Palladium-catalyzed cascade reaction of enynone and isocyanide: an access towards functionalized ketenimine and its application

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Supporting Information

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1 General Information

The NMR spectra were recorded on Bruker AC-500 spectrometer (500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR) with $CDCl_3$ as the solvent and TMS as internal reference. ^{1}H NMR spectral data were reported as follows: chemical shift (δ, ppm), multiplicity, integration, and coupling constant (Hz). ^{13}C NMR spectral data were reported in terms of the chemical shift. The following abbreviations were used to indicate multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet. Low-resolution mass spectra were obtained on a Shimadzu LCMS-2010EV spectrometer in ESI mode and reported as m/z. High-resolution mass spectra (HRMS) were recorded on a Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS instrument. Melting points were obtained on a X-4 digital melting point apparatus without correction. Purification of products was accomplished by column chromatography packed with silica gel. Dry THF was used as solvent and pretreated by sodium. Unless otherwise stated, all reagents were commercially purchased and used without further purification.

2 General Procedure

2.1 General procedure for the synthesis of ketenimine 3

Under nitrogen atmosphere, $Pd(PPh_3)_4$ (0.05 equiv) and PPh_3 (1.0 equiv) were added to a solution of enynone **1** (0.5 mmol) and isocyanide **2** (0.5 mmol) in 5 mL THF. The stirred mixture was stirred at room temperature for 3 hours and the progress was monitored using TLC detection. After completion of present reaction, the reaction mixture was concentrated under vacuum. The residue was purified by column chromatography on alumina [neutral alumina: 200-300; eluant: petroleum ether/ethyl acetate = 40:1] to afford the desired product **3**.

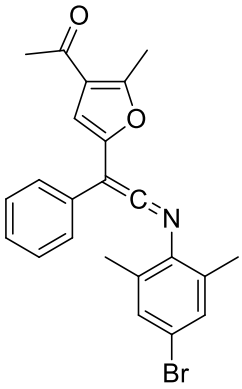
2.1 General procedure for the reaction of ketenimine and isocyanide

Under air atmosphere, ketenimine **3** (0.5 mmol) was added to a solution of isocyanide **2** (0.5 mmol) in 5 mL toluene. The stirred mixture was heated at 100 ^{o}C for 12 hours and the progress was monitored using TLC detection. After completion of present reaction, the reaction mixture was concentrated under vacuum. The residue was purified by column chromatography on alumina [neutral alumina: 200-300; eluant: petroleum ether/ethyl acetate = 50:1] to afford the desired product **4**.

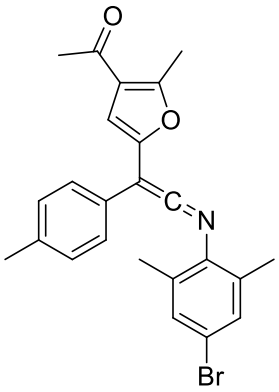
2.2 General procedure for the hydrolysis of indenone derivative

Under air atmosphere, indenone derivative **4** (0.5 mmol) was added to a solution of HCl (0.5 mmol) in 15 mL ethyl alcohol. The stirred mixture was stirred at room temperature for 4 hours and the progress was monitored using TLC detection. After completion of present reaction, the reaction mixture was concentrated under vacuum. The residue was purified by column chromatography on alumina [neutral alumina: 200-300; eluant: petroleum ether/ethyl acetate = 50:1] to afford the desired product **5**.

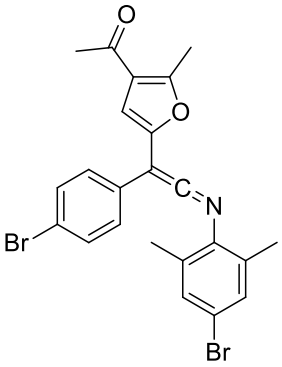
3 Characterization Data



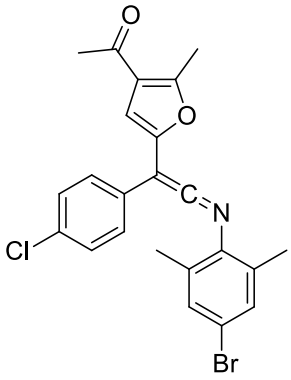
(**3a**): 159 mg, 76% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 4.4 Hz, 4H), 7.27-7.25 (m, 1H), 7.25-7.22 (m, 2H), 6.47 (s, 1H), 2.61 (s, 3H), 2.40 (s, 3H), 2.32 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.09, 183.65, 157.33, 145.49, 136.65, 133.68, 132.20, 131.38, 129.18, 127.10, 126.69, 123.36, 119.86, 107.19, 65.61, 29.34, 18.79, 14.59. HRMS (ESI): calcd. for $C_{23}H_{21}BrNO_2$ $[M+H]^+$ 422.0750, Found: 422.0753.



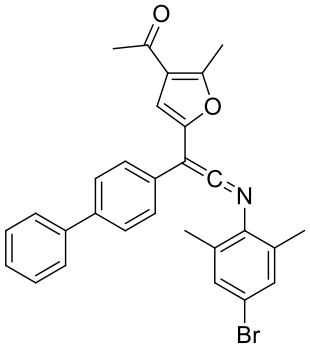
(**3b**): 128 mg, 59% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (t, *J* = 2.0 Hz, 1H), 7.28-7.27 (m, 1H), 7.22 (s, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.43 (s, 1H), 2.61 (s, 3H), 2.39 (s, 3H), 2.37 (s, 3H), 2.31 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.12, 184.71, 157.21, 145.76, 137.03, 136.67, 133.41, 131.32, 129.91, 128.75, 127.24, 123.35, 119.62, 106.94, 65.64, 29.32, 21.27, 18.76, 14.57. HRMS (ESI): calcd. for $C_{24}H_{23}BrNO_2$ $[M+H]^+$ 436.0907, Found: 436.0900.



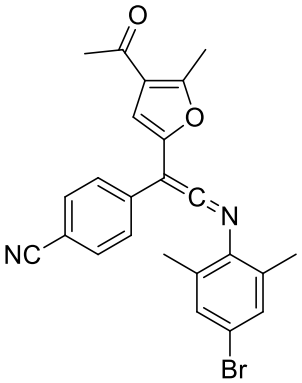
(**3c**): 101 mg, 41% yield, yellow solid: m. p. 164-165 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52-7.49 (m, 1H), 7.51-7.49 (m, 1H), 7.49-7.47 (m, 1H), 7.49-7.47 (m, 1H), 7.26-7.21 (m, 4H), 6.45 (s, 1H), 2.60 (s, 3H), 2.40 (s, 3H), 2.32 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.95, 182.09, 157.55, 144.96, 136.03, 133.97, 132.28, 131.53, 128.41, 123.37, 120.27, 120.00, 107.41, 64.68, 29.34, 18.82, 14.60. HRMS (ESI): calcd. for $C_{23}H_{20}Br_2NO_2$ $[M+H]^+$ 499.9855, Found: 499.9857.



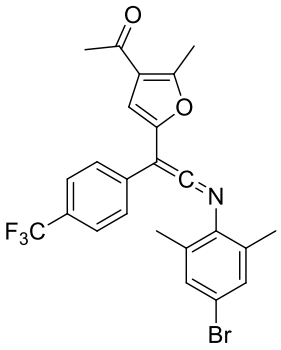
(**3d**): 160 mg, 70% yield, yellow solid: m. p. 142-143 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 7.24 (s, 2H), 6.44 (s, 1H), 2.60 (s, 3H), 2.40 (s, 3H), 2.32 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.97, 182.40, 157.53, 145.07, 136.14, 133.92, 132.14, 131.48, 130.98, 129.36, 128.14, 123.38, 120.22, 107.36, 64.68, 29.34, 18.82, 14.61. HRMS (ESI): calcd. for $C_{23}H_{20}ClBrNO_2$ $[M+H]^+$ 456.0360, Found: 456.0354.



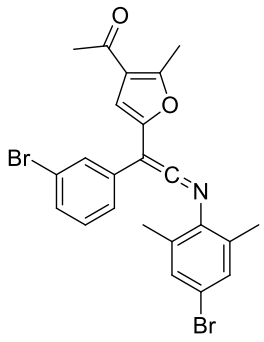
(**3e**): 139 mg, 56% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65-7.63 (m, 1H), 7.63 (d, *J* = 1.8 Hz, 2H), 7.61 (t, *J* = 2.4 Hz, 1H), 7.48-7.44 (m, 4H), 7.38-7.33 (m, 1H), 7.25 (s, 2H), 6.54 (s, 1H), 2.63 (s, 3H), 2.42 (s, 3H), 2.36 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.06, 183.33, 157.38, 145.36, 140.58, 139.41, 136.44, 133.79, 131.32, 128.92, 127.81, 127.46, 127.26, 126.99, 123.37, 119.98, 107.35, 65.28, 29.32, 18.83, 14.59. HRMS (ESI): calcd. for $C_{29}H_{25}BrNO_2$ $[M+H]^+$ 498.1063, Found: 498.1058.



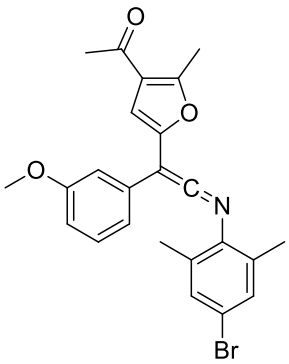
(**3f**): 152 mg, 63% yield, yellow, solid: m. p. 196-197 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 1.8 Hz, 1H), 7.59-7.57 (m, 1H), 7.39 (d, *J* = 8.6 Hz, 1H), 7.17-7.10 (m, 3H), 6.57 (s, 1H), 2.62 (s, 3H), 2.43 (s, 3H), 2.40 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.91, 174.91, 158.01, 144.38, 139.91, 134.83, 133.51, 132.75, 128.93, 128.08, 125.66, 123.31, 119.32, 108.41, 108.20, 63.00, 29.35, 19.15, 14.66. HRMS (ESI): calcd. for $C_{24}H_{20}BrN_2O_2$ $[M+H]^+$ 447.0703, Found: 447.0707.



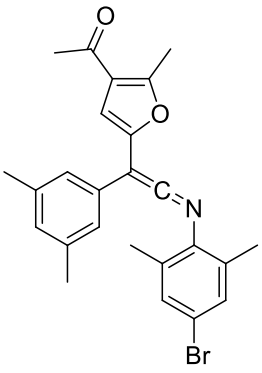
(**3g**): 176 mg, 72% yield, yellow solid: m. p. 130-131 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.26 (s, 2H), 6.54 (s, 1H), 2.62 (s, 3H), 2.42 (s, 3H), 2.35 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.87, 179.87, 157.78, 144.50, 137.27, 135.21, 134.53, 131.58, 130.67, 128.43, 128.17, 127.91, 127.59 (d, *J* = 17.1 Hz), 126.30, 126.04 (q, *J* = 3.6 Hz), 125.36, 123.37, 123.20, 120.77, 107.97, 64.28, 29.32, 18.87, 14.60. HRMS (ESI): calcd. for $C_{24}H_{20}BrF_3NO_2$ $[M+H]^+$ 490.0624, Found: 490.0619.



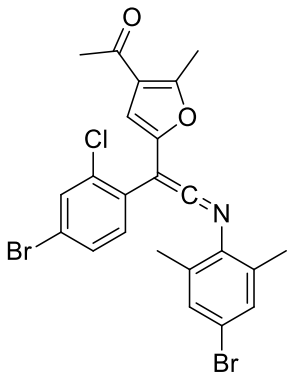
(**3h**): 148 mg, 59% yield, yellow solid: m. p. 108-109 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.34 (d, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.26 - 7.19 (m, 3H), 6.49 (s, 1H), 2.61 (s, 3H), 2.41 (s, 3H), 2.34 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.91, 181.11, 157.61, 144.67, 135.70, 135.01, 134.15, 131.47, 130.54, 129.32, 125.14, 123.29, 120.40, 107.64, 64.28, 29.57, 18.82, 14.59. HRMS (ESI): calcd. for $C_{23}H_{20}Br_2NO_2$ $[M+H]^+$ 499.9855, Found: 499.9829.



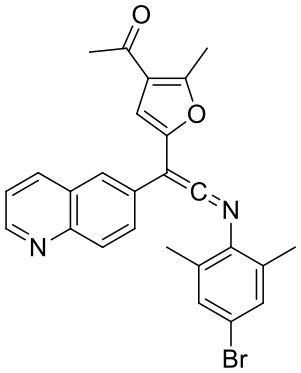
(**3i**): 111 mg, 49% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (t, *J* = 8.0 Hz, 1H), 7.20 (s, 2H), 6.95 (ddd, *J* = 7.8, 1.5, 0.9 Hz, 1H), 6.92- 6.87 (m, 1H), 6.77 (ddd, *J* = 8.2, 2.5, 0.6 Hz, 1H), 6.47 (s, 1H), 3.79 (s, 3H), 2.58 (s, 3H), 2.38 (s, 3H), 2.31 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.04, 183.18, 160.23, 157.32, 145.31, 136.49, 133.68, 131.36, 130.10, 123.33, 119.89, 119.49, 112.84, 111.83, 107.37, 65.50, 55.38, 29.31, 18.78, 14.56. HRMS (ESI): calcd. for $C_{24}H_{23}BrNO_3$ $[M+H]^+$ 452.0856, Found: 452.0853.



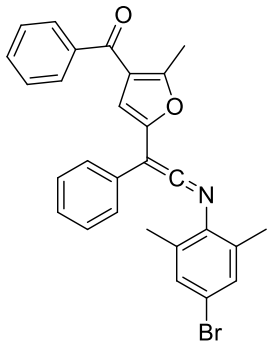
(**3j**): 115 mg, 46% yield, yellow solid: m. p. 109-110 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (s, 2H), 6.99 (s, 2H), 6.89 (s, 1H), 6.45 (s, 1H), 2.61 (s, 3H), 2.40 (s, 3H), 2.32 (d, *J* = 0.4 Hz, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.10, 184.21, 157.28, 145.69, 138.77, 136.90, 133.55, 131.84, 131.35, 128.58, 124.93, 123.39, 119.68, 107.23, 65.60, 29.35, 21.51, 18.77, 14.61. HRMS (ESI): calcd. for $C_{25}H_{25}BrNO_2$ $[M+H]^+$ 450.1063, Found: 450.1053.



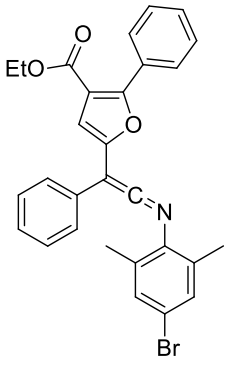
(**3k**):123 mg, 46% yield yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, ***J*** = 2.1 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.33 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.22 (s, 2H), 6.16 (s, 1H), 2.59 (s, 3H), 2.36 (s, 3H), 2.31 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.10, 184.21, 157.28, 145.69, 138.77, 136.90, 133.55, 131.84, 131.35, 128.58, 124.93, 123.39, 119.68, 107.23, 65.60, 29.35, 21.51, 18.77, 14.61. HRMS (ESI): calcd. for $C_{23}H_{19}Br_2ClNO_2$ $[M+H]^+$ 533.9466, Found: 533.9456.



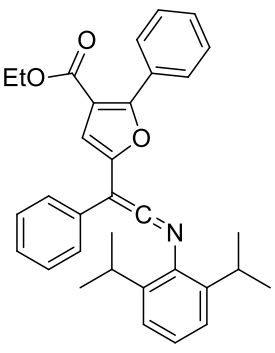
(**3l**): 144 mg, 61% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.11-8.09 (m, 1H), 8.09-8.07 (m, 1H), 7.74 (d, *J* = 2.0 Hz, 1H), 7.71 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.25 (s, 2H), 6.58 (d, *J* = 3.3 Hz, 1H), 2.64 (s, 3H), 2.42 (s, 3H), 2.36 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.99, 181.66, 157.72, 150.14, 147.18, 145.07, 135.69, 134.34, 131.55, 131.14, 130.32, 128.91, 128.74, 124.18, 123.44, 121.78, 120.49, 107.85, 64.99, 29.37, 18.90, 14.67. HRMS (ESI): calcd. for $C_{26}H_{22}BrN_2O_2$ $[M+H]^+$ 473.0859, Found: 473.0847.



(**3m**): 142 mg, 59% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 1.7, 1.1 Hz, 1H), 7.80 (t, *J* = 1.7 Hz, 1H), 7.57-7.53 (m, 1H), 7.48-7.44 (m, 2H), 7.41-7.35 (m, 4H), 7.25-7.21 (m, 3H), 6.46 (s, 1H), 2.54 (s, 3H), 2.34 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.21, 183.67, 158.37, 145.34, 139.24, 136.68, 133.62, 132.35, 132.20, 131.39, 129.17, 129.11, 128.52, 127.03, 126.64, 122.51, 119.85, 108.57, 65.65, 18.81, 14.45. HRMS (ESI): calcd. for $C_{28}H_{23}BrNO_2$ $[M+H]^+$ 484.0907, Found: 484.0902.

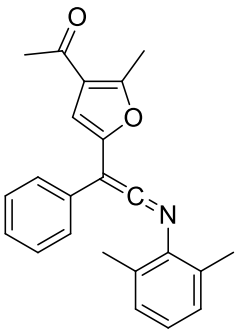


(**3n**): 185 mg, 72% yield, yellow solid: m. p. 101-102 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 1.5 Hz, 1H), 7.99 (s, 1H), 7.49-7.31 (m, 6H), 7.30-7.28 (m, 2H), 6.73 (s, 1H), 4.33 (q, *J* = 7.2 Hz, 2H), 2.37 (s, 6H), 1.36 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 183.19, 163.62, 155.93, 146.73, 136.44, 133.79, 132.03, 131.39, 129.25, 129.20, 128.29, 128.20, 127.32, 126.77, 120.00, 115.88, 109.66, 65.76, 60.73, 18.85, 14.39. HRMS (ESI): calcd. for $C_{29}H_{25}BrNO_3$ $[M+H]^+$ 514.1012, Found: 514.1017.

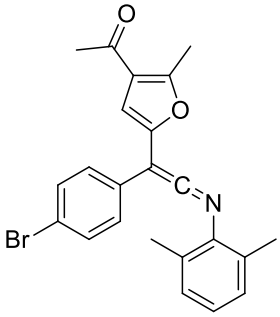


(**3o**): 147 mg, 60% yield, yellow solid: m. p. 108-109 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (dt, *J* = 3.3, 1.9 Hz, 2H), 7.51 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.47-7.36 (m, 5H), 7.31-7.26 (m, 1H), 7.25-7.17 (m, 3H), 6.70 (s, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.39 (dt, *J* = 13.7, 6.8 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.19 (d, *J* = 6.8 Hz, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.54, 163.69, 155.67, 147.45, 141.08, 135.15, 132.39, 129.13, 129.06, 128.28, 128.14, 127.48, 127.03, 126.59,

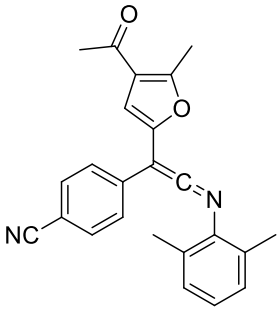
123.62, 115.82, 108.95, 64.31, 60.65, 28.94, 23.50, 14.38. HRMS (ESI): calcd. for $C_{33}H_{34}NO_3$ $[M+H]^+$ 492.2533, Found: 492.2538.



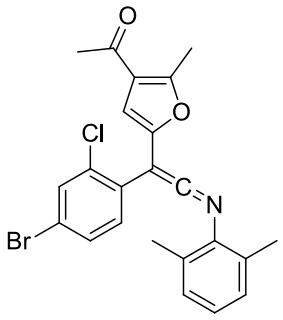
(**3p**): 113 mg, 52% yield yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.36 (m, 4H), 7.25-7.21 (m, 1H), 7.08 (s, 3H), 6.47 (s, 1H), 2.61 (s, 3H), 2.40 (s, 3H), 2.37 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.2, 181.8, 157.2, 146.0, 137.3, 132.7, 131.9, 129.1, 128.7, 126.9, 126.8, 126.4, 123.3, 106.9, 64.9, 29.3, 19.0, 14.6. HRMS (ESI): calcd. for $C_{23}H_{22}NO_2$ $[M+H]^+$ 344.1645, Found: 344.1648.



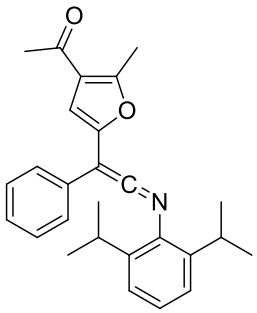
(**3q**): 122 mg, 62% yield yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 7.09 (s, 3H), 6.46 (s, 1H), 2.61 (s, 3H), 2.40 (s, 3H), 2.36 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.0, 180.2, 157.4, 145.4, 136.7, 132.2, 132.1, 128.7, 128.2, 127.1, 123.3, 119.6, 107.1, 63.9, 29.3, 19.0, 14.6. HRMS (ESI): calcd. for $C_{23}H_{21}BrNO_2$ $[M+H]^+$ 422.0750, Found: 422.0758.



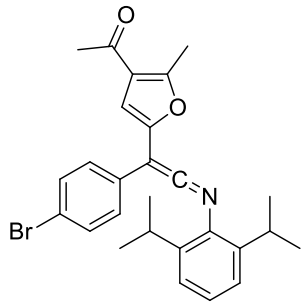
(**3r**): 104 mg, 56% yield, yellow solid: m. p. 129-130 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 1.8 Hz, 1H), 7.59-7.57 (m, 1H), 7.42-7.39 (m, 1H), 7.38 (d, *J* = 1.8 Hz, 1H), 7.18-7.08 (m, 3H), 6.57 (s, 1H), 2.62 (s, 3H), 2.43 (s, 3H), 2.40 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.91, 174.91, 158.01, 144.38, 139.91, 134.83, 133.51, 132.75, 128.93, 128.08, 125.66, 123.31, 119.32, 108.41, 108.20, 63.00, 29.35, 19.15, 14.66. HRMS (ESI): calcd. for $C_{24}H_{21}N_2O_2$ $[M+H]^+$ 369.1598, Found: 369.1592.



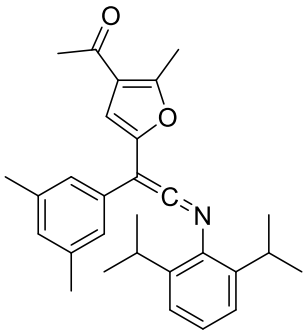
(**3s**): 96 mg, 48% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 2.0 Hz, 1H), 7.42 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.07 (s, 3H), 6.21 (s, 1H), 2.59 (s, 3H), 2.37 (s, 3H), 2.34 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.06, 177.41, 157.19, 145.98, 136.27, 134.79, 133.05, 132.17, 132.06, 130.55, 129.95, 128.66, 127.02, 123.40, 121.08, 105.89, 61.39, 29.31, 18.88, 14.57. HRMS (ESI): calcd. for $C_{23}H_{20}BrClNO_2$ $[M+H]^+$ 456.0360, Found:456.0363.



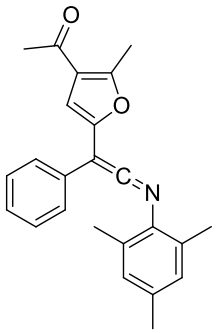
(**3t**): 106 mg, 53% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43-7.41 (m, 2H), 7.40-7.36 (m, 2H), 7.26-7.22 (m, 1H), 7.22-7.19 (m, 1H), 7.19-7.16 (m, 2H), 6.44 (s, 1H), 3.34 (dt, *J* = 13.7, 6.8 Hz, 2H), 2.61 (s, 3H), 2.40 (s, 3H), 1.20 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.18, 180.24, 156.96, 146.21, 140.91, 135.44, 132.50, 129.05, 127.26, 126.91, 126.52, 123.63, 123.30, 106.51, 64.27, 29.33, 28.88, 23.52, 14.52. HRMS (ESI): calcd. for $C_{27}H_{30}NO_2$ $[M+H]^+$ 400.2271, Found: 400.2264.



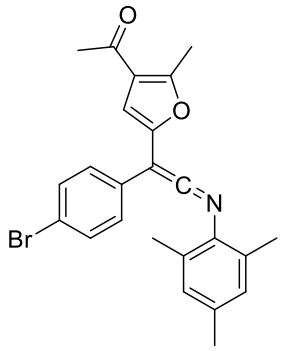
(**3u**): 117 mg, 47% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.49 (m, 1H), 7.49-7.47 (m, 1H), 7.28-7.27 (m, 1H), 7.23 (dd, *J* = 8.9, 6.2 Hz, 1H), 7.19-7.17 (m, 2H), 6.42 (s, 1H), 3.31 (dt, *J* = 13.7, 6.8 Hz, 2H), 2.60 (s, 3H), 2.39 (s, 3H), 1.20 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.06, 178.44, 157.20, 145.66, 141.22, 134.74, 132.16, 131.93, 128.51, 127.27, 123.72, 123.31, 119.72, 106.77, 63.20, 29.33, 28.99, 23.52, 14.53. HRMS (ESI): calcd. for $C_{27}H_{29}BrNO_2$ $[M+H]^+$ 478.1376, Found: 478.1382.



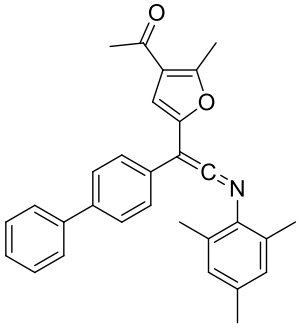
(**3v**): 94 mg, 44% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22-7.15 (m, 3H), 7.03 (s, 2H), 6.89 (s, 1H), 6.45 (s, 1H), 3.35 (dt, *J* = 13.7, 6.8 Hz, 2H), 2.62 (s, 3H), 2.40 (s, 3H), 2.32 (s, 6H), 1.21 (s, 6H), 1.19 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.21, 180.76, 156.94, 146.29, 140.59, 138.62, 138.29, 135.74, 132.15, 128.31, 126.69, 126.655, 124.95, 123.59, 123.31, 106.67, 64.33, 29.34, 28.84, 23.53, 21.48, 14.53. HRMS (ESI): calcd. for $C_{29}H_{34}NO_2$ $[M+H]^+$ 428.2584, Found: 428.2580.



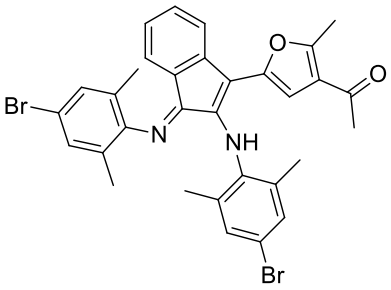
(**3w**): 100 mg, 50% yield, yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.33 (m, 4H), 7.23-7.18 (m, 1H), 6.91 (s, 2H), 6.47 (s, 1H), 2.61 (s, 3H), 2.40 (s, 3H), 2.35 (s, 6H), 2.29 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.21, 180.91, 157.17, 146.26, 137.05, 134.13, 133.19, 132.64, 129.44, 129.06, 128.86, 126.71, 126.10, 123.29, 106.73, 64.48, 29.34, 21.04, 19.00, 14.60. HRMS (ESI): calcd. for $C_{24}H_{24}NO_2$ $[M+H]^+$ 358.1802, Found: 358.1796.



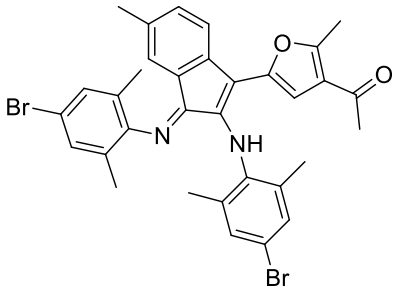
(**3x**): 116 mg, 53% yield, yellow solid: m. p. 110-111 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H), 6.91 (s, 2H), 6.45 (s, 1H), 2.60 (s, 3H), 2.40 (s, 3H), 2.34 (s, 6H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.07, 179.23, 157.38, 145.71, 137.46, 133.47, 132.97, 132.57, 132.11, 129.51, 127.97, 123.27, 119.24, 106.97, 63.51 29.33, 21.06, 19.02, 14.60. HRMS (ESI): calcd. for $C_{24}H_{23}BrNO_2$ $[M+H]^+$ 436.0907, Found: 436.0901.



(**3y**): 102 mg, 47% yield yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (dq, *J* = 4.6, 1.7 Hz, 4H), 7.45 (ddd, *J* = 6.1, 4.5, 2.3 Hz, 4H), 7.37-7.32 (m, 1H), 6.92 (s, 2H), 6.53 (s, 1H), 2.62 (s, 3H), 2.42 (s, 3H), 2.38 (s, 6H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.23, 180.53, 157.28, 146.15, 140.79, 138.82, 137.21, 133.92, 132.83, 132.34, 129.48, 128.95, 127.73, 127.35, 127.00, 126.89, 123.31, 106.93, 64.15, 29.36, 21.06, 19.06, 14.63. HRMS (ESI): calcd. for $C_{30}H_{28}NO_2$ $[M+H]^+$ 434.2115, Found: 434.2110.

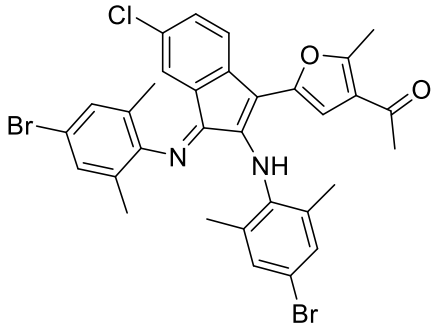


(**4a**): 195 mg, 62% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (s, 3H), 7.28 (s, 2H), 7.18-7.11 (m, 4H), 7.20-7.10 (m, 4H), 6.78 (s, 1H), 6.67 (td, *J* = 7.3, 1.5 Hz, 1H), 6.31 (d, *J* = 7.4 Hz, 1H), 5.82 (s, 1H), 2.39 (s, 3H), 2.24 (s, 3H), 2.21 (s, 6H), 2.07 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.18, 162.72, 157.22, 147.01, 146.81, 145.14, 137.34, 136.77, 132.92, 131.06, 130.67, 127.58, 125.91, 124.54, 124.08, 122.22, 119.36, 119.00, 116.69, 109.43, 105.09, 29.05, 18.49, 17.99, 14.19. HRMS (ESI): calcd. for $C_{32}H_{29}Br_2N_2O_2$ $[M+H]^+$ 631.0590, Found: 631.0595.

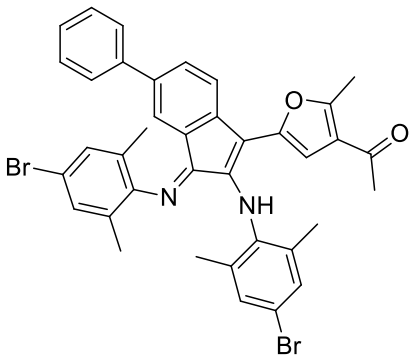


(**4b**): 158 mg, 49% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (s, 2H), 7.14 (s, 2H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.94 (ddd, *J* = 7.6, 1.5, 0.8 Hz, 1H), 6.71 (s, 1H), 6.12 (d, *J* = 0.8 Hz, 1H), 5.80 (s, 1H), 2.39 (s, 3H), 2.23 (s, 3H), 2.20 (s, 6H), 2.07 (s, 6H), 2.03 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.24, 162.85, 157.19 (s), 146.85, 145.38, 144.04, 137.26,

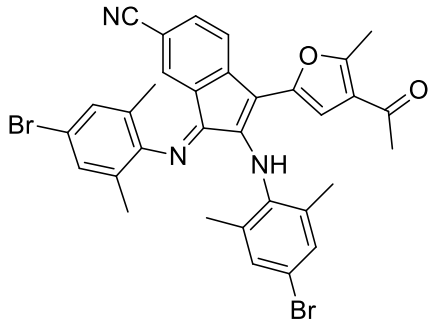
136.97, 136.08, 134.16, 132.96, 131.00, 130.67, 127.92, 127.60, 126.32, 125.12, 122.26, 119.15, 118.90, 116.59, 109.34, 105.46, 29.83, 29.06, 21.26, 18.53, 18.04, 14.21. HRMS (ESI): calcd. for $C_{33}H_{31}Br_2N_2O_2$ $[M+H]^+$ 645.0747, Found: 645.0740.



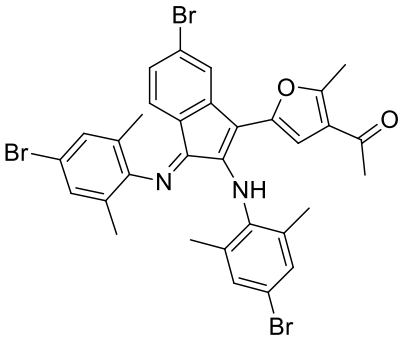
(**4c**): 98 mg, 41% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (s, 2H), 7.15 (s, 2H), 7.11 - 7.06 (m, 2H), 6.78 (s, 1H), 6.24 (dd, *J* = 1.6, 0.7 Hz, 1H), 5.77 (s, 1H), 2.40 (s, 3H), 2.23 (s, 3H), 2.20 (s, 6H), 2.07 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.09, 161.57, 157.39, 146.22, 145.41, 144.74, 137.34, 136.69, 136.47, 132.27, 131.23, 130.74, 129.80, 127.31, 124.19, 122.28, 119.82, 119.57, 117.15, 109.74, 104.84, 29.04, 18.48, 18.01, 14.22. HRMS (ESI): calcd. for $C_{32}H_{28}Br_2ClN_2O_2$ $[M+H]^+$ 665.0201, Found: 665.0211.



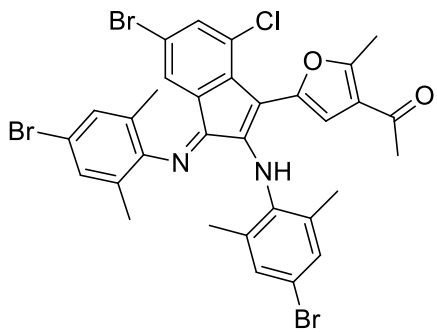
(**4d**): 180 mg, 51% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.38 - 7.34 (m, 2H), 7.32 (s, 2H), 7.29 - 7.37(m, 1H), 7.24-7.21 (m, 3H), 7.17 (s, 2H), 6.84 (s, 1H), 6.50 (d, *J* = 1.6 Hz, 1H), 5.84 (s, 1H), 2.42 (s, 3H), 2.25 (s, 3H), 2.23 (s, 6H), 2.10 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.20, 162.94, 157.33, 147.05, 145.86, 145.17, 139.95, 137.36, 136.73, 131.15, 130.97, 130.73, 129.05, 127.78, 127.31, 126.65, 126.05, 122.81, 122.31, 119.43,119.34, 109.55, 105.36, 29.08, 18.53, 18.03, 14.24. HRMS (ESI): calcd. for $C_{38}H_{33}Br_2N_2O_2$ $[M+H]^+$ 707.0903, Found: 707.0911.



(**4e**): 183 mg, 65% yield, purple solid: m. p. 108-109 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.32 (s, 2H), 7.19 (d, *J* = 7.9 Hz, 1H), 7.16 (s, 2H), 7.02 (s, 1H), 6.49 (d, *J* = 1.4 Hz, 1H), 5.79 (s, 1H), 2.40 (s, 3H), 2.23 (s, 3H), 2.20 (s, 6H), 2.06 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.88, 160.43, 157.61, 152.32, 145.69, 143.85, 139.42, 137.93, 137.49, 135.71, 131.49, 130.83, 127.02, 126.09, 125.94, 122.30, 120.28, 119.05, 117.76, 110.14, 107.03, 104.23, 29.06, 18.40, 18.00, 14.23. HRMS (ESI): calcd. for $C_{33}H_{28}Br_2N_3O_2$ $[M+H]^+$ 656.0543, Found: 656.0548.

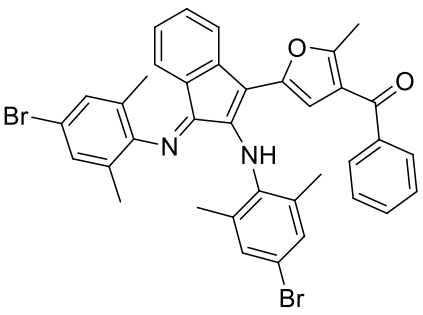


(**4f**): 148 mg, 42% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (s, 2H), 7.24 (d, *J* = 1.7 Hz, 1H), 7.15 (s, 2H), 6.85 (s, 1H), 6.80 (dd, *J* = 7.9, 1.7 Hz, 1H), 6.13 (d, *J* = 7.9 Hz, 1H), 5.79 (s, 1H), 2.40 (s, 3H), 2.24 (s, 3H), 2.20 (s, 6H), 2.06 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.08 , 161.65, 157.48, 149.26, 146.45, 144.46, 137.67, 137.38, 136.29, 131.18, 131.12, 130.75, 128.03, 127.49, 127.06, 124.95, 124.41, 122.32, 122.28, 119.73, 117.01, 109.70, 104.04, 29.80, 29.09, 18.44, 17.98, 15.89, 14.25. HRMS (ESI): calcd. for $C_{32}H_{28}Br_3N_2O_2$ $[M+H]^+$ 708.9695, Found: 708.9690.

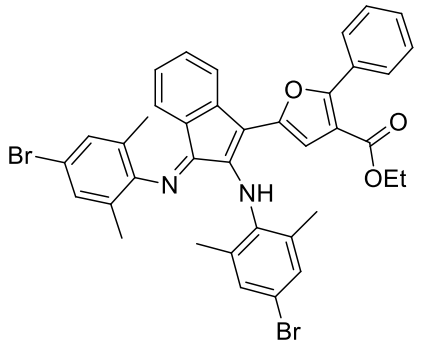


(**4g**): 119 mg, 32% yield. purple solid: m. p. 259-260 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (s, 2H), 7.20 (d, *J* = 1.8 Hz, 1H), 7.06 (s, 2H), 6.62 (s, 1H), 6.20 (d, *J* = 1.8 Hz, 1H), 5.78 (s, 1H), 2.47 (s, 3H), 2.23 (s, 3H), 2.22 (s, 6H), 2.07 (s, 6H). ^{13}C NMR

(125 MHz, $CDCl_3$) δ 193.81, 160.14, 157.48, 145.72, 144.47, 143.14, 141.05, 138.40, 137.10, 135.41, 131.38, 130.62, 129.58, 127.91, 126.95, 123.36, 122.41, 120.75, 117.52, 112.46, 112.27, 103.35, 28.98, 18.09 , 17.96, 14.40. HRMS (ESI): calcd. for $C_{32}H_{27}Br_3ClN_2O_2$ $[M+H]^+$ 743.9306, Found: 743.9310.

