

Supplementary Data

Iodine-catalyzed efficient synthesis of xanthene/thioxanthene-indole derivatives under mild conditions

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1. General Experimental

Melting points were determined on XT-4A melting-point apparatus and were uncorrected. The NMR spectra were recorded on a Bruker Avance 400 (^1H : 400 MHz, ^{13}C :100 MHz) spectrometer. HRMS were taken on AB QSTAR Pulsar mass spectrometer. The infrared (IR) spectra were acquired as thin films on a FT-IR spectrometer. Silica gel (200–300 mesh) for column chromatography and silica GF₂₅₄ for TLC were produced by Qingdao Marine Chemical Company (China). Starting materials and reagents used in the reactions were obtained from Acros, Aldrich, Adamas and Bidepharm without further purification.

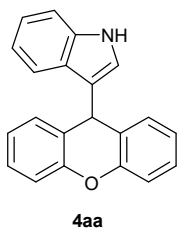
2. Experimental Procedures and Analytical Data

2.1 General procedure for the reaction of alcohols with nucleophiles

To a stirred solution of alcohol (1.0 mmol) and nucleophile (1.0 mmol) in EtOH (5 mL) at room temperature, I₂ (5 mol%) was added rapidly. Then being stirred at rt until complete consumption of starting material as monitored by TLC, the reaction mixture was quenched by the addition of saturated aq Na₂S₂O₃ (1 mL) and evaporated in vacuum. The residue was extracted with ethyl acetate (3×5 mL), and the combined extract was dried over anhydrous Na₂SO₄, filtered and concentrated under vacuum. The crude product was chromatographed on silica gel using petroleum ether/ethyl acetate as an eluent or purified by recrystallization from petroleum ether and ethyl acetate to afford the desired products.

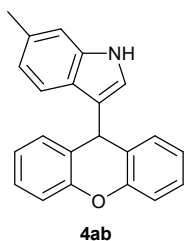
2.2 Spectroscopic data of the products of nucleophilic substitution

3-(9*H*-xanthen-9-yl)-1*H*-indole (4aa)



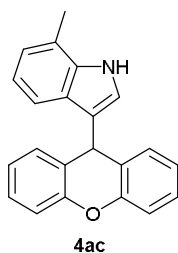
Yield 87%; White solid; Mp 148-149 °C; IR (KBr): 3425, 3052, 1599, 1481, 1446, 1312, 1258, 1096, 901, 756 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.92 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.18 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.15-7.07 (m, 6H), 7.03 (d, *J* = 2.4 Hz, 1H), 6.97-6.94 (m, 1H), 6.92-6.88 (m, 2H), 5.53 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 151.33, 136.75, 129.50, 127.73, 125.84, 124.44, 123.13, 122.83, 122.17, 120.38, 119.72, 119.65, 116.35, 111.25, 35.53; HRMS (ESI-TOF): *m/z* calcd for C₂₁H₁₅NONa [M+Na]⁺: 320.1046, found: 320.1047.

6-methyl-3-(9*H*-xanthen-9-yl)-1*H*-indole (4ab)



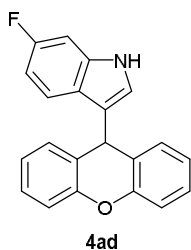
Yield 82%; Green solid; Mp 119-120 °C; IR (KBr): 3382, 3039, 2860, 1600, 1574, 1450, 1396, 1333, 1320, 1118, 1036, 903, 858, 765, 686, 512 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.78 (s, 1H), 7.23-7.10 (m, 8H), 7.01-6.96 (m, 1H), 6.95-6.89 (m, 2H), 6.84-6.79 (m, 1H), 5.52-5.50 (m, 1H), 2.42-2.39 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.36, 137.27, 132.01, 129.53, 127.71, 124.53, 123.69, 123.15, 122.28, 121.43, 120.08, 119.39, 116.33, 111.27, 35.58, 21.72; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{17}\text{NONa}$ $[\text{M}+\text{Na}]^+$: 334.1202, found: 334.1204.

7-methyl-3-(9H-xanthen-9-yl)-1H-indole (4ac)



Yield 84%; White solid; Mp 192-193 °C; IR (KBr): 3428, 3054, 2853, 1601, 1573, 1481, 1446, 1430, 1316, 1255, 1088, 902, 809, 750, 696 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.90 (s, 1H), 7.22-7.07 (m, 8H), 6.94-6.87 (m, 4H), 5.53 (s, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.30, 136.31, 129.49, 127.67, 125.39, 124.47, 123.10, 122.72, 122.54, 120.93, 120.35, 119.87, 117.46, 116.31, 35.59, 16.64; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{17}\text{NONa}$ $[\text{M}+\text{Na}]^+$: 334.1202, found: 334.1203.

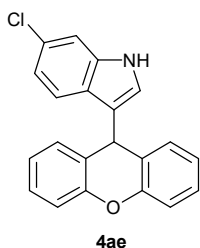
6-fluoro-3-(9H-xanthen-9-yl)-1H-indole (4ad)



Yield 97%; White solid; Mp 130-132 °C; IR (KBr): 3441, 3057, 1627, 1573, 1482, 1452, 1313, 1258, 1140, 1117, 1090, 847, 752 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.96 (s, 1H), 7.21-7.17 (m, 3H), 7.14 (dd, $J = 8.0, 0.8$ Hz, 2H), 7.08-7.07 (m, 3H), 6.97 (dd, $J = 9.6, 2.4$ Hz, 1H), 6.94-6.90 (m, 2H), 6.72-6.67 (m, 1H), 5.49 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 159.97 (d, $J = 236.7$ Hz), 151.28, 136.79 (d, $J = 12.3$ Hz), 129.39,

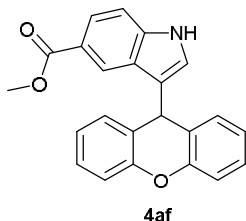
127.85, 124.08, 123.15, 122.95 (d, $J = 3.5$ Hz), 122.28, 120.50 (d, $J = 9.9$ Hz), 120.34, 116.41, 108.47 (d, $J = 24.3$ Hz), 97.54 (d, $J = 25.8$ Hz), 35.56; HRMS (ESI-TOF): m/z calcd for $C_{21}H_{13}FNO$ $[M-H]^-$: 314.0987, found: 314.0989.

6-chloro-3-(9H-xanthen-9-yl)-1H-indole (4ae)



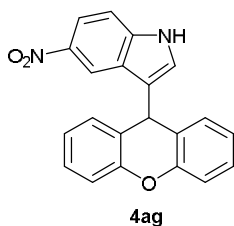
Yield 92%; White solid; Mp 151-152 °C; IR (KBr): 3432, 3064, 1599, 1572, 1474, 1447, 1307, 1250, 1093, 904, 798, 756 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 1H), 7.23 (s, 1H), 7.17-7.11 (m, 5H), 7.05-7.02 (m, 3H), 6.91-6.88 (m, 3H), 5.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.28, 137.17, 129.40, 128.18, 127.93, 124.33, 124.03, 123.37, 123.22, 120.60, 120.45, 116.46, 111.22, 35.49; HRMS (ESI-TOF): m/z calcd for $C_{21}H_{13}ClNO$ $[M-H]^-$: 330.0691, found: 330.0694.

Methyl 3-(9H-xanthen-9-yl)-1H-indole-5-carboxylate (4af)



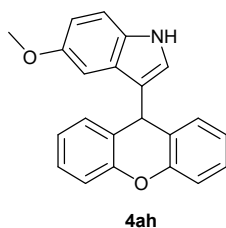
Yield 98%; Yellow solid; Mp 193-194 °C; IR (KBr): 3298, 2946, 2842, 1691, 1613, 1574, 1480, 1447, 1368, 1281, 1243, 1219, 1117, 902, 747 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): δ 8.29 (t, $J = 0.8$ Hz, 2H), 7.86 (dd, $J = 8.8, 1.6$ Hz, 1H), 7.33 (dd, $J = 8.8, 0.8$ Hz, 1H), 7.22-7.18 (m, 2H), 7.17-7.12 (m, 4H), 7.01 (d, $J = 2.0$ Hz, 1H), 6.96-6.92 (m, 2H), 5.61 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.09, 151.36, 139.05, 129.23, 127.86, 125.69, 124.40, 124.19, 123.60, 123.19, 122.35, 121.87, 116.53, 110.98, 51.93, 35.23; HRMS (ESI-TOF): m/z calcd for $C_{23}H_{17}NO_3Na$ $[M+Na]^+$: 378.1101, found: 378.1103.

5-nitro-3-(9*H*-xanthen-9-yl)-1*H*-indole (4ag)



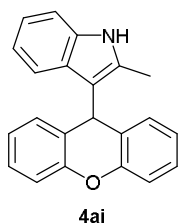
Yield 81%; Brown solid; Mp 234-235 °C; IR (KBr): 3334, 1601, 1460, 1448, 1325, 1290, 1254, 1093, 1040, 899, 749, 739 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 11.81 (s, 1H), 8.15 (s, 1H), 7.93 (t, $J = 8.8$ Hz, 1H), 7.67 (s, 1H), 7.53 (d, $J = 9.2$ Hz, 1H), 7.25 (s, 4H), 7.19 (d, $J = 7.2$ Hz, 2H), 7.03-7.00 (m, 2H), 5.78 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.03, 140.71, 140.38, 130.04, 128.57, 127.76, 124.78, 124.34, 123.92, 122.57, 117.07, 116.65, 116.05, 112.70, 34.81; HRMS (ESI-TOF): m/z calcd for $\text{C}_{21}\text{H}_{14}\text{N}_2\text{O}_3\text{Na}$ $[\text{M}+\text{Na}]^+$: 365.0897, found: 365.0898.

5-methoxy-3-(9*H*-xanthen-9-yl)-1*H*-indole (4ah)



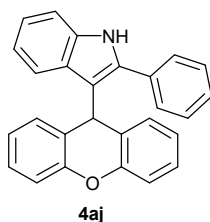
Yield 85%; White solid; Mp 179-180 °C; IR (KBr): 3332, 2831, 1578, 1479, 1465, 1322, 1254, 1211, 1172, 1064, 1029, 903, 837, 747 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.89 (s, 1H), 7.22-7.16 (m, 3H), 7.14-7.12 (m, 4H), 7.08 (d, $J = 2.4$ Hz, 1H), 6.95-6.91 (m, 2H), 6.79-6.77 (m, 2H), 5.51 (s, 1H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 153.83, 151.34, 131.84, 129.50, 127.70, 126.33, 124.32, 123.30, 123.12, 120.34, 116.26, 112.14, 111.83, 101.48, 55.69, 35.53; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{17}\text{NO}_2\text{Na}$ $[\text{M}+\text{Na}]^+$: 350.1151, found: 350.1148.

2-methyl-3-(9*H*-xanthen-9-yl)-1*H*-indole (4ai)



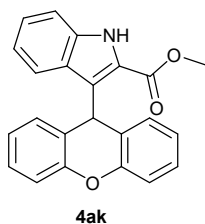
Yield 92%; Yellow solid; Mp 194-195 °C; IR (KBr): 3411, 3044, 2916, 1602, 1572, 1480, 1449, 1302, 1255, 1117, 1096, 902, 744, 595 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.81 (s, 1H), 7.26 (d, $J = 8.4$ Hz, 1H), 7.19-7.11 (m, 5H), 7.09-7.04 (m, 1H), 6.97-6.93 (m, 2H), 6.91-6.86 (m, 3H), 5.61 (s, 1H), 2.36 (d, $J = 1.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.29, 135.34, 132.29, 129.40, 127.62, 124.11, 123.06, 121.15, 119.47, 118.87, 116.15, 115.19, 110.23, 33.70, 12.04; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{17}\text{NONa}$ $[\text{M}+\text{Na}]^+$: 334.1202, found: 334.1200.

2-phenyl-3-(9H-xanthen-9-yl)-1H-indole (4aj)



Yield 86%; Green solid; Mp 234-236 °C; IR (KBr): 3392, 3022, 1570, 1457, 1447, 1314, 1250, 1094, 898, 747, 696 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.16 (s, 1H), 7.65-7.63 (m, 2H), 7.49-7.45 (m, 2H), 7.42-7.37 (m, 2H), 7.19-7.15 (m, 2H), 7.13-7.10 (m, 3H), 7.01-6.95 (m, 3H), 6.88-6.82 (m, 3H), 5.77 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.52, 137.18, 136.51, 132.66, 129.12, 129.03, 128.42, 128.39, 127.67, 126.93, 124.24, 123.08, 122.37, 120.96, 119.80, 116.16, 114.02, 110.82, 34.08; HRMS (ESI-TOF): m/z calcd for $\text{C}_{27}\text{H}_{19}\text{NONa}$ $[\text{M}+\text{Na}]^+$: 396.1359, found: 396.1357.

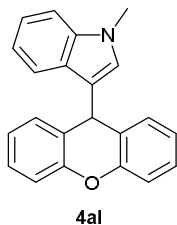
Methyl 3-(9H-xanthen-9-yl)-1H-indole-2-carboxylate (4ak)



Yield 90%; White solid; Mp 213-214 °C; IR (KBr): 3342, 1685, 1576, 1539, 1460, 1449, 1321, 1251, 1198, 1093, 902, 746 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.98 (s, 1H), 7.32 (d, $J = 8.0$ Hz, 1H), 7.22-7.11 (m, 6H), 6.98 (d, $J = 6.8$ Hz, 2H), 6.87-6.83 (m, 3H), 6.58 (s, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.99, 150.90, 136.44, 129.65, 127.90, 127.00, 125.71, 123.41, 123.35, 123.10, 122.20, 120.57, 116.30, 111.85,

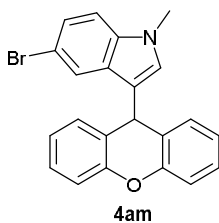
52.15, 33.62; HRMS (ESI-TOF): m/z calcd for $C_{23}H_{17}NO_3Na$ $[M+Na]^+$: 378.1101, found: 378.1102.

1-methyl-3-(9H-xanthen-9-yl)-1H-indole (4al)



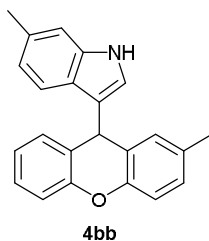
Yield 92%; Green solid; Mp 154-155 °C; IR (KBr): 3455, 3044, 2930, 2826, 1600, 1573, 1447, 1329, 1310, 1250, 1094, 896, 747, 679 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): δ 7.43-7.40 (m, 1H), 7.27-7.23 (m, 1H), 7.20-7.13 (m, 7H), 7.01-6.96 (m, 1H), 6.94-6.90 (m, 2H), 6.90-6.88 (m, 1H), 5.53 (d, $J = 3.2$ Hz, 1H), 3.71 (d, $J = 1.2$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.31, 137.38, 129.53, 127.64, 127.63, 127.48, 126.35, 124.77, 123.12, 121.67, 119.65, 119.19, 119.13, 116.34, 116.33, 109.34, 35.40, 32.76; HRMS (ESI-TOF): m/z calcd for $C_{22}H_{17}NONa$ $[M+Na]^+$: 334.1202, found: 334.1202.

5-bromo-1-methyl-3-(9H-xanthen-9-yl)-1H-indole (4am)



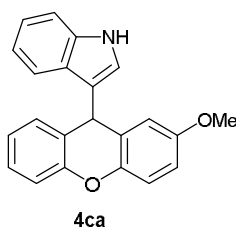
Yield 98%; White solid; Mp 178-180 °C; IR (KBr): 3447, 3059, 2917, 1599, 1571, 1445, 1421, 1377, 1294, 1213, 1148, 902, 790, 748, 647 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): δ 7.53 (t, $J = 1.6$ Hz, 1H), 7.23-7.16 (m, 3H), 7.14-7.12 (m, 2H), 7.08 (d, $J = 8.4$ Hz, 3H), 6.94-6.90 (m, 2H), 6.81 (s, 1H), 5.45 (s, 1H), 3.64 (t, $J = 2.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.29, 135.99, 129.31, 128.73, 127.97, 127.85, 124.60, 124.43, 123.22, 121.97, 118.91, 116.51, 112.68, 110.91, 35.22, 32.93; HRMS (ESI-TOF): m/z calcd for $C_{22}H_{16}BrNONa$ $[M+Na]^+$: 412.0307, found: 412.0304.

6-methyl-3-(2-methyl-9H-xanthen-9-yl)-1H-indole (4bb)



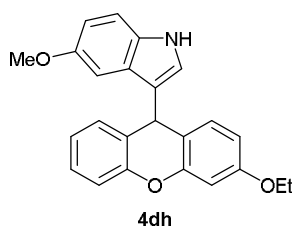
Yield 93%; Yellow solid; Mp 58-59 °C; IR (KBr): 3415, 1700, 1653, 1618, 1481, 1453, 1255, 1139, 1102, 799, 753 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.81 (s, 1H), 7.28-7.23 (m, 1H), 7.18-7.06 (m, 5H), 7.00-6.97 (m, 2H), 6.93-6.89 (m, 2H), 6.83 (d, $J = 8.4$ Hz, 1H), 5.46 (d, $J = 6.8$ Hz, 1H), 2.41-2.38 (m, 3H), 2.17-2.15 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.38, 149.17, 137.23, 132.40, 131.95, 129.81, 129.63, 128.44, 127.63, 124.51, 124.01, 123.73, 122.95, 122.05, 121.39, 120.56, 119.34, 116.29, 116.04, 111.25, 35.60, 21.73, 20.81; HRMS (ESI-TOF): m/z calcd for $\text{C}_{23}\text{H}_{18}\text{NO}$ $[\text{M}-\text{H}]^-$: 324.1394, found: 324.1395.

3-(2-methoxy-9H-xanthen-9-yl)-1H-indole (4ca)



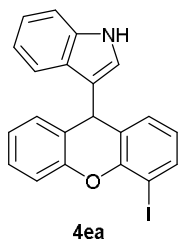
Yield 91%; Yellow solid; Mp 150-151 °C; IR (KBr): 3430, 2834, 1598, 1481, 1455, 1350, 1315, 1239, 1202, 1040, 945, 810, 747 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.99 (s, 1H), 7.37 (d, $J = 8.0$ Hz, 1H), 7.32 (dd, $J = 8.0, 0.4$ Hz, 1H), 7.17-7.06 (m, 6H), 6.99-6.95 (m, 1H), 6.92-6.88 (m, 1H), 6.76-6.73 (m, 1H), 6.65 (s, 1H), 5.51 (s, 1H), 3.63 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.20, 151.48, 145.48, 136.74, 129.48, 127.67, 125.81, 125.17, 123.87, 122.86, 122.65, 122.15, 120.36, 119.66, 119.64, 116.99, 116.26, 113.96, 113.44, 111.21, 55.56, 35.97; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{16}\text{NO}_2$ $[\text{M}-\text{H}]^-$: 326.1187, found: 326.1188.

3-(3-ethoxy-9H-xanthen-9-yl)-5-methoxy-1H-indole (4dh)



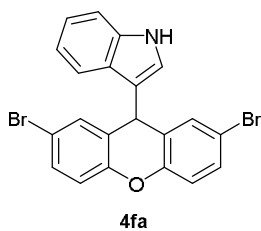
Yield 91%; White solid; Mp 146-147 °C; IR (KBr): 3344, 2975, 1629, 1607, 1509, 1485, 1431, 1312, 1283, 1233, 1154, 1113, 860, 780, 759 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.91 (s, 1H), 7.23-7.15 (m, 2H), 7.14-7.07 (m, 3H), 7.02-6.99 (m, 1H), 6.95 (m, 1H), 6.80-6.77 (m, 2H), 6.69-6.67 (m, 1H), 6.54-6.50 (m, 1H), 5.45 (s, 1H), 4.04-3.99 (m, 2H), 3.69-3.68 (m, 3H), 1.43-1.39 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.54, 153.74, 151.87, 151.24, 131.87, 130.10, 129.59, 127.61, 126.33, 124.51, 123.27, 123.12, 120.60, 116.19, 112.02, 111.84, 110.49, 101.53, 63.60, 55.69, 34.91, 14.86; HRMS (ESI-TOF): m/z calcd for $\text{C}_{24}\text{H}_{20}\text{NO}_3$ $[\text{M}-\text{H}]^-$: 370.1449, found: 370.1448.

3-(4-iodo-9H-xanthen-9-yl)-1H-indole (4ea)



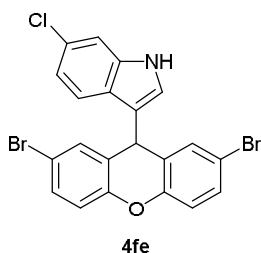
Yield 80%; Green oil; IR (KBr): 3415, 1618, 1558, 1485, 1455, 1438, 1354, 1245, 1101, 891, 742 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.02 (s, 1H), 7.65-7.63 (m, 1H), 7.32 (t, J = 7.2 Hz, 2H), 7.27 (dd, J = 8.0, 1.2 Hz, 1H), 7.22-7.18 (m, 1H), 7.16-7.12 (m, 1H), 7.09-7.05 (m, 3H), 7.00-6.96 (m, 1H), 6.96-6.92 (m, 1H), 6.65 (t, J = 8.0 Hz, 1H), 5.52 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.38, 150.42, 137.57, 136.72, 129.66, 129.12, 127.86, 125.79, 125.62, 124.64, 124.50, 123.74, 123.14, 122.29, 119.76, 119.68, 119.44, 116.73, 111.32, 84.62, 36.11; HRMS (ESI-TOF): m/z calcd for $\text{C}_{21}\text{H}_{13}\text{INO}$ $[\text{M}-\text{H}]^-$: 422.0047, found: 422.0051.

3-(2,7-dibromo-9H-xanthen-9-yl)-1H-indole (4fa)



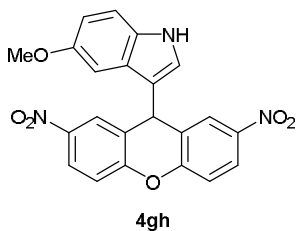
Yield 90%; White solid; Mp 216-217 °C; IR (KBr): 3436, 1616, 1542, 1472, 1405, 1297, 1251, 1181, 1099, 1012, 926, 765, 746 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.11 (s, 1H), 7.38 (d, $J = 8.0$ Hz, 1H), 7.29 (d, $J = 2.4$ Hz, 1H), 7.27 (d, $J = 2.4$ Hz, 1H), 7.24 (s, 1H), 7.19-7.14 (m, 4H), 7.02 (s, 1H), 7.00-6.96 (m, 2H), 5.46 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 149.87, 136.82, 132.18, 130.97, 125.59, 125.35, 122.77, 122.49, 119.96, 119.31, 119.16, 118.20, 115.60, 111.42, 35.31; HRMS (ESI-TOF): m/z calcd for $\text{C}_{21}\text{H}_{12}\text{Br}_2\text{NO}$ $[\text{M}-\text{H}]^-$: 451.9291, found: 451.9294.

6-chloro-3-(2,7-dibromo-9H-xanthen-9-yl)-1H-indole (4fe)



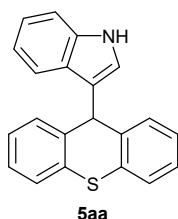
Yield 91%; White solid; Mp 210-211 °C; IR (KBr): 3457, 1616, 1466, 1401, 1278, 1249, 1179, 1064, 899, 803, 654 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.12 (s, 1H), 7.37 (d, $J = 1.2$ Hz, 1H), 7.31-7.28 (m, 2H), 7.20 (d, $J = 2.4$ Hz, 1H), 7.14 (dd, $J = 2.0, 0.8$ Hz, 2H), 7.09 (d, $J = 8.4$ Hz, 1H), 7.02 (d, $J = 8.8$ Hz, 2H), 6.93 (dd, $J = 8.4, 1.6$ Hz, 1H), 5.42 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 149.83, 137.26, 132.04, 131.13, 128.56, 125.19, 123.84, 123.39, 120.79, 120.23, 119.08, 118.29, 115.67, 111.41, 35.21; HRMS (ESI-TOF): m/z calcd for $\text{C}_{21}\text{H}_{11}\text{Br}_2\text{ClNO}$ $[\text{M}-\text{H}]^-$: 485.8901, found: 485.8900.

3-(2,7-dinitro-9H-xanthen-9-yl)-5-methoxy-1H-indole (4gh)



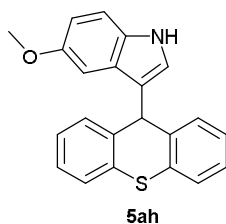
Yield 85%; White solid; Mp 172-173 °C; IR (KBr): 3415, 2935, 1637, 1618, 1471, 1410, 1256, 1110, 1058, 1019, 848, 820 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.00 (s, 1H), 7.25-7.22 (m, 1H), 7.15-7.11 (m, 3H), 7.06-7.04 (m, 4H), 6.83-6.80 (m, 1H), 6.68 (d, $J = 2.4$ Hz, 1H), 5.40 (1H, s), 3.68 (d, $J = 1.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 153.99, 149.54, 131.98, 129.24, 128.15, 128.08, 125.90, 125.07, 123.46, 118.81, 117.70, 112.30, 112.10, 101.31, 55.72, 35.52; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{14}\text{N}_3\text{O}_6$ [M-H] $^-$: 416.0888, found: 416.0890.

3-(9H-thioxanthen-9-yl)-1H-indole (5aa)



Yield 90%; White solid; Mp 158-159 °C; IR (KBr): 3388, 3052, 1462, 1456, 1418, 1348, 1253, 1122, 1077, 798, 760, 735 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.88 (s, 1H), 7.52 (d, $J = 8.0$ Hz, 1H), 7.46-7.44 (m, 2H), 7.38-7.36 (m, 2H), 7.30 (dd, $J = 8.0, 0.8$ Hz, 1H), 7.20-7.14 (m, 5H), 7.06-7.02 (m, 1H), 6.76 (s, 1H), 5.41 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 138.01, 136.62, 133.29, 128.78, 127.09, 126.59, 126.56, 126.48, 123.61, 121.98, 120.14, 119.58, 114.28, 111.40, 45.77; HRMS (ESI-TOF): m/z calcd for $\text{C}_{21}\text{H}_{15}\text{NSNa}$ [M+Na] $^+$: 336.0817, found: 336.0813.

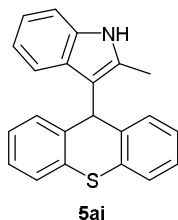
5-methoxy-3-(9H-thioxanthen-9-yl)-1H-indole (5ah)



Yield 91%; Yellow solid; Mp 166-168 °C; IR (KBr): 3436, 3038, 2952, 2827, 1625, 1584, 1486, 1463, 1440, 1257, 1208, 1237, 1175, 1044, 936, 822, 749 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.87 (s, 1H), 7.47-7.45 (m, 2H), 7.40-7.38 (m, 2H), 7.22-7.18 (m, 5H), 6.88 (s, 1H), 6.83-6.81 (m, 1H), 6.76 (s, 1H), 5.36 (s, 1H), 3.71 (d, $J = 1.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 153.81, 137.97, 133.41, 131.77, 128.71, 127.11, 126.93,

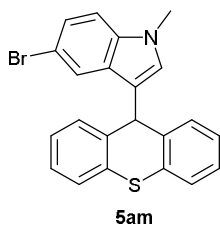
126.58, 126.49, 124.48, 113.88, 112.05, 102.09, 55.87, 45.88; HRMS (ESI-TOF): m/z calcd for $C_{22}H_{17}NOSNa$ $[M+Na]^+$: 366.0923, found: 366.0925.

2-methyl-3-(9*H*-thioxanthen-9-yl)-1*H*-indole (5ai)



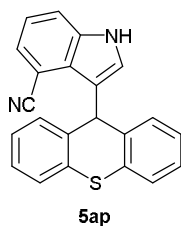
Yield 85%; Yellow solid; Mp 85-86 °C; IR (KBr): 3407, 3055, 1620, 1455, 1443, 1384, 1297, 1246, 1126, 1035, 775, 743, 509 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): δ 8.03 (s, 1H), 7.50 (d, $J = 7.6$ Hz, 2H), 7.40 (d, $J = 8.4$ Hz, 1H), 7.18-7.14 (m, 3H), 7.07 (d, $J = 8.0$ Hz, 1H), 7.03-6.92 (m, 5H), 4.99 (s, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.20, 135.74, 133.85, 133.67, 128.19, 127.98, 126.56, 126.29, 121.29, 120.96, 119.41, 110.53, 108.47, 42.99, 12.41; HRMS (ESI-TOF): m/z calcd for $C_{22}H_{17}NSNa$ $[M+Na]^+$: 350.0974, found: 350.0972.

5-bromo-1-methyl-3-(9*H*-thioxanthen-9-yl)-1*H*-indole (5am)



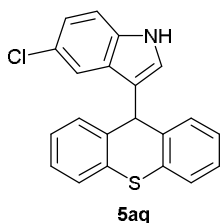
Yield 89%; White solid; Mp 184-185 °C; IR (KBr): 3423, 3058, 1653, 1473, 1463, 1419, 1197, 1141, 1078, 859, 770, 747 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): δ 7.64 (s, 1H), 7.45 (t, $J = 4.8$ Hz, 2H), 7.38 (t, $J = 4.8$ Hz, 2H), 7.25-7.19 (m, 5H), 7.08 (d, $J = 8.4$ Hz, 1H), 6.63 (s, 1H), 5.38 (s, 1H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.69, 135.93, 133.05, 129.10, 128.72, 128.45, 127.19, 126.72, 124.34, 122.33, 112.71, 112.57, 110.97, 45.54, 32.95; HRMS (ESI-TOF): m/z calcd for $C_{22}H_{16}BrNSNa$ $[M+Na]^+$: 428.0079, found: 428.0081.

3-(9*H*-thioxanthen-9-yl)-1*H*-indole-4-carbonitrile (5ap)



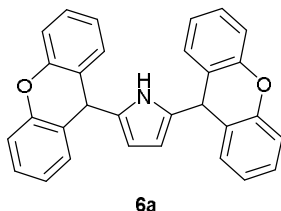
Yield 81%; White solid; Mp 266-267 °C; IR (KBr): 3325, 3053, 2225, 1650, 1457, 1442, 1343, 1276, 1175, 1113, 1045, 828, 791, 787 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.80 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.69 (s, 1H), 7.58-7.52 (m, 3H), 7.30-7.18 (m, 7H), 5.82 (s, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 138.72, 136.99, 131.74, 128.53, 127.27, 127.15, 127.12, 124.81, 121.55, 120.11, 118.03, 101.11, 42.95; HRMS (ESI-TOF): *m/z* calcd for C₂₂H₁₄N₂SNa [M+Na]⁺: 361.0770, found: 361.0771.

5-chloro-3-(9*H*-thioxanthen-9-yl)-1*H*-indole (5aq)



Yield 83%; Green oil; IR (KBr): 3397, 1719, 1565, 1461, 1415, 1315, 1214, 1082, 1062, 894, 859, 800, 741 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.82 (s, 1H), 7.45-7.41 (m, 3H), 7.34-7.32 (m, 2H), 7.19-7.15 (m, 4H), 7.10 (d, *J* = 8.4 Hz, 1H), 7.05 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.69 (d, *J* = 2.4 Hz, 1H), 5.34 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 137.61, 134.92, 133.21, 128.75, 127.51, 127.20, 126.79, 126.72, 125.31, 124.89, 122.31, 119.35, 114.33, 112.39, 45.66; HRMS (ESI-TOF): *m/z* calcd for C₂₁H₁₃ClNS [M-H]⁻: 346.0463, found: 346.0460.

