.455653
H	-0.387802	0.562433	2.363423
C	0.406325	1.737146	0.833408

C	0.268075	2.749610	-0.255712
O	-0.749788	3.354365	-0.563406
O	1.470806	3.027267	-0.831109
C	1.442324	3.986167	-1.899462
H	1.085525	4.973657	-1.541803
H	2.482675	4.069329	-2.264210
H	0.779234	3.638376	-2.717589
C	1.787680	1.477013	1.389080
O	-0.096894	0.240611	-1.905185
C	-0.874702	-0.750242	-1.878245
O	-1.672168	-1.162211	-2.744142
O	-0.771725	-1.466297	-0.630040
C	-1.548110	-2.666439	-0.364529
C	-3.055555	-2.365888	-0.400348
C	-1.168189	-3.773834	-1.360867
C	-1.141896	-3.075477	1.059065
H	-3.313551	-1.604889	0.363837
H	-3.333709	-1.979547	-1.398353
H	-3.642762	-3.283537	-0.184306
H	-0.073946	-3.962945	-1.325023
H	-1.688987	-4.724250	-1.117924
H	-1.438453	-3.461009	-2.387304
H	-1.718969	-3.965267	1.386794
H	-0.064557	-3.332749	1.113247
H	-1.343960	-2.251631	1.774466
H	1.733080	1.298881	2.479881
H	2.472537	2.321263	1.197019
C	2.548505	-2.241684	0.639345
C	1.733040	-1.019176	1.148913
H	1.944740	-2.800278	-0.103383
H	2.785390	-2.925776	1.478447
H	0.760945	-0.940537	0.622011
H	1.578776	-1.033542	2.244087
C	3.488009	-0.938128	-1.126802
H	4.434528	-0.645582	-1.624159
H	2.877741	-1.506196	-1.857457
C	2.707223	0.324124	-0.663720
H	3.257003	1.262301	-0.853430
H	1.689328	0.375924	-1.113510
C	3.866478	0.162755	1.510949
H	4.390776	1.108032	1.275976
H	3.676739	0.118323	2.599758
C	4.617831	-1.090994	0.976913

H	5.565955	-0.785909	0.491437
H	4.865541	-1.769715	1.817014
N	3.802511	-1.822657	0.002109
N	2.510538	0.242733	0.838325

TS2

E= −1342.349183

G= −1341.904626

C	3.443710	-2.429764	-1.984798
C	2.766715	-1.273659	-1.562280
C	1.603374	-1.362672	-0.764299
C	1.116355	-2.648507	-0.435223
C	1.787275	-3.805793	-0.864600
C	2.960710	-3.703493	-1.633703
H	4.354863	-2.334244	-2.597681
H	3.128892	-0.272964	-1.833527
H	0.199043	-2.739479	0.162985
H	1.389848	-4.797134	-0.592130
H	3.490611	-4.611516	-1.963904
C	0.805415	-0.135454	-0.417163
H	0.396882	0.296082	-1.344876
C	-0.126267	-0.072344	0.668251
C	0.100701	-0.738262	1.931409
O	1.041025	-1.477828	2.254419
O	-0.898692	-0.457146	2.861271
C	-0.740495	-1.076653	4.137751
H	0.189028	-0.741126	4.645042
H	-1.619907	-0.775254	4.739097
H	-0.708462	-2.183877	4.055426
C	-1.223815	0.929405	0.563352
O	1.303118	2.009354	-2.683998
C	1.260701	2.554784	-1.613608
O	0.949222	3.513050	-0.955299
O	2.039999	1.228192	-0.450947
C	2.784823	1.632204	0.719653
C	3.838504	2.638763	0.214538
C	1.895089	2.301501	1.789743
C	3.500891	0.407963	1.314308
H	4.447602	2.186047	-0.595240
H	3.360695	3.558895	-0.176678
H	4.522613	2.931548	1.039141
H	1.204560	1.575689	2.258147

H	2.525773	2.735729	2.594553
H	1.298578	3.114123	1.334167
H	4.089061	0.714174	2.206144
H	2.773729	-0.367596	1.630218
H	4.203259	-0.038870	0.580955
H	-0.950479	1.787535	-0.080723
H	-1.545660	1.311543	1.548304
C	-3.678177	-0.432663	-2.140065
C	-2.318117	-0.009238	-1.512544
H	-3.606517	-1.465017	-2.536042
H	-3.937833	0.241044	-2.980439
H	-1.590831	-0.840196	-1.476580
H	-1.855311	0.853948	-2.026631
C	-4.406863	-1.250201	-0.014886
H	-5.245491	-1.251981	0.709217
H	-4.277460	-2.283217	-0.394132
C	-3.104722	-0.766450	0.686159
H	-3.270422	-0.418257	1.721076
H	-2.306150	-1.530617	0.696149
C	-3.570739	1.527438	-0.061498
H	-3.674782	1.842623	0.993590
H	-3.133783	2.361152	-0.642833
C	-4.904238	1.000363	-0.667217
H	-5.706696	1.025191	0.096474
H	-5.216005	1.641429	-1.515485
N	-4.755963	-0.379929	-1.144952
N	-2.551409	0.412213	-0.080342

IM3

E= −1342.362461

G= −1341.920327

C	-3.556893	1.859405	-2.405341
C	-2.943703	0.839141	-1.655914
C	-1.703527	1.048744	-1.017203
C	-1.079063	2.305801	-1.171390
C	-1.680573	3.323365	-1.930803
C	-2.928297	3.109365	-2.546980
H	-4.529574	1.672305	-2.889743
H	-3.420275	-0.147346	-1.560113
H	-0.111848	2.482884	-0.678649
H	-1.174514	4.297443	-2.034730
H	-3.404368	3.910432	-3.135340

C	-0.983609	-0.110661	-0.326117
H	-0.415550	-0.576372	-1.161402
C	0.027595	0.224845	0.734015
C	-0.190360	1.244285	1.702958
O	-1.128917	2.062175	1.786774
O	0.825072	1.289015	2.686499
C	0.654285	2.291286	3.679292
H	-0.313284	2.188947	4.217411
H	1.488653	2.166742	4.398193
H	0.693773	3.317984	3.251642
C	1.146505	-0.713574	0.890159
O	-1.079743	-2.824700	-2.341722
C	-0.855673	-3.346367	-1.312351
O	-0.583906	-3.955821	-0.342955
O	-1.903785	-1.227516	-0.053041
C	-2.689635	-1.348652	1.163217
C	-3.679188	-2.474337	0.818500
C	-1.815479	-1.793818	2.354241
C	-3.458798	-0.064162	1.507619
H	-4.284570	-2.203215	-0.071200
H	-3.142312	-3.419690	0.597522
H	-4.371403	-2.663891	1.665181
H	-1.174438	-0.973398	2.726080
H	-2.458154	-2.138301	3.192627
H	-1.162273	-2.637169	2.052262
H	-4.010274	-0.207883	2.461727
H	-2.773030	0.800303	1.631134
H	-4.202739	0.179426	0.722411
H	0.925679	-1.726257	0.497130
H	1.520953	-0.794764	1.927304
C	3.547923	0.006942	-2.144226
C	2.220420	-0.308044	-1.394425
H	3.434987	0.927728	-2.750314
H	3.806978	-0.824903	-2.829140
H	1.449396	0.470595	-1.543247
H	1.797523	-1.292870	-1.669706
C	4.314337	1.303769	-0.288265
H	5.164814	1.470633	0.402538
H	4.177506	2.224413	-0.890106
C	3.023357	0.988646	0.520625
H	3.196219	0.922180	1.609456
H	2.205675	1.712100	0.344541
C	3.535610	-1.402426	0.358942

H	3.682242	-1.427724	1.455535
H	3.104222	-2.369140	0.035193
C	4.836903	-1.031614	-0.414873
H	5.674450	-0.878726	0.294543
H	5.117358	-1.852219	-1.104833
N	4.652634	0.198837	-1.196531
N	2.493880	-0.351279	0.085329

IM4

E= −1725.119217

G= −1724.535441

C	1.983953	4.352565	-0.521063
C	0.732128	3.832478	-1.291837
H	1.987377	5.460928	-0.510614
H	2.912834	4.010557	-1.019971
H	0.004611	4.634721	-1.520331
H	0.997065	3.311107	-2.231897
C	0.726694	4.224004	1.513881
H	0.769972	3.916943	2.578128
H	0.619636	5.326974	1.482000
C	-0.480027	3.540636	0.810211
H	-0.965978	2.767367	1.428894
H	-1.260766	4.248184	0.477847
C	1.000838	1.763073	-0.030765
H	0.432232	0.957129	0.471091
H	1.399059	1.363711	-0.980345
C	2.111995	2.393277	0.848055
H	2.043536	2.025307	1.891793
H	3.107981	2.112816	0.452191
N	1.994403	3.859350	0.864237
N	0.019201	2.834611	-0.420911
C	-1.207518	2.177420	-1.219103
H	-0.681664	1.718808	-2.082459
H	-1.771570	3.074421	-1.541532
C	-2.047353	1.231223	-0.468767
C	-1.673038	-0.222906	-0.516179
C	-3.204228	1.804945	0.141724
O	-3.548128	3.004431	0.136385
O	-4.011498	0.873689	0.809998
C	-5.205939	1.394018	1.382074
H	-5.907463	1.776299	0.607836
H	-5.685488	0.553675	1.922198

H	-4.999096	2.222124	2.093166
C	-2.717792	-1.243911	-0.986490
C	-2.433822	-2.626657	-0.907701
C	-3.901423	-0.847506	-1.641640
C	-3.318591	-3.581219	-1.436381
H	-1.504717	-2.954083	-0.418077
C	-4.792411	-1.799138	-2.169971
H	-4.119985	0.225604	-1.742232
C	-4.509404	-3.172638	-2.065442
H	-3.073941	-4.653270	-1.358205
H	-5.715925	-1.462077	-2.668920
H	-5.207260	-3.919257	-2.477686
H	-0.905168	-0.270661	-1.322453
C	-1.256102	-0.926840	1.970331
C	-1.290085	0.434129	2.689611
H	-2.094094	1.079047	2.292463
H	-1.476351	0.281418	3.773571
H	-0.318665	0.958338	2.585654
C	-2.604776	-1.643926	2.138550
H	-3.409509	-1.084536	1.626131
H	-2.568002	-2.677425	1.743082
H	-2.855619	-1.700351	3.219042
C	-0.131644	-1.784180	2.570346
H	-0.099569	-2.779932	2.085878
H	0.852745	-1.291794	2.430574
H	-0.291966	-1.934173	3.658053
O	-0.845221	-0.787371	0.579381
C	3.494805	-1.049795	-0.609129
C	4.638997	-0.598688	0.094076
C	5.316488	0.530640	-0.379899
C	4.869166	1.206817	-1.538251
C	3.736702	0.763408	-2.243312
C	3.048447	-0.367569	-1.779798
H	4.988937	-1.110027	1.001233
H	6.201425	0.901770	0.159364
H	5.414331	2.097037	-1.889617
H	3.391152	1.298341	-3.141411
C	1.819351	-1.022962	-2.353039
C	1.425620	-2.073164	-1.292355
C	2.596038	-2.167751	-0.352620
C	2.712689	-3.182668	0.594368
C	3.786131	-3.284904	1.530179
N	4.666273	-3.377883	2.305267

C	1.702552	-4.193327	0.663178
N	0.848234	-5.001726	0.697978
H	1.011144	-0.288562	-2.552009
H	2.056475	-1.500848	-3.328365
H	0.561888	-1.719069	-0.672757
H	1.131749	-3.056299	-1.710457

TS3

E= −1725.106903

G= −1724.523112

C	1.179091	4.645188	-0.243217
C	-0.046759	4.121590	-1.047572
H	1.050150	5.724129	-0.025499
H	2.109068	4.521954	-0.833147
H	-0.885234	4.843275	-1.069761
H	0.210429	3.835762	-2.084598
C	0.070187	3.979420	1.770350
H	0.213042	3.499663	2.759197
H	-0.184015	5.044724	1.940696
C	-1.077624	3.265037	1.002041
H	-1.391933	2.328486	1.491455
H	-1.966414	3.901737	0.845720
C	0.573293	1.894109	-0.221930
H	0.161891	0.922491	0.143444
H	0.964079	1.751077	-1.245745
C	1.635775	2.504134	0.725252
H	1.671313	1.945820	1.682954
H	2.637438	2.437843	0.257427
N	1.331759	3.912710	1.021218
N	-0.569507	2.876546	-0.365697
C	-1.691415	2.257983	-1.229842
H	-1.183326	2.007400	-2.180515
H	-2.401605	3.090478	-1.398725
C	-2.406861	1.079509	-0.644713
C	-1.935683	-0.212529	-0.926229
C	-3.569823	1.411063	0.175797
O	-4.110867	2.521094	0.239796
O	-4.012982	0.363943	0.946180
C	-5.192643	0.611914	1.716440
H	-6.057296	0.863190	1.066455
H	-5.401546	-0.324494	2.267192
H	-5.038528	1.443658	2.434843

C	-2.747489	-1.442409	-1.128740
C	-2.104968	-2.699514	-1.240269
C	-4.141107	-1.388051	-1.371517
C	-2.829910	-3.863097	-1.533365
H	-1.023822	-2.743594	-1.052853
C	-4.871090	-2.553683	-1.657492
H	-4.659294	-0.418638	-1.361986
C	-4.222537	-3.799533	-1.730608
H	-2.305217	-4.829695	-1.603566
H	-5.956184	-2.484525	-1.837575
H	-4.796221	-4.713257	-1.954482
H	-1.035470	-0.216530	-1.560169
C	-0.735150	-1.232676	1.820444
C	-1.085611	0.031689	2.641788
H	-2.018012	0.485825	2.254551
H	-1.246909	-0.210788	3.714772
H	-0.264992	0.776825	2.584116
C	-1.887799	-2.250777	1.974484
H	-2.826916	-1.826903	1.567542
H	-1.664967	-3.189315	1.427077
H	-2.056313	-2.508572	3.042906
C	0.560386	-1.847645	2.401997
H	0.806479	-2.796983	1.886017
H	1.412576	-1.148818	2.270564
H	0.457794	-2.066611	3.487137
O	-0.483254	-0.907935	0.469988
C	3.570432	-0.509436	-0.699956
C	4.652080	0.218863	-0.148896
C	5.013423	1.437145	-0.739189
C	4.316409	1.928406	-1.866076
C	3.243276	1.208394	-2.420878
C	2.869767	-0.011357	-1.837304
H	5.197280	-0.148526	0.731378
H	5.844904	2.021468	-0.315789
H	4.616847	2.889444	-2.312700
H	2.704373	1.596269	-3.299538
C	1.773856	-0.960858	-2.243537
C	1.711374	-1.965970	-1.075339
C	2.980229	-1.795251	-0.324718
C	3.483093	-2.736918	0.581454
C	4.660206	-2.540367	1.361749
N	5.629758	-2.388154	2.012786
C	2.816659	-3.989039	0.752009

N	2.263682	-5.021124	0.878180
H	0.812068	-0.437945	-2.426897
H	2.041750	-1.466558	-3.197931
H	0.853384	-1.635359	-0.362586
H	1.487917	-3.013072	-1.359009

IM5

E= −1491.615689

G= −1491.157386

C	5.865142	-0.468703	-1.258573
C	4.498405	0.222676	-1.524088
H	6.664906	0.295159	-1.193782
H	6.114685	-1.158951	-2.088350
H	4.548696	1.324185	-1.438016
H	4.064111	-0.040503	-2.506297
C	5.439640	-0.346605	1.093929
H	5.491416	-0.908533	2.047256
H	6.164026	0.490009	1.147312
C	3.997886	0.205042	0.888600
H	3.286681	-0.204747	1.629324
H	3.943612	1.307764	0.907661
C	3.438143	-1.750441	-0.493869
H	2.660260	-2.046376	0.232565
H	3.108584	-2.033352	-1.511334
C	4.842453	-2.314520	-0.130558
H	4.797438	-2.863666	0.830413
H	5.175880	-3.021271	-0.915787
N	5.829330	-1.235032	-0.007311
N	3.503499	-0.236809	-0.473588
C	2.138977	0.375122	-0.820663
H	1.865644	-0.080819	-1.789498
H	2.324049	1.454264	-0.973201
C	1.061905	0.169186	0.210185
C	0.202778	-0.893692	0.037263
C	1.046876	1.212240	1.273842
O	1.596171	2.305863	1.164023
O	0.440395	0.813811	2.415056
C	0.298252	1.817535	3.437701
H	-0.302875	2.668537	3.058309
H	-0.227981	1.322157	4.274371
H	1.289217	2.183504	3.775145
C	-1.000541	-1.364320	0.727876

C	-1.350768	-2.729133	0.535559
C	-1.876744	-0.557611	1.499184
C	-2.499830	-3.276760	1.123186
H	-0.695685	-3.364895	-0.082005
C	-3.025782	-1.106148	2.082618
H	-1.673531	0.512145	1.617531
C	-3.342468	-2.465787	1.904796
H	-2.744616	-4.338655	0.962530
H	-3.696739	-0.456796	2.666024
H	-4.251558	-2.887668	2.361824
H	0.484783	-1.561994	-0.793638
C	-3.280377	0.506033	-1.047644
C	-4.241203	1.133276	-0.229567
C	-5.448784	0.461913	0.038853
C	-5.703255	-0.814812	-0.500222
C	-4.754767	-1.435616	-1.340353
C	-3.555388	-0.770841	-1.616782
H	-4.051770	2.121790	0.213200
H	-6.201700	0.939902	0.686074
H	-6.650172	-1.328700	-0.269642
H	-4.956904	-2.429698	-1.771232
C	-2.391155	-1.191119	-2.480568
C	-1.427066	-0.046995	-2.326195
C	-1.931343	0.931352	-1.488230
C	-1.246864	2.148035	-1.067534
C	-1.599828	2.848421	0.104271
N	-1.889465	3.415767	1.105136
C	-0.105094	2.587855	-1.771369
N	0.840433	2.938069	-2.394799
H	-1.955488	-2.156788	-2.128419
H	-2.702619	-1.376323	-3.535914
H	-0.446664	-0.004541	-2.821010

TS4

E= −1491.602552

G= −1491.141586

C	-4.650117	2.150012	-0.288406
C	-3.309856	1.456922	-0.674335
H	-5.035931	2.729523	-1.150427
H	-4.488019	2.852023	0.553284
H	-3.067325	1.558377	-1.748767
H	-2.457366	1.822135	-0.073986

C	-5.851151	0.196283	-0.972243
H	-6.662858	-0.504030	-0.692286
H	-6.169055	0.745332	-1.880779
C	-4.541189	-0.594691	-1.248470
H	-4.618316	-1.664369	-0.977357
H	-4.204899	-0.517682	-2.299479
C	-3.795277	-0.198882	1.063226
H	-3.763598	-1.282670	1.269890
H	-2.986445	0.286446	1.639464
C	-5.183900	0.455973	1.311884
H	-5.930083	-0.316656	1.584548
H	-5.115746	1.177378	2.150347
N	-5.659180	1.163194	0.115486
N	-3.431010	-0.022188	-0.394298
C	-2.112381	-0.775695	-0.745092
H	-1.965335	-0.549066	-1.819811
H	-2.380275	-1.841950	-0.632213
C	-0.919694	-0.418822	0.074039
C	-0.059937	0.610156	-0.470410
C	-0.736491	-1.272166	1.236418
O	-1.523317	-2.162840	1.596077
O	0.395404	-1.015224	1.974170
C	0.582126	-1.823851	3.138226
H	1.572146	-1.544453	3.547218
H	-0.202244	-1.624763	3.899834
H	0.571955	-2.904606	2.893885
C	0.784159	1.601828	0.276227
C	0.584769	2.969861	-0.041656
C	1.810324	1.290611	1.199794
C	1.358779	3.984302	0.546263
H	-0.196453	3.239107	-0.771832
C	2.589391	2.301017	1.785093
H	1.997199	0.244210	1.453937
C	2.371254	3.652764	1.463544
H	1.173716	5.037130	0.278814
H	3.387246	2.023961	2.492730
H	2.988821	4.442191	1.921172
H	-0.609824	1.165722	-1.249644
C	3.212996	-0.543588	-0.816890
C	4.252640	-0.986249	0.030603
C	5.374799	-0.161267	0.210831
C	5.475338	1.082332	-0.449288
C	4.451906	1.519509	-1.312958

C	3.328040	0.706074	-1.497056
H	4.181979	-1.944633	0.564015
H	6.185353	-0.487887	0.881588
H	6.362374	1.715034	-0.286612
H	4.529646	2.490942	-1.826850
C	2.097523	0.944999	-2.336596
C	1.147293	-0.146638	-1.866582
C	1.910291	-1.129995	-1.151014
C	1.389932	-2.400491	-0.788243
C	2.004302	-3.239950	0.178077
N	2.502224	-3.931180	0.995232
C	0.217057	-2.911653	-1.411117
N	-0.717794	-3.373088	-1.967670
H	1.697929	1.974697	-2.228661
H	2.330133	0.811913	-3.418357
H	0.341349	-0.478253	-2.540098

IM6

E= −1491.607771

G= −1491.14706

C	-4.689229	1.884068	-0.316585
C	-3.334768	1.220012	-0.701810
H	-5.104367	2.429823	-1.187070
H	-4.538504	2.612086	0.505107
H	-3.103961	1.310121	-1.780071
H	-2.484938	1.614366	-0.115973
C	-5.842080	-0.120849	-0.936119
H	-6.624716	-0.840429	-0.623771
H	-6.195789	0.395755	-1.850603
C	-4.509992	-0.873581	-1.221189
H	-4.549895	-1.942009	-0.936291
H	-4.193382	-0.799984	-2.278766
C	-3.748649	-0.414585	1.069423
H	-3.689548	-1.493786	1.293894
H	-2.939556	0.093043	1.625059
C	-5.148400	0.212611	1.330025
H	-5.870149	-0.570771	1.636111
H	-5.084055	0.957310	2.148402
N	-5.663629	0.877751	0.125366
N	-3.411385	-0.253029	-0.393361
C	-2.047733	-0.970885	-0.739006
H	-1.967361	-0.816227	-1.834515

H	-2.272621	-2.035619	-0.534269
C	-0.852067	-0.503586	-0.008880
C	0.022554	0.496982	-0.712106
C	-0.569025	-1.221535	1.201293
O	-1.283624	-2.097916	1.725437
O	0.630815	-0.865250	1.807592
C	0.965440	-1.591822	2.985622
H	1.972438	-1.245334	3.290763
H	0.244395	-1.396523	3.809240
H	0.991501	-2.686504	2.804207
C	0.556161	1.701304	0.064131
C	-0.010209	2.964829	-0.232683
C	1.602648	1.665913	1.014830
C	0.427625	4.141231	0.400188
H	-0.808031	3.025916	-0.991306
C	2.052730	2.840413	1.641839
H	2.064465	0.708442	1.272304
C	1.468061	4.084172	1.343742
H	-0.039723	5.106024	0.144545
H	2.875852	2.779215	2.372297
H	1.824476	5.002126	1.838261
H	-0.627021	0.951921	-1.485118
C	3.305651	-0.443989	-0.680519
C	4.375775	-0.777478	0.182628
C	5.448207	0.118338	0.302416
C	5.469910	1.324753	-0.431792
C	4.417722	1.653097	-1.307761
C	3.340687	0.767821	-1.434990
H	4.363617	-1.703923	0.773277
H	6.280593	-0.119056	0.983398
H	6.319881	2.015852	-0.315709
H	4.437184	2.595960	-1.876840
C	2.105132	0.884469	-2.289752
C	1.153987	-0.179012	-1.693960
C	2.044739	-1.119272	-0.962604
C	1.642725	-2.418187	-0.632509
C	2.400109	-3.262188	0.232522
N	3.011675	-3.957424	0.960634
C	0.453213	-3.004023	-1.166382
N	-0.456353	-3.586059	-1.642643
H	1.679704	1.907593	-2.297933
H	2.348969	0.625289	-3.343843
H	0.545324	-0.698142	-2.459075

TS5

E= −1491.603271

G= −1491.144763

C	-5.205588	1.035650	-0.968652
C	-3.857745	0.348013	-1.367516
H	-5.995357	0.805754	-1.712525
H	-5.082579	2.137064	-0.928933
H	-3.949583	-0.244296	-2.299047
H	-3.037565	1.079089	-1.497766
C	-5.841184	-0.893585	0.300171
H	-6.187497	-1.239309	1.295318
H	-6.638063	-1.120675	-0.436827
C	-4.504924	-1.611491	-0.093274
H	-4.155719	-2.303659	0.697700
H	-4.593021	-2.178276	-1.041517
C	-3.266474	0.174502	0.982260
H	-2.942383	-0.552218	1.750309
H	-2.435486	0.887889	0.818406
C	-4.610594	0.883800	1.343657
H	-4.962940	0.558353	2.343572
H	-4.478127	1.984683	1.369925
N	-5.650254	0.564449	0.350726
N	-3.458571	-0.578782	-0.279499
C	-1.778288	-1.432518	-0.734883
H	-1.935087	-1.368436	-1.825491
H	-2.059831	-2.399455	-0.287666
C	-0.645284	-0.795054	-0.185028
C	0.056530	0.289333	-0.983134
C	-0.255548	-1.254027	1.135879
O	-0.860071	-2.073425	1.842753
O	0.925705	-0.691469	1.580795
C	1.417238	-1.160585	2.835379
H	2.331070	-0.574688	3.051298
H	0.675923	-1.004765	3.647138
H	1.670428	-2.240916	2.796988
C	0.172512	1.659624	-0.307414
C	-0.726231	2.665968	-0.735525
C	1.102071	2.006362	0.701270
C	-0.727252	3.952036	-0.169605
H	-1.440213	2.432535	-1.542574
C	1.112744	3.294704	1.263975

H	1.819373	1.261481	1.057826
C	0.196965	4.273481	0.839709
H	-1.446825	4.706307	-0.526976
H	1.852057	3.533880	2.045636
H	0.207911	5.280371	1.287022
H	-0.619806	0.478637	-1.839752
C	3.394879	-0.166976	-0.434659
C	4.347276	-0.339527	0.595870
C	5.246865	0.703272	0.857394
C	5.212736	1.894658	0.098416
C	4.277192	2.064985	-0.938416
C	3.367034	1.034100	-1.203890
H	4.372733	-1.255664	1.201810
H	5.983961	0.595903	1.668326
H	5.925902	2.702628	0.326723
H	4.251330	2.998789	-1.521451
C	2.269019	0.972566	-2.234459
C	1.387374	-0.206471	-1.750759
C	2.309650	-1.023330	-0.894854
C	2.110841	-2.383376	-0.668176
C	2.926604	-3.142777	0.224353
N	3.585957	-3.769605	0.971187
C	1.084222	-3.119844	-1.341189
N	0.307260	-3.791219	-1.918373
H	1.716894	1.927176	-2.336159
H	2.700278	0.735891	-3.232102
H	1.000569	-0.819779	-2.587284

IM7

E= −1491.60573

G= −1491.152912

C	-4.885904	0.898194	-0.532304
C	-4.037680	-0.263268	-1.150541
H	-5.881564	0.979188	-1.018600
H	-4.369816	1.874727	-0.652045
H	-4.587913	-0.784881	-1.962153
H	-3.087413	0.118212	-1.575688
C	-5.793018	-0.624253	1.090133
H	-5.954860	-0.782429	2.177842
H	-6.791289	-0.545861	0.609011
C	-4.950069	-1.790737	0.465100
H	-4.682196	-2.550647	1.229759
H	-5.510014	-2.307175	-0.343444
C	-2.933887	-0.584583	0.958963

H	-2.674754	-1.344551	1.725201
H	-1.988675	-0.206580	0.522499
C	-3.773680	0.586947	1.570846
H	-3.936202	0.442422	2.660294
H	-3.258470	1.560908	1.431387
N	-5.090334	0.660012	0.909399
N	-3.703227	-1.250874	-0.107222
C	-0.966900	-2.190172	-1.713424
H	-1.248064	-1.907017	-2.739926
H	-1.358873	-3.134271	-1.307398
C	-0.158839	-1.403696	-0.964373
C	0.377975	-0.090905	-1.536753
C	0.126224	-1.912051	0.421702
O	-0.114038	-3.045110	0.814989
O	0.677343	-0.965669	1.219263
C	1.011255	-1.365446	2.558705
H	1.397212	-0.459419	3.059685
H	0.114884	-1.741971	3.090937
H	1.786330	-2.158076	2.551419
C	-0.222778	1.181110	-0.927199
C	-1.162101	1.879614	-1.722065
C	0.088809	1.716035	0.343309
C	-1.786236	3.052717	-1.266217
H	-1.401778	1.493832	-2.726359
C	-0.529571	2.892470	0.801202
H	0.812880	1.210438	0.988860
C	-1.472562	3.564591	0.004897
H	-2.513498	3.570758	-1.911154
H	-0.265830	3.286088	1.795788
H	-1.957009	4.483844	0.370532
H	-0.008711	-0.087323	-2.573726
C	3.235196	0.668999	0.101412
C	3.758765	0.824313	1.405390
C	4.026846	2.120328	1.865072
C	3.797212	3.242064	1.036232
C	3.291315	3.091135	-0.267248
C	3.002664	1.802030	-0.732789
H	3.925574	-0.041534	2.061063
H	4.413584	2.267437	2.885271
H	4.011906	4.251320	1.421903
H	3.107806	3.971055	-0.902873
C	2.450606	1.367476	-2.066233
C	1.948560	-0.075333	-1.788438

C	2.804254	-0.518163	-0.622667
C	3.157765	-1.844531	-0.400064
C	3.976762	-2.254009	0.697579
N	4.641710	-2.598604	1.604465
C	2.727763	-2.884858	-1.285015
N	2.395857	-3.741338	-2.019268
H	1.664472	2.042363	-2.455597
H	3.266939	1.338755	-2.820791
H	2.108385	-0.753838	-2.648610

TS6

E= −1491.59548

G= −1491.142831

C	-4.705209	-0.212703	-0.306696
C	-3.174508	0.094772	-0.355664
H	-5.085336	-0.429378	-1.325674
H	-5.269553	0.654738	0.091788
H	-2.739303	-0.114826	-1.350285
H	-2.939532	1.142767	-0.087115
C	-4.169105	-2.516425	0.080046
H	-4.438895	-3.415861	0.670347
H	-4.436575	-2.710006	-0.978681
C	-2.642046	-2.213923	0.217728
H	-2.167426	-2.834698	1.000394
H	-2.090993	-2.364071	-0.730527
C	-3.073193	-0.593311	1.978567
H	-2.471237	-1.179287	2.700247
H	-2.981286	0.480468	2.229729
C	-4.568496	-1.051653	1.935379
H	-4.722058	-1.951071	2.565571
H	-5.227661	-0.247428	2.321201
N	-4.966869	-1.375070	0.557052
N	-2.483978	-0.790726	0.625351
C	0.596659	-3.283018	0.867681
H	-0.035503	-3.236025	1.768055
H	0.739290	-4.260600	0.381069
C	1.189097	-2.175532	0.369050
C	1.051835	-0.825719	1.074152
C	2.099288	-2.371112	-0.812715
O	2.443136	-3.453812	-1.265883
O	2.526327	-1.189916	-1.313546
C	3.342644	-1.245605	-2.491223

H	3.603117	-0.198706	-2.731214
H	4.263476	-1.836048	-2.309191
H	2.783123	-1.701125	-3.334118
C	2.454225	-0.261923	1.367261
C	3.282695	-0.963862	2.268724
C	2.957289	0.906848	0.763314
C	4.582209	-0.512444	2.557526
H	2.903242	-1.882334	2.746832
C	4.253255	1.365485	1.052620
H	2.330059	1.462249	0.050670
C	5.073625	0.656498	1.949186
H	5.212705	-1.075454	3.264617
H	4.626045	2.283370	0.570025
H	6.090747	1.014957	2.174659
H	0.647008	-1.109135	2.069145
C	-0.295087	2.373407	-0.452543
C	-0.527180	3.438137	-1.354359
C	-0.855799	4.703380	-0.843590
C	-0.971399	4.916492	0.546676
C	-0.754096	3.860044	1.449277
C	-0.405916	2.598099	0.946935
H	-0.458782	3.294551	-2.440589
H	-1.032845	5.538126	-1.539991
H	-1.235073	5.916729	0.925780
H	-0.849682	4.021198	2.534951
C	-0.127654	1.331153	1.690728
C	0.048408	0.255772	0.595306
C	0.010933	0.945420	-0.683670
C	0.059242	0.365276	-1.986062
C	0.223331	1.114939	-3.180710
N	0.390409	1.693495	-4.197378
C	-0.152218	-1.016707	-2.211546
N	-0.404614	-2.150003	-2.429077
H	0.795302	1.436486	2.304072
H	-0.932724	1.084801	2.416357
H	-1.196971	-0.369144	0.597390

IM8

E= -1491.618758

G= -1491.16331

C	4.725774	-0.062731	0.503315
C	3.247249	0.427824	0.510241

H	5.223570	0.214026	1.453606
H	5.284166	0.409759	-0.328823
H	2.930762	0.848269	1.481919
H	3.021080	1.159278	-0.287149
C	4.040919	-2.173101	1.426351
H	4.147708	-3.271162	1.325217
H	4.489497	-1.870872	2.393223
C	2.536569	-1.772875	1.379914
H	1.871412	-2.625496	1.149176
H	2.176836	-1.276346	2.301352
C	2.732750	-1.410939	-1.061657
H	2.011915	-2.232468	-1.227932
H	2.581894	-0.634477	-1.834709
C	4.207800	-1.898633	-0.956822
H	4.257911	-3.000480	-1.060621
H	4.816534	-1.448456	-1.765654
N	4.789083	-1.522405	0.340300
N	2.377803	-0.779521	0.259266
C	-2.802811	-0.464524	2.804095
H	-2.252754	-1.254266	3.339870
H	-3.600571	0.069897	3.343895
C	-2.508773	-0.153362	1.523786
C	-1.399346	-0.881369	0.753836
C	-3.290594	0.962361	0.890839
O	-3.907377	1.825160	1.500075
O	-3.256998	0.899882	-0.463962
C	-3.908486	1.970724	-1.167360
H	-3.731551	1.781042	-2.241676
H	-4.997453	1.980439	-0.956817
H	-3.475645	2.949715	-0.878146
C	-1.869680	-2.118528	-0.010337
C	-0.915079	-3.100977	-0.352869
C	-3.205903	-2.311246	-0.412795
C	-1.279884	-4.240036	-1.088195
H	0.131535	-2.964343	-0.036203
C	-3.576629	-3.452470	-1.147723
H	-3.968244	-1.561622	-0.156637
C	-2.616297	-4.419395	-1.491519
H	-0.518013	-4.993999	-1.343508
H	-4.627018	-3.583938	-1.453910
H	-2.907689	-5.312000	-2.067766
H	-0.715718	-1.259255	1.546524
C	0.364141	2.018472	-0.951946

C	1.019334	3.257714	-1.101412
C	1.363727	3.689590	-2.396311
C	1.073525	2.897353	-3.525476
C	0.429410	1.651167	-3.378023
C	0.068687	1.221918	-2.094803
H	1.259583	3.881706	-0.228386
H	1.872404	4.658251	-2.527107
H	1.355146	3.252488	-4.529683
H	0.212950	1.026375	-4.259792
C	-0.583082	-0.059050	-1.649676
C	-0.615696	0.065879	-0.140810
C	-0.076520	1.285566	0.257788
C	0.083229	1.778082	1.629312
C	0.118338	3.155296	1.937148
N	0.138393	4.312449	2.194711
C	0.297615	0.868046	2.682579
N	0.520529	0.054309	3.517832
H	-1.616509	-0.167543	-2.047497
H	-0.033369	-0.954743	-2.017975
H	1.372270	-0.458486	0.212737

TS7

E= -1491.594081

G= -1491.139203

C	0.082452	-1.830665	0.479783
H	0.527875	-1.998788	1.475438
H	0.149369	-2.704203	-0.189563
C	0.307847	-0.545917	-0.130845
C	-0.166309	0.594001	0.800302
C	-0.027344	-0.519401	-1.563564
O	-0.035684	-1.495505	-2.318262
O	-0.313566	0.740963	-2.037518
C	-0.649003	0.827352	-3.426284
H	-0.867955	1.893877	-3.623267
H	0.191930	0.494502	-4.070367
H	-1.540837	0.211619	-3.665657
C	0.464537	1.976824	0.746430
C	0.163161	2.887781	1.785299
C	1.361403	2.387200	-0.258860
C	0.734500	4.170333	1.814724
H	-0.526371	2.578715	2.588562
C	1.942704	3.668468	-0.230504

H	1.591477	1.702004	-1.083728
C	1.630727	4.566780	0.804100
H	0.485382	4.862071	2.635583
H	2.642756	3.965116	-1.028368
H	2.083699	5.570894	0.825454
H	0.041489	0.229125	1.832205
C	-3.776421	-0.315922	0.155175
C	-4.909383	-1.140661	0.008857
C	-6.097481	-0.575958	-0.494948
C	-6.164440	0.789189	-0.837392
C	-5.035810	1.622159	-0.676204
C	-3.849204	1.069173	-0.184433
H	-4.875561	-2.206828	0.278769
H	-6.988512	-1.212366	-0.619419
H	-7.104028	1.210065	-1.229622
H	-5.089709	2.691740	-0.937353
C	-2.511322	1.713136	0.090597
C	-1.666832	0.574558	0.603927
C	-2.411039	-0.587607	0.633441
C	-1.820761	-1.904061	1.047237
C	-2.361489	-3.082515	0.410835
N	-2.741643	-4.045368	-0.148892
C	-1.685241	-2.052454	2.478259
N	-1.509112	-2.125130	3.640081
H	-2.047732	2.152229	-0.820279
H	-2.585698	2.548137	0.823296
C	3.420997	-2.212369	0.017446
C	4.966883	-2.414914	0.040785
H	2.930507	-2.535006	0.954658
H	2.928920	-2.718674	-0.834061
H	5.278812	-2.892446	0.990850
H	5.282250	-3.072376	-0.793715
C	3.738213	0.010062	1.023738
H	3.476771	1.075126	0.879946
H	3.233120	-0.359452	1.936343
C	5.276365	-0.246842	1.028469
H	5.826218	0.710371	0.931092
H	5.585954	-0.725802	1.978797
C	5.286823	-0.492404	-1.361362
H	5.831942	0.468052	-1.452904
H	5.608256	-1.150352	-2.193060
C	3.747538	-0.250479	-1.423588
H	3.485863	0.819918	-1.513877

H	3.252415	-0.808639	-2.240313
N	3.158647	-0.743238	-0.135746
N	5.661228	-1.125032	-0.087585
H	2.049134	-0.599999	-0.152739