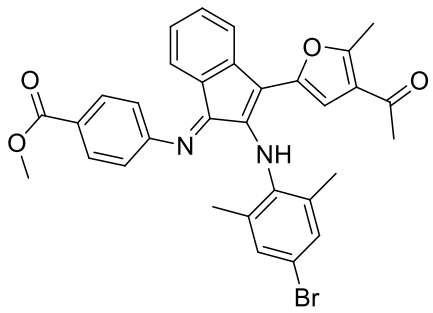


(**4h**): 135 mg, 39% yield. purple solid: m. p. 179-180 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 7.66 (q, *J* = 1.6 Hz, 1H), 7.64 (t, *J* = 1.7 Hz, 1H), 7.60-7.56 (m, 1H), 7.53-7.47 (m, 2H), 7.28 (s, 2H), 7.15-7.08 (m, 4H), 6.72 (s, 1H), 6.66 (td, *J* = 7.3, 1.5 Hz, 1H), 6.30 (d, *J* = 7.4 Hz, 1H), 6.19 (s, 1H), 2.23 (s, 6H), 2.20 (s, 3H), 2.07 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.35, 162.79, 158.08, 146.90, 146.82, 145.17, 139.24, 137.36, 137.04, 136.85, 132.95, 132.25, 131.07, 130.75, 128.96, 128.56, 127.60, 125.95, 124.58, 124.16, 121.77, 119.21, 118.63, 116.72, 110.73, 105.29, 18.60, 18.02, 14.05. HRMS (ESI): calcd. for $C_{37}H_{31}Br_2N_2O_2$ $[M+H]^+$ 693.0747, Found: 693.0742.

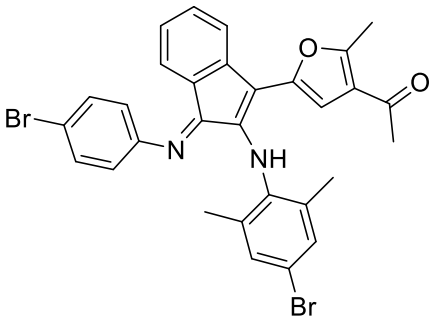


(**4i**): 227 mg, 63% yield, purple solid: m. p. 153-154 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 7.9, 1.5 Hz, 2H), 7.50 -7.39 (m, 3H), 7.32 (s, 2H), 7.29-7.25 (m, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 6.92 (s, 2H), 6.80 (s, 1H), 6.71 (t, *J* = 7.5 Hz, 1H), 6.36 (d, *J* = 7.5 Hz, 1H), 6.20 (s, 1H), 5.32 (s, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 2.21 (s, 6H), 2.12 (s, 6H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.45, 162.71, 155.93, 146.97, 146.84, 145.92, 137.55, 136.68, 136.32, 133.00, 131.05, 130.77, 129.52, 129.29, 128.44,

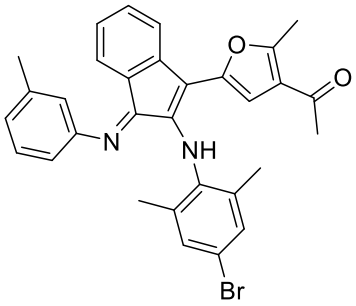
128.01, 127.55, 125.89, 124.52, 124.15, 119.33, 118.82, 116.68, 114.71, 112.02, 104.90, 60.70, 53.55, 18.54, 18.01, 14.37. HRMS (ESI): calcd. for $C_{38}H_{33}Br_2N_2O_3$ $[M+H]^+$ 723.08526, Found: 723.0856.



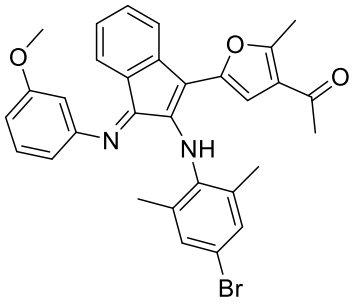
(**4j**): 125 mg, 43% yield, purple solid: m. p. 259-260 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19-8.06 (m, 2H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.14-7.05 (m, 5H), 6.60 (m, 2H), 6.34 (d, *J* = 7.4 Hz, 1H), 5.80 (s, 1H), 3.95 (s, 3H), 2.38 (s, 3H), 2.23 (s, 3H), 2.20 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.11, 166.91, 162.05, 157.26, 154.62, 147.70, 144.97, 137.17, 136.65, 136.57, 132.84, 131.23, 130.65, 126.49, 125.53, 125.06, 123.93, 122.20, 119.27, 119.20, 118.57, 109.62, 105.33, 52.23, 29.02, 18.60, 14.18. HRMS (ESI): calcd. for $C_{32}H_{28}BrN_2O_4$ $[M+H]^+$ 583.1227, Found: 583.1222.



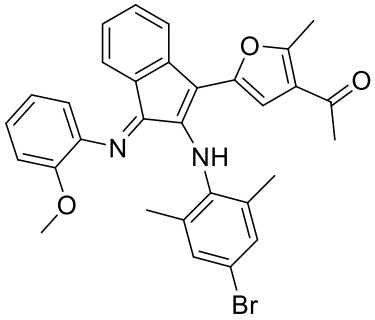
(**4k**): 150mg, 50% yield, purple solid: m. p. 208-209 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57-7.52 (m, 2H), 7.17-7.10 (m, 4H), 6.97-6.88 (m, 2H), 6.66 (m, 1H), 6.61 (s, 1H), 6.48 (d, *J* = 7.3 Hz, 1H), 5.79 (s, 1H), 2.38 (s, 3H), 2.23 (s, 3H), 2.19 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.15, 162.30, 157.23, 149.15, 147.75, 145.02, 137.18, 136.89, 136.61, 132.76, 132.52, 130.64, 125.43, 125.02, 123.90, 122.19, 120.66, 119.18, 118.92, 117.84, 109.55, 105.07, 29.05, 18.62, 14.20. HRMS (ESI): calcd. for $C_{30}H_{25}Br_2N_2O_2$ $[M+H]^+$ 603.0277, Found: 603.0270.



(**4l**): 150 mg, 56% yield, purple solid: m. p. 149-150 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.7 Hz, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 7.13 - 7.08 (m, 3H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.86 (s, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.69 (s, 1H), 6.63 (m, 1H), 6.46 (d, *J* = 7.5 Hz, 1H), 5.79 (s, 1H), 2.40 (s, 3H), 2.38 (s, 3H), 2.23 (s, 3H), 2.20 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.24, 161.64, 157.15, 150.17, 147.70, 145.23, 139.40, 137.24, 137.18, 136.78, 132.40, 130.61, 129.29, 125.57, 125.50, 125.18, 123.78, 122.18, 119.26, 119.15, 118.90, 115.67, 109.37, 104.70, 29.05, 21.60, 18.62, 14.20. HRMS (ESI): calcd. for $C_{31}H_{28}BrN_2O_2$ $[M+H]^+$ 539.1329, Found: 539.1333.

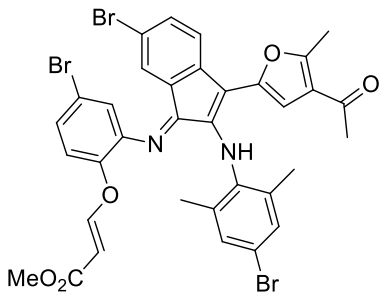


(**4m**): 116 mg, 42% yield, purple solid: m. p. 76-77 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (t, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 1H), 7.13 - 7.08 (m, 3H), 6.78 (ddd, *J* = 8.3, 2.5, 0.8 Hz, 1H), 6.66-6.59 (m, 3H), 6.59-6.57 (m, 1H), 6.50 (d, *J* = 7.1 Hz, 1H), 5.78 (s, 1H), 3.84 (s, 3H), 2.38 (s, 3H), 2.23 (s, 3H), 2.20 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.24, 161.84, 160.70, 157.17, 151.57, 147.67, 145.18, 137.23, 137.09, 136.72, 132.50, 130.62, 130.37, 125.63, 125.07, 123.86, 122.18, 119.18, 118.93, 110.86, 110.67, 109.40, 104.79, 104.12, 55.52, 29.06, 18.64, 14.20. HRMS (ESI): calcd. for $C_{31}H_{28}BrN_2O_3$ $[M+H]^+$ 555.1278, Found: 555.1279.

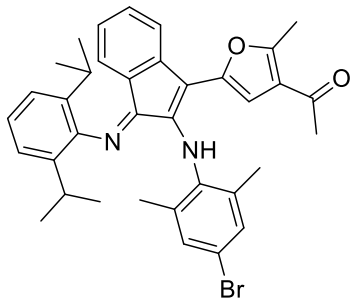


(**4n**): 94 mg, 34% yield, purple solid: m. p. 108-109 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24-7.19 (m, 1H), 7.15 (d, *J* = 7.1 Hz, 1H), 7.13 -7.08 (m, 3H), 7.03 (m, 2H), 6.96 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.74 (d, *J* = 13.8 Hz, 1H), 6.63 (m, 1H), 6.49 (d, *J* = 7.3 Hz, 1H), 5.79 (s, 1H),

3.80 (s, 3H), 2.38 (s, 3H), 2.23 (s, 3H), 2.21 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.28, 162.79, 157.11, 149.02, 147.40, 145.34, 139.18, 137.34, 137.28, 136.89, 132.36, 130.60, 125.86, 124.89, 123.93, 122.19, 121.29, 119.89, 119.07, 118.81, 112.03, 109.32, 104.82, 55.97, 29.05, 18.63, 14.20. HRMS (ESI): calcd. for $C_{31}H_{28}BrN_2O_3$ $[M+H]^+$ 555.1278, Found: 555.1273.

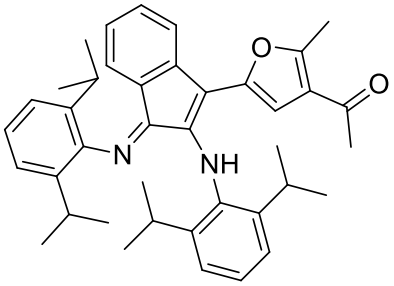


(**4o**): 72 mg, 33% yield, purple solid: m. p. 137-138 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 12.2 Hz, 1H), 7.40 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.26 (dd, *J* = 6.2, 2.2 Hz, 2H), 7.14-7.08 (m, 3H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.65-6.48 (m, 2H), 5.73 (s, 1H), 5.42 (d, *J* = 12.3 Hz, 1H), 3.63 (s, 3H), 2.39 (s, 3H), 2.21 (s, 3H), 2.14 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.07, 167.27, 163.12, 159.26, 157.56, 146.44, 144.46, 143.56, 141.69, 137.24, 136.32, 136.22, 135.53, 130.72, 129.13, 127.77, 127.16, 123.52, 122.28, 121.75, 120.61, 119.54, 118.92, 117.07, 110.14, 105.56, 101.95, 51.48, 29.02, 18.43, 14.23. HRMS (ESI): calcd. for $C_{34}H_{28}Br_3N_2O_5$ $[M+H]^+$ 780.9543, Found:780.9522.

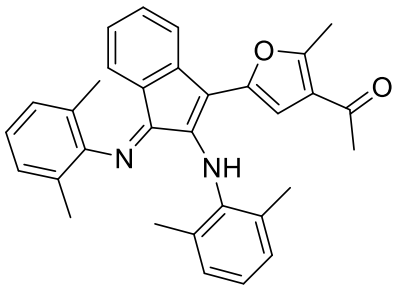


(**4p**): 164 mg, 54% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24-7.19 (m, 3H), 7.16 (t, *J* = 3.6 Hz, 3H), 7.09 (m, 1H), 6.86 (s, 1H), 6.60 (m, 1H), 6.19 (d, *J* = 7.2 Hz, 1H), 5.84 (s, 1H), 2.90-2.83 (m, 2H), 2.40 (s, 3H), 2.25 (s, 3H), 2.23 (s, 6H), 1.19 (d, *J* = 6.9 Hz, 6H), 1.08 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.31, 162.19, 157.15, 147.03, 145.92, 145.41, 137.47, 136.96, 136.82, 135.49, 132.49, 130.66, 125.74, 124.84, 124.67, 124.08, 123.50, 122.21, 119.32, 118.83, 109.24, 104.65, 28.73, 23.03, 22.99, 18.45, 14.20. HRMS (ESI): calcd. for

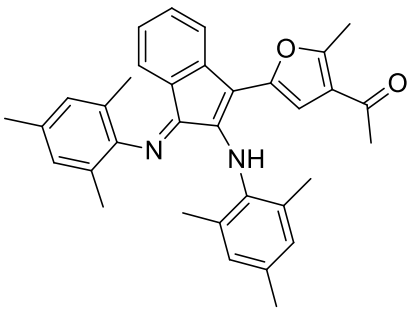
$C_{36}H_{38}BrN_2O_2$ $[M+H]^+$ 609.2111, Found: 609.2107.



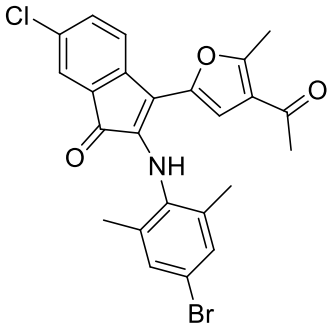
(**4q**): 129 mg, 44% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 - 7.19 (m, 4H), 7.13 (s, 1H), 7.11 (s, 1H), 7.11-7.05 (m, 3H), 6.58 (td, *J* = 7.3, 1.6 Hz, 1H), 6.24 (d, *J* = 7.3 Hz, 1H), 5.53 (s, 1H), 3.30 (dt, *J* = 13.7, 6.9 Hz, 2H), 2.98-2.87 (m, 2H), 2.35 (s, 3H), 2.13 (s, 3H), 1.20 (dd, *J* = 8.5, 6.9 Hz, 12H), 1.13 (dd, *J* = 6.8, 5.2 Hz, 12H). ^{13}C NMR (125MHz, $CDCl_3$) δ 194.50, 162.04, 156.77, 148.21, 146.56, 145.88, 145.42, 138.08, 135.53, 135,48, 132.60, 127.72, 125.64, 124.72, 124.59, 123.62, 123.45, 123.01, 121.87, 118.73, 109.40, 102.49, 29.15, 28.94, 28.79, 24.24, 22.93, 22.83, 22.26, 14.08. HRMS (ESI): calcd. for $C_{40}H_{47}N_2O_2$ $[M+H]^+$ 587.3632, Found: 587.3638.



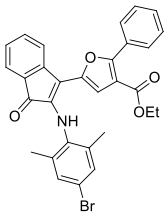
(**4r**): 98 mg, 41% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 7.4 Hz, 1H), 7.15 - 7.09 (m, 3H), 7.05 (dd, *J* = 7.9, 7.1 Hz, 1H), 7.01 (s, 3H), 6.96 (s, 1H), 6.61 (td, *J* = 7.5, 1.0 Hz, 1H), 6.25 (d, *J* = 7.3 Hz, 1H), 5.68 (s, 1H), 2.39 (s, 3H), 2.26 (s, 6H), 2.16 (s, 3H), 2.12 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.44, 162.34, 156.99, 147.86, 147.35, 145.52, 137.58, 137.30, 135.29, 132.58, 128.36, 128.01, 126.23, 126.12, 125.30 , 124.16, 124.07, 124.03, 122.01, 118.77, 109.18, 104.25, 29.12, 18.68, 18.16, 14.19. HRMS (ESI): calcd. for $C_{32}H_{31}N_2O_2$ $[M+H]^+$ 475.2380, Found: 475.2389.



(**4s**): 143 mg, 57% yield, purple oil.[1]H NMR (500 MHz, $CDCl_3$) δ 7.16 (d, *J* = 7.3 Hz, 1H), 7.09 (td, *J* = 7.6, 1.1 Hz, 1H), 6.94 (s, 2H), 6.92 (s, 1H), 6.81 (s, 2H), 6.61 (td, *J* = 7.5, 1.0 Hz, 1H), 6.30 (d, *J* = 7.1 Hz, 1H), 5.60 (s, 1H), 2.40 (s, 3H), 2.35 (s, 3H), 2.24 (s, 3H), 2.20 (s, 6H), 2.14 (s, 3H), 2.07 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.54, 162.48, 156.85, 147.61, 145.73, 145.33, 137.68, 135.73, 135.29, 135.00, 133.38, 132.49, 129.05, 128.60, 126.15, 125.12, 124.05, 123.99, 121.95, 118.68, 109.11, 103.57, 31.76, 29.80, 28.86, 21.00, 20.94, 18.54, 18.08, 14.15. HRMS (ESI): calcd. for $C_{34}H_{35}N_2O_2$ $[M+H]^+$ 503.2693, Found: 503.2690.



(**5b**): 154 mg, 64% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 1.9 Hz, 1H), 7.22 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.20-7.14 (m, 3H), 6.13 (s, 1H), 5.72 (s, 1H), 2.44 (s, 3H), 2.20 (s, 3H), 2.12 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.92, 191.47, 158.14, 145.77, 144.66, 137.22, 135.69, 134.24, 132.75, 131.31, 130.83, 129.88, 123.71, 122.55, 120.92, 119.85, 110.92, 109.12, 29.00, 18.54, 14.34. HRMS (ESI): calcd. for $C_{24}H_{20}BrClNO_3$ $[M+H]^+$ 484.0313, Found: 484.0310.

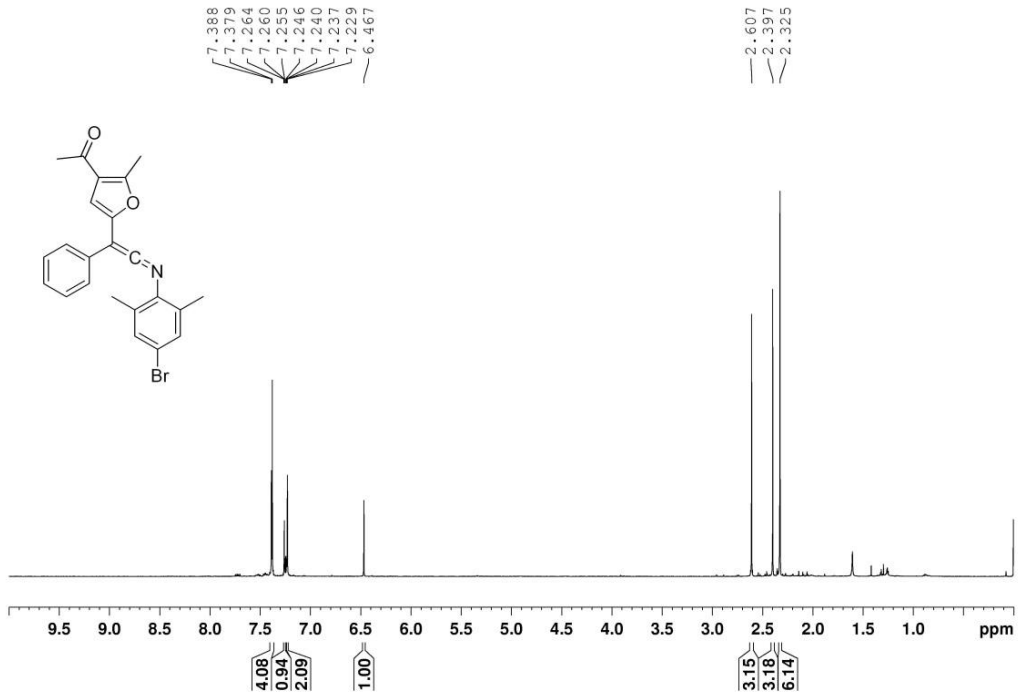


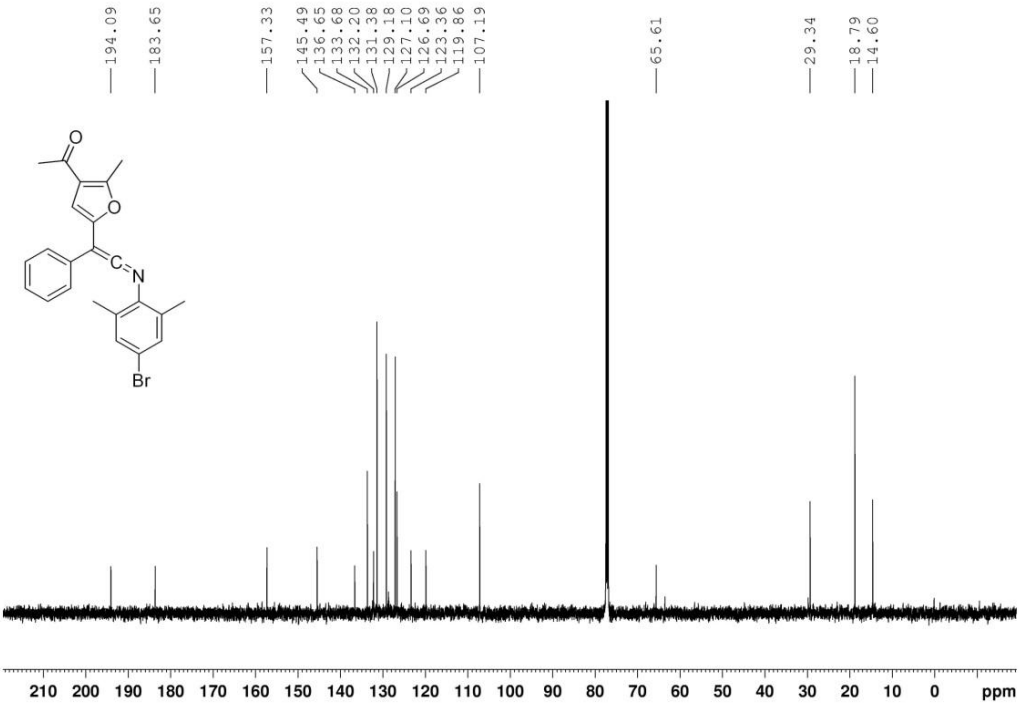
(**5h**): 116 mg, 55% yield, purple oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 - 7.74 (m, 2H), 7.48-7.39 (m, 3H), 7.40-7.36 (m, 1H), 7.33-7.27 (m, 2H), 7.02 -6.97 (m, 1H), 6.95 (s, 2H), 6.17 (s, 1H), 6.16 (s, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.13 (s, 6H), 1.34 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.67, 163.26, 156.44, 147.73, 145.83, 136.60, 135.64, 135.48, 133.84, 130.93, 129.61, 129.30, 128.44, 128.19, 125.55, 123.53, 119.77, 119.66,

115.21, 113.05, 108.85, 18.60, 14.38. HRMS (ESI): calcd. for $C_{30}H_{25}Br_3NO_4$ $[M+H]^+$ 542.0967, Found: 542.0961.

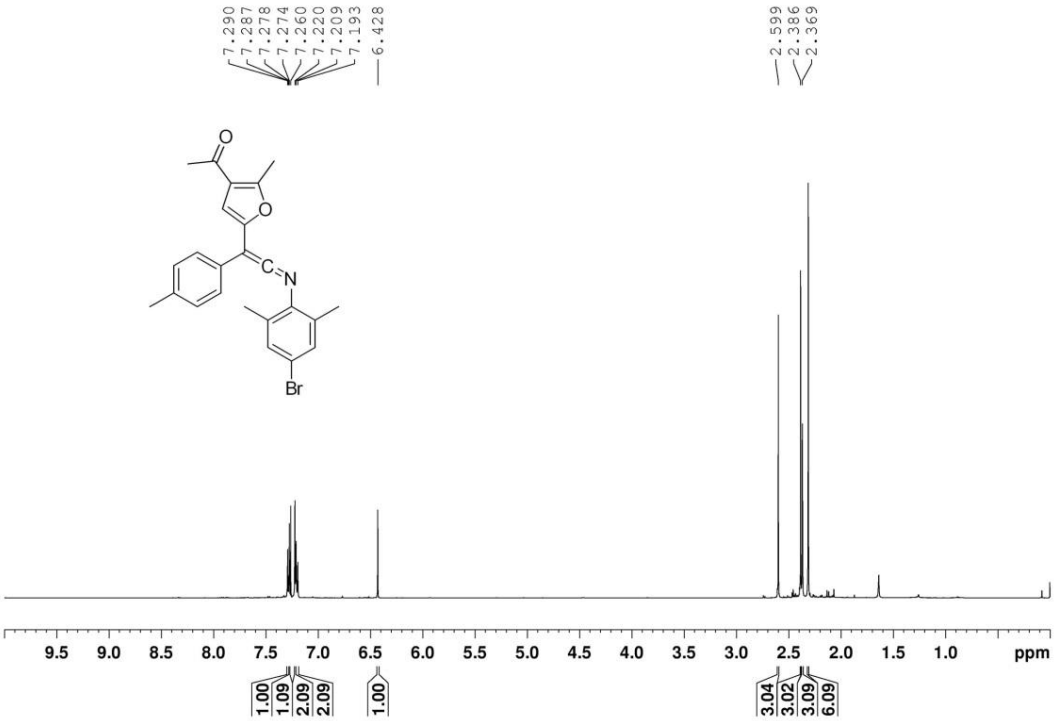
4 ^{1}H NMR and ^{13}C NMR Spectra of All Compounds

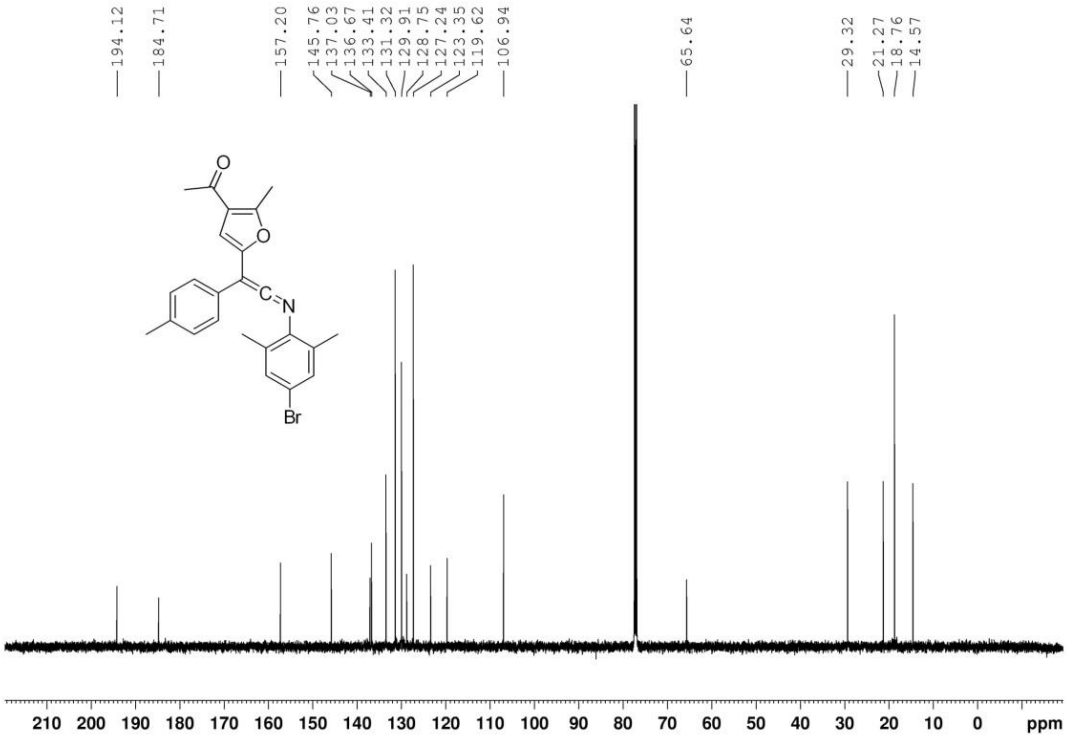
Compound **3a**



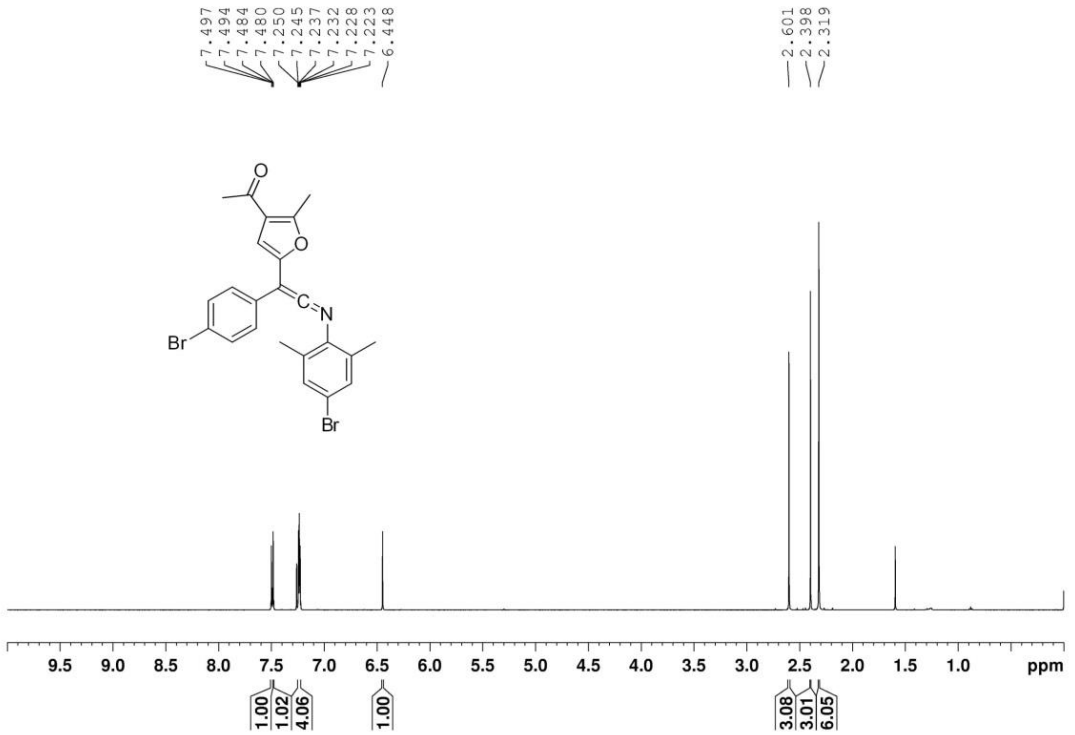


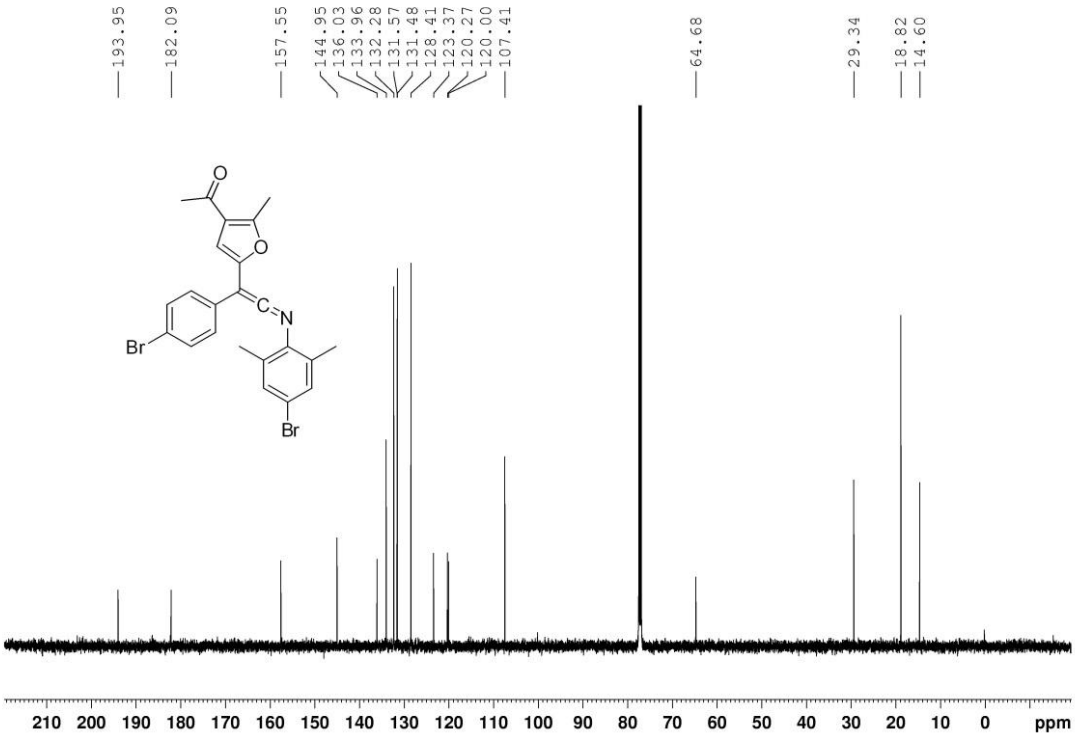
Compound **3b**


7.290
7.287
7.278
7.274
7.260
7.220
7.209
7.193
6.428
2.599
2.386
2.369
O
O
C=N
Br
9.5 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 ppm
1.00
1.09
2.09
2.09
1.00
3.04
3.02
3.09
6.09

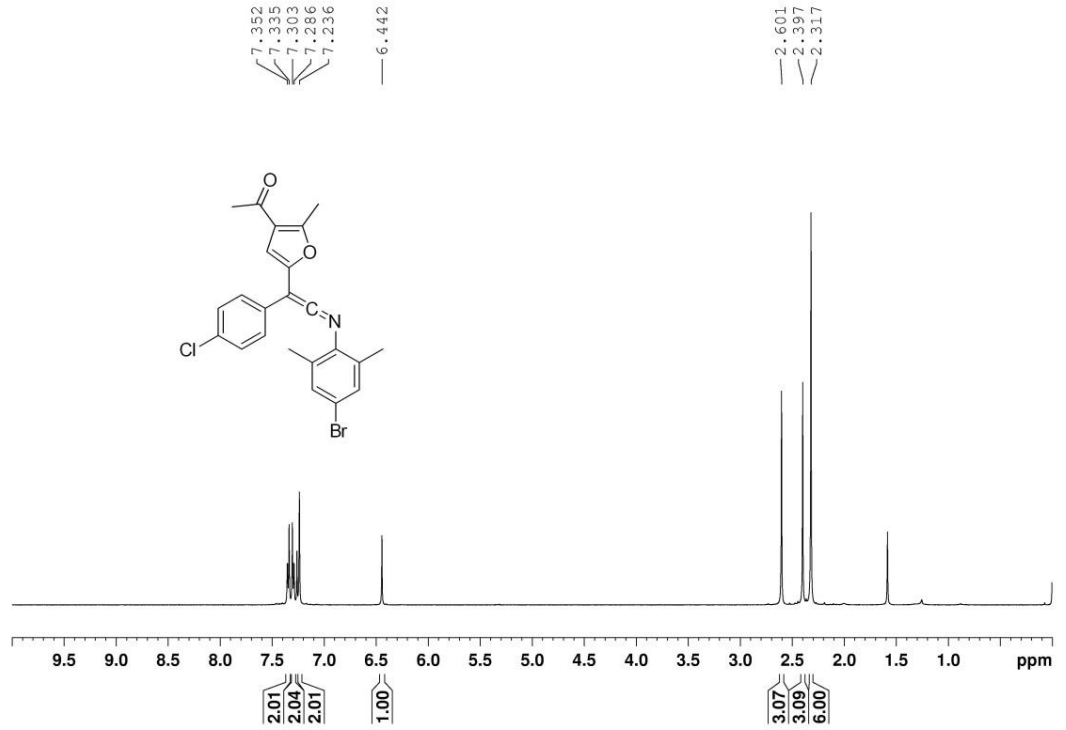

194.12
184.71
157.20
145.76
137.03
136.67
133.41
131.32
129.91
128.75
127.24
123.35
119.62
106.94
65.64
29.32
21.27
18.76
14.57
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

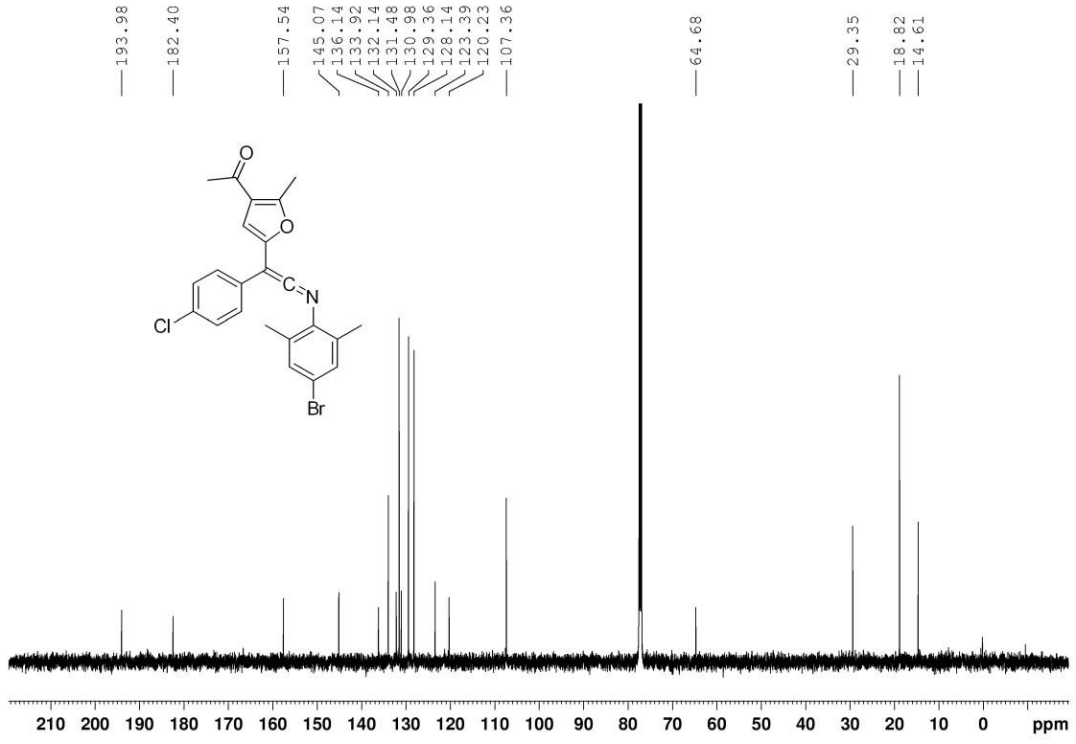
Compound **3c**


7.497
7.494
7.484
7.480
7.250
7.245
7.237
7.232
7.228
7.223
6.448
2.601
2.398
2.319
O
O
C=N
Br
Br
9.5 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 ppm
1.00
1.02
4.06
1.00
3.08
3.01
6.05

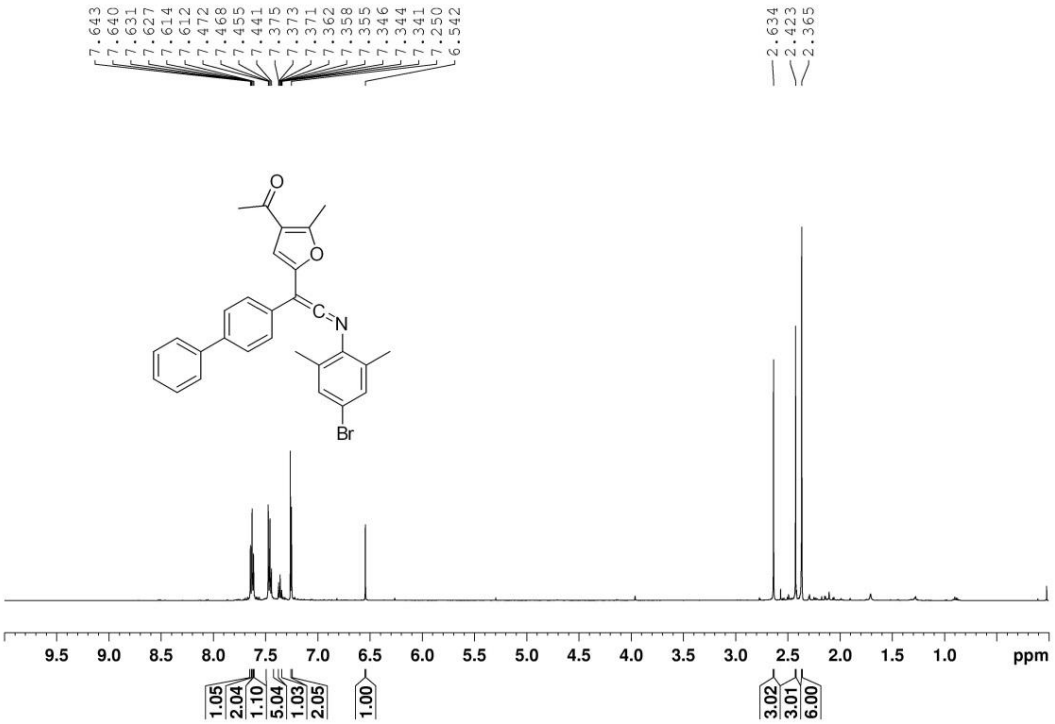

193.95
182.09
157.55
144.95
136.03
133.96
132.28
131.57
131.48
128.41
123.37
120.27
120.00
107.41
64.68
29.34
18.82
14.60
O
O
C=N
Br
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound **3d**