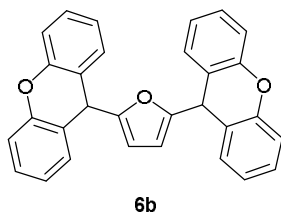
2,5-di(9*H*-xanthen-9-yl)-1*H*-pyrrole (6a)



Yield 92%; White solid; Mp 198-200 °C; IR (KBr): 3379, 2845, 1601, 1573, 1481, 1447, 1317, 1256, 1120, 1035, 900, 764, 747 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.35 (s,

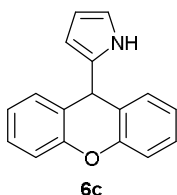
1H), 7.20-7.15 (m, 4H), 7.03 (d, $J = 8.4$ Hz, 8H), 6.96 (t, $J = 7.2$ Hz, 4H), 6.02-6.01 (m, 2H), 5.23 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ ; HRMS (ESI-TOF): m/z calcd for $\text{C}_{30}\text{H}_{20}\text{NO}_2$ $[\text{M}-\text{H}]^-$: 426.1500, found: 426.1502.

2,5-di(9H-xanthen-9-yl)furan (6b)



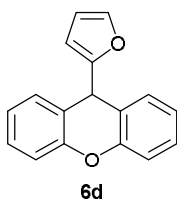
Yield 80%; Pink solid; Mp 113-114 °C; IR (KBr): 3410, 1618, 1480, 1451, 1257, 1119, 1012, 903, 746 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.23-7.22 (m, 8H), 7.13-7.11 (m, 4H), 7.04-7.01 (m, 4H), 5.63-5.61 (m, 2H), 5.29 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.49, 151.33, 129.67, 128.32, 123.09, 121.27, 116.60, 107.02, 37.83; HRMS (ESI-TOF): m/z calcd for $\text{C}_{30}\text{H}_{20}\text{KO}_3$ $[\text{M}+\text{K}]^+$: 467.1044, found: 467.1047.

2-(9H-xanthen-9-yl)-1H-pyrrole (6c)



Yield 83%; White solid; Mp 112-113 °C; IR (KBr): 3403, 1600, 1576, 1481, 1452, 1254, 1186, 1124, 1094, 1027, 902, 756, 734, 716 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.68 (s, 1H), 7.26-7.21 (m, 2H), 7.16-7.10 (m, 4H), 7.06-7.01 (m, 2H), 6.64-6.62 (m, 1H), 6.18-6.16 (m, 1H), 6.15-6.12 (m, 1H), 5.37 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.25, 134.25, 129.48, 129.45, 128.23, 123.42, 122.87, 118.15, 116.67, 107.95, 107.27, 37.24; HRMS (ESI-TOF): m/z calcd for $\text{C}_{17}\text{H}_{12}\text{NO}$ $[\text{M}-\text{H}]^-$: 246.0924, found: 246.0921.

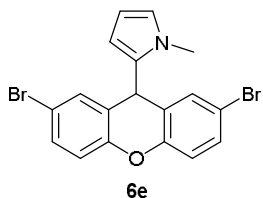
9-(furan-2-yl)-9H-xanthene (6d)



Yield 81%; White solid; Mp 96-97 °C; IR (KBr): 3464, 3040, 1604, 1577, 1481, 1451, 1318, 1255, 1208, 1141, 1070, 1008, 926, 903, 748, 687 cm^{-1} ; ^1H NMR (400 MHz,

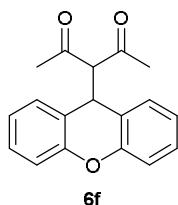
CDCl₃): δ 7.29-7.28 (m, 1H), 7.27-7.23 (m, 4H), 7.12 (d, J = 8.4 Hz, 2H), 7.07-7.03 (m, 2H), 6.24-6.23 (m, 1H), 5.91-5.90 (m, 1H), 5.37 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 156.98, 151.40, 142.20, 129.49, 128.40, 123.20, 121.35, 116.74, 110.15, 106.56, 37.95; HRMS (ESI-TOF): m/z calcd for C₁₇H₁₂KO₂ [M+K]⁺: 287.0469, found: 287.0465.

2-(2,7-dibromo-9H-xanthen-9-yl)-1-methyl-1H-pyrrole (6e)



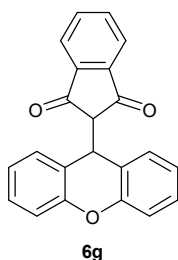
Yield 80%; White solid; Mp 142-143 °C; IR (KBr): 3458, 1466, 1406, 1300, 1253, 1182, 1111, 809, 719 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.33-7.30 (m, 2H), 7.09-7.08 (m, 2H), 6.96 (d, J = 8.8 Hz, 2H), 6.55 (t, J = 2.4 Hz, 1H), 6.24-6.23 (m, 1H), 6.12-6.10 (m, 1H), 5.42 (s, 1H), 3.07 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 149.58, 131.80, 131.41, 124.09, 123.87, 118.27, 115.92, 111.16, 106.61, 36.38, 34.71; HRMS (ESI-TOF): m/z calcd for C₁₈H₁₄Br₂NO [M+H]⁺: 417.9437, found: 417.9440.

3-(9H-xanthen-9-yl)pentane-2,4-dione (6f)



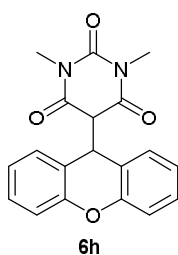
Yield 88%; White solid; Mp 136-137 °C; IR (KBr): 3462, 1725, 1701, 1639, 1478, 1459, 1354, 1278, 1253, 1146, 1118, 766, 746 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.27-7.23 (m, 2H), 7.20 (dd, J = 7.6, 1.6 Hz, 2H), 7.16 (dd, J = 8.4, 1.2 Hz, 2H), 7.06-7.02 (m, 2H), 4.84 (d, J = 9.6 Hz, 1H), 4.11 (d, J = 10 Hz, 1H), 1.87 (s, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 201.86, 153.29, 129.11, 128.43, 123.76, 123.30, 116.82, 73.64, 40.22, 32.04; HRMS (ESI-TOF): m/z calcd for C₁₈H₁₅O₃ [M-H]⁻: 279.1027, found: 279.1025.

2-(9H-xanthen-9-yl)-1H-indene-1,3(2H)-dione (6g)



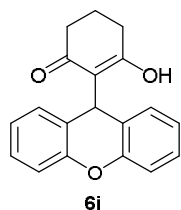
Yield 81%; Brown solid; Mp 140-141 °C; IR (KBr): 3440, 2924, 1745, 1710, 1599, 1574, 1486, 1456, 1347, 1284, 1223, 1124, 912, 873, 759, 586 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.82-7.78 (m, 2H), 7.72-7.68 (m, 2H), 7.18-7.13 (m, 4H), 7.08 (d, J = 8.0 Hz, 2H), 6.93-6.89 (m, 2H), 5.05 (d, J = 3.2 Hz, 1H), 3.37 (d, J = 2.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 198.75, 152.45, 142.78, 135.55, 128.59, 128.15, 123.27, 122.98, 120.65, 116.81, 62.36, 37.79; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{14}\text{O}_3\text{Na}$ $[\text{M}+\text{Na}]^+$: 349.0835, found: 349.0837.

1,3-dimethyl-5-(9H-xanthen-9-yl)pyrimidine-2,4,6(1H,3H,5H)-trione (6h)



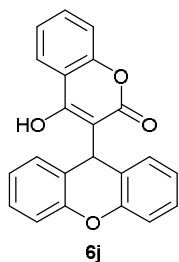
Yield 93%; White solid; Mp 179-180 °C; IR (KBr): 3413, 2967, 1749, 1679, 1601, 1478, 1379, 1283, 1257, 1121, 1109, 990, 764, 514 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.34-7.30 (m, 2H), 7.20-7.18 (m, 2H), 7.13-7.09 (m, 4H), 5.00 (d, J = 4.0 Hz, 1H), 3.73 (d, J = 3.6 Hz, 1H), 3.07 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 166.75, 152.82, 150.94, 129.57, 127.96, 123.66, 119.40, 116.80, 58.76, 44.54, 28.32; HRMS (ESI-TOF): m/z calcd for $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$: 359.1002, found: 359.1005.

3-hydroxy-2-(9H-xanthen-9-yl)cyclohex-2-en-1-one (6i)



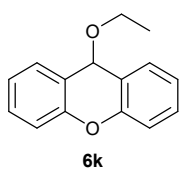
Yield 90%; White solid; Mp 242-243 °C; IR (KBr): 3416, 2509, 1616, 1569, 1447, 1375, 1256, 1194, 1087, 988, 905, 774, 750 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.12 (t, $J = 7.2$ Hz, 2H), 6.98-6.91 (m, 6H), 5.51 (s, 1H), 2.36 (s, 4H), 1.85 (t, $J = 6.0$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.41, 128.39, 127.39, 124.85, 123.08, 115.70, 30.79, 20.92; HRMS (ESI-TOF): m/z calcd for $\text{C}_{19}\text{H}_{15}\text{O}_3$ $[\text{M}-\text{H}]^-$: 291.1027, found: 291.1022.

4-hydroxy-3-(9H-xanthen-9-yl)-2H-chromen-2-one (6j)



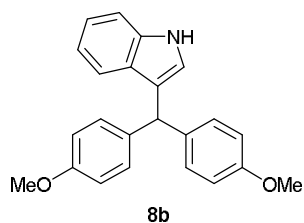
Yield 92%; White solid; Mp 218-219 °C; IR (KBr): 3231, 1685, 1628, 1566, 1497, 1483, 1455, 1396, 1302, 1267, 1201, 1168, 1066, 900, 747 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.07 (s, 1H), 7.60 (t, $J = 8.0$ Hz, 1H), 7.35 (d, $J = 8.4$ Hz, 2H), 7.19 (t, $J = 7.6$ Hz, 2H), 7.10-7.05 (m, 4H), 6.96 (t, $J = 7.2$ Hz, 2H), 5.92 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 161.26, 152.84, 151.44, 132.62, 128.64, 128.26, 124.41, 123.36, 122.74, 116.76, 116.60, 116.14, 32.83; HRMS (ESI-TOF): m/z calcd for $\text{C}_{22}\text{H}_{13}\text{O}_4$ $[\text{M}-\text{H}]^-$: 341.0819, found: 341.0820.

9-ethoxy-9H-xanthene (6k)



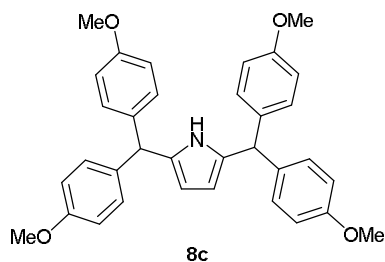
Yield 94%; Colorless oil; IR (KBr): 3414, 2974, 1607, 1480, 1340, 1257, 1213, 1062, 984, 904, 755 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.52 (d, $J = 7.6$ Hz, 2H), 7.34 (t, $J = 7.6$ Hz, 2H), 7.17-7.13 (m, 4H), 5.76 (s, 1H), 3.17-3.12 (m, 2H), 1.05 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.35, 129.96, 129.46, 123.19, 120.35, 116.59, 69.96, 59.54, 15.39; HRMS (ESI-TOF): m/z calcd for $\text{C}_{15}\text{H}_{15}\text{O}_2$ $[\text{M}+\text{H}]^+$: 227.1067, found: 227.1069.

3-(bis(4-methoxyphenyl)methyl)-1H-indole (8b)



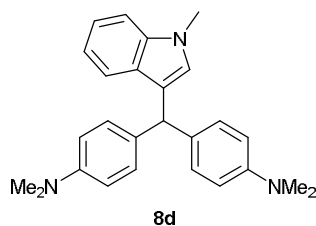
Yield 99%; Brown oil; IR (KBr): 3417, 2834, 1608, 1507, 1456, 1337, 1300, 1245, 1173, 1109, 1032, 815, 742 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.97 (s, 1H), 7.35-7.33 (m, 1H), 7.22 (d, $J = 8.0$ Hz, 1H), 7.18-7.12 (m, 5H), 7.00-6.97 (m, 1H), 6.83-6.80 (m, 4H), 6.54 (d, $J = 1.2$ Hz, 1H), 5.57 (s, 1H), 3.78 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.88, 136.74, 136.51, 129.83, 126.96, 123.93, 122.05, 120.63, 120.03, 119.33, 113.60, 111.04, 55.25, 47.11; HRMS (ESI-TOF): m/z calcd for $\text{C}_{23}\text{H}_{20}\text{NO}_2$ [M-H]: 342.1500, found: 342.1502.

2,5-bis(bis(4-methoxyphenyl)methyl)-1H-pyrrole (8c)



Yield 80%; Yellow solid; Mp 147-148 $^{\circ}\text{C}$; IR (KBr): 3416, 3339, 2835, 1700, 1610, 1507, 1464, 1302, 1249, 1174, 1111, 1032, 801, 786 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.48 (s, 1H), 7.05 (d, $J = 8.4$ Hz, 8H), 6.79 (d, $J = 8.4$ Hz, 8H), 5.57 (d, $J = 2.4$ Hz, 2H), 5.25 (s, 2H), 3.76 (s, 12H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.15, 135.67, 134.11, 129.72, 113.72, 107.67, 55.28, 48.96; HRMS (ESI-TOF): m/z calcd for $\text{C}_{34}\text{H}_{33}\text{NO}_4\text{K}$ [M+K] $^+$: 558.2041, found: 558.2041.

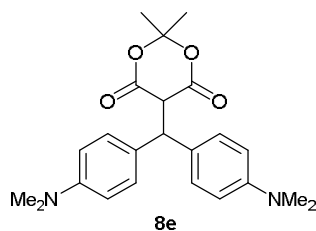
4,4'-((1-methyl-1H-indol-3-yl)methylene)bis(N,N-dimethylaniline) (8d)



Yield 84%; Purple solid; Mp 172-173 $^{\circ}\text{C}$; IR (KBr): 3416, 2854, 1611, 1517, 1474, 1442, 1328, 1227, 1199, 1165, 1116, 1056, 944, 814, 802, 743 cm^{-1} ; ^1H NMR (400 MHz,

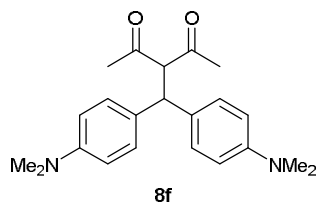
CDCl₃): δ 7.27-7.24 (m, 2H), 7.17-7.16 (m, 1H), 7.11-7.08 (m, 4H), 6.98-6.95 (m, 1H), 6.68-6.65 (m, 4H), 6.43 (d, J = 3.6 Hz, 1H), 5.50 (d, J = 4.0 Hz, 1H), 3.66-3.65 (m, 3H), 2.90-2.89 (m, 12H); ¹³C NMR (100 MHz, CDCl₃): δ 148.94, 137.48, 133.32, 129.54, 128.66, 127.61, 121.41, 120.36, 119.73, 118.64, 112.68, 109.03, 46.84, 40.92, 32.71; HRMS (ESI-TOF): m/z calcd for C₂₆H₂₉N₃Na [M+Na]⁺: 406.2254, found: 406.2252.

5-(bis(4-(dimethylamino)phenyl)methyl)-2,2-dimethyl-1,3-dioxane-4,6-dione (8e)



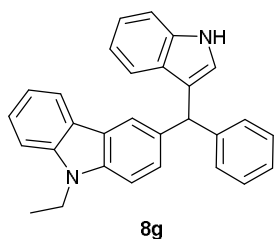
Yield 95%; Green solid; Mp 163-164 °C; IR (KBr): 3419, 2869, 1782, 1748, 1617, 1521, 1397, 1325, 1297, 1203, 1180, 1059, 1017, 902, 814 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.19 (d, J = 8.4 Hz, 4H), 6.66 (d, J = 8.8 Hz, 4H), 5.21 (d, J = 2.0 Hz, 1H), 4.24 (d, J = 2.4 Hz, 1H), 2.91 (s, 12H), 1.71 (s, 3H), 1.48 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 165.25, 149.40, 129.87, 128.40, 112.35, 105.01, 51.53, 48.21, 40.64, 28.30, 27.88; HRMS (ESI-TOF): m/z calcd for C₂₃H₂₇N₂O₄ [M-H]⁻: 395.1976, found: 395.1975.

3-(bis(4-(dimethylamino)phenyl)methyl)pentane-2,4-dione (8f)



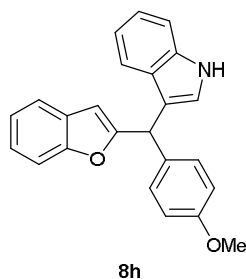
Yield 82%; Blue solid; Mp 148-149 °C; IR (KBr): 3426, 1734, 1692, 1613, 1521, 1446, 1356, 1226, 1166, 1062, 950, 830, 795, 543 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.09 (d, J = 8.0 Hz, 4H), 6.61 (d, J = 8.0 Hz, 4H), 4.65-4.58 (m, 2H), 2.85 (s, 12H), 1.99 (s, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 204.00, 149.32, 129.98, 128.26, 112.93, 75.05, 49.90, 40.55, 29.79; HRMS (ESI-TOF): m/z calcd for C₂₂H₂₇N₂O₂ [M-H]⁻: 351.2078, found: 351.2079.

3-((1*H*-indol-3-yl)(phenyl)methyl)-9-ethyl-9*H*-carbazole (8g)



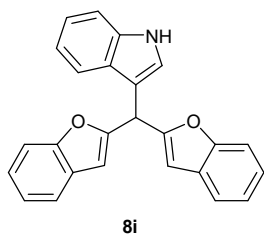
Yield 85%; White solid; Mp 194-195 °C; IR (KBr): 3397, 2973, 1598, 1470, 1417, 1331, 1231, 1146, 1090, 762, 743, 710 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.99-7.95 (m, 3H), 7.46-7.30 (m, 10H), 7.25-7.22 (m, 1H), 7.19-7.14 (m, 2H), 7.01-6.95 (m, 1H), 6.57 (s, 1H), 5.89 (t, $J = 4.8$ Hz, 1H), 4.36-4.31 (m, 2H), 1.44-1.40 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 144.75, 140.21, 138.75, 136.76, 134.59, 129.11, 128.29, 127.12, 127.03, 126.11, 125.48, 124.25, 122.86, 122.06, 120.83, 120.62, 120.52, 120.12, 119.37, 118.58, 111.04, 108.41, 108.22, 48.83, 37.60, 13.96; HRMS (ESI-TOF): m/z calcd for $\text{C}_{29}\text{H}_{23}\text{N}_2$ $[\text{M}-\text{H}]^-$: 399.1867, found: 399.1864.

3-(benzofuran-2-yl(4-methoxyphenyl)methyl)-1H-indole (8h)



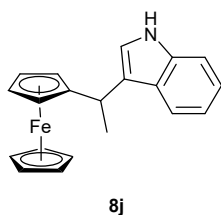
Yield 96%; Yellow solid; Mp 67-68 °C; IR (KBr): 3417, 1656, 1639, 1509, 1454, 1247, 1175, 1094, 814, 742 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.98 (s, 1H), 7.45-7.43 (m, 3H), 7.35 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.27-7.24 (m, 2H), 7.21-7.17 (m, 3H), 7.06-7.04 (m, 1H), 6.88-6.84 (m, 2H), 6.77 (s, 1H), 6.33-6.32 (m, 1H), 5.76 (d, $J = 3.2$ Hz, 1H), 3.80-3.79 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 160.46, 158.49, 155.06, 136.55, 133.19, 129.63, 128.70, 126.66, 123.55, 122.56, 122.28, 120.67, 119.64, 117.02, 113.92, 111.22, 104.55, 55.32, 42.31; HRMS (ESI-TOF): m/z calcd for $\text{C}_{24}\text{H}_{18}\text{NO}_2$ $[\text{M}-\text{H}]^-$: 352.1343, found: 352.1345.

3-(di(benzofuran-2-yl)methyl)-1H-indole (8i)



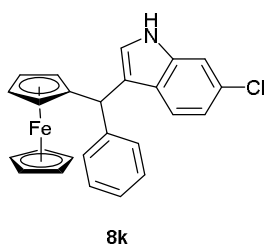
Yield 96%; Red solid; Mp 155-156 °C; IR (KBr): 3416, 3056, 1617, 1453, 1414, 1254, 1163, 1102, 953, 804, 747 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 8.04 (s, 1H), 7.56 (d, $J = 7.6$ Hz, 1H), 7.46 (dd, $J = 7.6, 0.8$ Hz, 2H), 7.43 (d, $J = 8.0$ Hz, 2H), 7.35 (d, $J = 8.4$ Hz, 1H), 7.25-7.22 (m, 1H), 7.21-7.16 (m, 4H), 7.09-7.05 (m, 2H), 6.52 (d, $J = 0.8$ Hz, 2H), 5.99 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.94, 155.02, 136.39, 128.53, 126.35, 123.90, 123.49, 122.75, 122.46, 120.90, 119.91, 119.38, 113.25, 111.40, 111.28, 104.61, 37.56; HRMS (ESI-TOF): m/z calcd for $\text{C}_{25}\text{H}_{16}\text{NO}_2$ $[\text{M-H}]^-$: 362.1187, found: 362.1190.

1-(3-indolethyl)ferrocene (8j)



Yield 92%; Yellow solid; Mp 121-122 °C; IR (KBr): 3418, 2973, 1637, 1454, 1417, 1335, 1219, 1102, 998, 836, 744 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 7.84 (s, 1H), 7.65 (d, $J = 8.0$ Hz, 1H), 7.32 (d, $J = 8.0$ Hz, 1H), 7.19-7.08 (m, 2H), 6.75 (d, $J = 2.4$ Hz, 1H), 4.25-4.08 (m, 10H), 1.70 (d, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 136.29, 126.47, 123.27, 121.81, 120.67, 119.36, 119.12, 111.16, 94.78, 68.64, 68.13, 67.37, 66.80, 66.45, 30.69, 21.74; HRMS (ESI-TOF): m/z calcd for $\text{C}_{20}\text{H}_{18}\text{FeN}$ $[\text{M-H}]^-$: 328.0794, found: 328.0782.

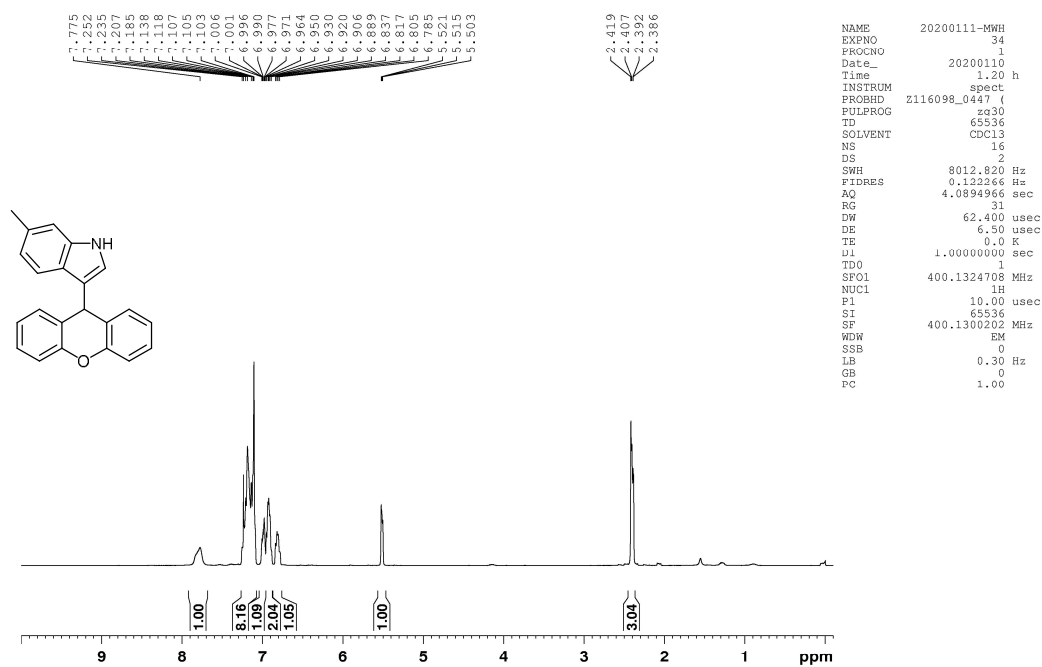
(6-chloro-2-3-indol phenylmethyl)ferrocene (8k)



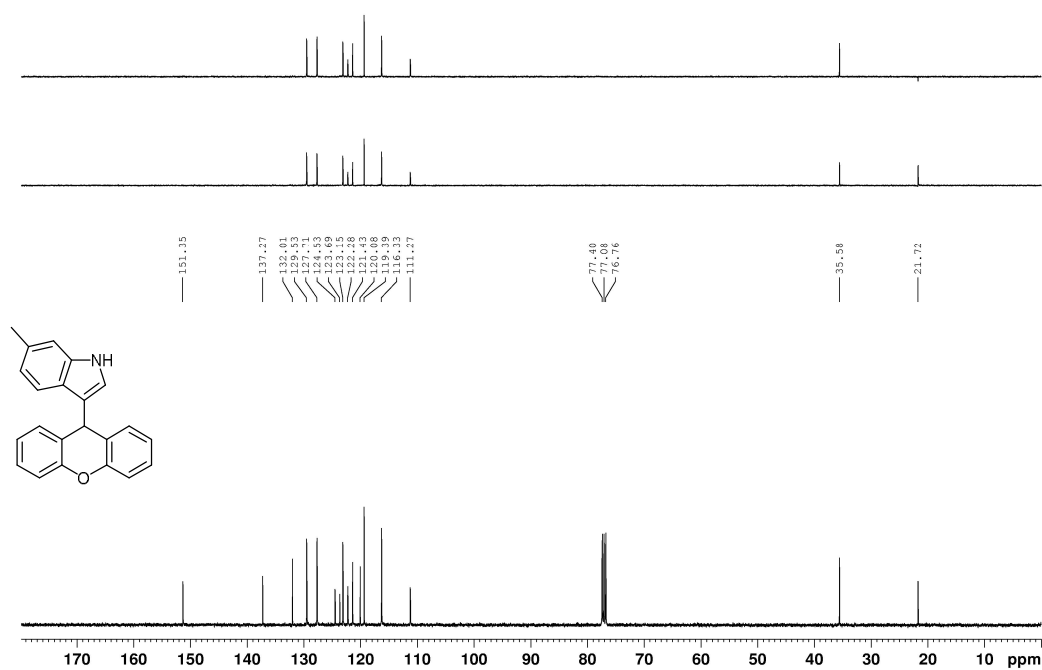
Yield 98%; Yellow solid; Mp 202-203 °C; IR (KBr): 3399, 2860, 1700, 1653, 1451, 1395, 1332, 1224, 1104, 1094, 1038, 906, 844, 808, 744, 705 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 7.89 (s, 1H), 7.33-7.27 (m, 5H), 7.23-7.21 (m, 1H), 7.11 (d, J = 8.4 Hz, 1H), 6.90 (dd, J = 8.4, 1.6 Hz, 1H), 6.81 (s, 1H), 5.26 (s, 1H), 4.22-4.16 (m, 3H), 4.03-3.99 (m, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 144.05, 136.78, 128.68, 128.07, 127.80, 126.33, 125.26, 123.23, 121.54, 120.62, 120.03, 110.93, 92.44, 69.05, 68.95, 68.53, 67.78, 67.57, 43.44; HRMS (ESI-TOF): *m/z* calcd for C₂₅H₁₉ClFeN [M-H]⁻: 424.0561, found: 424.0544.