IM9

E= -1491.62654

G= -1491.170255

C	0.439262	-2.022031	-0.383719
H	0.137258	-2.063857	-1.448726
H	0.145021	-2.978458	0.089081
C	-0.266977	-0.823220	0.276431
C	0.084595	0.461665	-0.505815
C	0.010332	-0.823231	1.776833
O	-0.594170	-1.525070	2.573548
O	1.021959	0.002791	2.132650
C	1.379149	0.005595	3.527233
H	2.191742	0.747153	3.630397
H	0.513433	0.295206	4.156646
H	1.737349	-0.996948	3.837501
C	-0.667485	1.725691	-0.100777
C	-0.746627	2.784261	-1.034744
C	-1.342366	1.874489	1.127559
C	-1.452466	3.961902	-0.742789
H	-0.259464	2.672863	-2.016896
C	-2.058535	3.049331	1.421716
H	-1.352090	1.065298	1.870108
C	-2.111968	4.100972	0.492166
H	-1.498469	4.770219	-1.490050
H	-2.583452	3.135465	2.386386
H	-2.673202	5.020243	0.723226
H	-0.262145	0.254729	-1.546611
C	3.843288	0.020822	-0.623976
C	5.073075	-0.663094	-0.594123
C	6.260861	0.090713	-0.664168
C	6.222514	1.495759	-0.763545
C	4.988944	2.182055	-0.791460
C	3.804196	1.442685	-0.719492
H	5.117995	-1.760536	-0.516442
H	7.232833	-0.427444	-0.641101
H	7.164464	2.064431	-0.817367
H	4.962767	3.281375	-0.863817

C	2.362377	1.893640	-0.711052
C	1.584578	0.605458	-0.601452
C	2.454478	-0.450299	-0.559389
C	2.011354	-1.897875	-0.349189
C	2.539937	-2.371499	0.955917
N	2.935604	-2.714280	2.003405
C	2.574733	-2.763735	-1.410379
N	3.006477	-3.422406	-2.276783
H	2.130242	2.561393	0.149023
H	2.092990	2.476104	-1.619906
C	-3.773596	-2.060043	-0.765472
C	-5.290712	-2.120317	-1.151194
H	-3.121160	-2.274901	-1.638230
H	-3.524695	-2.792569	0.031304
H	-5.423577	-2.366406	-2.226186
H	-5.826151	-2.892846	-0.559382
C	-3.732255	0.283835	-1.317601
H	-3.450749	1.285194	-0.931202
H	-3.081365	0.064222	-2.190277
C	-5.250055	0.218593	-1.698938
H	-5.753534	1.190942	-1.512187
H	-5.386660	-0.030785	-2.772741
C	-5.784823	-0.483137	0.536669
H	-6.291392	0.488194	0.720953
H	-6.315871	-1.258474	1.128796
C	-4.267843	-0.414414	0.920675
H	-3.986505	0.593918	1.289557
H	-4.010166	-1.148733	1.712471
N	-3.443941	-0.711061	-0.266249
N	-5.927786	-0.815554	-0.893845
H	-1.368050	-0.981090	0.174849

TS8

E= −1491.616646

G= −1491.162141

C	-0.679036	0.229732	-2.257180
H	0.013605	-0.620254	-2.390984
H	-0.927146	0.622164	-3.261805
C	0.021743	1.303626	-1.402241
C	0.399779	0.785751	-0.008704
C	-0.824683	2.585668	-1.423605
O	-0.875766	3.352092	-2.374187

O	-1.537595	2.755612	-0.290204
C	-2.420089	3.890994	-0.267249
H	-2.874821	3.903116	0.739834
H	-1.858599	4.830342	-0.444956
H	-3.209747	3.784818	-1.039036
C	1.269439	1.692414	0.797560
C	1.750532	1.340188	2.091736
C	1.752492	2.921563	0.265223
C	2.635638	2.162269	2.804904
H	1.460804	0.384353	2.543744
C	2.641564	3.742906	0.978061
H	1.440008	3.259238	-0.733226
C	3.091662	3.375971	2.258000
H	2.981464	1.840501	3.801027
H	2.982579	4.686680	0.521596
H	3.787703	4.020767	2.817382
H	1.368049	-0.236758	-0.274287
C	-2.670666	-1.221249	0.807926
C	-3.900068	-1.879564	0.590820
C	-4.563229	-2.455199	1.693607
C	-4.019854	-2.379326	2.990779
C	-2.792242	-1.710993	3.211065
C	-2.131222	-1.132745	2.125602
H	-4.343410	-1.944718	-0.415162
H	-5.523690	-2.972421	1.535667
H	-4.554542	-2.837254	3.838115
H	-2.369581	-1.642373	4.227026
C	-0.834589	-0.360416	2.066469
C	-0.672596	0.009959	0.597774
C	-1.753304	-0.535207	-0.093820
C	-1.974071	-0.343191	-1.586069
C	-3.134585	0.560171	-1.800996
N	-4.035679	1.299012	-1.926905
C	-2.272078	-1.644427	-2.232767
N	-2.459882	-2.695519	-2.714671
H	-0.852565	0.549521	2.706874
H	0.014106	-0.974767	2.434591
C	2.164035	-1.894237	-1.711823
C	3.322658	-2.937824	-1.820983
H	1.167407	-2.376206	-1.682557
H	2.180877	-1.163586	-2.543914
H	2.916862	-3.968856	-1.866739
H	3.917950	-2.763494	-2.740187

C	2.277181	-2.073526	0.713339
H	2.360260	-1.471253	1.637421
H	1.280631	-2.556382	0.699175
C	3.444189	-3.101260	0.568559
H	4.131230	-3.037093	1.436806
H	3.050474	-4.136966	0.520944
C	4.779492	-1.477773	-0.595845
H	5.474854	-1.422947	0.266371
H	5.366807	-1.300007	-1.519569
C	3.641295	-0.418316	-0.451379
H	3.713311	0.152622	0.493313
H	3.620479	0.303303	-1.291144
N	2.331568	-1.132209	-0.441797
N	4.215247	-2.836325	-0.656793
H	0.936411	1.565803	-1.972614

IM10

E= −1491.623291

G= −1491.164961

C	-0.819765	0.554483	-2.142156
H	-0.129151	-0.279722	-2.363254
H	-1.076069	1.046600	-3.099974
C	-0.107468	1.539407	-1.194141
C	0.234670	0.936281	0.161332
C	-0.916229	2.843157	-1.135544
O	-1.008928	3.628023	-2.072079
O	-1.542718	3.020723	0.043238
C	-2.403552	4.172774	0.135720
H	-2.807706	4.164594	1.164021
H	-1.831808	5.105221	-0.045373
H	-3.228833	4.094542	-0.600939
C	1.283530	1.598221	0.936359
C	1.784358	1.117487	2.190572
C	1.920652	2.783030	0.437734
C	2.838110	1.749912	2.864586
H	1.364750	0.211751	2.641196
C	2.973906	3.409798	1.117265
H	1.588904	3.235311	-0.508087
C	3.454369	2.902339	2.339382
H	3.186965	1.326401	3.821335
H	3.424325	4.317714	0.682207
H	4.282835	3.395360	2.871819

H	1.487062	-0.425162	-0.329483
C	-2.648003	-1.361142	0.728896
C	-3.865939	-2.034999	0.470156
C	-4.443168	-2.815791	1.491896
C	-3.834444	-2.933613	2.756517
C	-2.621453	-2.250541	3.022616
C	-2.044397	-1.469858	2.021427
H	-4.366312	-1.953215	-0.507619
H	-5.391688	-3.342618	1.294487
H	-4.303385	-3.549588	3.540340
H	-2.144714	-2.330252	4.014149
C	-0.782998	-0.634798	2.040995
C	-0.706487	-0.009799	0.646826
C	-1.814224	-0.501543	-0.084820
C	-2.101622	-0.085404	-1.513973
C	-3.246263	0.863301	-1.543147
N	-4.133245	1.629508	-1.497335
C	-2.448888	-1.265638	-2.341249
N	-2.668042	-2.229379	-2.971106
H	-0.813978	0.150593	2.828819
H	0.105755	-1.260159	2.272087
C	2.034623	-1.765937	-1.881302
C	3.199956	-2.766821	-2.136722
H	1.044921	-2.256501	-1.827160
H	1.994767	-0.955277	-2.632332
H	2.805868	-3.797406	-2.235464
H	3.724949	-2.511009	-3.078173
C	2.314250	-2.163385	0.534949
H	2.439162	-1.628384	1.493889
H	1.327822	-2.663376	0.527363
C	3.495446	-3.127810	0.217828
H	4.237573	-3.109290	1.040169
H	3.125349	-4.167008	0.115206
C	4.712972	-1.377836	-0.889778
H	5.464015	-1.378131	-0.075268
H	5.230375	-1.104269	-1.830459
C	3.580792	-0.356984	-0.575480
H	3.691013	0.126089	0.412444
H	3.477717	0.429379	-1.345927
N	2.281792	-1.117873	-0.547521
N	4.169581	-2.738634	-1.030947
H	0.815672	1.822739	-1.741387

TS9

E= −1491.592759

G= −1491.136419

C	0.386280	-0.889778	-0.182660
H	0.526546	-0.960858	-1.279496
H	1.230031	-1.417157	0.301207
C	-0.946334	-1.564999	0.186743
C	-2.135947	-0.868442	-0.457367
C	-1.012831	-1.682123	1.721136
O	-0.175013	-2.278512	2.380966
O	-2.072578	-1.046577	2.258360
C	-2.147071	-1.053084	3.696879
H	-3.063295	-0.492504	3.957308
H	-2.210705	-2.088999	4.087226
H	-1.258660	-0.553445	4.133976
C	-3.317598	-1.665909	-0.799137
C	-4.302392	-1.222384	-1.729558
C	-3.530815	-2.944365	-0.202612
C	-5.436227	-1.994080	-2.021569
H	-4.159673	-0.275818	-2.266603
C	-4.668746	-3.710177	-0.492646
H	-2.802495	-3.347509	0.516430
C	-5.636371	-3.241458	-1.401074
H	-6.169533	-1.618578	-2.753881
H	-4.801551	-4.687105	0.000236
H	-6.529004	-3.844896	-1.629734
H	2.976562	0.196057	-0.755324
C	-1.198726	2.646707	0.060176
C	-0.406968	3.747046	0.464797
C	-0.962132	5.040181	0.398465
C	-2.275203	5.241622	-0.068594
C	-3.062164	4.144835	-0.493578
C	-2.524211	2.857912	-0.429868
H	0.615674	3.600433	0.841387
H	-0.359407	5.905814	0.717939
H	-2.691759	6.260828	-0.109037
H	-4.083199	4.308479	-0.875686
C	-3.118978	1.538353	-0.878292
C	-2.041944	0.513558	-0.534102
C	-0.890857	1.233895	-0.023801
C	0.386610	0.610496	0.186663
C	1.026693	0.946661	1.444815

N	1.542009	1.195401	2.472384
C	1.642802	1.349590	-0.952526
N	1.823942	2.440874	-1.403169
H	-4.087789	1.304248	-0.384388
H	-3.334169	1.572513	-1.969466
C	4.981548	0.585211	-1.217273
C	6.353083	-0.128562	-1.024702
H	4.717298	0.745870	-2.279356
H	4.911182	1.551098	-0.683024
H	6.853618	-0.269707	-2.003046
H	7.018206	0.481524	-0.381984
C	3.881978	-1.621166	-1.371811
H	3.079209	-2.223365	-0.907545
H	3.605098	-1.397266	-2.419030
C	5.291819	-2.273999	-1.233145
H	5.204722	-3.278938	-0.774399
H	5.762575	-2.389927	-2.229368
C	5.560778	-1.273475	0.934948
H	5.432204	-2.273203	1.394932
H	6.252508	-0.687460	1.571878
C	4.185171	-0.547872	0.824601
H	3.343003	-1.150805	1.212501
H	4.169172	0.440628	1.319936
N	3.925374	-0.312359	-0.636238
N	6.168795	-1.444279	-0.393522
H	-0.873952	-2.611867	-0.173836

IM11

E= −1398.257874

G= −1397.726376

C	0.441376	-0.230740	-1.262978
H	0.266124	-0.331868	-2.359136
H	1.526964	-0.408751	-1.087317
C	-0.407276	-1.288349	-0.528570
C	-1.899857	-0.972968	-0.579776
C	0.126853	-1.458224	0.901325
O	1.163966	-2.053292	1.168052
O	-0.641318	-0.857935	1.826219
C	-0.183054	-0.935162	3.192635
H	-0.981463	-0.476432	3.803051
H	-0.023931	-1.989971	3.492703
H	0.761635	-0.367632	3.313841

C	-2.845899	-2.102489	-0.511795
C	-4.162371	-2.015849	-1.037730
C	-2.454725	-3.331330	0.086933
C	-5.051499	-3.096383	-0.946669
H	-4.482821	-1.107033	-1.563702
C	-3.351234	-4.404679	0.190313
H	-1.440052	-3.457054	0.493172
C	-4.655885	-4.293677	-0.323359
H	-6.062594	-3.003990	-1.374451
H	-3.024444	-5.339305	0.673280
H	-5.357260	-5.139773	-0.248581
C	-1.928616	2.668023	-0.106846
C	-1.415121	3.954857	0.162951
C	-2.306756	4.971595	0.539570
C	-3.690523	4.714977	0.644756
C	-4.207107	3.433741	0.373532
C	-3.323547	2.412299	0.000520
H	-0.338119	4.164122	0.088311
H	-1.921172	5.980053	0.757752
H	-4.373250	5.526598	0.943135
H	-5.288151	3.237596	0.454684
C	-3.635098	0.976131	-0.355144
C	-2.261796	0.353060	-0.547603
C	-1.253442	1.425529	-0.501240
C	0.064107	1.173729	-0.830115
C	1.057403	2.182640	-0.851795
N	1.912683	2.996329	-0.876789
H	-4.232893	0.454415	0.423476
H	-4.243310	0.941770	-1.286343
C	4.581024	0.573774	-1.436914
C	6.053024	0.541042	-0.906265
H	4.516729	0.199325	-2.480739
H	4.162966	1.602041	-1.422628
H	6.752377	0.155869	-1.678593
H	6.399306	1.556832	-0.619924
C	4.239084	-1.663629	-0.619504
H	3.564894	-2.290965	-0.000601
H	4.176388	-2.033476	-1.665060
C	5.712230	-1.692366	-0.090315
H	5.805546	-2.344084	0.804415
H	6.410053	-2.083256	-0.861271
C	5.244827	0.188519	1.326422
H	5.338761	-0.460927	2.222688

H	5.592871	1.203745	1.613003
C	3.771704	0.220798	0.800742
H	3.103776	-0.416052	1.416177
H	3.358879	1.250772	0.808934
N	3.725707	-0.279332	-0.588881
N	6.148930	-0.331682	0.281397
H	-0.207188	-2.259181	-1.023014

TS10

E= −1398.231534

G= −1397.796358

C	-0.612234	0.296227	-1.061106
H	-0.897336	0.640803	-2.077540
H	-2.006834	0.387101	-0.549829
C	0.280448	1.238411	-0.252261
C	1.767434	0.877877	-0.391942
C	-0.093354	1.219974	1.240341
O	-0.969168	0.542850	1.759613
O	0.692528	2.061659	1.950050
C	0.469460	2.103410	3.371536
H	1.204262	2.824199	3.774542
H	-0.560454	2.443455	3.603554
H	0.629654	1.104508	3.825945
C	2.772351	1.935854	-0.581582
C	4.083395	1.658231	-1.064400
C	2.468447	3.299494	-0.304180
C	5.032280	2.675133	-1.241360
H	4.358855	0.632200	-1.339481
C	3.417203	4.316083	-0.485889
H	1.479326	3.565091	0.093060
C	4.710100	4.013949	-0.951226
H	6.034006	2.418050	-1.622382
H	3.144204	5.358026	-0.252309
H	5.456185	4.812360	-1.090271
C	1.494604	-2.777413	0.041535
C	0.867226	-4.032355	0.200335
C	1.642535	-5.135252	0.602575
C	3.024299	-4.998623	0.847118
C	3.655937	-3.745658	0.688453
C	2.892196	-2.643173	0.290265
H	-0.212568	-4.150102	0.021826
H	1.160390	-6.117521	0.733927

H	3.613974	-5.872977	1.165829
H	4.736958	-3.639686	0.876917
C	3.333889	-1.220823	0.009903
C	2.026495	-0.478427	-0.248384
C	0.963810	-1.470352	-0.342302
C	-0.246865	-1.104622	-0.960533
C	-1.079173	-2.088449	-1.567395
N	-1.793494	-2.876454	-2.079473
H	3.931745	-0.768494	0.831060
H	3.994886	-1.220915	-0.885782
C	-3.935325	0.373756	-1.644639
C	-5.475780	0.404407	-1.388341
H	-3.588880	1.232591	-2.252305
H	-3.604467	-0.561424	-2.136049
H	-5.943472	1.253226	-1.927168
H	-5.948589	-0.531526	-1.748636
C	-3.585324	1.736051	0.351018
H	-3.037793	1.752273	1.310907
H	-3.206702	2.559231	-0.286126
C	-5.135103	1.785769	0.542375
H	-5.388267	1.906302	1.615227
H	-5.571242	2.642558	-0.010169
C	-5.188757	-0.602574	0.773140
H	-5.405925	-0.478458	1.853518
H	-5.696034	-1.525748	0.426524
C	-3.649087	-0.700114	0.529056
H	-3.051021	-0.638261	1.456005
H	-3.367806	-1.624061	-0.011198
N	-3.244017	0.452688	-0.325377
N	-5.757001	0.546951	0.049066
H	0.111009	2.278076	-0.599083

IM12

E= −1398.240352

G= −1397.796795

C	-0.050335	-0.790265	-1.616931
H	0.427679	-1.371988	-2.418108
H	2.109376	-1.521664	0.092836
C	-1.104484	-1.410225	-0.732051
C	-2.267545	-0.434215	-0.510891
C	-0.496826	-1.891367	0.602671
O	0.705258	-2.057706	0.822409

O	-1.420752	-2.148831	1.533009
C	-0.947009	-2.609780	2.816585
H	-1.850396	-2.762454	3.433718
H	-0.389823	-3.562121	2.710855
H	-0.288745	-1.849917	3.283305
C	-3.638204	-0.942294	-0.487241
C	-4.781000	-0.083314	-0.526140
C	-3.915702	-2.343940	-0.425521
C	-6.088910	-0.585368	-0.493065
H	-4.643276	1.001358	-0.616950
C	-5.225485	-2.843162	-0.401463
H	-3.084833	-3.060935	-0.364967
C	-6.331026	-1.971651	-0.428254
H	-6.935136	0.120723	-0.530174
H	-5.384330	-3.933078	-0.348395
H	-7.359924	-2.363921	-0.400954
C	-0.336714	2.674936	0.029571
C	0.786544	3.536684	0.064768
C	0.662669	4.801609	0.672577
C	-0.554999	5.221951	1.243491
C	-1.683427	4.366870	1.206782
C	-1.571676	3.109969	0.609314
H	1.748521	3.228461	-0.373242
H	1.537672	5.472013	0.703813
H	-0.629996	6.213321	1.718166
H	-2.641731	4.693583	1.644546
C	-2.627200	2.039439	0.407214
C	-1.859718	0.877176	-0.220292
C	-0.524907	1.332712	-0.493348
C	0.287257	0.539406	-1.380080
C	1.330705	1.163121	-2.131974
N	2.205253	1.674037	-2.735061
H	-3.151768	1.750168	1.344860
H	-3.417996	2.434070	-0.269399
C	3.674258	-1.367121	-1.339151
C	5.189274	-1.008378	-1.287382
H	3.480744	-2.396618	-1.693386
H	3.089983	-0.658784	-1.951925
H	5.797899	-1.843342	-1.687789
H	5.389303	-0.109555	-1.903911
C	3.856256	-2.285213	0.939719
H	3.399375	-2.216003	1.944237
H	3.646529	-3.286379	0.518554

C	5.371075	-1.920774	0.928398
H	5.722118	-1.708489	1.957697
H	5.967340	-2.764497	0.528233
C	4.853742	0.406636	0.626655
H	5.204249	0.616423	1.656577
H	5.065049	1.296697	0.001646
C	3.326946	0.100911	0.625603
H	2.879888	0.099054	1.637052
H	2.749026	0.788964	-0.016785
N	3.146550	-1.284773	0.066164
N	5.613811	-0.734543	0.093678
H	-1.473480	-2.341966	-1.214297

TS11

E= −1398.230914

G= −1397.796251

C	-0.430304	1.998724	1.604772
H	-0.788507	2.397778	2.564448
C	-1.361269	1.299359	0.747606
C	-0.929626	1.016889	-0.628503
C	-2.792107	1.786009	0.943566
O	-3.410208	2.459110	0.134890
O	-3.268712	1.461774	2.166407
C	-4.574289	1.980261	2.486328
H	-4.797520	1.631887	3.511271
H	-4.580067	3.088847	2.451621
H	-5.335024	1.592491	1.778713
C	-1.891137	0.392235	-1.562185
C	-1.802914	0.550599	-2.969717
C	-2.925649	-0.444158	-1.060745
C	-2.694710	-0.103801	-3.832673
H	-1.049846	1.227997	-3.395135
C	-3.807555	-1.109902	-1.925594
H	-3.022492	-0.597395	0.024828
C	-3.699109	-0.945290	-3.318081
H	-2.609543	0.052521	-4.920210
H	-4.590862	-1.761364	-1.505142
H	-4.398257	-1.458779	-3.997126
H	-1.024371	-1.033810	1.334115
C	2.754407	1.353373	-0.470890
C	4.029859	1.592250	0.088189
C	5.174013	1.253298	-0.657359
C	5.063000	0.683978	-1.941999

C	3.790630	0.445866	-2.506678
C	2.647640	0.775885	-1.772324
H	4.137420	2.030965	1.091025
H	6.172108	1.433584	-0.226248
H	5.971699	0.422673	-2.507269
H	3.700629	0.001358	-3.511373
C	1.190600	0.634790	-2.151768
C	0.444033	1.090999	-0.906651
C	1.402631	1.550295	0.050336
C	0.933052	2.071830	1.291683
C	1.828943	2.670922	2.233420
N	2.563803	3.161078	3.010692
H	0.965035	1.276348	-3.030756
H	0.913693	-0.398139	-2.459243
C	-0.753432	-3.111449	2.081822
C	0.249081	-4.306480	1.994366
H	-0.841724	-2.701288	3.106770
H	-1.766455	-3.375338	1.719342
H	0.705669	-4.505599	2.985000
H	-0.273949	-5.227650	1.667104
C	1.117900	-1.601029	1.649255
H	1.420175	-0.737983	1.024405
H	1.030867	-1.261127	2.699573
C	2.072760	-2.824646	1.489706
H	2.866820	-2.605908	0.747557
H	2.563456	-3.061787	2.455335
C	0.733633	-3.731664	-0.283474
H	1.551905	-3.558980	-1.011518
H	0.166352	-4.626444	-0.610484
C	-0.197767	-2.480951	-0.211439
H	0.180118	-1.638196	-0.817858
H	-1.236530	-2.698021	-0.525257
N	-0.240870	-2.020160	1.206119
N	1.325395	-4.009475	1.035240
H	-1.571621	-0.124951	1.415972

IM13

E= −1398.239427

G= −1397.798573

C	-1.234351	-2.461316	-0.193305
H	-1.597857	-3.306156	-0.793733
C	-2.083871	-1.367788	0.050934

C	-1.633401	-0.256438	0.825319
C	-3.488291	-1.412822	-0.472300
O	-4.465937	-0.945327	0.090597
O	-3.548102	-2.066797	-1.658696
C	-4.863307	-2.219985	-2.227868
H	-4.716165	-2.722410	-3.201023
H	-5.506408	-2.842761	-1.572976
H	-5.345299	-1.232643	-2.375819
C	-2.433529	0.989970	0.974381
C	-2.755911	1.505633	2.248377
C	-2.818189	1.712069	-0.178541
C	-3.461553	2.714603	2.366066
H	-2.468367	0.944741	3.151217
C	-3.513123	2.925277	-0.057858
H	-2.557804	1.318830	-1.173999
C	-3.839288	3.429017	1.214966
H	-3.718442	3.100985	3.365234
H	-3.800565	3.482130	-0.963888
H	-4.387058	4.380042	1.309854
H	-0.630467	-0.493892	-2.974838
C	1.871396	-1.083661	1.637901
C	3.085221	-1.800566	1.610948
C	4.228178	-1.206260	2.170730
C	4.165771	0.080036	2.747279
C	2.954452	0.797812	2.779032
C	1.808680	0.214054	2.224189
H	3.147735	-2.798622	1.154562
H	5.186018	-1.749369	2.153450
H	5.076569	0.529732	3.173313
H	2.911012	1.803908	3.225038
C	0.411622	0.772816	2.108162
C	-0.327274	-0.303224	1.343916
C	0.545999	-1.395580	1.090151
C	0.081202	-2.493884	0.320477
C	0.923449	-3.611441	0.023157
N	1.618235	-4.526986	-0.223969
H	-0.038847	0.961451	3.106791
H	0.382437	1.748669	1.576151
C	2.078670	1.400417	-3.626356
C	3.283928	2.187538	-3.005082
H	2.419657	0.676302	-4.396366
H	1.349271	2.087099	-4.106050
H	4.248309	1.868227	-3.454505

H	3.179477	3.280963	-3.170641
C	2.321480	-0.292359	-1.937177
H	1.772087	-0.869535	-1.167086
H	2.664825	-1.009350	-2.712510
C	3.518447	0.498350	-1.310317
H	3.575310	0.334135	-0.214218
H	4.487702	0.181024	-1.750457
C	2.085480	2.385198	-0.931548
H	2.160701	2.212217	0.162189
H	1.979089	3.478777	-1.094993
C	0.881837	1.597075	-1.549865
H	0.334627	1.017986	-0.779376
H	0.154148	2.280158	-2.036397
N	1.376655	0.650024	-2.567613
N	3.348724	1.943723	-1.551732
H	-1.317026	-0.860232	-2.965529

TS12

E= −1398. 20583

G= −1397. 773702

C	-4.123302	1.366923	-0.147853
H	-5.197922	1.591974	-0.200945
C	-3.702145	0.023594	-0.070130
C	-2.320331	-0.316846	0.008880
C	-4.795980	-1.003972	-0.061231
O	-5.863387	-0.862893	0.520128
O	-4.489422	-2.085802	-0.810072
C	-5.418281	-3.182177	-0.749857
H	-4.995436	-3.974226	-1.394164
H	-5.518478	-3.554302	0.290582
H	-6.418194	-2.881047	-1.123065
C	-1.899999	-1.737331	0.189804
C	-1.132282	-2.402772	-0.787515
C	-2.319617	-2.449398	1.336135
C	-0.798851	-3.756907	-0.626174
H	-0.800885	-1.856291	-1.681284
C	-1.978121	-3.801244	1.501353
H	-2.921477	-1.933783	2.102021
C	-1.218454	-4.460647	0.517405
H	-0.204563	-4.267682	-1.400932
H	-2.308546	-4.343301	2.401940
H	-0.954199	-5.523060	0.641833

C	-0.626233	2.974296	0.039081
C	-0.475140	4.379705	0.047692
C	0.800083	4.924839	0.258693
C	1.922396	4.083937	0.459628
C	1.792294	2.686946	0.426939
C	0.520215	2.126601	0.204445
H	-1.340548	5.043084	-0.096596
H	0.928986	6.018568	0.276113
H	2.911582	4.534474	0.641475
H	2.666872	2.036457	0.577392
C	0.102495	0.722811	0.040638
C	-1.375657	0.738244	-0.005622
C	-1.797651	2.113308	-0.074811
C	-3.182872	2.417464	-0.172302
C	-3.648611	3.767282	-0.266431
N	-4.034348	4.875597	-0.346183
C	4.528628	-2.093589	-0.626384
C	6.070003	-2.108111	-0.394812
H	3.987012	-2.814351	0.015313
H	4.250397	-2.279364	-1.681434
H	6.340854	-2.867285	0.366025
H	6.600765	-2.360588	-1.334531
C	4.326973	-0.426692	1.164506
H	3.889922	0.562111	1.396600
H	3.807232	-1.191275	1.771953
C	5.875450	-0.459288	1.341784
H	6.246131	0.527540	1.684396
H	6.162984	-1.215619	2.099259
C	6.206313	0.229947	-0.936282
H	6.591360	1.208476	-0.585871
H	6.726006	-0.024098	-1.881756
C	4.665393	0.300369	-1.161534
H	4.233999	1.282551	-0.890989
H	4.370051	0.059802	-2.200796
N	4.025089	-0.724366	-0.273533
N	6.535839	-0.792227	0.069610
H	2.911747	-0.712467	-0.447503
O	0.841107	-0.325955	0.601509
O	1.469193	-0.815866	-0.706270
H	0.708060	0.201054	-1.072928

IM14

E= -1398.251304

G= -1397.825095

C	0.951442	2.407482	-1.198992
H	1.293927	3.024829	-2.041138
C	1.851903	1.482870	-0.609811
C	1.448509	0.636078	0.455900
C	3.228069	1.460008	-1.196090
O	3.476845	1.617469	-2.385320
O	4.187319	1.297834	-0.253413
C	5.530508	1.147928	-0.741807
H	6.166439	1.009306	0.151454
H	5.612916	0.261537	-1.404237
H	5.855123	2.047449	-1.303588
C	2.317052	-0.450722	0.981265
C	2.547917	-0.588290	2.369086
C	2.904868	-1.391454	0.101645
C	3.353430	-1.628296	2.862091
H	2.107785	0.142673	3.064602
C	3.704332	-2.434169	0.595010
H	2.726109	-1.304087	-0.981671
C	3.932963	-2.556481	1.978158
H	3.533523	-1.711545	3.945949
H	4.150361	-3.158262	-0.105525
H	4.561502	-3.373940	2.365912
C	-2.064267	1.619317	1.059161
C	-3.313384	2.270471	0.898931
C	-4.409323	1.852611	1.660730
C	-4.279016	0.781517	2.593049
C	-3.062539	0.118843	2.772021
C	-1.928966	0.516979	2.008085
H	-3.426242	3.096071	0.179302
H	-5.382811	2.354725	1.542394
H	-5.157918	0.472491	3.182846
H	-2.979188	-0.711296	3.492898
C	-0.602665	-0.019561	1.920981
C	0.117213	0.762438	0.958528
C	-0.794673	1.760276	0.396473
C	-0.356392	2.558864	-0.698726
C	-1.236645	3.498489	-1.322011
N	-1.970588	4.263360	-1.833463
H	-0.191695	-0.821324	2.547124
C	-2.126346	-2.832426	0.066725
C	-2.580206	-3.663784	-1.169761

H	-1.303747	-3.306104	0.634582
H	-2.953991	-2.596069	0.761733
H	-1.985541	-4.595530	-1.248403
H	-3.647570	-3.944705	-1.072102
C	-0.447303	-1.739188	-1.378686
H	-0.068533	-0.740198	-1.663204
H	0.335768	-2.265159	-0.801783
C	-0.982279	-2.563005	-2.588198
H	-0.868288	-1.985647	-3.526966
H	-0.410568	-3.506423	-2.692407
C	-3.190670	-1.647188	-2.325051
H	-3.092967	-1.099078	-3.283070
H	-4.257432	-1.913105	-2.187238
C	-2.695093	-0.757355	-1.145228
H	-2.253404	0.198296	-1.480232
H	-3.479172	-0.543791	-0.395936
N	-1.603178	-1.517657	-0.443956
N	-2.405695	-2.888851	-2.407683
H	-1.252099	-0.965003	0.403408

3aa

E= -1397.077938

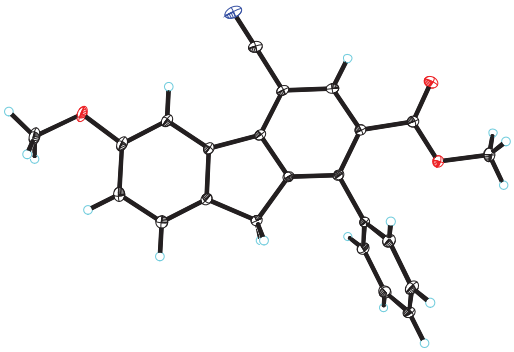
G= -1396.660891

C	-2.531314	2.371410	0.933786
H	-3.125855	3.052019	1.560276
C	-3.045398	1.103320	0.621818
C	-2.289531	0.182762	-0.170363
C	-4.412313	0.788921	1.160297
O	-4.807601	1.127129	2.266460
O	-5.167014	0.133628	0.255057
C	-6.465017	-0.299839	0.703675
H	-6.923617	-0.821859	-0.155447
H	-6.369083	-0.995428	1.562176
H	-7.090843	0.565045	1.003296
C	-2.748983	-1.214262	-0.400793
C	-2.885341	-1.731788	-1.706543
C	-3.047237	-2.044476	0.703348
C	-3.314134	-3.054625	-1.903301
H	-2.677565	-1.086200	-2.573521
C	-3.468780	-3.367874	0.504422
H	-2.931783	-1.649923	1.725557
C	-3.604325	-3.877332	-0.800214

H	-3.425637	-3.444349	-2.927643
H	-3.691337	-4.006381	1.374064
H	-3.937137	-4.915702	-0.956773
C	0.798769	2.045834	-1.002105
C	1.715871	3.112962	-1.026338
C	2.917442	2.948368	-1.740758
C	3.191177	1.750797	-2.430431
C	2.272964	0.680229	-2.407974
C	1.088612	0.829473	-1.680350
H	1.507579	4.059471	-0.507275
H	3.647507	3.772403	-1.768864
H	4.132058	1.650052	-2.993942
H	2.484295	-0.255720	-2.943285
C	-0.017381	-0.183856	-1.441663
C	-1.046774	0.621348	-0.657176
C	-0.524883	1.909294	-0.370756
C	-1.277921	2.798810	0.436414
C	-0.802302	4.108907	0.760288
N	-0.413100	5.185901	1.025254
C	3.507479	-2.455203	1.308398
C	4.688462	-2.170298	2.292395
H	2.533172	-2.506631	1.835654
H	3.647337	-3.408544	0.758598
H	4.324559	-2.086000	3.337849
H	5.439866	-2.986944	2.260631
C	3.195749	-0.075083	1.011481
H	3.112494	0.720286	0.246134
H	2.221156	-0.145480	1.533940
C	4.380230	0.192245	1.995799
H	4.902124	1.138399	1.740687
H	4.018749	0.277311	3.042042
C	5.875166	-1.014950	0.554334
H	6.399601	-0.069142	0.303542
H	6.623212	-1.834719	0.524214
C	4.702141	-1.286922	-0.442588
H	4.603762	-0.477136	-1.192793
H	4.833680	-2.244553	-0.987338
N	3.426220	-1.361273	0.308663
N	5.358493	-0.908529	1.930671
H	2.212171	-1.755646	-0.681145
O	0.367391	-1.259075	-0.570376
O	1.386078	-2.047751	-1.252161
H	-0.417144	-0.597812	-2.395212

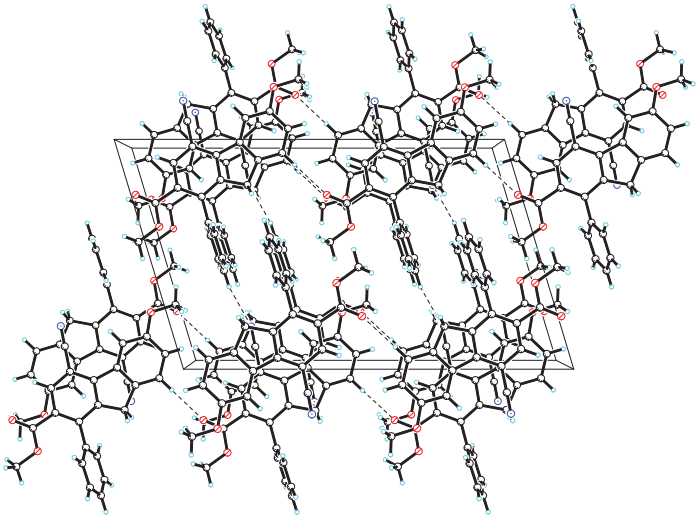
6. X-ray crystal structure of compound 3ba

Crystal data for mo_hd_fjy1_0m: $C_{23}H_{17}NO_3$, M = 355.38, a = 13.0762(14) Å, b = 6.6583(7) Å, c = 21.175(2) Å, α = 90°, β = 106.715(2)°, γ = 90°, V = 1765.7(3) Å^3, T = 100(2) K, space group $P21/c$, Z = 4, μ(MoKα) = 0.089 mm^{-1}, 19366 reflections measured, 5260 independent reflections (R_{int} = 0.0386). The final R_1 values were 0.0479 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1326 ($I > 2\sigma(I)$). The final R_1 values were 0.0693 (all data). The final $wR(F^2)$ values were 0.1474 (all data). The goodness of fit on F^2 was 1.033.



View of a molecule of hd_fjy1 with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of hd_fjy1.

Hydrogen-bonds are shown as dashed lines.

Table S2. Crystal data and structure refinement for mo_hd_fjy1_0m.

Identification code	mo_hd_fjy1_0m	
Empirical formula	C23 H17 N O3	
Formula weight	355.38	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.0762(14) Å	α= 90°.
	b = 6.6583(7) Å	β= 106.715(2)°.
	c = 21.175(2) Å	γ = 90°.
Volume	1765.7(3) $Å^3$	
Z	4	
Density (calculated)	1.337 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	744	
Crystal size	0.670 x 0.350 x 0.180 mm^3	
Theta range for data collection	1.626 to 31.139°.	
Index ranges	-18<=h<=18, -9<=k<=9, -30<=l<=30	
Reflections collected	19366	
Independent reflections	5260 [R(int) = 0.0386]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5260 / 0 / 246	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.1326	
R indices (all data)	R1 = 0.0693, wR2 = 0.1474	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.715 and -0.252 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for mo_hd_fjy1_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3774(1)	2909(1)	4596(1)	28(1)
O(2)	-2422(1)	2664(1)	515(1)	28(1)
O(3)	2364(1)	2503(1)	4982(1)	28(1)
N(1)	-1802(1)	2740(2)	2989(1)	29(1)
C(1)	4452(1)	2767(2)	5267(1)	33(1)
C(2)	2729(1)	2696(2)	4521(1)	19(1)
C(3)	2056(1)	2726(2)	3819(1)	17(1)
C(4)	954(1)	2729(2)	3734(1)	18(1)
C(5)	225(1)	2748(2)	3109(1)	17(1)
C(6)	600(1)	2759(2)	2552(1)	16(1)
C(7)	40(1)	2743(2)	1841(1)	17(1)
C(8)	-1042(1)	2725(2)	1502(1)	19(1)
C(9)	-1340(1)	2697(2)	816(1)	22(1)
C(10)	-2761(1)	2605(2)	-190(1)	31(1)
C(11)	2448(1)	2738(2)	3263(1)	16(1)
C(12)	1707(1)	2761(2)	2639(1)	16(1)
C(13)	1928(1)	2743(2)	1978(1)	18(1)
C(14)	822(1)	2737(2)	1500(1)	19(1)
C(15)	514(1)	2710(2)	818(1)	24(1)
C(16)	-572(1)	2691(2)	474(1)	26(1)
C(17)	3600(1)	2695(2)	3289(1)	18(1)
C(18)	4161(1)	889(2)	3384(1)	25(1)
C(19)	5218(1)	846(2)	3370(1)	34(1)
C(20)	5721(1)	2596(2)	3266(1)	36(1)
C(21)	5166(1)	4388(2)	3169(1)	32(1)
C(22)	4105(1)	4449(2)	3177(1)	25(1)
C(23)	-902(1)	2744(2)	3045(1)	21(1)

Table S4. Bond lengths [Å] and angles [°] for mo_hd_fjy1_0m.