7.352
7.335
7.303
7.286
7.236
6.442
2.601
2.397
2.317
O
O
C=N
Cl
Br
9.5 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 ppm
2.01
2.04
2.01
1.00
3.07
3.09
6.00


193.98
182.40
157.54
145.07
136.14
133.92
132.14
131.48
130.98
129.36
128.14
123.39
120.23
107.36
64.68
29.35
18.82
14.61
O
O
C=N
Cl
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound **3e**


7.643
7.640
7.631
7.627
7.614
7.612
7.472
7.468
7.455
7.441
7.375
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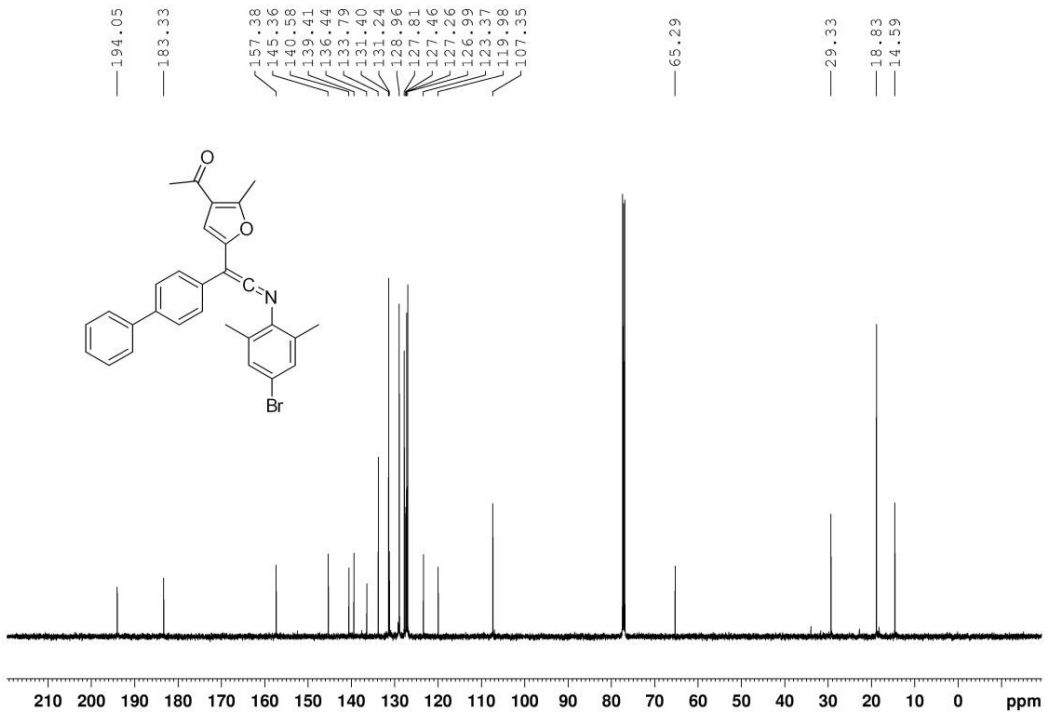
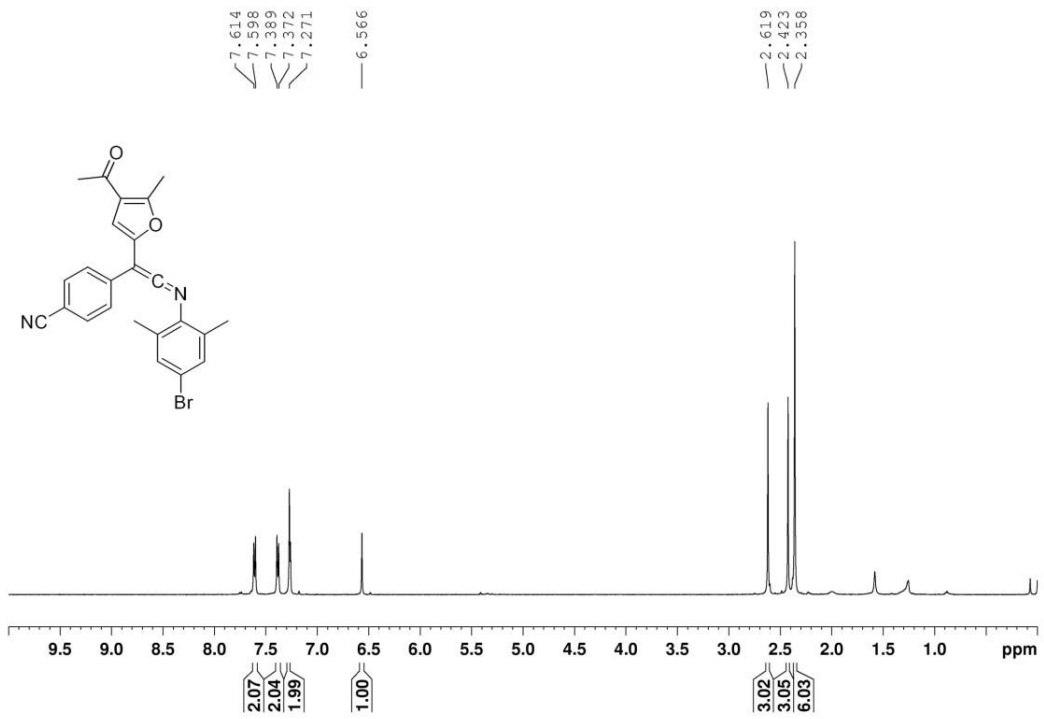
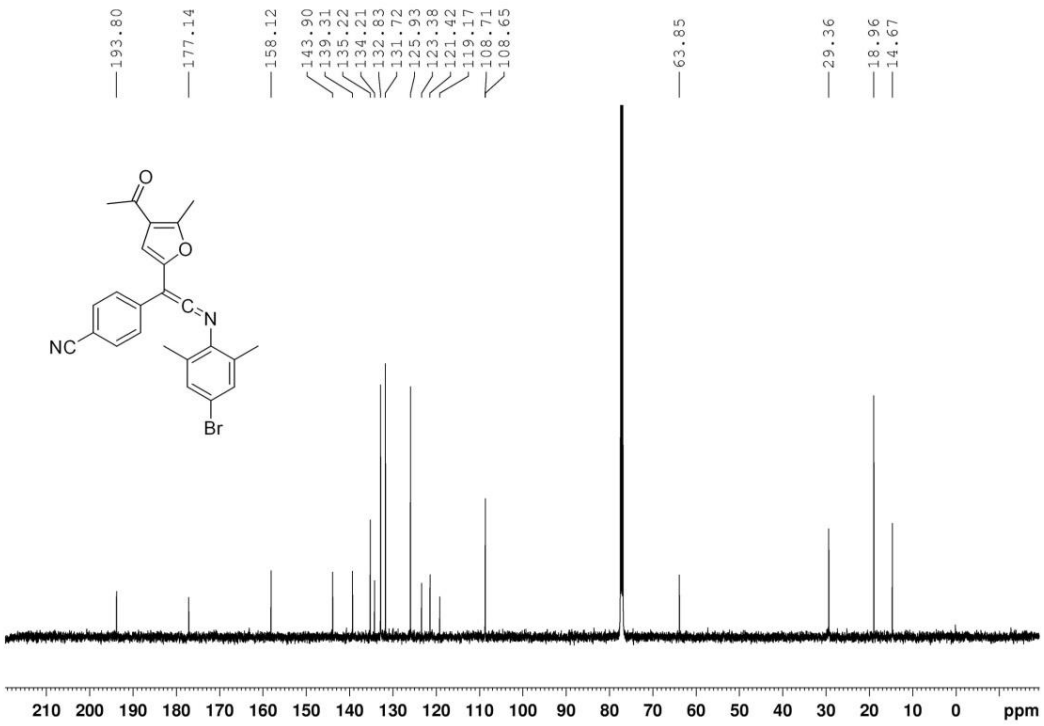
7.371
7.362
7.358
7.355
7.346
7.344
7.341
7.250
6.542
2.634
2.423
2.365
O
O
C=N
Br
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.05
2.04
1.10
5.04
1.03
2.05
1.00
3.02
3.01
6.00

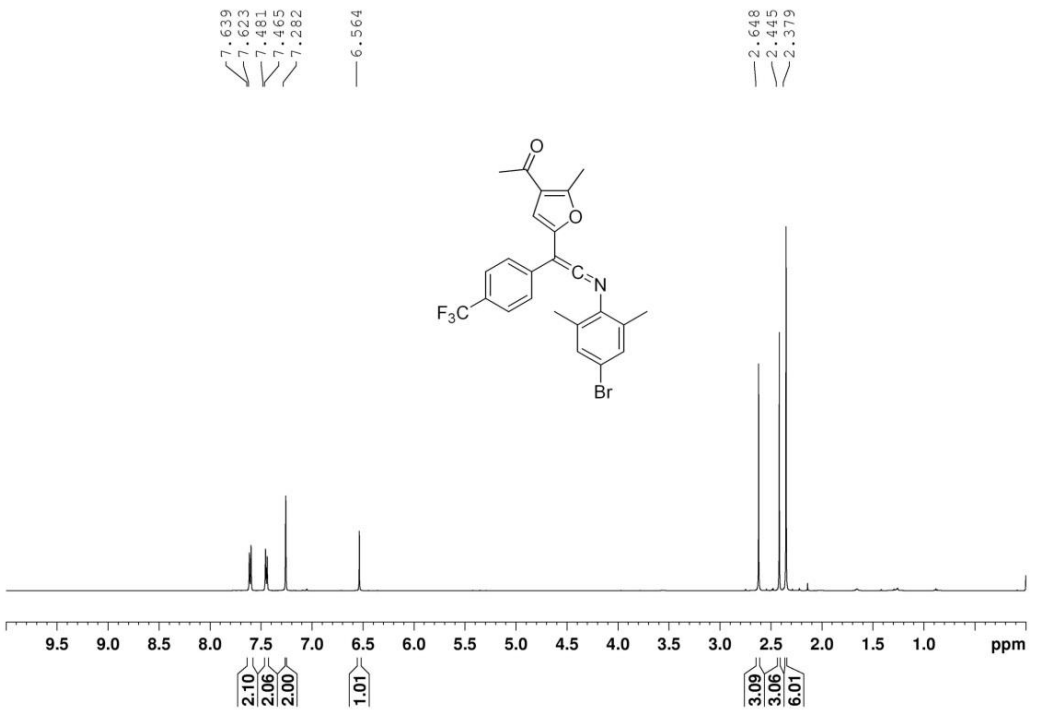

194.05
183.33
157.38
145.36
140.58
139.41
136.44
133.79
131.40
131.24
128.96
127.81
127.46
127.26
126.99
123.37
119.98
107.35
65.29
29.33
18.83
14.59
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

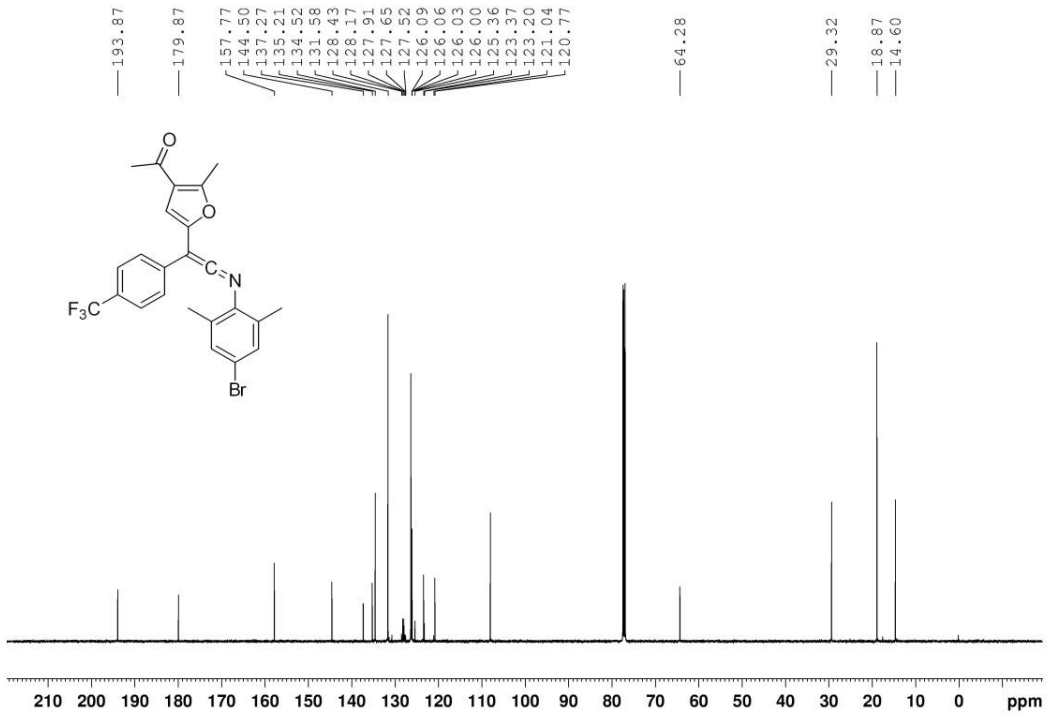
Compound **3f**


7.614
7.598
7.389
7.372
7.271
6.566
2.619
2.423
2.358
O
O
C=N
NC
Br
9.5 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 ppm
2.07
2.04
1.99
1.00
3.02
3.05
6.03

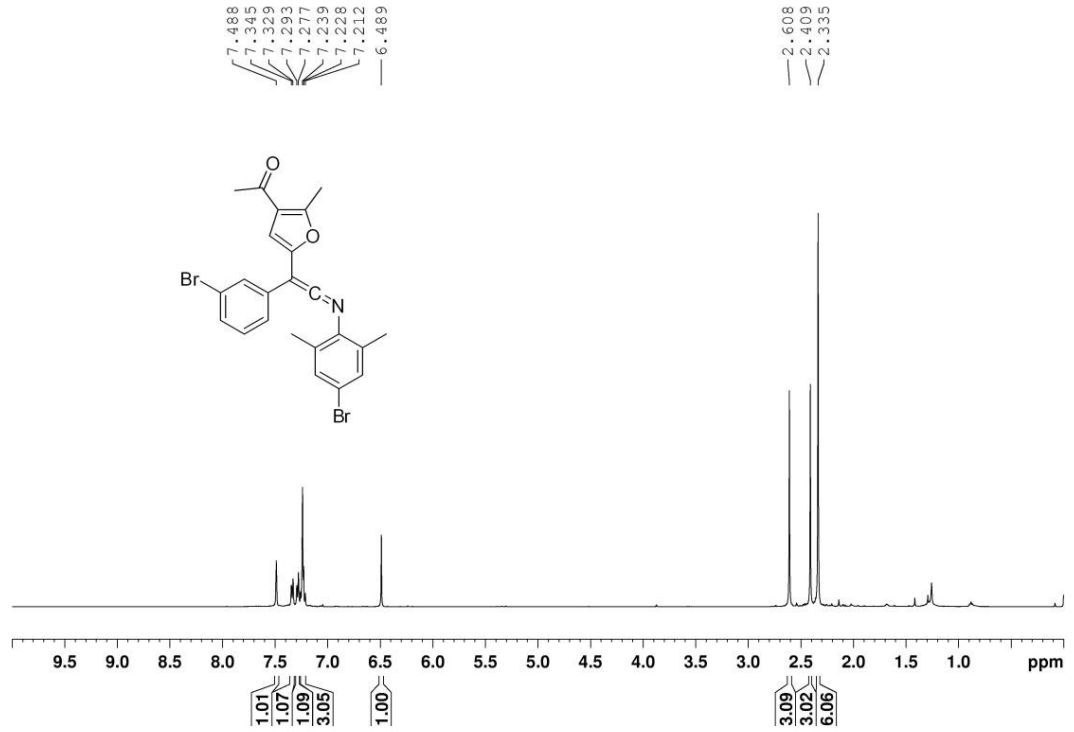

193.80
177.14
158.12
143.90
139.31
135.22
134.21
132.83
131.72
125.93
123.38
121.42
119.17
108.71
108.65
63.85
29.36
18.96
14.67
O
O
C=N
NC
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

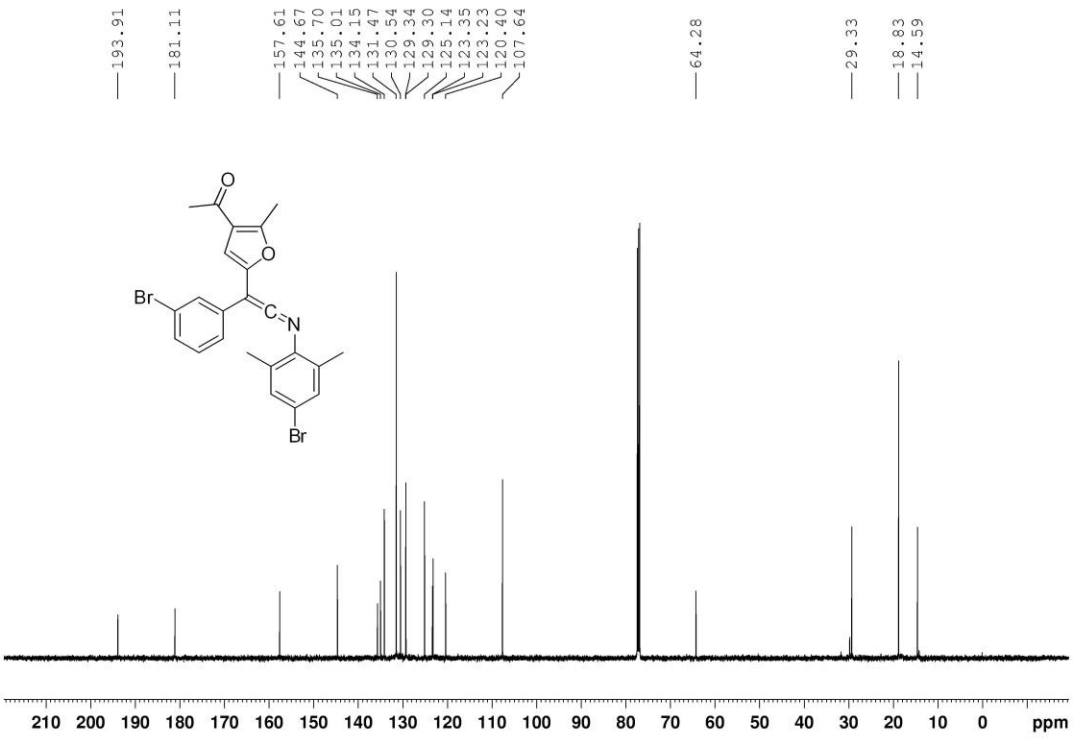
Compound **3g**


7.639
7.623
7.481
7.465
7.282
6.564
2.648
2.445
2.379
O
O
C=N
F3C
Br
9.5 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 ppm
2.10
2.06
2.00
1.01
3.09
3.06
6.01

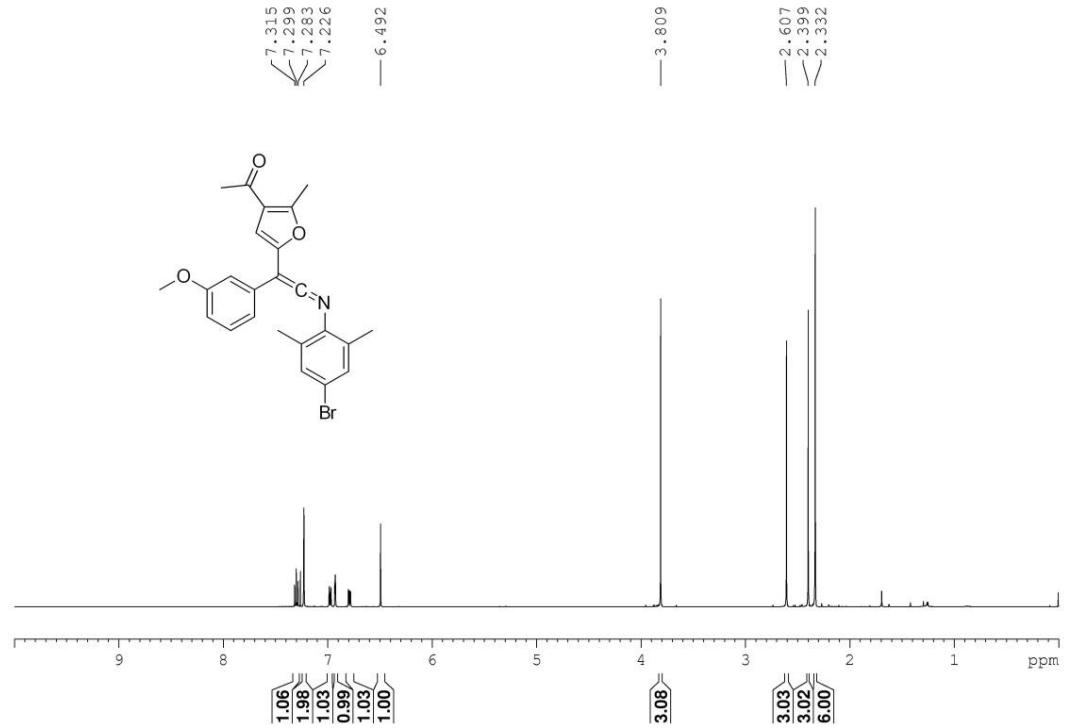

193.87
179.87
157.77
144.50
137.27
135.21
134.52
131.58
128.43
128.17
127.91
127.65
127.52
126.09
126.06
126.03
126.00
125.36
123.37
123.20
121.04
120.77
64.28
29.32
18.87
14.60
O
O
C=N
F3C
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

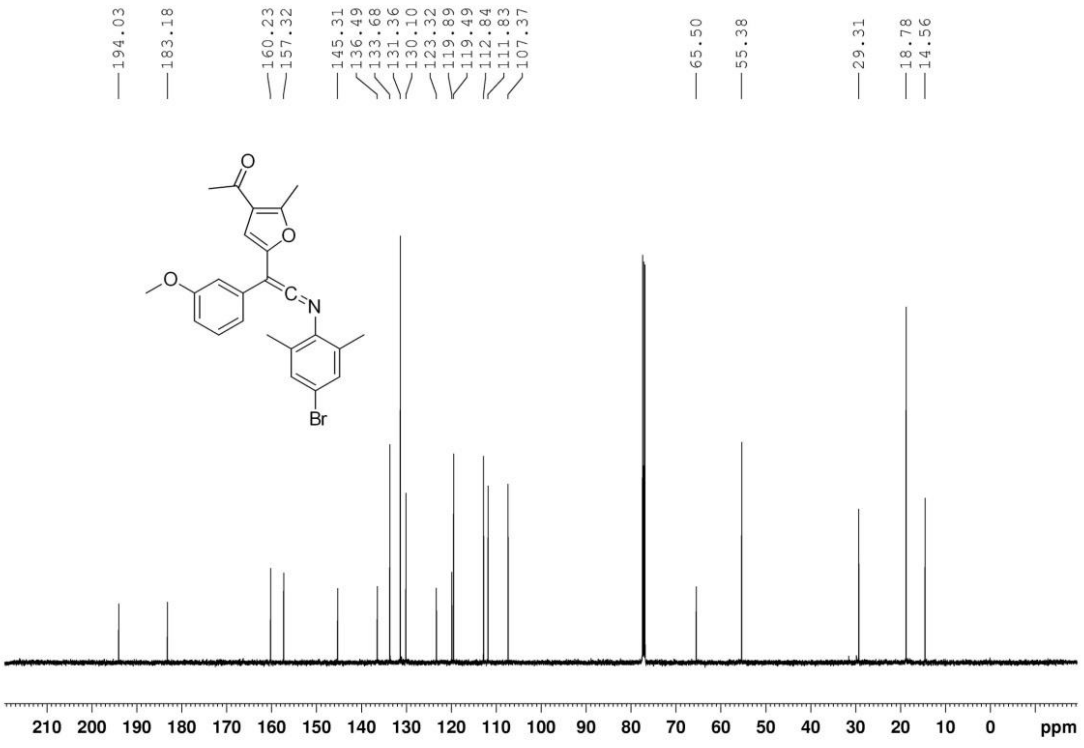
Compound **3h**


7.488
7.345
7.329
7.293
7.277
7.239
7.228
7.212
6.489
2.608
2.409
2.335
O
O
Br
C=N
Br
9.5 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 ppm
1.01
1.07
1.09
3.05
1.00
3.09
3.02
6.06

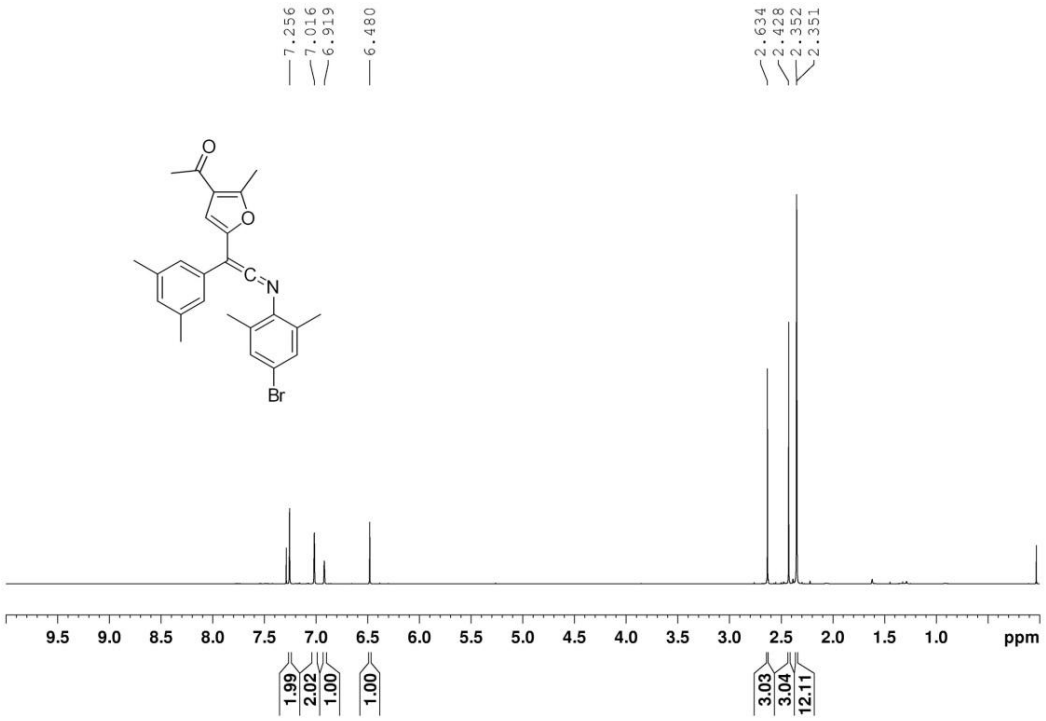

193.91
181.11
157.61
144.67
135.70
135.01
134.15
131.47
130.54
129.34
129.30
125.14
123.35
123.23
120.40
107.64
64.28
29.33
18.83
14.59
O
O
Br
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

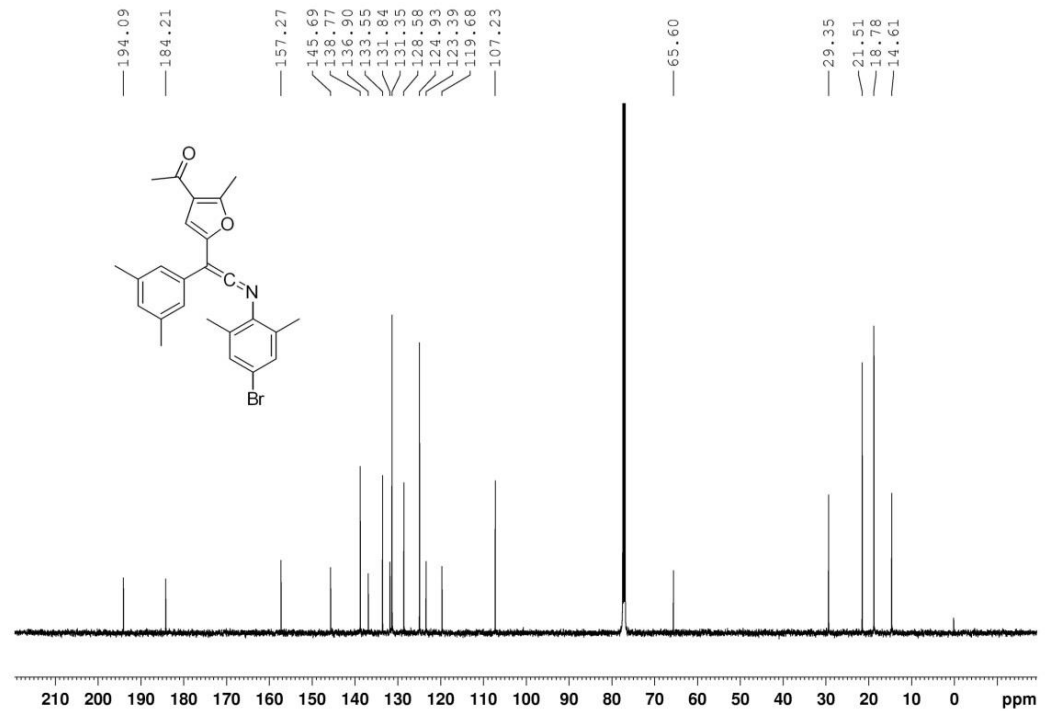
Compound **3i**


7.315
7.299
7.283
7.226
6.492
3.809
2.607
2.399
2.332
O
O
O
C=N
Br
9
8
7
6
5
4
3
2
1
ppm
1.06
1.98
1.03
0.99
1.03
1.00
3.08
3.03
3.02
6.00

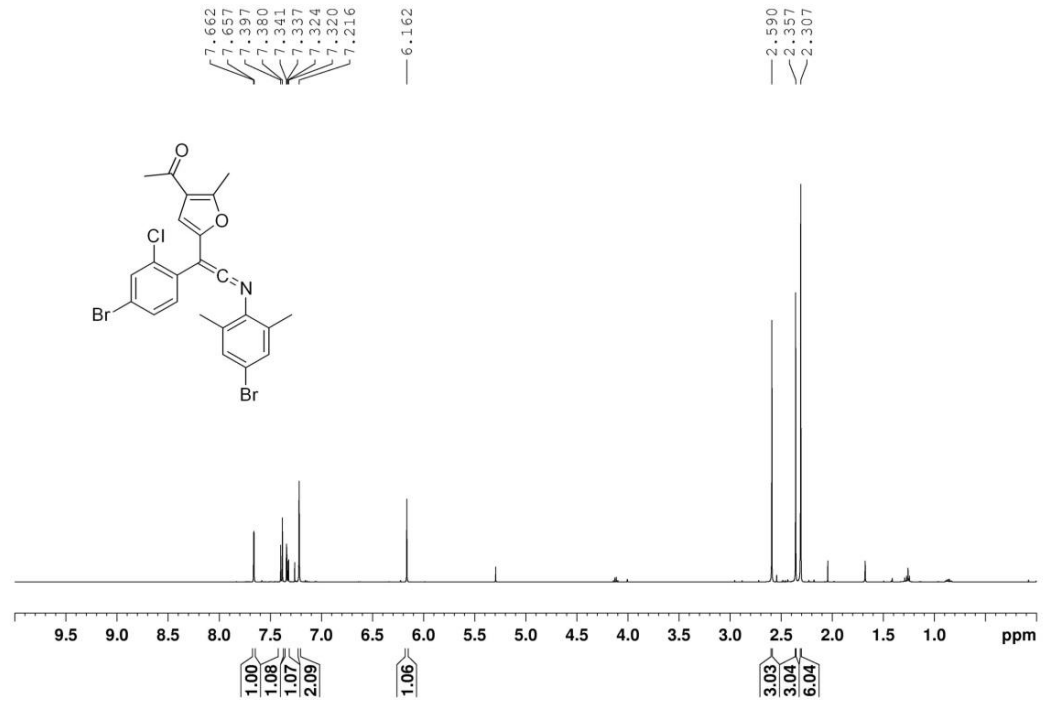

194.03
183.18
160.23
157.32
145.31
136.49
133.68
131.36
130.10
123.32
119.89
119.49
112.84
111.83
107.37
65.50
55.38
29.31
18.78
14.56
O
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

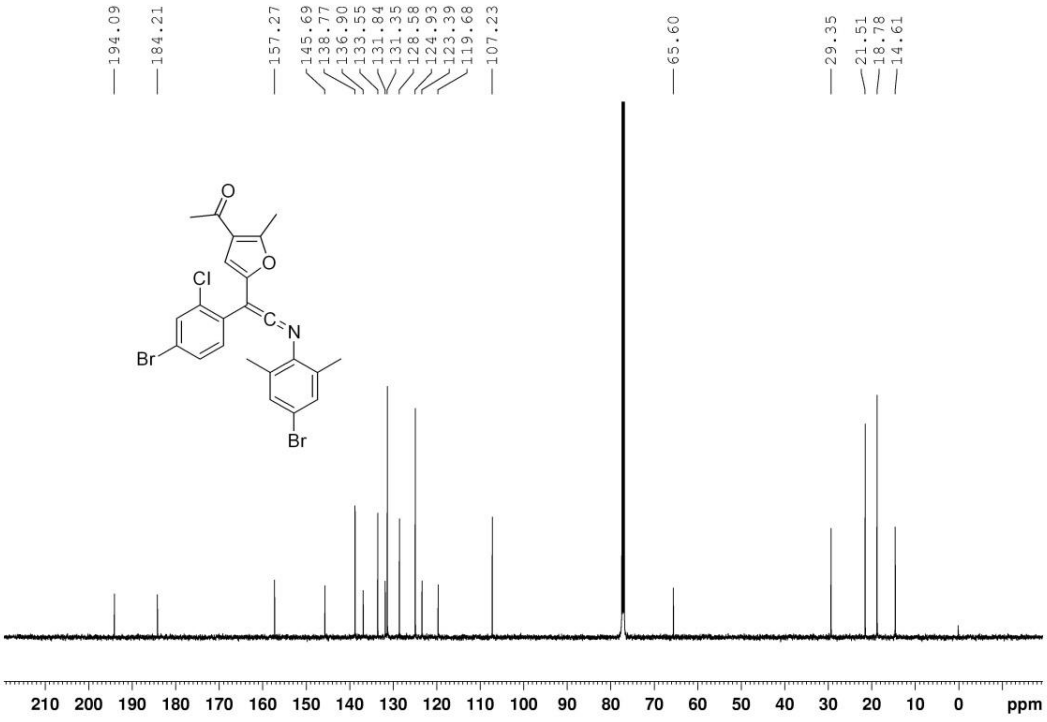
Compound **3j**


7.256
7.016
6.919
6.480
2.634
2.428
2.352
2.351
O
O
C=N
Br
9.5 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 ppm
1.99
2.02
1.00
1.00
3.03
3.04
12.11

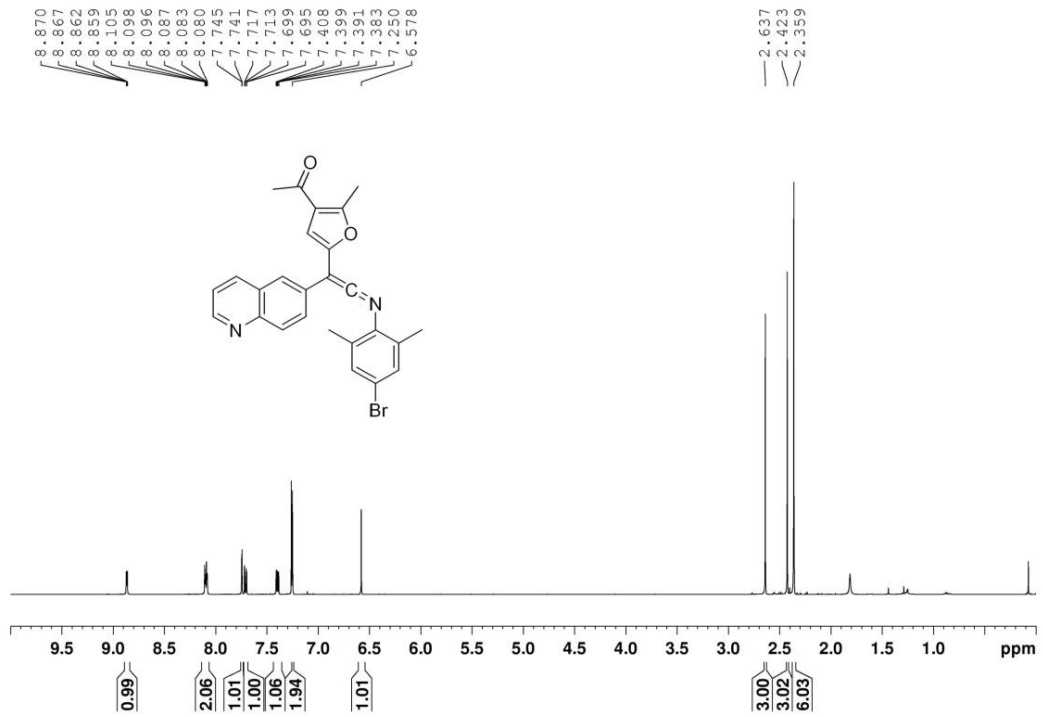

194.09
184.21
157.27
145.69
138.77
136.90
133.55
131.84
131.35
128.58
124.93
123.39
119.68
107.23
65.60
29.35
21.51
18.78
14.61
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