¹H-NMR and ¹³C-NMR spectral of compound 4ab

M-6

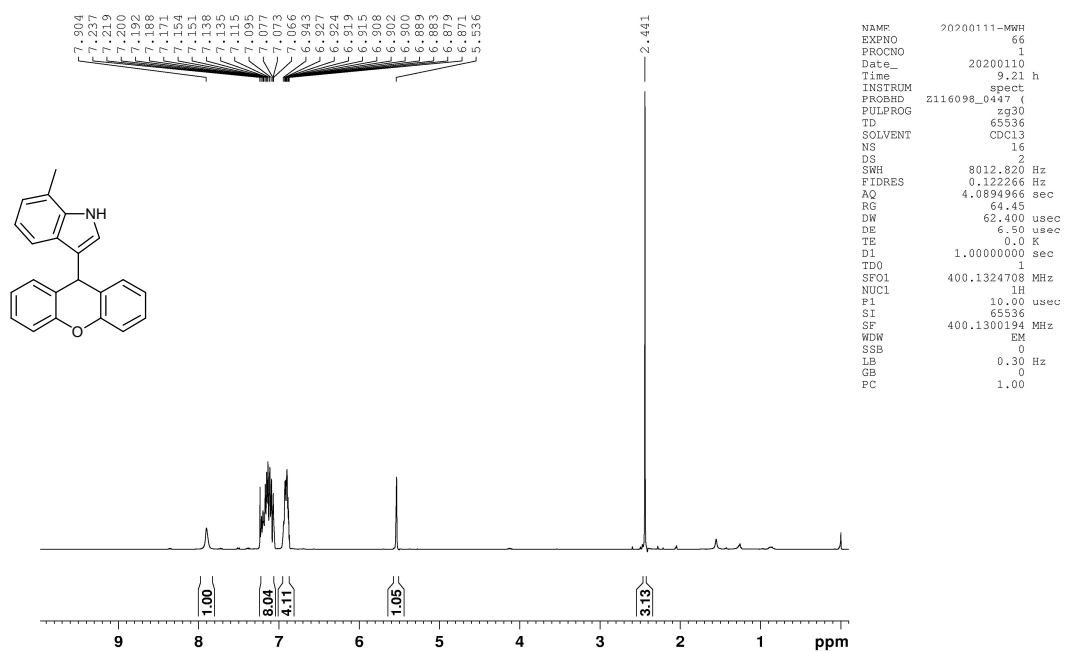


M-6

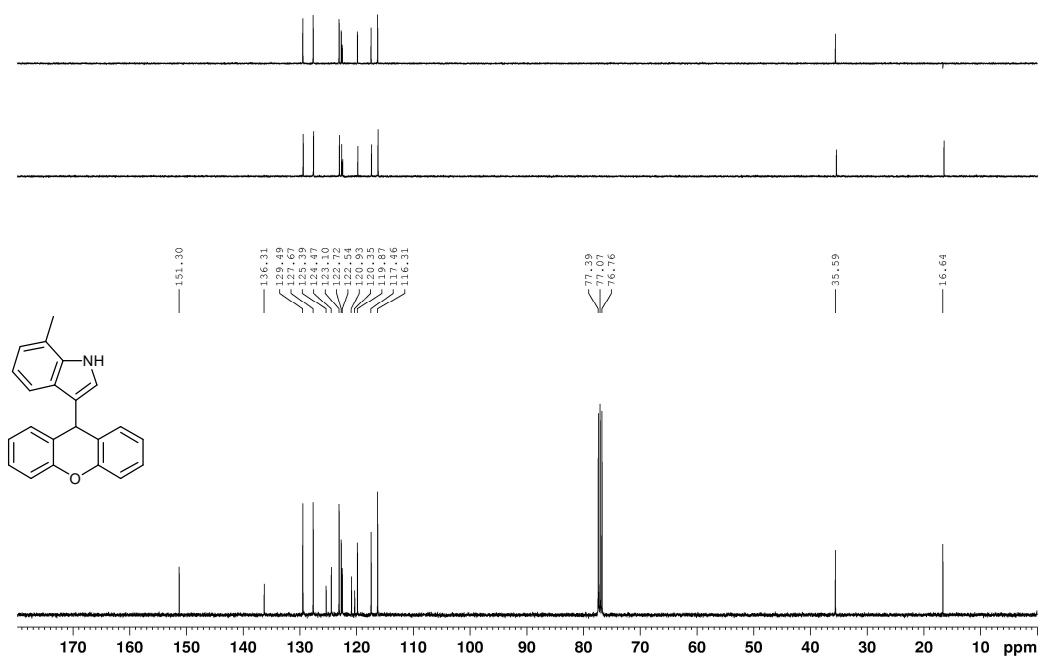


¹H-NMR and ¹³C-NMR spectral of compound 4ac

M-7

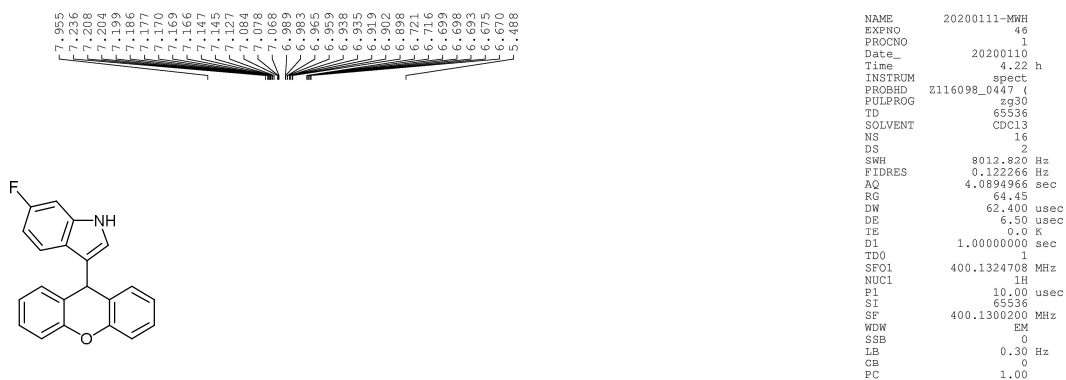


M-7

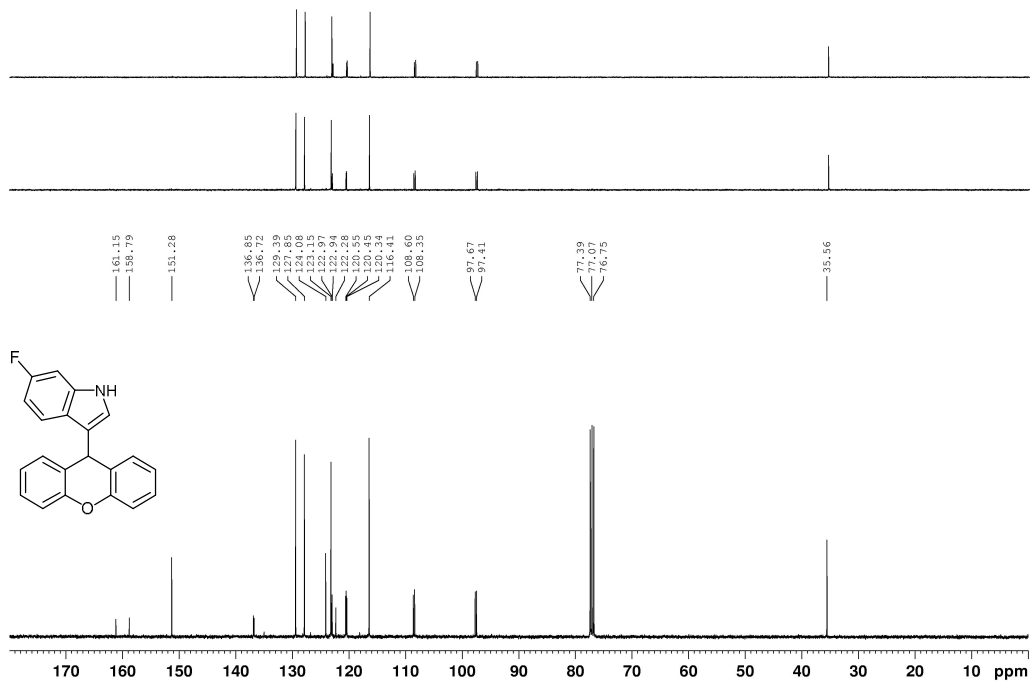


¹H-NMR and ¹³C-NMR spectral of compound 4ad

M-5

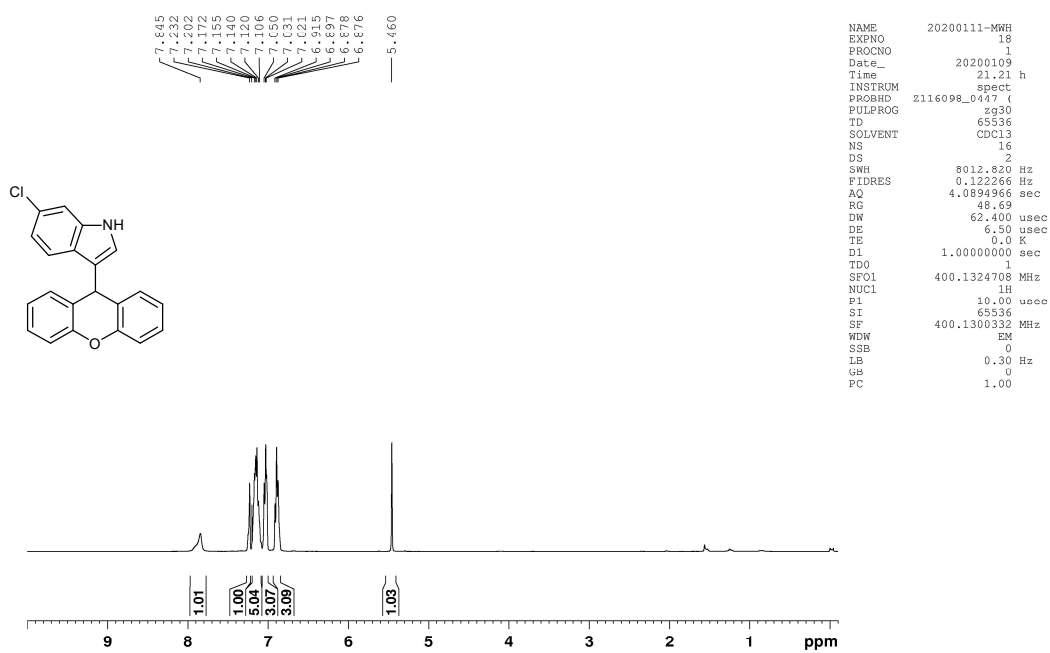


M-5

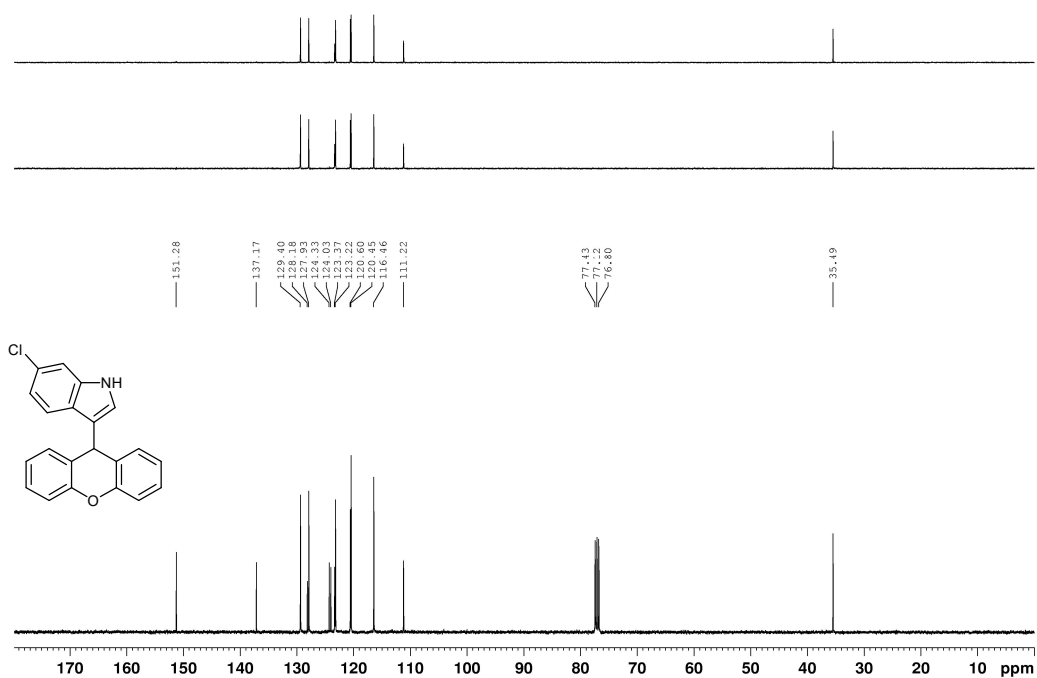


¹H-NMR and ¹³C-NMR spectral of compound 4ae

M-15

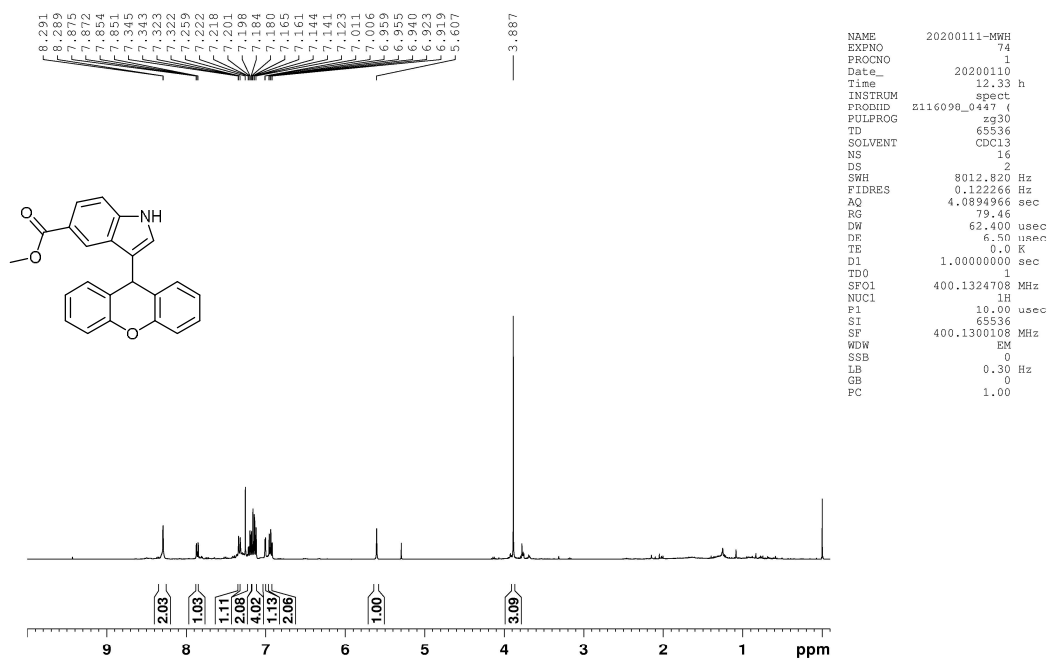


M-15

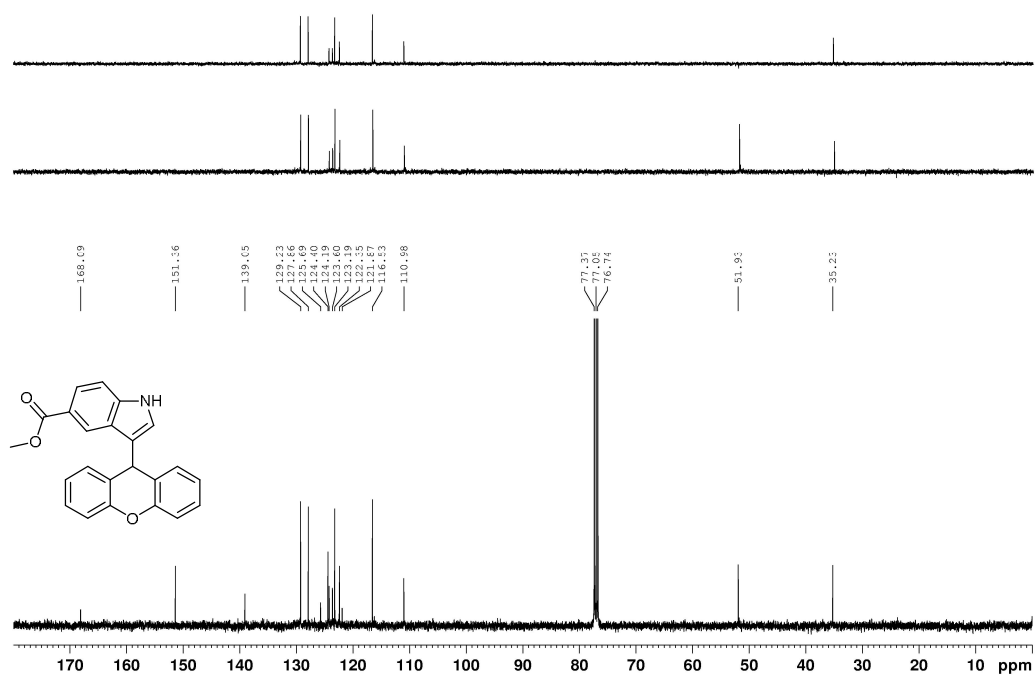


¹H-NMR and ¹³C-NMR spectral of compound 4af

M-11

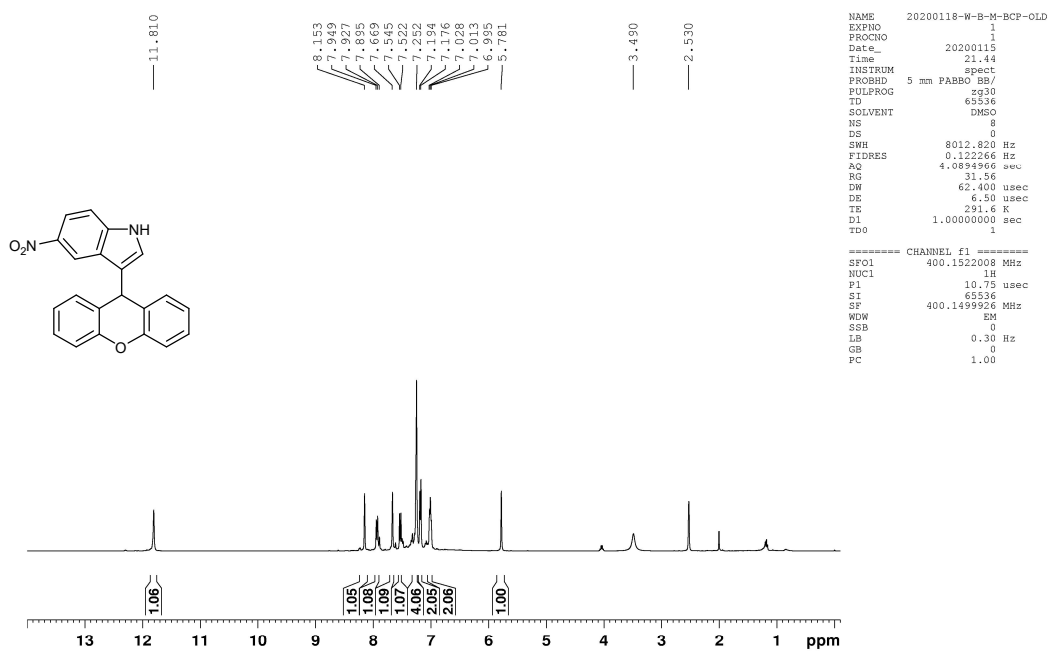


M-11



¹H-NMR and ¹³C-NMR spectral of compound 4ag

M-9

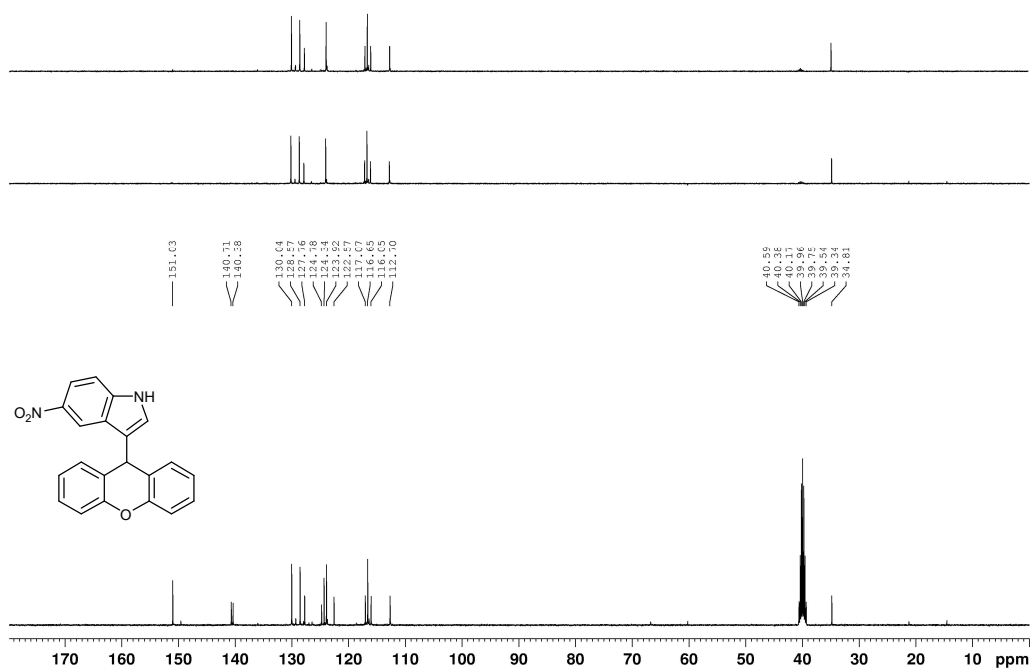


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PROCNO   1
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TD       65536
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NS       0
DS       0
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       31.56
DW       62.400 usec
DE       6.50 usec
TE       291.6 K
D1       1.00000000 sec
TD0      1

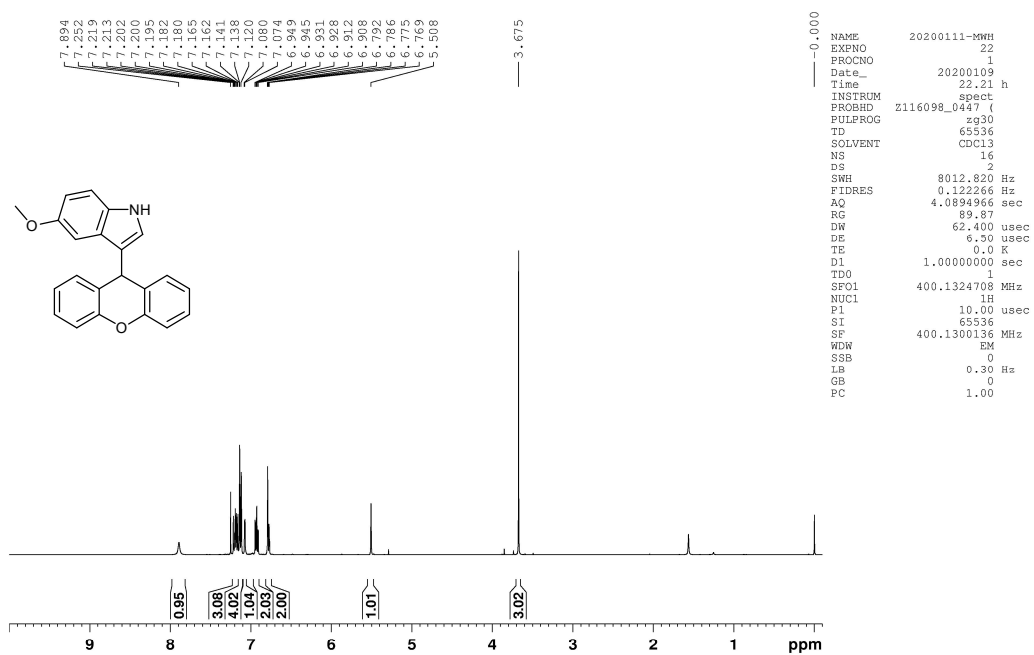
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P1      10.75 usec
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SF      400.1499526 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
    
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M-9

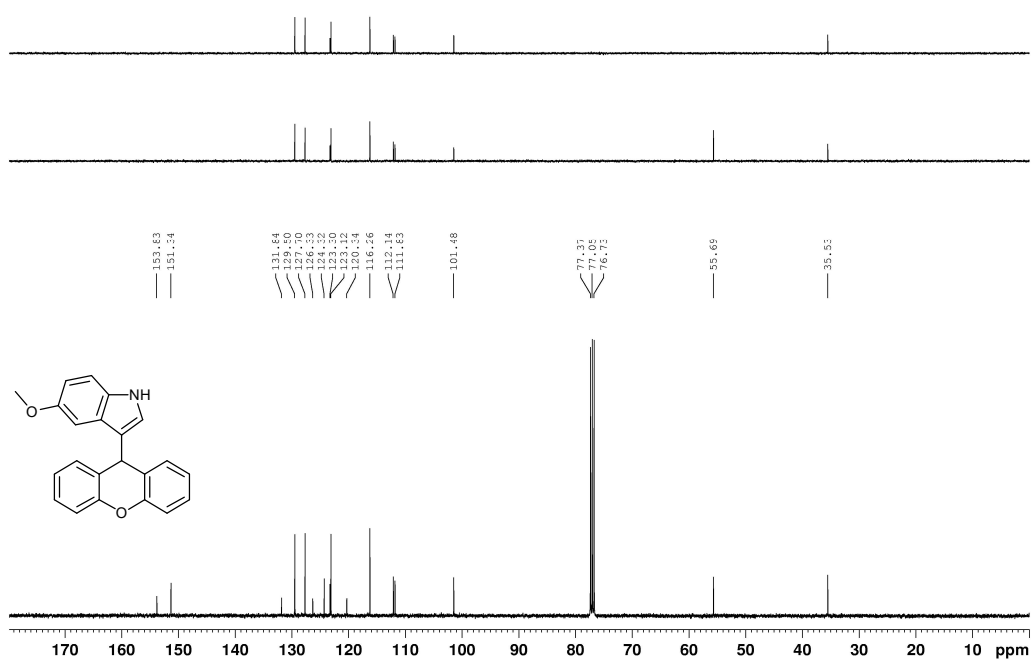


¹H-NMR and ¹³C-NMR spectral of compound 4ah

M-19

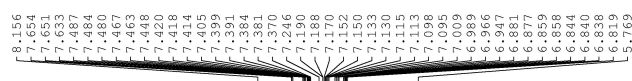


M-19



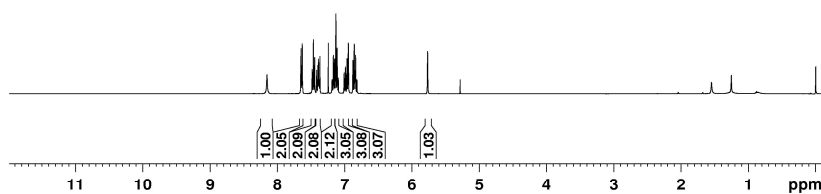
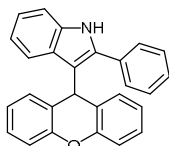
¹H-NMR and ¹³C-NMR spectral of compound 4aj

M-17

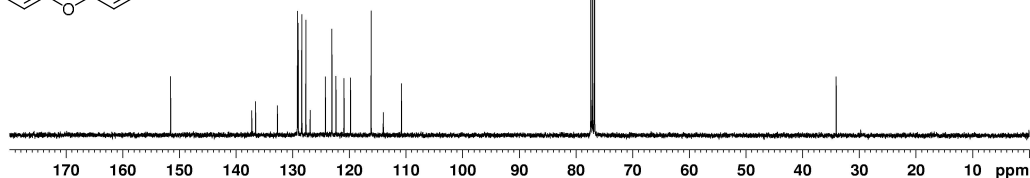
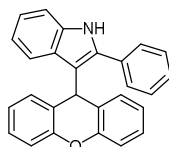
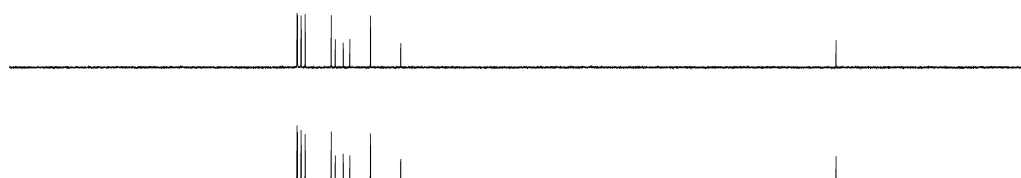


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PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         79.48
DW         62.400 usec
DE         6.50 usec
TE         0.0 K
D1         1.00000000 sec
TDO        1
SF01      400.1324708 MHz
NUC1       1H
P1         10.00 usec
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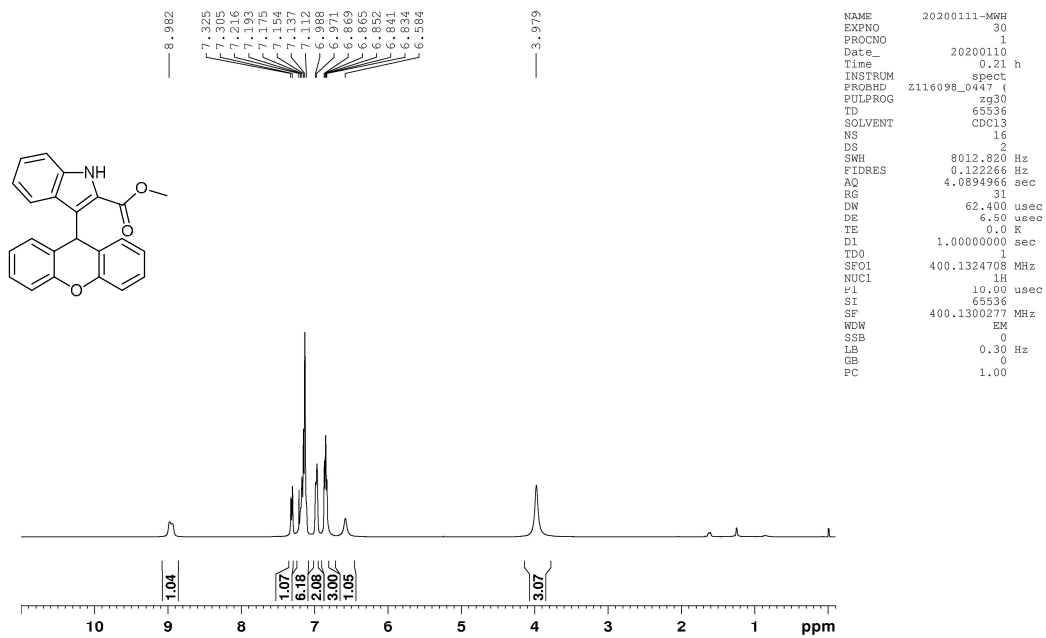


M-17

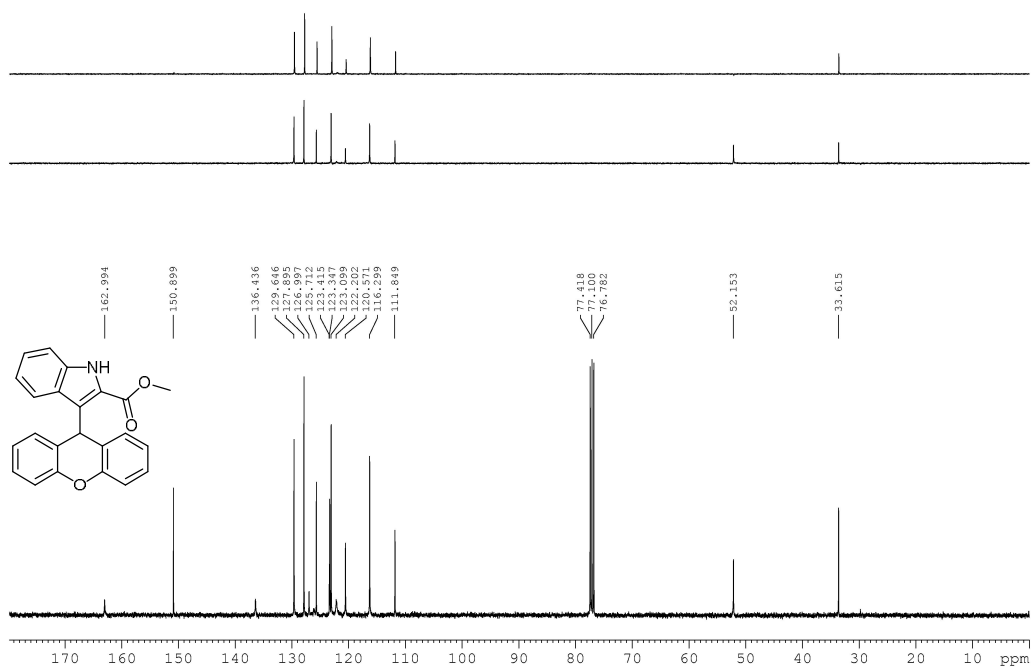


¹H-NMR and ¹³C-NMR spectral of compound 4ak

M-18

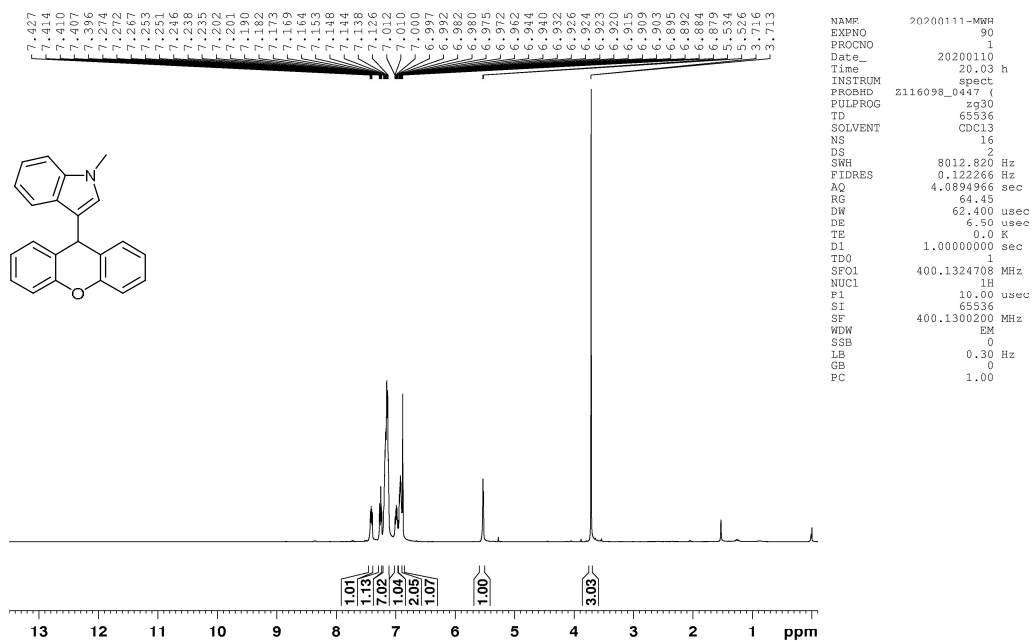


M-18



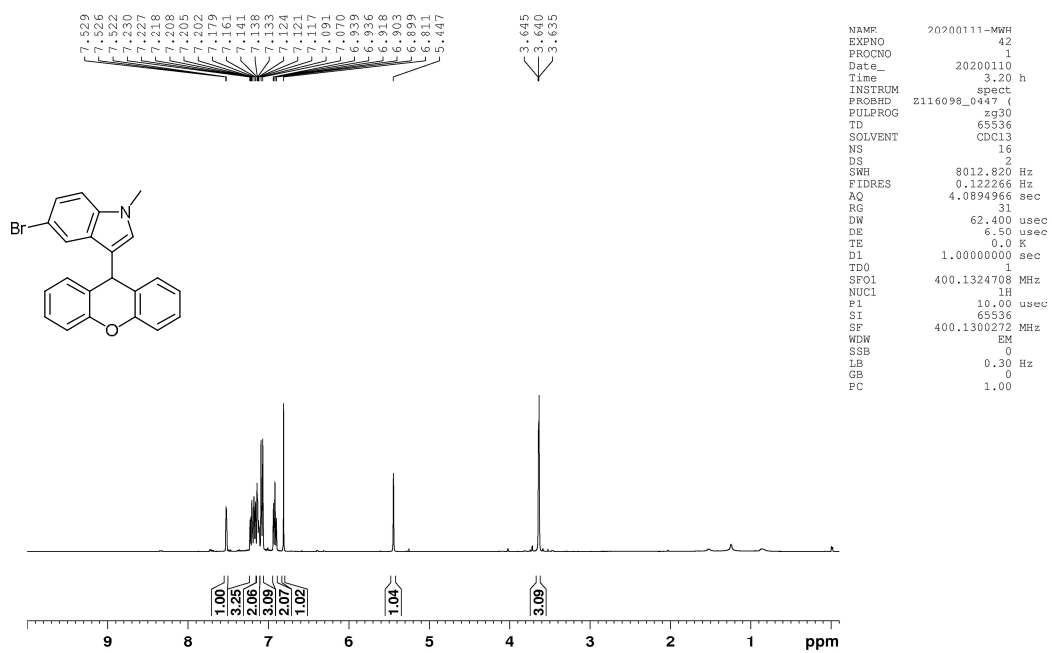
¹H-NMR and ¹³C-NMR spectral of compound 4al