O(1)-C(2)	1.3371(14)
O(1)-C(1)	1.4451(15)
O(2)-C(9)	1.3737(14)
O(2)-C(10)	1.4318(16)
O(3)-C(2)	1.2085(14)
N(1)-C(23)	1.1487(16)
C(1)-H(4)	0.9800
C(1)-H(1)	0.9800
C(1)-H(5)	0.9800
C(2)-C(3)	1.4946(16)
C(3)-C(4)	1.4002(16)
C(3)-C(11)	1.4131(15)
C(4)-C(5)	1.3901(16)
C(4)-H(15)	0.9500
C(5)-C(6)	1.4012(15)
C(5)-C(23)	1.4405(16)
C(6)-C(12)	1.4060(15)
C(6)-C(7)	1.4723(15)
C(7)-C(8)	1.3902(16)
C(7)-C(14)	1.4112(16)
C(8)-C(9)	1.3925(17)
C(8)-H(16)	0.9500
C(9)-C(16)	1.3978(19)
C(10)-H(17)	0.9800
C(10)-H(3)	0.9800
C(10)-H(2)	0.9800
C(11)-C(12)	1.3960(15)
C(11)-C(17)	1.4920(15)
C(12)-C(13)	1.5085(15)
C(13)-C(14)	1.5068(16)
C(13)-H(9)	0.9900
C(13)-H(8)	0.9900
C(14)-C(15)	1.3832(16)
C(15)-C(16)	1.3968(18)
C(15)-H(7)	0.9500

C(16)-H(6)	0.9500
C(17)-C(18)	1.3923(16)
C(17)-C(22)	1.3950(16)
C(18)-C(19)	1.3911(16)
C(18)-H(14)	0.9500
C(19)-C(20)	1.386(2)
C(19)-H(13)	0.9500
C(20)-C(21)	1.381(2)
C(20)-H(12)	0.9500
C(21)-C(22)	1.3934(16)
C(21)-H(11)	0.9500
C(22)-H(10)	0.9500

C(2)-O(1)-C(1)	115.30(10)
C(9)-O(2)-C(10)	116.92(11)
O(1)-C(1)-H(4)	109.5
O(1)-C(1)-H(1)	109.5
H(4)-C(1)-H(1)	109.5
O(1)-C(1)-H(5)	109.5
H(4)-C(1)-H(5)	109.5
H(1)-C(1)-H(5)	109.5
O(3)-C(2)-O(1)	122.80(11)
O(3)-C(2)-C(3)	123.28(11)
O(1)-C(2)-C(3)	113.92(9)
C(4)-C(3)-C(11)	119.95(10)
C(4)-C(3)-C(2)	114.68(10)
C(11)-C(3)-C(2)	125.37(10)
C(5)-C(4)-C(3)	121.42(10)
C(5)-C(4)-H(15)	119.3
C(3)-C(4)-H(15)	119.3
C(4)-C(5)-C(6)	119.40(10)
C(4)-C(5)-C(23)	119.48(10)
C(6)-C(5)-C(23)	121.12(10)
C(5)-C(6)-C(12)	119.10(10)
C(5)-C(6)-C(7)	132.01(10)
C(12)-C(6)-C(7)	108.88(9)
C(8)-C(7)-C(14)	121.04(11)

C(8)-C(7)-C(6)	131.33(10)
C(14)-C(7)-C(6)	107.63(10)
C(7)-C(8)-C(9)	118.49(11)
C(7)-C(8)-H(16)	120.8
C(9)-C(8)-H(16)	120.8
O(2)-C(9)-C(8)	115.21(11)
O(2)-C(9)-C(16)	123.89(12)
C(8)-C(9)-C(16)	120.90(11)
O(2)-C(10)-H(17)	109.5
O(2)-C(10)-H(3)	109.5
H(17)-C(10)-H(3)	109.5
O(2)-C(10)-H(2)	109.5
H(17)-C(10)-H(2)	109.5
H(3)-C(10)-H(2)	109.5
C(12)-C(11)-C(3)	118.00(10)
C(12)-C(11)-C(17)	117.05(10)
C(3)-C(11)-C(17)	124.95(10)
C(11)-C(12)-C(6)	122.14(10)
C(11)-C(12)-C(13)	127.74(10)
C(6)-C(12)-C(13)	110.11(9)
C(14)-C(13)-C(12)	102.68(9)
C(14)-C(13)-H(9)	111.2
C(12)-C(13)-H(9)	111.2
C(14)-C(13)-H(8)	111.2
C(12)-C(13)-H(8)	111.2
H(9)-C(13)-H(8)	109.1
C(15)-C(14)-C(7)	119.81(11)
C(15)-C(14)-C(13)	129.48(11)
C(7)-C(14)-C(13)	110.70(10)
C(14)-C(15)-C(16)	119.55(12)
C(14)-C(15)-H(7)	120.2
C(16)-C(15)-H(7)	120.2
C(15)-C(16)-C(9)	120.20(12)
C(15)-C(16)-H(6)	119.9
C(9)-C(16)-H(6)	119.9
C(18)-C(17)-C(22)	119.52(11)
C(18)-C(17)-C(11)	120.42(10)

C(22)-C(17)-C(11)	119.94(10)
C(19)-C(18)-C(17)	119.97(12)
C(19)-C(18)-H(14)	120.0
C(17)-C(18)-H(14)	120.0
C(20)-C(19)-C(18)	120.41(13)
C(20)-C(19)-H(13)	119.8
C(18)-C(19)-H(13)	119.8
C(21)-C(20)-C(19)	119.75(12)
C(21)-C(20)-H(12)	120.1
C(19)-C(20)-H(12)	120.1
C(20)-C(21)-C(22)	120.42(13)
C(20)-C(21)-H(11)	119.8
C(22)-C(21)-H(11)	119.8
C(21)-C(22)-C(17)	119.92(12)
C(21)-C(22)-H(10)	120.0
C(17)-C(22)-H(10)	120.0
N(1)-C(23)-C(5)	179.49(14)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_hd_fjy1_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(1)	51(1)	16(1)	0(1)	3(1)	-3(1)
O(2)	15(1)	38(1)	24(1)	3(1)	-5(1)	-1(1)
O(3)	26(1)	42(1)	20(1)	1(1)	11(1)	-2(1)
N(1)	18(1)	30(1)	43(1)	-1(1)	13(1)	-1(1)
C(1)	20(1)	58(1)	18(1)	1(1)	0(1)	-2(1)
C(2)	16(1)	23(1)	18(1)	0(1)	6(1)	-1(1)
C(3)	15(1)	19(1)	17(1)	0(1)	5(1)	-1(1)
C(4)	16(1)	20(1)	21(1)	0(1)	9(1)	-1(1)
C(5)	12(1)	16(1)	22(1)	0(1)	6(1)	0(1)
C(6)	12(1)	15(1)	19(1)	1(1)	4(1)	0(1)
C(7)	14(1)	17(1)	19(1)	1(1)	2(1)	-1(1)
C(8)	13(1)	19(1)	22(1)	2(1)	2(1)	0(1)
C(9)	15(1)	23(1)	24(1)	2(1)	-1(1)	0(1)
C(10)	23(1)	37(1)	24(1)	3(1)	-6(1)	-3(1)
C(11)	13(1)	17(1)	18(1)	1(1)	4(1)	-1(1)
C(12)	13(1)	17(1)	17(1)	0(1)	5(1)	0(1)
C(13)	14(1)	24(1)	17(1)	0(1)	5(1)	0(1)
C(14)	14(1)	22(1)	19(1)	1(1)	4(1)	-1(1)
C(15)	19(1)	34(1)	19(1)	1(1)	5(1)	0(1)
C(16)	22(1)	33(1)	18(1)	1(1)	1(1)	-1(1)
C(17)	11(1)	29(1)	14(1)	-1(1)	3(1)	-1(1)
C(18)	19(1)	34(1)	22(1)	1(1)	5(1)	5(1)
C(19)	18(1)	55(1)	26(1)	-2(1)	4(1)	12(1)
C(20)	13(1)	76(1)	18(1)	-5(1)	4(1)	-1(1)
C(21)	19(1)	57(1)	20(1)	-1(1)	5(1)	-14(1)
C(22)	17(1)	34(1)	22(1)	1(1)	5(1)	-6(1)
C(23)	18(1)	20(1)	26(1)	0(1)	9(1)	0(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_hd_fjy1_0m.

	x	y	z	U(eq)
H(4)	4219	3747	5542	50
H(1)	5193	3048	5278	50
H(5)	4405	1411	5436	50
H(15)	698	2718	4111	22
H(16)	-1565	2732	1734	22
H(17)	-2490	3791	-364	46
H(3)	-3543	2594	-347	46
H(2)	-2482	1389	-343	46
H(9)	2332	3951	1919	22
H(8)	2332	1528	1925	22
H(7)	1036	2704	586	29
H(6)	-788	2673	5	31
H(14)	3822	-314	3458	30
H(13)	5597	-389	3432	40
H(12)	6445	2562	3261	43
H(11)	5510	5586	3096	38
H(10)	3725	5684	3106	30

Table S7. Torsion angles [°] for mo_hd_fjy1_0m.

C(1)-O(1)-C(2)-O(3)	3.74(16)
C(1)-O(1)-C(2)-C(3)	-176.50(10)
O(3)-C(2)-C(3)-C(4)	6.50(16)
O(1)-C(2)-C(3)-C(4)	-173.26(9)
O(3)-C(2)-C(3)-C(11)	-173.05(11)
O(1)-C(2)-C(3)-C(11)	7.19(15)
C(11)-C(3)-C(4)-C(5)	-0.15(15)
C(2)-C(3)-C(4)-C(5)	-179.72(9)
C(3)-C(4)-C(5)-C(6)	0.15(15)
C(3)-C(4)-C(5)-C(23)	179.84(9)
C(4)-C(5)-C(6)-C(12)	-0.30(15)
C(23)-C(5)-C(6)-C(12)	-179.99(9)
C(4)-C(5)-C(6)-C(7)	178.76(10)
C(23)-C(5)-C(6)-C(7)	-0.93(17)
C(5)-C(6)-C(7)-C(8)	0.52(19)
C(12)-C(6)-C(7)-C(8)	179.65(10)
C(5)-C(6)-C(7)-C(14)	-179.18(11)
C(12)-C(6)-C(7)-C(14)	-0.05(11)
C(14)-C(7)-C(8)-C(9)	0.15(15)
C(6)-C(7)-C(8)-C(9)	-179.51(10)
C(10)-O(2)-C(9)-C(8)	-179.12(10)
C(10)-O(2)-C(9)-C(16)	0.46(16)
C(7)-C(8)-C(9)-O(2)	179.47(9)
C(7)-C(8)-C(9)-C(16)	-0.13(16)
C(4)-C(3)-C(11)-C(12)	0.29(15)
C(2)-C(3)-C(11)-C(12)	179.82(10)
C(4)-C(3)-C(11)-C(17)	-178.69(9)
C(2)-C(3)-C(11)-C(17)	0.83(16)
C(3)-C(11)-C(12)-C(6)	-0.45(15)
C(17)-C(11)-C(12)-C(6)	178.61(9)
C(3)-C(11)-C(12)-C(13)	-178.92(10)
C(17)-C(11)-C(12)-C(13)	0.15(15)
C(5)-C(6)-C(12)-C(11)	0.46(15)
C(7)-C(6)-C(12)-C(11)	-178.80(9)
C(5)-C(6)-C(12)-C(13)	179.17(9)

C(7)-C(6)-C(12)-C(13)	-0.09(11)
C(11)-C(12)-C(13)-C(14)	178.80(10)
C(6)-C(12)-C(13)-C(14)	0.18(11)
C(8)-C(7)-C(14)-C(15)	-0.12(16)
C(6)-C(7)-C(14)-C(15)	179.61(10)
C(8)-C(7)-C(14)-C(13)	-179.56(9)
C(6)-C(7)-C(14)-C(13)	0.17(12)
C(12)-C(13)-C(14)-C(15)	-179.58(11)
C(12)-C(13)-C(14)-C(7)	-0.21(11)
C(7)-C(14)-C(15)-C(16)	0.08(17)
C(13)-C(14)-C(15)-C(16)	179.40(10)
C(14)-C(15)-C(16)-C(9)	-0.06(17)
O(2)-C(9)-C(16)-C(15)	-179.48(10)
C(8)-C(9)-C(16)-C(15)	0.08(17)
C(12)-C(11)-C(17)-C(18)	-98.17(12)
C(3)-C(11)-C(17)-C(18)	80.82(14)
C(12)-C(11)-C(17)-C(22)	77.72(13)
C(3)-C(11)-C(17)-C(22)	-103.29(13)
C(22)-C(17)-C(18)-C(19)	0.36(17)
C(11)-C(17)-C(18)-C(19)	176.27(11)
C(17)-C(18)-C(19)-C(20)	0.36(18)
C(18)-C(19)-C(20)-C(21)	-0.60(19)
C(19)-C(20)-C(21)-C(22)	0.13(19)
C(20)-C(21)-C(22)-C(17)	0.59(17)
C(18)-C(17)-C(22)-C(21)	-0.83(17)
C(11)-C(17)-C(22)-C(21)	-176.76(10)

Symmetry transformations used to generate equivalent atoms:

Table S8. Hydrogen bonds for mo_hd_fjy1_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4
C(10)-H(17)...O(3)#1	0.98	2.59	3.3120(15)	130.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+1/2

8. The fluorescence properties of compound 6.

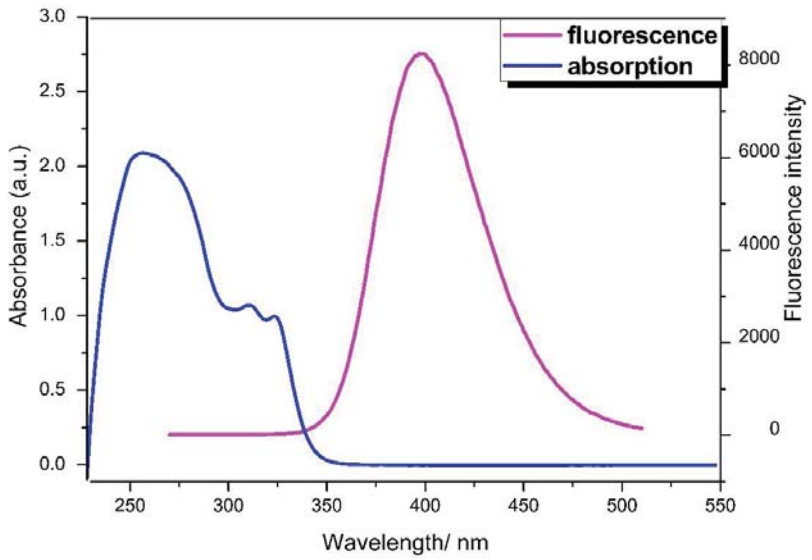
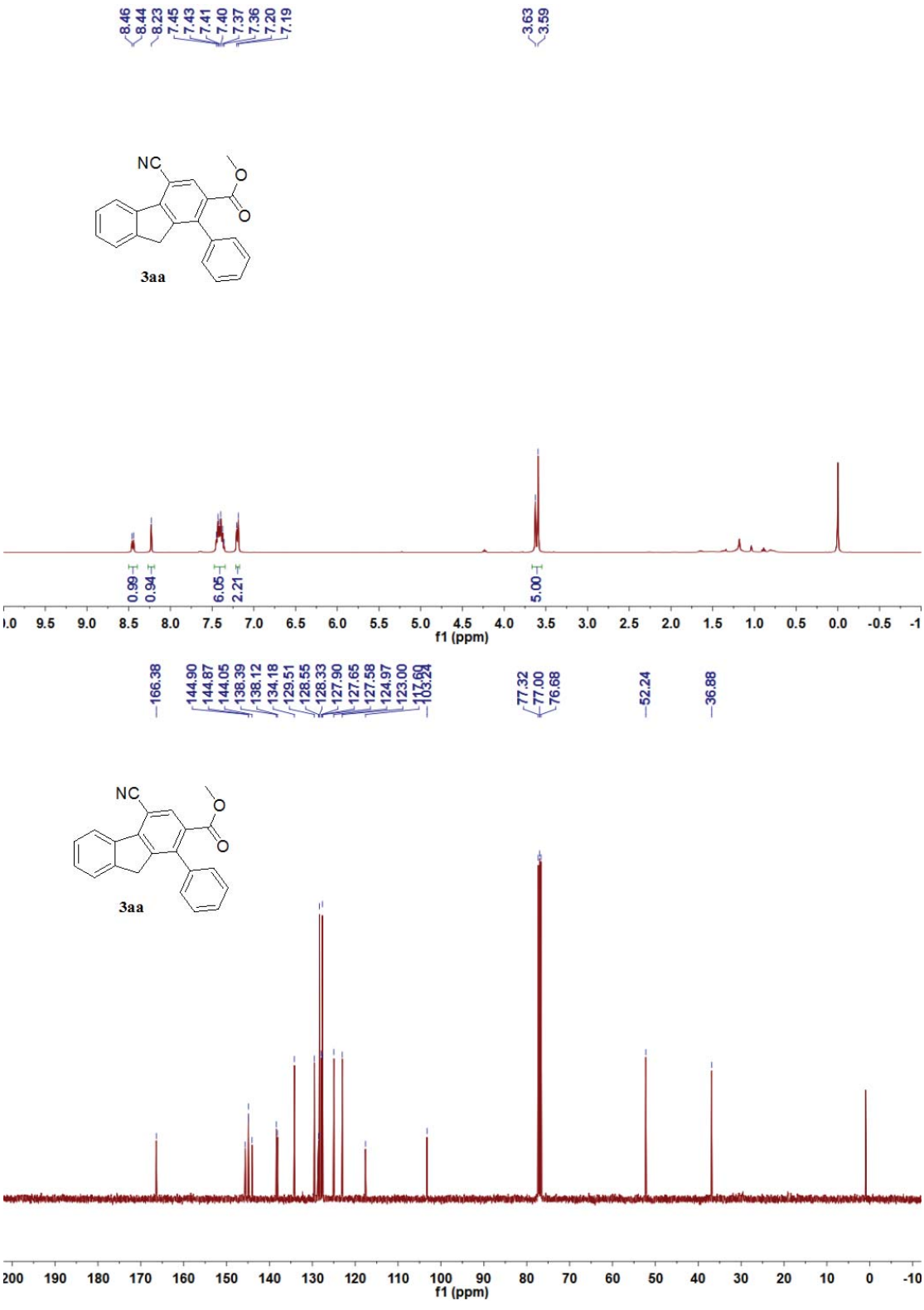
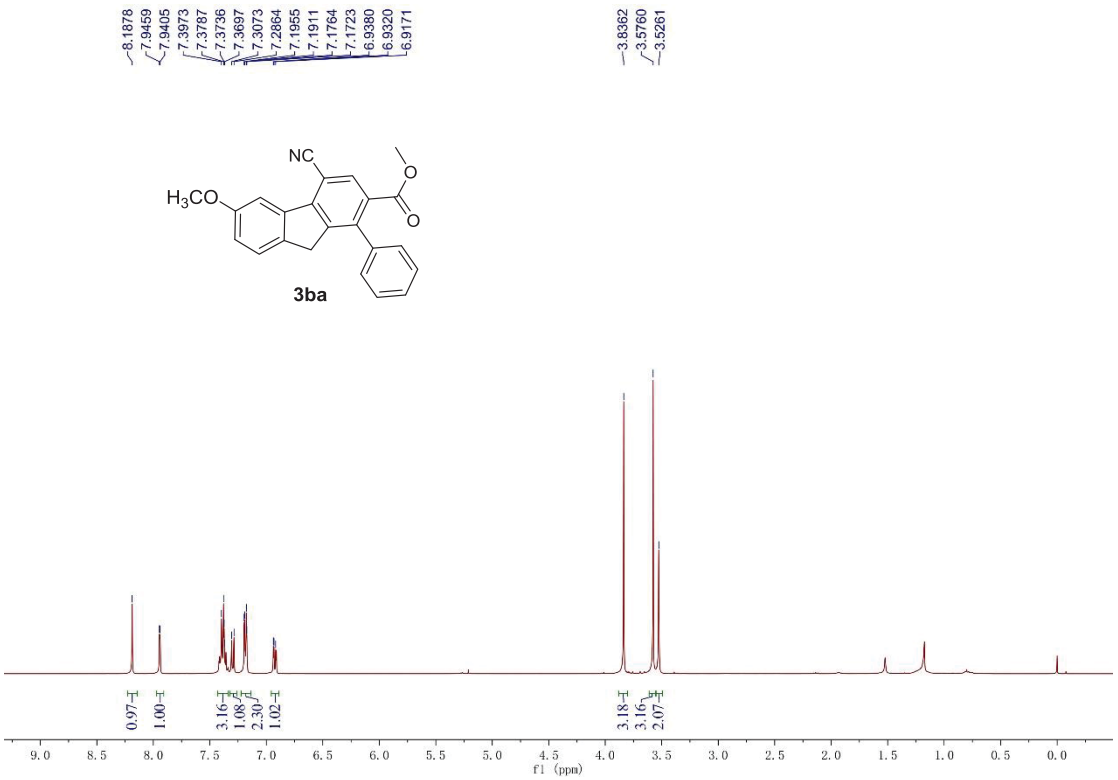


Figure S8. UV-vis absorption and fluorescence spectra of **6** ($5 * 10^{-5}$ mol L^{-1}) in THF

7. ^{1}H and ^{13}C NMR spectra for compounds **3aa-aq** and compounds **4aa-ap** and derivatives **5** and **6**.

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7.9459
7.9405
7.3973
7.3787
7.3736
7.3697
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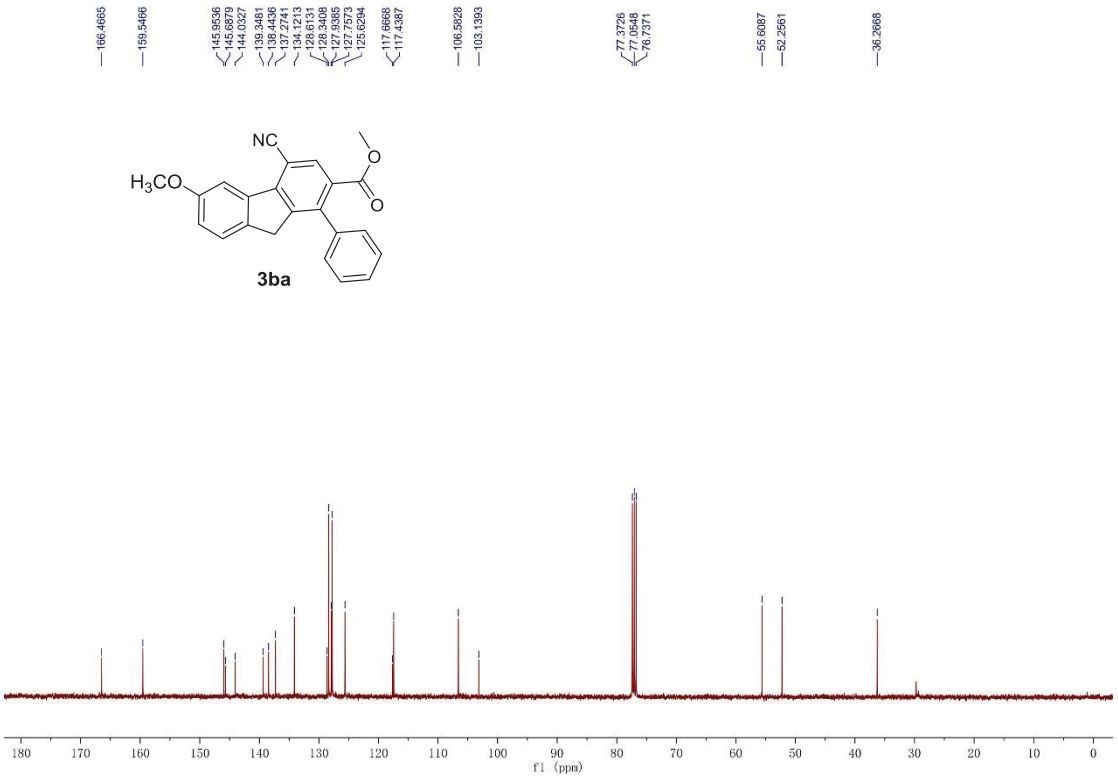
7.2864
7.1955
7.1911
7.1764
7.1723
6.9380
6.9320
6.9171
3.8362
3.5760
3.5261
NC
O
O
H3CO
3ba
0.97
1.00
3.16
1.08
2.30
1.02
3.18
3.16
2.07
f1 (ppm)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159.5466
145.9536
145.6879
144.0327
139.3481
138.4436
137.2741
134.1213
128.6131
128.3408
127.9385
127.7573
125.6294
117.6668
117.4387
106.5628
103.1393
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77.0548
76.7371
55.6087
52.2561
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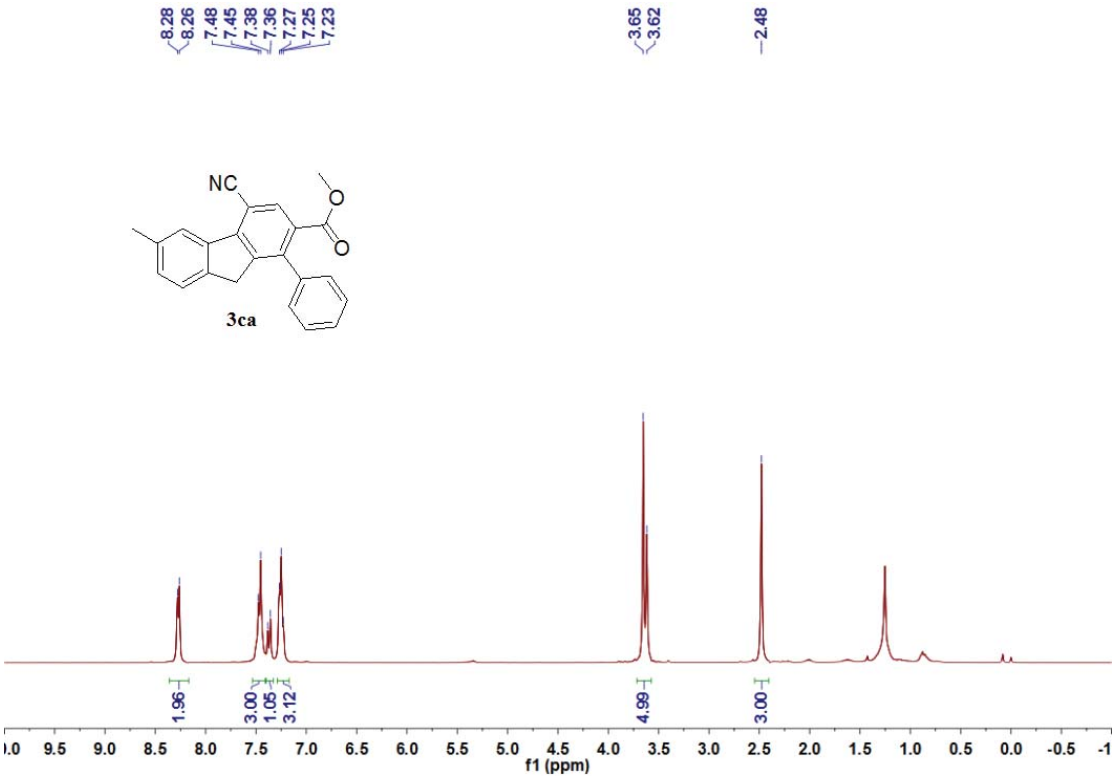
NC
O
O
H3CO
3ba
f1 (ppm)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8.26
7.48
7.45
7.38
7.36
7.27
7.25
7.23
3.65
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2.48
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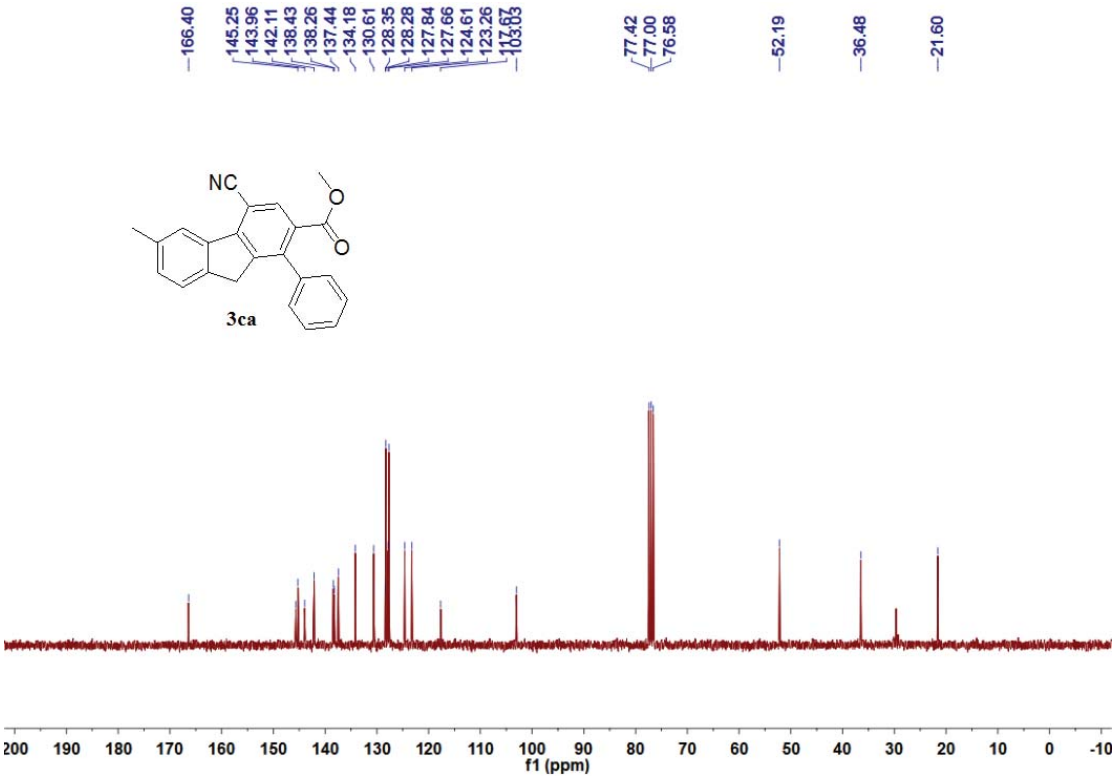
O
O
1.96
3.00
1.05
3.12
4.99
3.00
f1 (ppm)

3ca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145.25
143.96
142.11
138.43
138.26
137.44
134.18
130.61
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128.28
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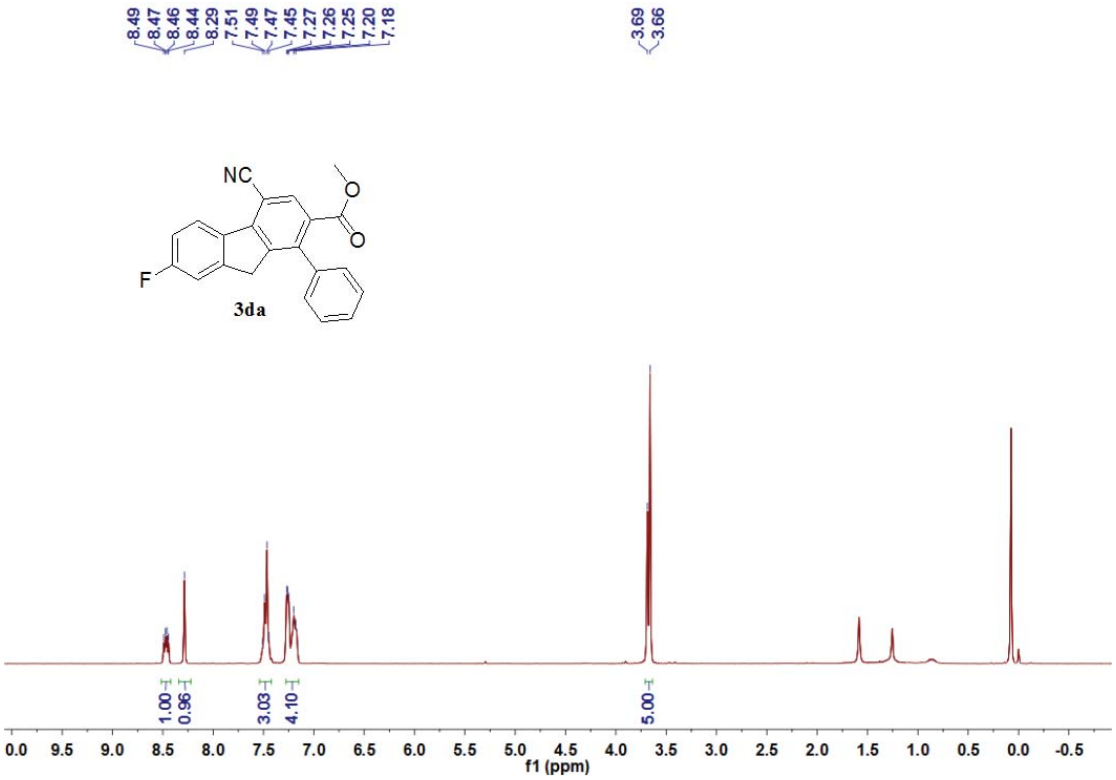
127.66
124.61
123.26
77.42
77.00
76.58
52.19
36.48
21.60
NC
O
O
f1 (ppm)