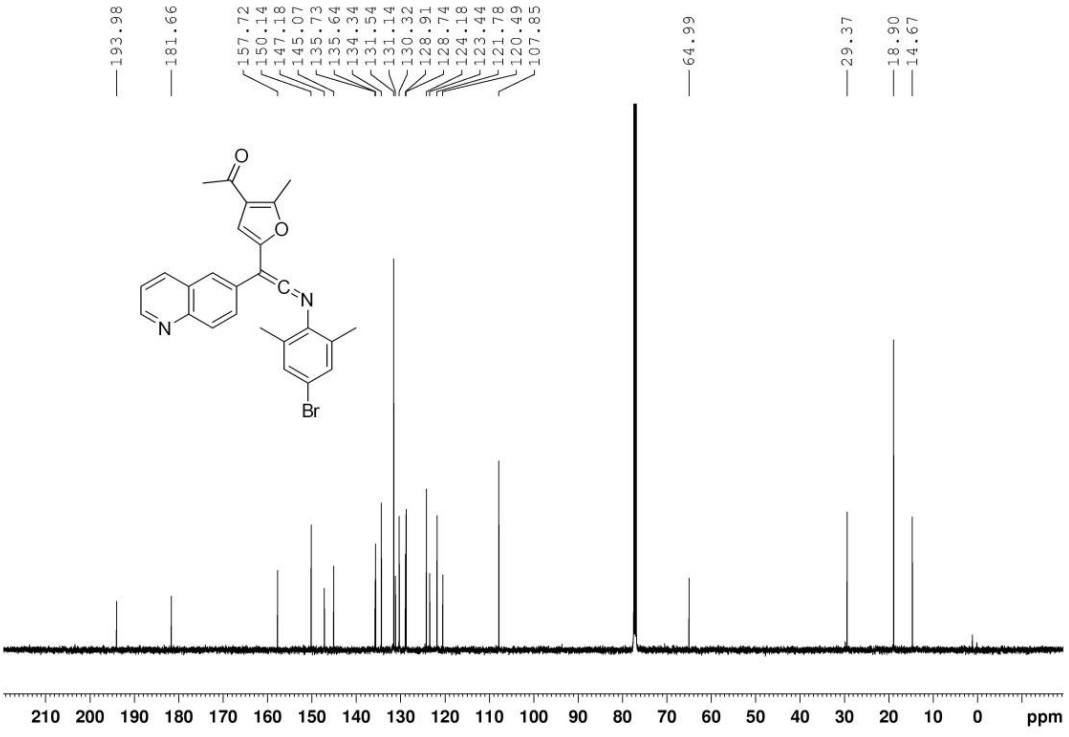
Compound **3k**


7.662
7.657
7.397
7.380
7.341
7.337
7.324
7.320
7.216
6.162
2.590
2.357
2.307
O
O
Cl
C=N
Br
Br
9.5 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 ppm
1.00
1.08
1.07
2.09
1.06
3.03
3.04
6.04

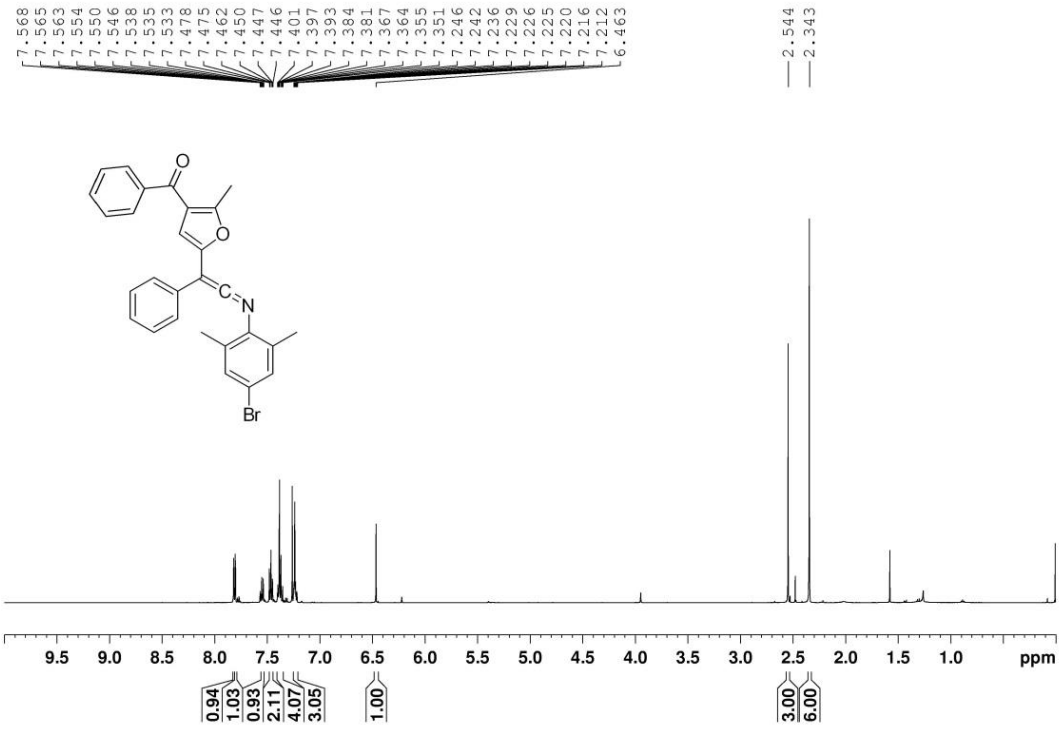

194.09
184.21
157.27
145.69
138.77
136.90
133.55
131.84
131.35
128.58
124.93
123.39
119.68
107.23
65.60
29.35
21.51
18.78
14.61
O
O
Cl
C=N
Br
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

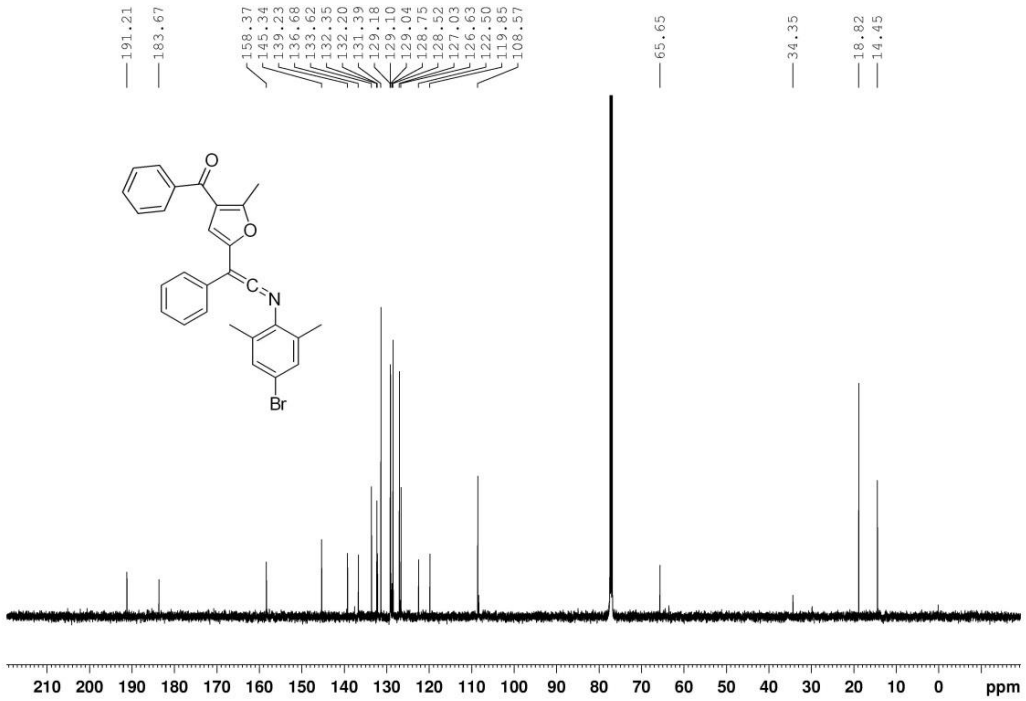
Compound **3l**


8.870
8.867
8.862
8.859
8.105
8.098
8.096
8.087
8.083
8.080
7.745
7.741
7.717
7.713
7.699
7.695
7.408
7.399
7.391
7.383
7.250
6.578
2.637
2.423
2.359
O
O
C=N
N
Br
9.5 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 ppm
0.99
2.06
1.01
1.00
1.06
1.94
1.01
3.00
3.02
6.03

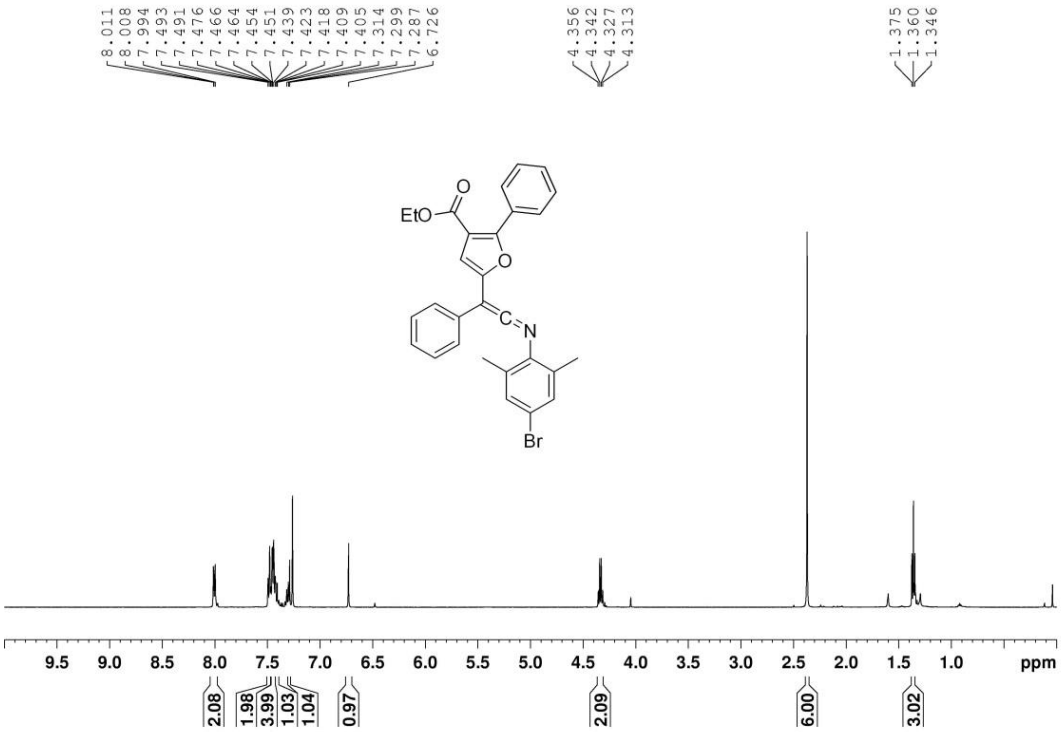

193.98
181.66
157.72
150.14
147.18
145.07
135.73
135.64
134.34
131.54
131.14
130.32
128.91
128.74
124.18
123.44
121.78
120.49
107.85
64.99
29.37
18.90
14.67
O
O
C=N
N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

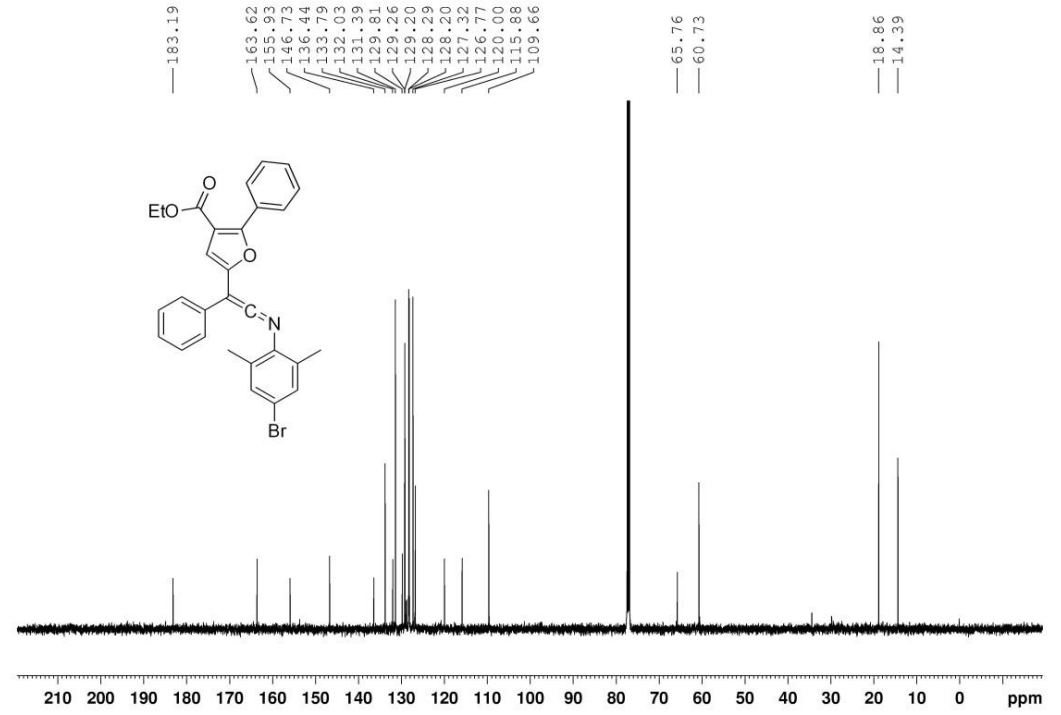
Compound **3m**


7.568
7.565
7.563
7.554
7.550
7.546
7.538
7.535
7.533
7.478
7.475
7.462
7.450
7.447
7.446
7.401
7.397
7.393
7.384
7.381
7.367
7.364
7.355
7.351
7.246
7.242
7.236
7.229
7.226
7.225
7.220
7.216
7.212
6.463
2.544
2.343
O
O
C=N
Br
9.5 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 ppm
0.94
1.03
0.93
2.11
4.07
3.05
1.00
3.00
6.00

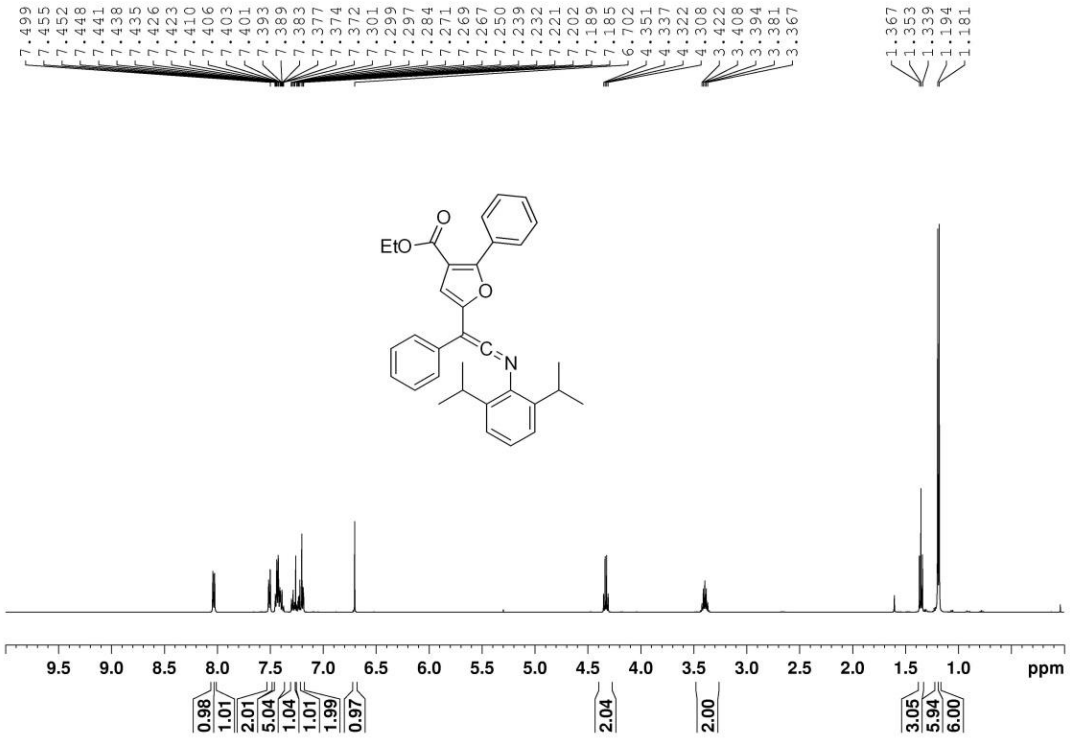

191.21
183.67
158.37
145.34
139.23
136.68
133.62
132.35
132.20
131.39
129.18
129.10
129.04
128.75
128.52
127.03
126.63
122.50
119.85
108.57
65.65
34.35
18.82
14.45
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

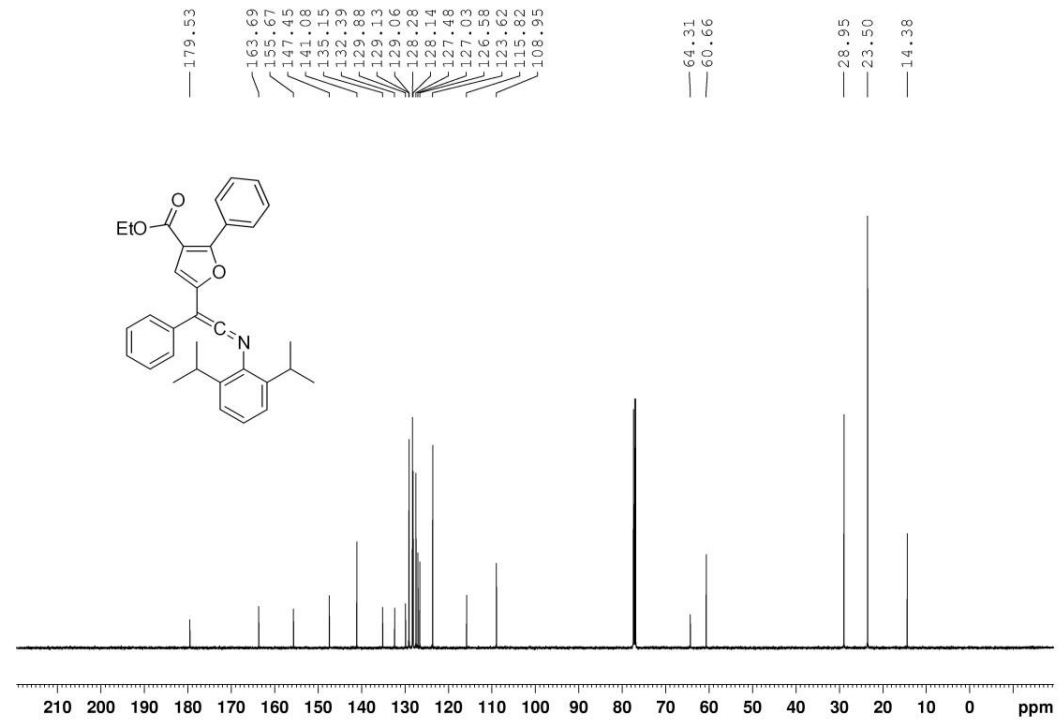
Compound **3n**


8.011
8.008
7.994
7.493
7.491
7.476
7.466
7.464
7.454
7.451
7.439
7.423
7.418
7.409
7.405
7.314
7.299
7.287
6.726
4.356
4.342
4.327
4.313
1.375
1.360
1.346
EtO
O
O
C=N
Br
9.5 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 ppm
2.08
1.98
3.99
1.03
1.04
0.97
2.09
6.00
3.02

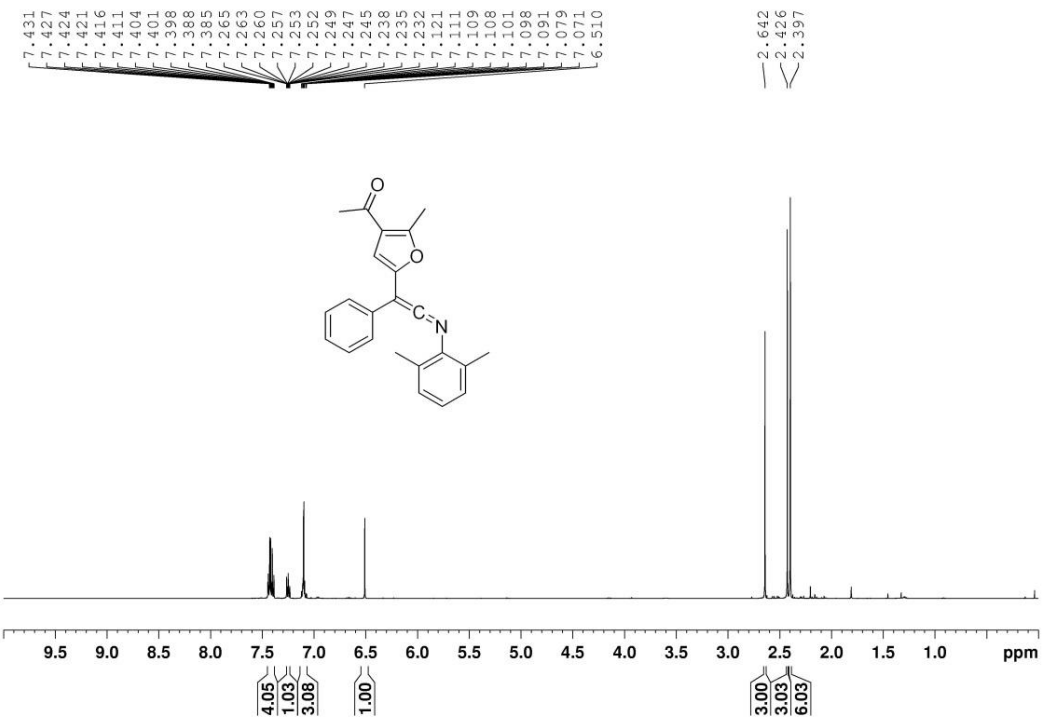

183.19
163.62
155.93
146.73
136.44
133.79
132.03
131.39
129.81
129.26
129.20
128.29
128.20
127.32
126.77
120.00
115.88
109.66
65.76
60.73
18.86
14.39
EtO
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

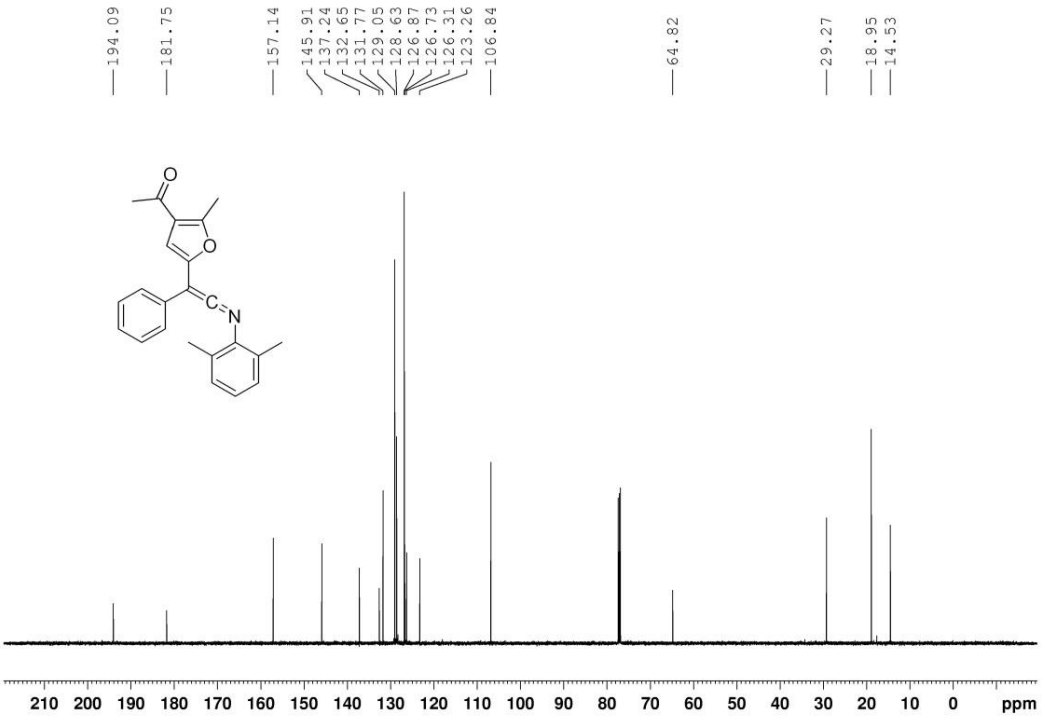
Compound **3o**


7.499
7.455
7.452
7.448
7.441
7.438
7.435
7.426
7.423
7.410
7.406
7.403
7.401
7.393
7.389
7.383
7.377
7.374
7.372
7.301
7.299
7.297
7.284
7.271
7.269
7.267
7.250
7.239
7.232
7.221
7.202
7.189
7.185
6.702
4.351
4.337
4.322
4.308
3.422
3.408
3.394
3.381
3.367
1.367
1.353
1.339
1.194
1.181
EtO
O
O
C=N
9.5 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 ppm
0.98
1.01
2.01
5.04
1.04
1.01
1.99
0.97
2.04
2.00
3.05
5.94
6.00

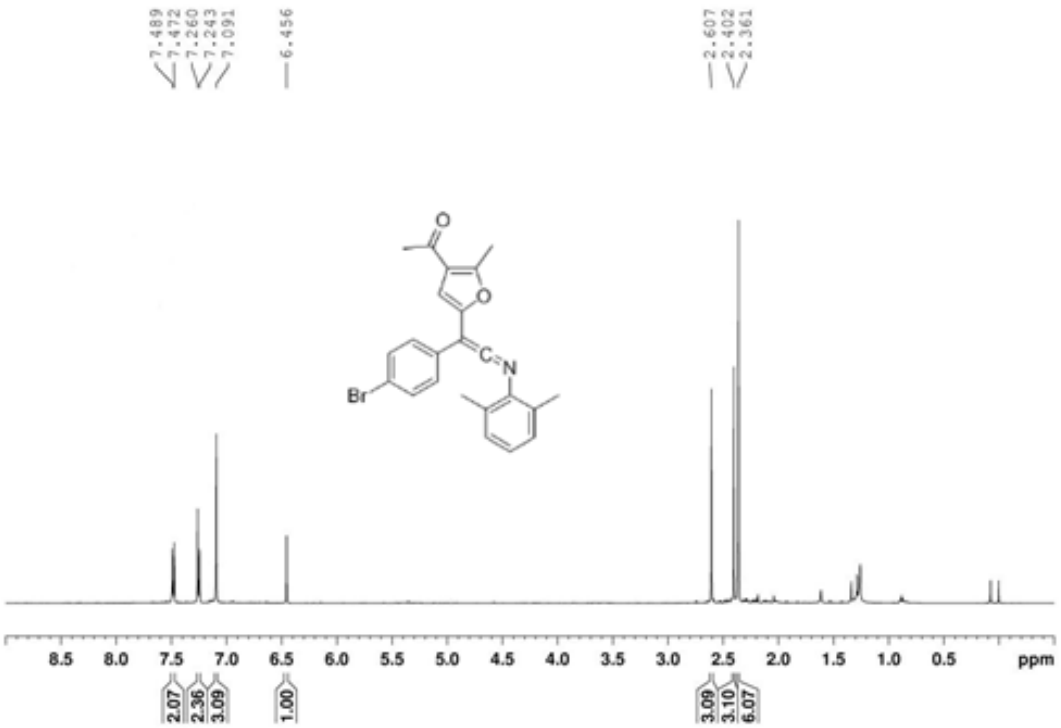

179.53
163.69
155.67
147.45
141.08
135.15
132.39
129.88
129.13
129.06
128.28
128.14
127.48
127.03
126.58
123.62
115.82
108.95
64.31
60.66
28.95
23.50
14.38
EtO
O
O
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

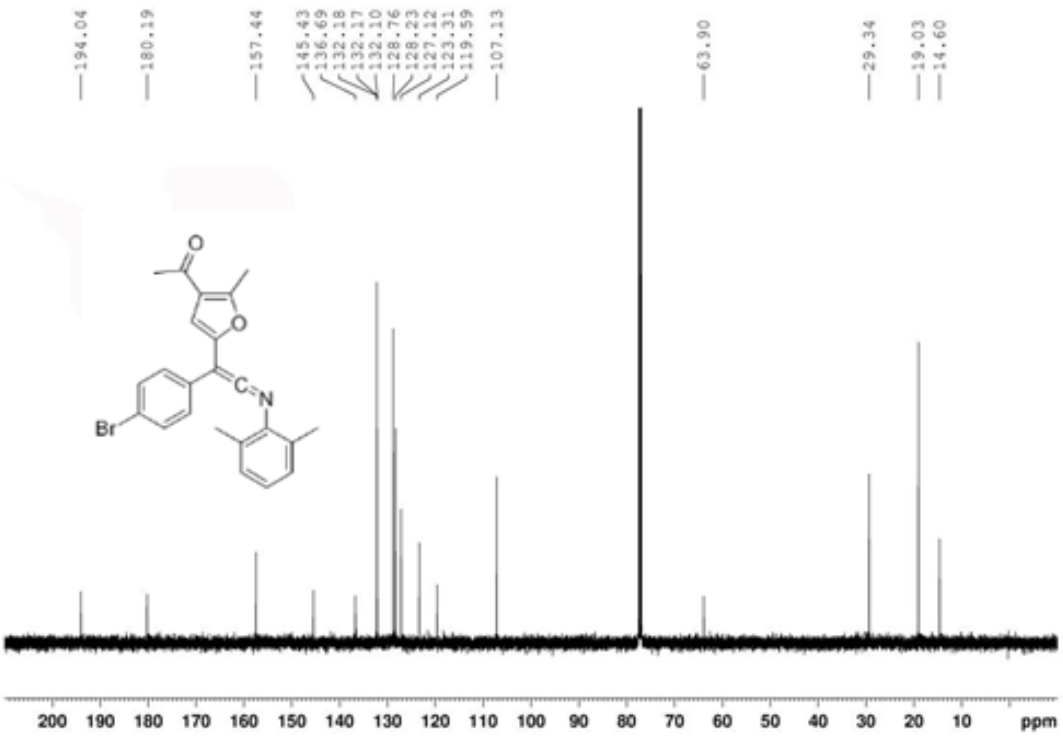
Compound **3p**


7.431
7.427
7.424
7.421
7.416
7.411
7.404
7.401
7.398
7.388
7.385
7.265
7.263
7.260
7.257
7.253
7.252
7.249
7.247
7.245
7.238
7.235
7.232
7.121
7.111
7.109
7.108
7.101
7.098
7.091
7.079
7.071
6.510
2.642
2.426
2.397
O
O
C=N
9.5 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 ppm
4.05
1.03
3.08
1.00
3.00
3.03
6.03

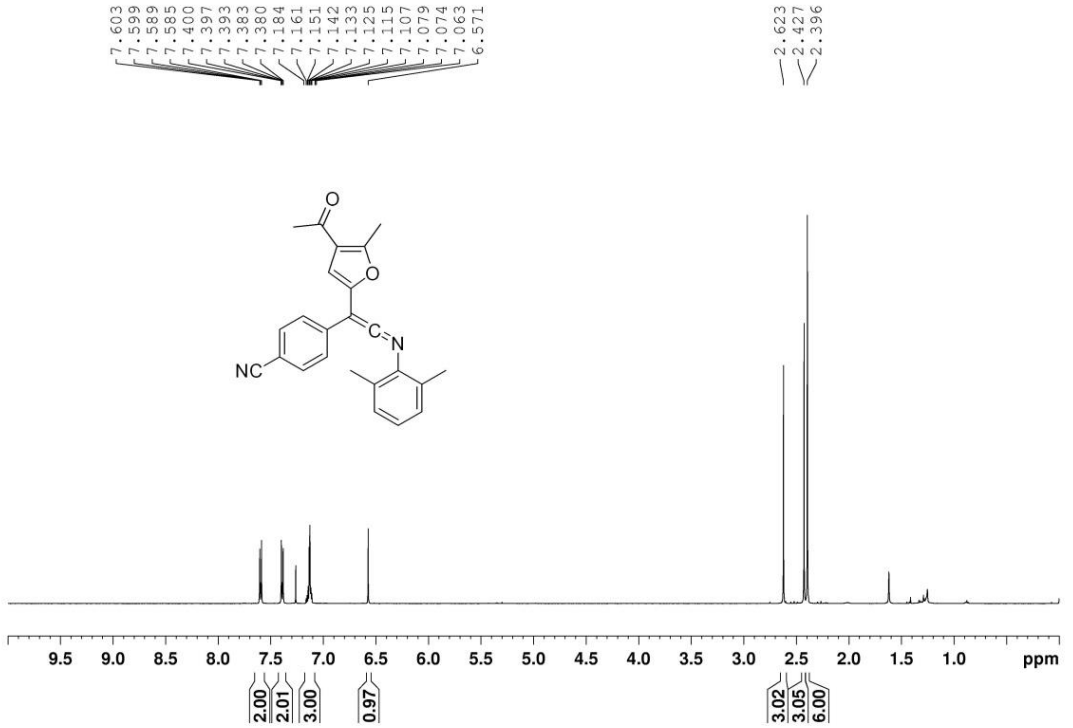

194.09
181.75
157.14
145.91
137.24
132.65
131.77
129.05
128.63
126.87
126.73
126.31
123.26
106.84
64.82
29.27
18.95
14.53
O
O
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

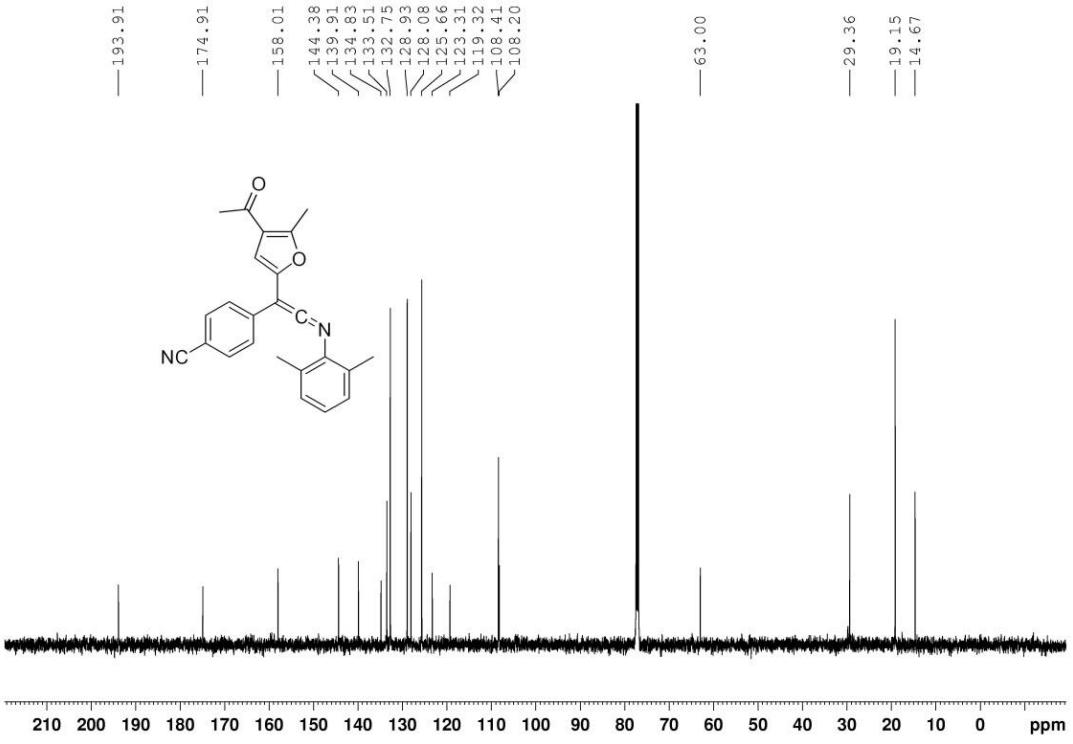
Compound **3q**


7.489
7.472
7.260
7.243
7.091
6.456
2.607
2.402
2.361
O
O
C=N
Br
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 ppm
2.07
2.36
3.09
1.00
3.09
3.10
6.07

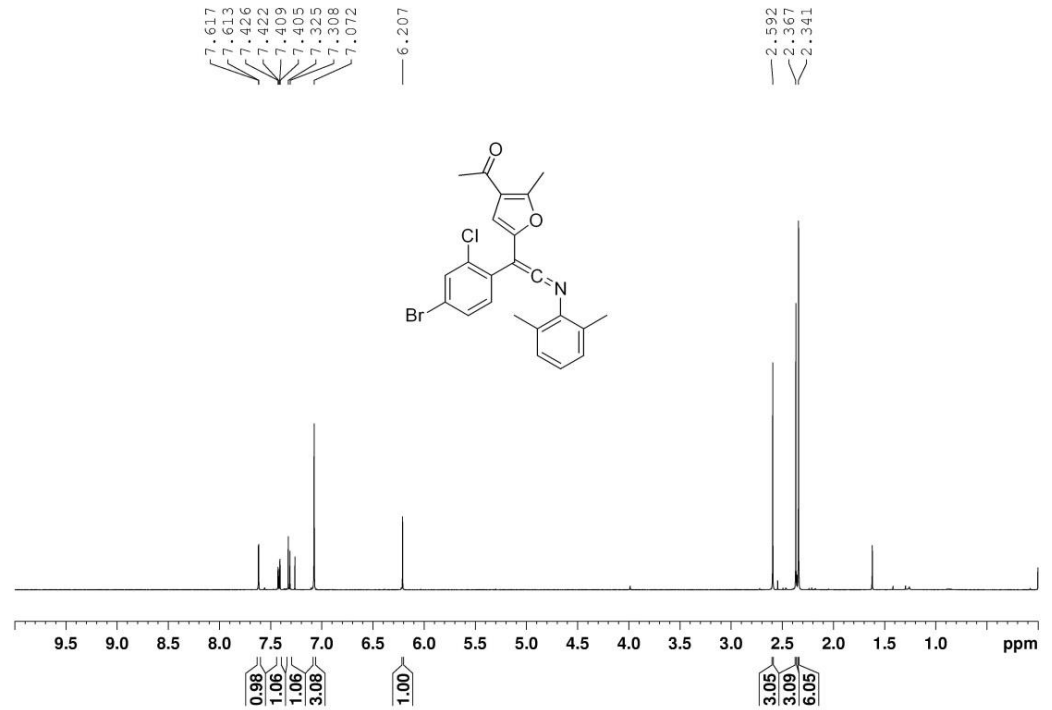

194.04
180.19
157.44
145.43
136.69
132.18
132.17
132.10
128.76
128.23
127.12
123.31
119.59
107.13
63.90
29.34
19.03
14.60
O
O
C=N
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

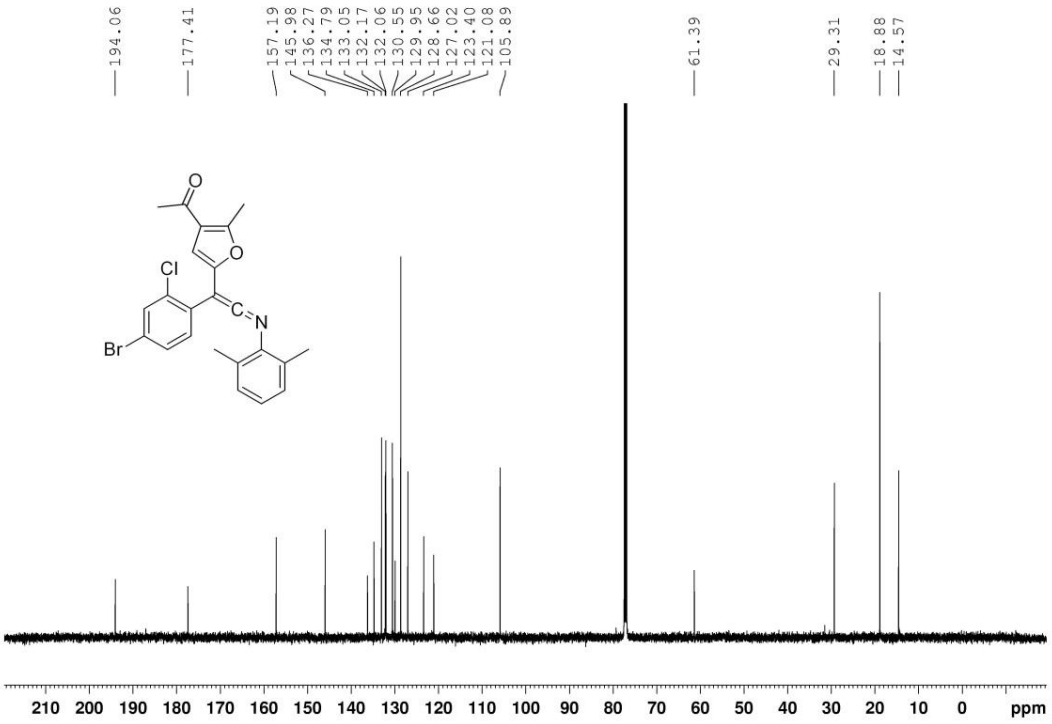
Compound **3r**


7.603
7.599
7.589
7.585
7.400
7.397
7.393
7.383
7.380
7.184
7.161
7.151
7.142
7.133
7.125
7.115
7.107
7.079
7.074
7.063
6.571
2.623
2.427
2.396
O
O
C=N
NC
9.5 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 ppm
2.00
2.01
3.00
0.97
3.02
3.05
6.00