M-1

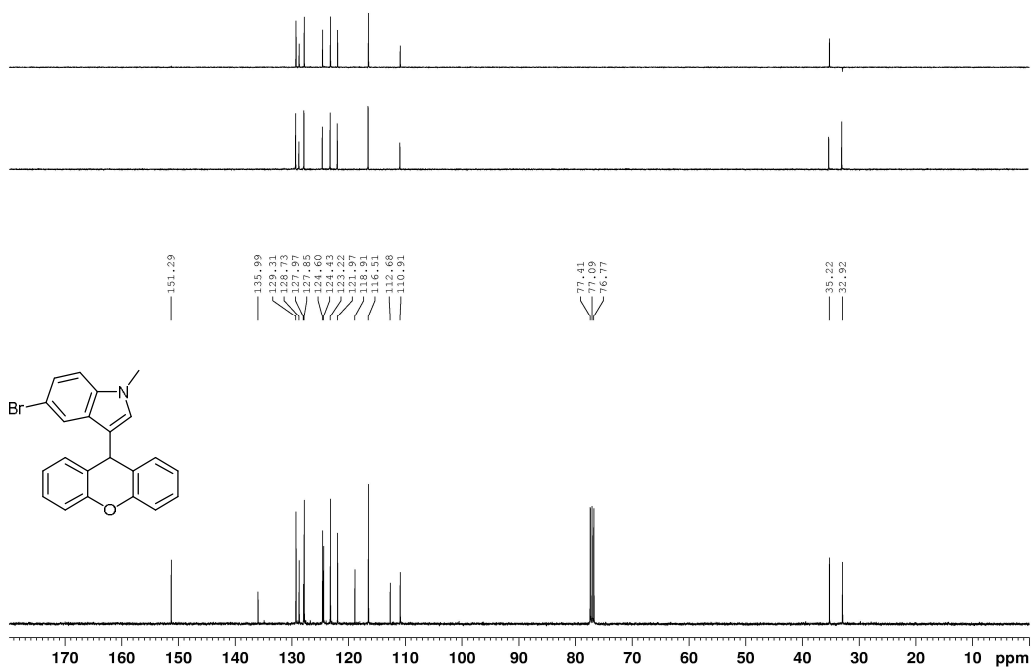


¹H-NMR and ¹³C-NMR spectral of compound 4am

M-8

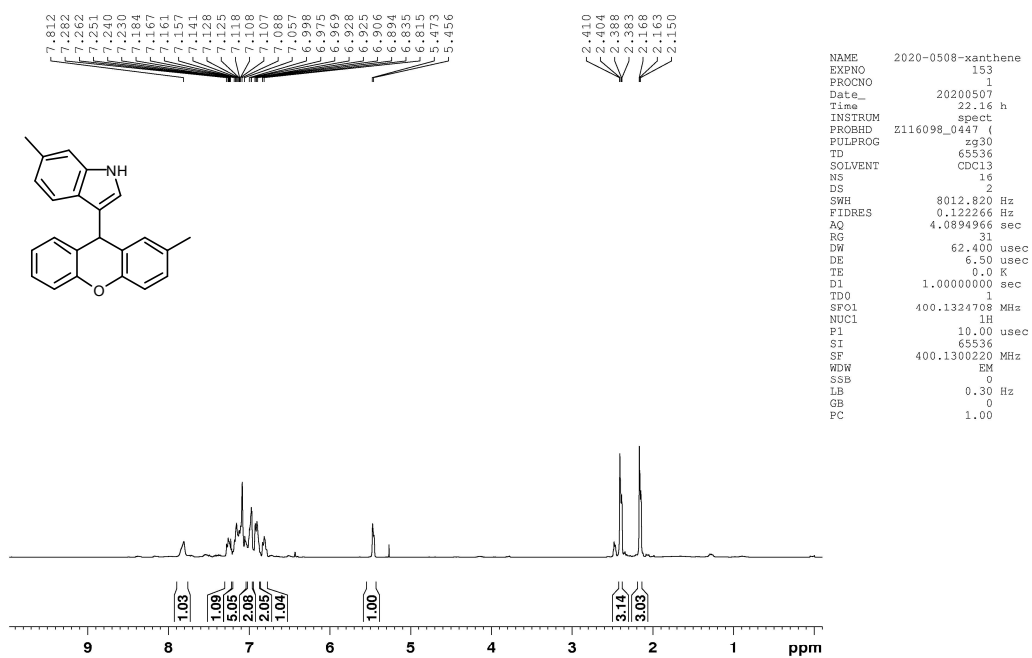


M-8

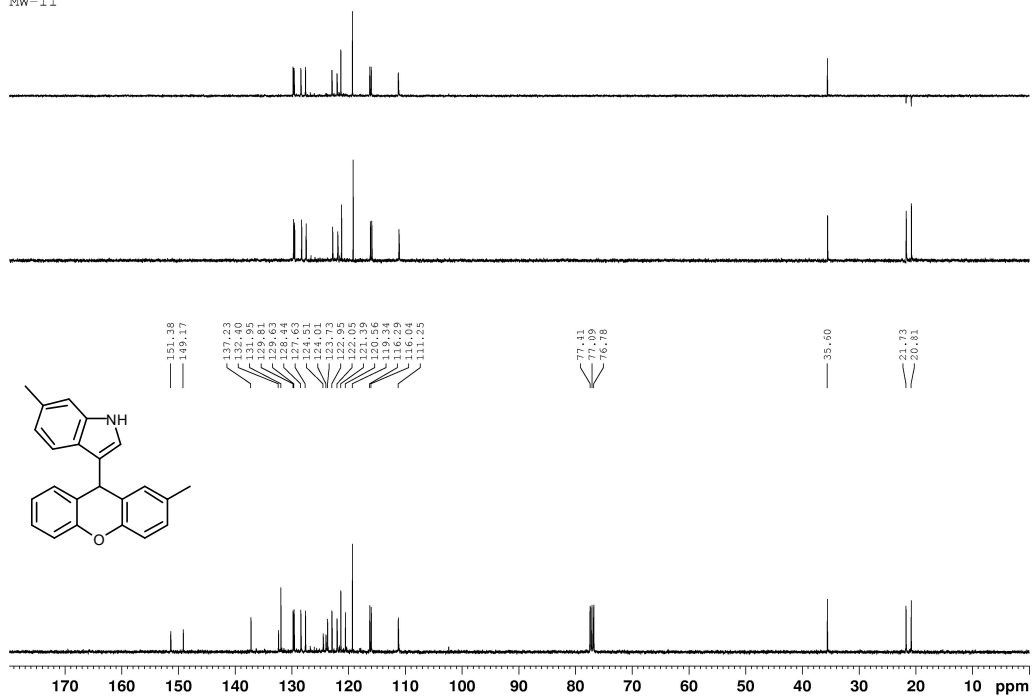


¹H-NMR and ¹³C-NMR spectral of compound 4bb

MW-11

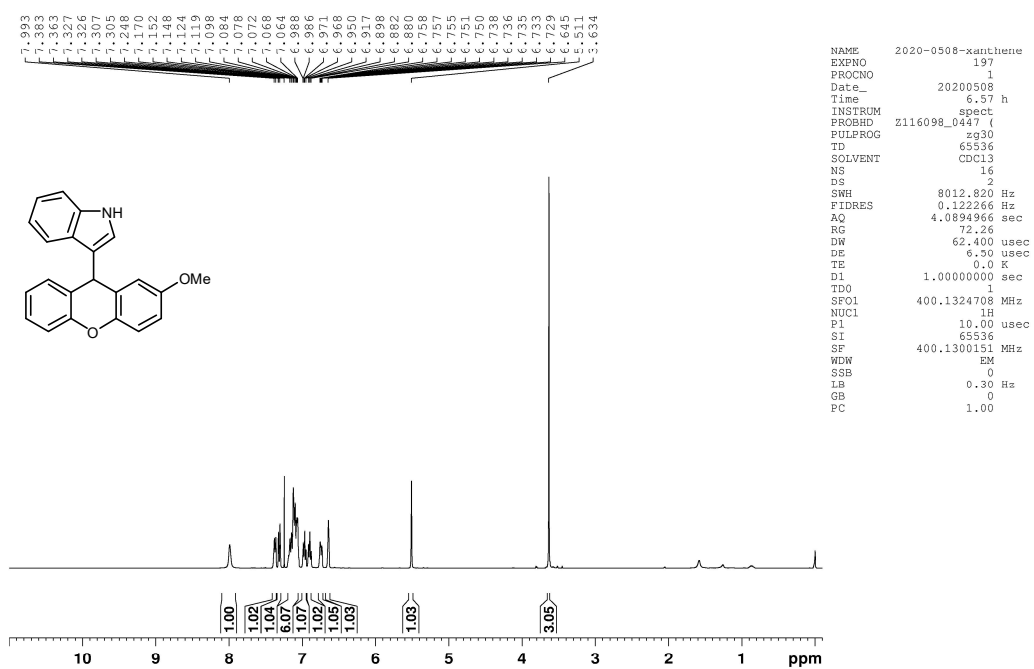


MW-11

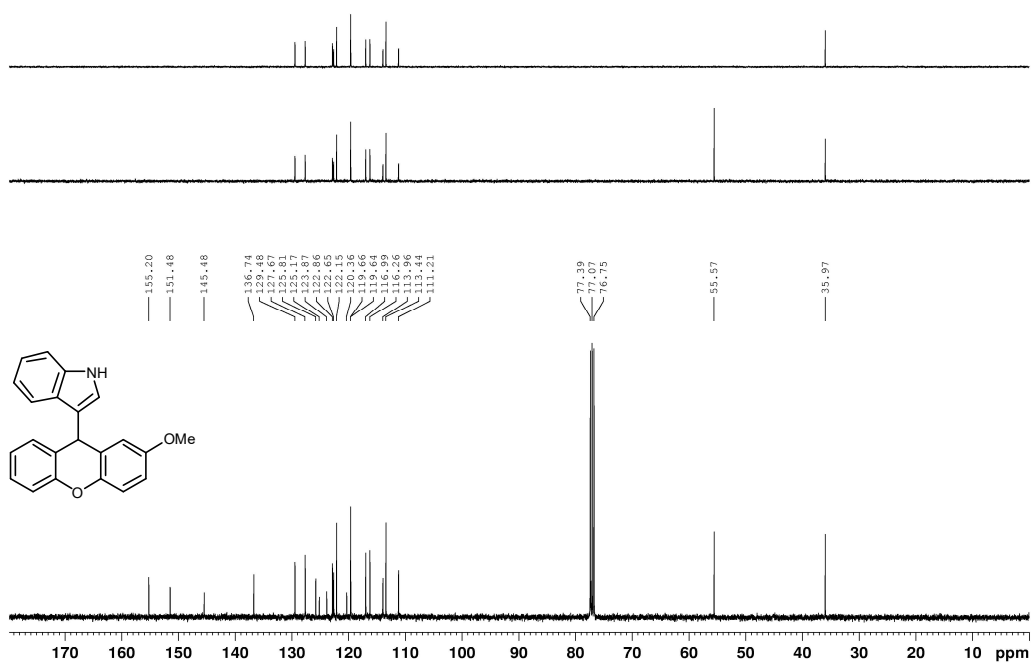


¹H-NMR and ¹³C-NMR spectral of compound 4ca

MW-10

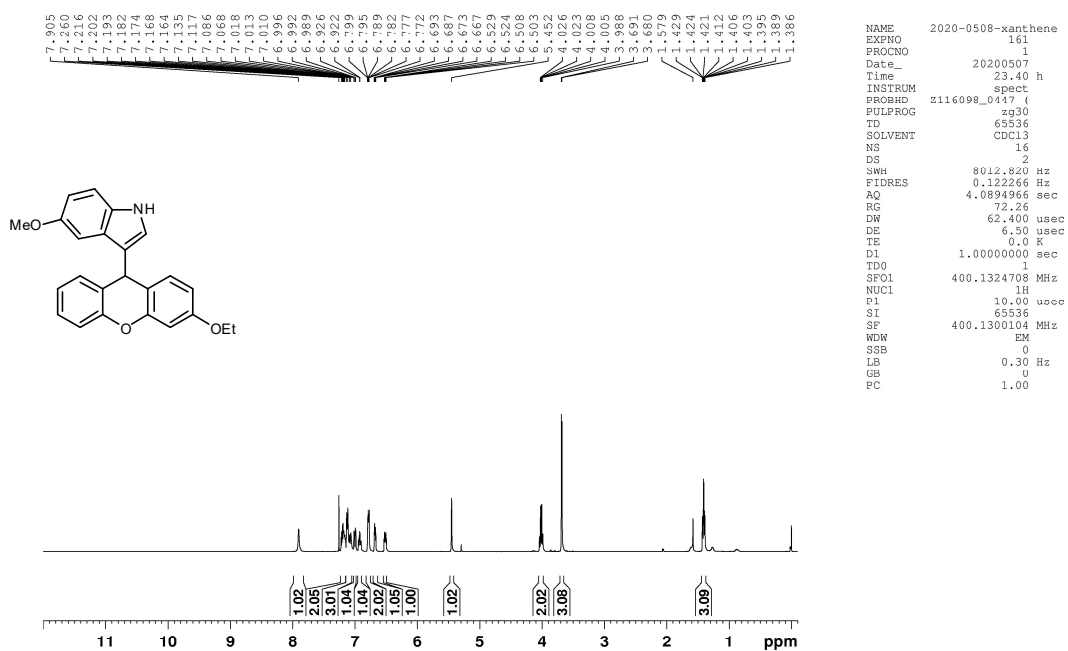


MW-10

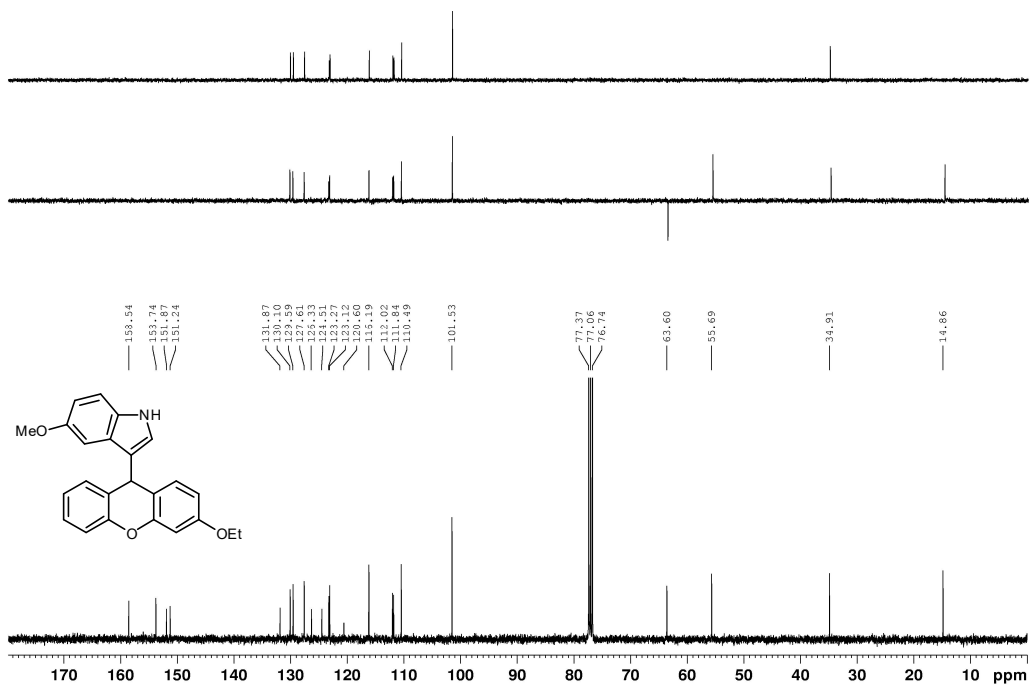


¹H-NMR and ¹³C-NMR spectral of compound 4dh

MW-9

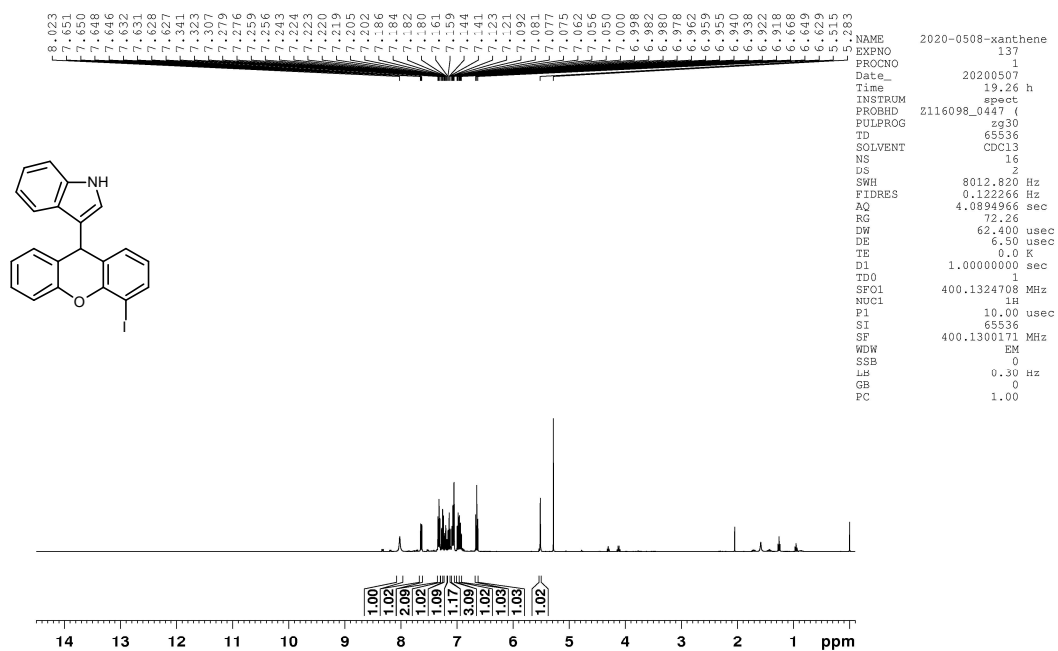


MW-9

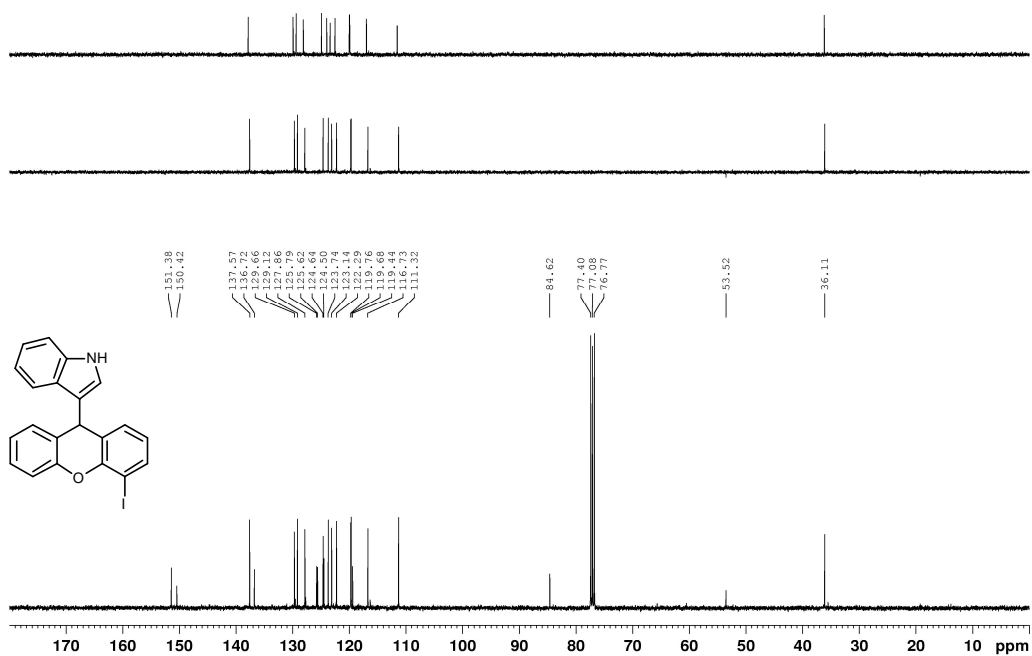


¹H-NMR and ¹³C-NMR spectral of compound 4ea

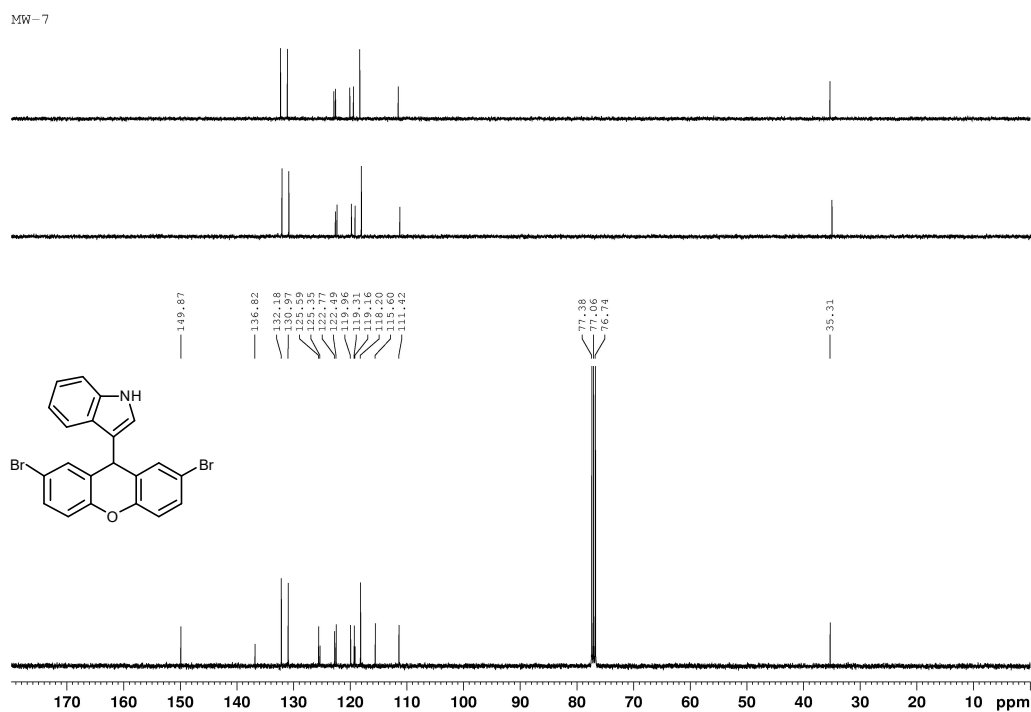
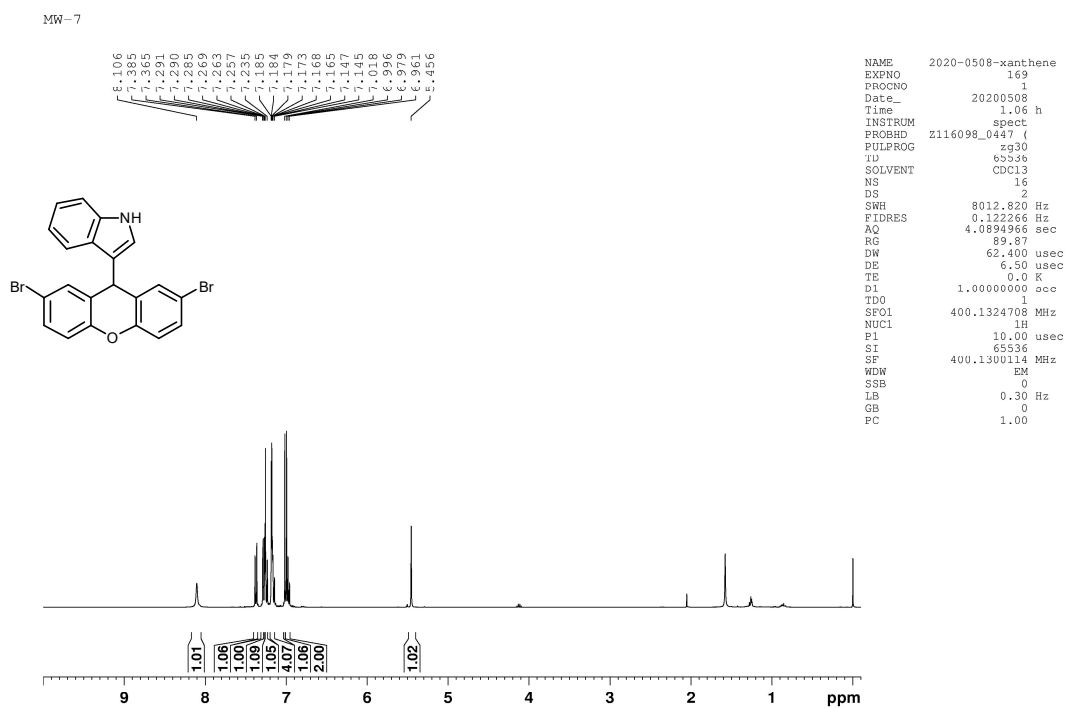
MW-13



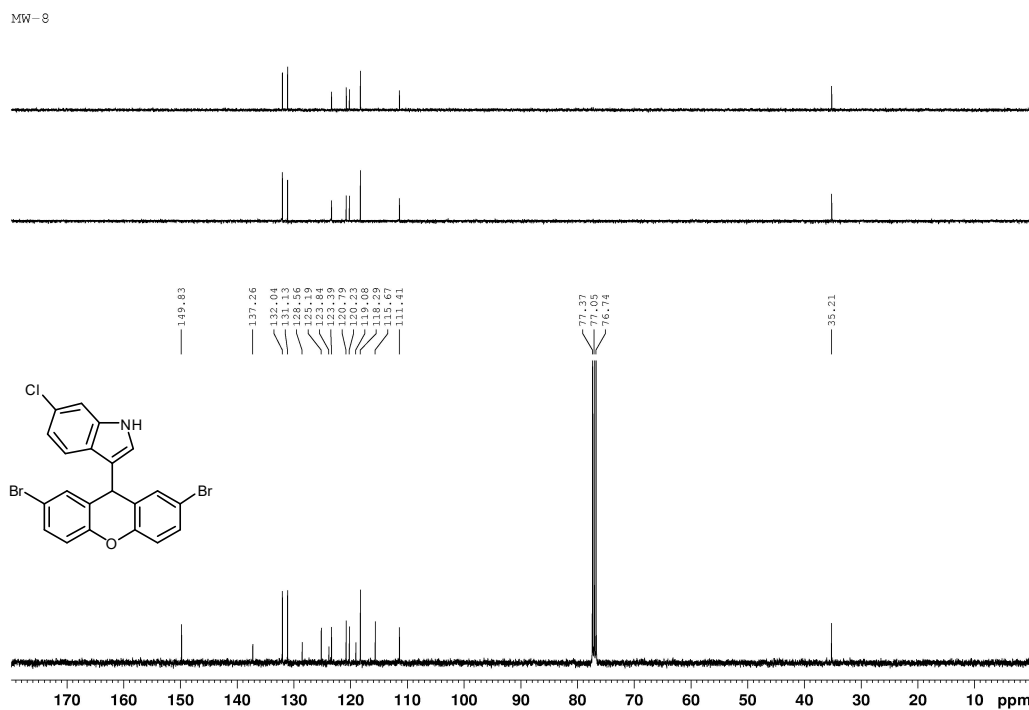
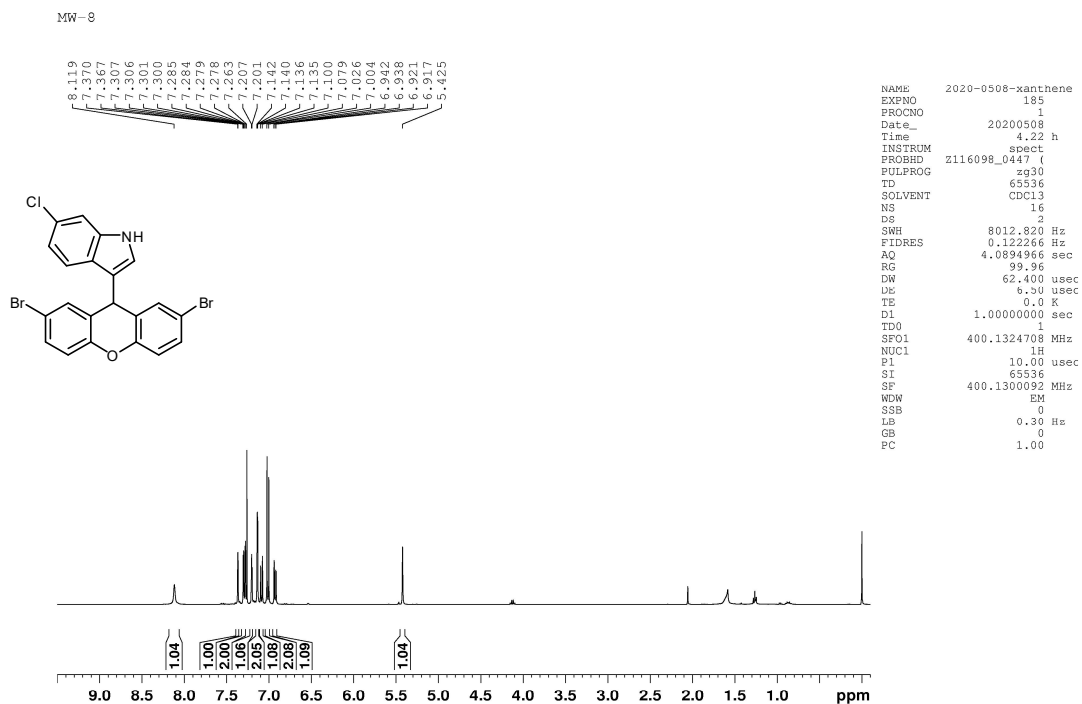
MW-13