3ca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8.46
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7.49
7.47
7.45
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7.26
7.25
7.20
7.18
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O
F
3da
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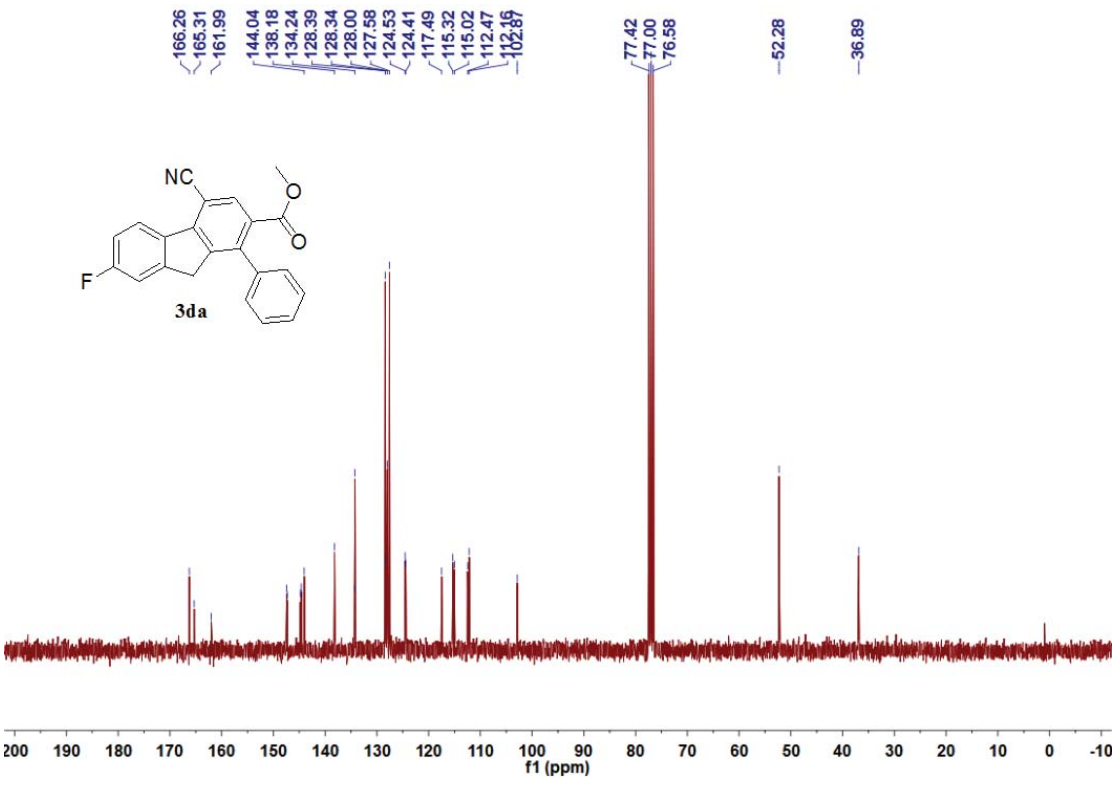
3.03
4.10
5.00
f1 (ppm)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138.18
134.24
128.39
128.34
128.00
127.58
124.53
124.41
117.49
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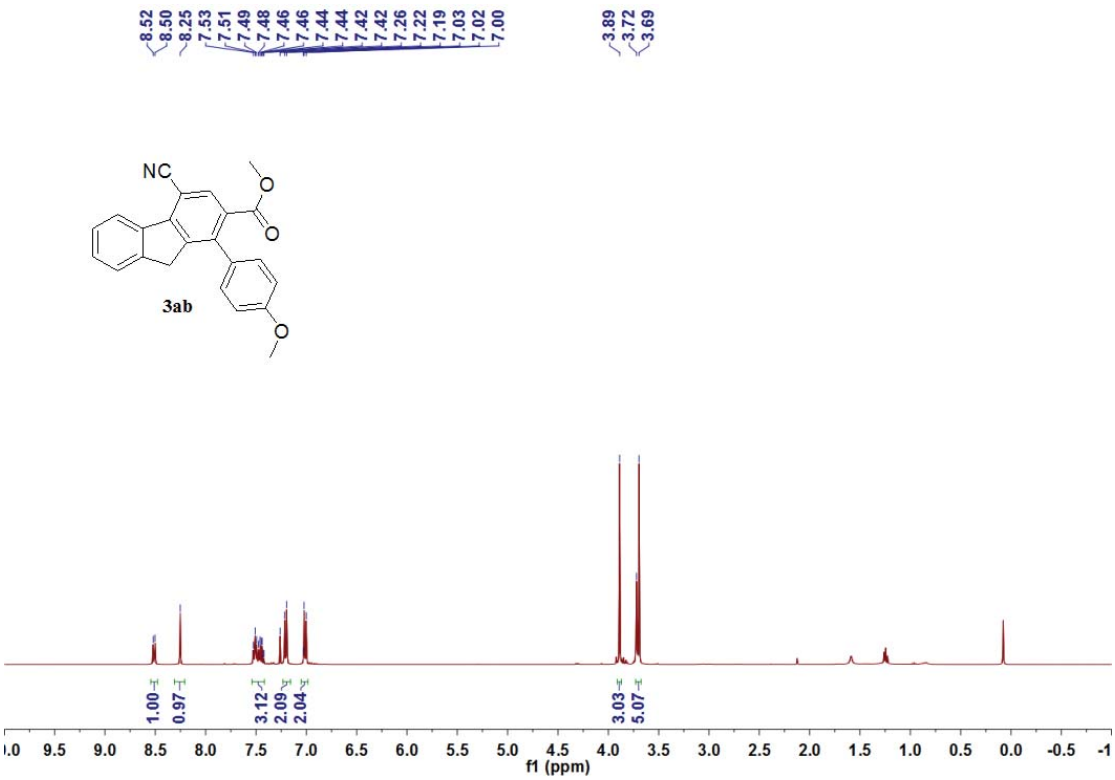
115.02
112.47
77.42
77.00
76.58
52.28
36.89
NC
O
O
F
3da
f1 (ppm)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7.44
7.42
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7.26
7.22
7.19
7.03
7.02
7.00
3.89
3.72
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O
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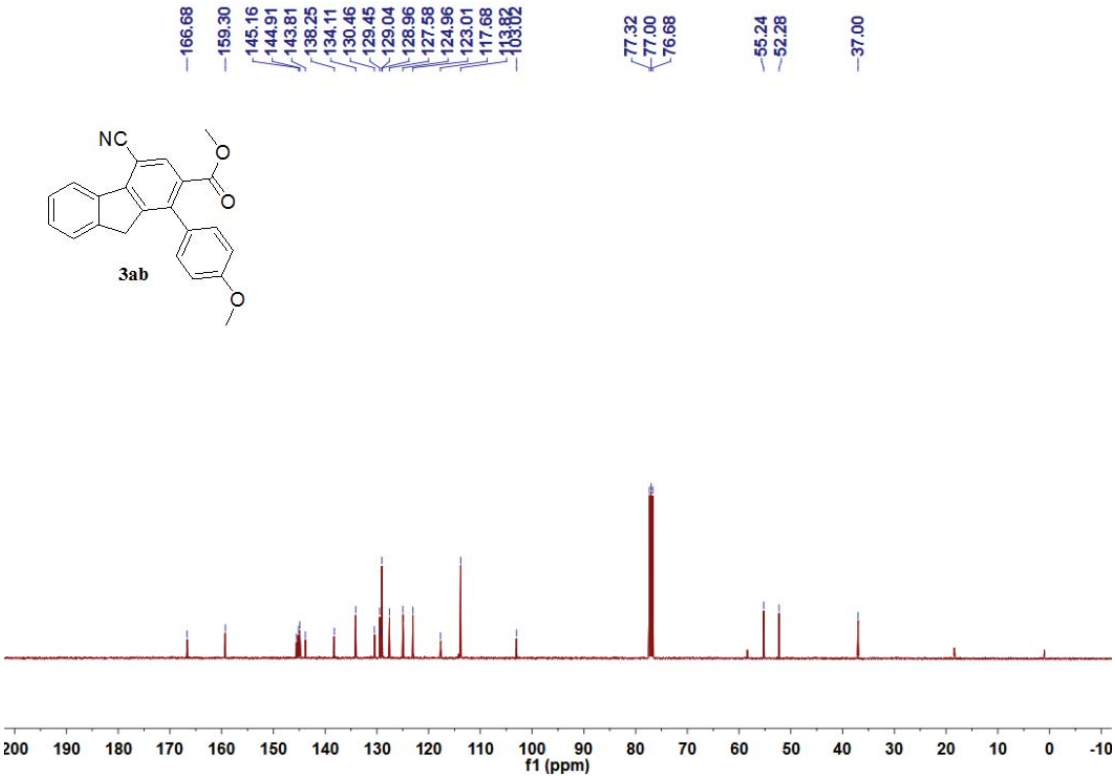
O
3ab
1.00
0.97
3.12
2.09
2.04
3.03
5.07
f1 (ppm)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138.25
134.11
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127.58
124.96
123.01
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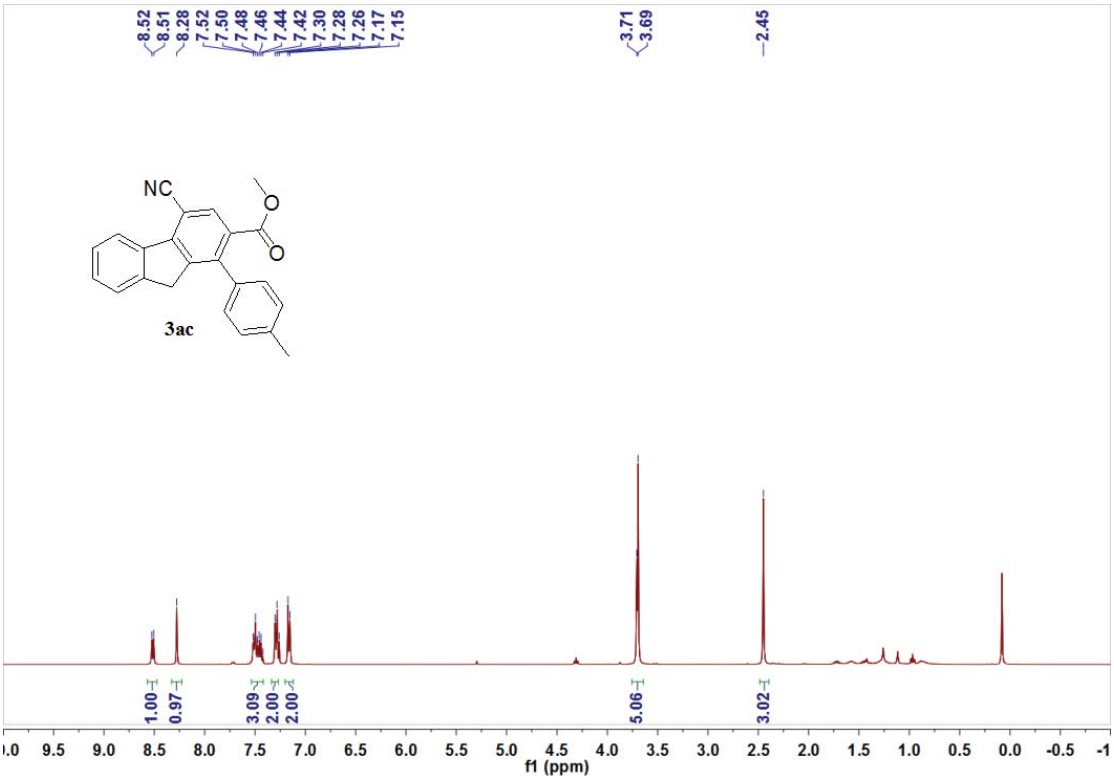
77.32
77.00
76.68
55.24
52.28
37.00
NC
O
O
O
3ab
f1 (ppm)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7.28
7.26
7.17
7.15
3.71
3.69
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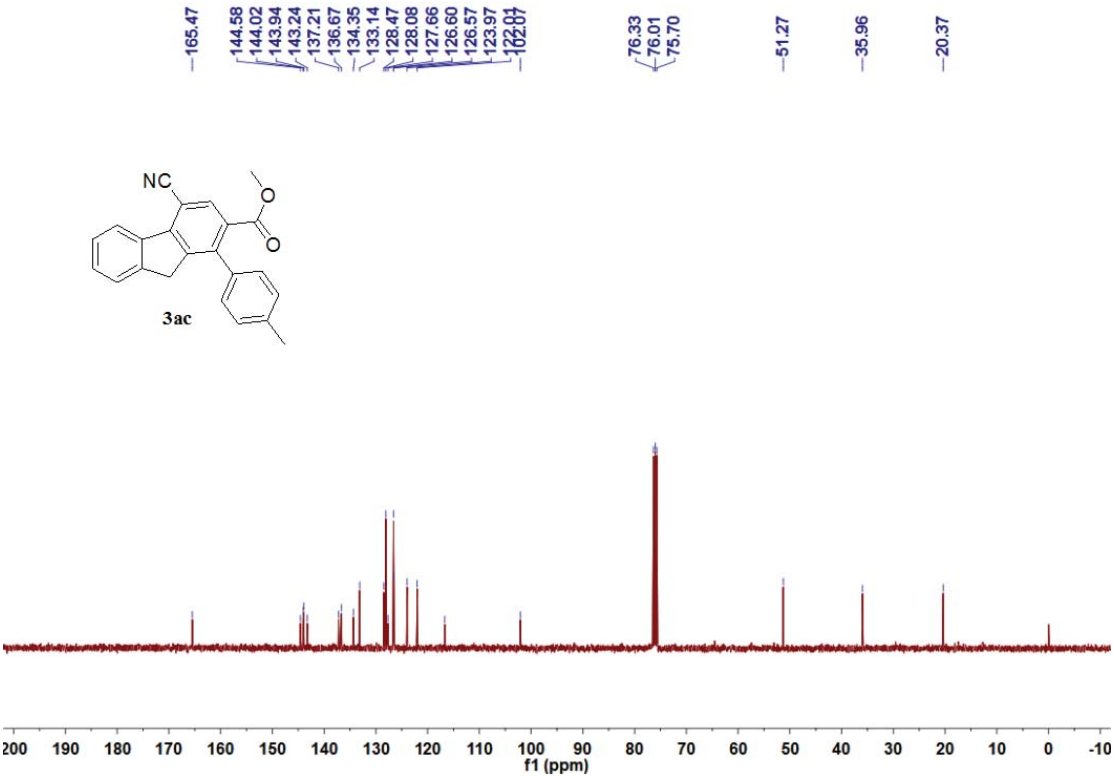
2.00
5.06
3.02
f1 (ppm)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134.35
133.14
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128.08
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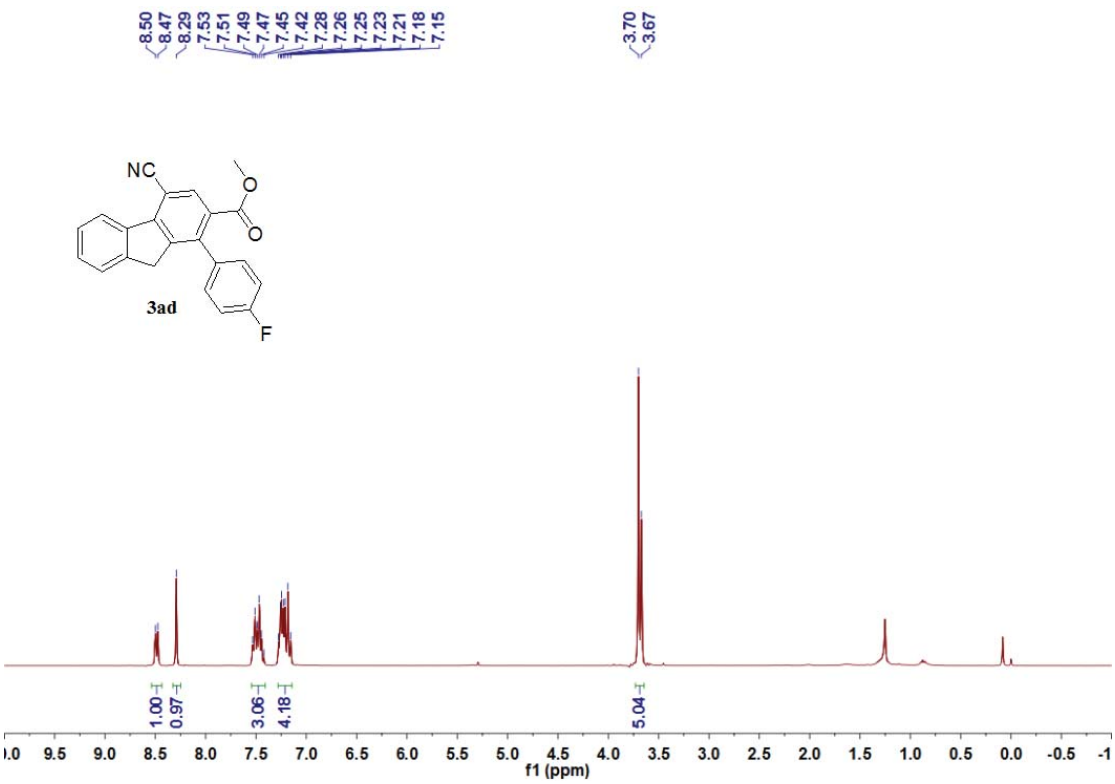
126.60
126.57
123.97
76.33
76.01
75.70
51.27
35.96
20.37
NC
O
O
3ac
f1 (ppm)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8.29
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7.49
7.47
7.45
7.42
7.28
7.26
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7.23
7.21
7.18
7.15
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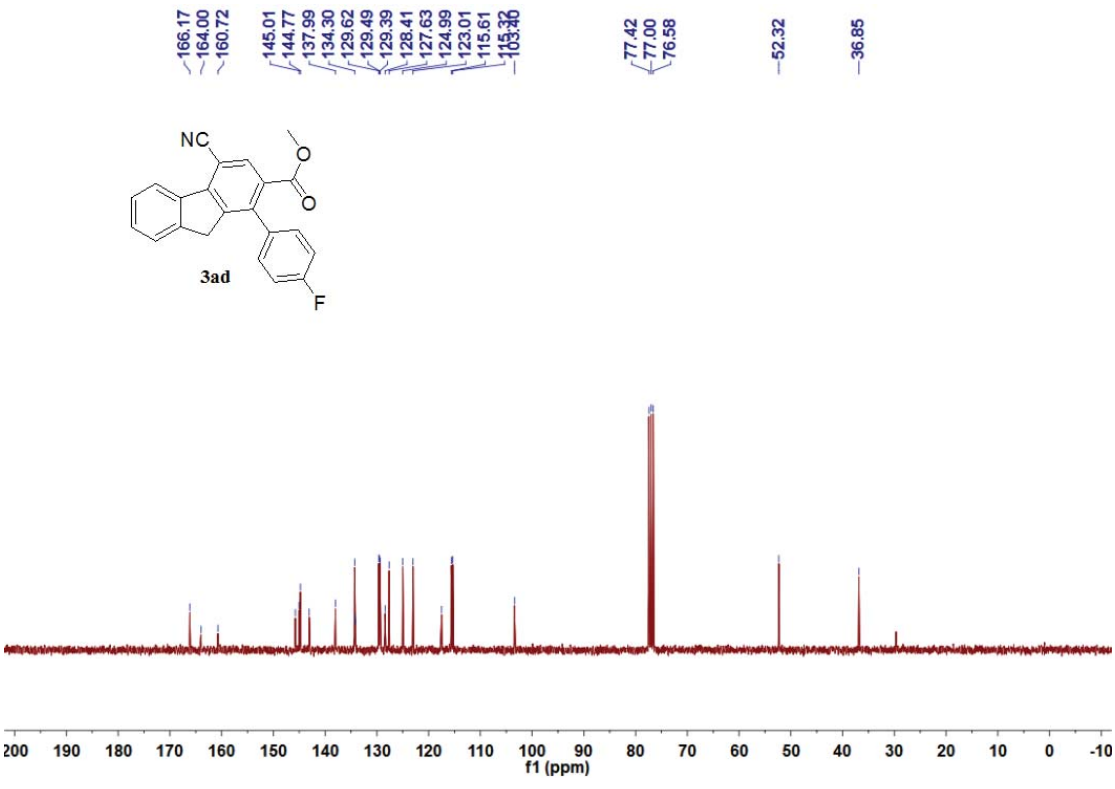
3ad
1.00
0.97
3.06
4.18
5.04
f1 (ppm)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129.39
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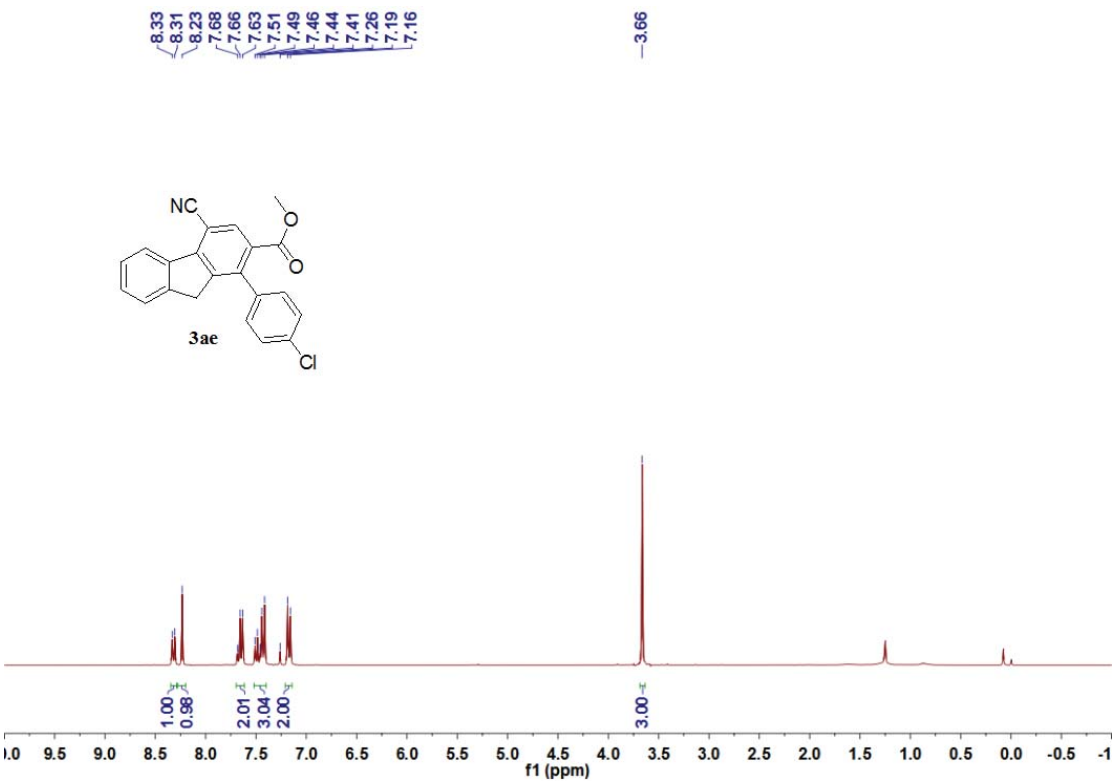
77.00
76.58
52.32
36.85
NC
O
O
F
3ad
f1 (ppm)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7.49
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7.41
7.26
7.19
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O
Cl
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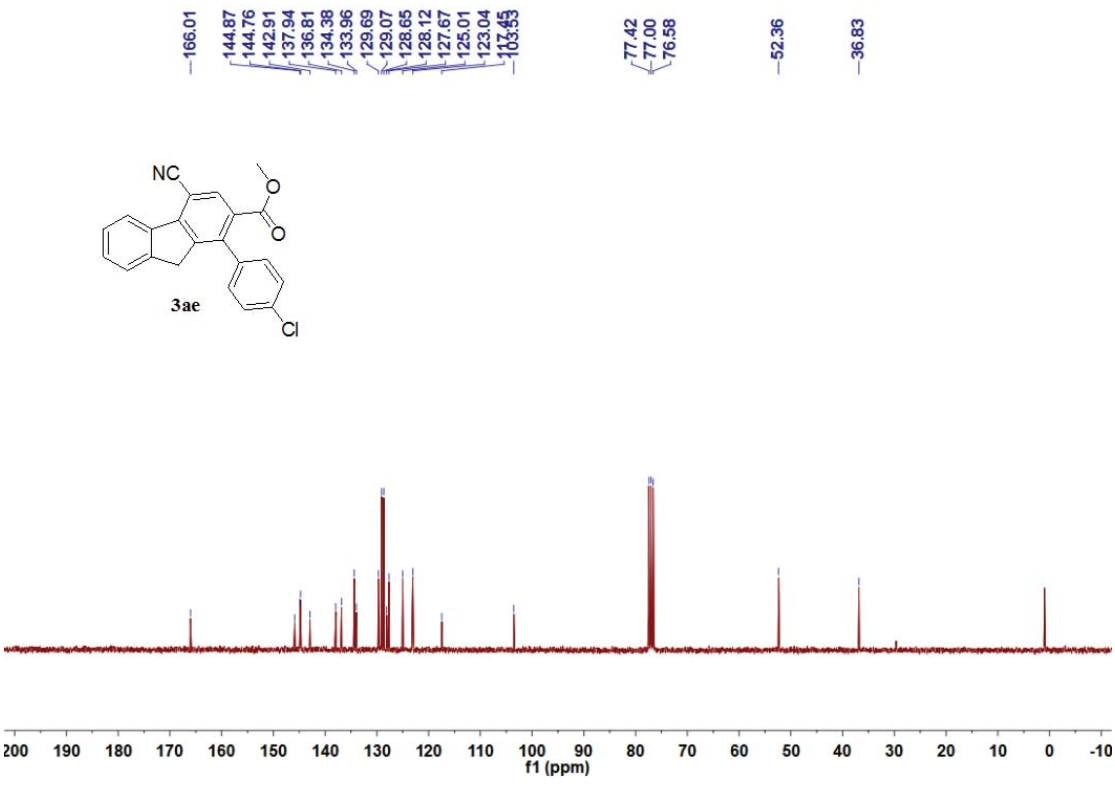
2.01
3.04
2.00
3.00
f1 (ppm)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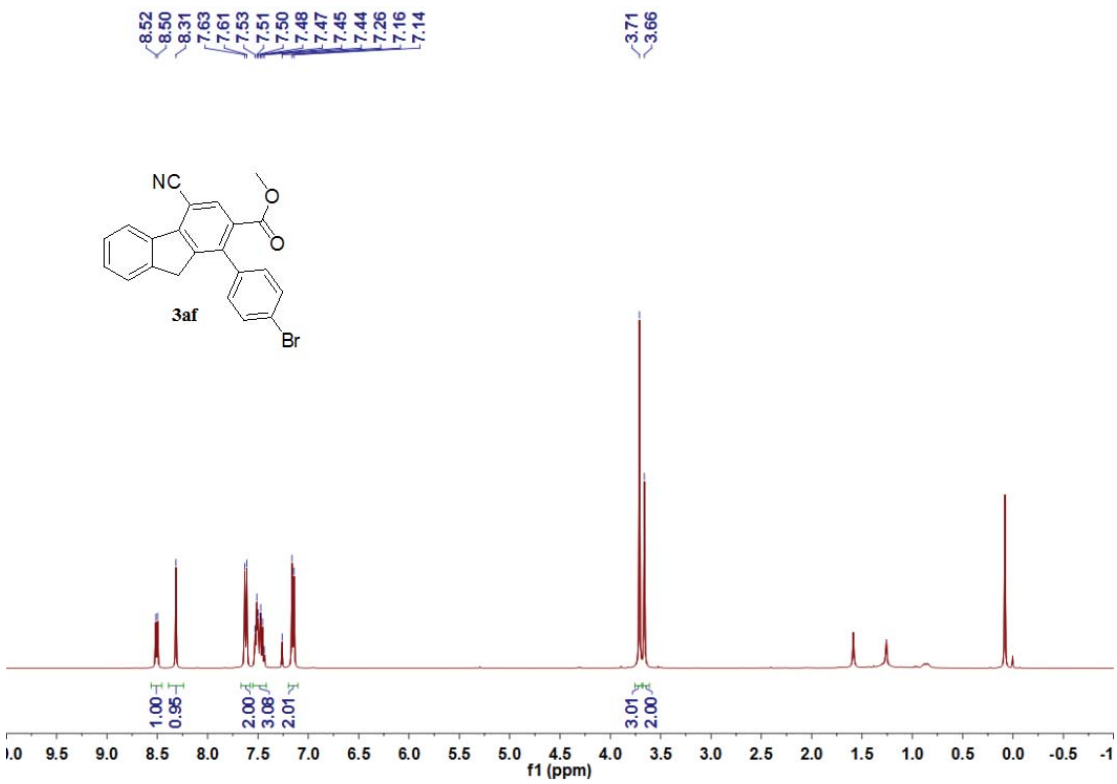
O
Cl
3ae
f1 (ppm)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7.50
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7.47
7.45
7.44
7.26
7.16
7.14
3.71
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Br
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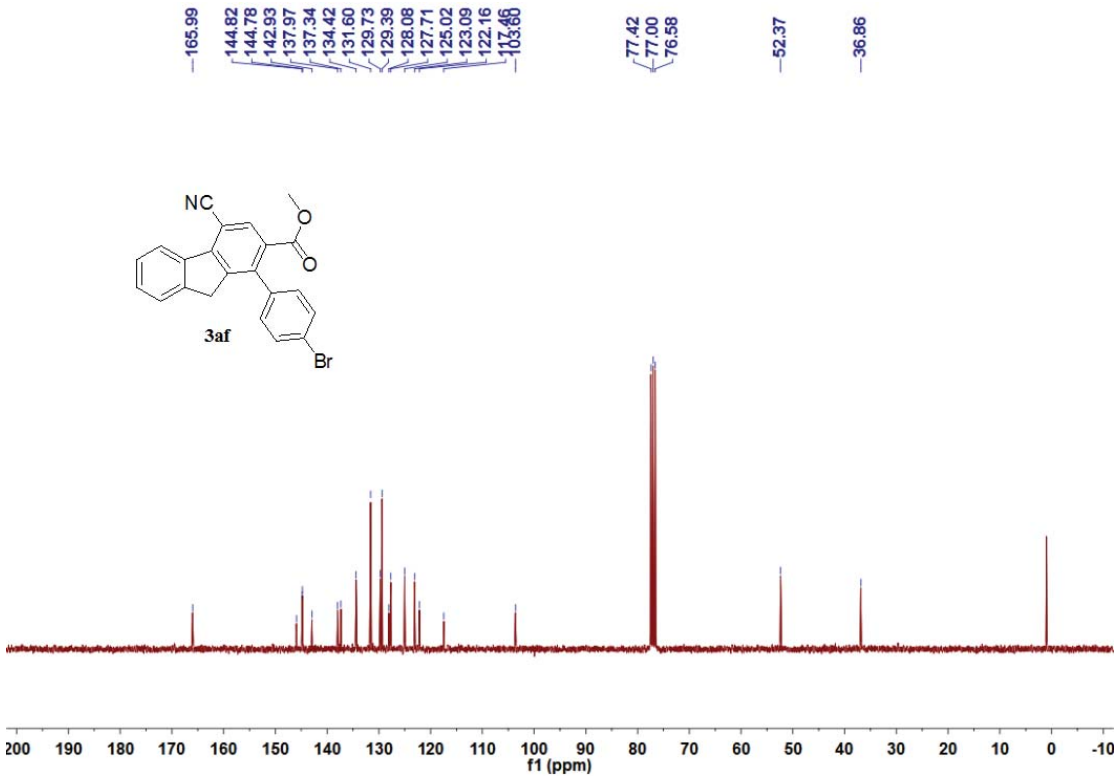
3.08
2.01
3.01
2.00
f1 (ppm)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77.00
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36.86
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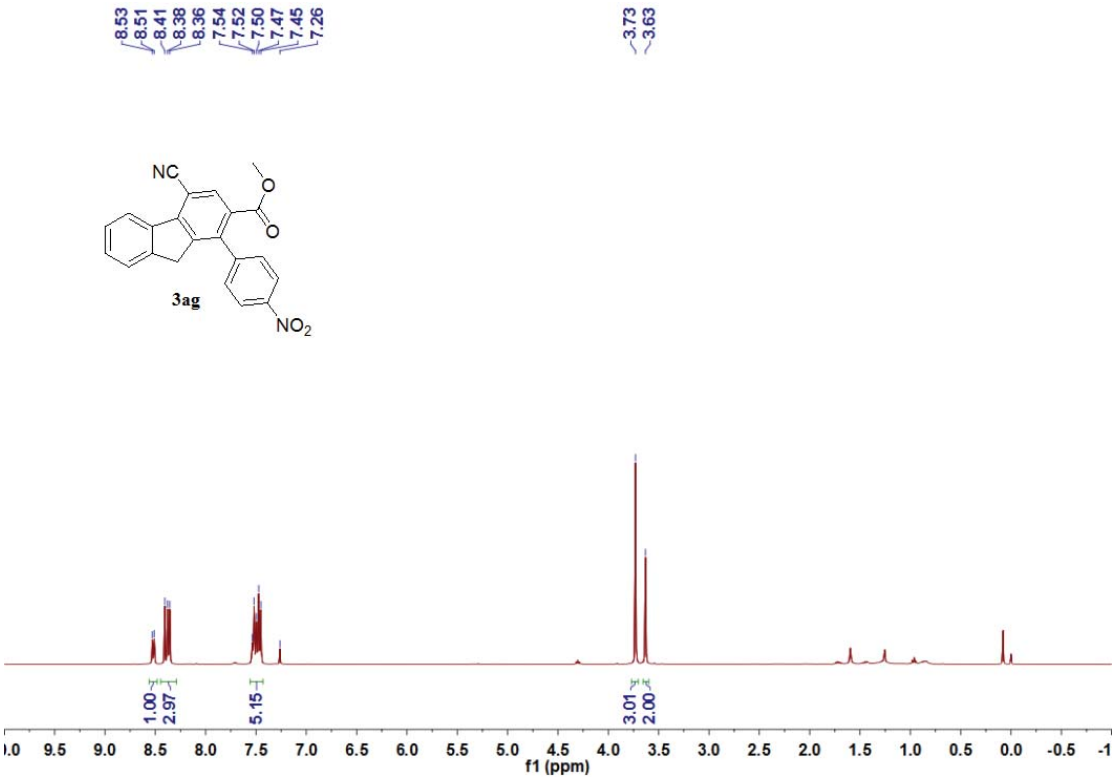
3af
Br
f1 (ppm)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7.47
7.45
7.26
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O
O
3ag
NO2
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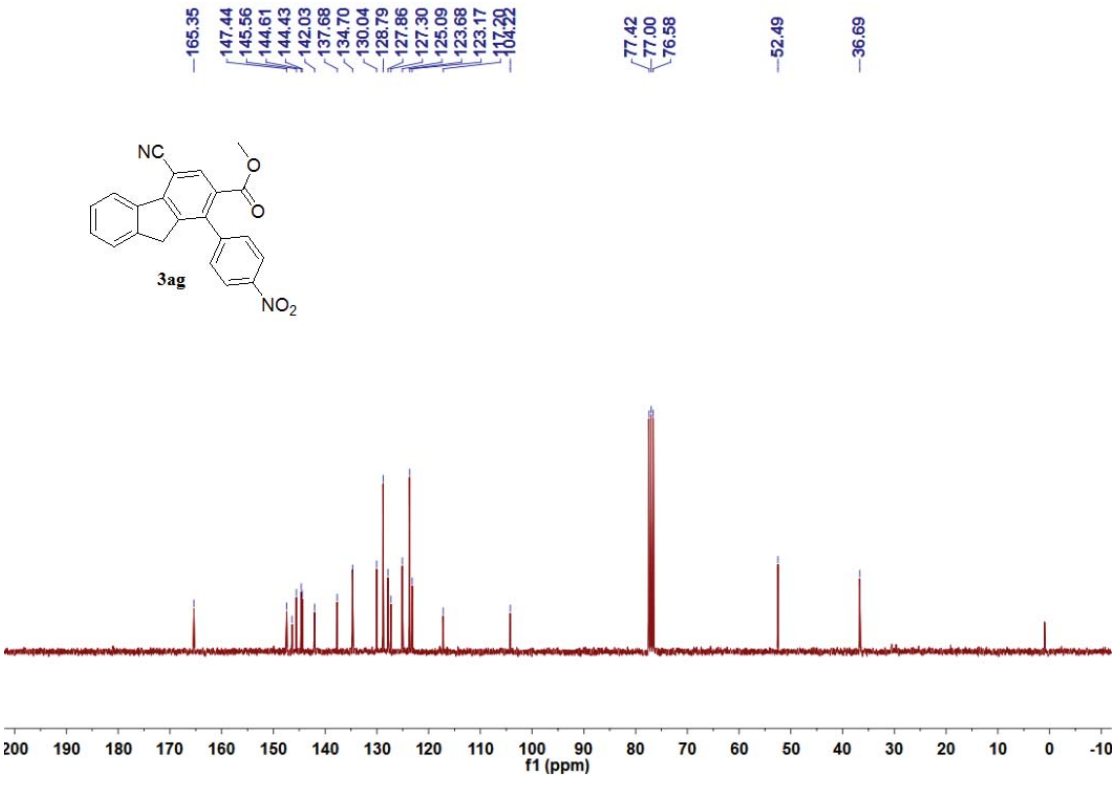
5.15
3.01
2.00
f1 (ppm)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142.03
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134.70
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128.79
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127.30
125.09
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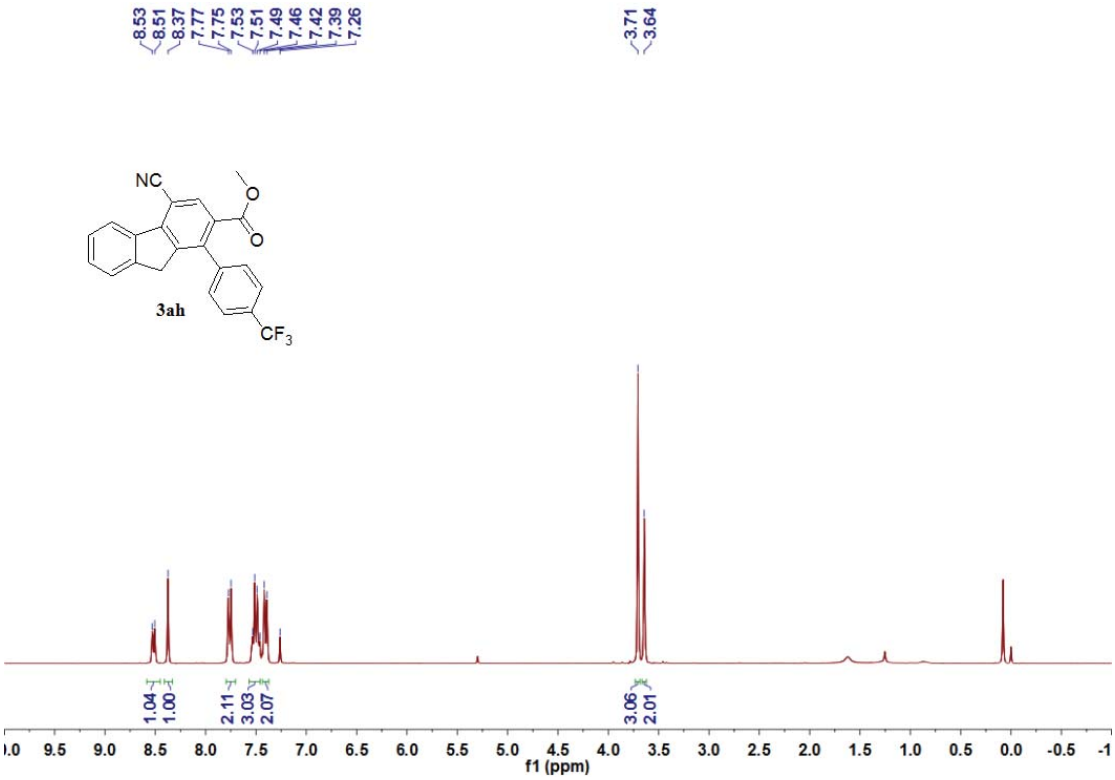
123.17
77.42
77.00
76.58
52.49
36.69
NC
O
O
3ag
NO2
f1 (ppm)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7.51
7.49
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7.42
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3.64
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O
O
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CF3
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1.00
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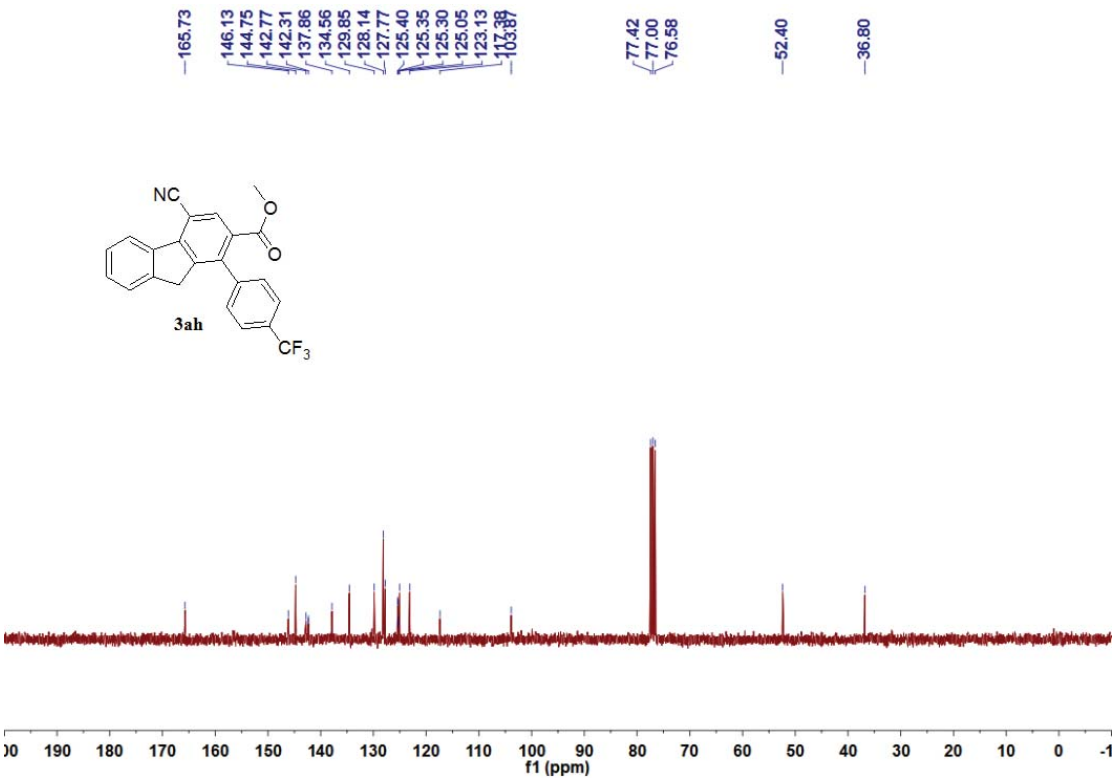
3.03
2.07
3.06
2.01
f1 (ppm)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128.14
127.77
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O
O
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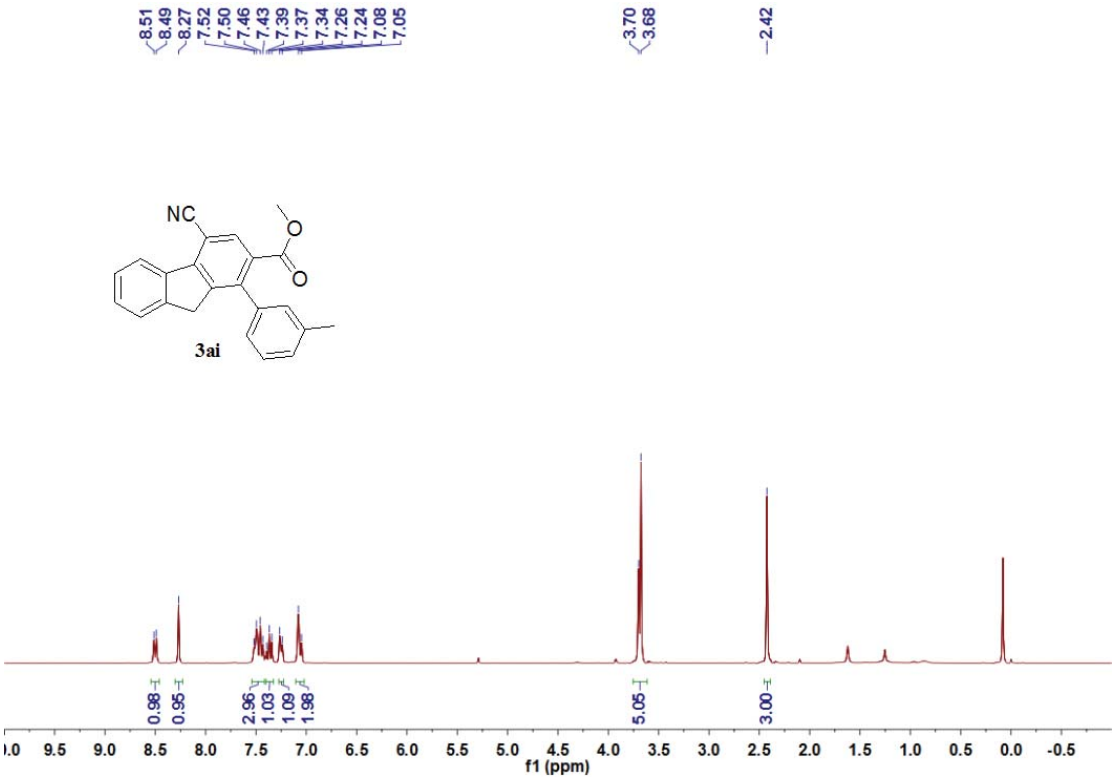
CF3
f1 (ppm)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7.08
7.05
3.70
3.68
2.42
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0.95
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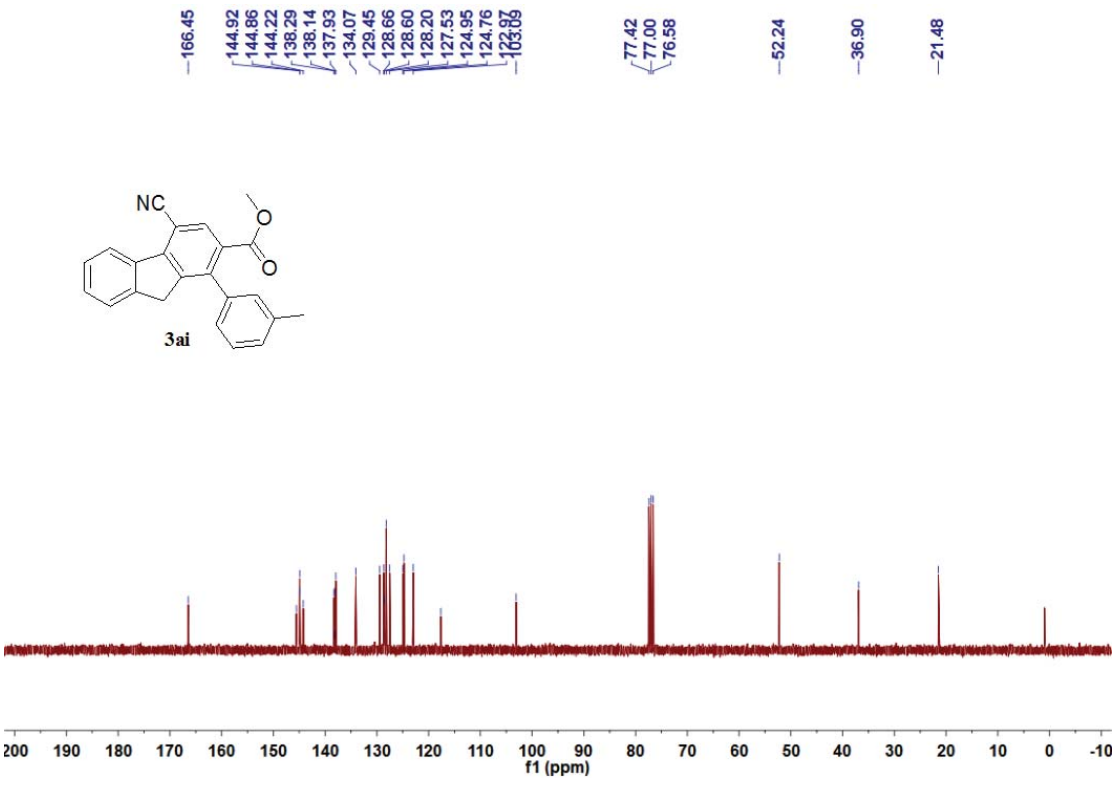
1.03
1.09
1.98
5.05
3.00
f1 (ppm)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127.53
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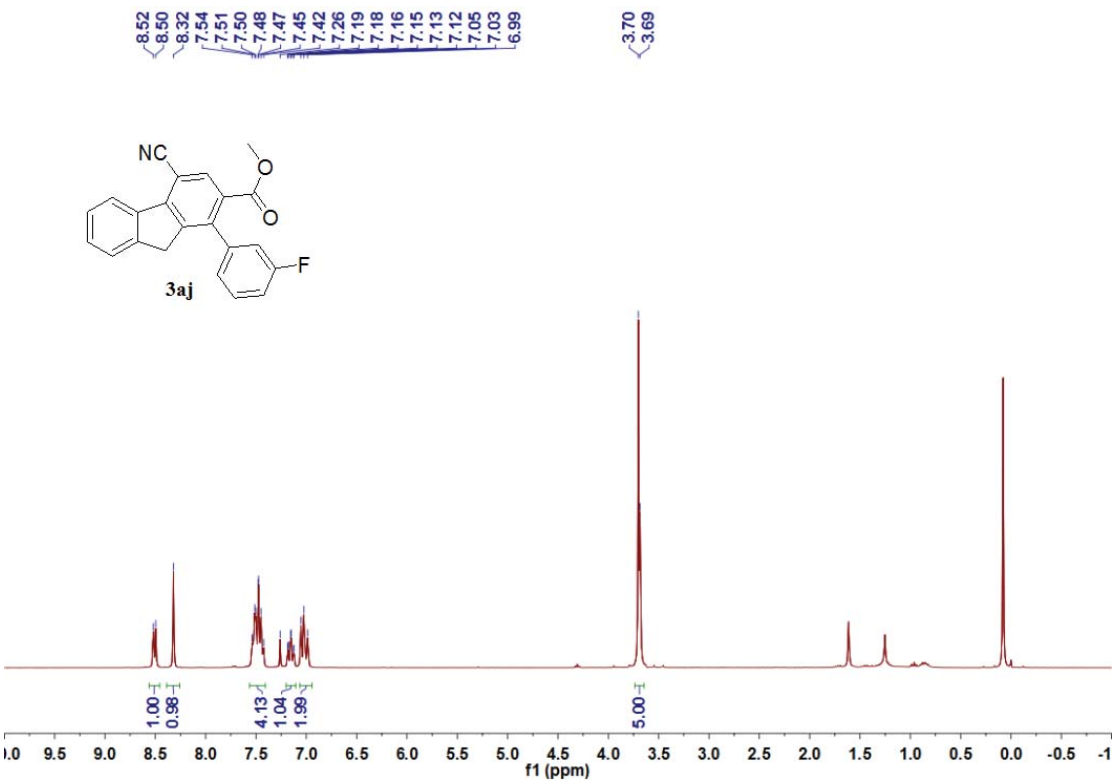
3ai
f1 (ppm)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8.32
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7.51
7.50
7.48
7.47
7.45
7.42
7.26
7.19
7.18
7.16
7.15
7.13
7.12
7.05
7.03
6.99
3.70
3.69
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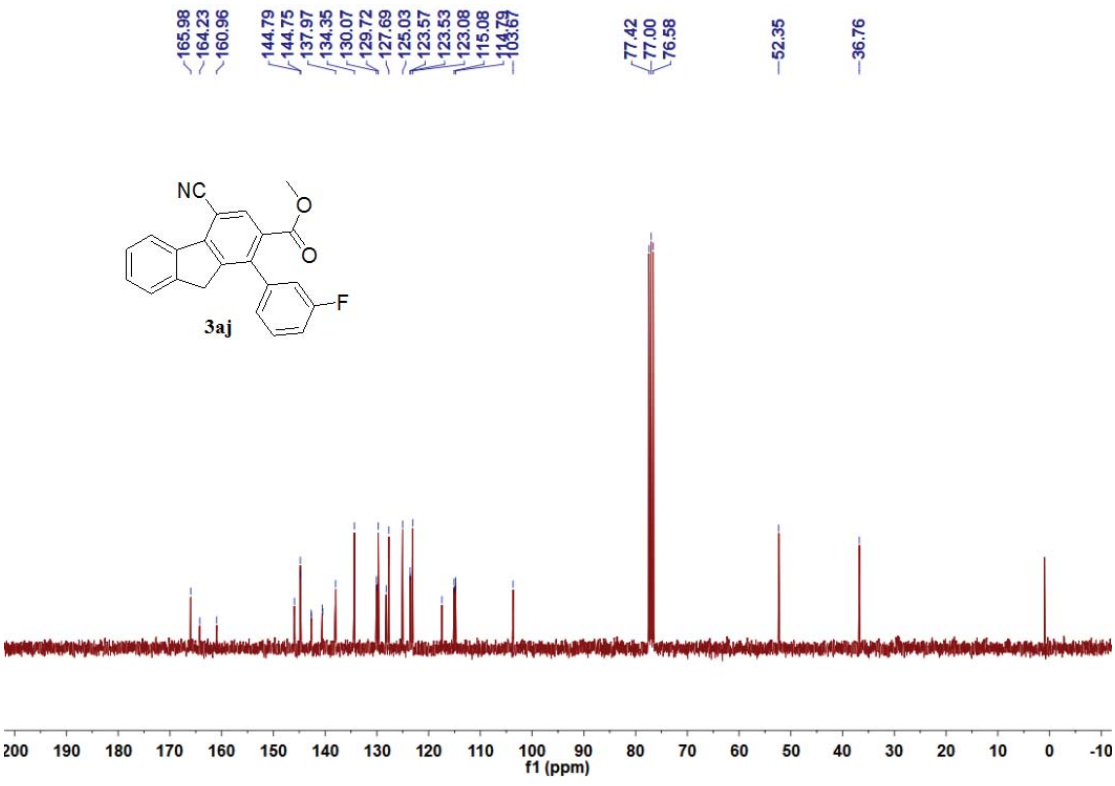
O
O
F
3aj
1.00
0.98
4.13
1.04
1.99
5.00
f1 (ppm)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164.23
160.96
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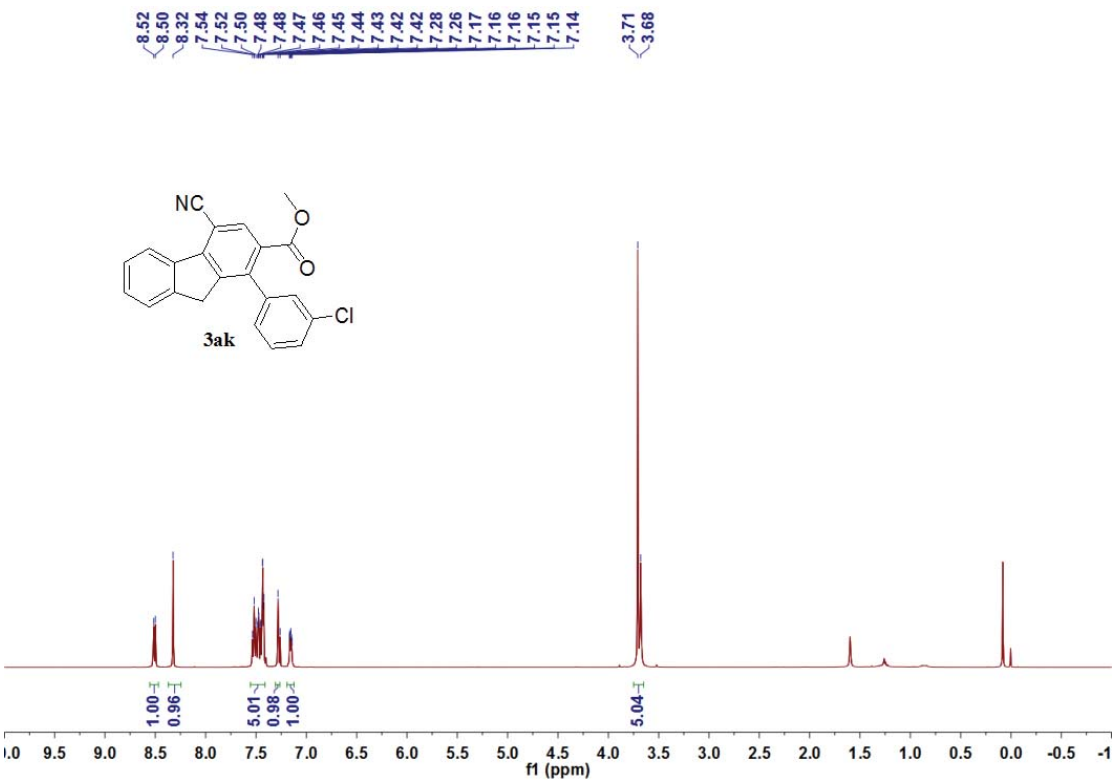
144.75
137.97
134.35
130.07
129.72
127.69
125.03
123.57
123.53
123.08
115.08
77.42
77.00
76.58
52.35
36.76
NC
O
O
F
3aj
f1 (ppm)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8.32
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7.50
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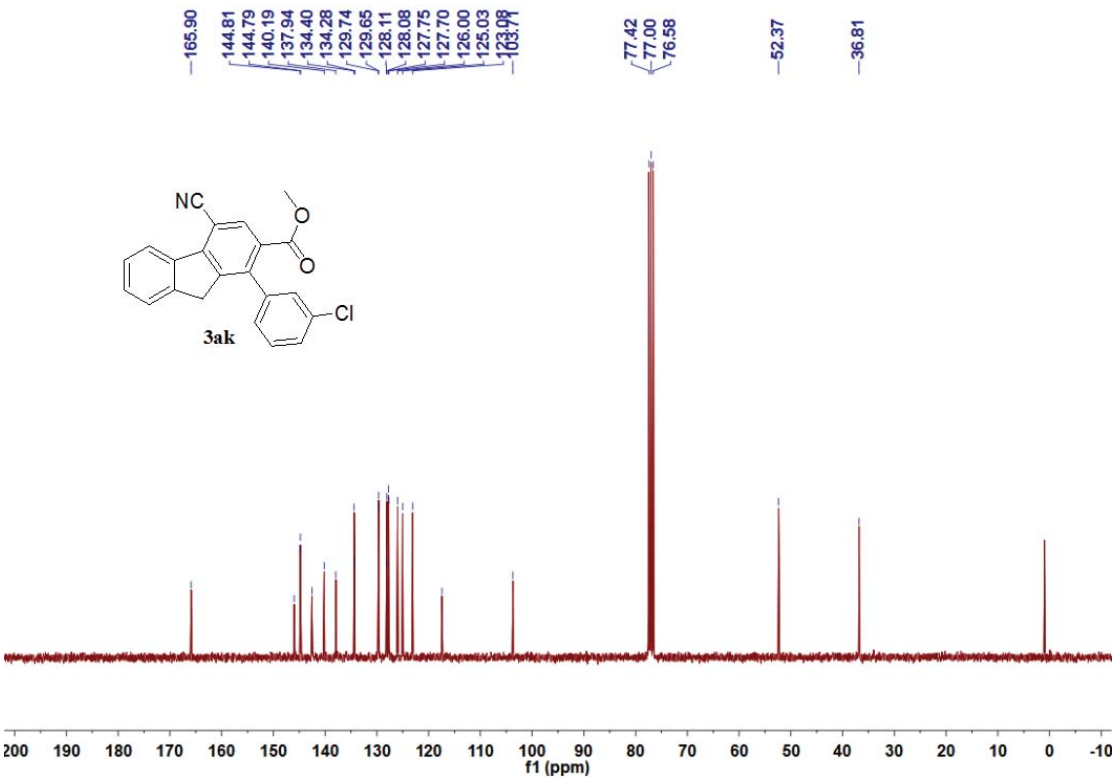
7.48
7.47
7.46
7.45
7.44
7.43
7.42
7.42
7.28
7.26
7.17
7.16
7.16
7.15
7.15
7.14
3.71
3.68
NC
O
O
Cl
3ak
1.00
0.96
5.01
0.98
1.00
5.04
f1 (ppm)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129.74
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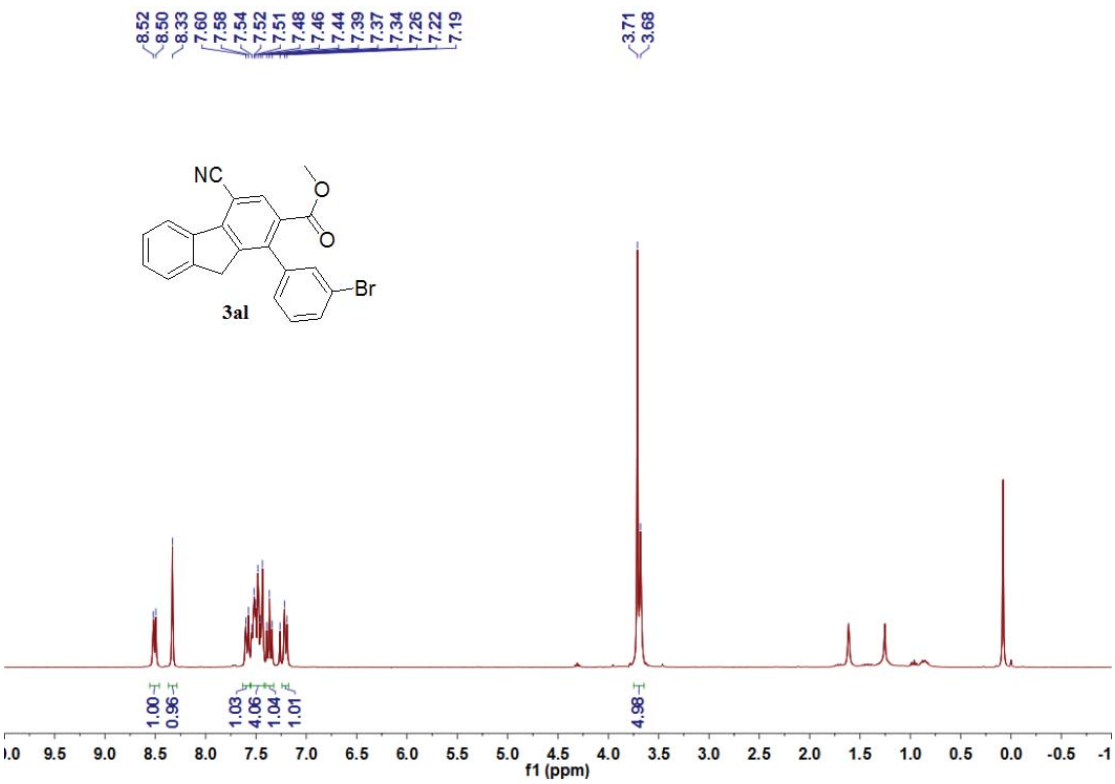
128.11
128.08
127.75
127.70
126.00
125.03
77.42
77.00
76.58
52.37
36.81
NC
O
O
Cl
3ak
f1 (ppm)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8.50
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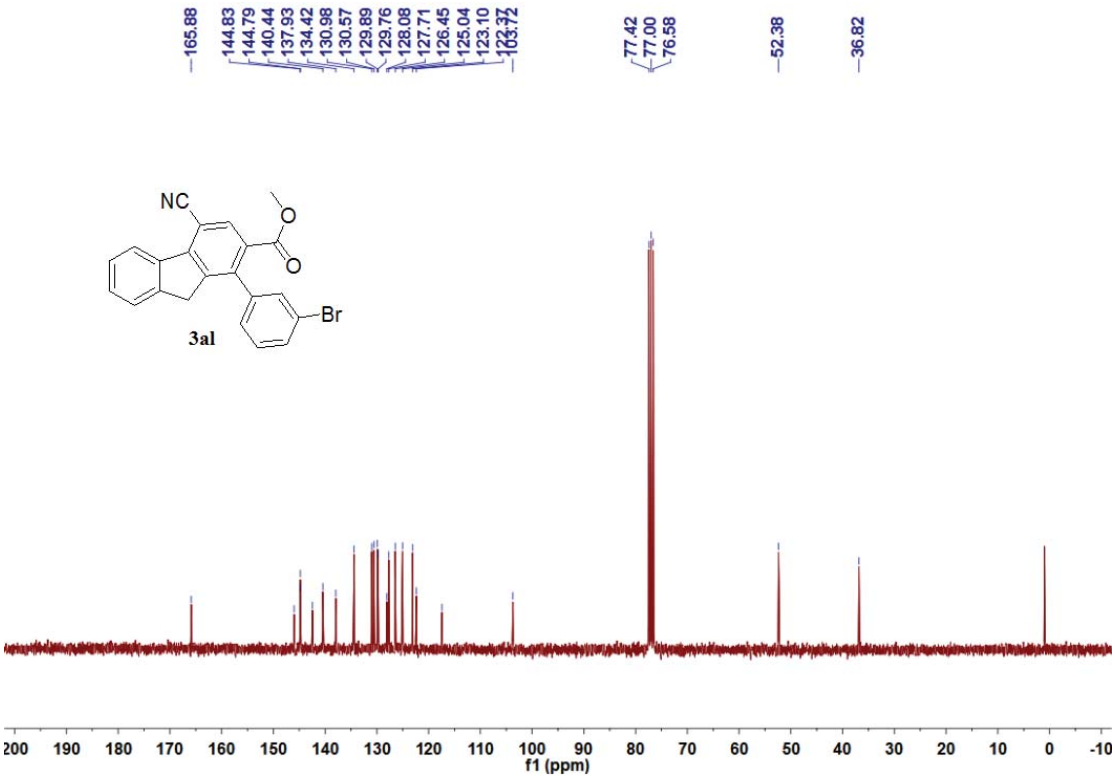
7.54
7.52
7.51
7.48
7.46
7.44
7.39
7.37
7.34
7.26
7.22
7.19
3.71
3.68
NC
O
O
Br
3al
1.00
0.96
1.03
4.06
1.04
1.01
4.98
f1 (ppm)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144.79
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134.42
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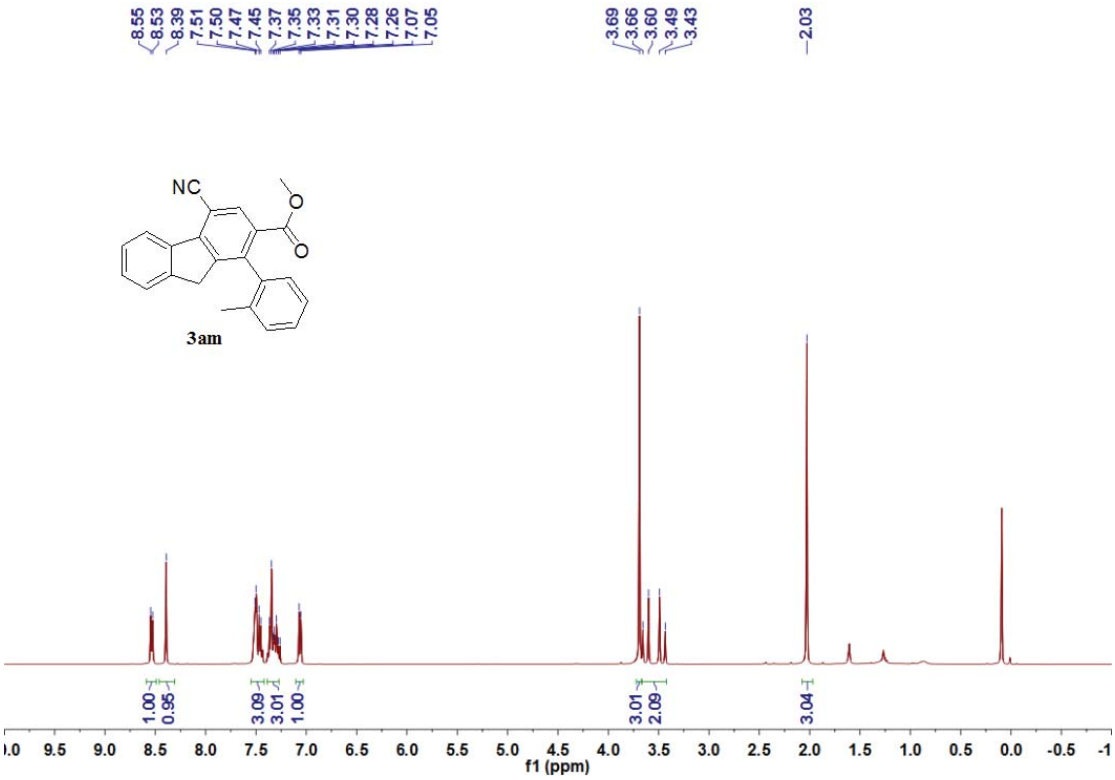
130.57
129.89
129.76
128.08
127.71
126.45
125.04
123.10
77.42
77.00
76.58
52.38
36.82
NC
O
O
Br
3al
f1 (ppm)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8.53
8.39
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7.47
7.45
7.37
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7.33
7.31
7.30
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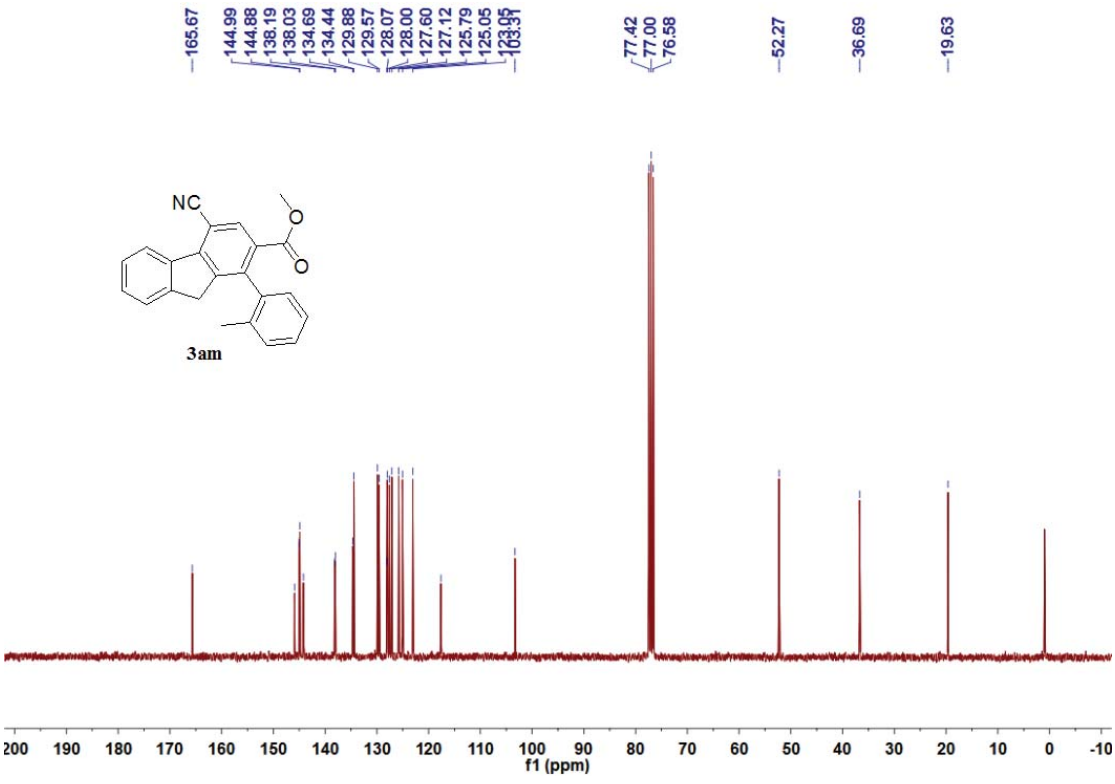
7.26
7.07
7.05
3.69
3.66
3.60
3.49
3.43
2.03
NC
O
O
3am
1.00
0.96
3.09
3.01
1.00
3.01
2.09
3.04
f1 (ppm)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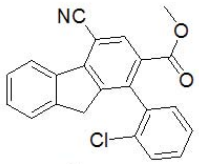
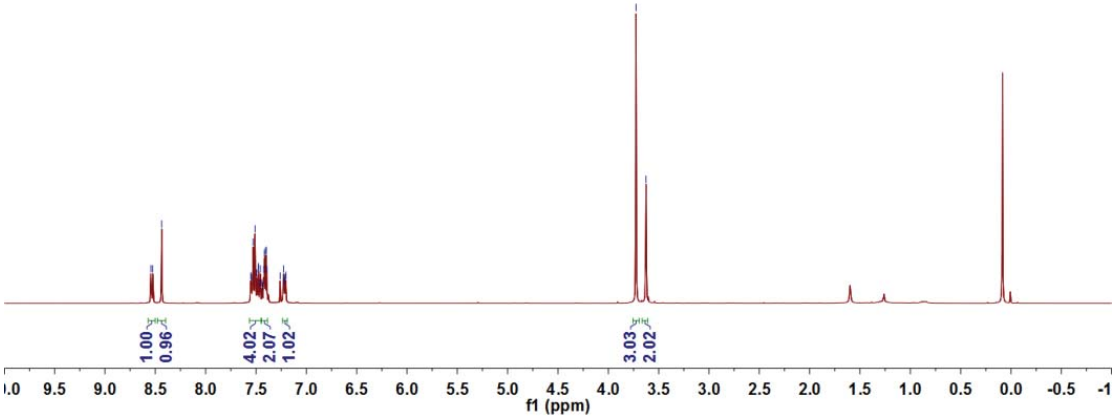
138.03
134.69
134.44
129.88
129.57
128.07
128.00
127.60
127.12
125.79
125.05
123.05
103.31
77.42
77.00
76.58
52.27
36.69
19.63
NC
O
O
3am
f1 (ppm)