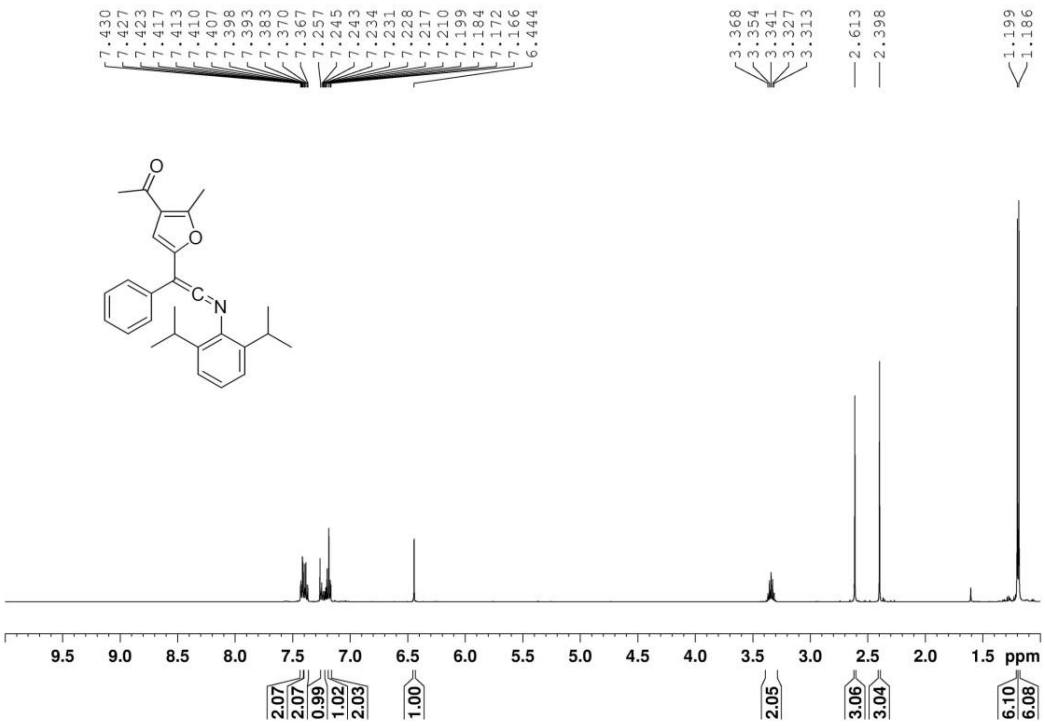

193.91
174.91
158.01
144.38
139.91
134.83
133.51
132.75
128.93
128.08
125.66
123.31
119.32
108.41
108.20
63.00
29.36
19.15
14.67
O
O
C=N
NC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

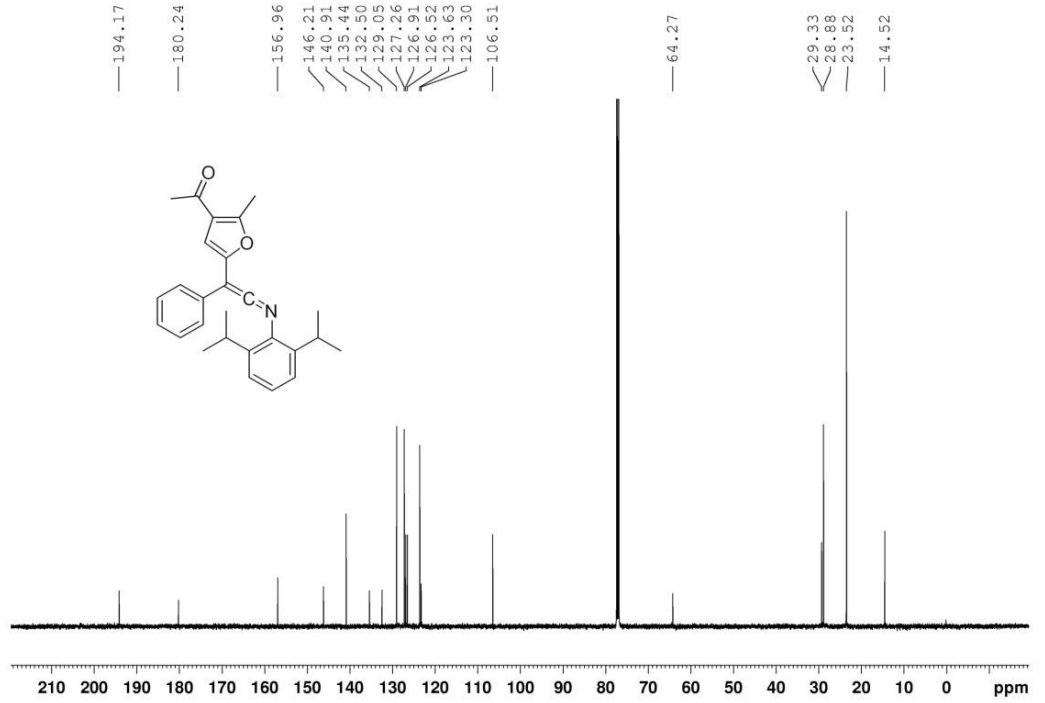
Compound **3s**


7.617
7.613
7.426
7.422
7.409
7.405
7.325
7.308
7.072
6.207
2.592
2.367
2.341
O
Cl
Br
C=N
9.5 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 ppm
0.98
1.06
1.06
3.08
1.00
3.05
3.09
6.05

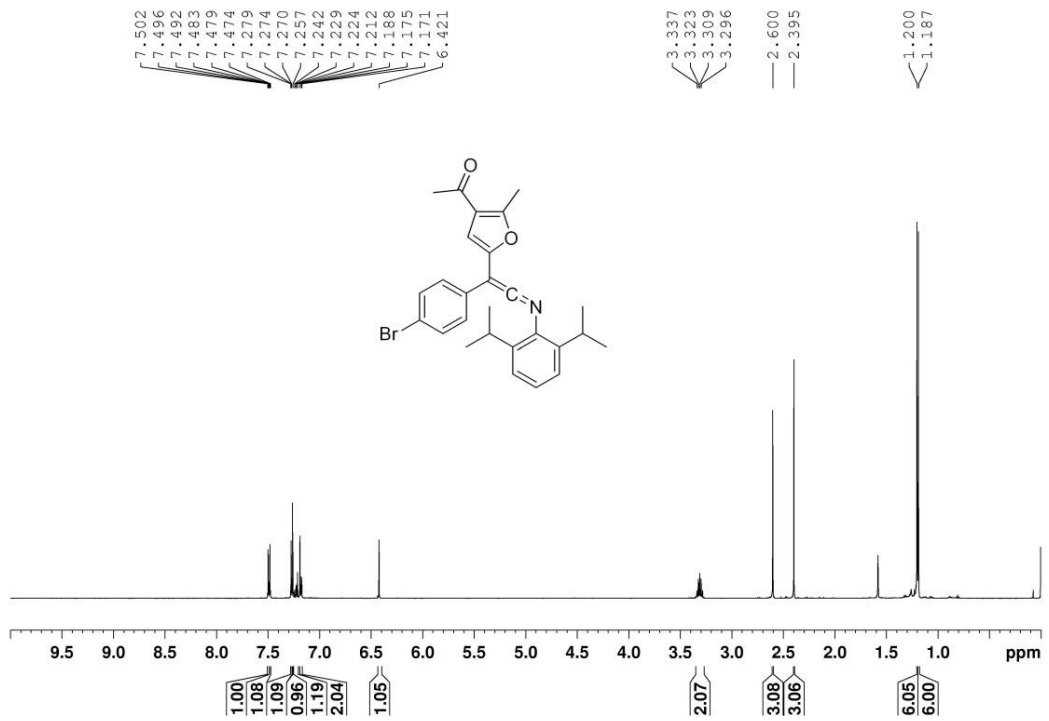

194.06
177.41
157.19
145.98
136.27
134.79
133.05
132.17
132.06
130.55
129.95
128.66
127.02
123.40
121.08
105.89
61.39
29.31
18.88
14.57
O
Cl
Br
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

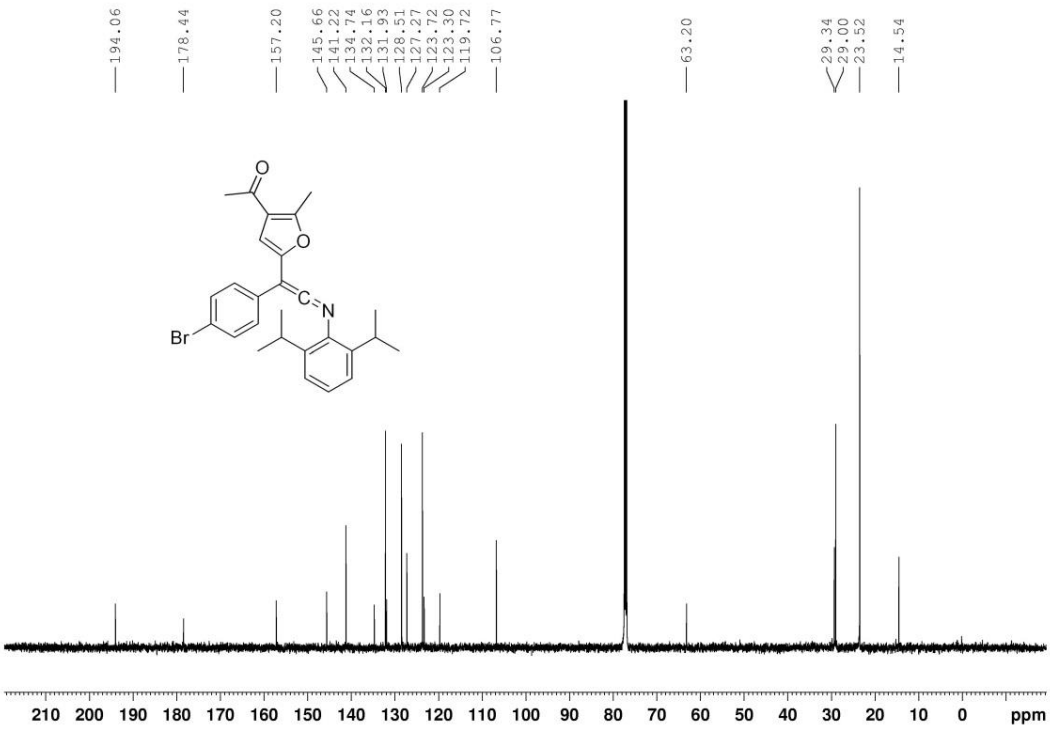
Compound **3t**


7.430
7.427
7.423
7.417
7.413
7.410
7.407
7.398
7.393
7.383
7.370
7.367
7.257
7.245
7.243
7.234
7.231
7.228
7.217
7.210
7.199
7.184
7.172
7.166
6.444
3.368
3.354
3.341
3.327
3.313
2.613
2.398
1.199
1.186
O
O
C=N
9.5 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 ppm
2.07
2.07
0.99
1.02
2.03
1.00
2.05
3.06
3.04
6.10
6.08

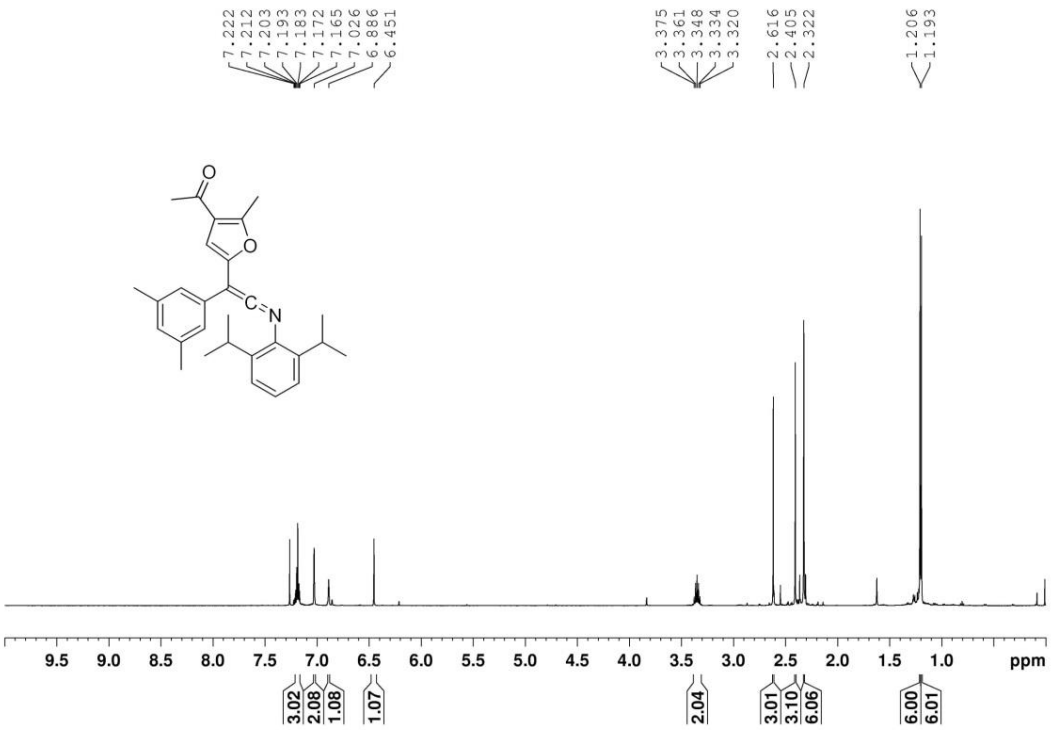

194.17
180.24
156.96
146.21
140.91
135.44
132.50
129.05
127.26
126.91
126.52
123.63
123.30
106.51
64.27
29.33
28.88
23.52
14.52
O
O
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

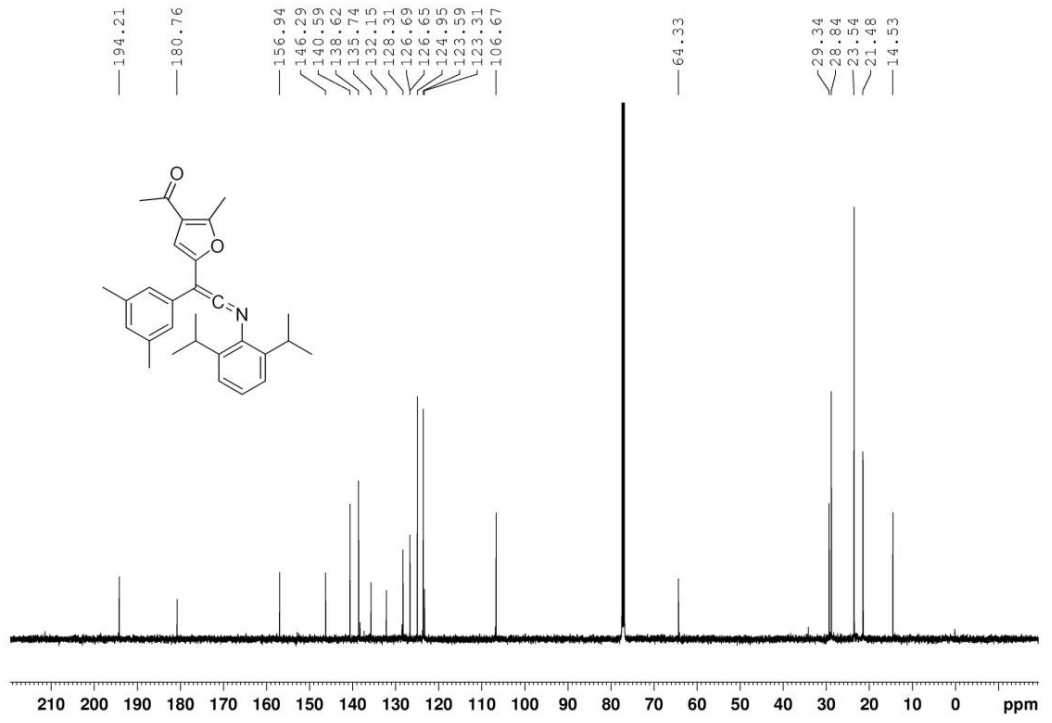
Compound **3u**


7.502
7.496
7.492
7.483
7.479
7.474
7.279
7.274
7.270
7.257
7.242
7.229
7.224
7.212
7.188
7.175
7.171
6.421
3.337
3.323
3.309
3.296
2.600
2.395
1.200
1.187
O
O
C=N
Br
9.5 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 ppm
1.00
1.08
1.09
0.96
1.19
2.04
1.05
2.07
3.08
3.06
6.05
6.00

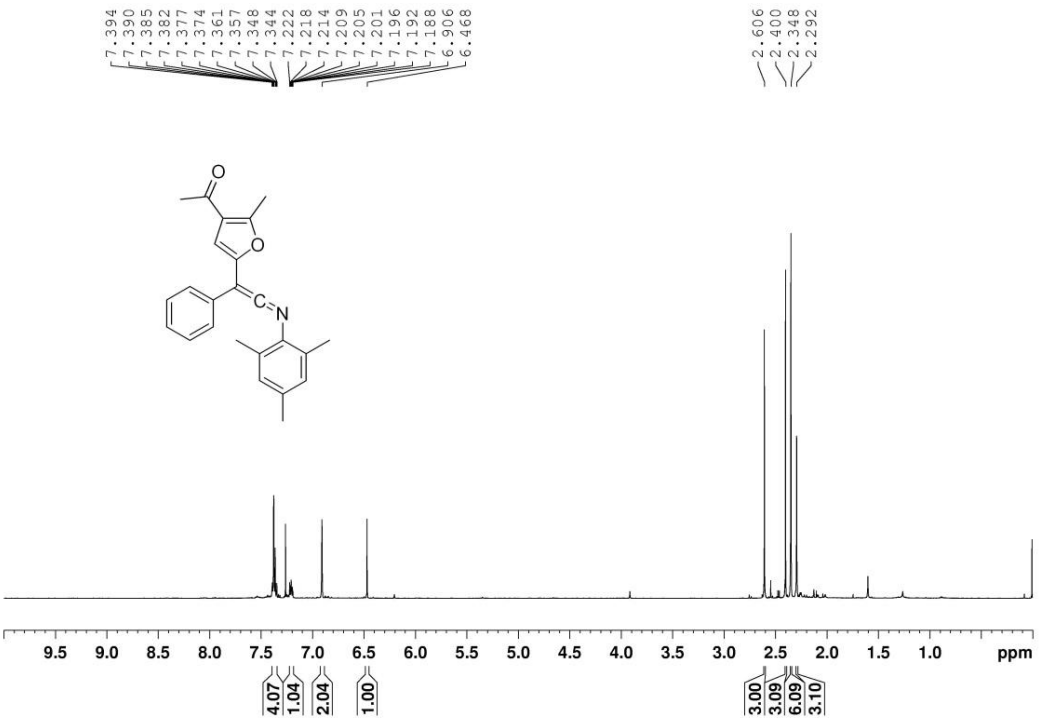

194.06
178.44
157.20
145.66
141.22
134.74
132.16
131.93
128.51
127.27
123.72
123.30
119.72
106.77
63.20
29.34
29.00
23.52
14.54
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

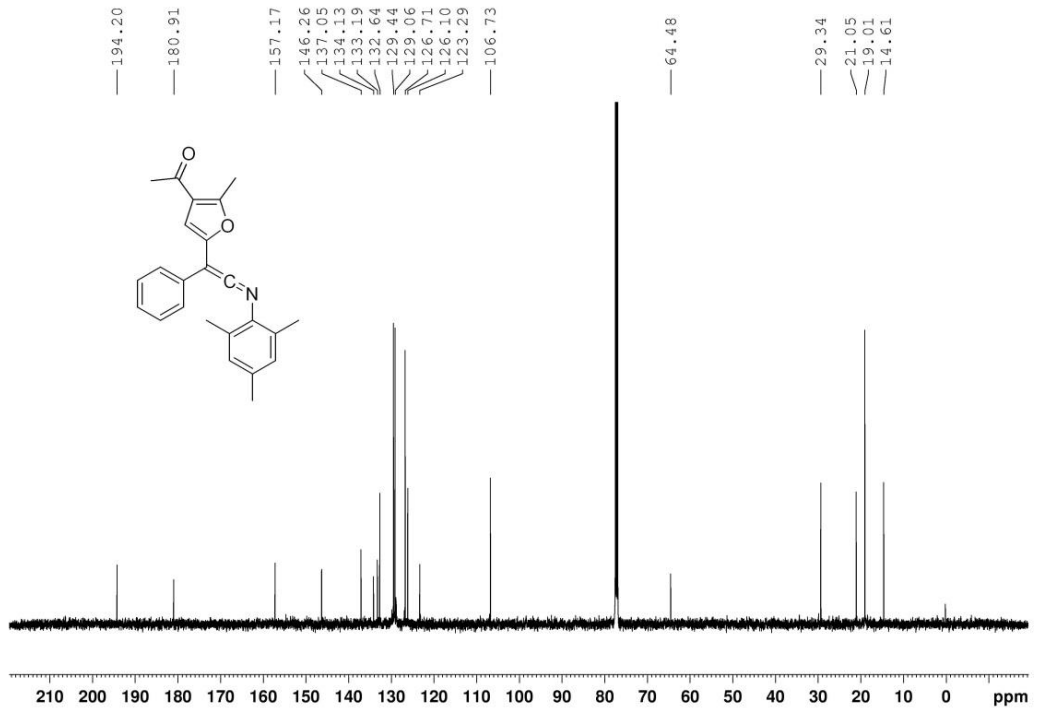
Compound **3v**


7.222
7.212
7.203
7.193
7.183
7.172
7.165
7.026
6.886
6.451
3.375
3.361
3.348
3.334
3.320
2.616
2.405
2.322
1.206
1.193
O
O
C=N
9.5 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 ppm
3.02
2.08
1.08
1.07
2.04
3.01
3.10
6.06
6.00
6.01

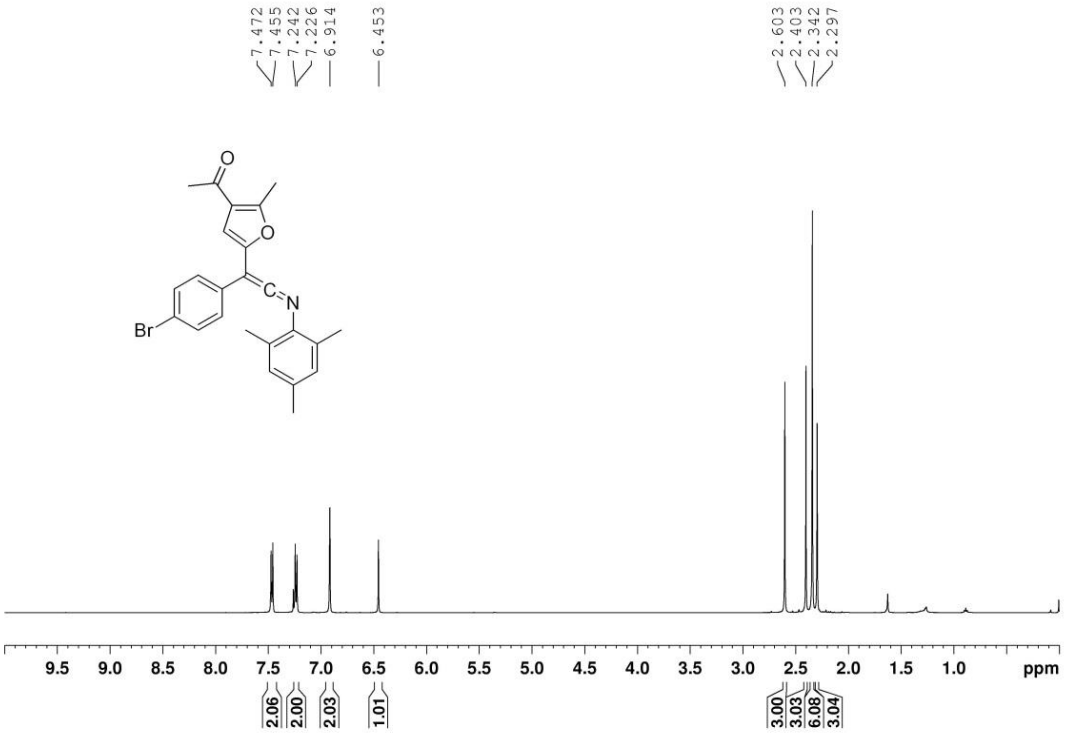

194.21
180.76
156.94
146.29
140.59
138.62
135.74
132.15
128.31
126.69
126.65
124.95
123.59
123.31
106.67
64.33
29.34
28.84
23.54
21.48
14.53
O
O
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

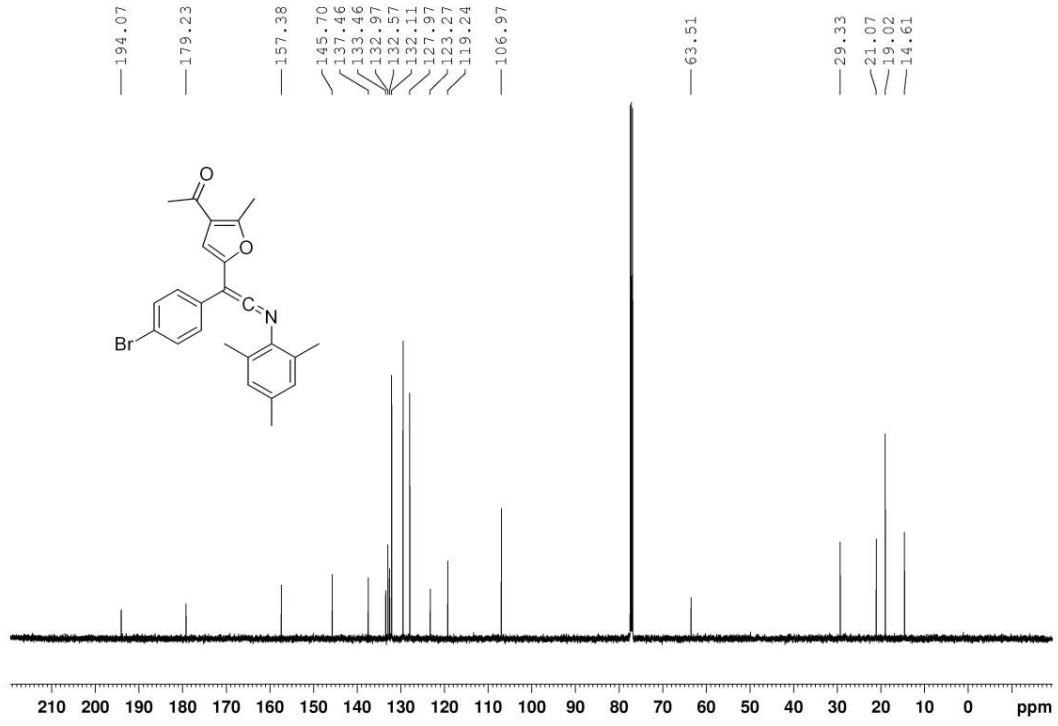
Compound **3w**


7.394
7.390
7.385
7.382
7.377
7.374
7.361
7.357
7.348
7.344
7.222
7.218
7.214
7.209
7.205
7.201
7.196
7.192
7.188
6.906
6.468
2.606
2.400
2.348
2.292
O
O
C=N
9.5 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 ppm
4.07
1.04
2.04
1.00
3.00
3.09
6.09
3.10

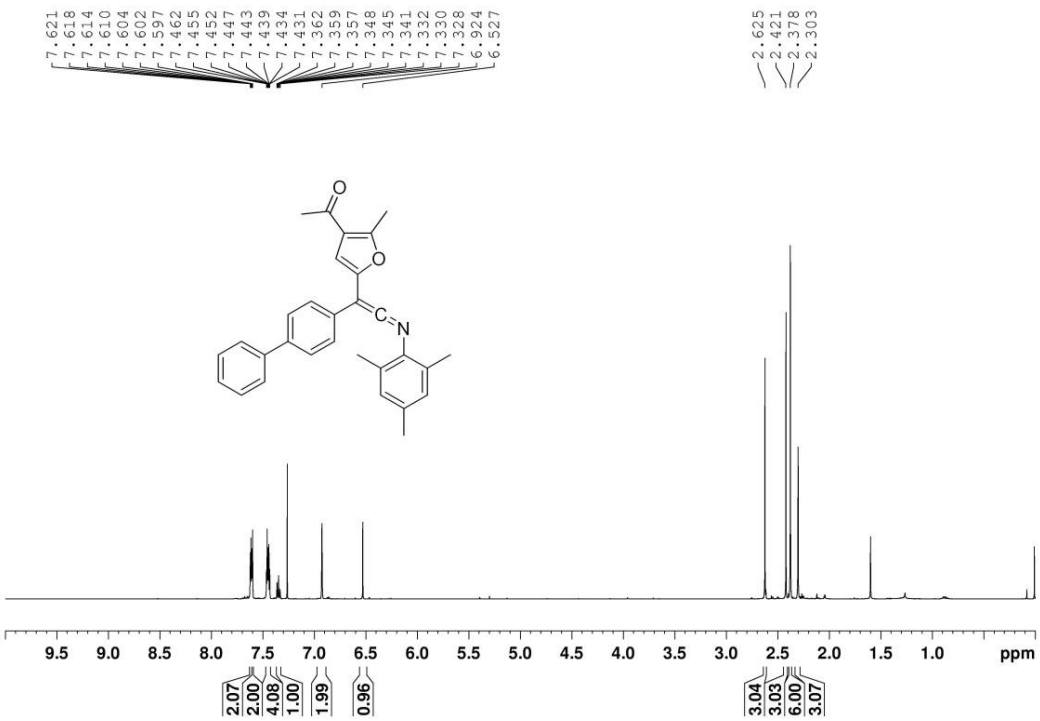

194.20
180.91
157.17
146.26
137.05
134.13
133.19
132.64
129.44
129.06
126.71
126.10
123.29
106.73
64.48
29.34
21.05
19.01
14.61
O
O
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

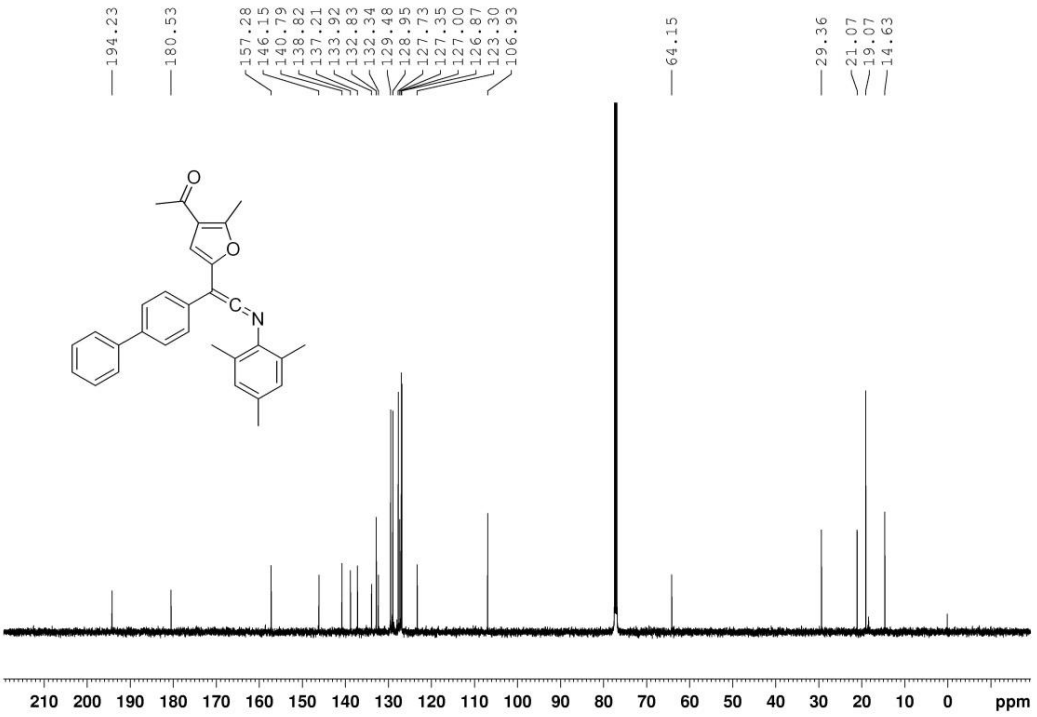
Compound **3x**


7.472
7.455
7.242
7.226
6.914
6.453
2.603
2.403
2.342
2.297
O
O
C=N
Br
9.5 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 ppm
2.06
2.00
2.03
1.01
3.00
3.03
6.08
3.04

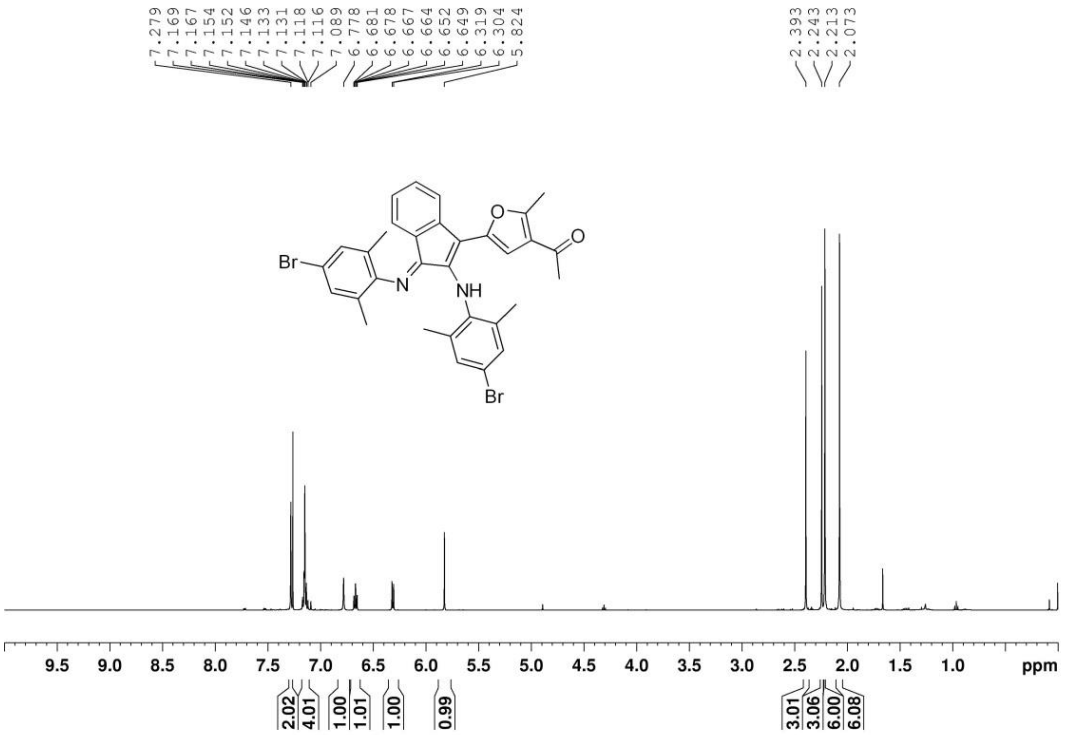

194.07
179.23
157.38
145.70
137.46
133.46
132.97
132.57
132.11
127.97
123.27
119.24
106.97
63.51
29.33
21.07
19.02
14.61
O
O
C=N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

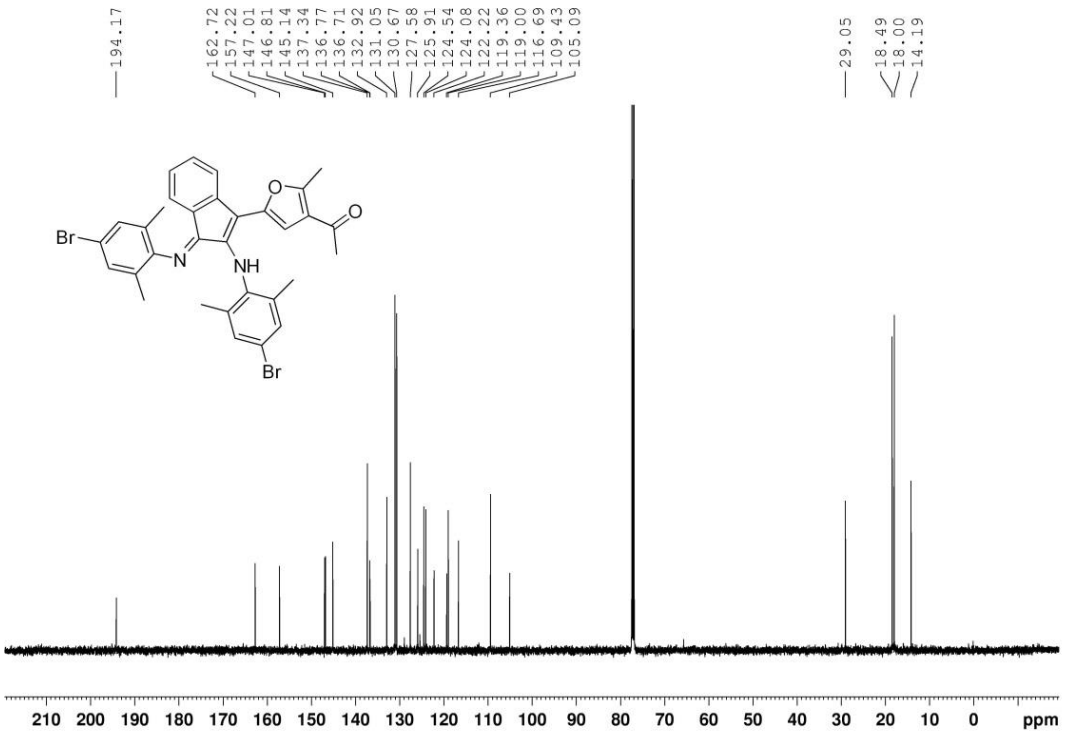
Compound **3y**


7.621
7.618
7.614
7.610
7.604
7.602
7.597
7.462
7.455
7.452
7.447
7.443
7.439
7.434
7.431
7.362
7.359
7.357
7.348
7.345
7.341
7.332
7.330
7.328
6.924
6.527
2.625
2.421
2.378
2.303
O
O
C=N
9.5 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 ppm
2.07
2.00
4.08
1.00
1.99
0.96
3.04
3.03
6.00
3.07