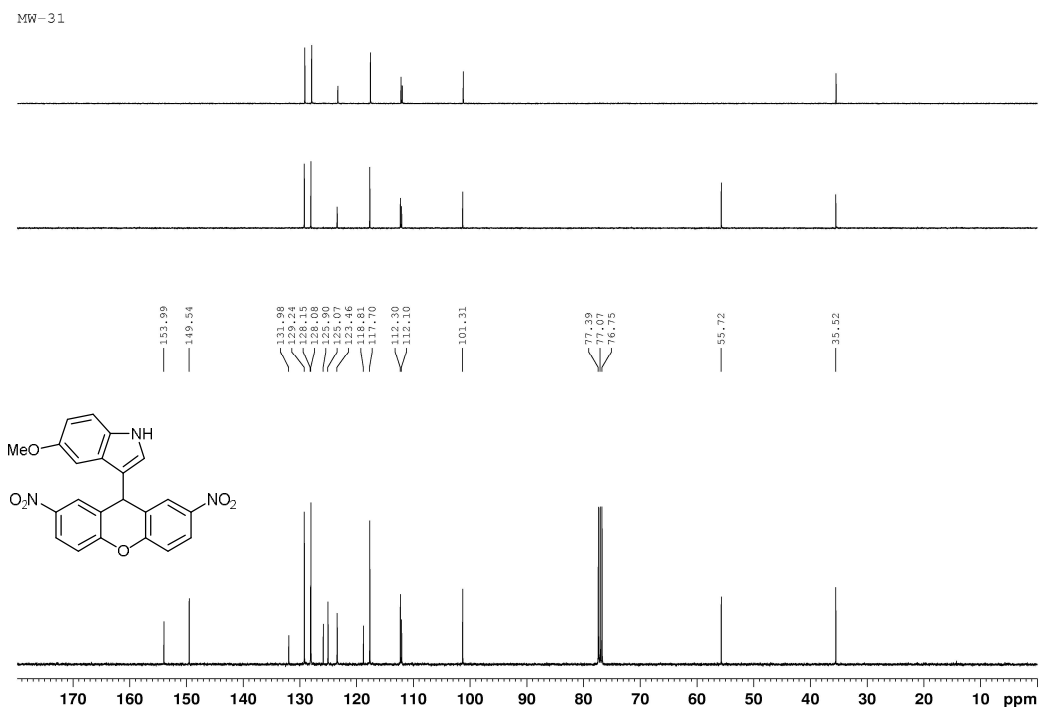
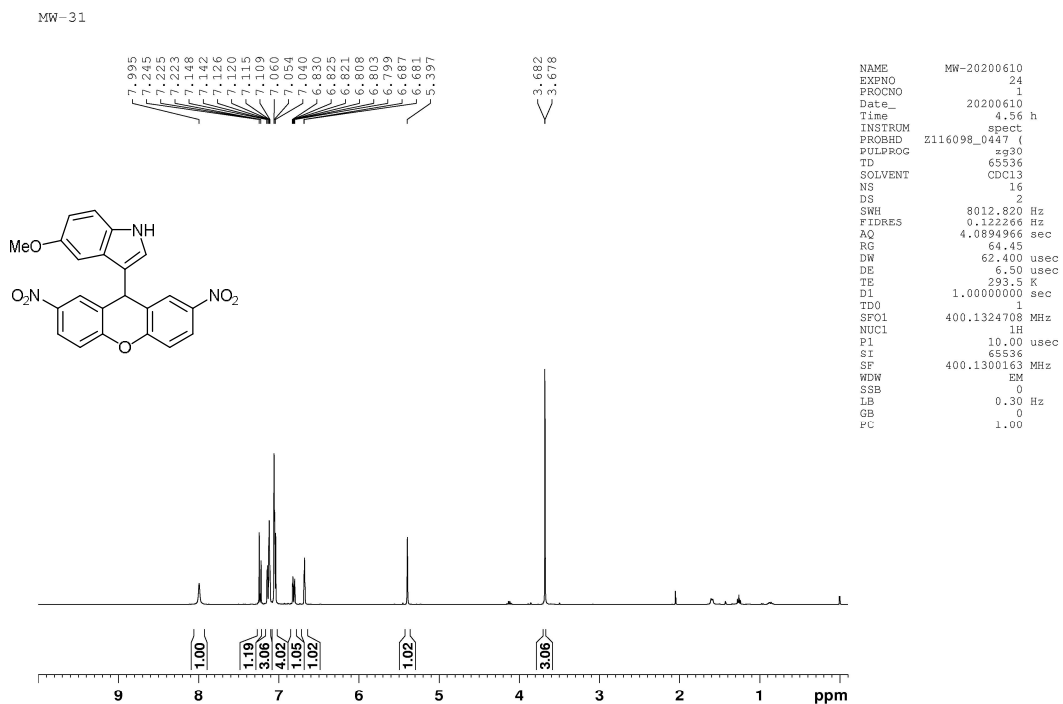
¹H-NMR and ¹³C-NMR spectral of compound 4fa



¹H-NMR and ¹³C-NMR spectral of compound 4fe

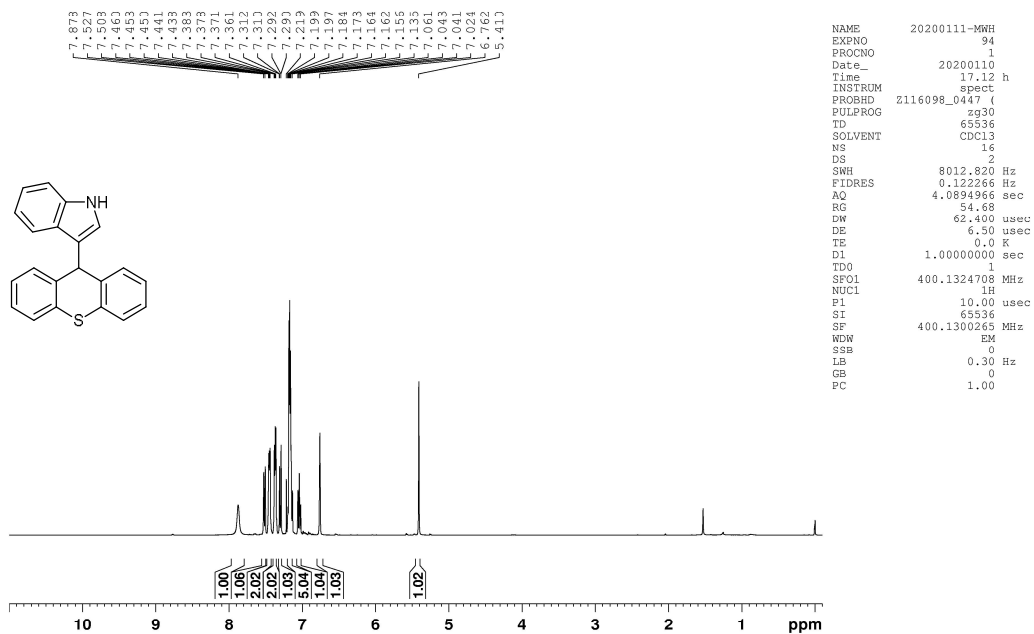


¹H-NMR and ¹³C-NMR spectral of compound 4gh

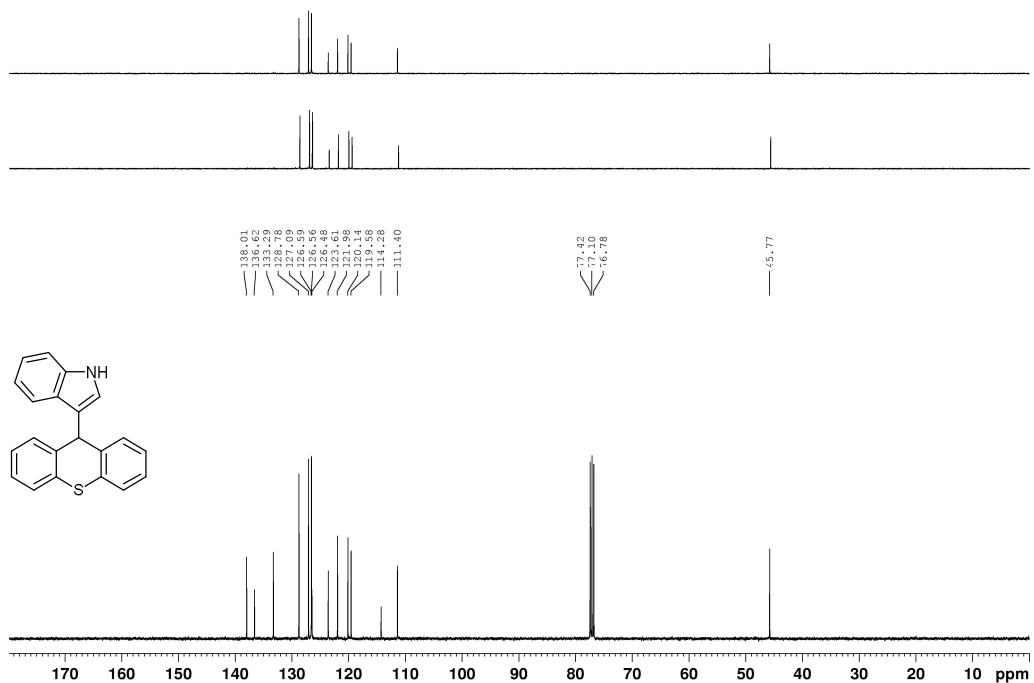


¹H-NMR and ¹³C-NMR spectral of compound 5aa

M-16

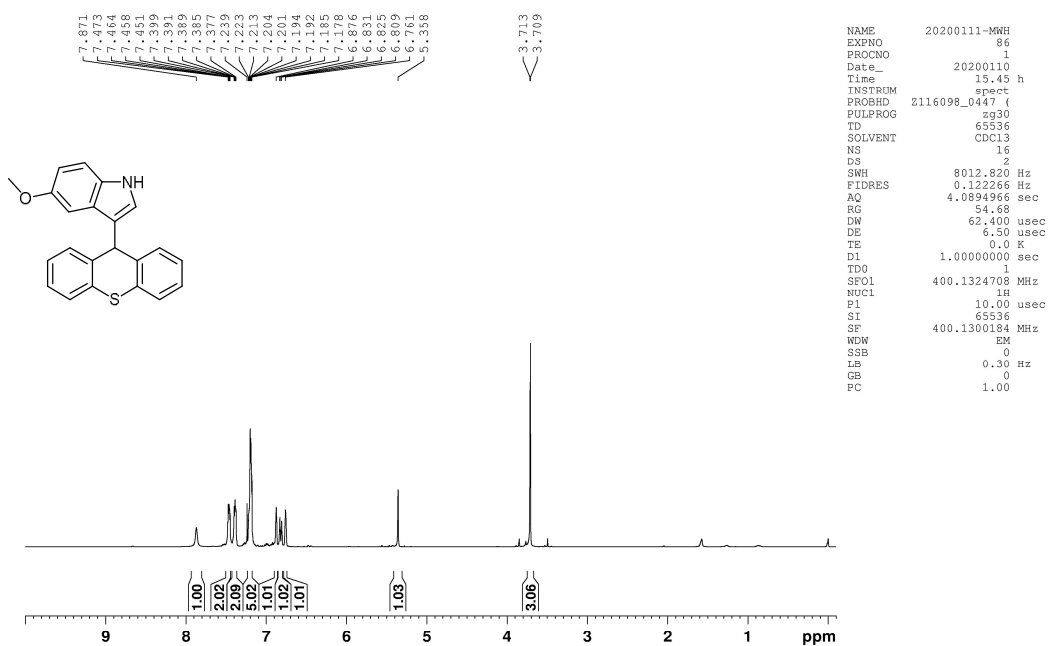


M-16

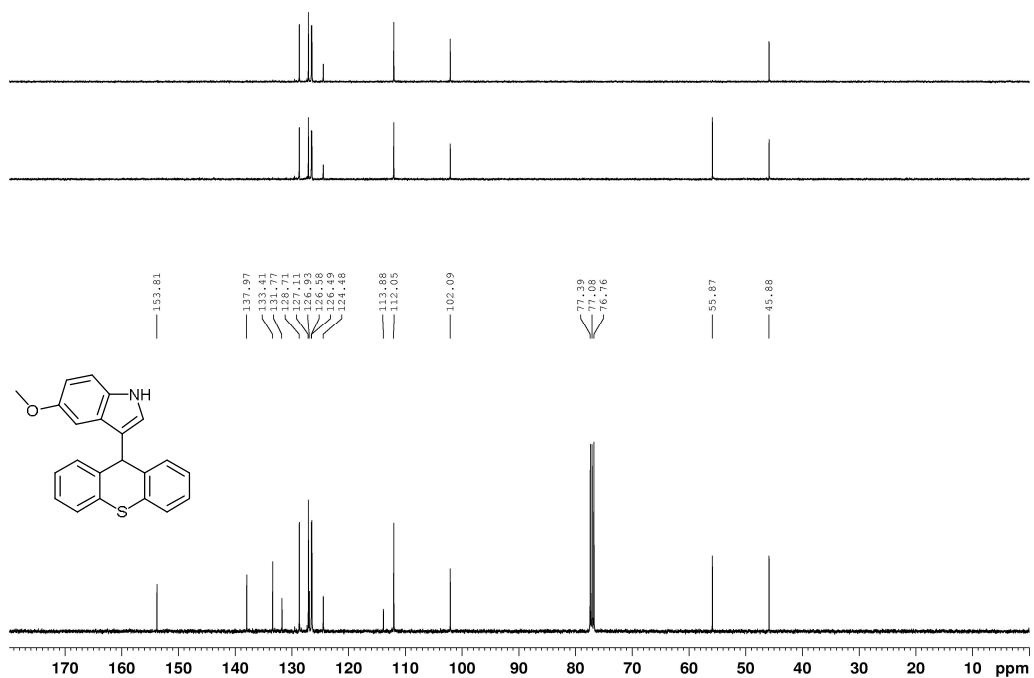


¹H-NMR and ¹³C-NMR spectral of compound 5ah

M-23

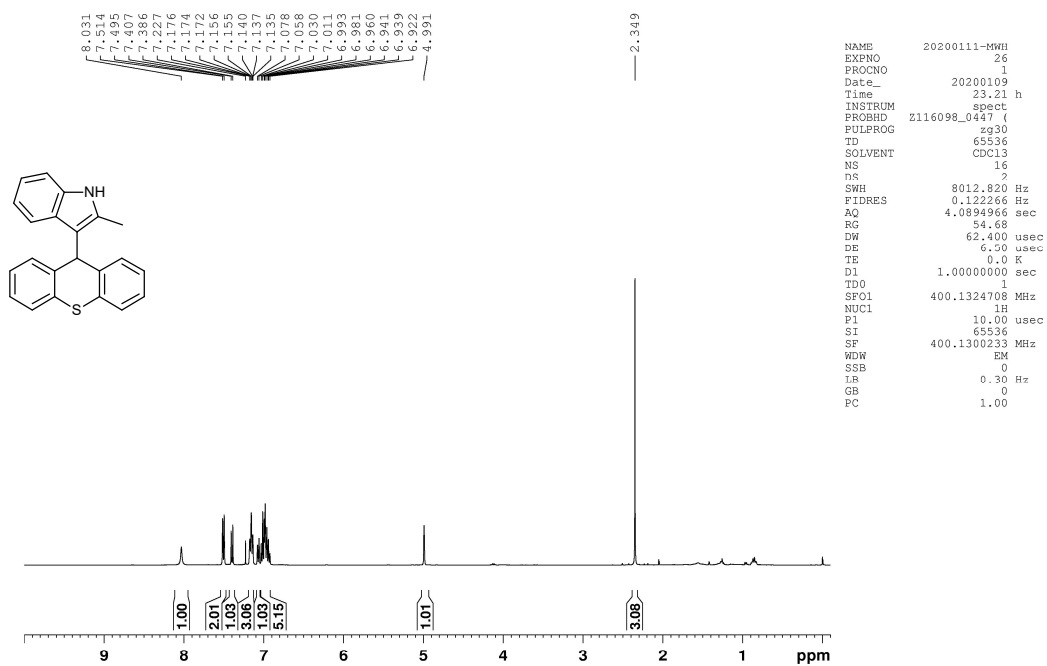


M-23

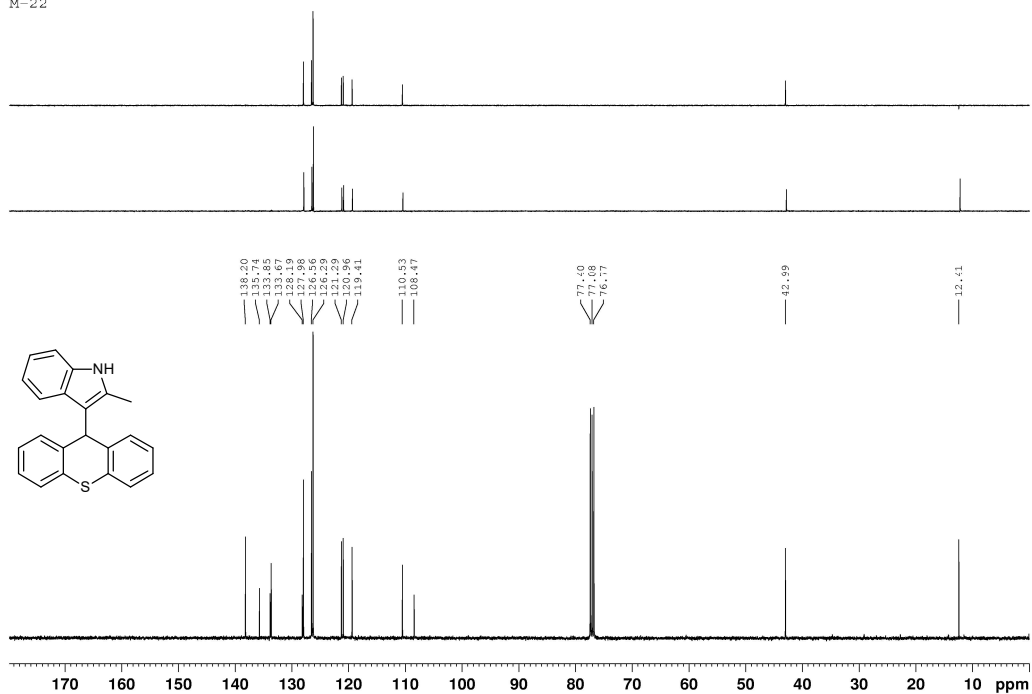


¹H-NMR and ¹³C-NMR spectral of compound 5ai

M-22

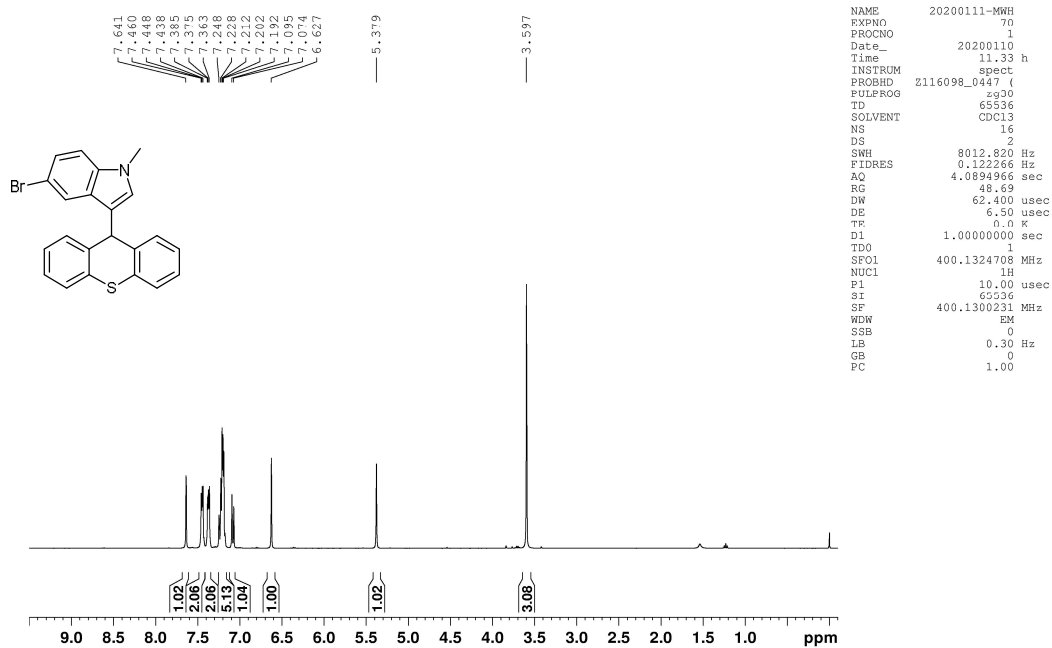


M-22

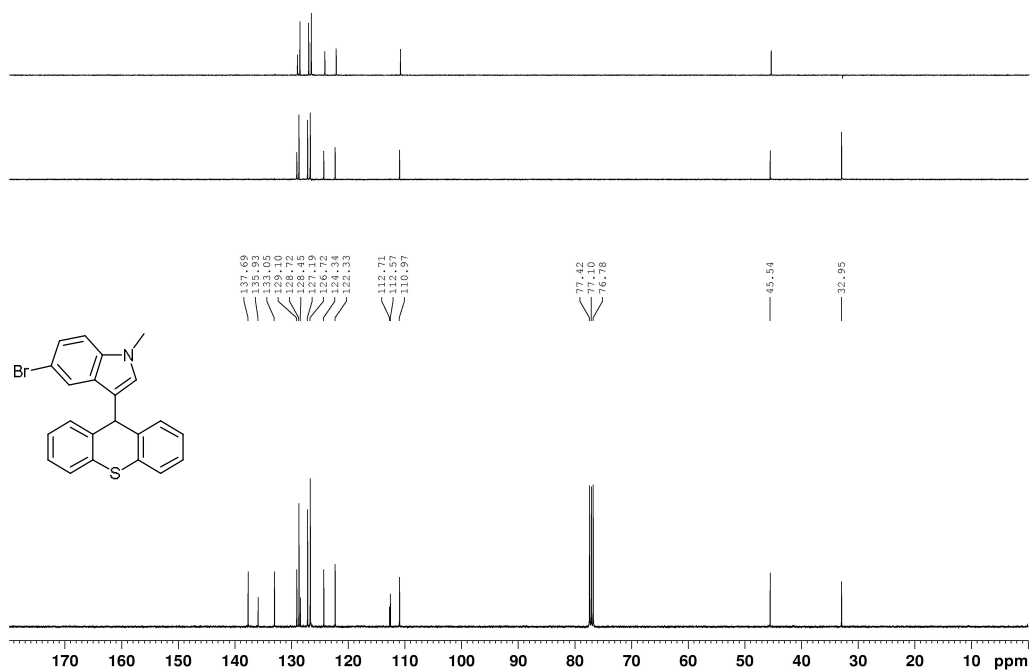


¹H-NMR and ¹³C-NMR spectral of compound 5am

M-20

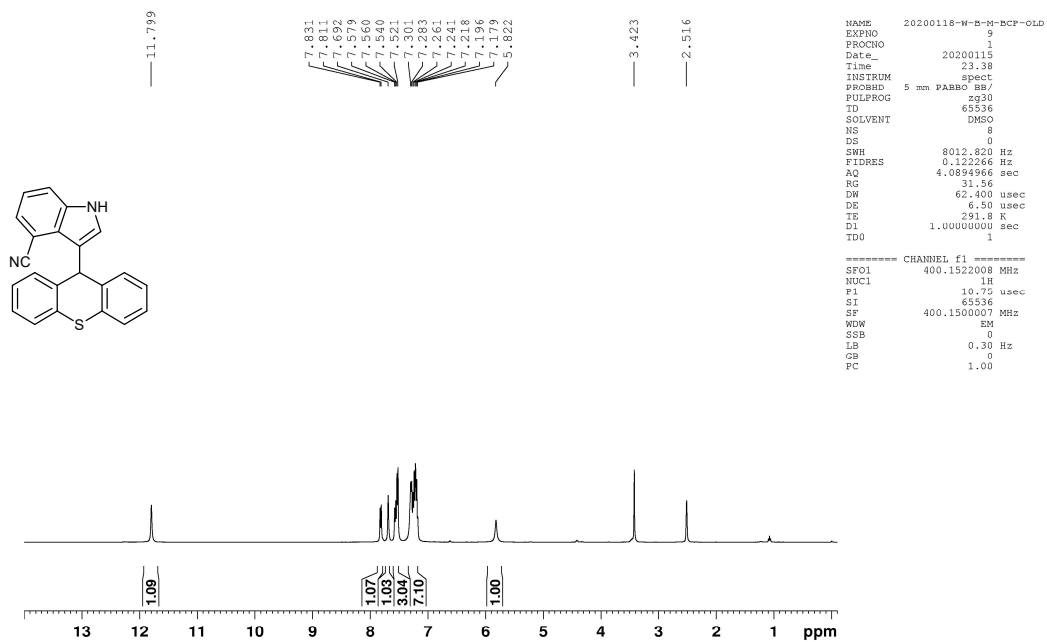


M-20



¹H-NMR and ¹³C-NMR spectral of compound 5ap

M-24

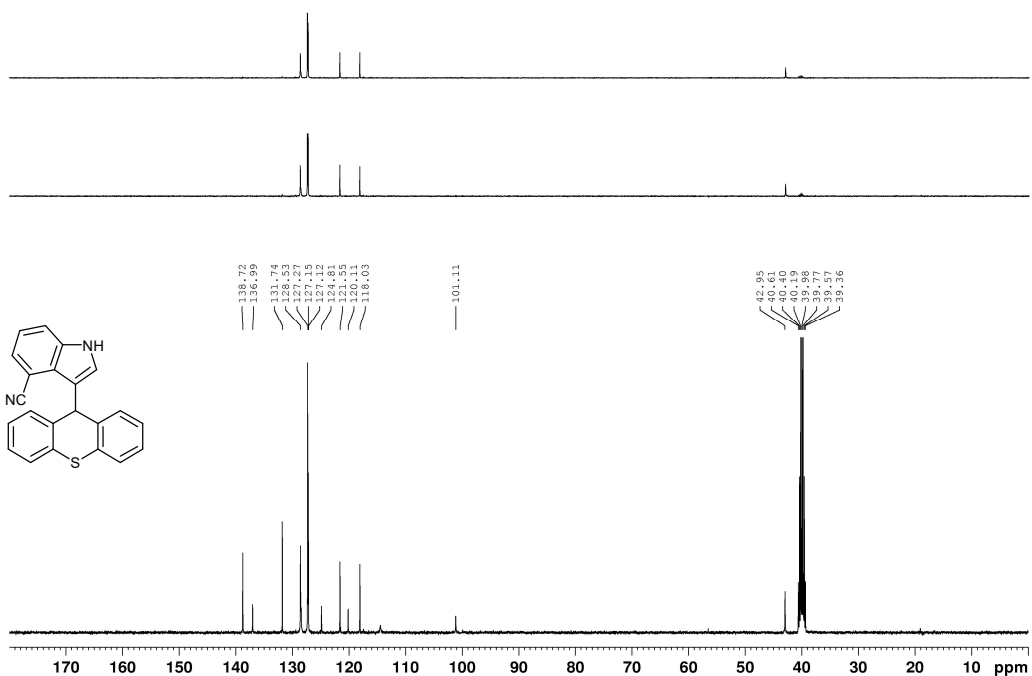


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NAME      20200118-W-B-M-BCP-OLD
EXPNO     9
PROCNO    1
Date_     20200115
Time      23.38
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0834966 sec
RG         31.56
DW         62.400 usec
DE         6.50 usec
TE         291.8 K
D1         1.0000000 sec
TD0        1

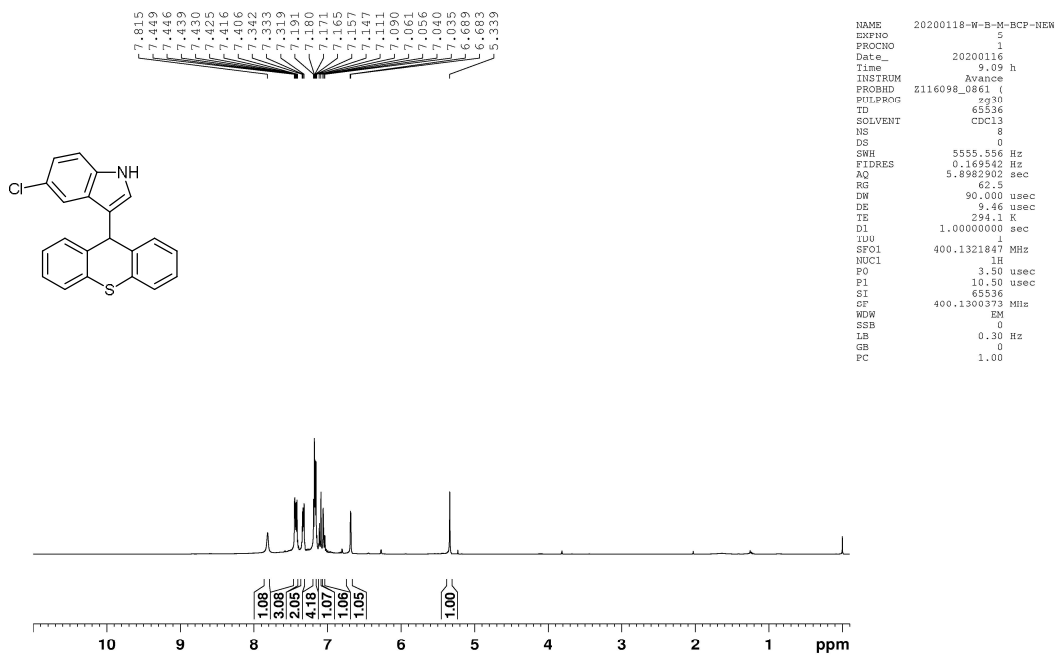
===== CHANNEL f1 =====
SFO1      400.1522008 MHz
NUC1      1H
P1         10.75 usec
SI         65536
SF         400.1500007 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