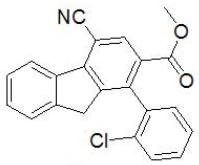

8.54
8.53
8.44
7.55
7.55
7.53
7.51
7.49
7.48
7.47
7.46
7.46
7.44
7.43
7.42
7.42
7.41
7.40
7.39
7.26
7.23
7.22
7.22
7.21
7.20
3.72
3.63


NC
O
O
Cl

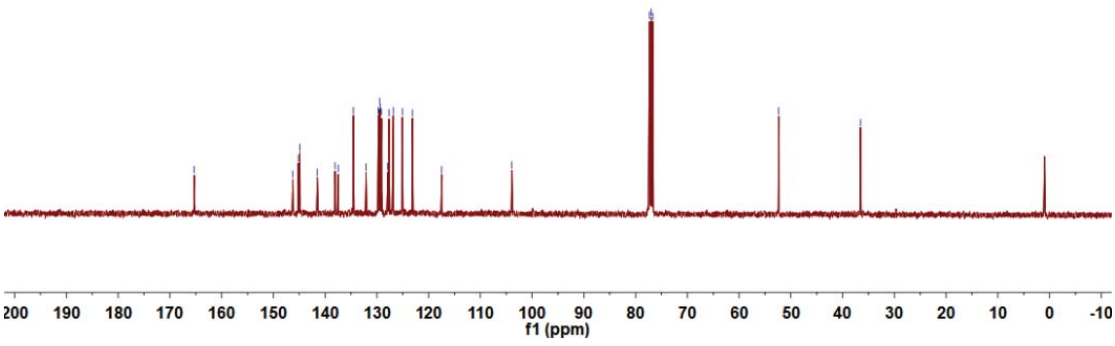
3an


1.00
0.96
4.02
2.07
1.02
3.03
2.02
f1 (ppm)


165.30
145.16
144.88
138.09
137.46
134.55
132.09
129.72
129.45
129.36
129.09
127.91
127.66
126.83
125.07
77.32
77.00
76.68
52.35
36.53


NC
O
O
Cl

3an


f1 (ppm)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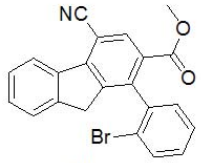
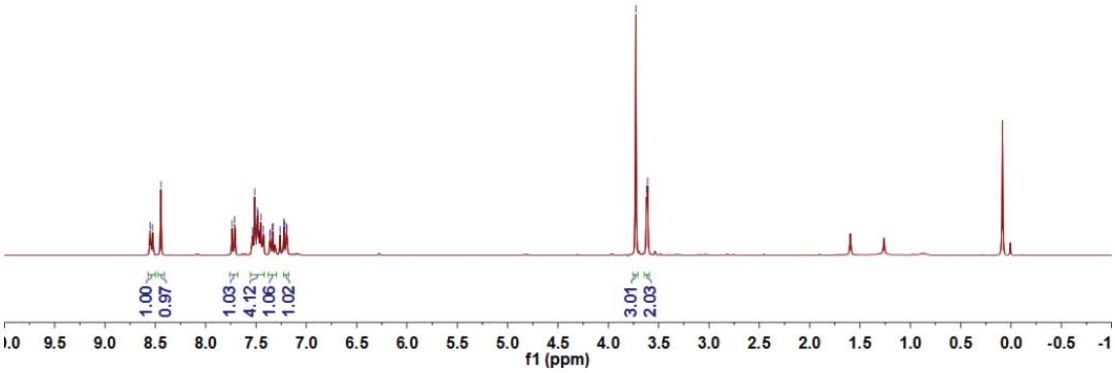
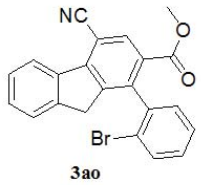
8.53
8.44
7.74
7.71
7.53
7.51
7.49
7.48
7.47
7.45
7.43
7.36
7.36
7.34
7.33
7.26
7.22
7.22
7.20
7.19
3.73
3.62
3.61


NC
O
O
Br

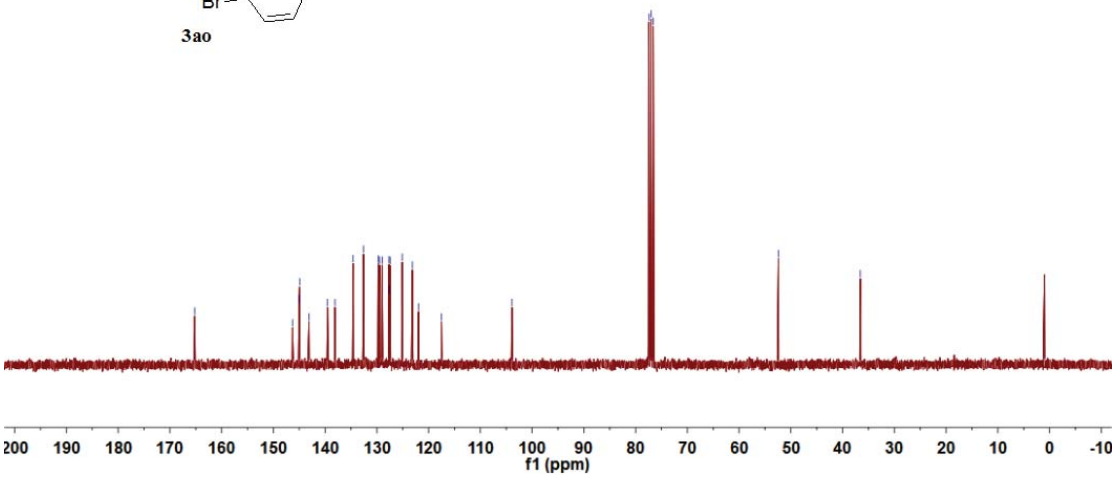
3ao


1.00
0.97
1.03
4.12
1.06
1.02
3.01
2.03
f1 (ppm)

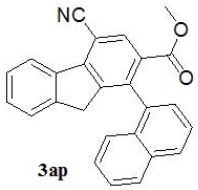

165.21
145.03
144.92
139.54
138.09
134.60
132.58
129.74
129.46
128.97
127.67
127.65
127.44
125.10
123.14
77.42
77.00
76.58
52.40
36.57


NC
O
O
Br

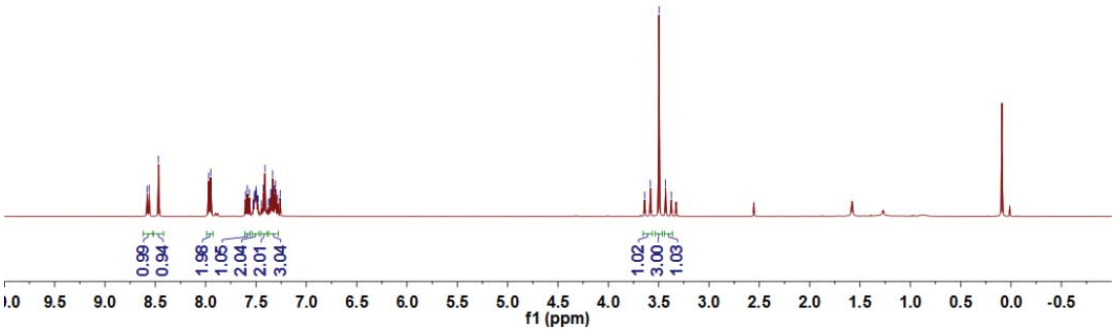
3ao


f1 (ppm)

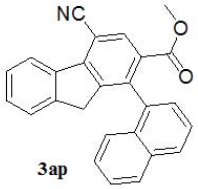

8.58
8.56
8.47
7.97
7.95
7.60
7.59
7.57
7.52
7.51
7.50
7.50
7.50
7.49
7.48
7.43
7.41
7.35
7.35
7.33
7.32
7.30
7.28
3.64
3.58
3.50
3.43
3.37