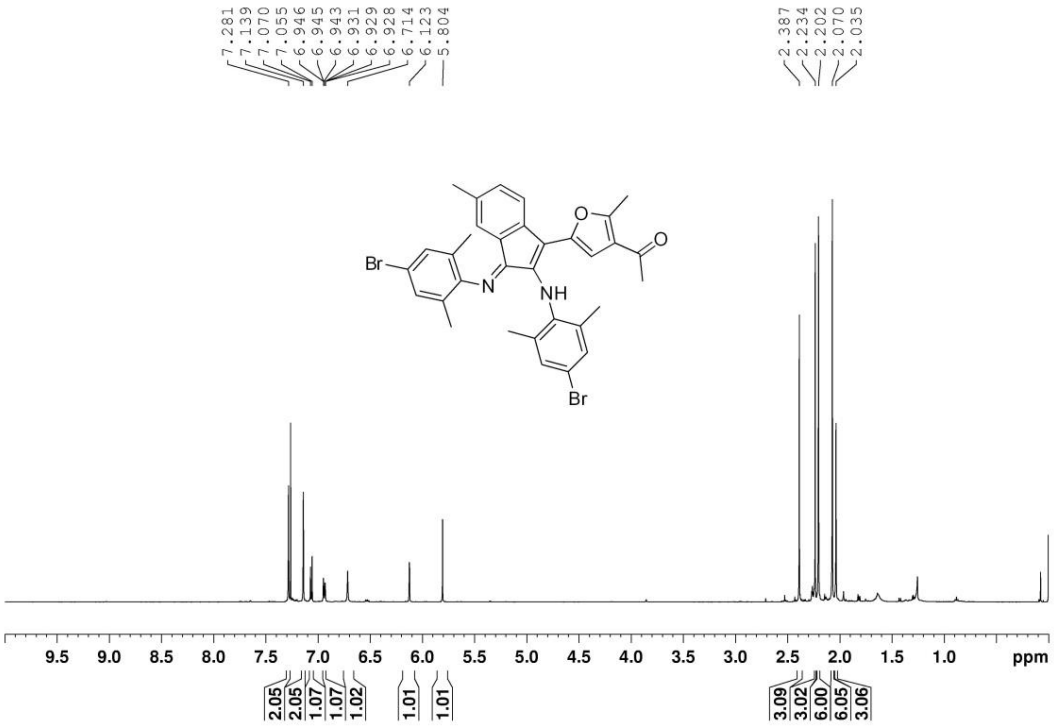

194.23
180.53
157.28
146.15
140.79
138.82
137.21
133.92
132.83
132.34
129.48
128.95
127.73
127.35
127.00
126.87
123.30
106.93
64.15
29.36
21.07
19.07
14.63
O
O
C=N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

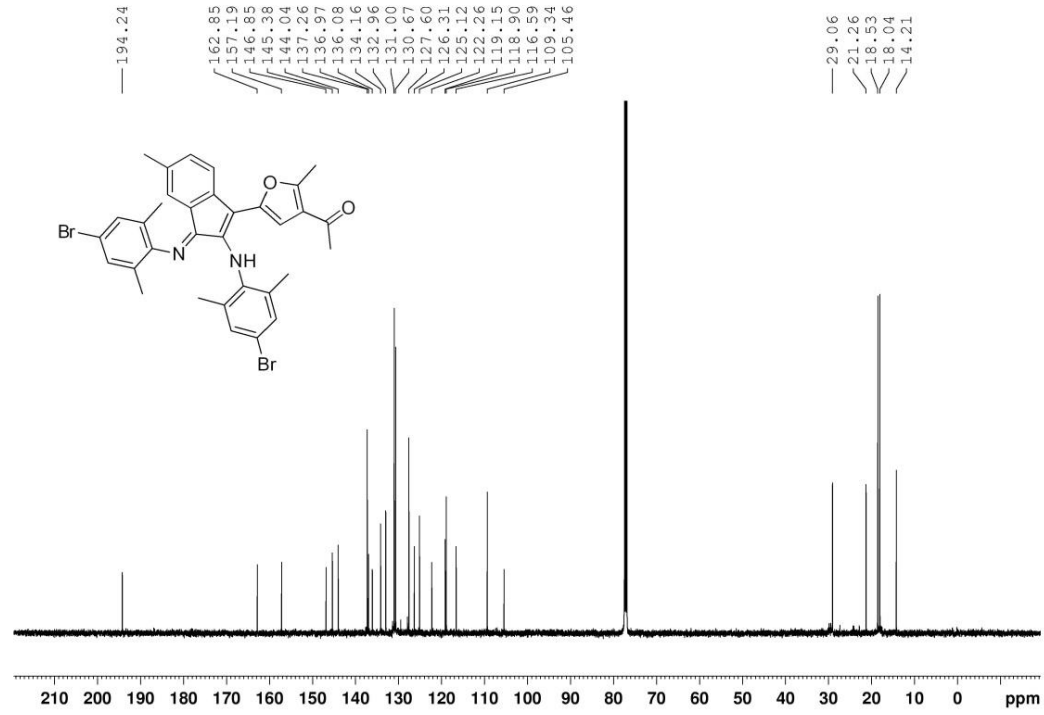
Compound **4a**


7.279
7.169
7.167
7.154
7.152
7.146
7.133
7.131
7.118
7.116
7.089
6.778
6.681
6.678
6.667
6.664
6.652
6.649
6.319
6.304
5.824
2.393
2.243
2.213
2.073
Br
N
NH
O
O
Br
9.5 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 ppm
2.02
4.01
1.00
1.01
1.00
0.99
3.01
3.06
6.00
6.08

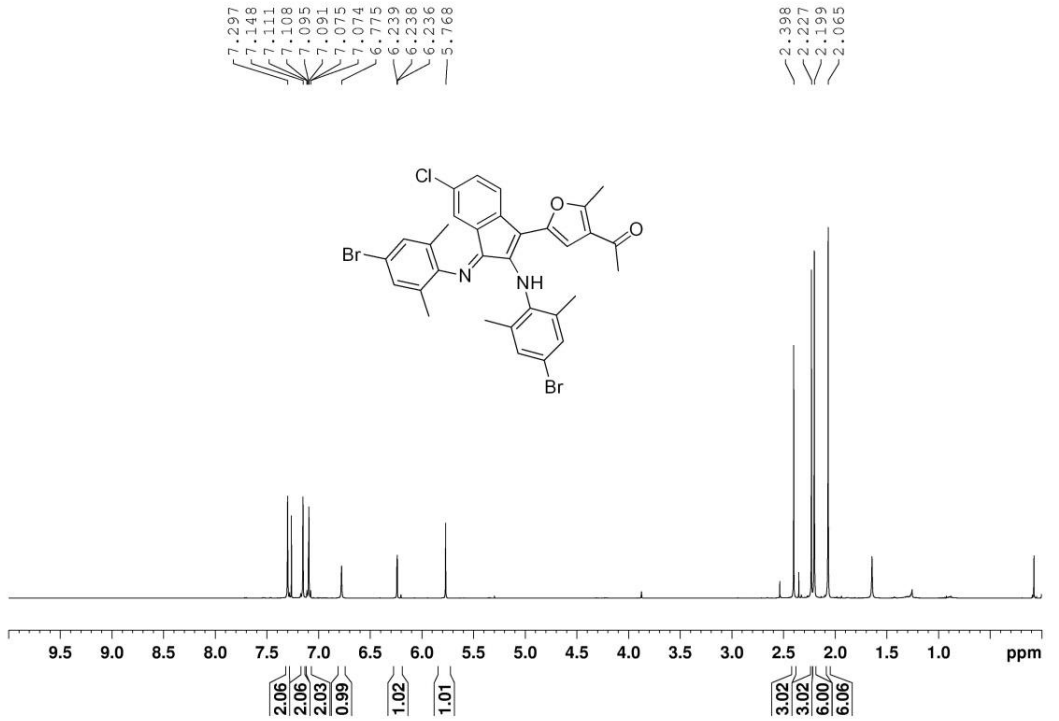

194.17
162.72
157.22
147.01
146.81
145.14
137.34
136.77
136.71
132.92
131.05
130.67
127.58
125.91
124.54
124.08
122.22
119.36
119.00
116.69
109.43
105.09
29.05
18.49
18.00
14.19
Br
N
NH
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

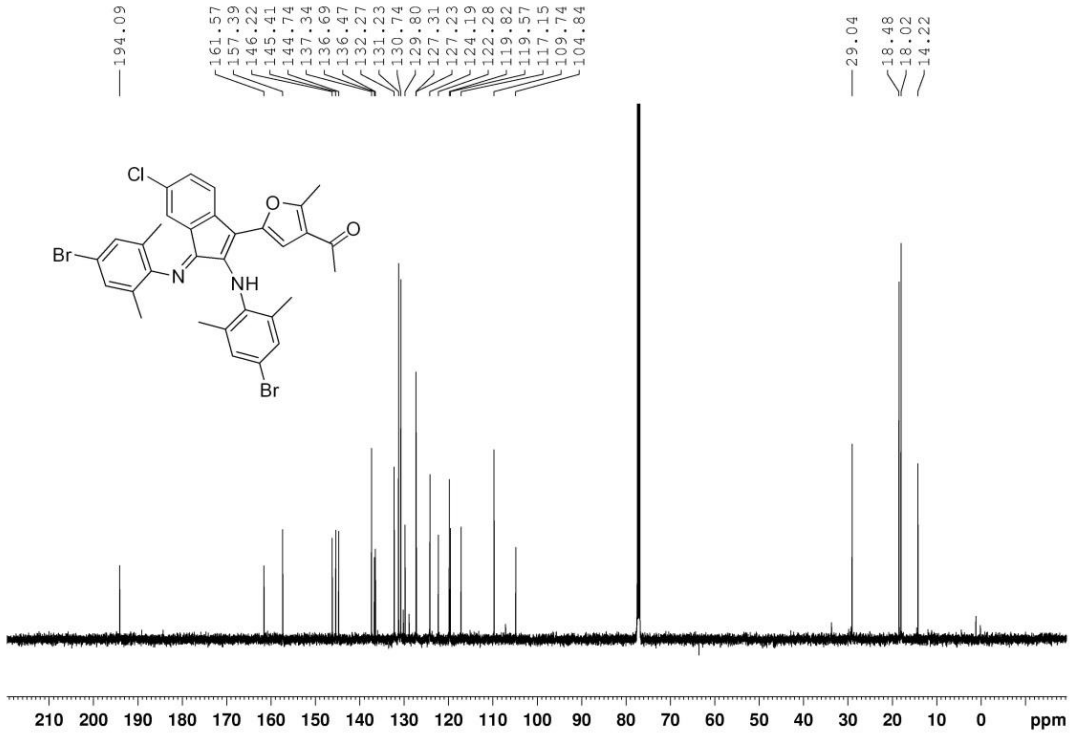
Compound **4b**


7.281
7.139
7.070
7.055
6.946
6.945
6.943
6.931
6.929
6.928
6.714
6.123
5.804
2.387
2.234
2.202
2.070
2.035
Br
N
NH
O
O
Br
9.5 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 ppm
2.05
2.05
1.07
1.07
1.02
1.01
1.01
3.09
3.02
6.00
6.05
3.06

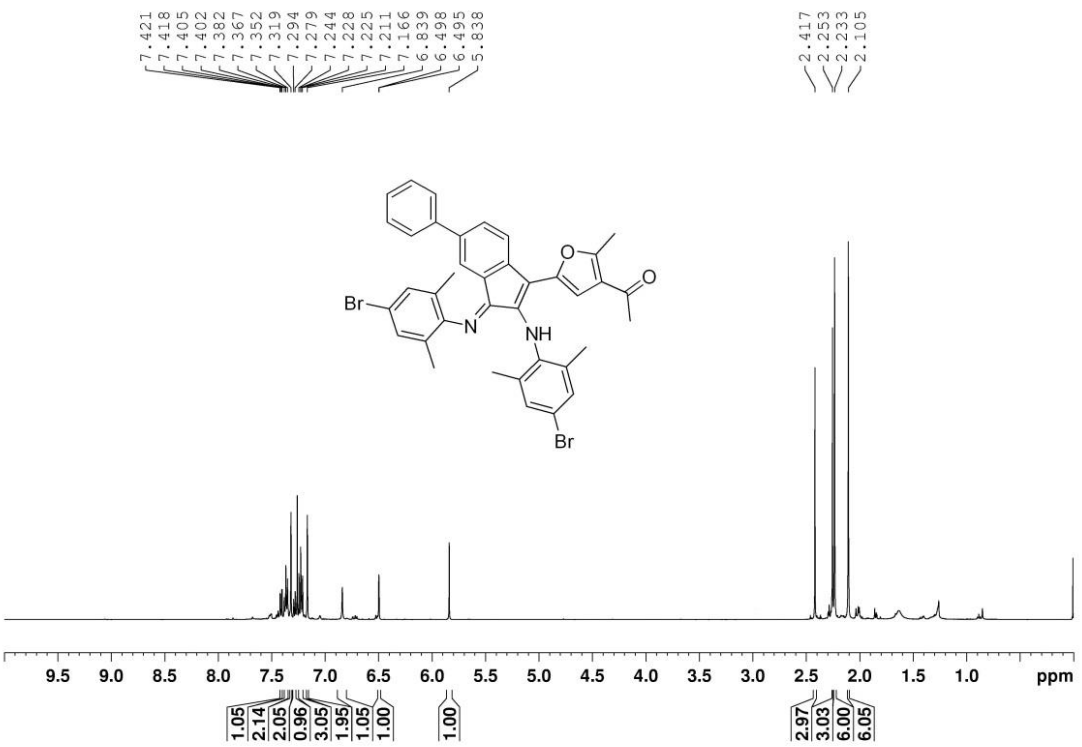

194.24
162.85
157.19
146.85
145.38
144.04
137.26
136.97
136.08
134.16
132.96
131.00
130.67
127.60
126.31
125.12
122.26
119.15
118.90
116.59
109.34
105.46
29.06
21.26
18.53
18.04
14.21
Br
N
NH
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

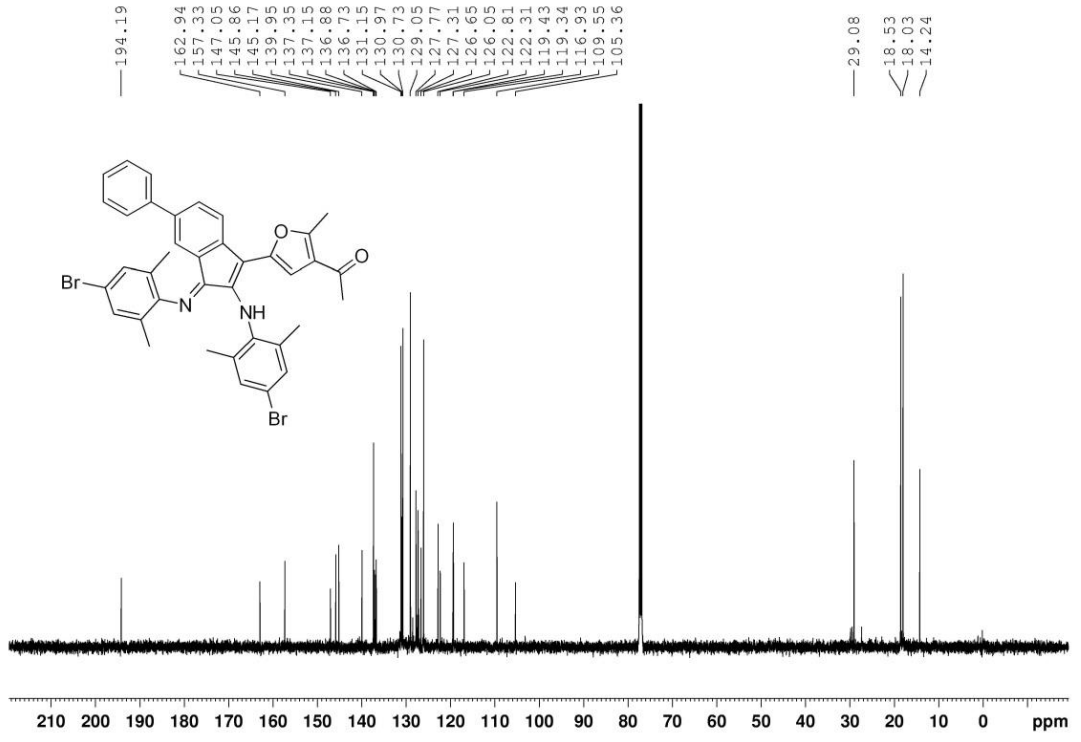
Compound **4c**


7.297
7.148
7.111
7.108
7.095
7.091
7.075
7.074
6.775
6.239
6.238
6.236
5.768
2.398
2.227
2.199
2.065
Cl
O
O
Br
N
NH
Br
9.5 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 ppm
2.06
2.06
2.03
0.99
1.02
1.01
3.02
3.02
6.00
6.06

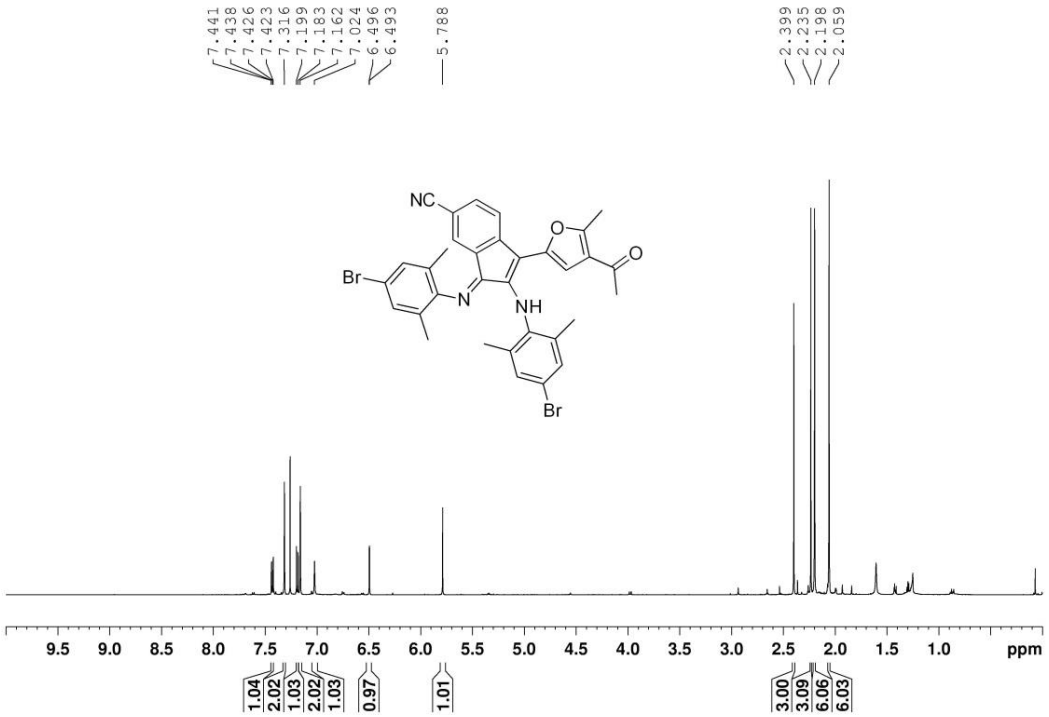

194.09
161.57
157.39
146.22
145.41
144.74
137.34
136.69
136.47
132.27
131.23
130.74
129.80
127.31
127.23
124.19
122.28
119.82
119.57
117.15
109.74
104.84
29.04
18.48
18.02
14.22
Cl
O
O
Br
N
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

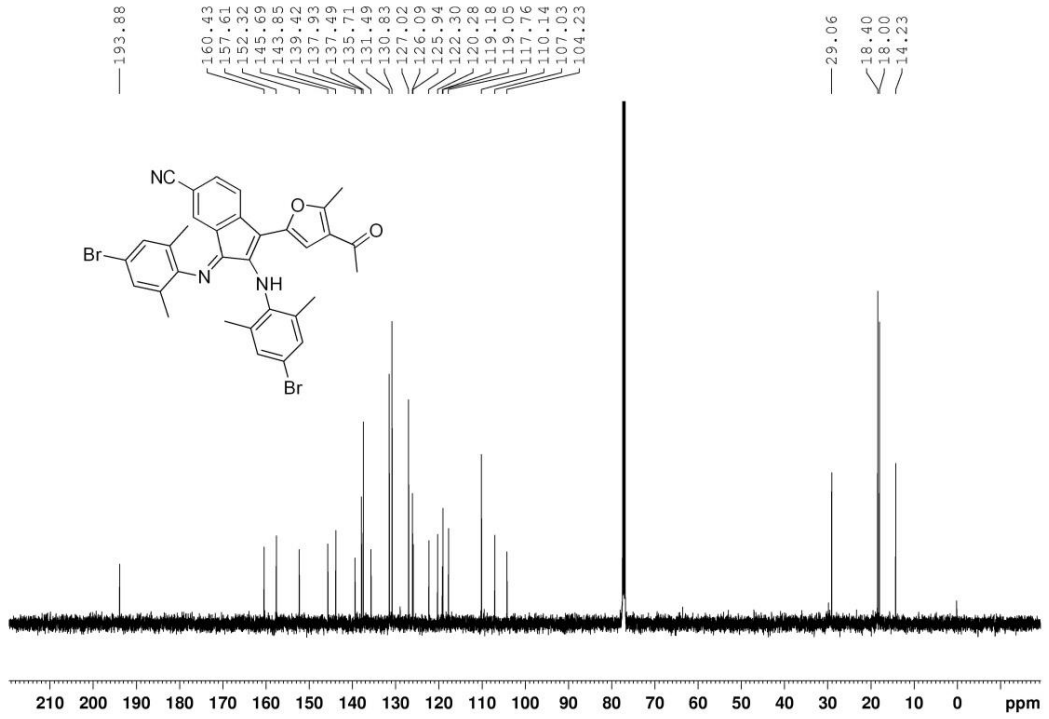
Compound **4d**


7.421
7.418
7.405
7.402
7.382
7.367
7.352
7.319
7.294
7.279
7.244
7.228
7.225
7.211
7.166
6.839
6.498
6.495
5.838
2.417
2.253
2.233
2.105
Br
N
NH
O
O
Br
9.5 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 ppm
1.05
2.14
2.05
0.96
3.05
1.95
1.05
1.00
1.00
2.97
3.03
6.00
6.05

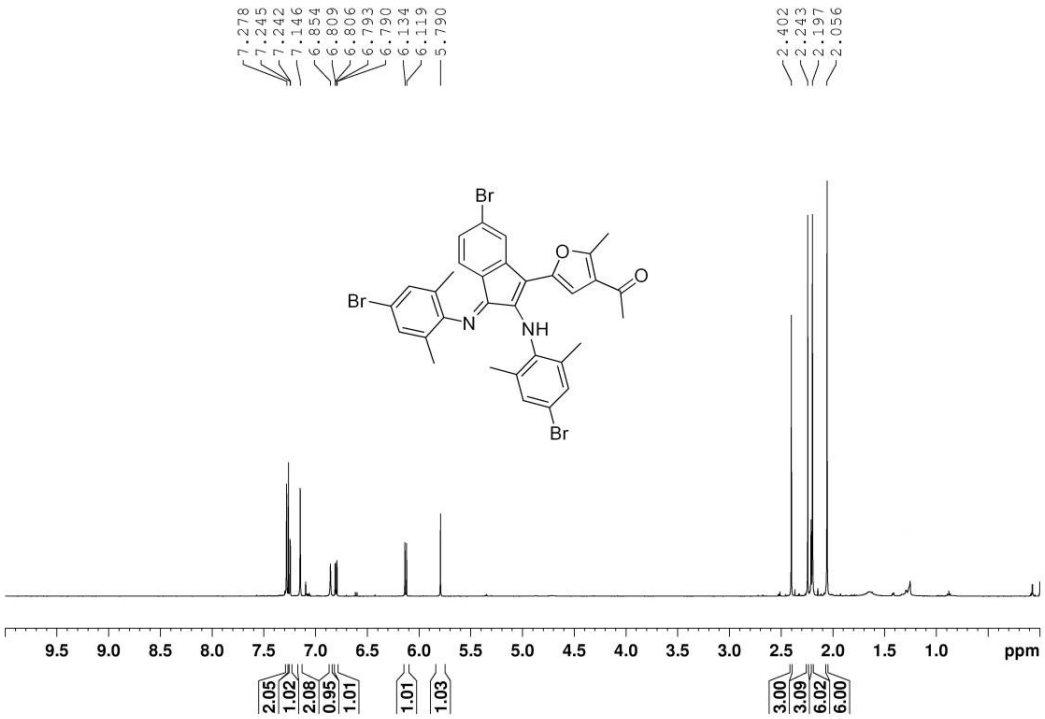

194.19
162.94
157.33
147.05
145.86
145.17
139.95
137.35
137.15
136.88
136.73
131.15
130.97
130.73
129.05
127.77
127.31
126.65
126.05
122.81
122.31
119.43
119.34
116.93
109.55
105.36
29.08
18.53
18.03
14.24
Br
N
NH
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

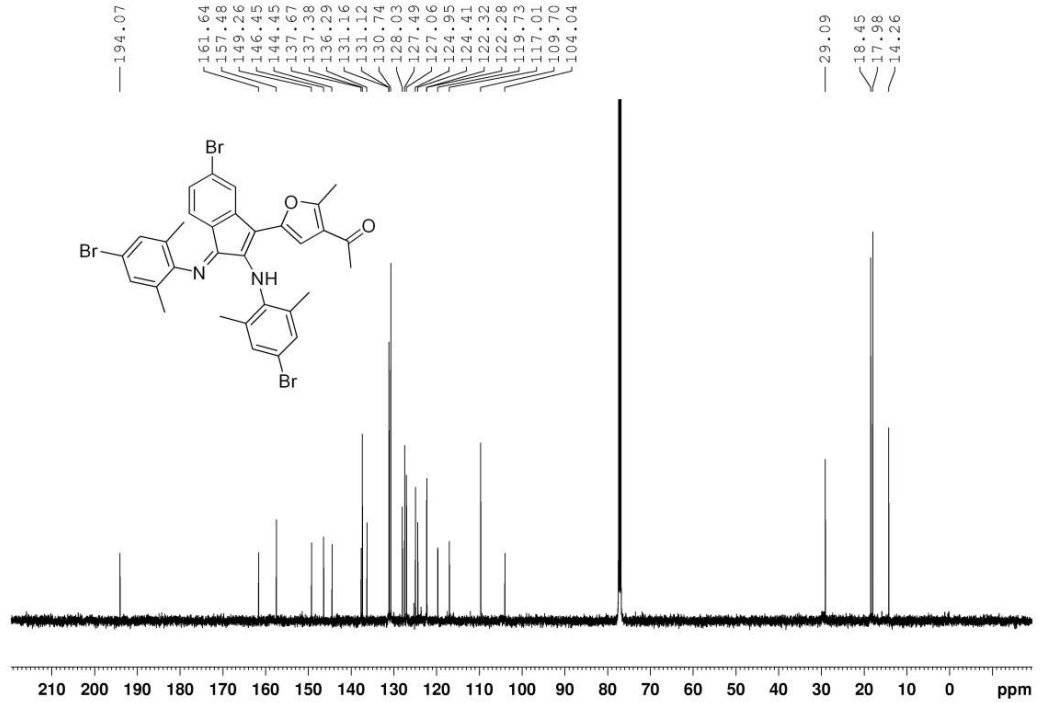
Compound **4e**


7.441
7.438
7.426
7.423
7.316
7.199
7.183
7.162
7.024
6.496
6.493
5.788
2.399
2.235
2.198
2.059
NC
O
Br
N
NH
Br
9.5 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 ppm
1.04 2.02 1.03 2.02 1.03 0.97 1.01 3.00 3.09 6.06 6.03

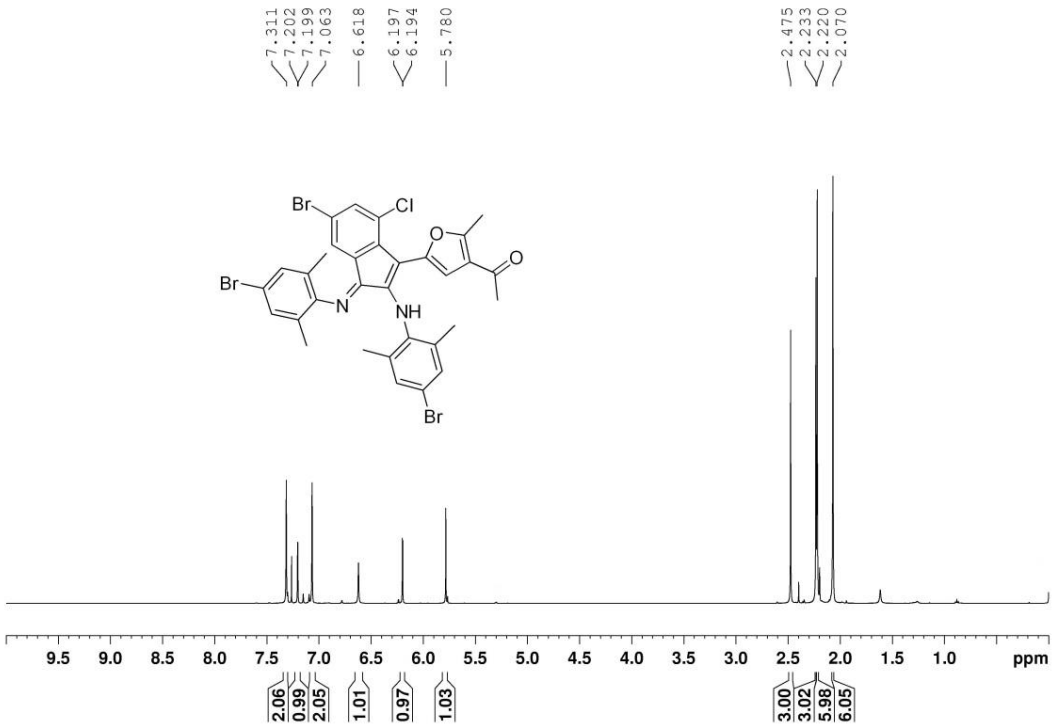

193.88
160.43
157.61
152.32
145.69
143.85
139.42
137.93
137.49
135.71
131.49
130.83
127.02
126.09
125.94
122.30
120.28
119.18
119.05
117.76
110.14
107.03
104.23
29.06
18.40
18.00
14.23
NC
O
Br
N
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

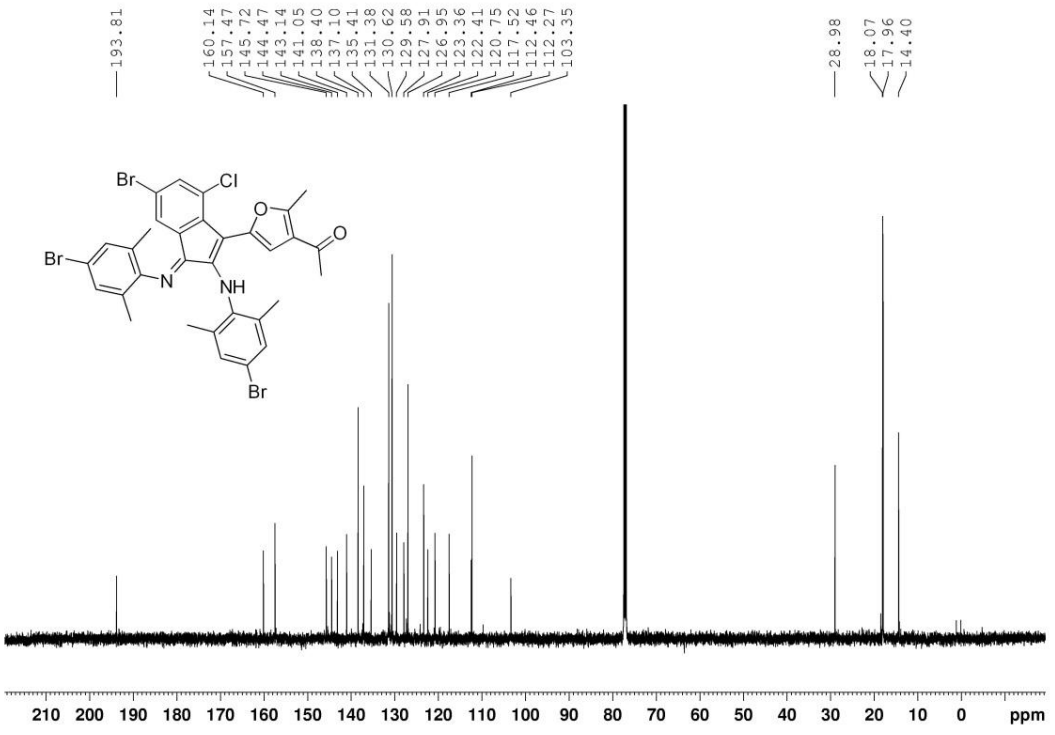
Compound **4f**


7.278
7.245
7.242
7.146
6.854
6.809
6.806
6.793
6.790
6.134
6.119
5.790
2.402
2.243
2.197
2.056
Br
Br
N
NH
O
O
Br
9.5 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 ppm
2.05
1.02
2.08
0.95
1.01
1.01
1.03
3.00
3.09
6.02
6.00

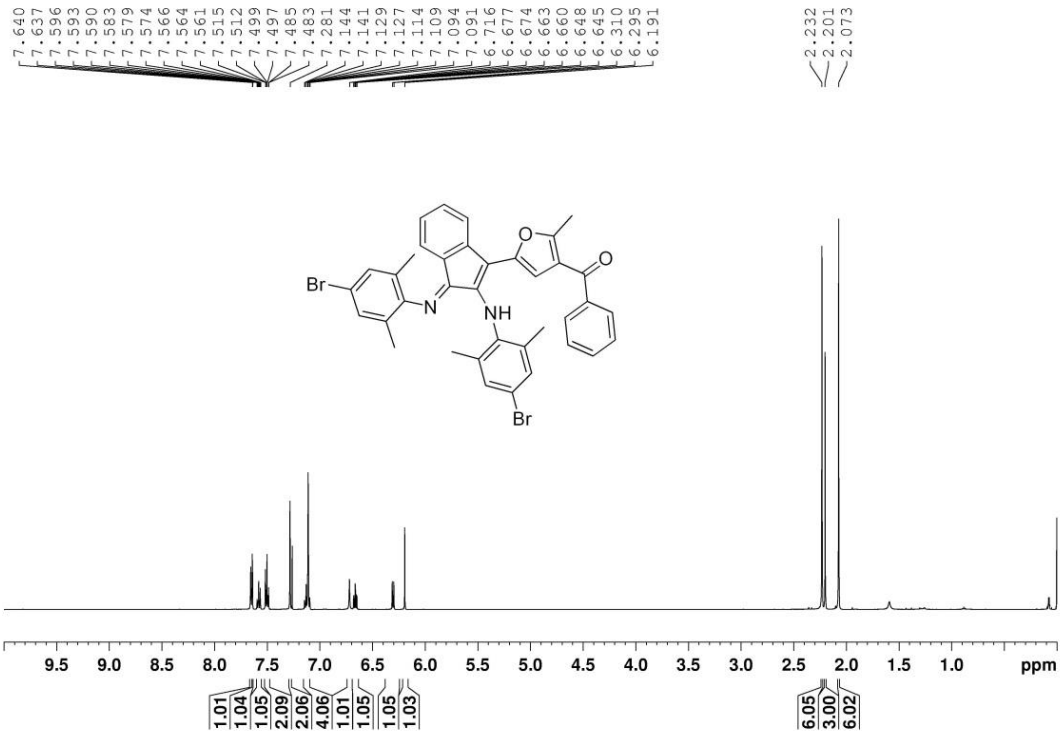

194.07
161.64
157.48
149.26
146.45
144.45
137.67
137.38
136.29
131.16
131.12
130.74
128.03
127.49
127.06
124.95
124.41
122.32
122.28
119.73
117.01
109.70
104.04
29.09
18.45
17.98
14.26
Br
Br
N
NH
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

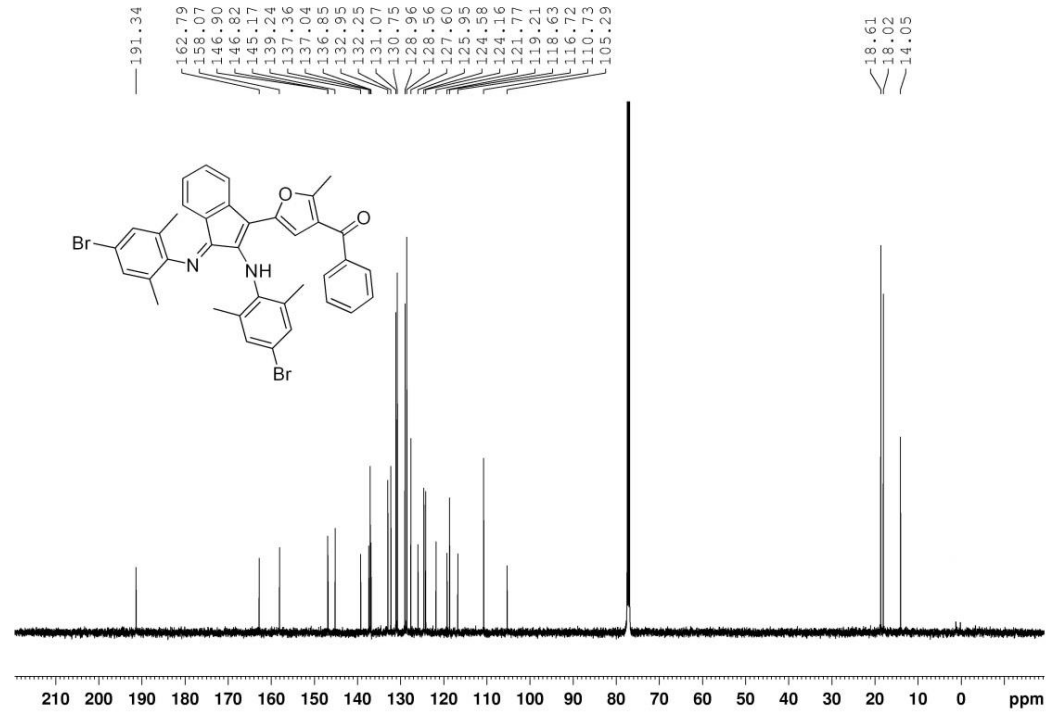
Compound **4g**


7.311
7.202
7.199
7.063
6.618
6.197
6.194
5.780
2.475
2.233
2.220
2.070
Br
Cl
O
Br
N
NH
O
Br
9.5 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 ppm
2.06
0.99
2.05
1.01
0.97
1.03
3.00
3.02
5.98
6.05