M-24



¹H-NMR and ¹³C-NMR spectral of compound 5aq

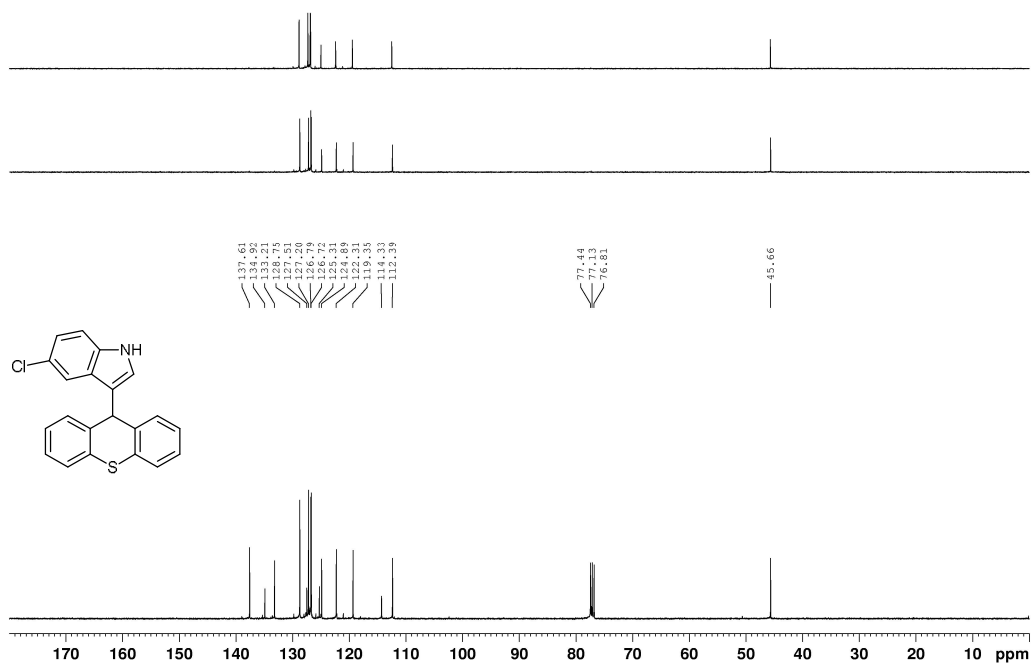
M-21



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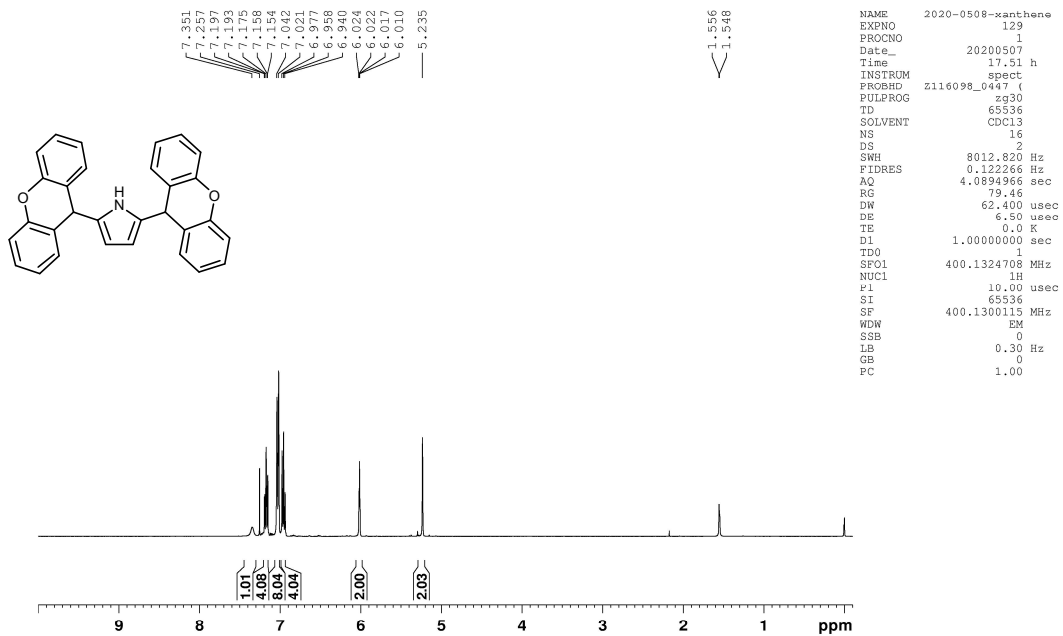
NAME      20200118-W-B-M-BCP-NEW
EXPNO    5
PROCNO   1
Date_    20200116
Time     9.09 h
INSTRUM  Avance
PROBHD   z116098_0861 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        0
SHH       5555.556 Hz
FIDRES   0.169542 Hz
AQ        5.8982502 sec
RG         62.5
DW         90.000 usec
DE         9.46 usec
TE        294.1 K
D1         1.00000000 sec
IDU        4
SFO1     400.1321847 MHz
NUC1      1H
PO         3.50 usec
P1         10.50 usec
SI         65536
SF         400.1300373 MHz
WDW       EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

M-21

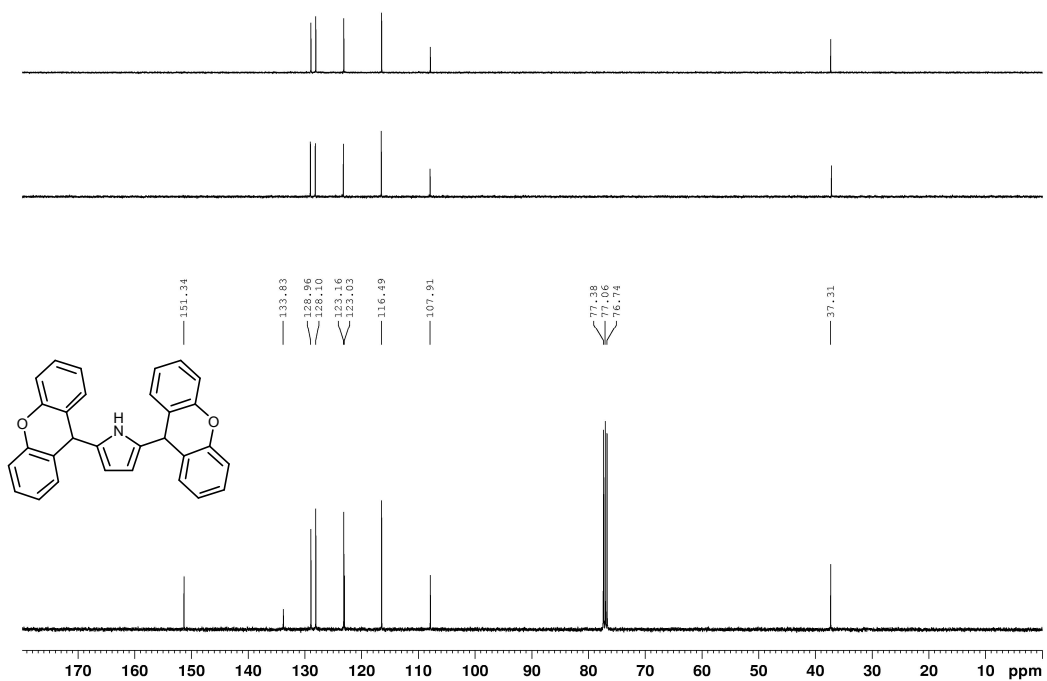


¹H-NMR and ¹³C-NMR spectral of compound 6a

MW-17-1

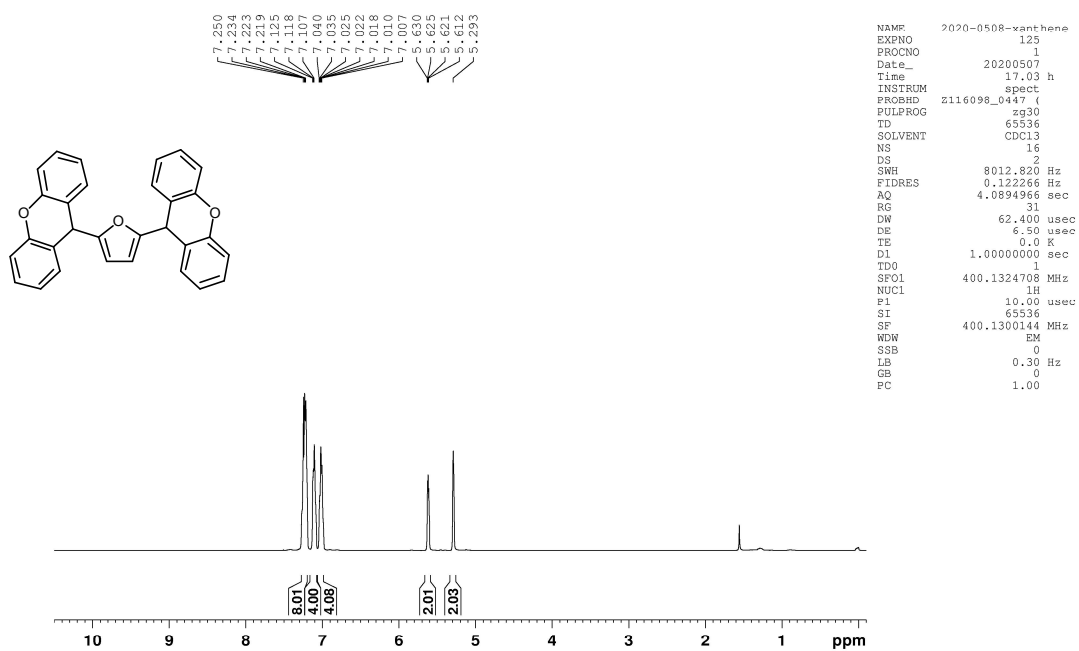


MW-17-1

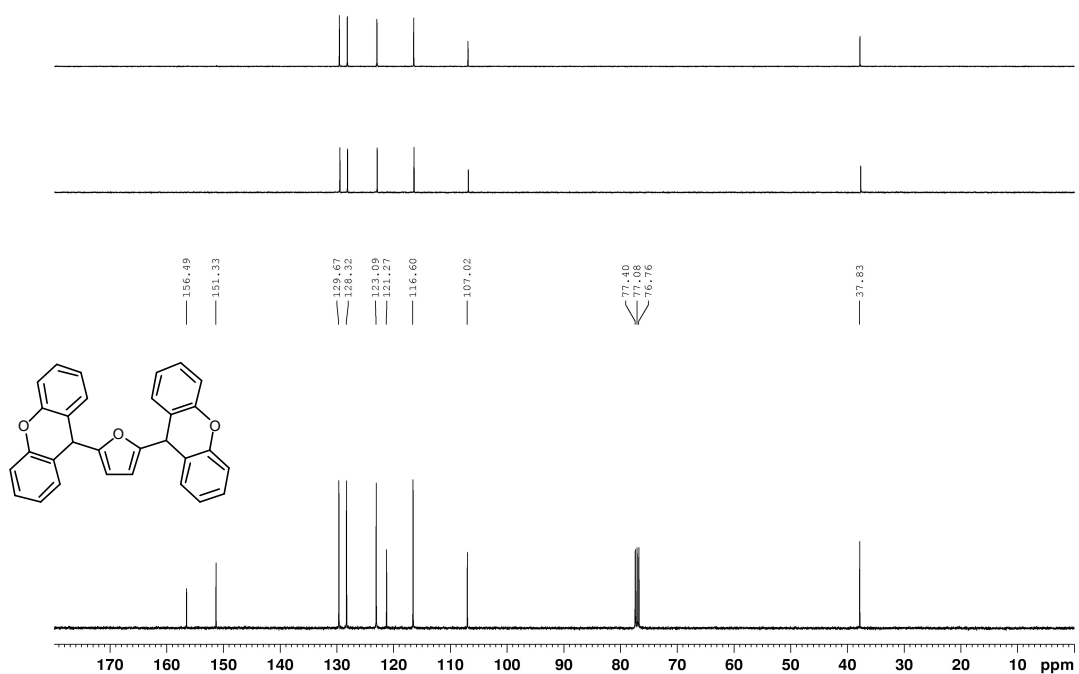


¹H-NMR and ¹³C-NMR spectral of compound 6b

MW-15-2

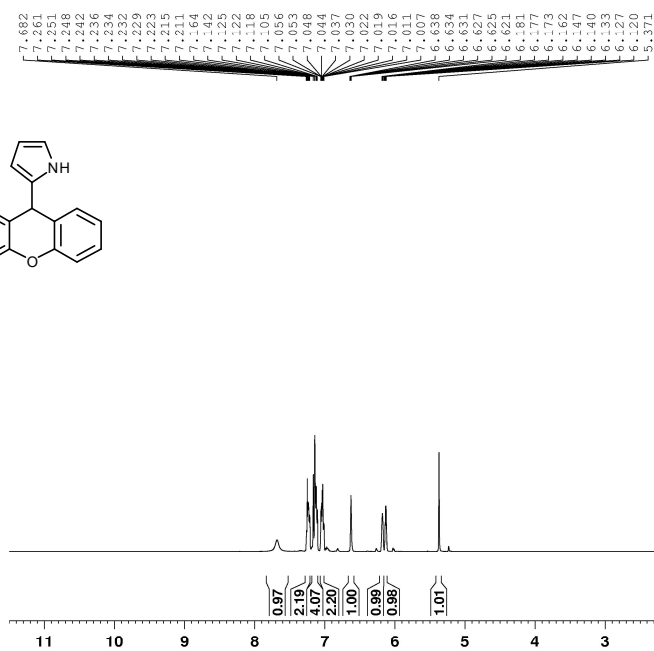
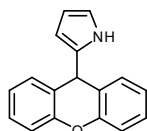


MW-15-2



¹H-NMR and ¹³C-NMR spectral of compound 6c

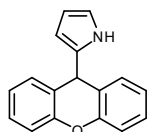
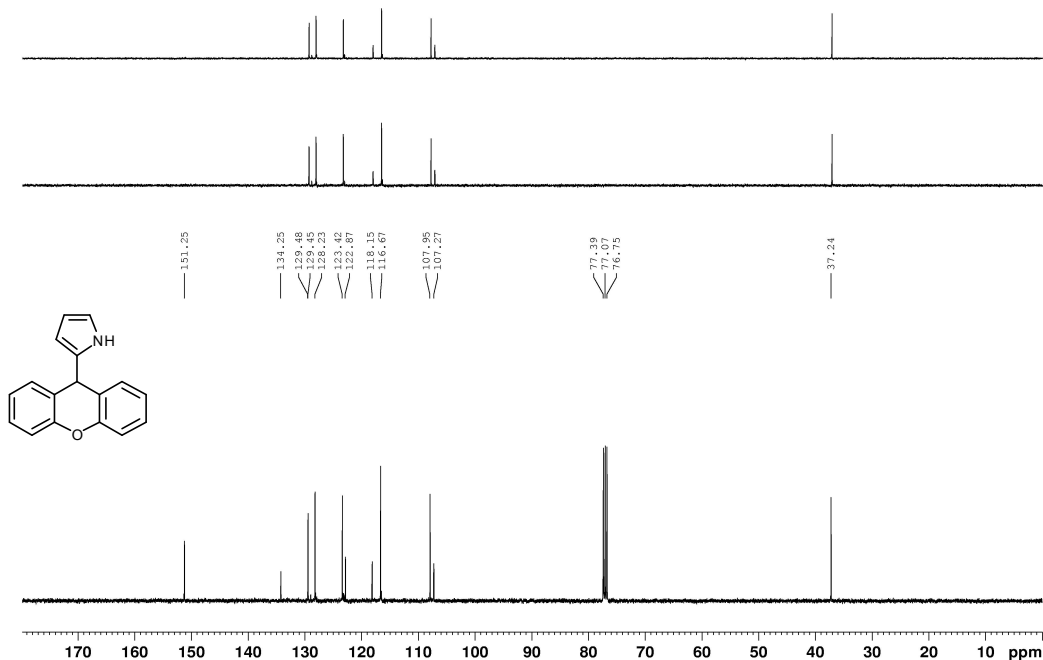
MW-17-2



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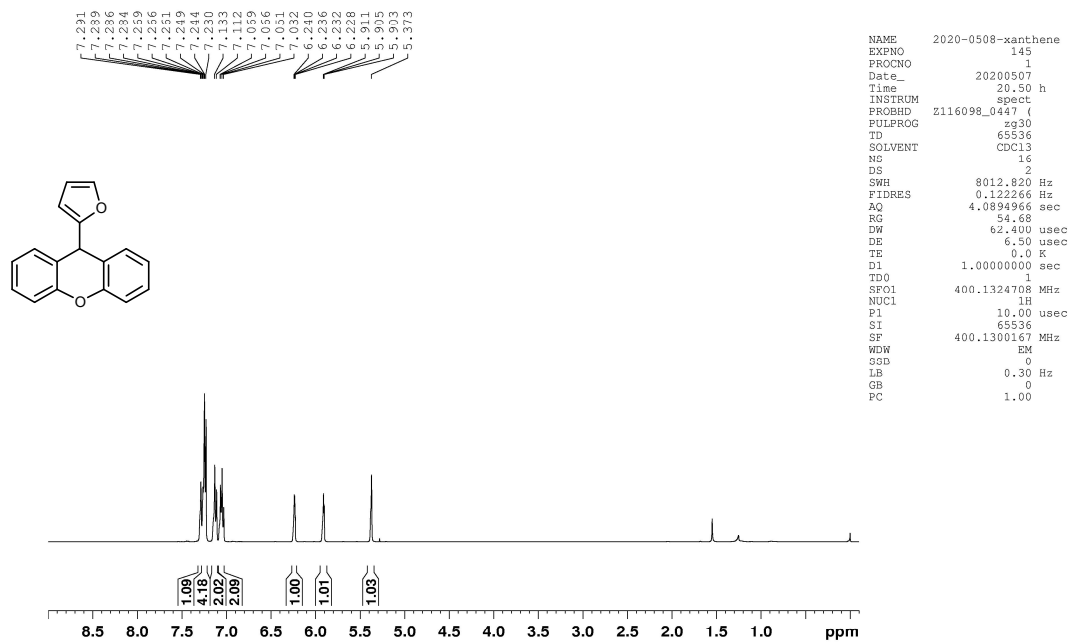
NAME      2020-0508-xanthene
EXPNO     141
PROCNO    1
Date_     20200507
Time      20.06 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SFO1      8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         64.45
NW         62.400 usec
DE         6.50 usec
TE         0.0 K
D1         1.0000000 sec
TDO        1
SFO1      400.1324708 MHz
NUC1      1H
P1         10.00 usec
SI         65536
SF         400.1300138 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

MW-17-2

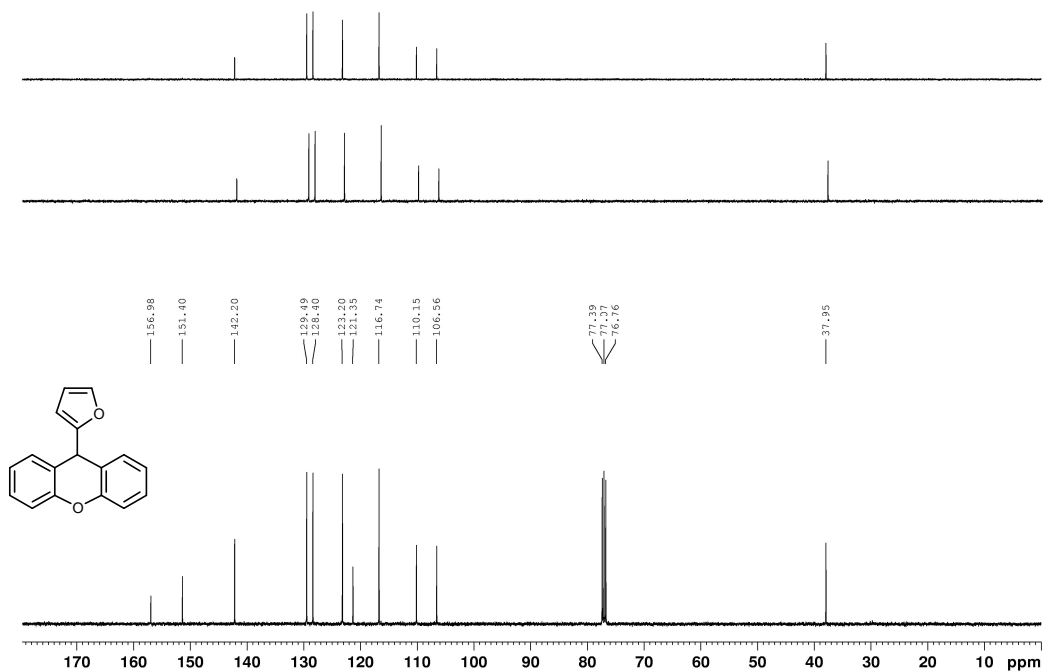


¹H-NMR and ¹³C-NMR spectral of compound 6d

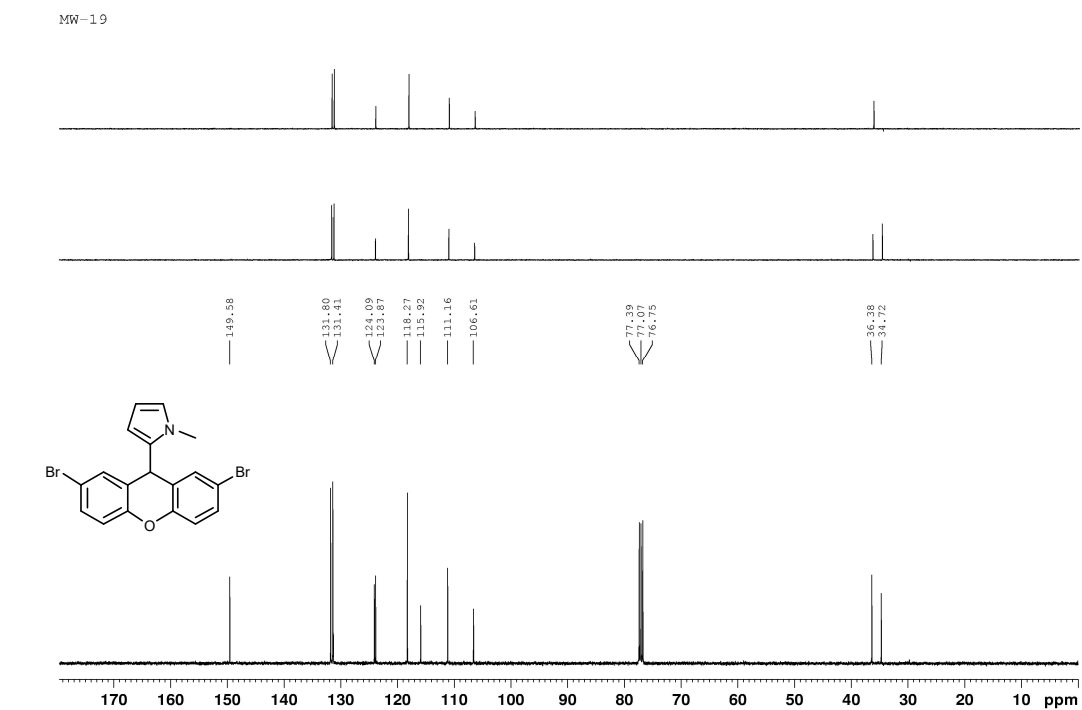
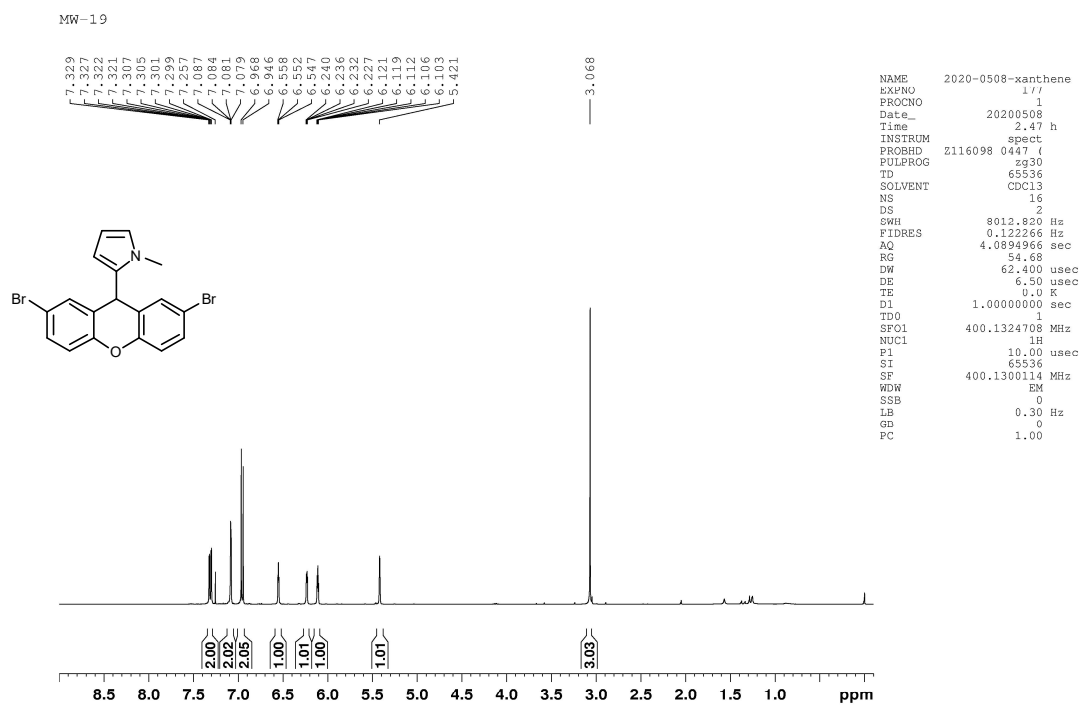
MW-15-1