NC
O
O

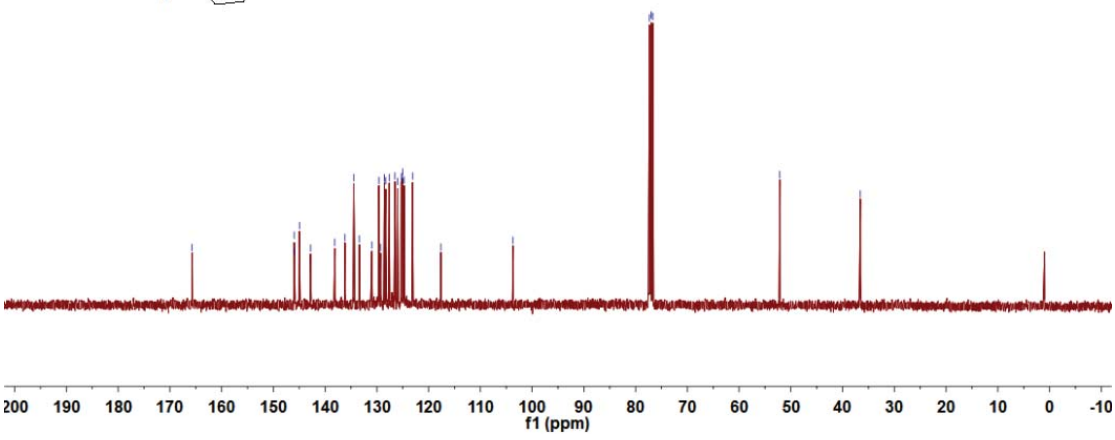
3ap

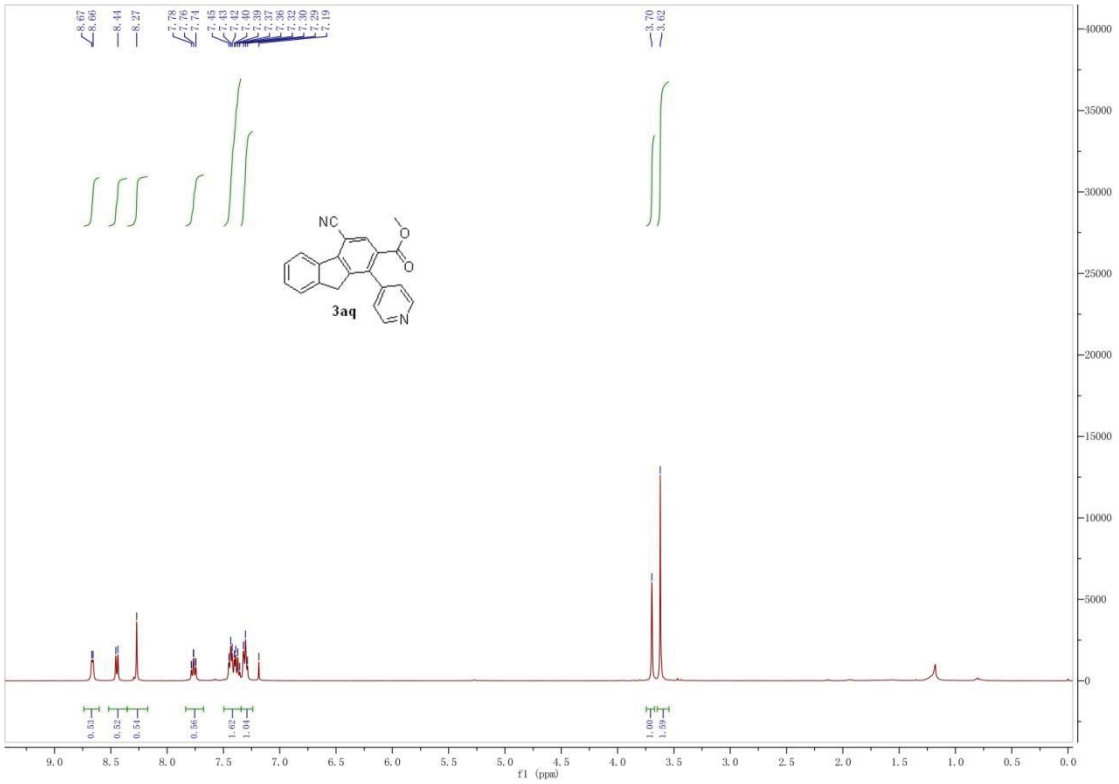

0.99
0.94
1.98
1.05
2.04
2.01
3.04
1.02
3.00
1.03
f1 (ppm)


165.72
145.97
144.95
136.17
134.47
129.62
128.55
128.29
127.61
126.52
126.01
125.26
125.13
125.02
124.73
77.32
77.00
76.68
52.15
36.58


NC
O
O

3ap


f1 (ppm)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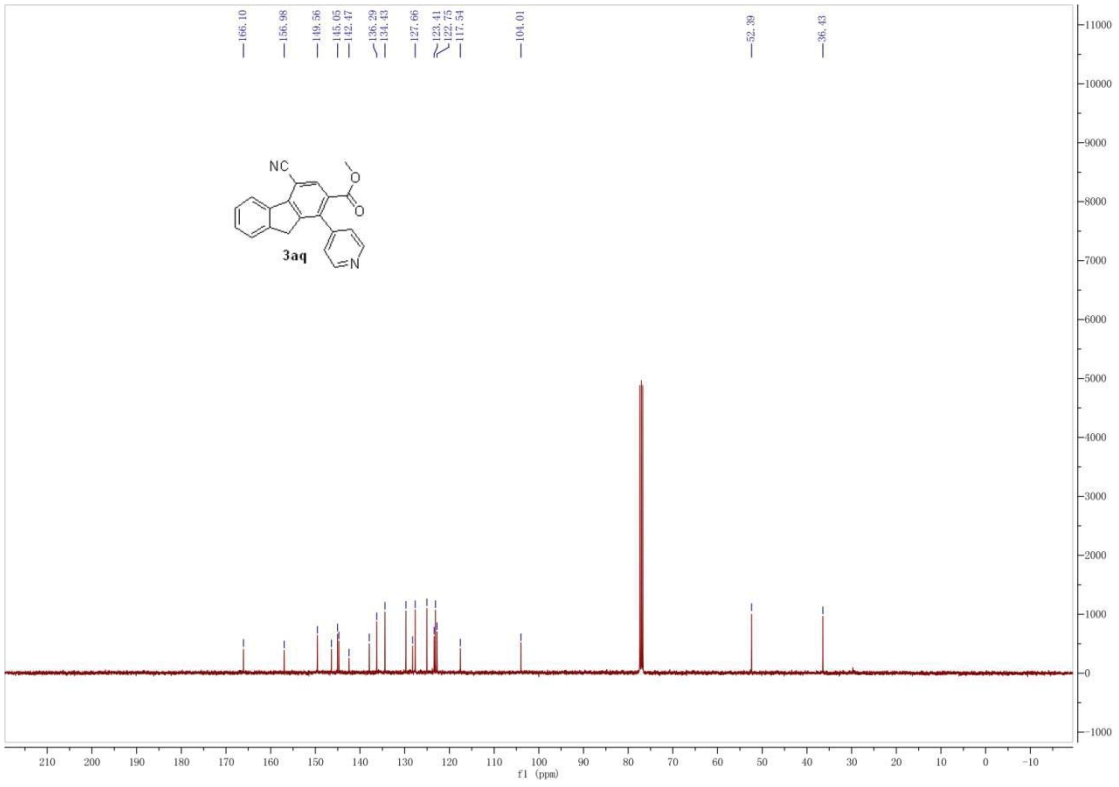
8.66
8.44
8.27
7.78
7.76
7.74
7.45
7.43
7.42
7.40
7.39
7.37
7.36
7.32
7.30
7.29
7.19
3.70
3.62
NC
O
O
N
3aq
0.53
0.52
0.54
0.58
1.62
1.04
1.00
1.59
f1 (ppm)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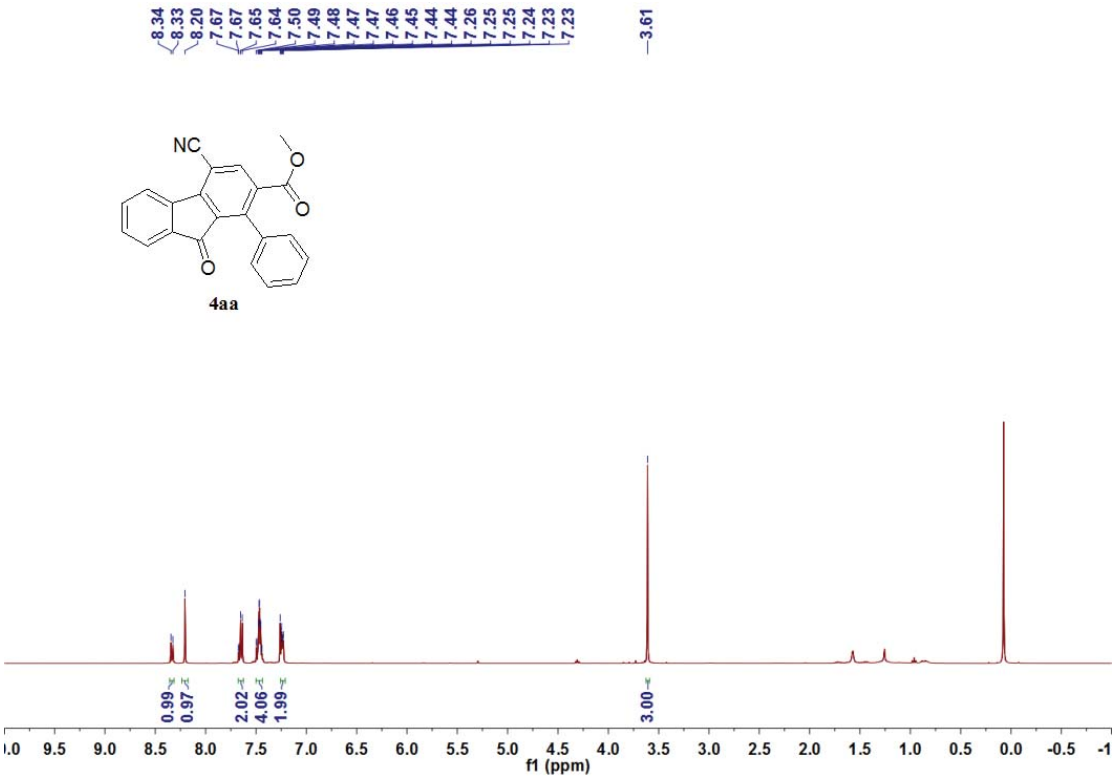
156.98
149.56
145.05
142.47
136.29
134.43
127.66
123.41
122.75
117.54
104.01
52.39
36.43
NC
O
O
N
3aq
f1 (ppm)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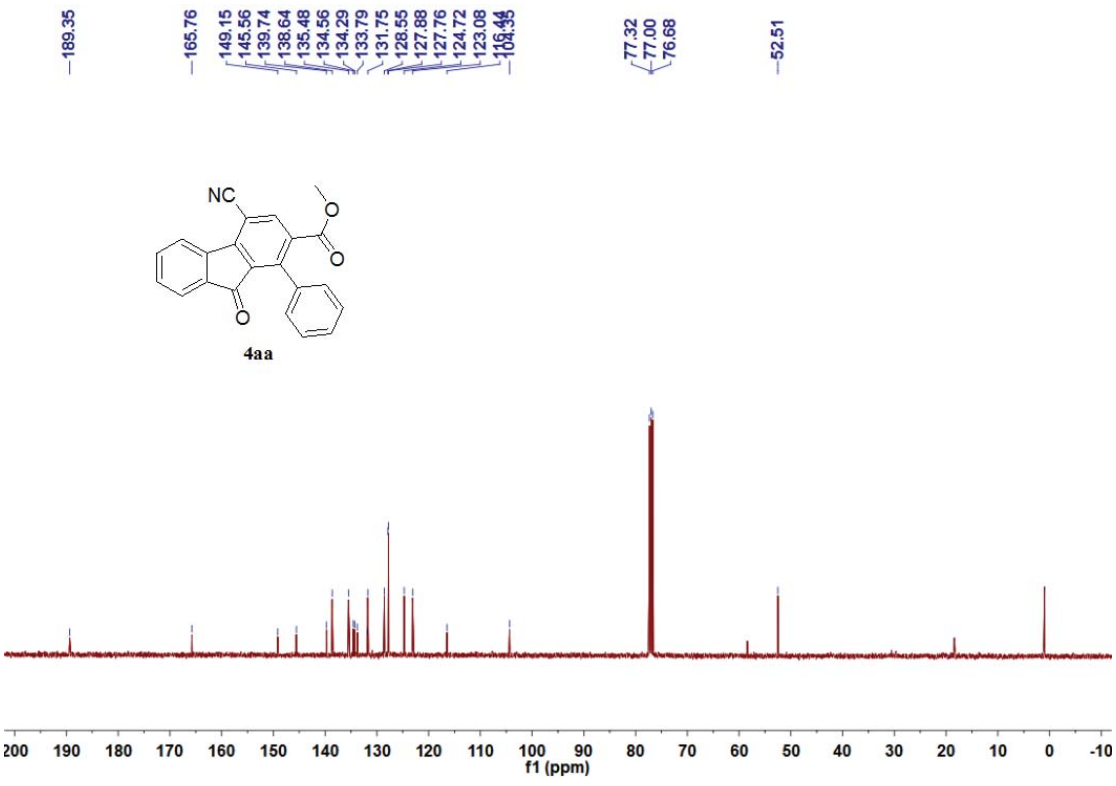
7.50
7.49
7.48
7.47
7.47
7.46
7.45
7.44
7.44
7.26
7.25
7.25
7.24
7.23
7.23
3.61
NC
O
O
O
4aa
0.99
0.97
2.02
4.06
1.99
3.00
f1 (ppm)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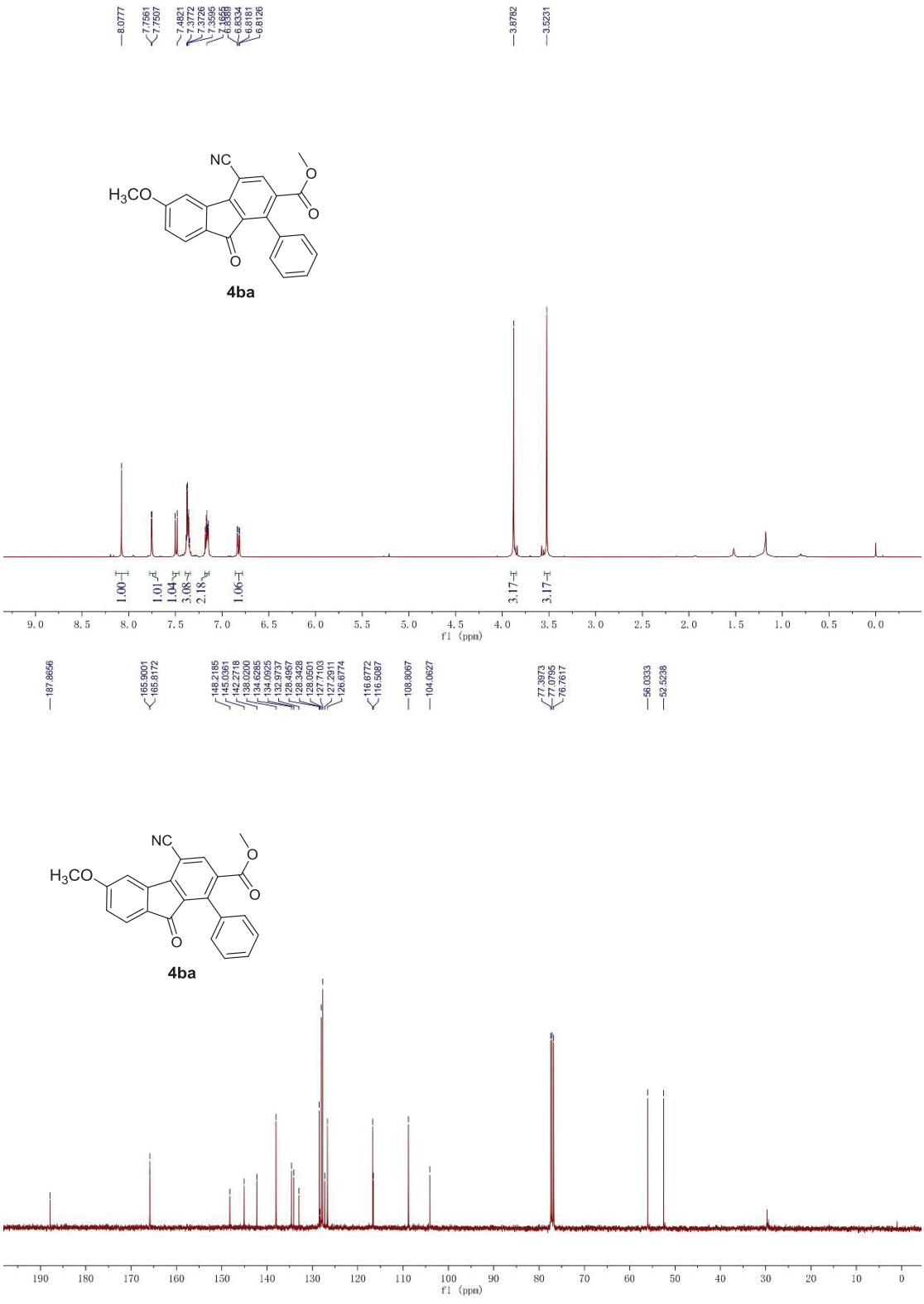
145.56
139.74
138.64
135.48
134.56
134.29
133.79
131.75
128.55
127.88
127.76
124.72
123.08
77.32
77.00
76.68
52.51
NC
O
O
O
4aa
f1 (ppm)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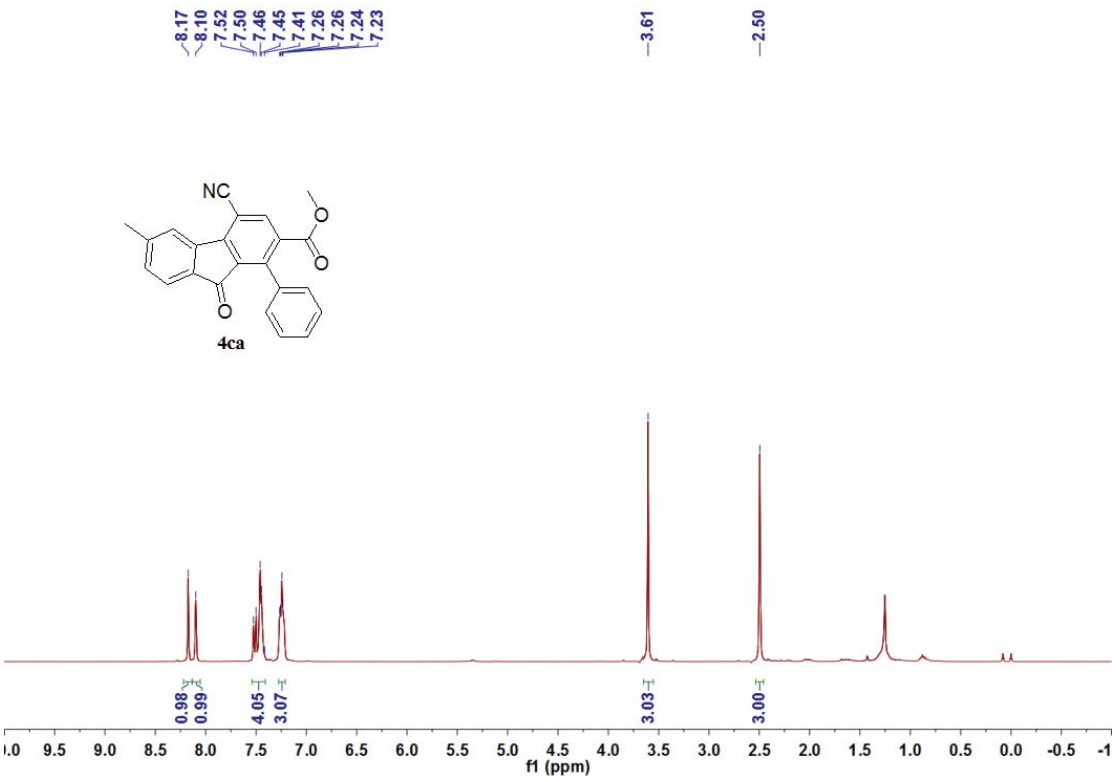
7.7507
7.4821
7.3772
7.3726
7.3595
7.3555
6.8368
6.8334
6.8181
6.8126
3.8782
3.5231
NC
O
H3CO
O
O
4ba
1.00
1.01
1.04
3.08
2.18
1.06
3.17
3.17
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
187.8656
165.9001
165.8172
148.2185
145.0361
142.2718
138.0200
134.2255
134.0525
132.9737
128.4957
128.3428
128.0501
127.7103
127.2911
126.6774
116.8772
116.5087
108.8067
104.0627
77.3973
77.0795
76.7617
56.0333
52.5238
NC
O
H3CO
O
O
4ba
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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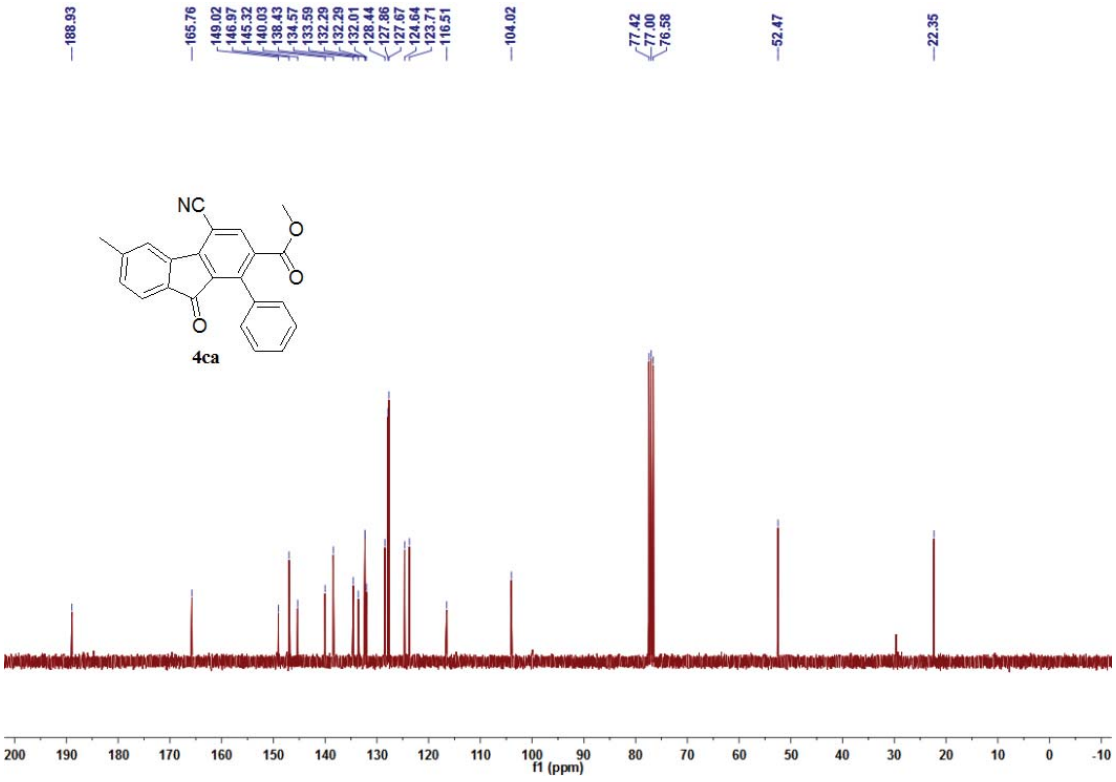
8.10
7.52
7.50
7.46
7.45
7.41
7.26
7.26
7.24
7.23
3.61
2.50
NC
O
O
O
4ca
0.98
0.99
4.05
3.07
3.03
3.00
f1 (ppm)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134.57
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132.29
132.29
132.01
128.44
127.86
127.67
124.64
123.71
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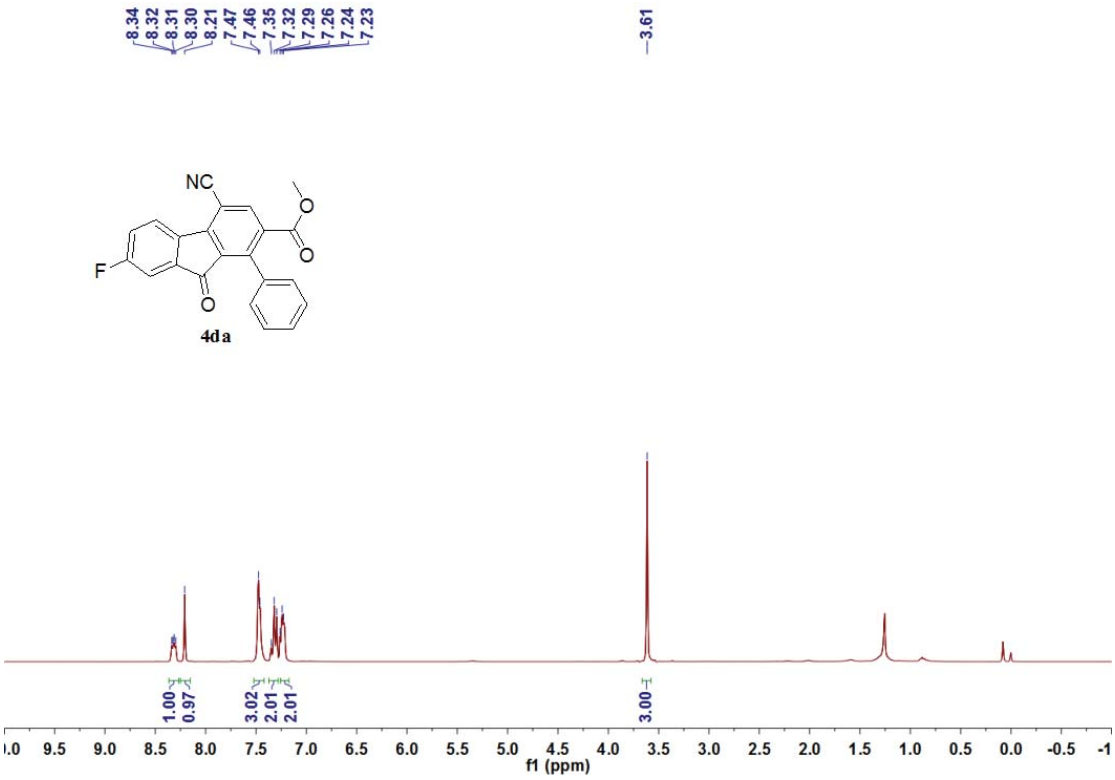
77.42
77.00
76.58
52.47
22.35
NC
O
O
O
4ca
f1 (ppm)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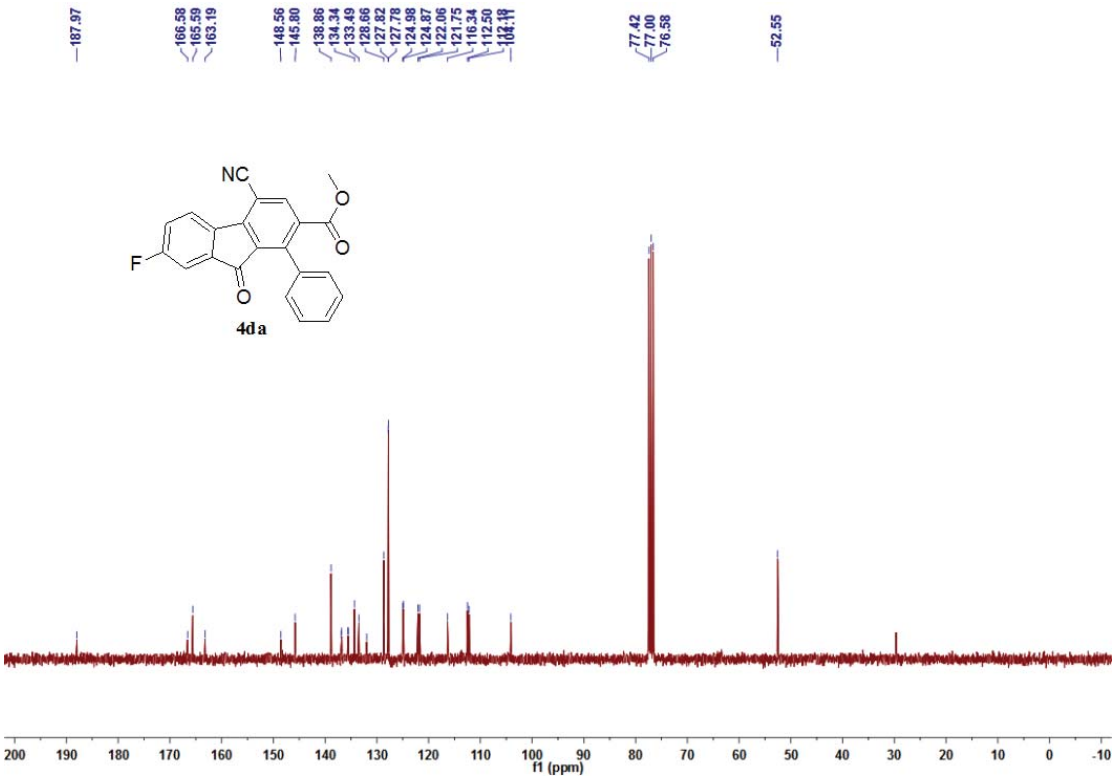
8.32
8.31
8.30
8.21
7.47
7.46
7.35
7.32
7.29
7.26
7.24
7.23
3.61
NC
O
O
F
O
4da
1.00
0.97
3.02
2.01
2.01
3.00
f1 (ppm)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166.58
165.59
163.19
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145.80
138.86
134.34
133.49
128.66
127.82
127.78
124.98
124.87
122.06
121.75
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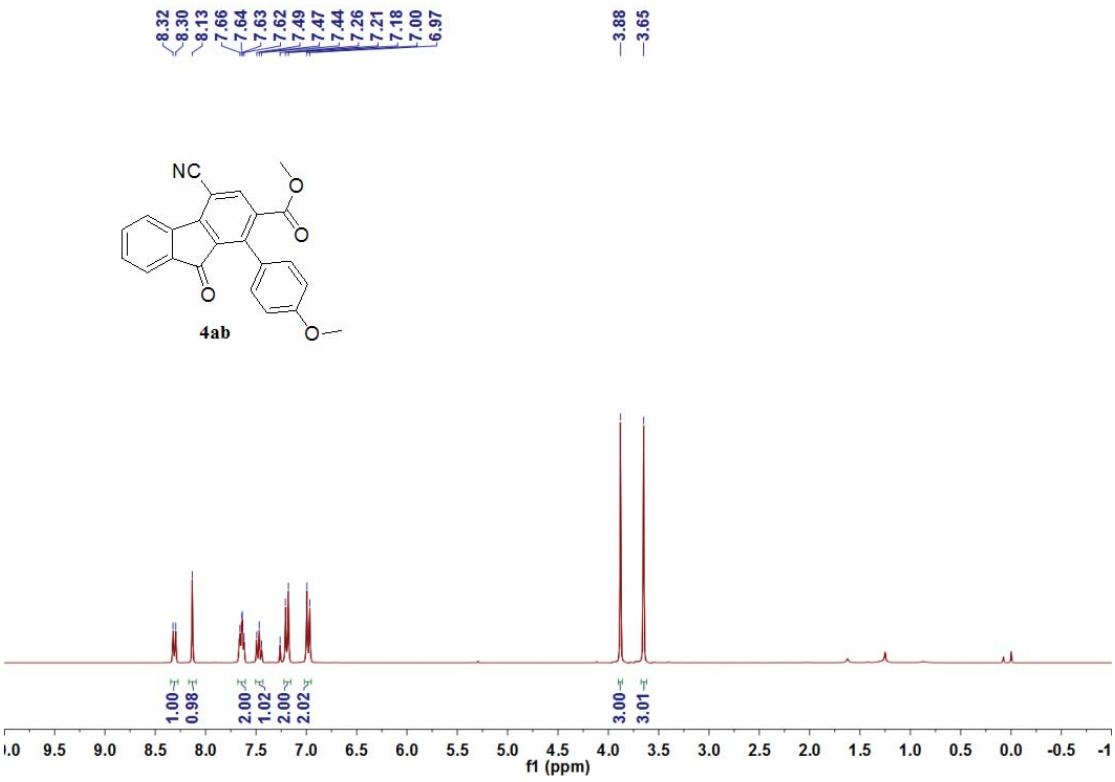
77.42
77.00
76.58
52.55
NC
O
O
F
O
4da
f1 (ppm)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8.30
8.13
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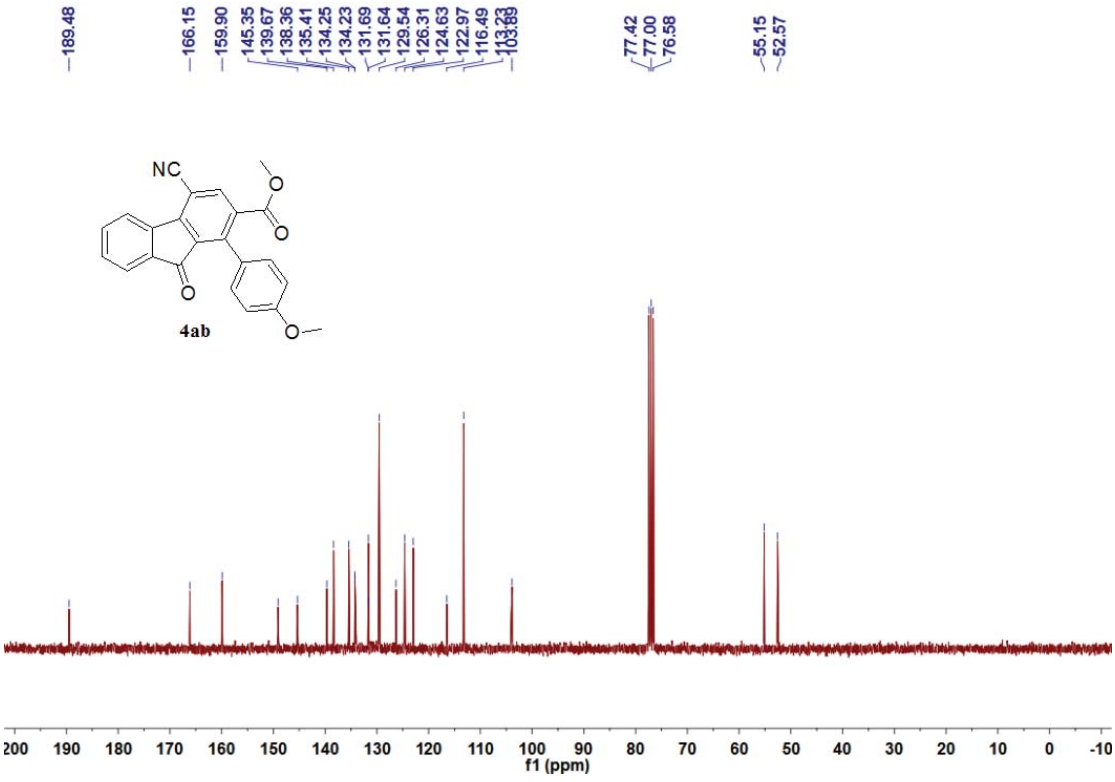
7.64
7.63
7.62
7.49
7.47
7.44
7.26
7.21
7.18
7.00
6.97
3.88
3.65
NC
O
O
O
O
4ab
1.00
0.98
2.00
1.02
2.00
2.02
3.00
3.01
f1 (ppm)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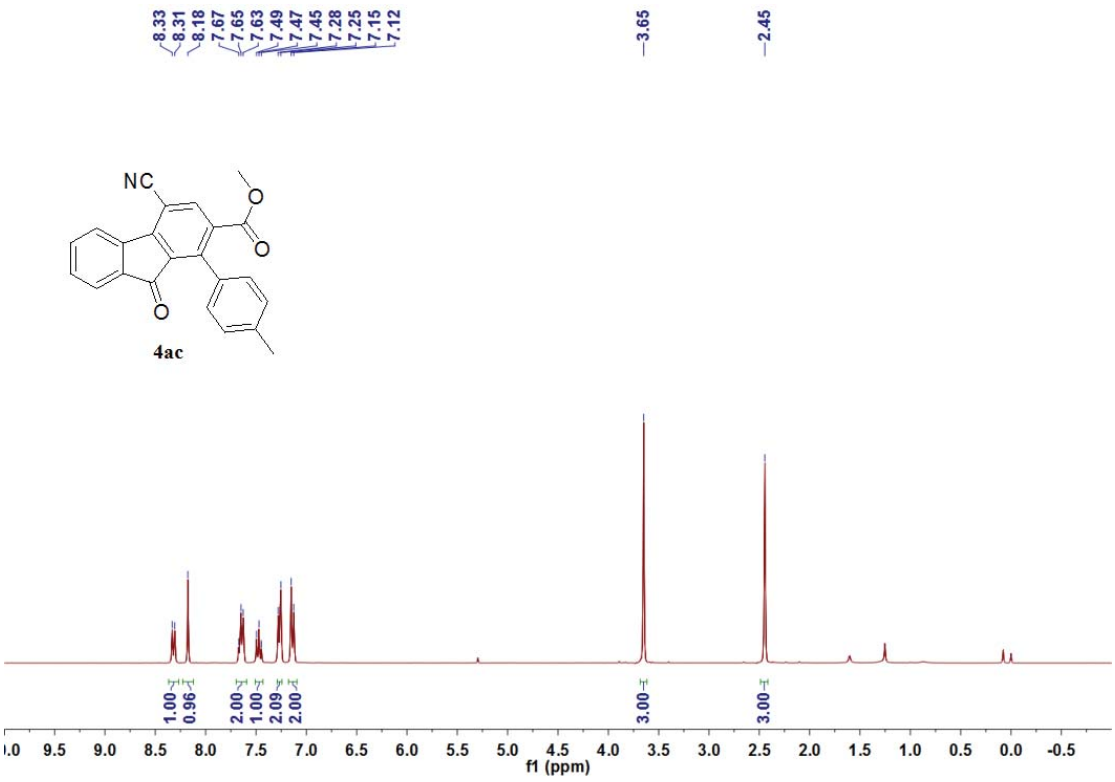
131.69
131.64
129.54
126.31
124.63
122.97
116.49
77.42
77.00
76.58
55.15
52.57
NC
O
O
O
O
4ab
f1 (ppm)