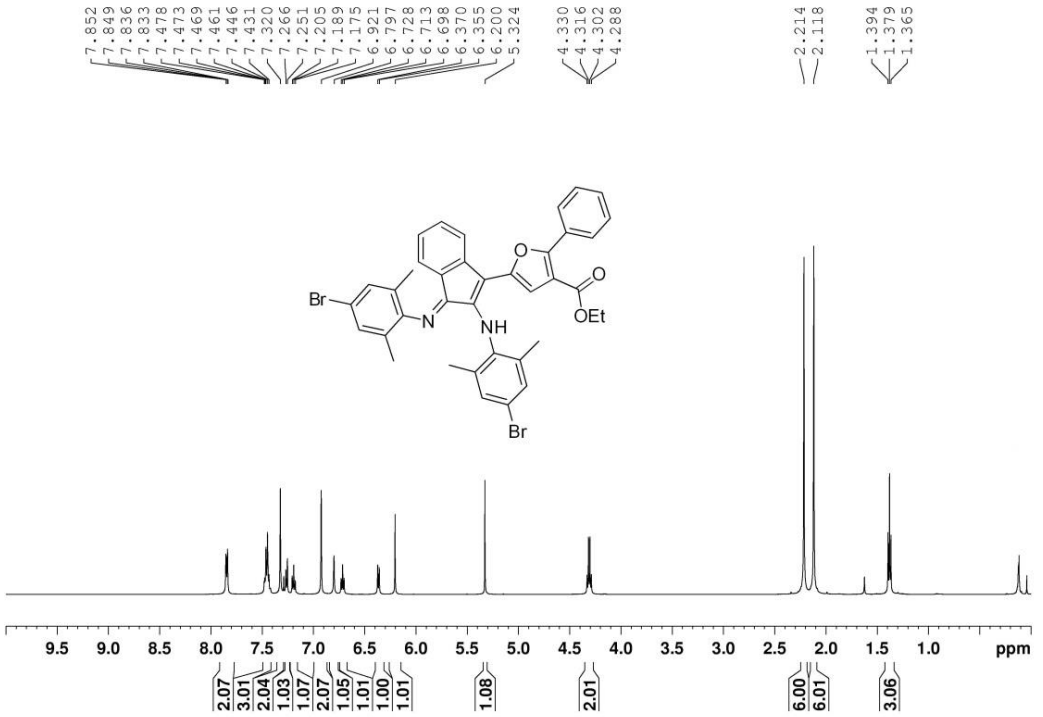

193.81
160.14
157.47
145.72
144.47
143.14
141.05
138.40
137.10
135.41
131.38
130.62
129.58
127.91
126.95
123.36
122.41
120.75
117.52
112.46
112.27
103.35
28.98
18.07
17.96
14.40
Br
Cl
O
Br
N
NH
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

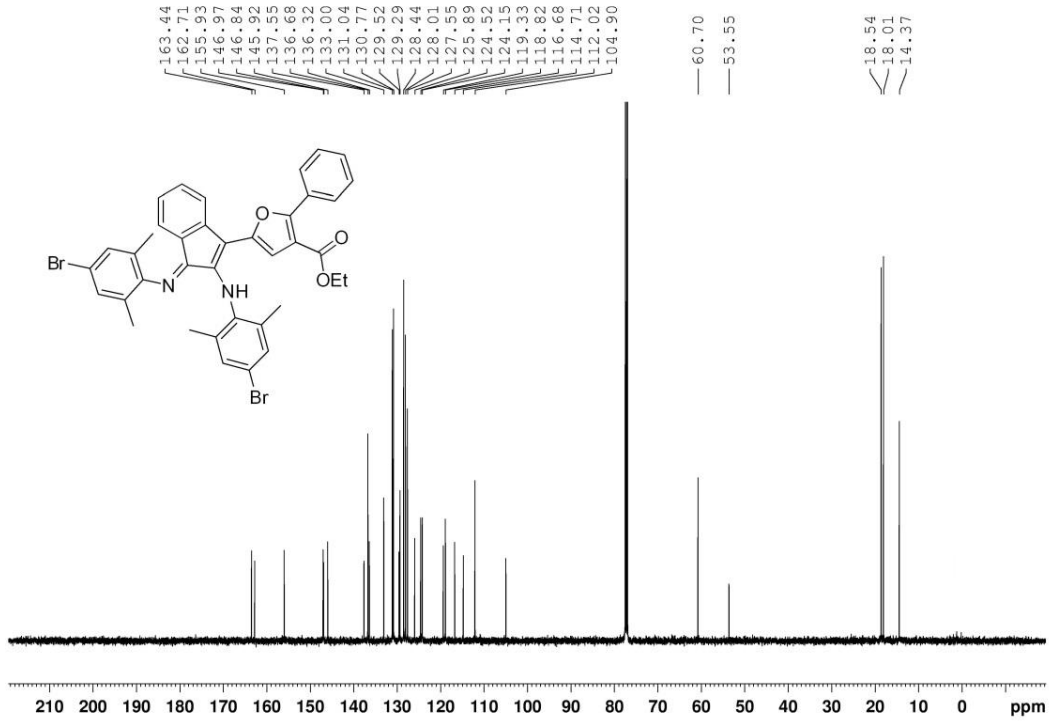
Compound **4h**


7.640
7.637
7.596
7.593
7.590
7.583
7.579
7.574
7.566
7.564
7.561
7.515
7.512
7.499
7.497
7.485
7.483
7.281
7.144
7.141
7.129
7.127
7.114
7.109
7.094
7.091
6.716
6.677
6.674
6.663
6.660
6.648
6.645
6.310
6.295
6.191
2.232
2.201
2.073
Br
N
NH
O
O
Br
9.5 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 ppm
1.01 1.04 1.05 2.09 2.06 4.06 1.01 1.05 1.05 1.03
6.05 3.00 6.02

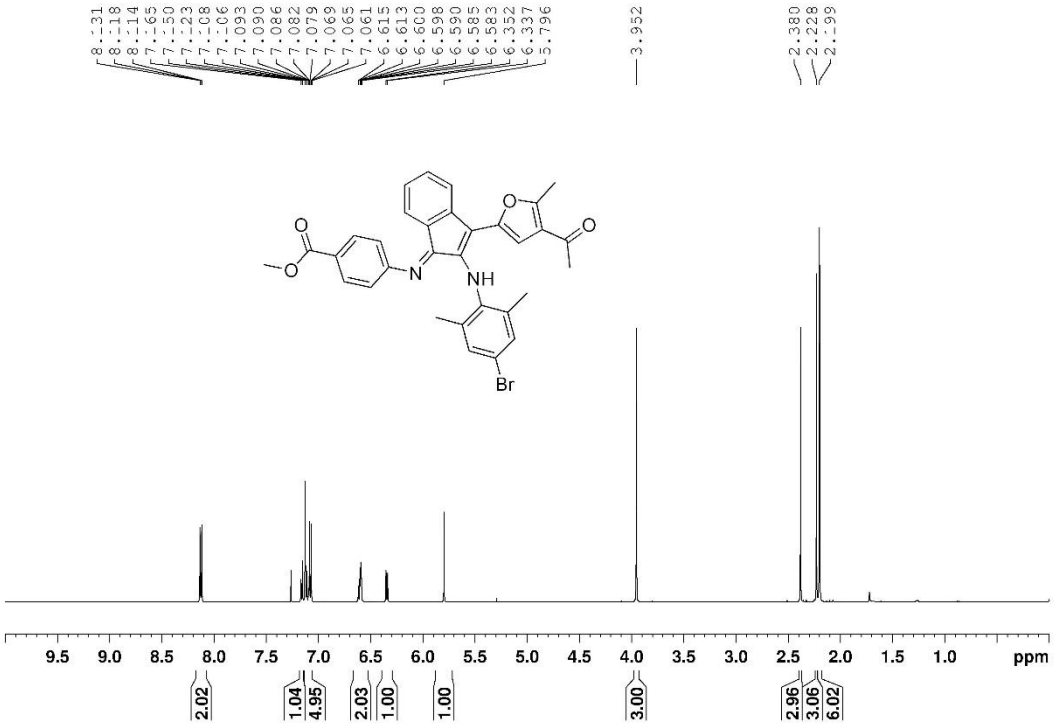

191.34
162.79
158.07
146.90
146.82
145.17
139.24
137.36
137.04
136.85
132.95
132.25
131.07
130.75
128.96
128.56
127.60
125.95
124.58
124.16
121.77
119.21
118.63
116.72
110.73
105.29
18.61
18.02
14.05
Br
N
NH
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

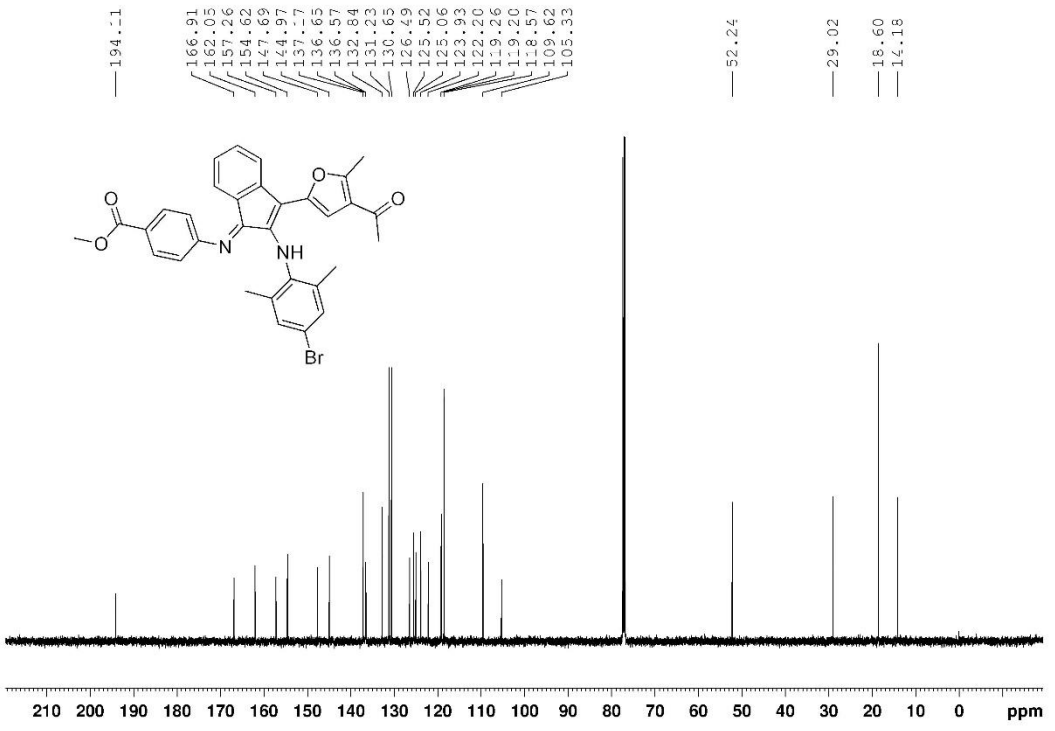
Compound **4i**


7.852
7.849
7.836
7.833
7.478
7.473
7.469
7.461
7.446
7.431
7.320
7.266
7.251
7.205
7.189
7.175
6.921
6.797
6.728
6.713
6.698
6.370
6.355
6.200
5.324
4.330
4.316
4.302
4.288
2.214
2.118
1.394
1.379
1.365
Br
N
NH
O
O
OEt
Br
9.5 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 ppm
2.07 3.01 2.04 1.03 1.07 2.07 1.05 1.01 1.00 1.01 1.08 2.01 6.00 6.01 3.06

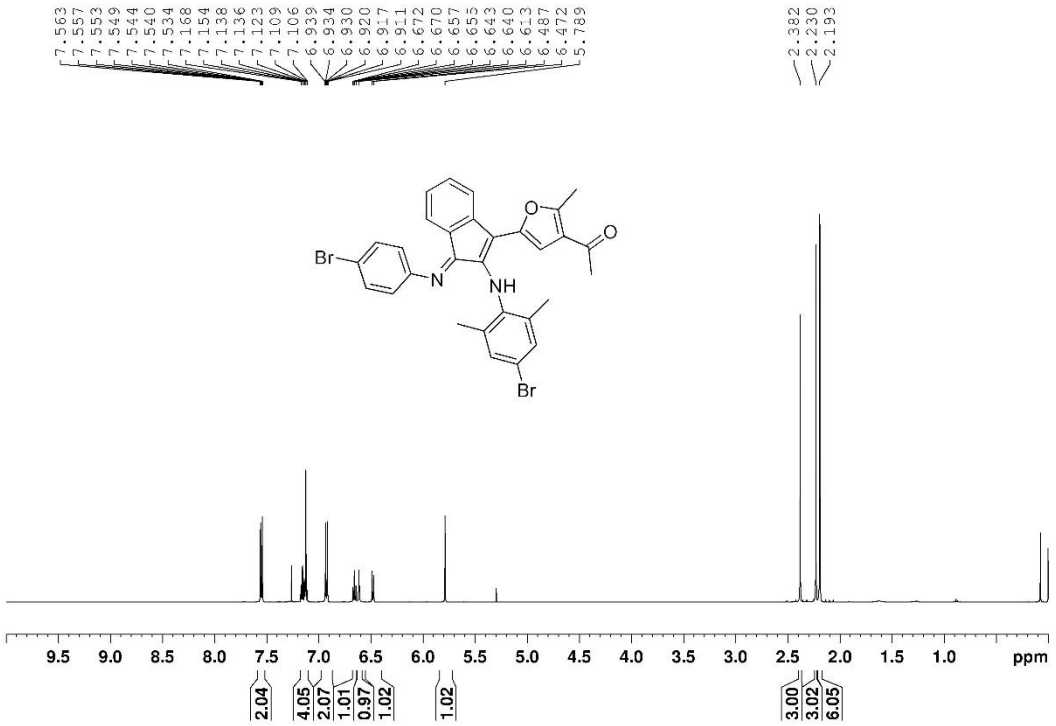

163.44
162.71
155.93
146.97
146.84
145.92
137.55
136.68
136.32
133.00
131.04
130.77
129.52
129.29
128.44
128.01
127.55
125.89
124.52
124.15
119.33
118.82
116.68
114.71
112.02
104.90
60.70
53.55
18.54
18.01
14.37
Br
N
NH
O
O
OEt
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

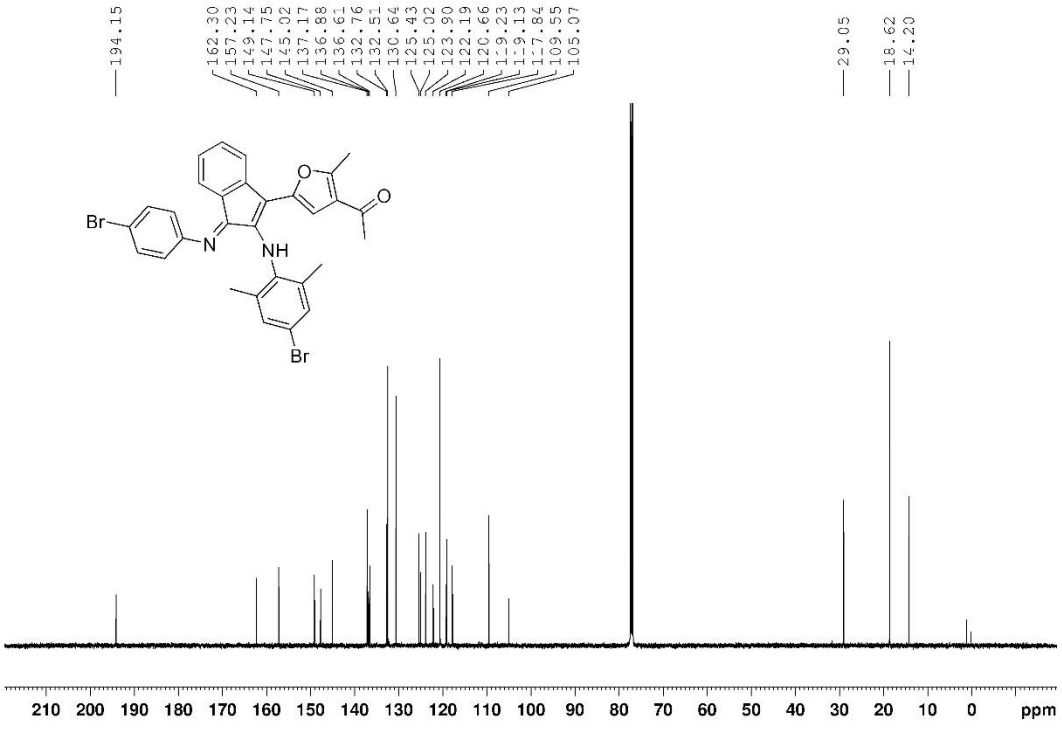
Compound **4j**


8.31
8.18
8.14
7.65
7.50
7.23
7.08
7.06
7.03
7.00
7.086
7.082
7.079
7.069
7.065
7.061
6.615
6.613
6.600
6.598
6.590
6.585
6.583
6.352
6.337
5.796
3.952
2.380
2.228
2.99
O
O
O
N
NH
Br
9.5 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 ppm
2.02
1.04
4.95
2.03
1.00
1.00
3.00
2.96
3.06
6.02

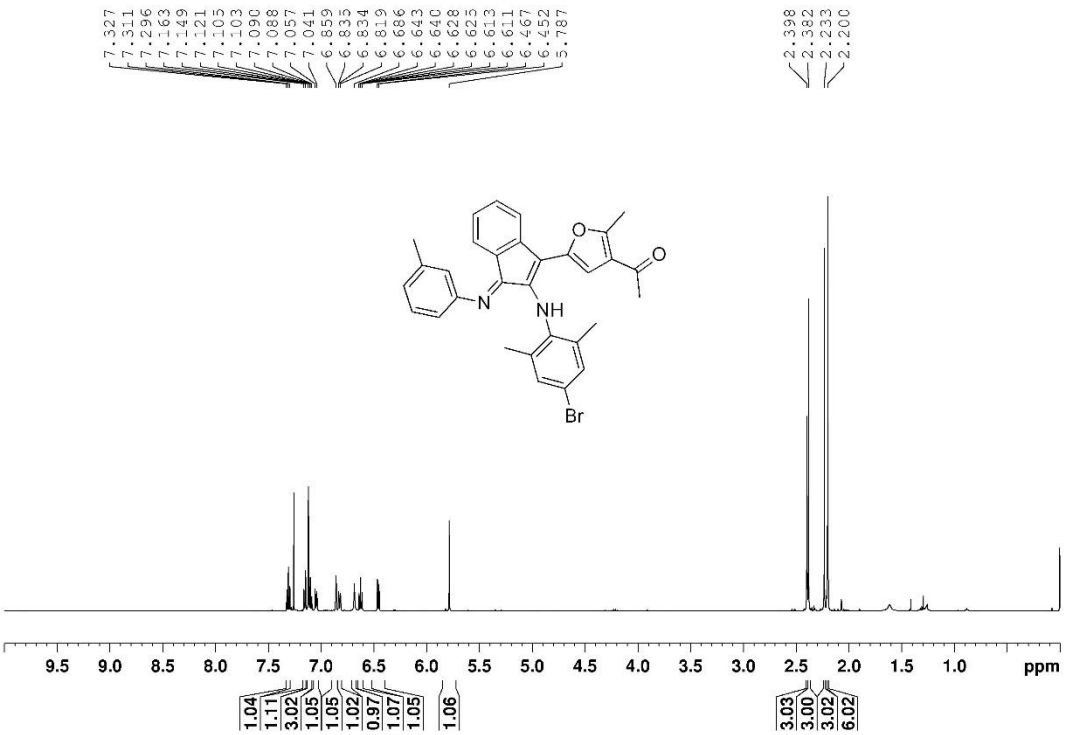

194.11
166.91
162.05
157.26
154.62
147.69
144.97
137.17
136.65
136.57
132.84
131.23
130.65
126.49
125.52
125.06
123.93
122.20
119.26
118.57
109.62
105.33
52.24
29.02
18.60
14.18
O
O
O
N
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

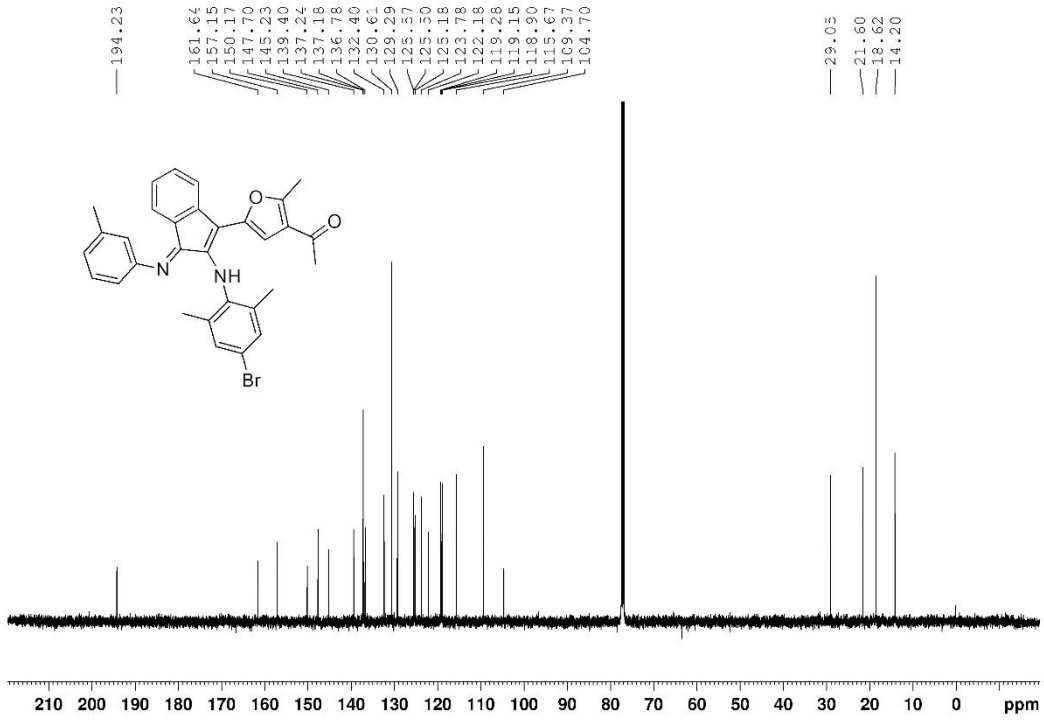
Compound **4k**


7.563
7.557
7.553
7.549
7.544
7.540
7.534
7.168
7.154
7.138
7.136
7.123
7.109
7.106
6.939
6.934
6.930
6.920
6.917
6.911
6.672
6.670
6.657
6.655
6.643
6.640
6.613
6.487
6.472
5.789
2.382
2.230
2.193
Br
N
NH
O
Br
9.5 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 ppm
2.04
4.05
2.07
1.01
0.97
1.02
1.02
3.00
3.02
6.05

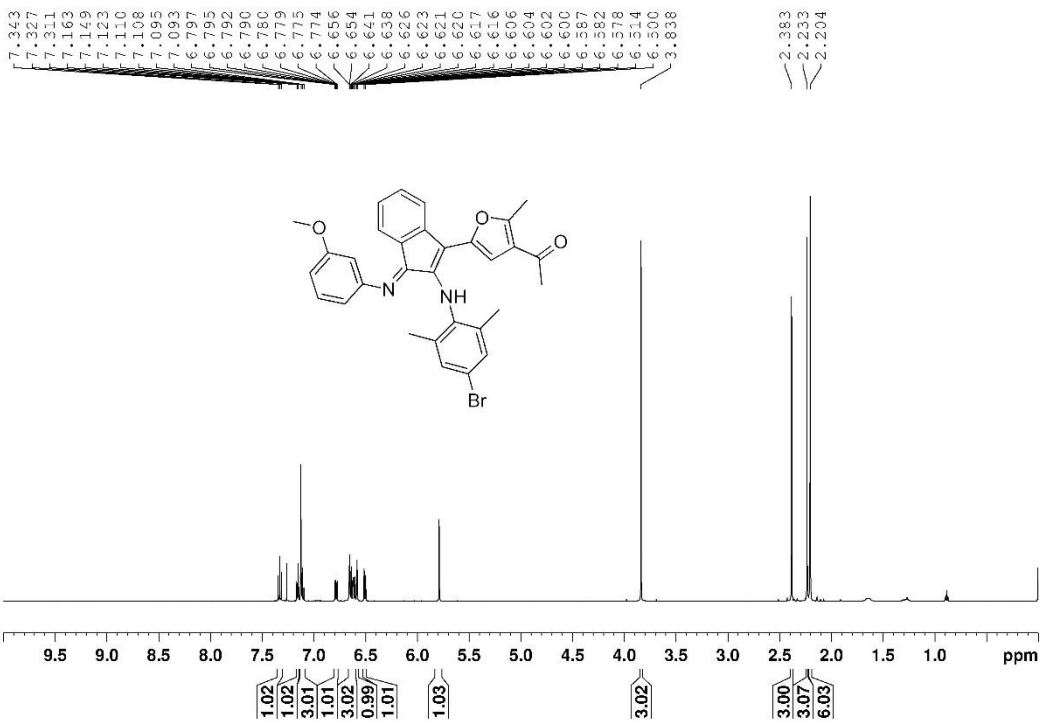

194.15
162.30
157.23
149.14
147.75
145.02
137.17
136.88
136.61
132.76
132.51
130.64
125.43
125.02
123.90
122.19
120.66
29.05
18.62
14.20
Br
N
NH
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

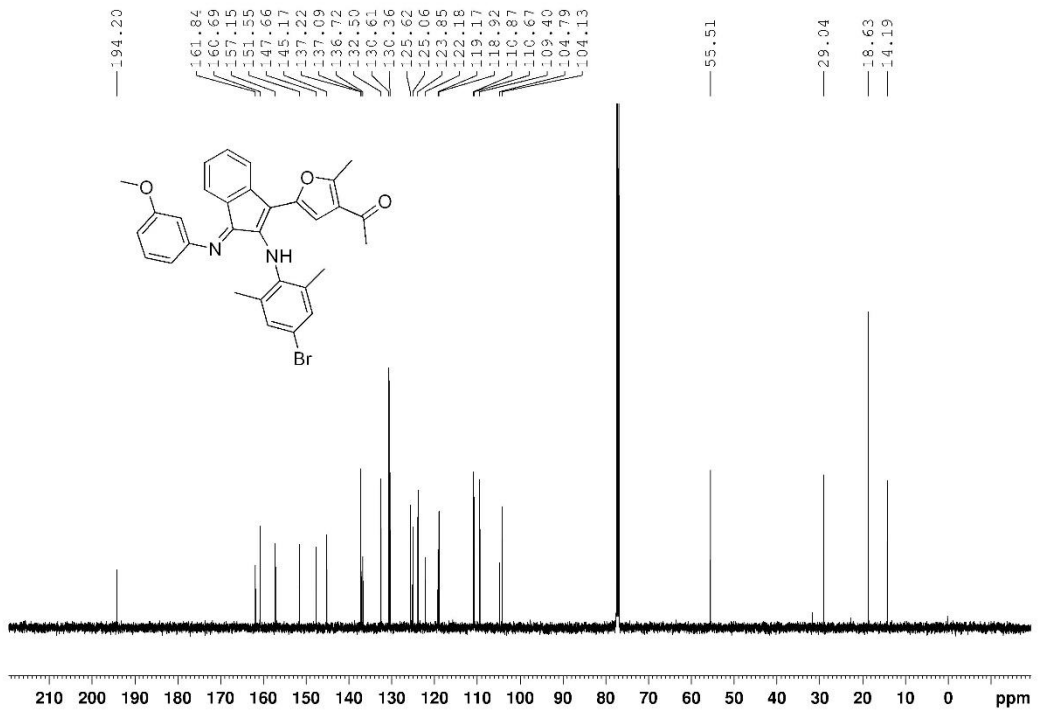
Compound **4l**


7.327
7.311
7.296
7.163
7.149
7.121
7.103
7.090
7.088
7.057
7.041
6.859
6.835
6.834
6.819
6.686
6.643
6.640
6.628
6.623
6.613
6.611
6.467
6.452
5.787
2.398
2.382
2.233
2.200
O
N
NH
Br
9.5 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 ppm
1.04
1.11
3.02
1.05
1.05
1.02
0.97
1.07
1.05
1.06
3.03
3.00
3.02
6.02

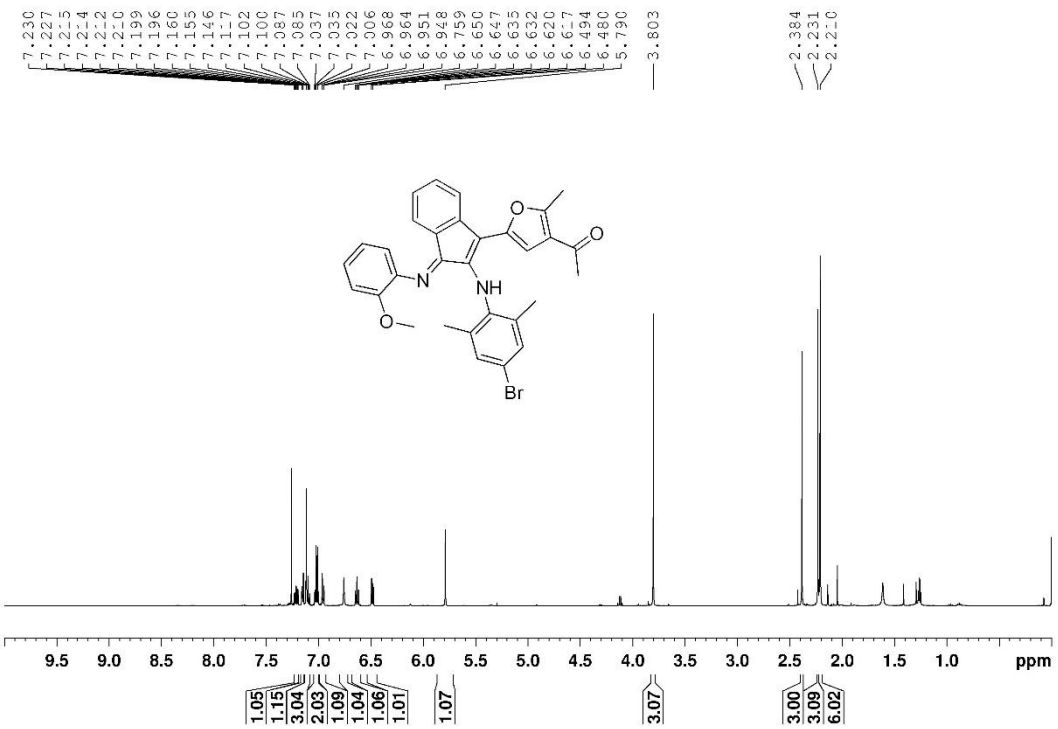

194.23
161.64
157.15
150.17
147.70
145.23
139.40
137.24
137.18
136.78
132.40
130.61
129.29
125.57
125.30
125.18
123.78
122.18
119.28
119.15
118.90
115.67
109.37
104.70
29.05
21.60
18.62
14.20
O
N
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

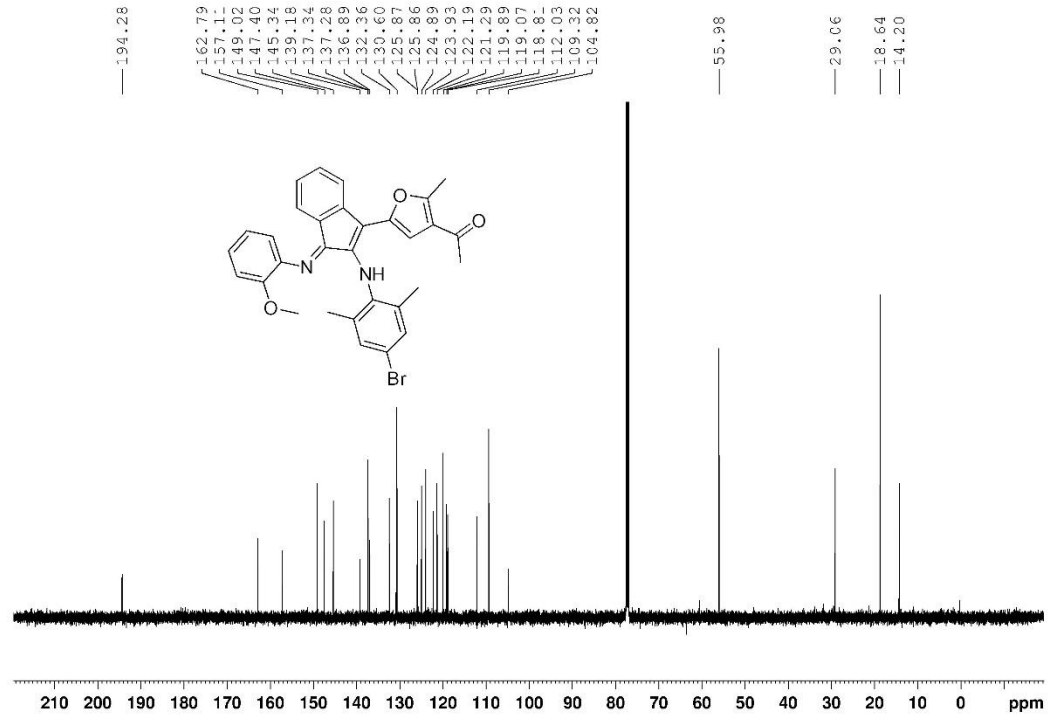
Compound **4m**


7.343
7.327
7.311
7.163
7.149
7.123
7.110
7.108
7.095
7.093
6.797
6.795
6.792
6.790
6.780
6.779
6.775
6.774
6.656
6.654
6.641
6.638
6.626
6.623
6.621
6.620
6.617
6.616
6.606
6.604
6.602
6.600
6.387
6.382
6.378
6.314
6.300
3.838
2.383
2.233
2.204
O
N
NH
Br
O
O
9.5 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 ppm
1.02
1.02
3.01
1.01
3.02
0.99
1.01
1.03
3.02
3.00
3.07
6.03

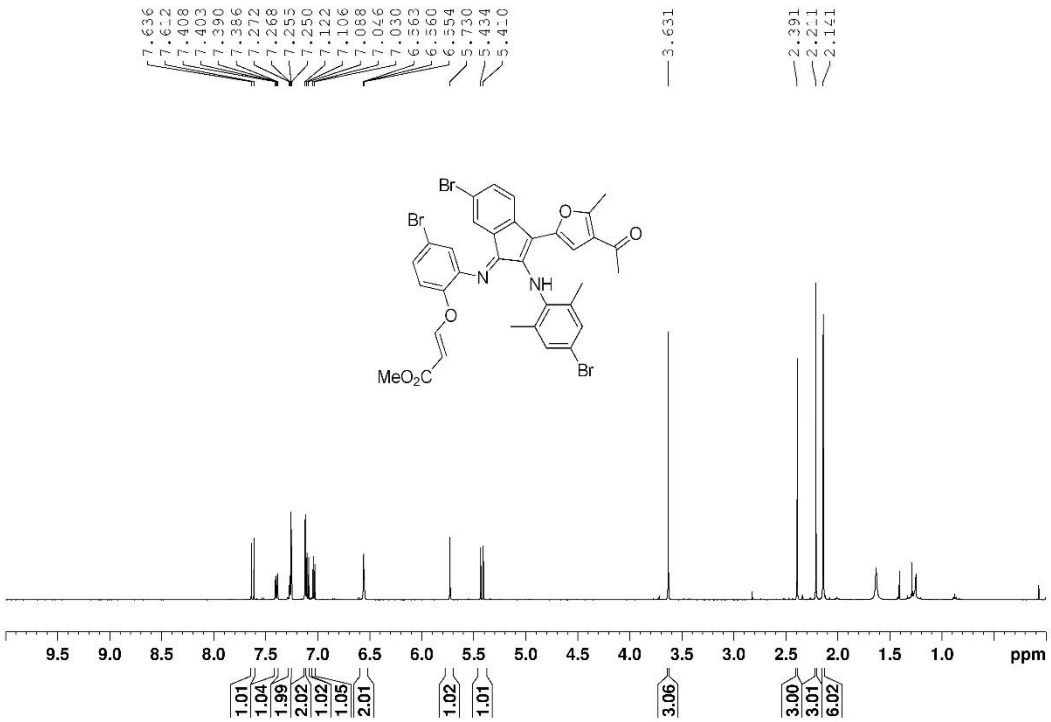

194.20
161.84
160.69
157.15
151.55
147.66
145.17
137.22
137.09
136.72
132.50
130.61
130.36
125.62
125.06
123.85
122.18
119.17
118.92
110.87
110.67
109.40
104.79
104.13
55.51
29.04
18.63
14.19
O
N
NH
Br
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

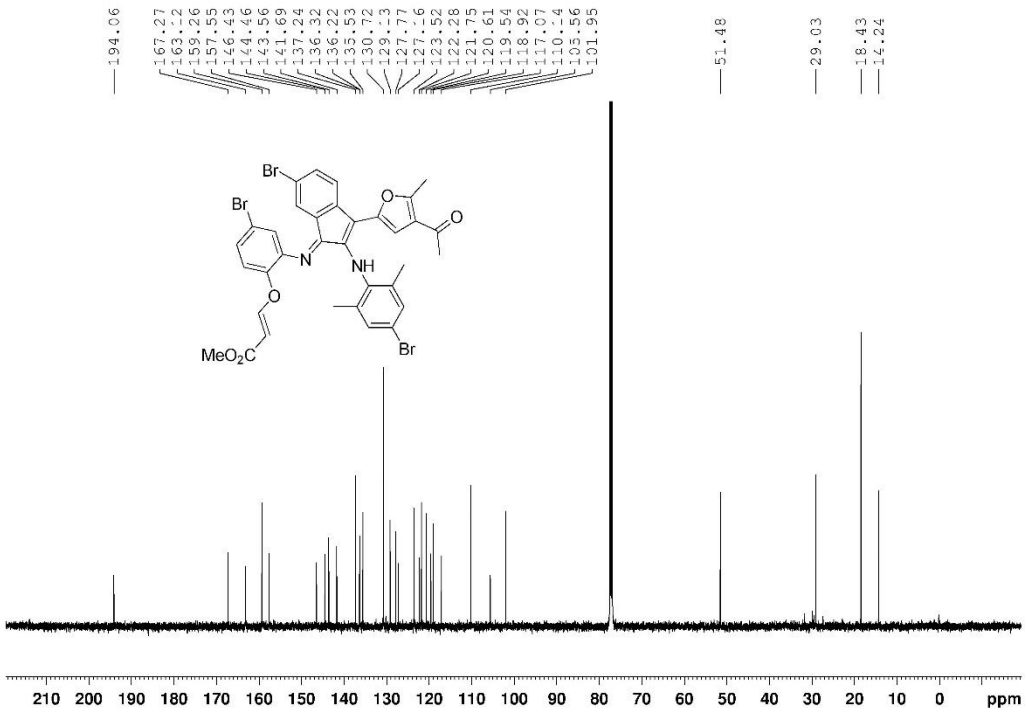
Compound **4n**


7.230
7.227
7.225
7.224
7.222
7.220
7.199
7.196
7.160
7.155
7.146
7.117
7.102
7.100
7.087
7.085
7.037
7.035
7.022
7.006
6.968
6.964
6.951
6.948
6.759
6.650
6.647
6.635
6.632
6.620
6.617
6.494
6.480
5.790
3.803
2.384
2.231
2.220
O
O
N
NH
O
Br
9.5 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 ppm
1.05
1.15
3.04
2.03
1.09
1.04
1.06
1.01
1.07
3.07
3.00
3.09
6.02