MW-15-1

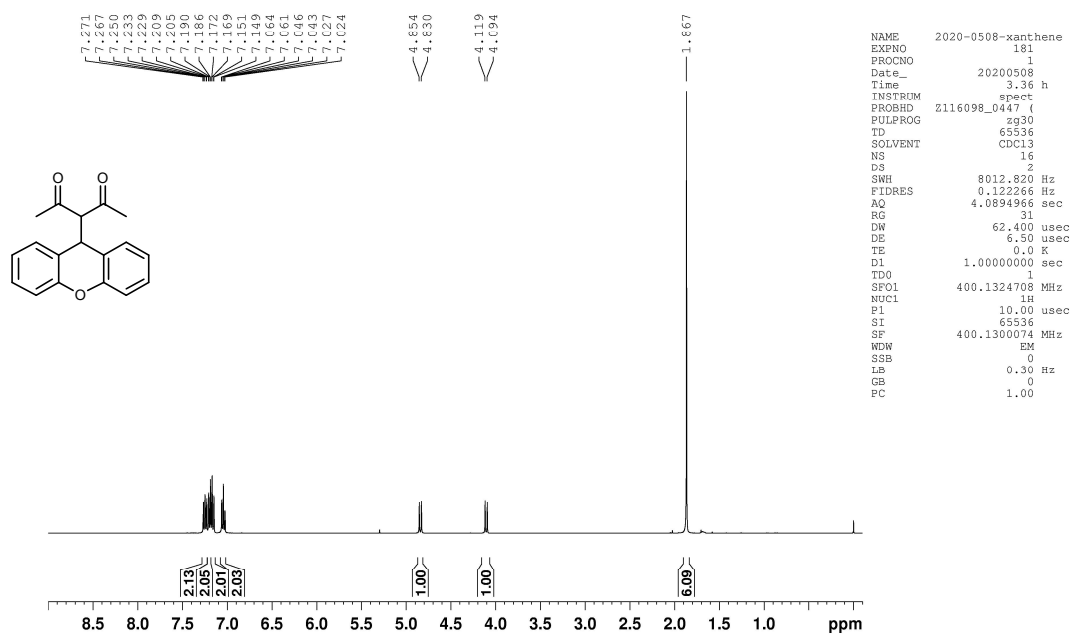


¹H-NMR and ¹³C-NMR spectral of compound 6e

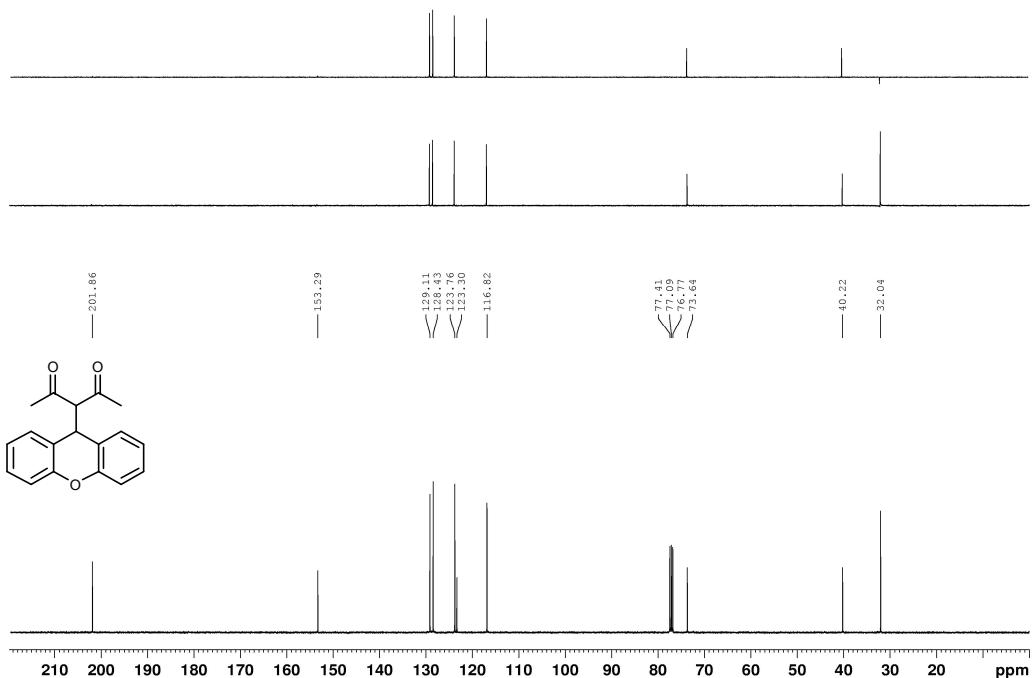


¹H-NMR and ¹³C-NMR spectral of compound 6f

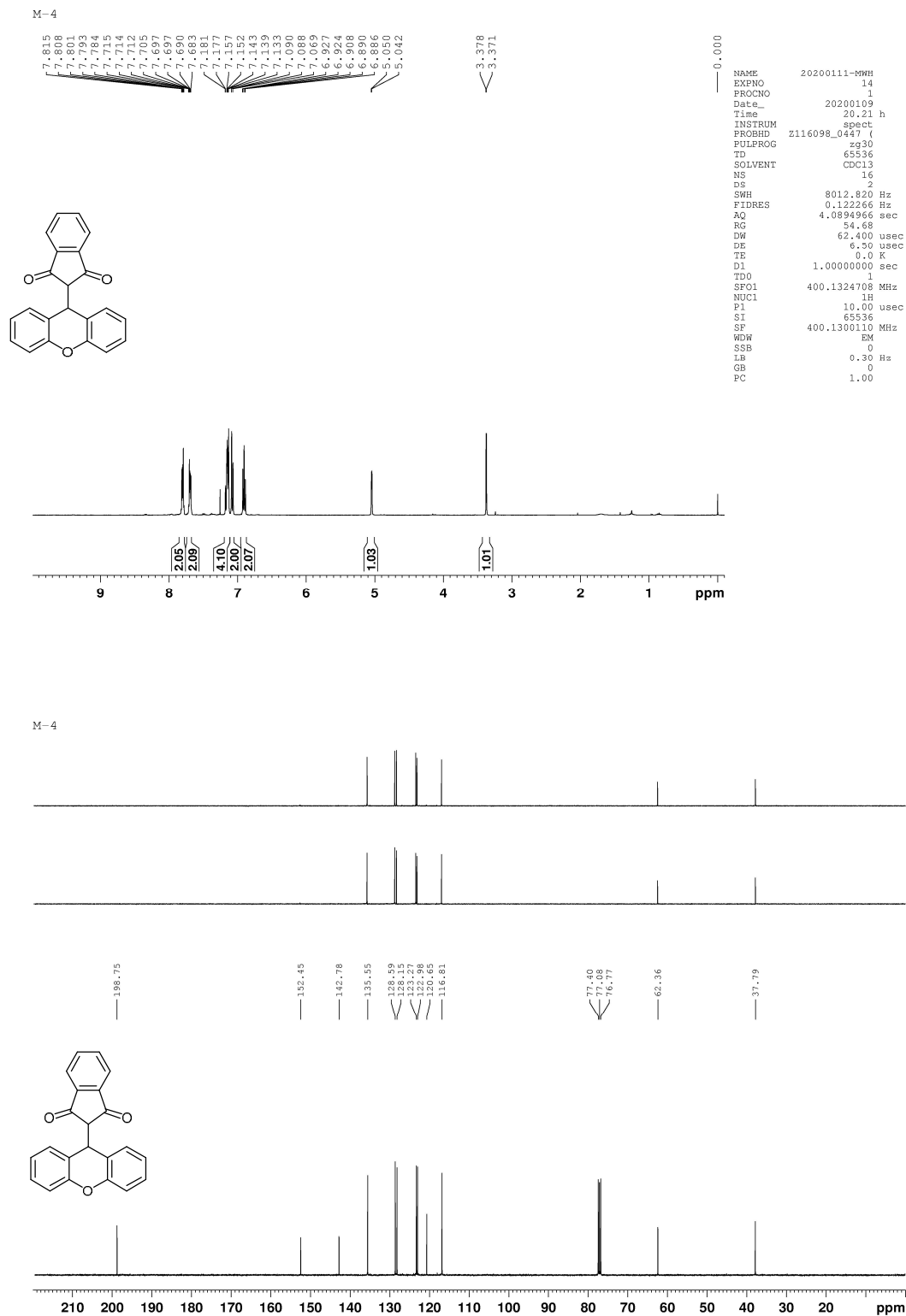
MW-26



MW-26

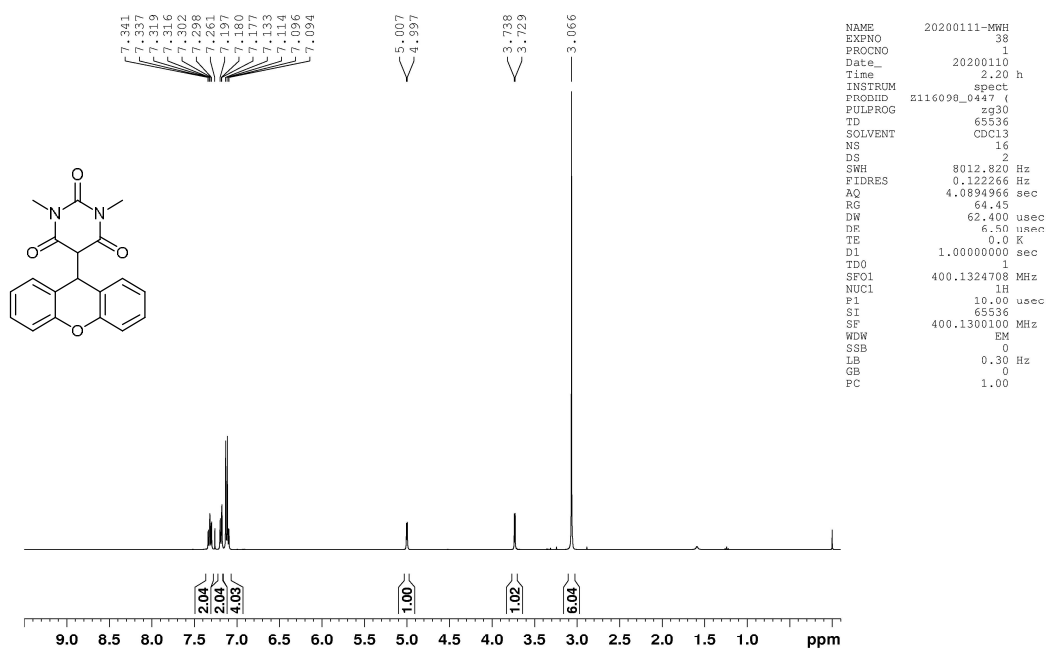


¹H-NMR and ¹³C-NMR spectral of compound 6g



¹H-NMR and ¹³C-NMR spectral of compound 6h

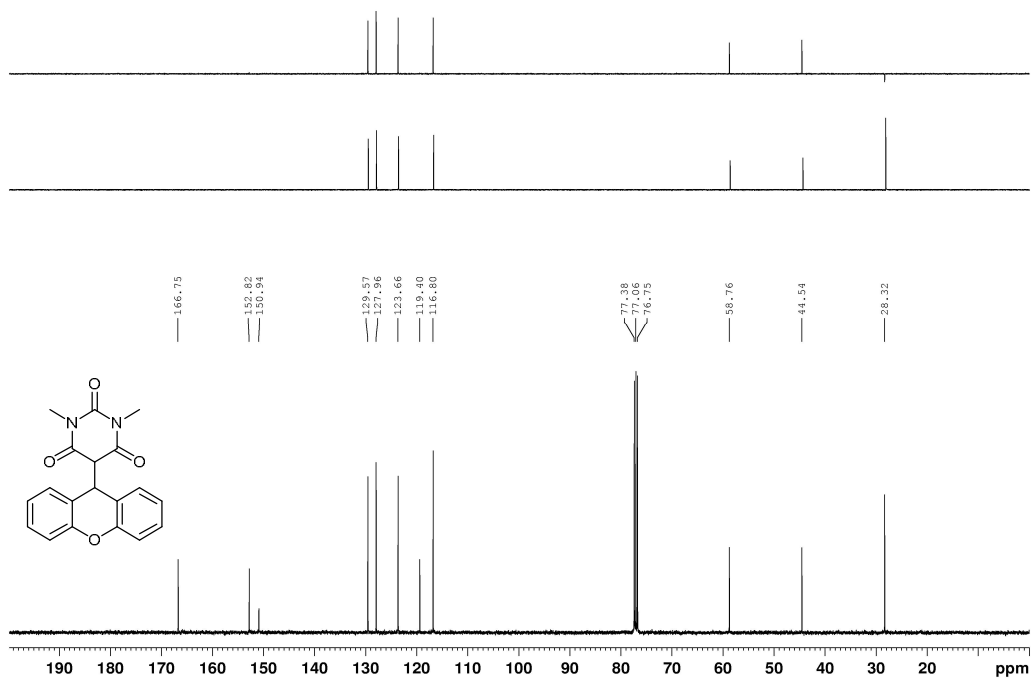
M-14



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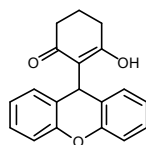
NAME      20200111-MWH
EXPNO    38
PROCNO   1
Date_    20200110
Time     2.20 h
INSTRUM  spect
PROBHD   z116098_0447 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         64.45
DM         62.400 usec
DE         6.50 usec
TE         0.0 K
D1         1.00000000 sec
TDO        1
SFO1      400.1324708 MHz
NUC1      1H
P1         10.00 usec
SI         65536
SF         400.1300100 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