8.33
8.31
8.18
7.67
7.65
7.63
7.49
7.47
7.45
7.28
7.25
7.15
7.12
3.65
2.45
NC
O
O
O
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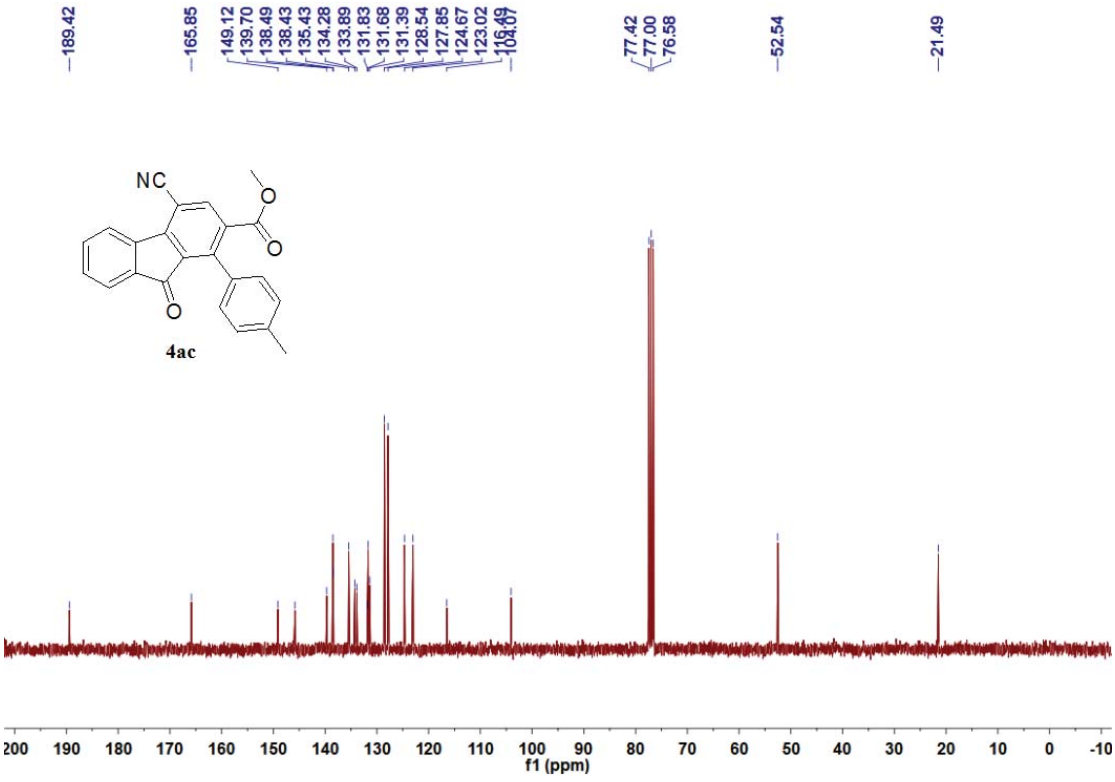
1.00
0.96
2.00
1.00
2.09
2.00
3.00
3.00
f1 (ppm)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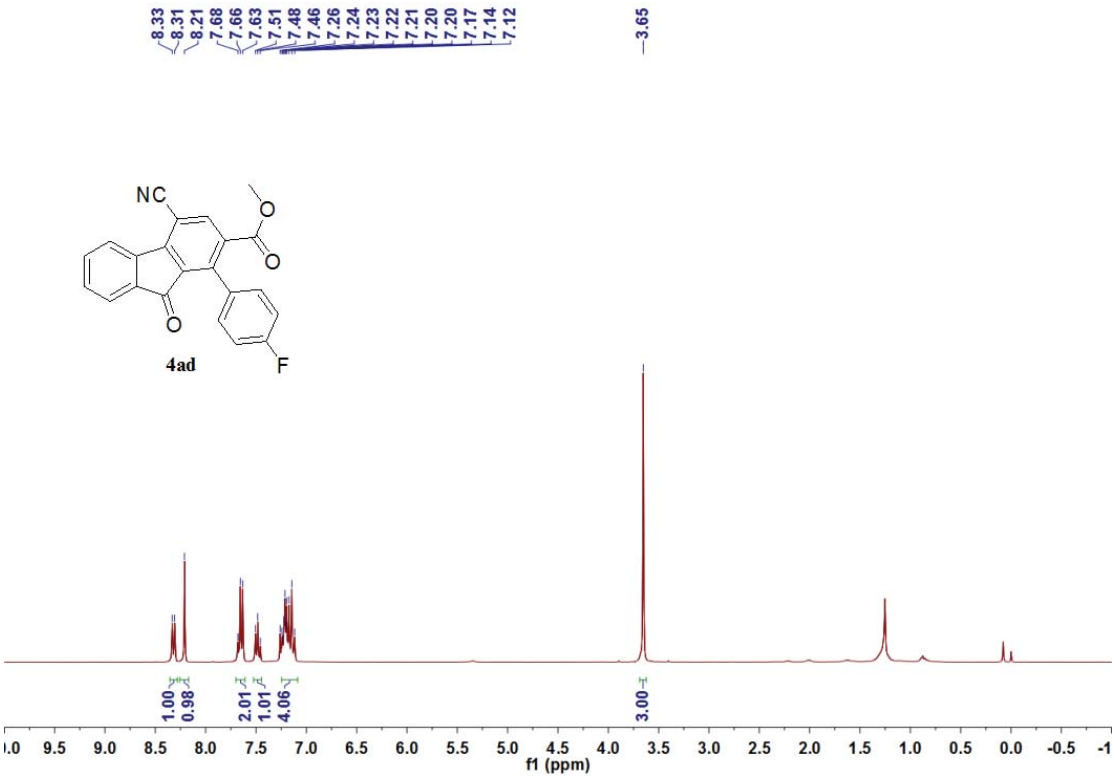
139.70
138.49
138.43
135.43
134.28
133.89
131.83
131.68
131.39
128.54
127.85
124.67
123.02
77.42
77.00
76.58
52.54
21.49
NC
O
O
O
4ac
f1 (ppm)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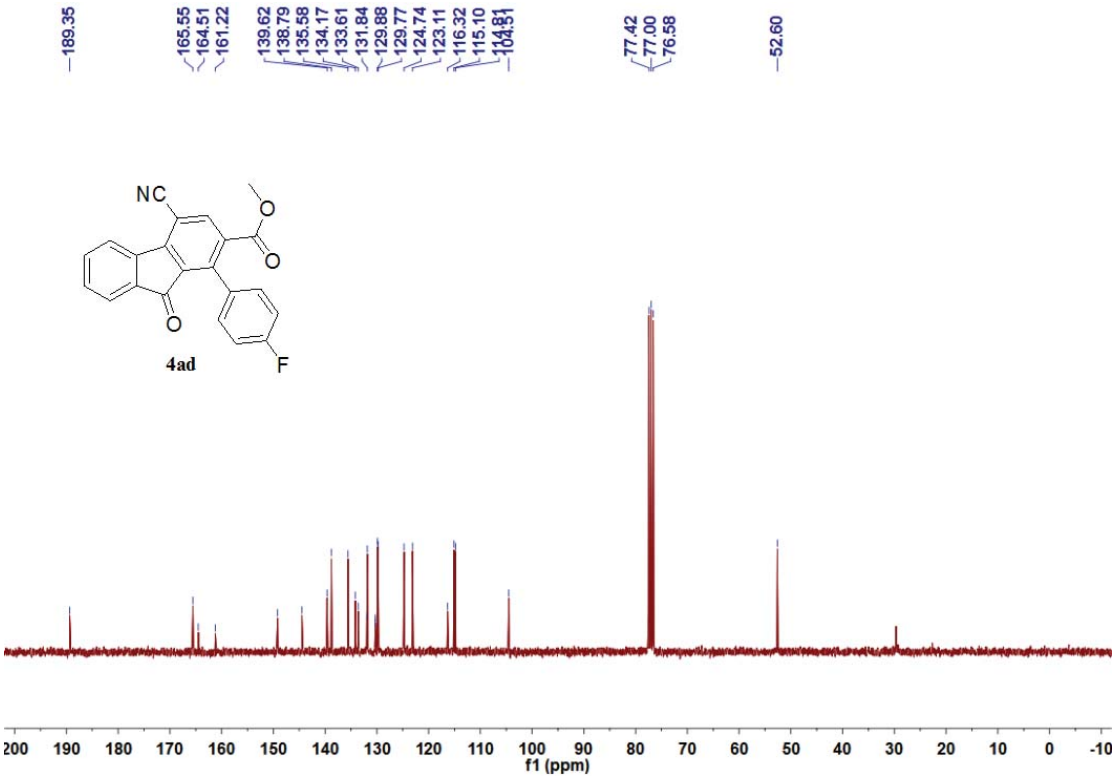
7.63
7.51
7.48
7.46
7.26
7.24
7.23
7.22
7.21
7.20
7.20
7.17
7.14
7.12
3.65
NC
O
O
O
F
4ad
1.00
0.98
2.01
1.01
4.06
3.00
f1 (ppm)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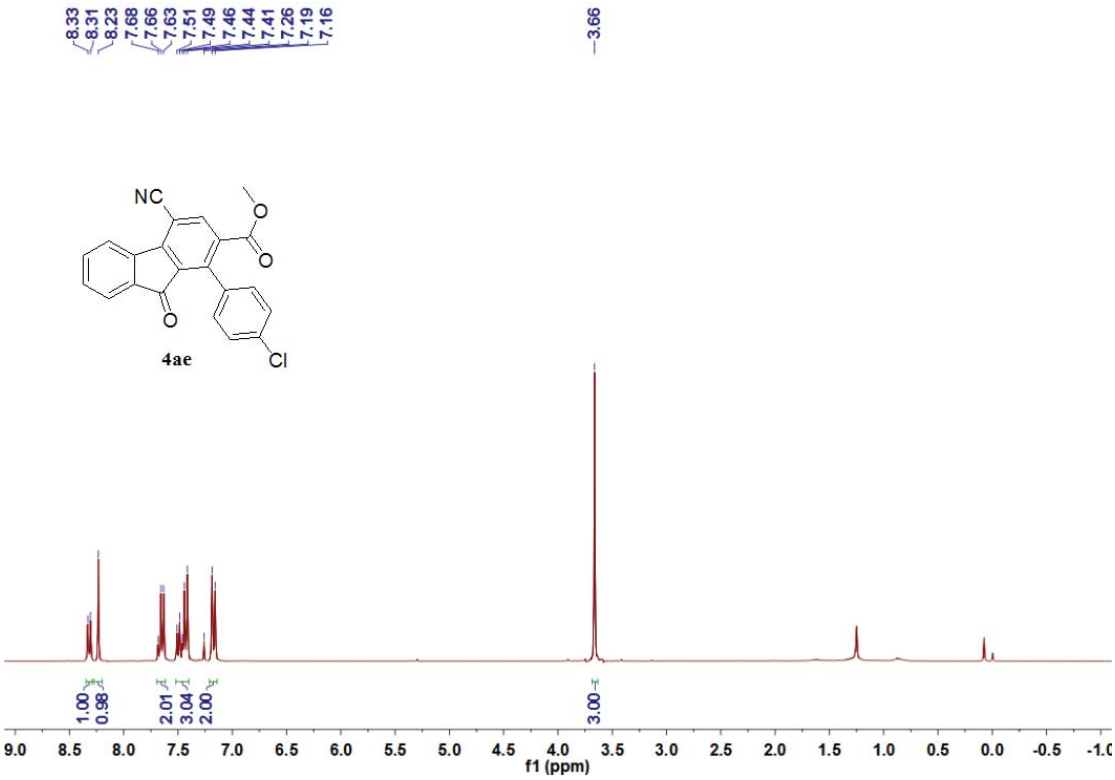
138.79
135.58
134.17
133.61
131.84
129.88
129.77
124.74
123.11
116.32
115.10
77.42
77.00
76.58
52.60
NC
O
O
O
F
4ad
f1 (ppm)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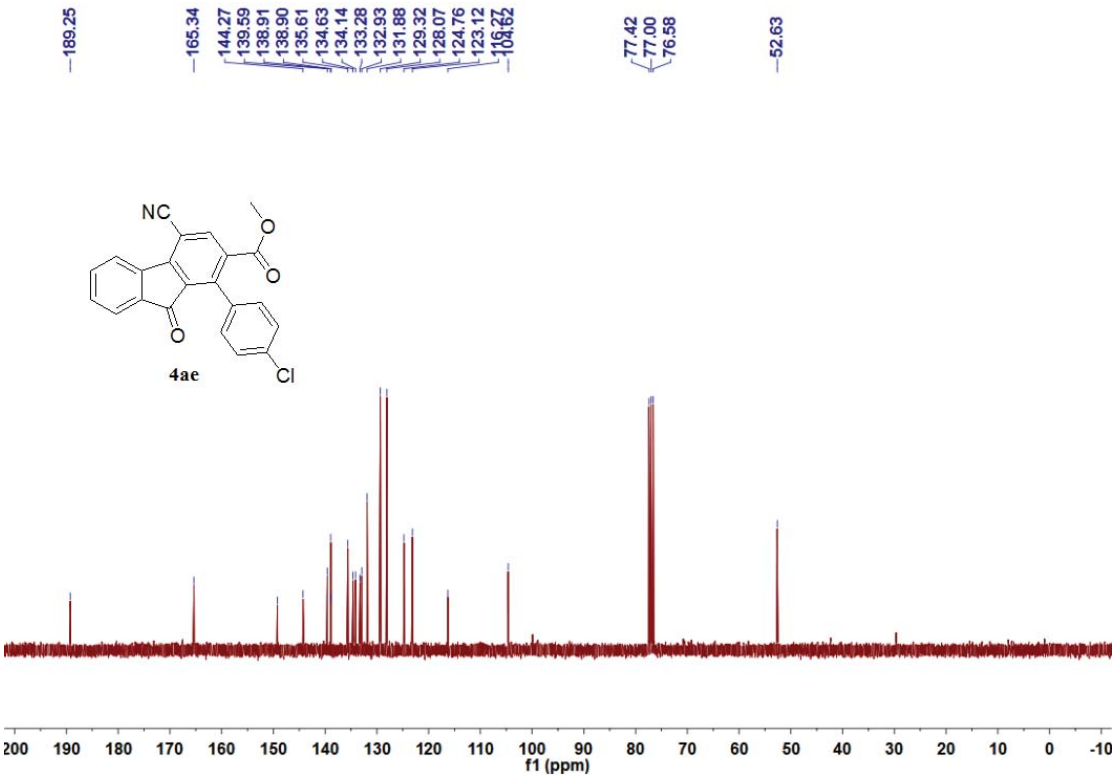
8.31
8.23
7.68
7.66
7.63
7.51
7.49
7.46
7.44
7.41
7.26
7.19
7.16
3.66
NC
O
O
O
Cl
4ae
1.00
0.98
2.01
3.04
2.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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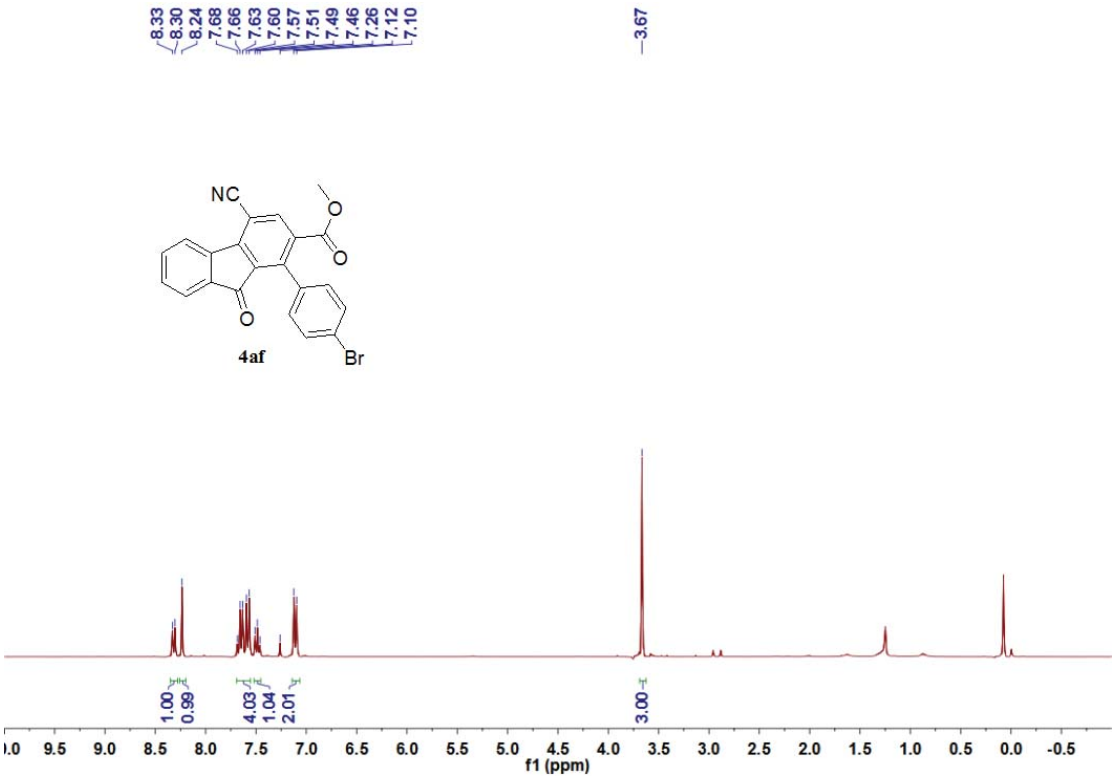
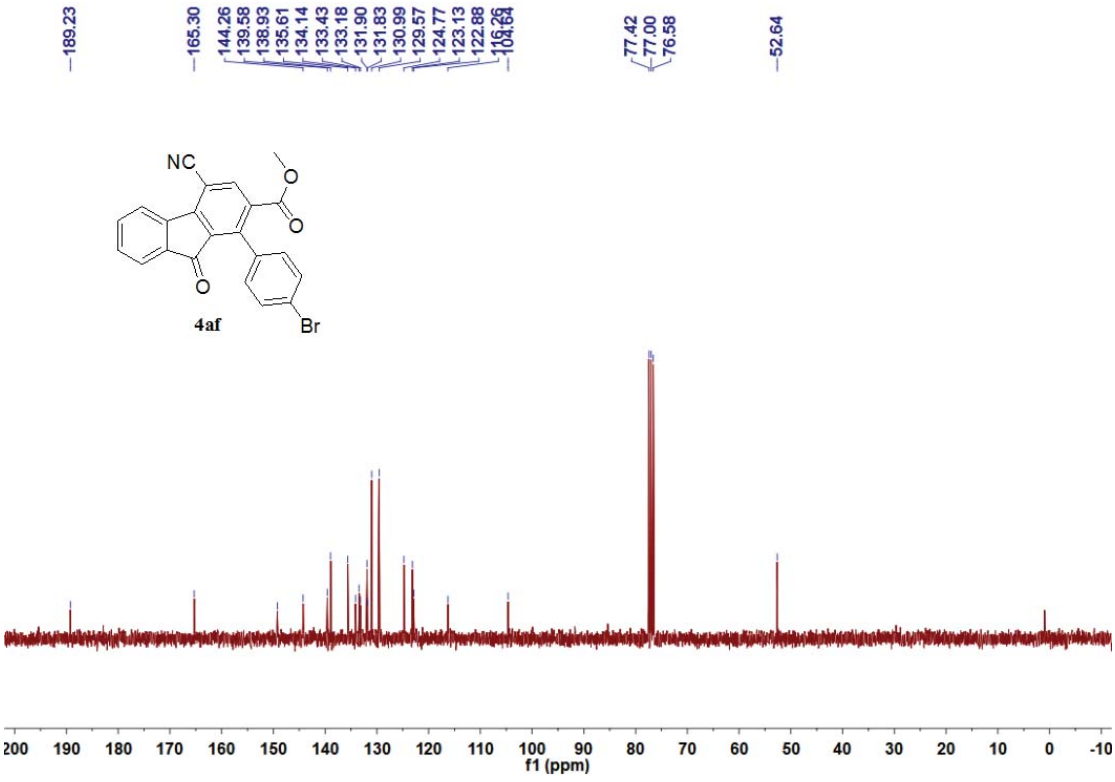
138.91
138.90
135.61
134.63
134.14
133.28
132.93
131.88
129.32
128.07
124.76
123.12
116.27
104.62
77.42
77.00
76.58
52.63
NC
O
O
O
Cl
4ae
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.33
8.30
8.24
7.68
7.66
7.63
7.60
7.57
7.51
7.49
7.46
7.26
7.12
7.10
3.67
NC
O
O
O
Br
4af
1.00
0.99
4.03
1.04
2.01
3.00
f1 (ppm)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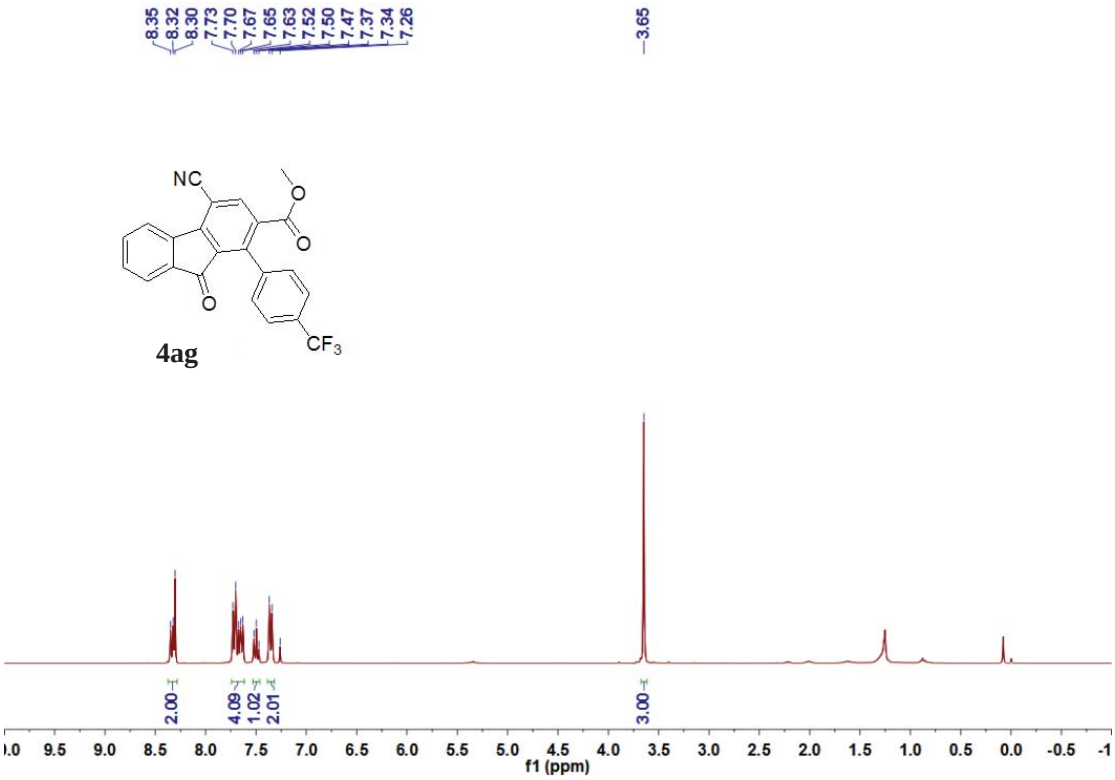
165.30
144.26
139.58
138.93
135.61
134.14
133.43
133.18
131.90
131.83
130.99
129.57
124.77
123.13
122.88
77.42
77.00
76.58
52.64
NC
O
O
O
Br
4af
f1 (ppm)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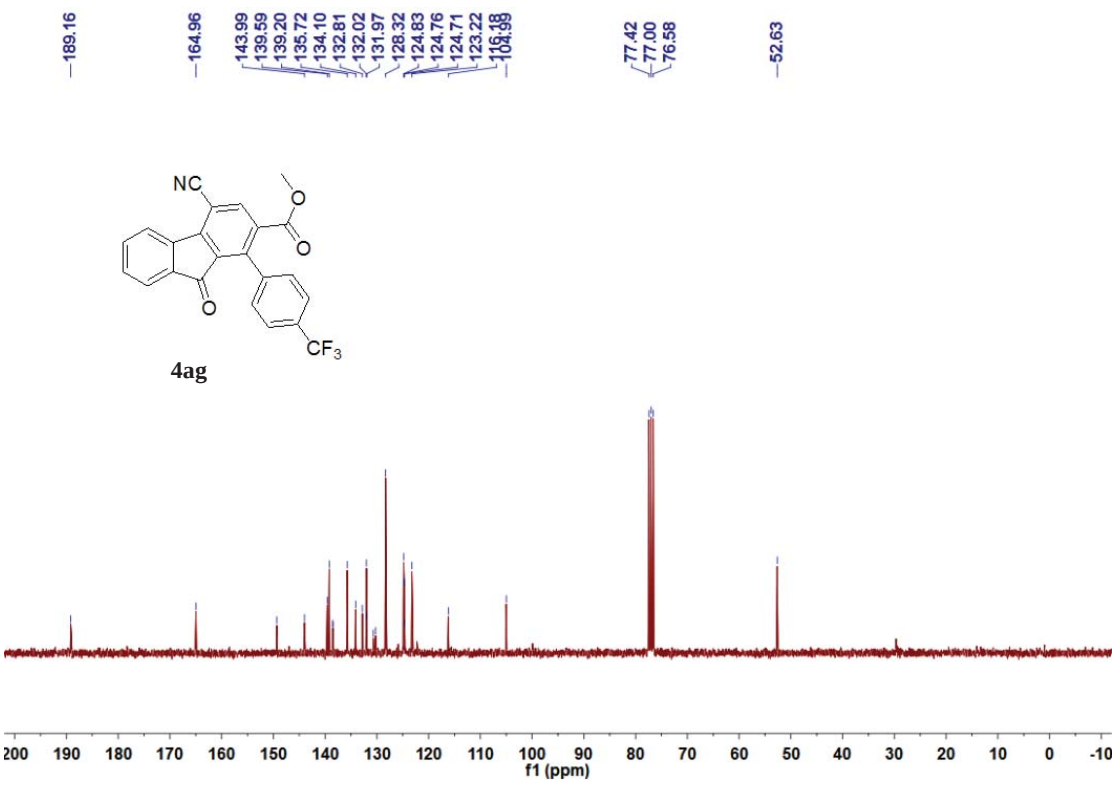
8.32
8.30
7.73
7.70
7.67
7.65
7.63
7.52
7.50
7.47
7.37
7.34
7.26
3.65
NC
O
O
O
CF3
2.00
4.09
1.02
2.01
3.00
f1 (ppm)

4ag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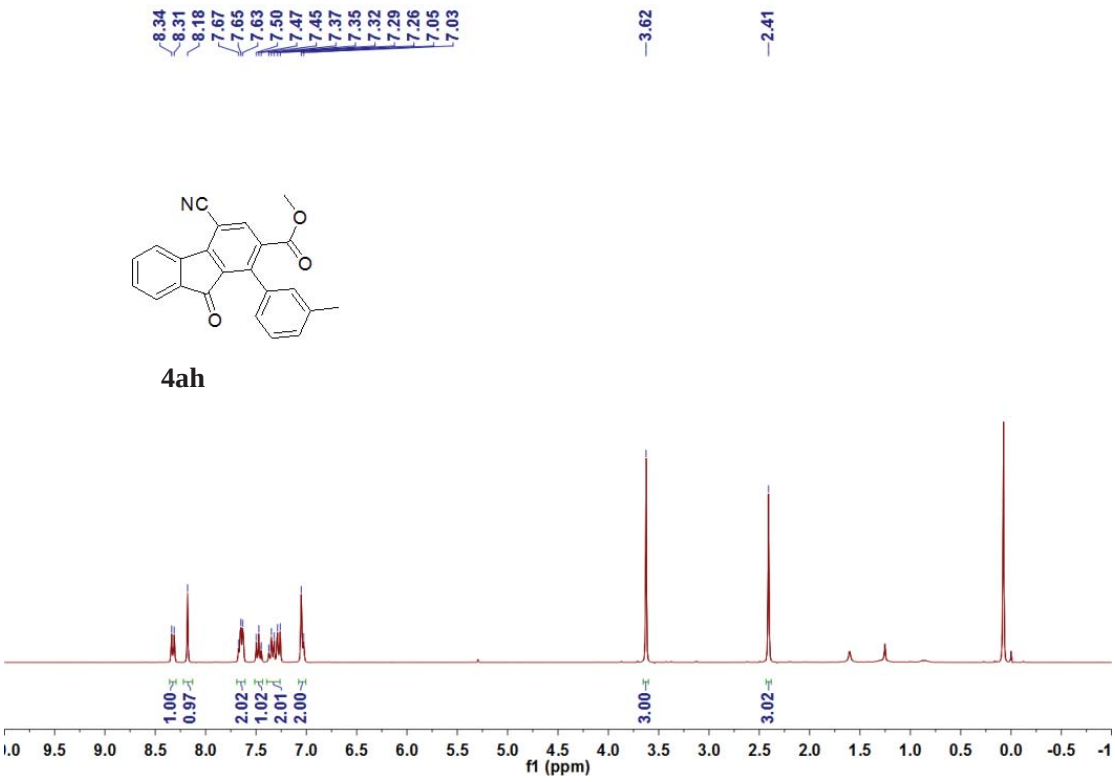
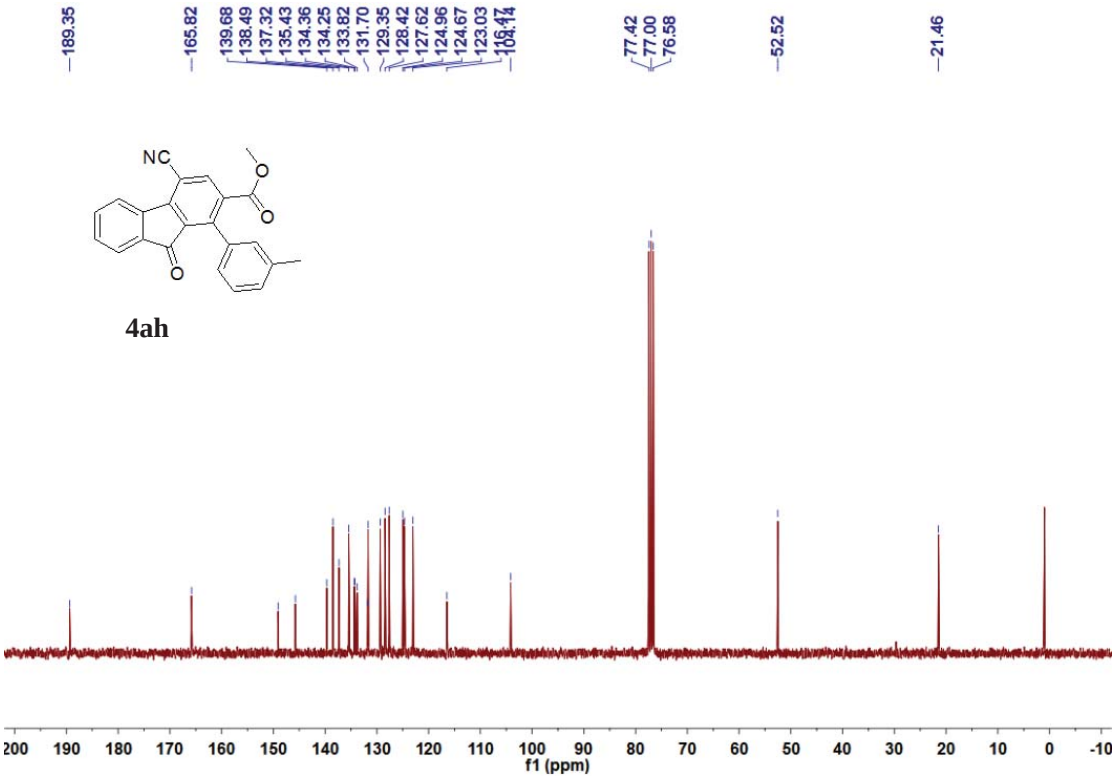
164.96
143.99
139.59
139.20
135.72
134.10
132.81
132.02
131.97
128.32
124.83
124.76
124.71
123.22
77.42
77.00
76.58
52.63
NC
O
O
O
CF3
f1 (ppm)

4ag


8.34
8.31
8.18
7.67
7.65
7.63
7.50
7.47
7.45
7.37
7.35
7.32
7.29
7.26
7.05
7.03
3.62
2.41
NC
O
O
O
1.00
0.97
2.02
1.02
2.01
2.00
3.00
3.02
f1 (ppm)

4ah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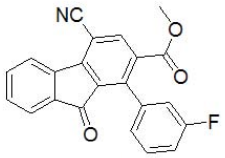
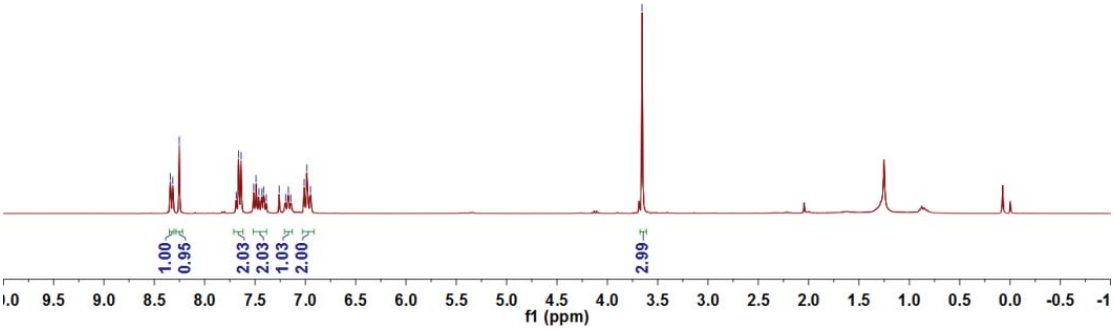
139.68
138.49
137.32
135.43
134.36
134.25
133.82
131.70
129.35
128.42
127.62
124.96
124.67
123.03
116.47
104.14
77.42
77.00
76.58
52.52
21.46
NC
O
O
O
f1 (ppm)

4ah


8.34
8.32
8.25
7.69
7.66
7.64
7.51
7.49
7.46
7.43
7.41
7.39
7.26
7.20
7.17
7.15
7.01
6.98
6.95
3.66


NC
O
O
O
F

4ai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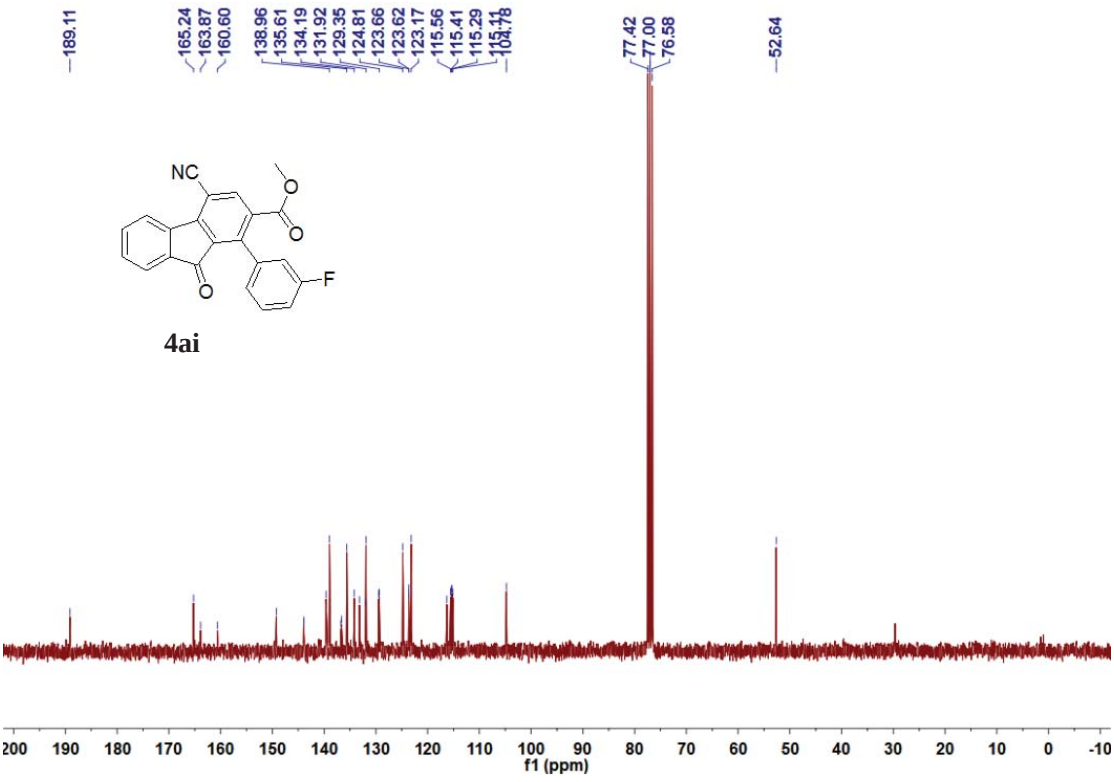
0.95
2.03
2.03
1.03
2.00
2.99
f1 (ppm)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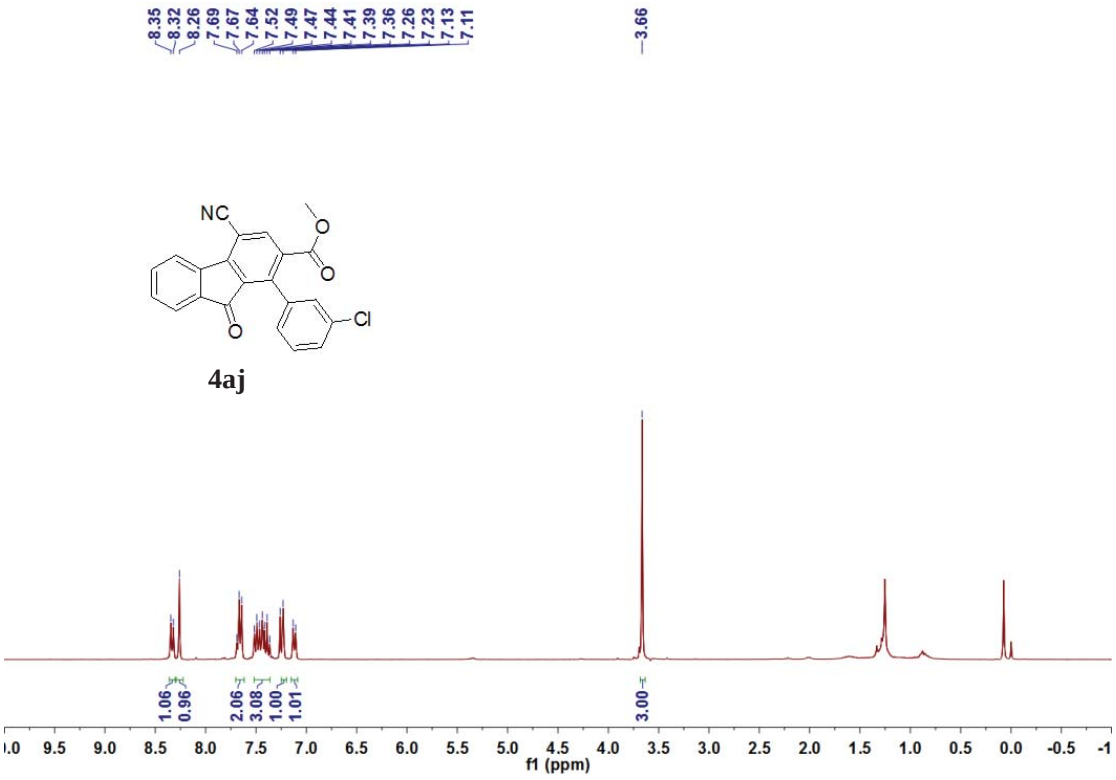
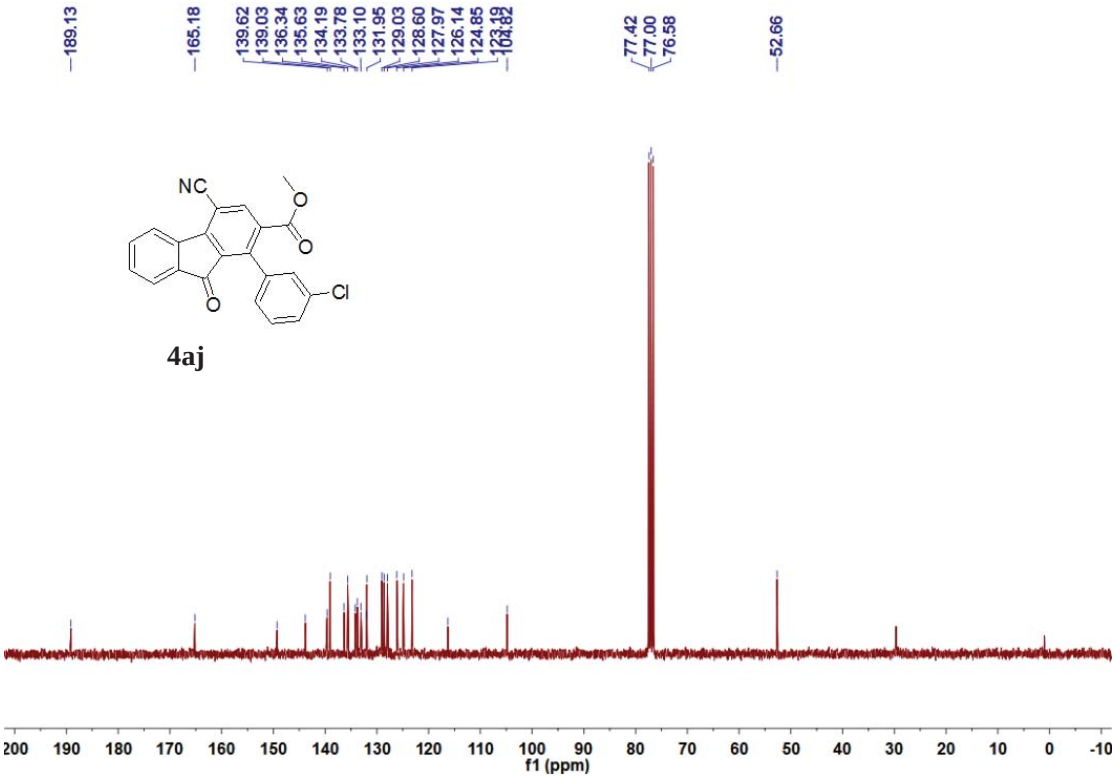
165.24
163.87
160.60
138.96
135.61
134.19
131.92
129.35
124.81
123.66
123.62
123.17
115.56
115.41
115.29
77.42
77.00
76.58
52.64
f1 (ppm)