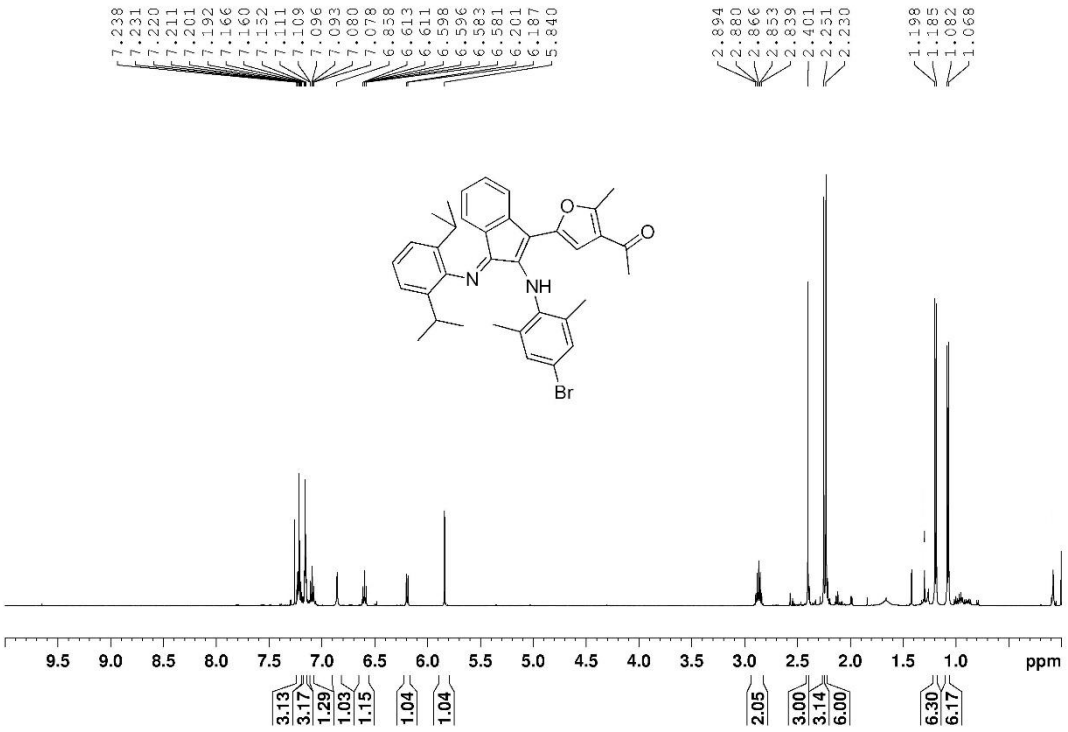

194.28
162.79
157.1-
149.02
147.40
145.34
139.18
137.34
137.28
136.89
132.36
130.60
125.87
125.86
124.89
123.93
122.19
121.29
119.89
119.07
118.8-
112.03
109.32
104.82
55.98
29.06
18.64
14.20
O
O
N
NH
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

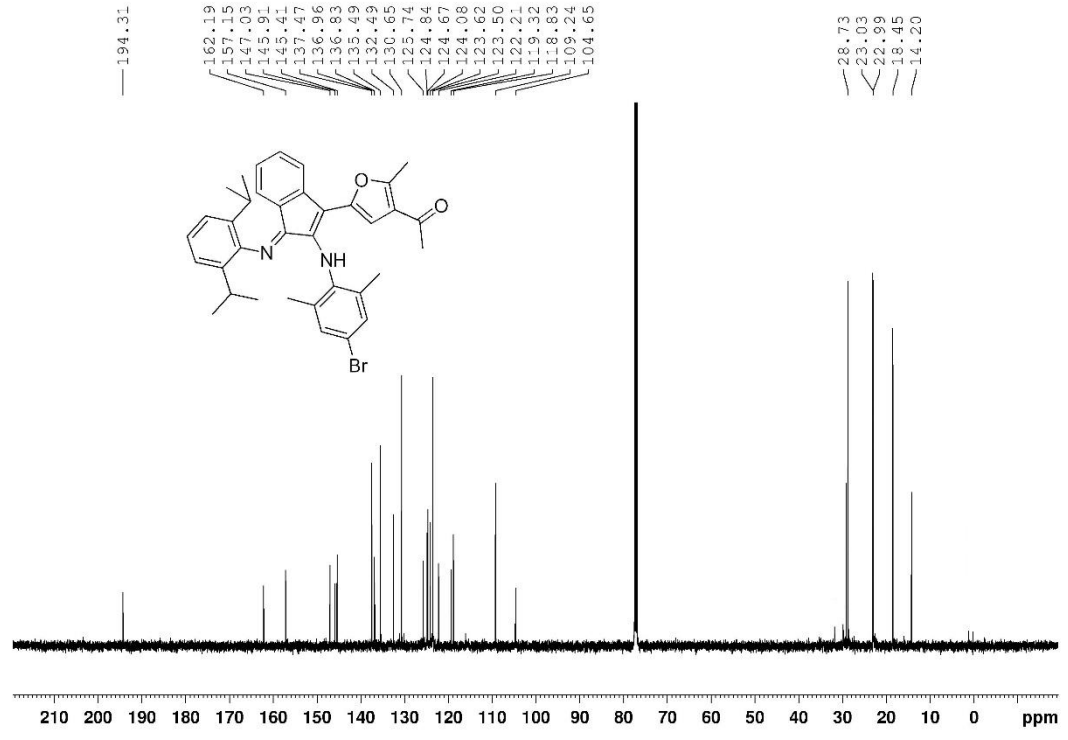
Compound **4o**


7.636
7.612
7.408
7.403
7.390
7.386
7.272
7.268
7.255
7.250
7.122
7.106
7.088
7.046
7.030
6.563
6.560
6.354
5.730
5.434
5.410
3.631
2.391
2.211
2.141
Br
Br
O
O
N
NH
O
MeO2C
Br
9.5 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 ppm
1.01
1.04
1.99
2.02
1.02
1.05
2.01
1.02
1.01
3.06
3.00
3.01
6.02

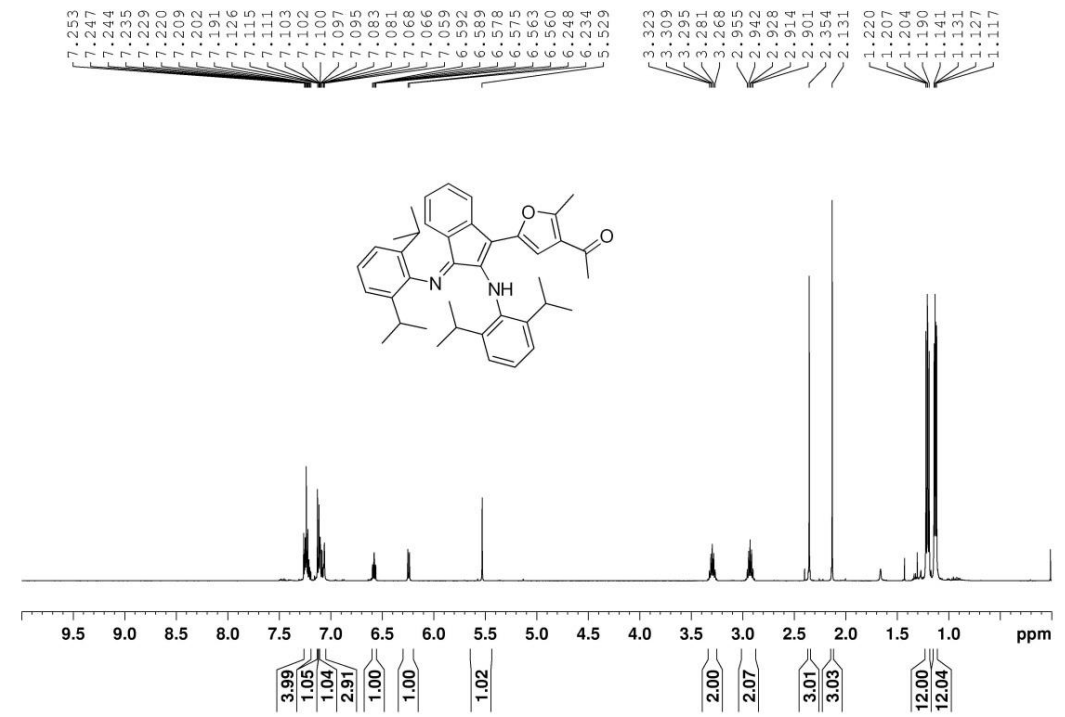

194.06
167.27
163.12
159.26
157.55
146.43
144.46
143.56
141.69
137.24
136.32
136.22
133.53
130.72
129.13
127.77
127.16
123.52
122.28
121.75
120.61
119.54
118.92
117.07
110.14
105.56
101.95
51.48
29.03
18.43
14.24
Br
Br
O
O
N
NH
O
MeO2C
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

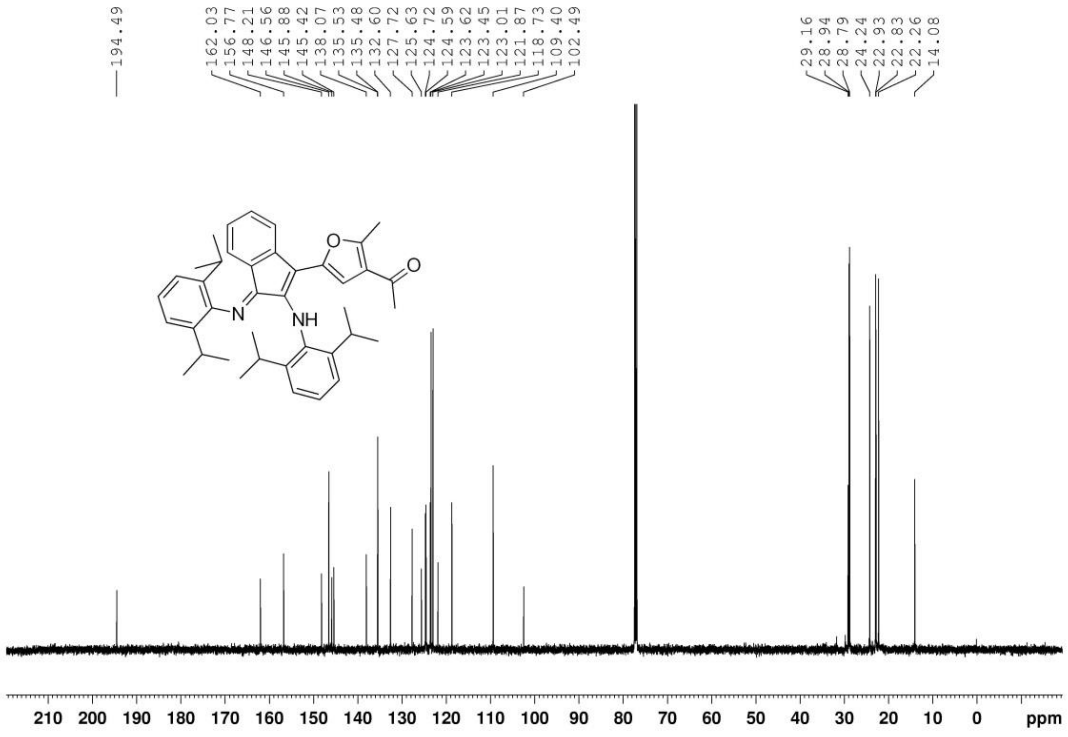
Compound **4p**


7.238
7.231
7.220
7.211
7.201
7.192
7.166
7.160
7.152
7.111
7.109
7.096
7.093
7.080
7.078
6.858
6.613
6.611
6.598
6.596
6.583
6.581
6.201
6.187
5.840
2.894
2.880
2.866
2.853
2.839
2.401
2.231
2.230
1.198
1.185
1.082
1.068
O
N
NH
Br
9.5 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 ppm
3.13
3.17
1.29
1.03
1.15
1.04
1.04
2.05
3.00
3.14
6.00
6.30
6.17

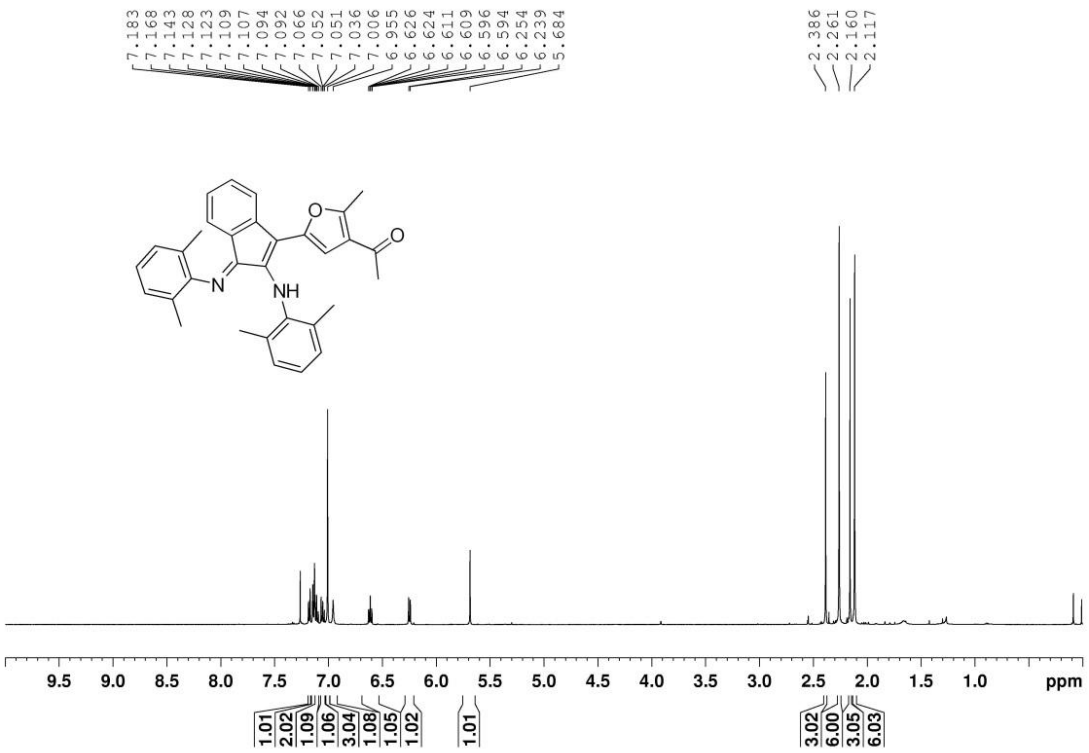

194.31
162.19
157.15
147.03
145.91
145.41
137.47
136.96
136.83
135.49
132.49
130.65
125.74
124.84
124.67
124.08
123.62
123.50
122.21
119.32
118.83
109.24
104.65
28.73
23.03
22.99
18.45
14.20
O
N
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

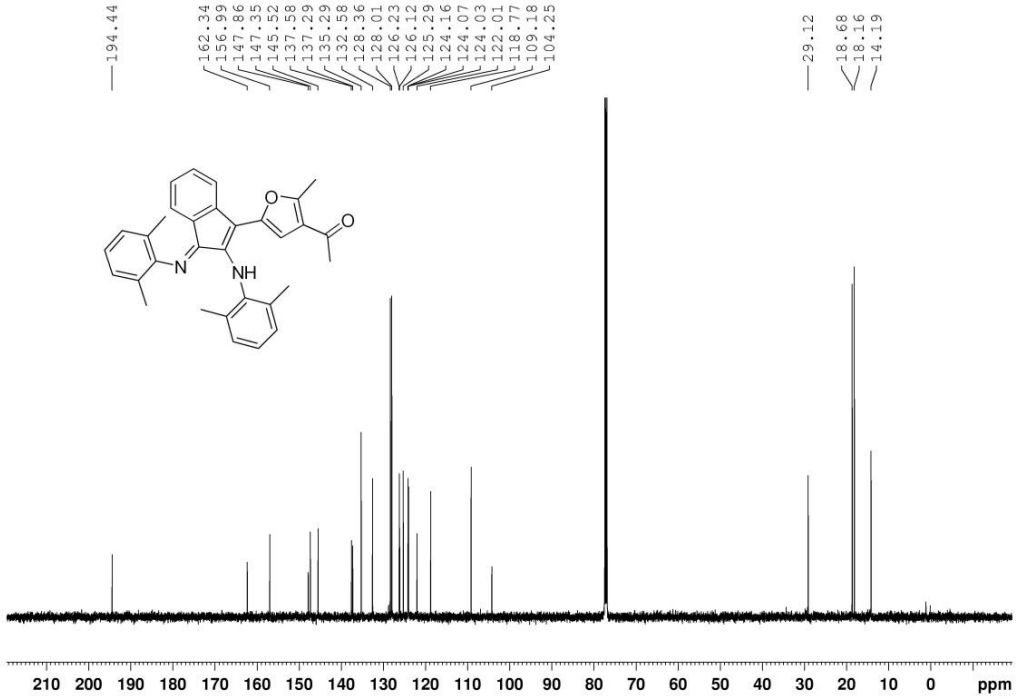
Compound **4q**


7.253
7.247
7.244
7.235
7.229
7.220
7.209
7.202
7.191
7.126
7.115
7.111
7.103
7.102
7.100
7.097
7.095
7.083
7.081
7.068
7.066
7.059
6.592
6.589
6.578
6.575
6.563
6.560
6.248
6.234
5.529
3.323
3.309
3.295
3.281
3.268
2.955
2.942
2.928
2.914
2.901
2.354
2.131
1.220
1.207
1.204
1.190
1.141
1.131
1.127
1.117
O
N
NH
O
9.5 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 ppm
3.99
1.05
1.04
2.91
1.00
1.00
1.02
2.00
2.07
3.01
3.03
12.00
12.04

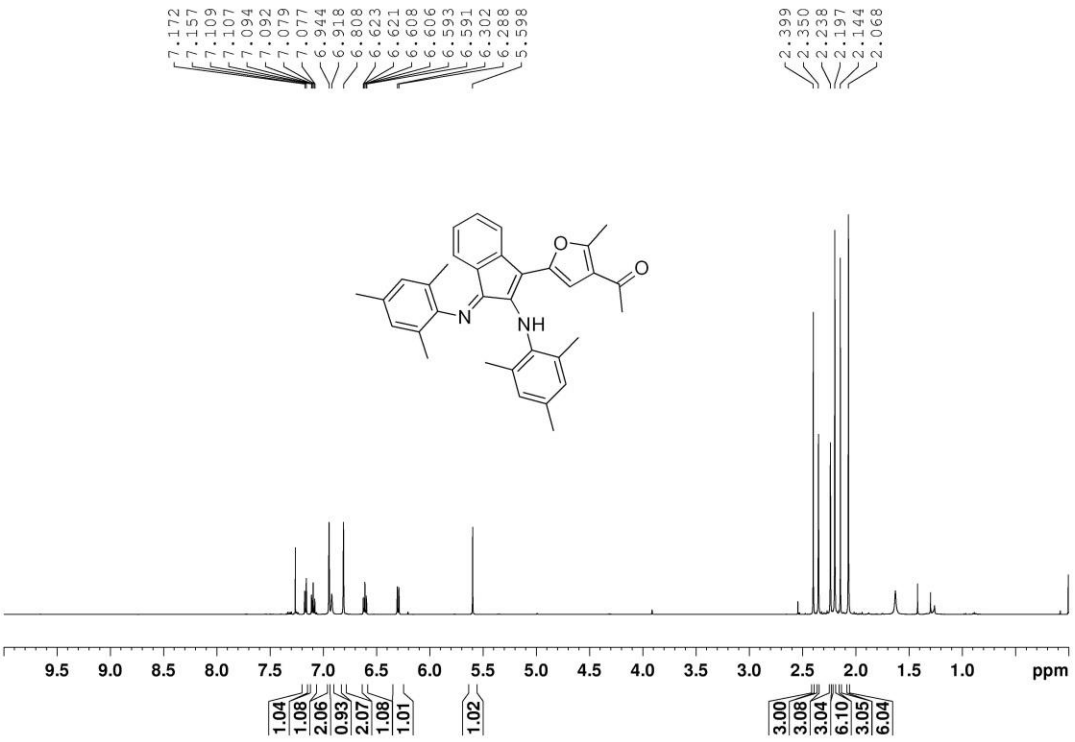

194.49
162.03
156.77
148.21
146.56
145.88
145.42
138.07
135.53
135.48
132.60
127.72
125.63
124.72
124.59
123.62
123.45
123.01
121.87
118.73
109.40
102.49
29.16
28.94
28.79
24.24
22.93
22.83
22.26
14.08
O
N
NH
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

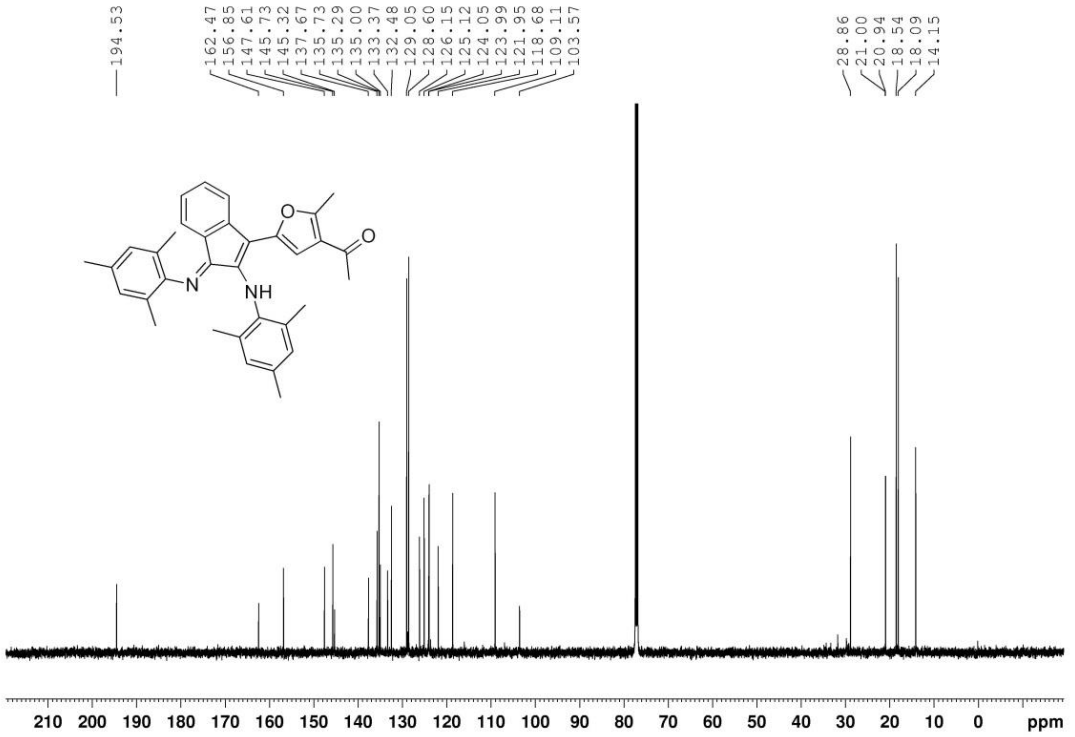
Compound **4r**


7.183
7.168
7.143
7.128
7.123
7.109
7.107
7.094
7.092
7.066
7.052
7.051
7.036
7.006
6.955
6.626
6.624
6.611
6.609
6.596
6.594
6.254
6.239
5.684
2.386
2.261
2.160
2.117
O
O
N
NH
9.5 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 ppm
1.01
2.02
1.09
1.06
3.04
1.08
1.05
1.02
1.01
3.02
6.00
3.05
6.03

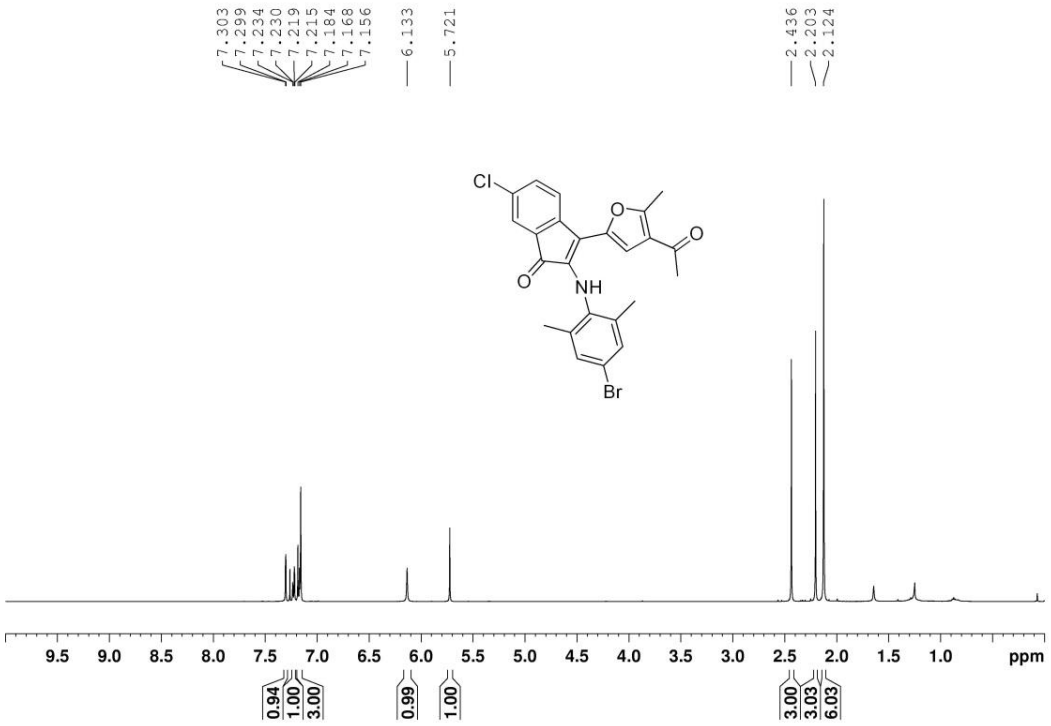

194.44
162.34
156.99
147.86
147.35
145.52
137.58
137.29
135.29
132.58
128.36
128.01
126.23
126.12
125.29
124.16
124.07
124.03
122.01
118.77
109.18
104.25
29.12
18.68
18.16
14.19
O
O
N
NH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

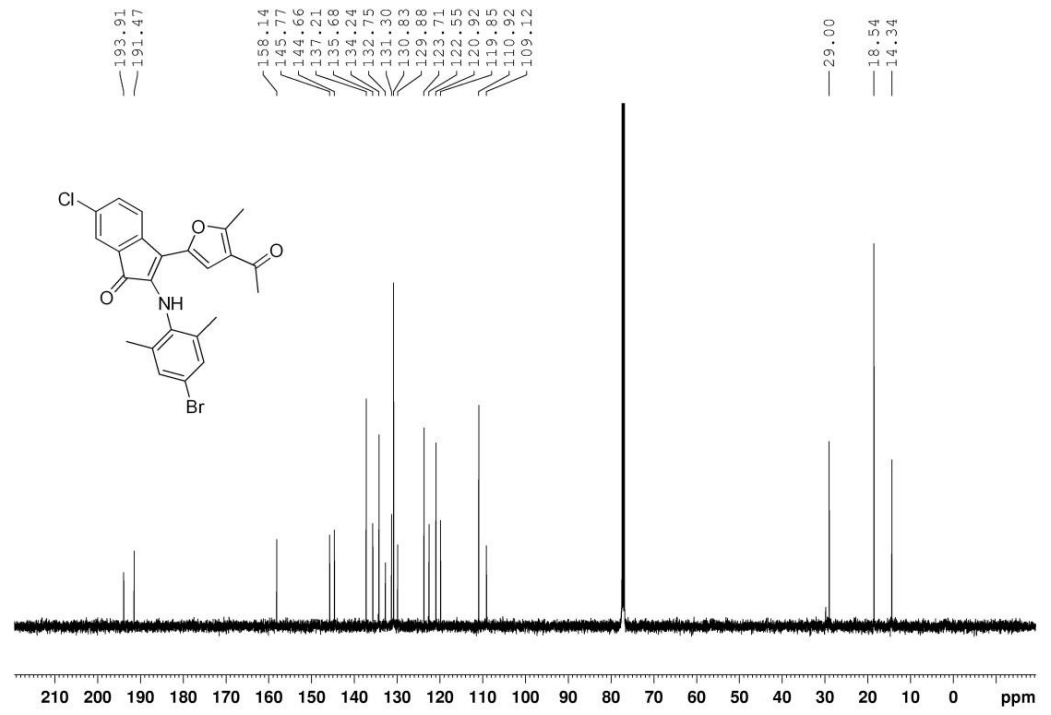
Compound **4s**


7.172
7.157
7.109
7.107
7.094
7.092
7.079
7.077
6.944
6.918
6.808
6.623
6.621
6.608
6.606
6.593
6.591
6.302
6.288
5.598
2.399
2.350
2.238
2.197
2.144
2.068
O
N
NH
O
9.5 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 ppm
1.04 1.08 2.06 0.93 2.07 1.08 1.01 1.02 3.00 3.08 3.04 6.10 3.05 6.04

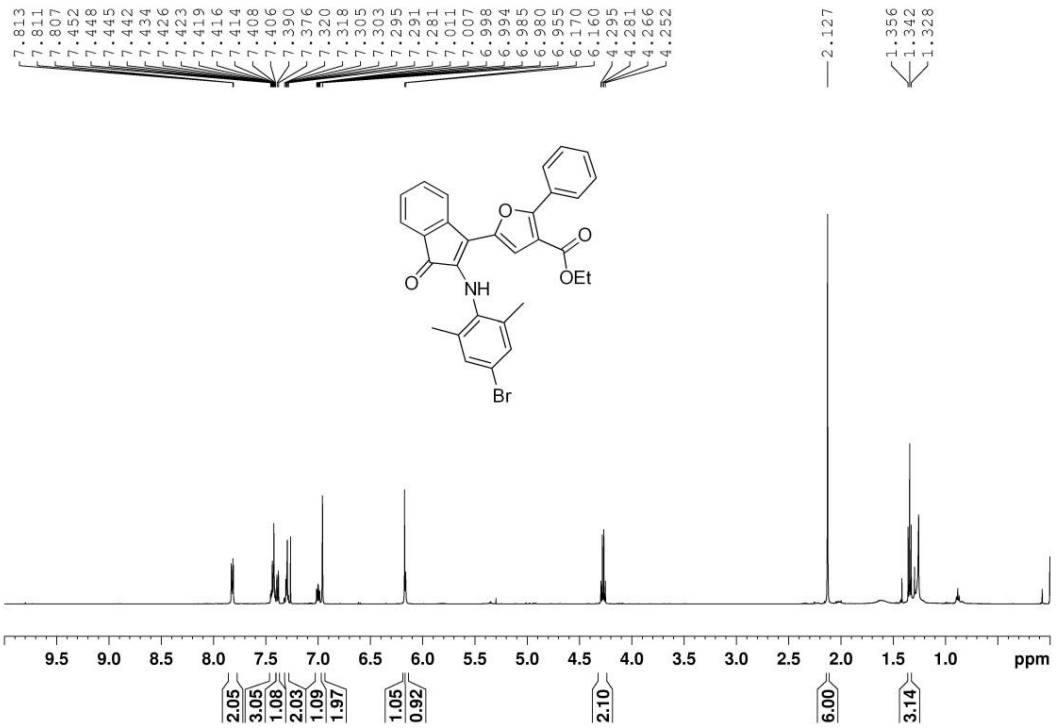

194.53
162.47
156.85
147.61
145.73
145.32
137.67
135.73
135.29
135.00
133.37
132.48
129.05
128.60
126.15
125.12
124.05
123.99
121.95
118.68
109.11
103.57
28.86
21.00
20.94
18.54
18.09
14.15
O
N
NH
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

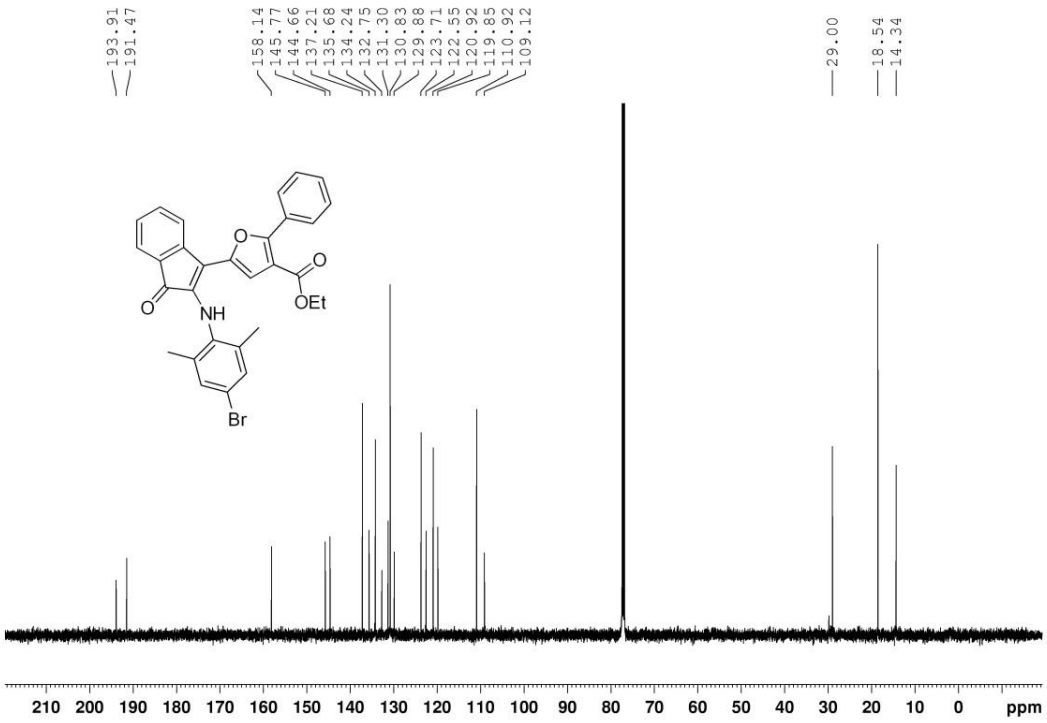
Compound **5b**


7.303
7.299
7.234
7.230
7.219
7.215
7.184
7.168
7.156
6.133
5.721
2.436
2.203
2.124
Cl
O
O
NH
Br
9.5 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 ppm
0.94
1.00
3.00
0.99
1.00
3.00
3.03
6.03


193.91
191.47
158.14
145.77
144.66
137.21
135.68
134.24
132.75
131.30
130.83
129.88
123.71
122.55
120.92
119.85
110.92
109.12
29.00
18.54
14.34
Cl
O
O
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound **5h**


7.813
7.811
7.807
7.452
7.448
7.445
7.442
7.434
7.426
7.423
7.419
7.416
7.414
7.408
7.406
7.390
7.376
7.320
7.318
7.305
7.303
7.295
7.291
7.281
7.011
7.007
6.998
6.994
6.985
6.980
6.955
6.170
6.160
4.295
4.281
4.266
4.252
2.127
1.356
1.342
1.328
O
O
OEt
O
NH
Br
9.5 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 ppm
2.05
3.05
1.08
2.03
1.09
1.97
1.05
0.92
2.10
6.00
3.14


193.91
191.47
158.14
145.77
144.66
137.21
135.68
134.24
132.75
131.30
130.83
129.88
123.71
122.55
120.92
119.85
110.92
109.12
29.00
18.54
14.34
O
O
OEt
O
NH
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

5 Crystal Structure of Compound 3g and 4o

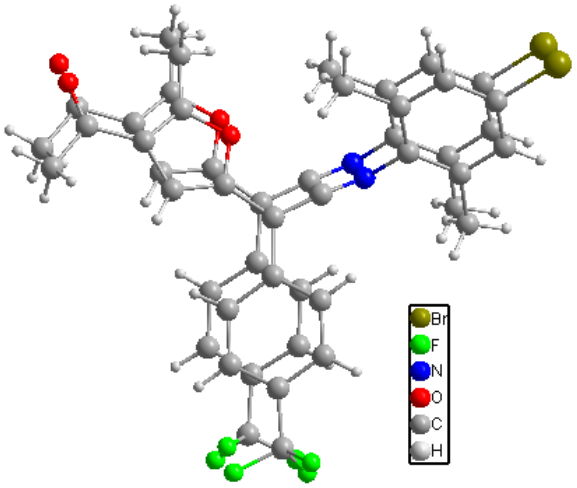


Figure 1 Single Crystal X-Ray structure for 3g

Table 1. Crystal data and structure refinement for 3g.

Identification code	3g	
Empirical formula	C24 H19 Br F3 N O2	
Formula weight	490.31	
Temperature	173(2) K	
Wavelength	1.34138 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.2620(6) Å	α= 91.776(2)°.
	b = 11.3867(8) Å	β= 94.224(2)°.
	c = 22.2514(15) Å	γ = 94.328(2)°.
Volume	2080.3(3) Å^3	
Z	4	
Density (calculated)	1.566 Mg/m^3	
Absorption coefficient	2.052 mm^{-1}	
F(000)	992	
Crystal size	0.250 x 0.220 x 0.180 mm^3	
Theta range for data collection	3.389 to 58.999°.	
Index ranges	-10<=h<=10, -14<=k<=14, -28<=l<=28	
Reflections collected	24072	
Independent reflections	9035 [R(int) = 0.0553]	
Completeness to theta = 53.594°	99.00%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.752 and 0.403	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9035 / 0 / 567	
Goodness-of-fit on F^2	1.103	
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1508	

R indices (all data)	R1 = 0.0568, wR2 = 0.1576
Extinction coefficient	n/a
Largest diff. peak and hole	0.735 and -0.773 e.Å^{-3}

6 Crystal Structure of Compound 4o

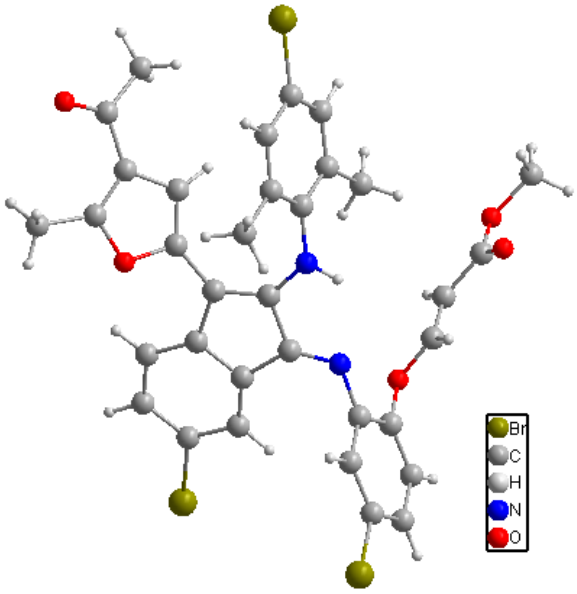


Figure 2 Single Crystal X-Ray structure for 4o

Table 2. Crystal data and structure refinement for 4o.

Identification code	4o	
Empirical formula	C34 H27 Br3 N2 O5	
Formula weight	783.3	
Temperature	193(2) K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.8209(9) Å	α= 90°.
	b = 13.1614(9) Å	β= 103.056(5)°.
	c = 23.1775(18) Å	γ = 90°.
Volume	3215.6(4) Å^3	
Z	4	
Density (calculated)	1.618 Mg/m^3	
Absorption coefficient	3.317 mm^{-1}	
F(000)	1560	
Crystal size	0.190 x 0.170 x 0.120 mm^3	
Theta range for data collection	3.382 to 52.989°.	
Index ranges	-12<=h<=10, -12<=k<=15, -27<=l<=27	

Reflections collected	18635
Independent reflections	5658 [R(int) = 0.0704]
Completeness to theta = 52.989°	99.40%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5658 / 0 / 402
Goodness-of-fit on F^2	0.983
Final R indices [I>2sigma(I)]	R1 = 0.0492, wR2 = 0.1084
R indices (all data)	R1 = 0.0917, wR2 = 0.1267
Extinction coefficient	n/a
Largest diff. peak and hole	0.656 and -0.519 e.$Å^{-3}$