M-14



¹H-NMR and ¹³C-NMR spectral of compound 6i

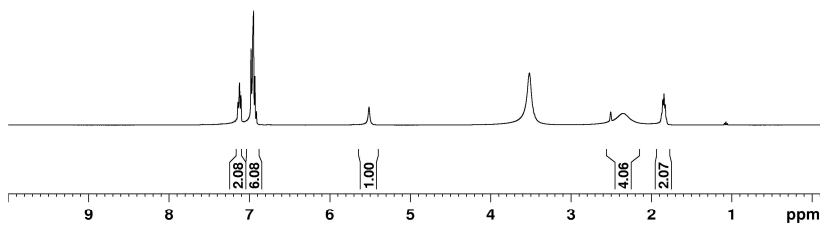
w-16



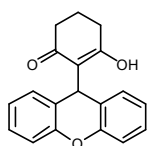
7.141
7.123
7.123
7.079
6.949
6.931
6.912
5.911
3.920
2.357
1.850
1.845
1.850

```

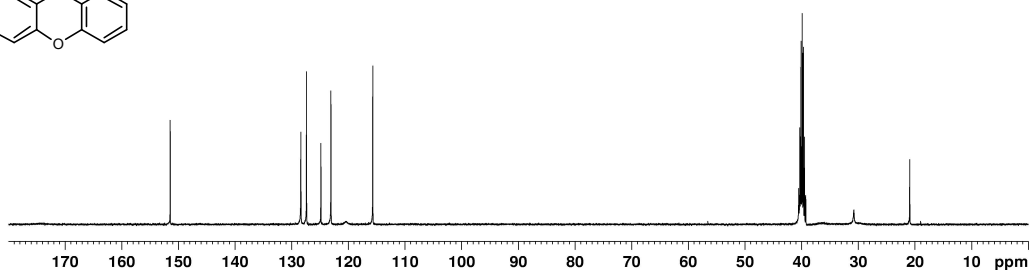
NAME      MW-20200531-YD
EXPNO     21
PROCNO    1
Date_     20200528
Time      13.44 h
INSTRUM   Avance
PROBHD    Z116098_0861 (
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        5555.556 Hz
FIDRES     0.169542 Hz
AQ          5.8982902 sec
RG          48.7805
DW          90.000 usec
DE          9.46 usec
TE          296.1 K
D1          1.00000000 sec
TD0         1
SF01       400.1321847 MHz
NUC1       1H
PC         3.50 usec
P1         10.50 usec
SI         65536
SF         400.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



w-16

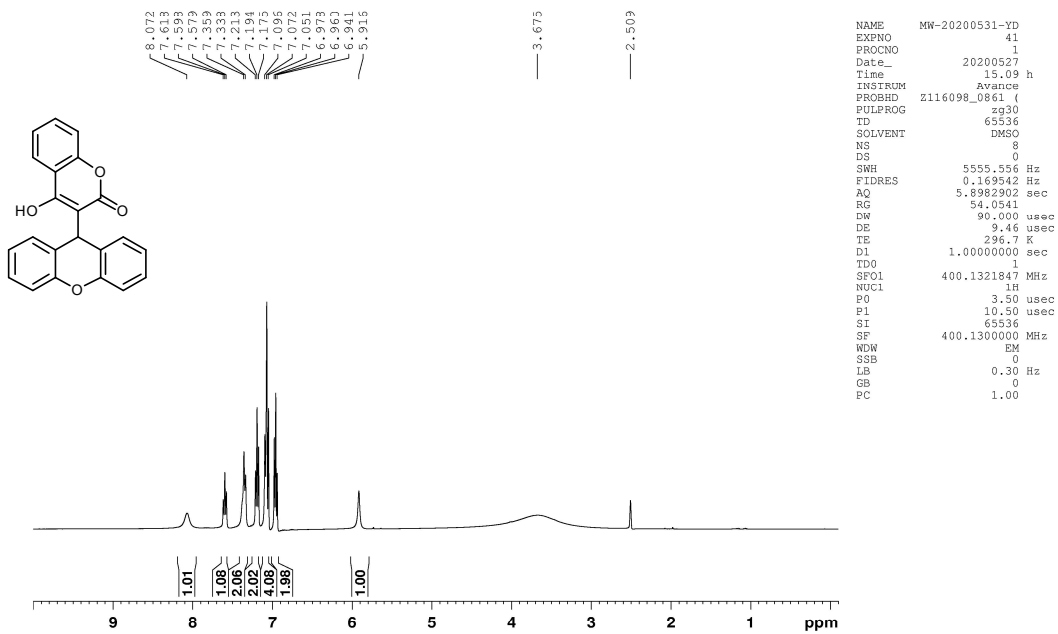


151.41
128.99
127.99
124.85
123.08
115.70
40.52
40.32
39.60
39.60
39.69
39.48
39.27
30.79
20.92

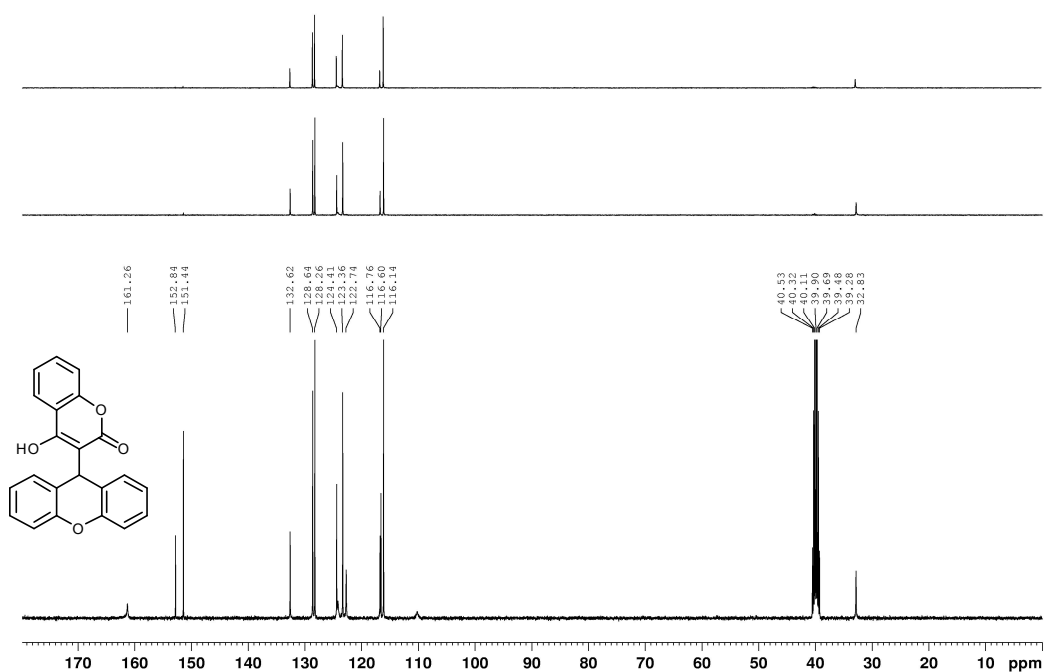


¹H-NMR and ¹³C-NMR spectral of compound 6j

w-22

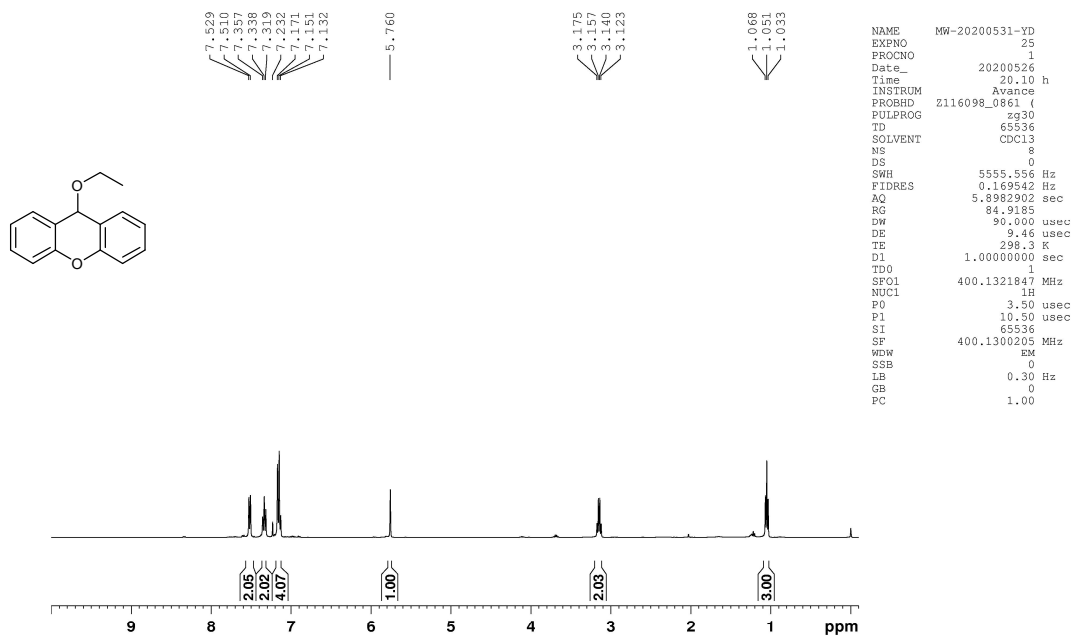


w-22

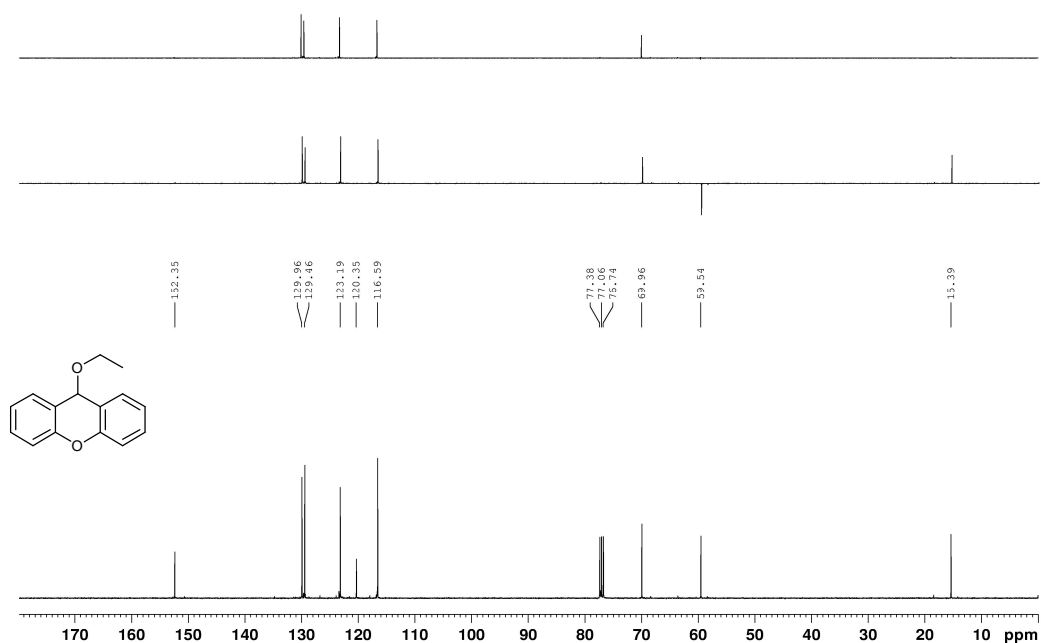


¹H-NMR and ¹³C-NMR spectral of compound 6k

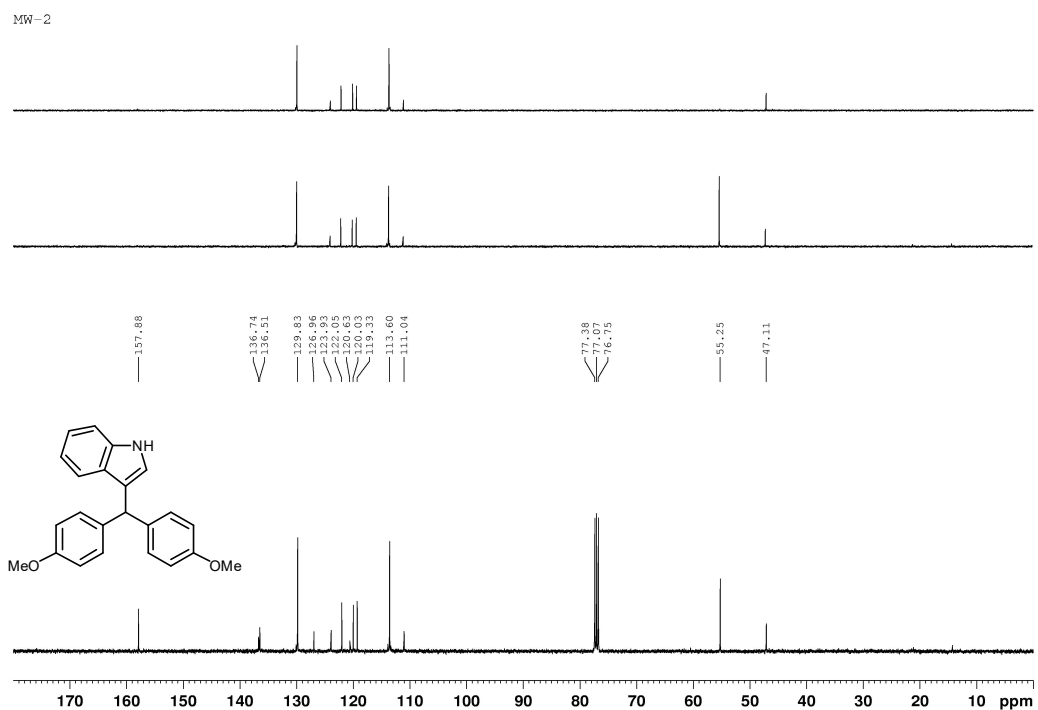
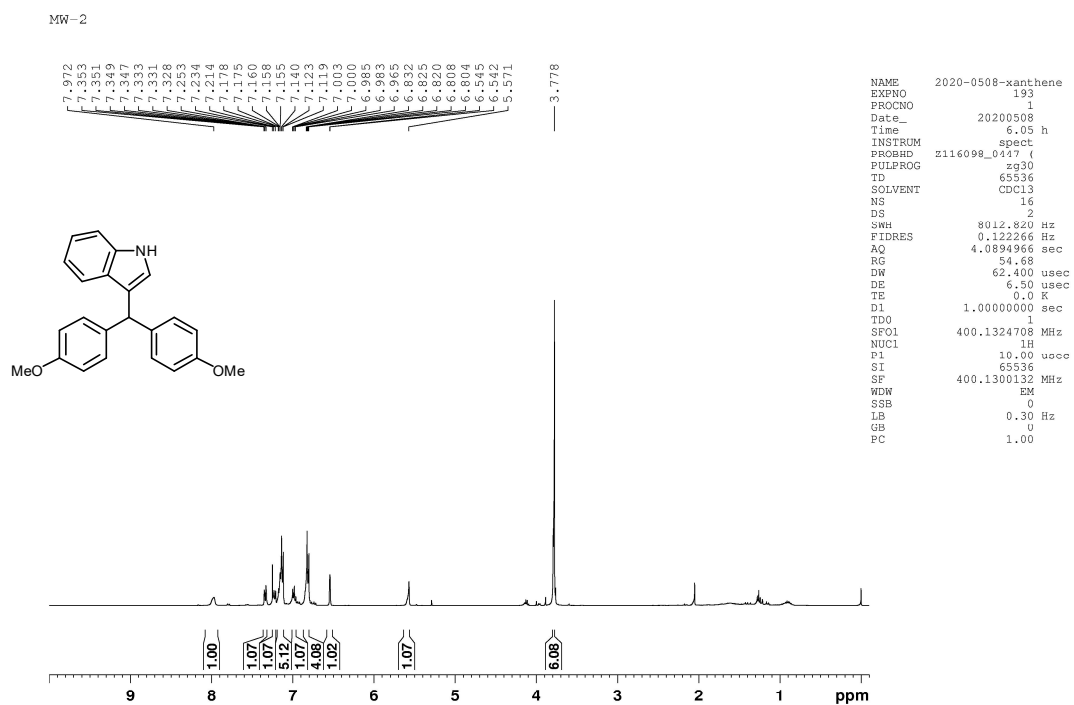
w-18



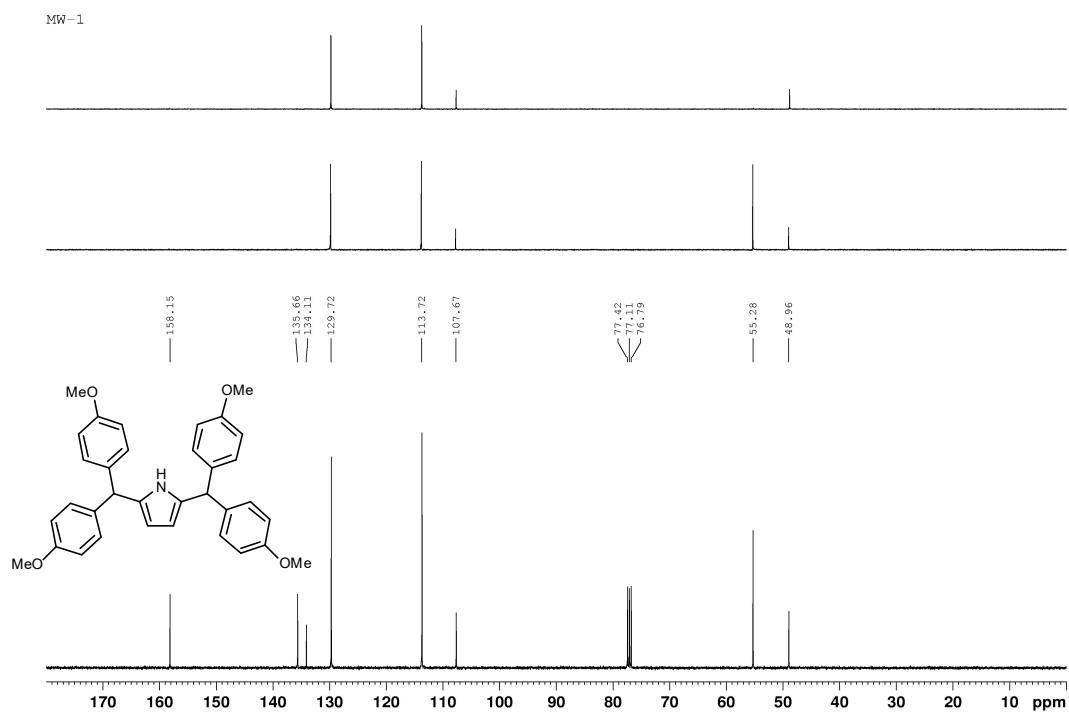
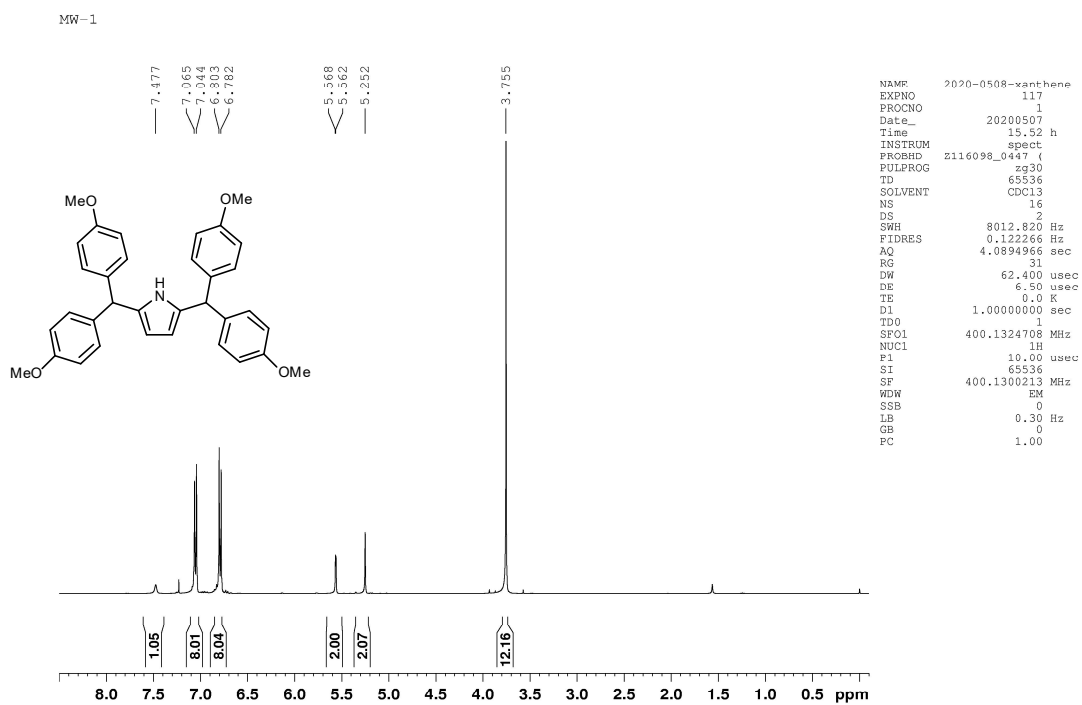
w-18



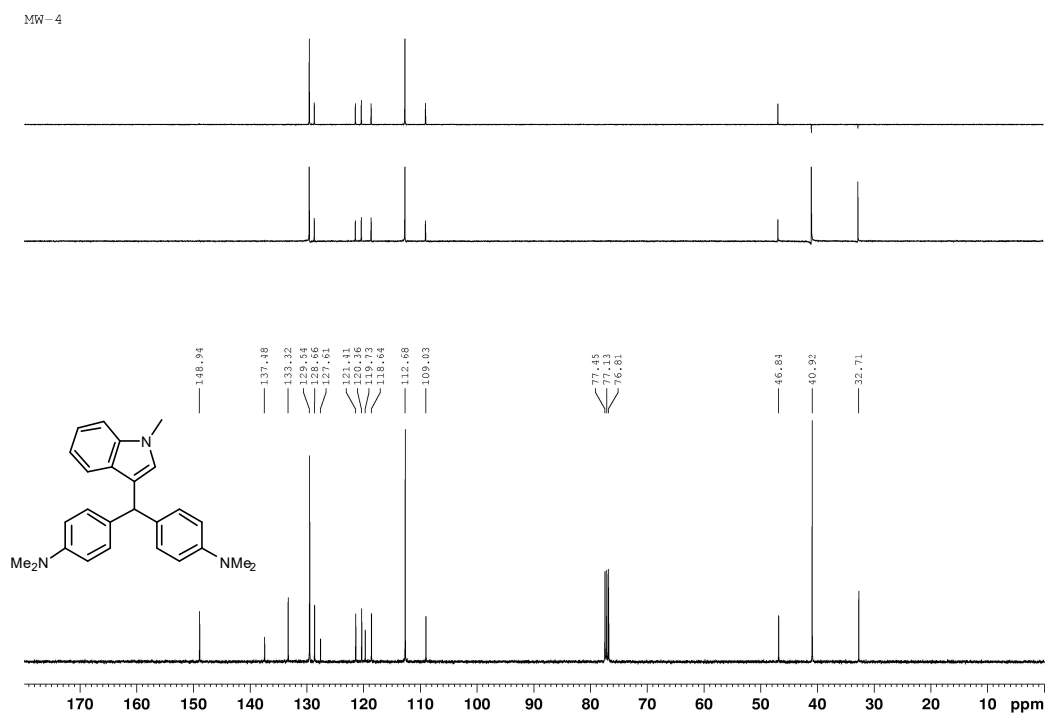
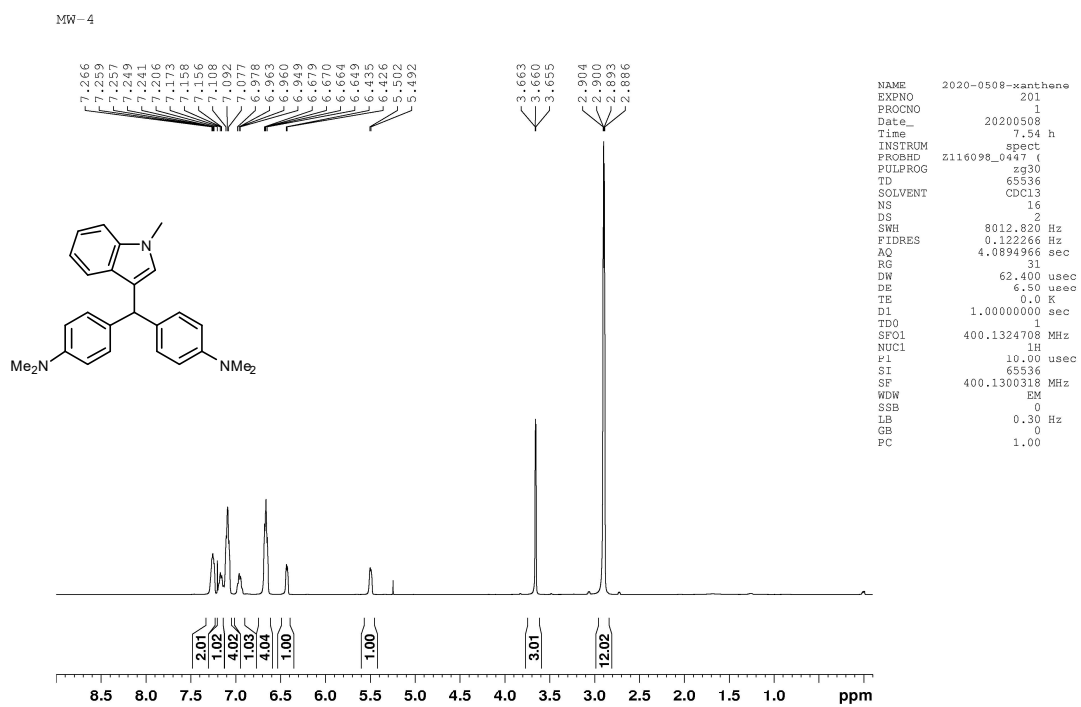
¹H-NMR and ¹³C-NMR spectral of compound 8b



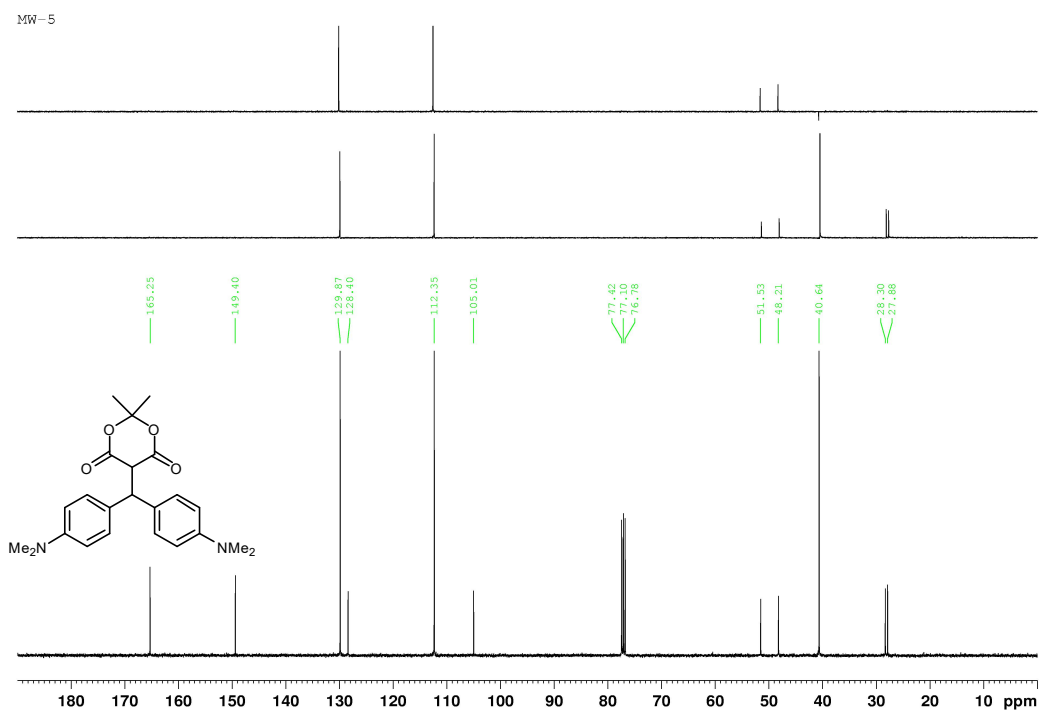
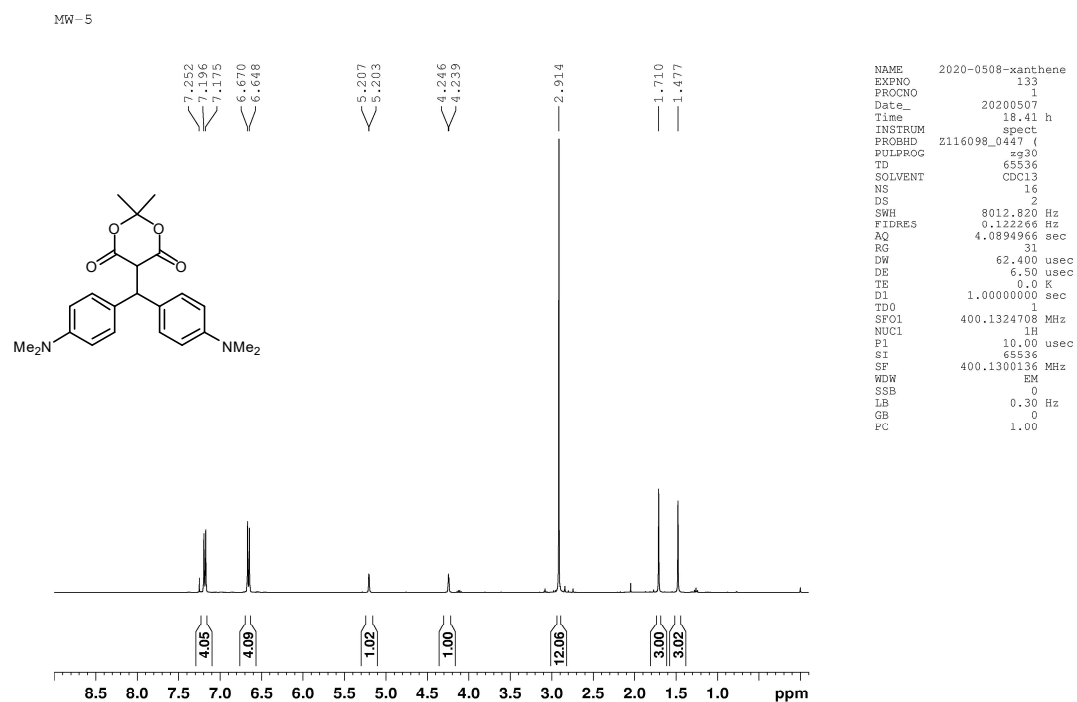
¹H-NMR and ¹³C-NMR spectral of compound 8c



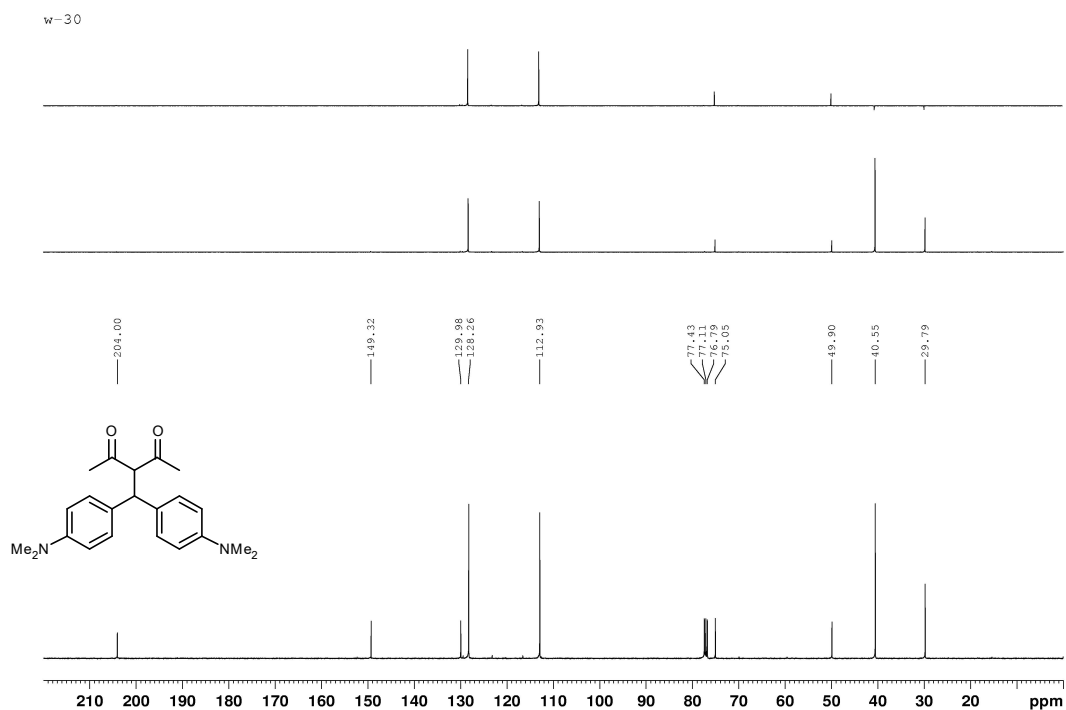
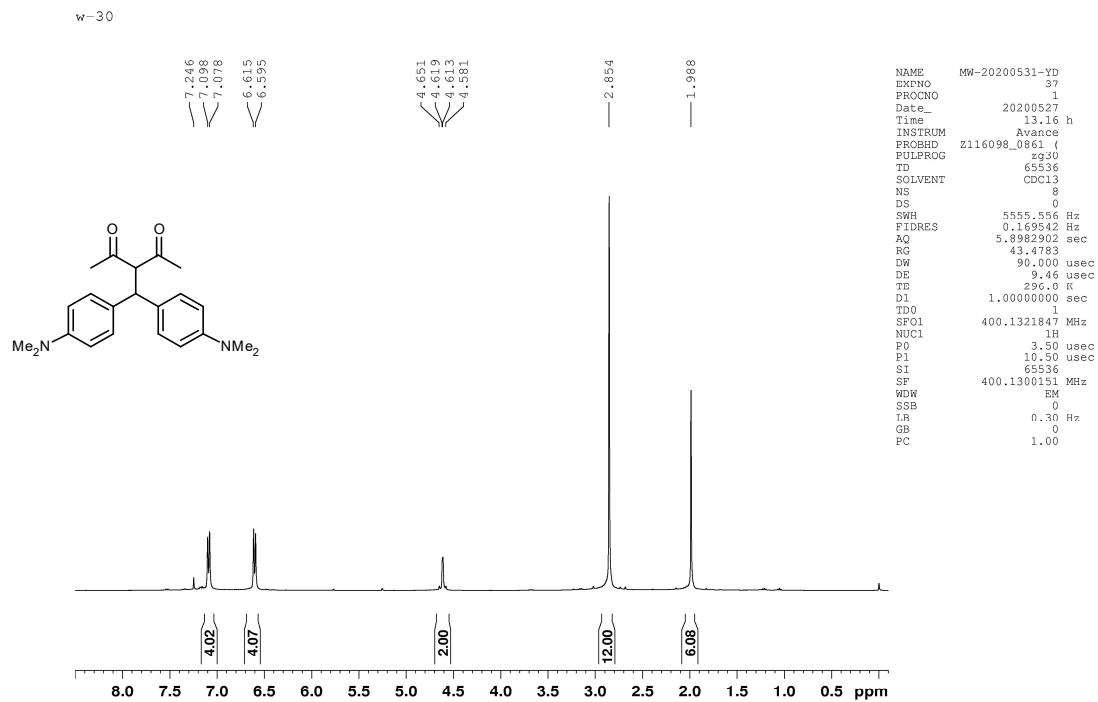
¹H-NMR and ¹³C-NMR spectral of compound 8d



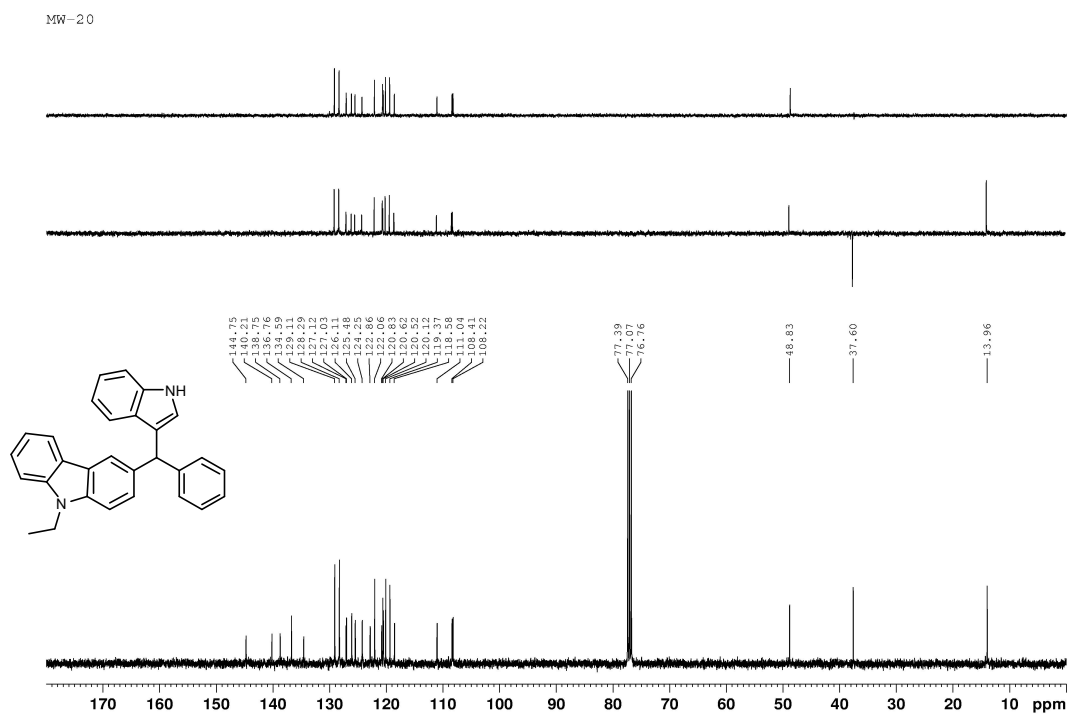
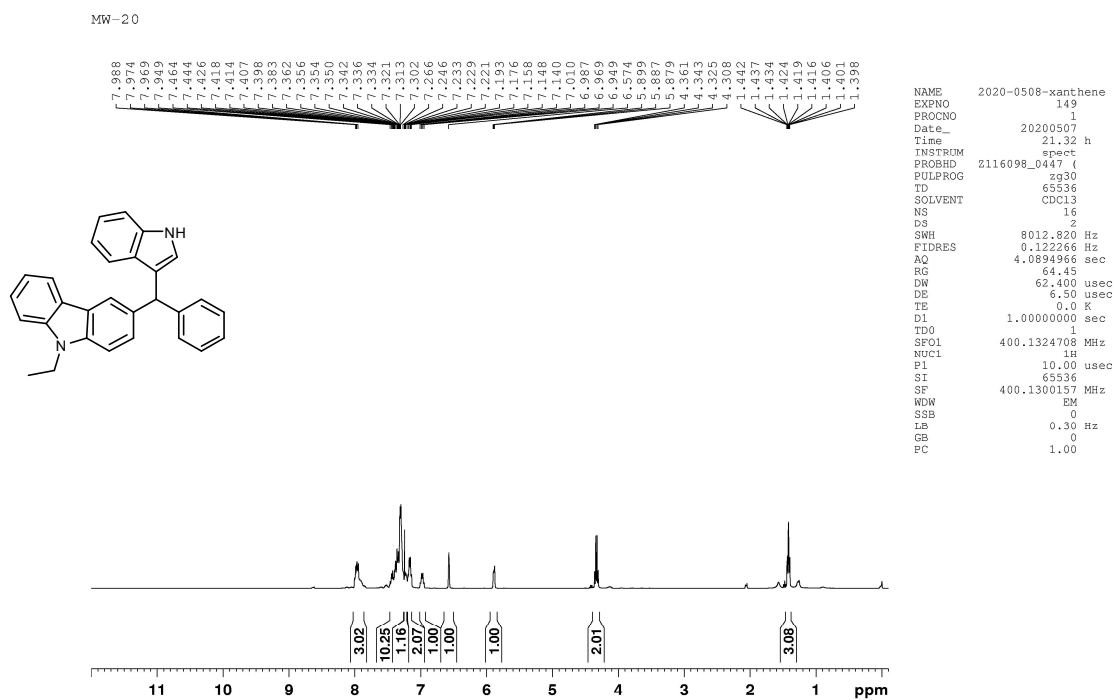
¹H-NMR and ¹³C-NMR spectral of compound 8e



¹H-NMR and ¹³C-NMR spectral of compound 8f

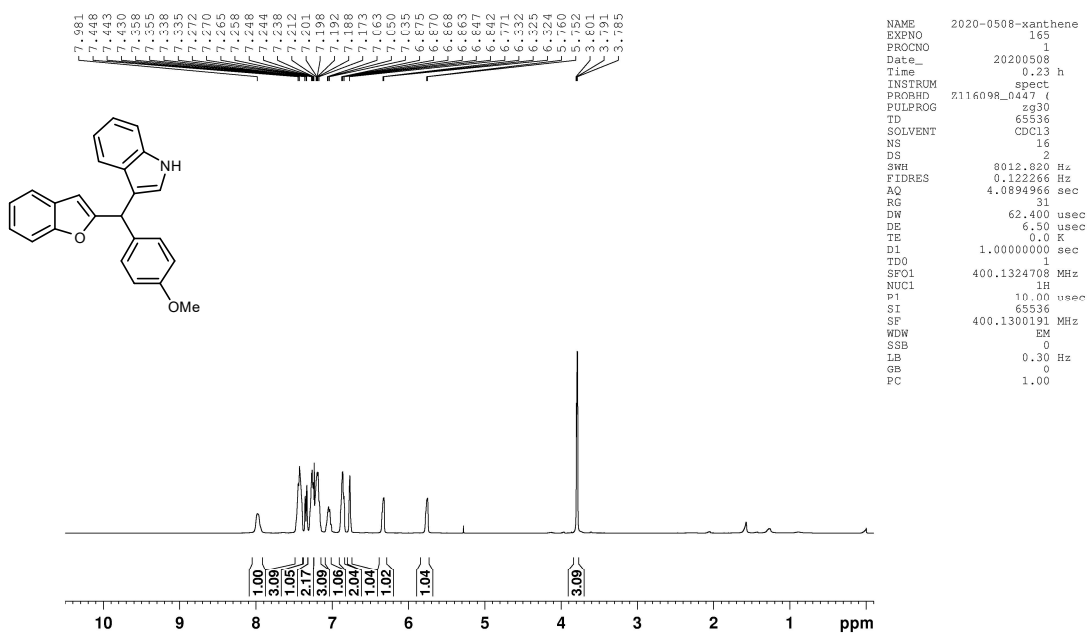


¹H-NMR and ¹³C-NMR spectral of compound 8g

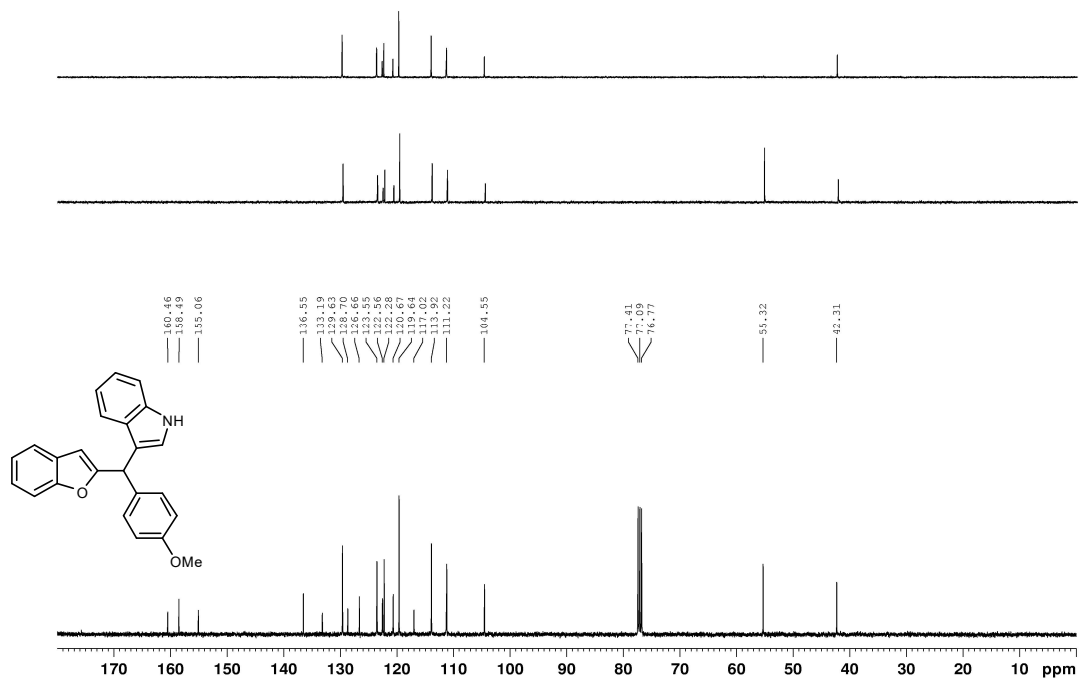


¹H-NMR and ¹³C-NMR spectral of compound 8h

MW-21

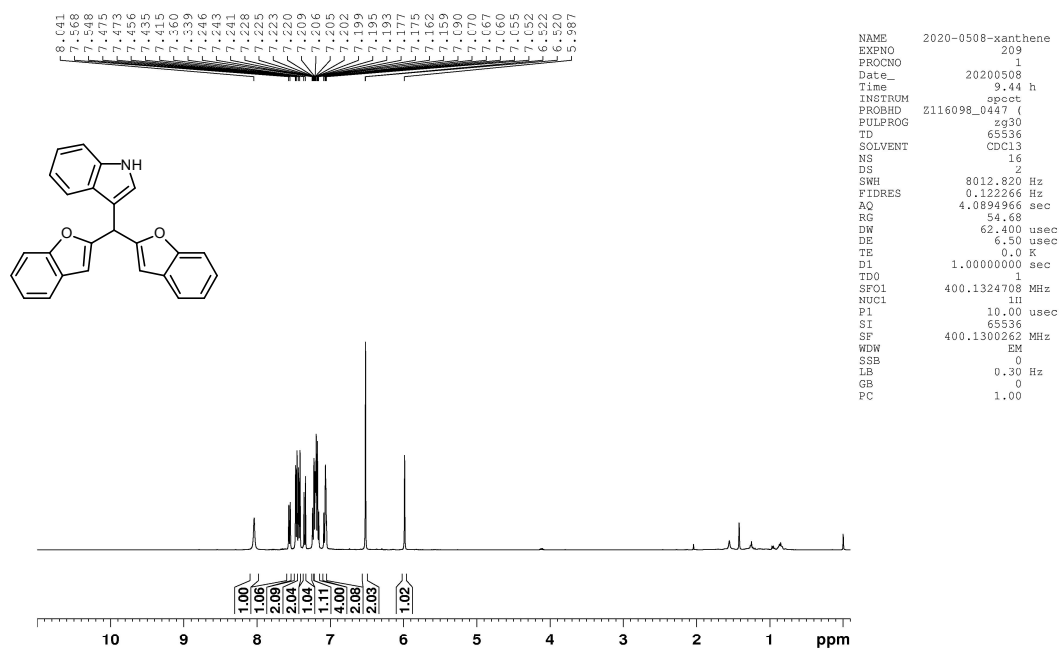


MW-21

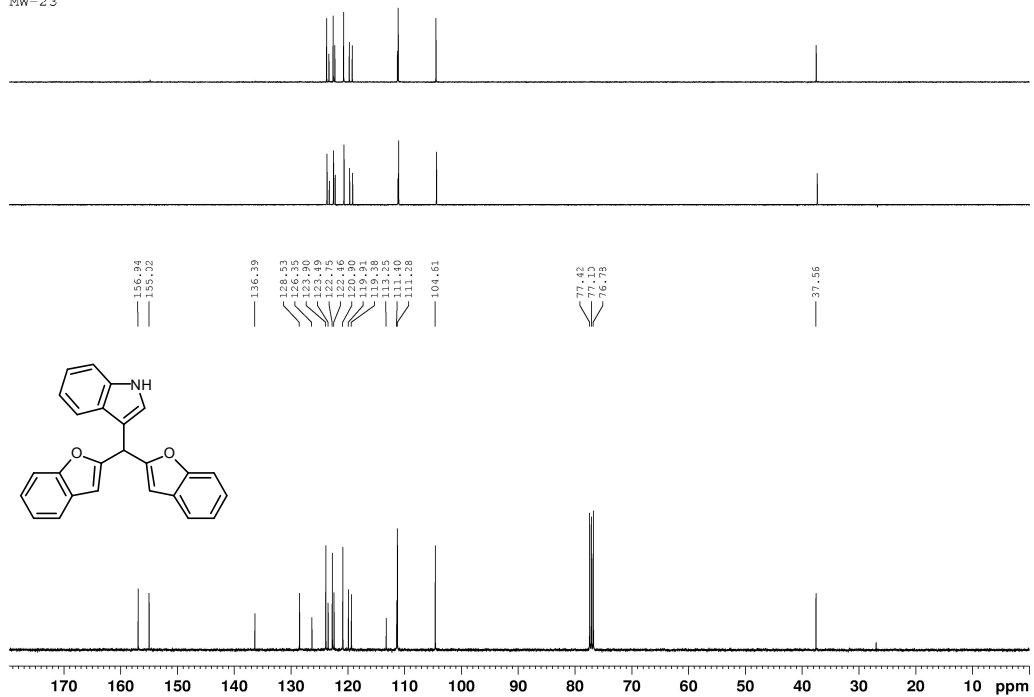


¹H-NMR and ¹³C-NMR spectral of compound 8i

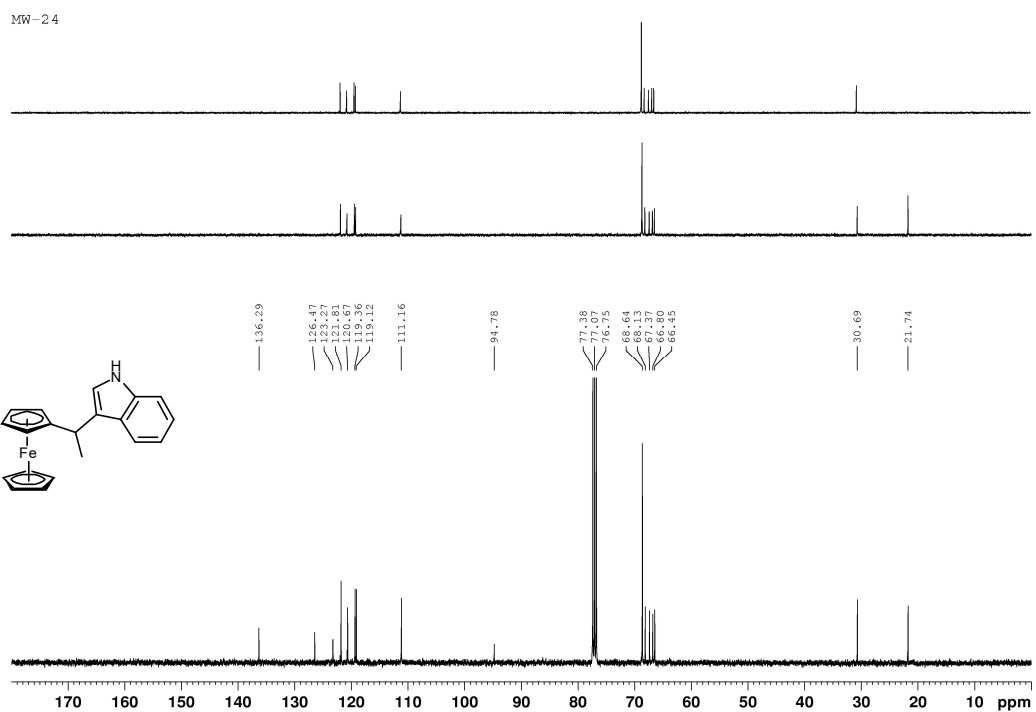
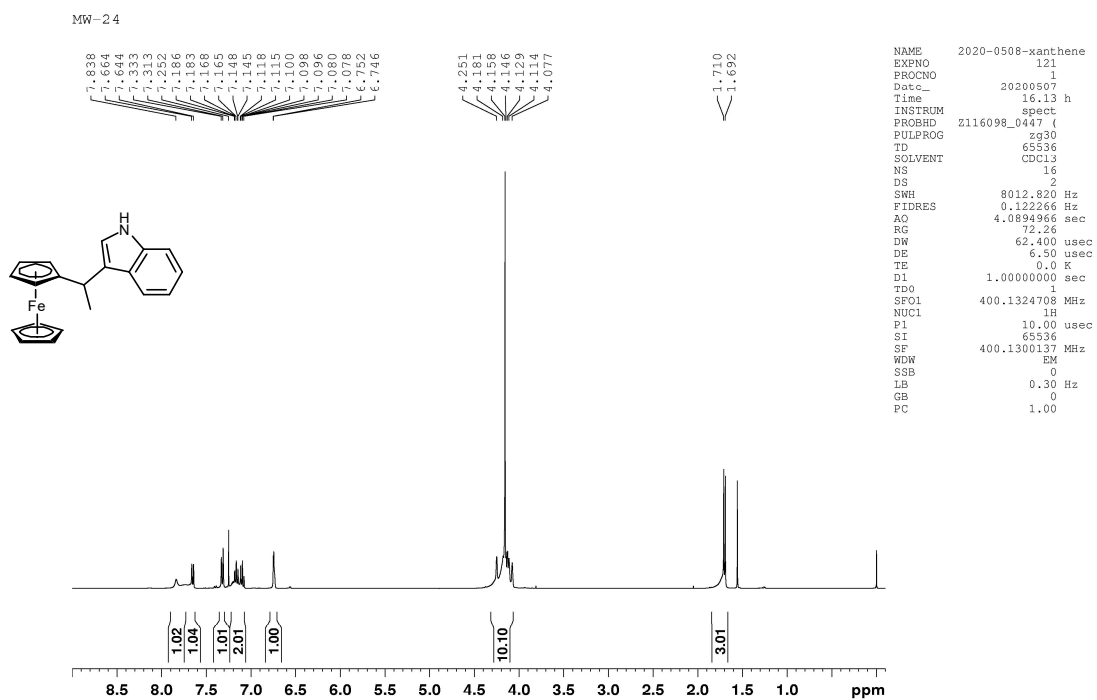
MW-23



MW-23



¹H-NMR and ¹³C-NMR spectral of compound 8j



¹H-NMR and ¹³C-NMR spectral of compound 8k