NC
O
O
O
F

4ai


8.35
8.32
8.26
7.69
7.67
7.64
7.52
7.49
7.47
7.44
7.41
7.39
7.36
7.26
7.23
7.13
7.11
3.66
NC
O
O
O
Cl
1.06
0.96
2.06
3.08
1.00
1.01
3.00
f1 (ppm)

4aj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165.18
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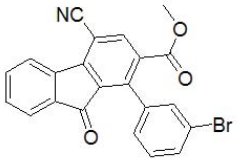
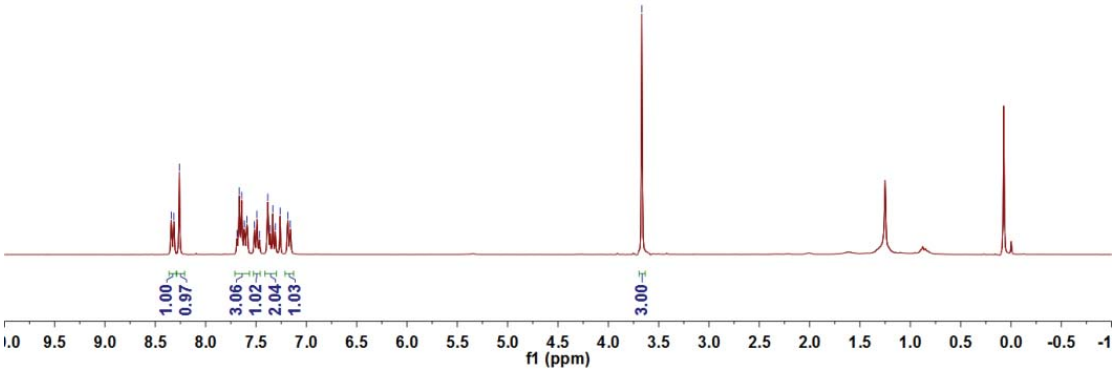
139.03
136.34
135.63
134.19
133.78
133.10
131.95
129.03
128.60
127.97
126.14
124.85
77.42
77.00
76.58
52.66
NC
O
O
O
Cl
f1 (ppm)

4aj


8.34
8.32
8.26
7.69
7.67
7.64
7.62
7.59
7.52
7.49
7.47
7.38
7.36
7.33
7.31
7.26
7.18
7.16
3.67


NC
O
O
O
Br

4ak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3.06
1.02
2.04
1.03
3.00
f1 (ppm)


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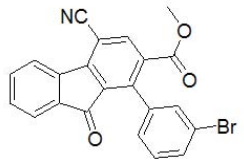
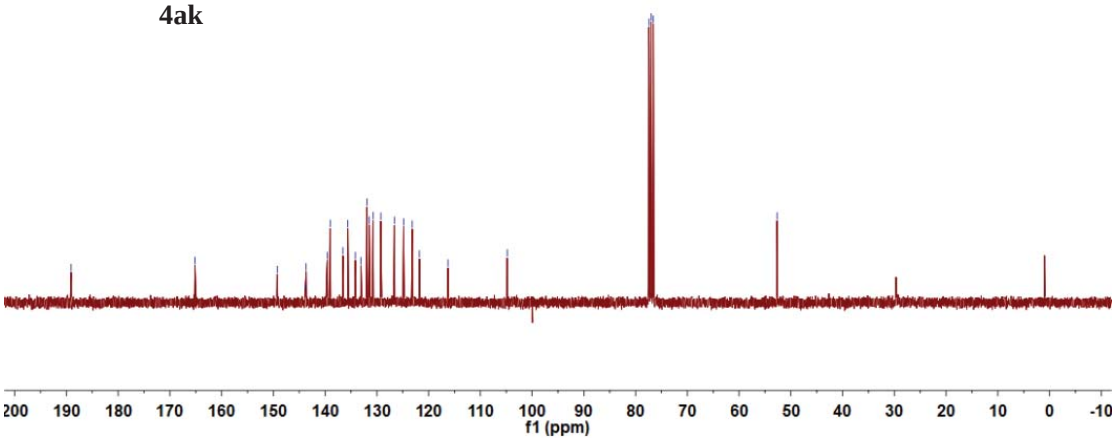
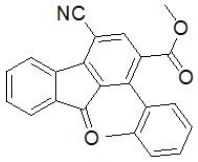
165.15
139.59
139.01
136.55
135.61
134.16
133.07
131.93
131.48
130.74
129.23
126.61
124.83
123.17
77.42
77.00
76.58
52.66


NC
O
O
O
Br

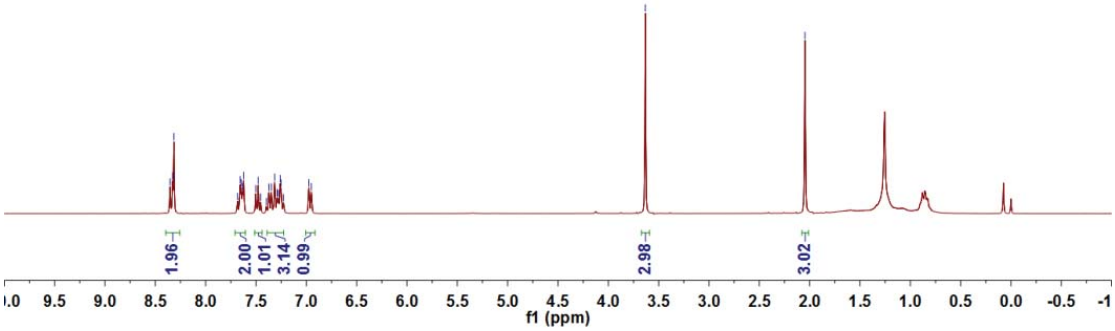
4ak


f1 (ppm)


8.35
8.33
8.32
7.68
7.66
7.65
7.63
7.62
7.50
7.48
7.45
7.40
7.37
7.35
7.31
7.29
7.28
7.26
7.25
7.23
6.97
6.95
3.63
2.05


NC
O
O
O

4al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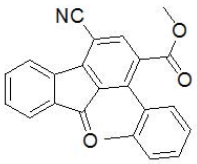
2.00
1.01
3.14
0.99
2.98
3.02
f1 (ppm)


189.35
165.06
139.87
139.13
135.46
135.08
134.77
134.31
133.17
131.79
129.44
128.45
126.89
125.37
124.73
123.17
77.42
77.00
76.58
52.54
19.87


NC
O
O
O

4al

f1 (ppm)


8.42
8.36
8.33
7.69
7.66
7.64
7.51
7.49
7.46
7.45
7.43
7.43
7.41
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7.37
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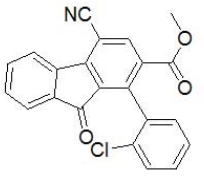
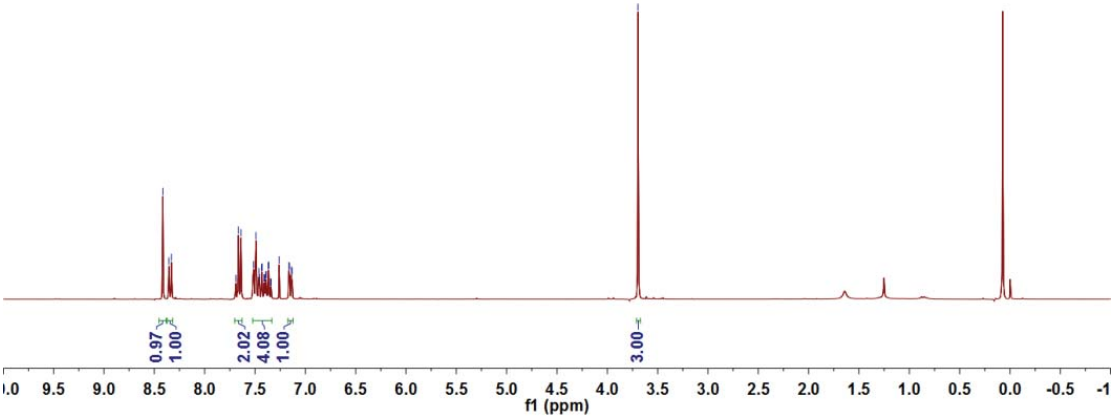
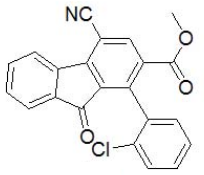
7.34
7.26
7.16
7.14
7.13
3.70


NC
O
O
O
Cl

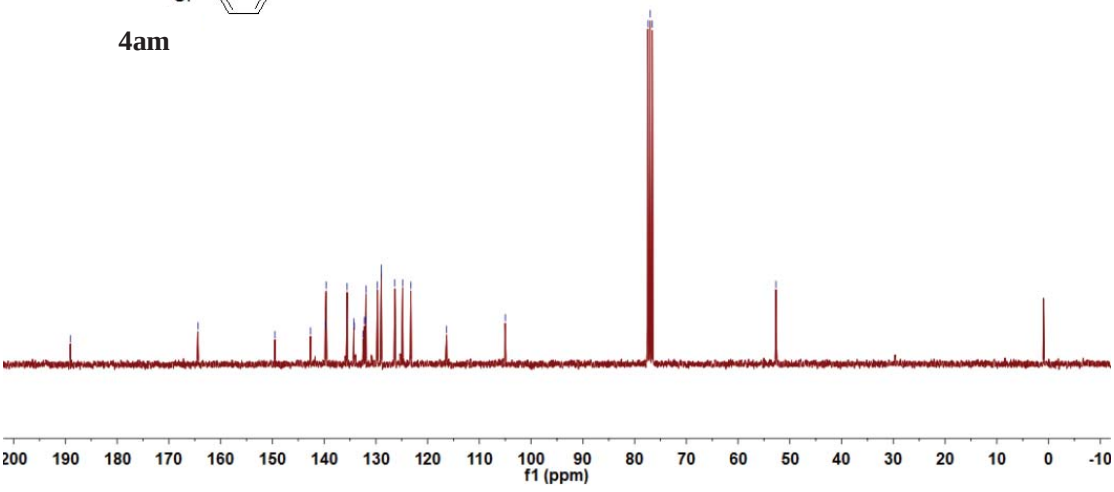
4am


0.97
1.00
2.02
4.08
1.00
3.00
f1 (ppm)


189.03
164.39
139.80
139.62
135.56
134.27
134.17
132.22
131.98
131.91
129.70
128.95
128.92
126.35
124.83
77.42
77.00
76.58
52.68


NC
O
O
O
Cl

4am


f1 (ppm)


8.42
8.35
8.33
7.70
7.66
7.64
7.51
7.49
7.46
7.42
7.40
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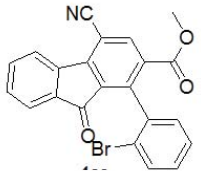
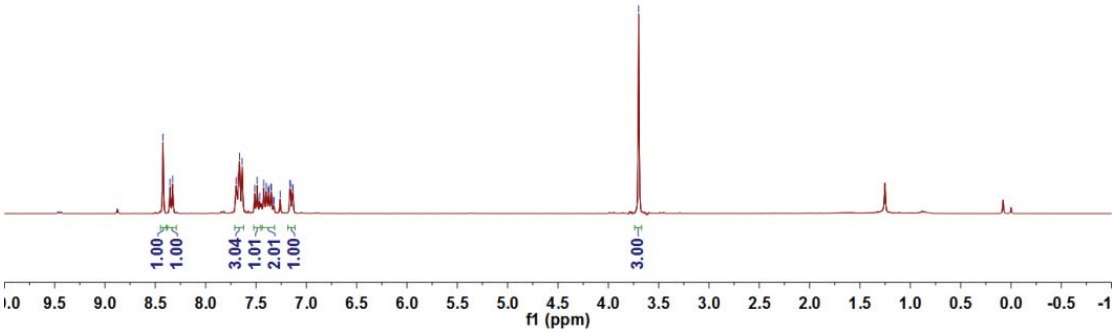
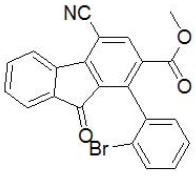
7.26
7.16
7.16
7.14
7.13
3.70


NC
O
O
O
Br

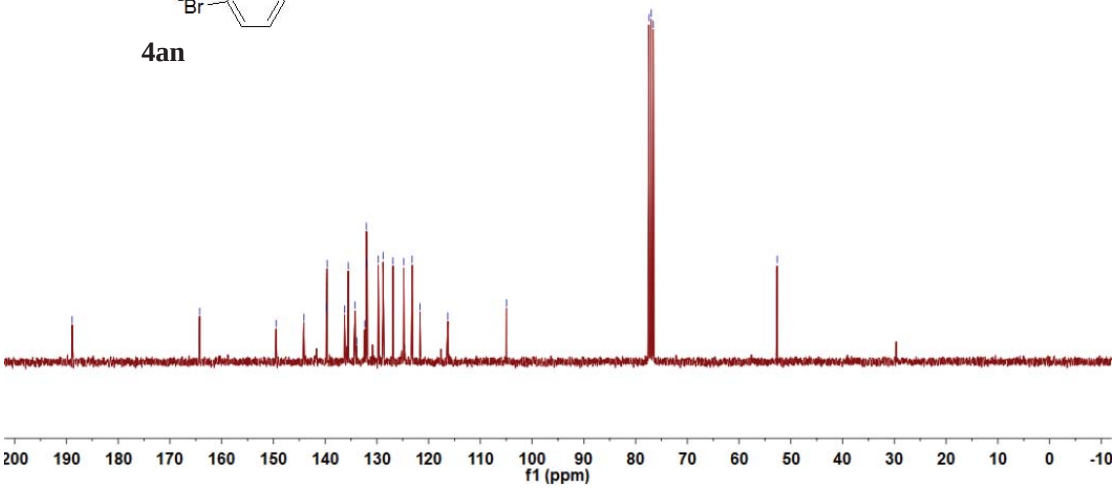
4an

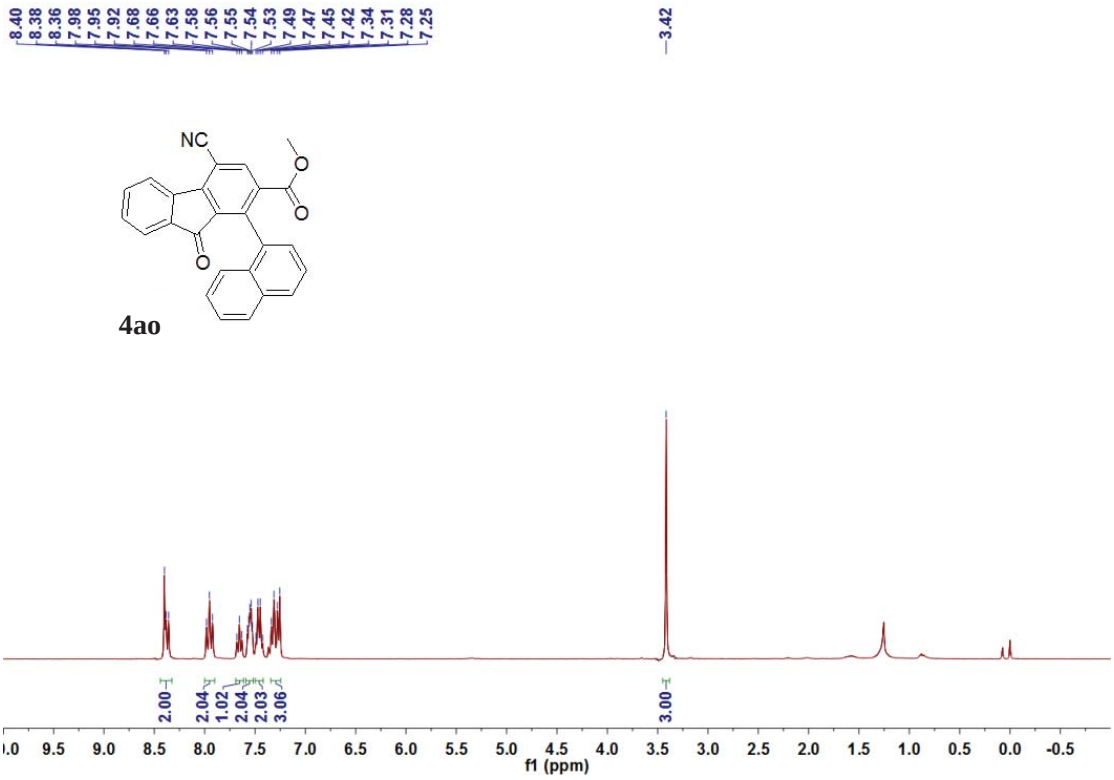

1.00
1.00
3.04
1.01
2.01
1.00
3.00
f1 (ppm)


188.90
164.25
139.78
139.62
136.24
135.52
134.22
132.03
131.88
129.73
128.79
126.90
124.81
123.19
121.67
77.42
77.00
76.58
52.65


NC
O
O
O
Br

4an


f1 (ppm)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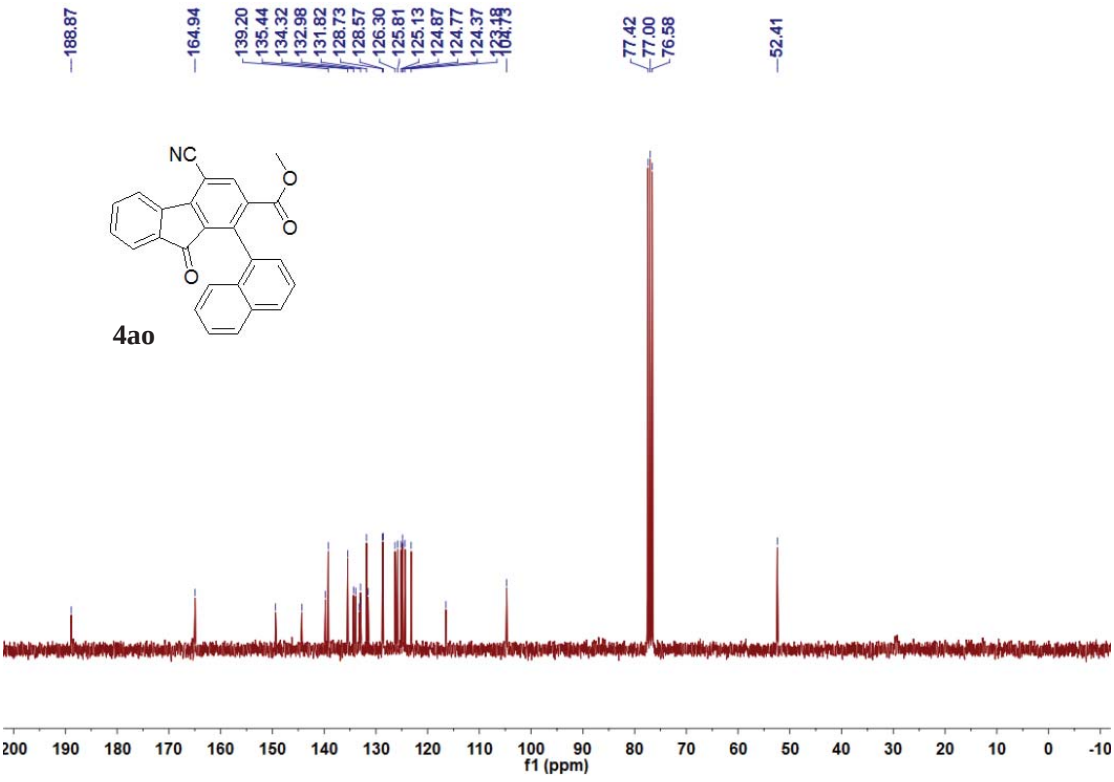
7.92
7.68
7.66
7.63
7.58
7.56
7.55
7.54
7.53
7.49
7.47
7.45
7.42
7.34
7.31
7.28
7.25
3.42
NC
O
O
O
4ao
2.00
2.04
1.02
2.04
2.03
3.06
3.00
f1 (ppm)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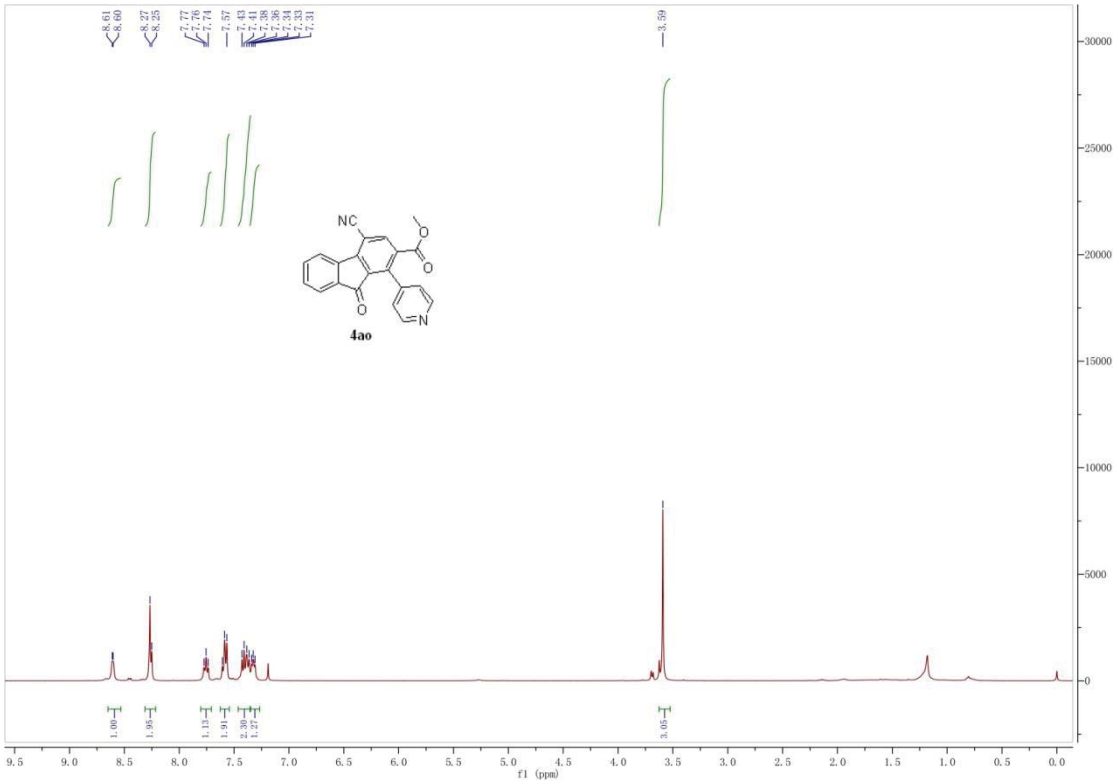
135.44
134.32
132.98
131.82
128.73
128.57
126.30
125.81
125.13
124.87
124.77
124.37
77.42
77.00
76.58
52.41
NC
O
O
O
4ao
f1 (ppm)


8.61
8.60
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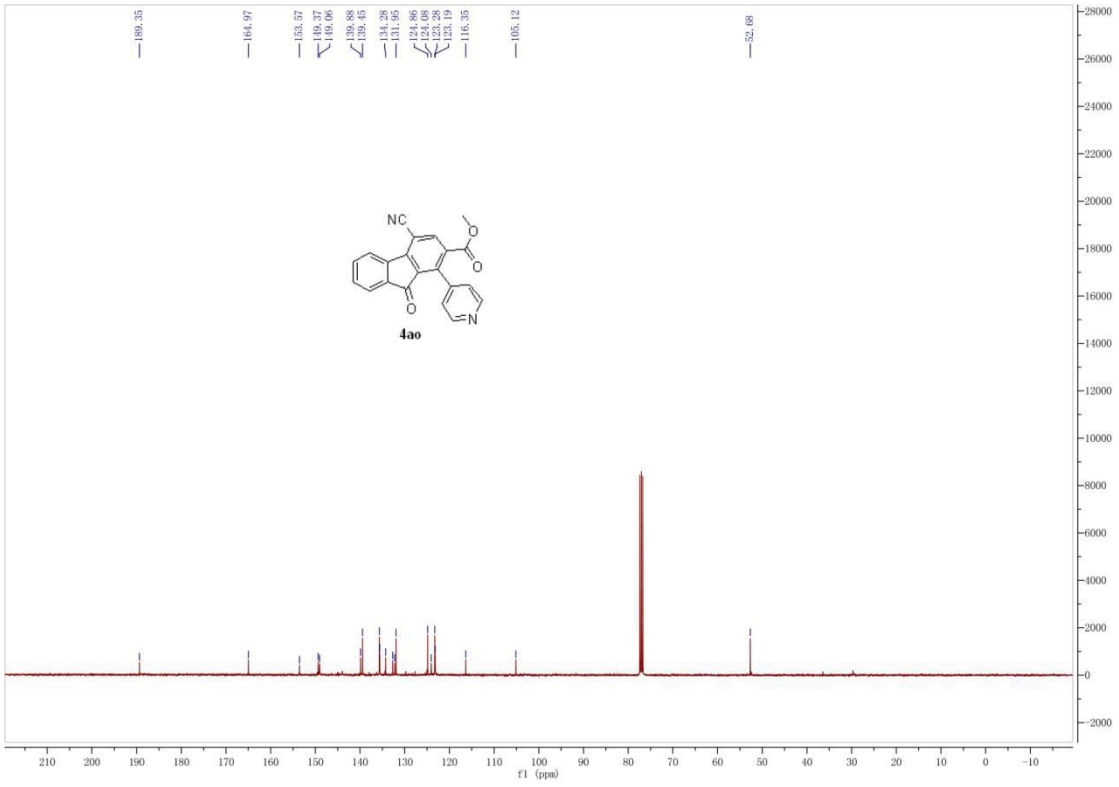
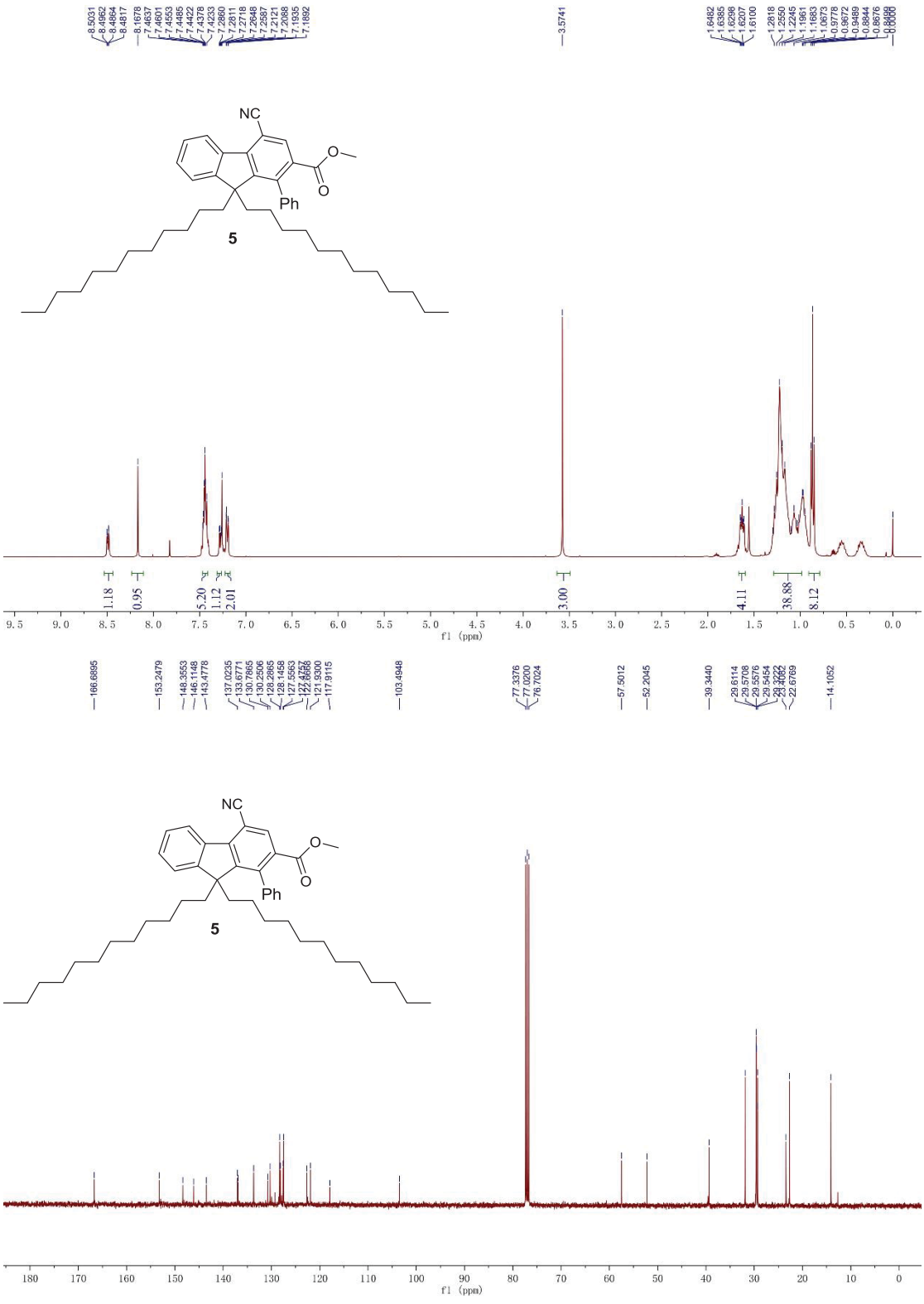
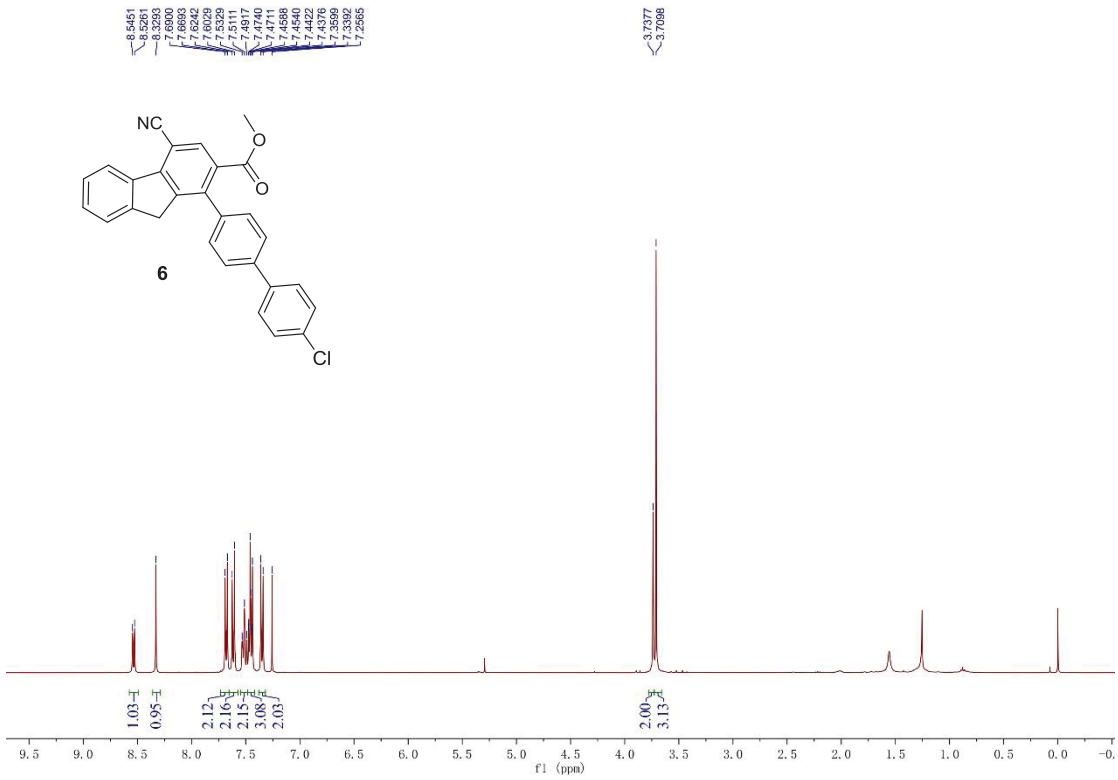
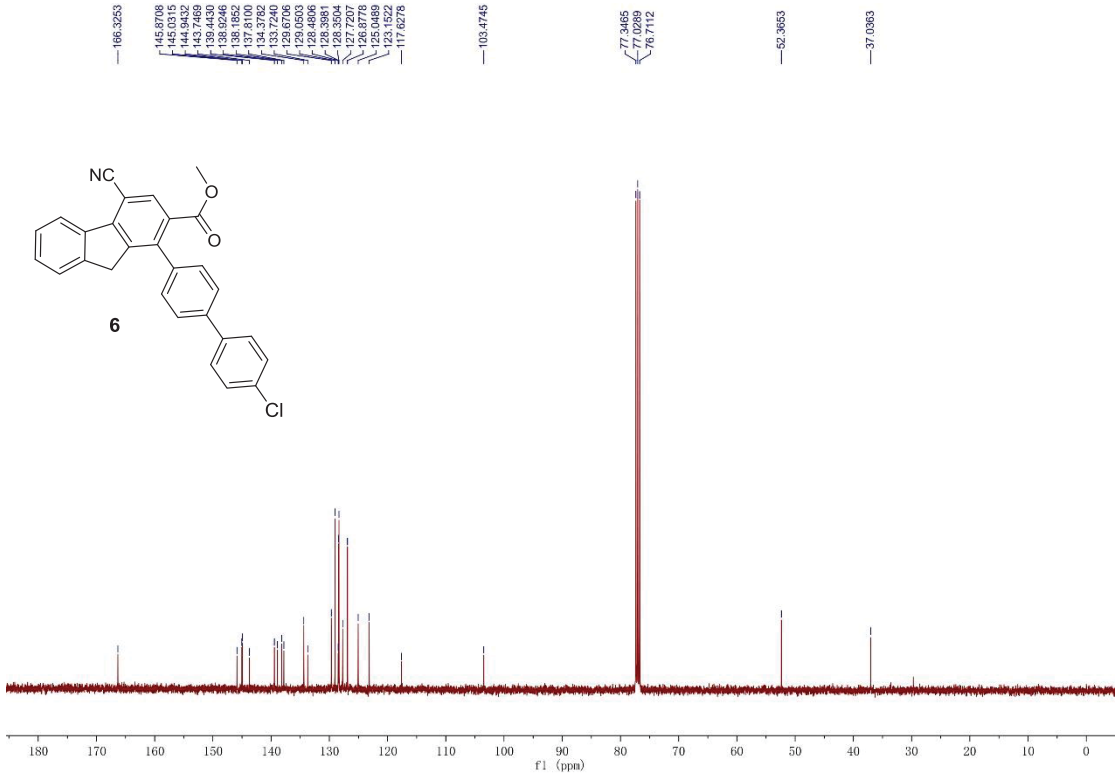
8.25
7.77
7.76
7.74
7.57
7.43
7.41
7.38
7.36
7.34
7.33
7.31
3.59
NC
O
O
O
N
4ao
1.00
1.95
1.13
1.91
2.39
1.27
3.05
f1 (ppm)


189.35
164.97
153.57
149.37
149.06
139.88
139.45
134.28
131.95
124.86
124.08
123.28
123.19
116.35
105.12
52.68
NC
O
O
O
N
4ao
f1 (ppm)


NC
O
O
Ph
5
1.18
0.95
5.20
1.12
2.01
3.00
4.11
38.88
8.12
f1 (ppm)
NC
O
O
Ph
5
f1 (ppm)


8.5451
8.5261
8.3293
7.6900
7.6693
7.6242
7.6029
7.5329
7.5111
7.4917
7.4740
7.4711
7.4588
7.4540
7.4422
7.4376
7.3599
7.3392
7.2565
3.7377
3.7098
NC
O
O
6
Cl
1.03
0.95
2.12
2.16
2.15
3.08
2.03
2.00
3.13
f1 (ppm)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145.8708
145.0315
144.9432
143.7469
139.4430
138.9246
138.1852
137.8100
134.3782
133.7240
129.6706
129.1553
128.4806
128.3981
128.3504
127.7207
126.8778
125.0489
123.1522
117.6278
103.4745
77.3465
77.0289
76.7112
52.3653
37.0363
NC
O
O
6
Cl
f1 (ppm)