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Cascade cyclization and acyl migration of propargylic esters with isocyanides: a rapid access to substituted furans

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Supporting Information

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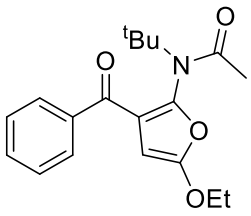
1 General Information

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. Chemical yields referred to pure isolated product. Purification of products was accomplished by column chromatography packed with silica gel.

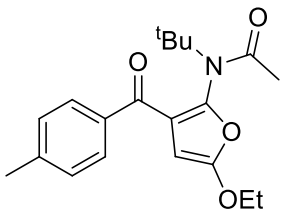
2 General Procedure

To a solution of the propargylic ester **1** (0.5 mmol) in 3 mL acetone was added isocyanide **2** (0.5 mmol). The stirred mixture was heated at 120 ^{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 = 40:1] to afford the desired product.

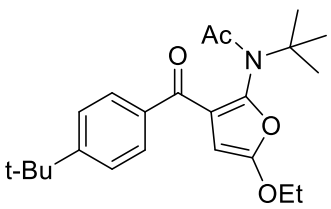
3 Characterization Data



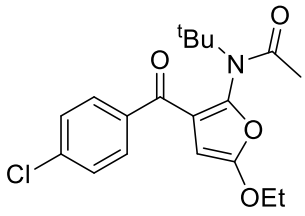
(**3a**): 130 mg, 79% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.97 - 7.76 (m, 2H), 7.68 - 7.56 (m, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 5.39 (s, 1H), 4.19 - 4.13 (m, 2H), 1.99 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.17, 172.08, 156.43, 142.41, 138.02, 133.00, 129.24, 128.69, 120.99, 82.77, 67.26, 60.71, 28.34, 24.78, 14.57. HRMS (ESI): Calcd. for $C_{19}H_{24}NO_4$ $[M+H]^+$ 330.1700, Found: 330.1705.



(**3b**): 94 mg, 55% yield, white solid: m. p. 80 - 81 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 - 7.72 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.38 (s, 1H), 4.19 - 4.13 (m, 2H), 2.46 (s, 3H), 1.98 (s, 3H), 1.47 (t, *J* = 7.0 Hz, 3H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 188.84, 172.18, 156.36, 143.92, 142.13, 135.40, 129.46, 129.38, 121.14, 82.87, 67.23, 60.67, 28.34, 24.80, 21.82, 14.58. HRMS (ESI): Calcd. for $C_{20}H_{25}NNaO_4$ $[M+Na]^+$ 366.1676, Found: 366.1663.

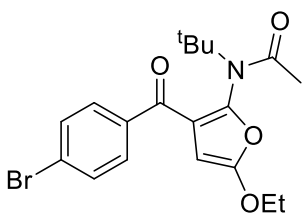


(3c): 104 mg, 54% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 - 7.80 (m, 2H), 7.54 - 7.49 (m, 2H), 5.41 (s, 1H), 4.18 - 4.12 (m, 2H), 1.98 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.37 (s, 18H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 188.78, 172.18, 156.84, 156.35, 142.14, 135.27, 129.28, 125.65, 121.12, 82.85, 67.21, 60.63, 35.29, 31.22, 28.32, 24.78, 14.56. HRMS (ESI): Calcd. for $C_{23}H_{31}NO_4$ $[M+Na]^+$ 408.2145, Found: 408.2135.

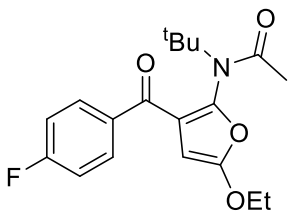


(**3d**): 125 mg, 69% yield, white solid: m. p. 90 - 91 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.86 - 7.76 (m, 2H), 7.51 - 7.47 (m, 2H), 5.35 (s, 1H), 4.19 - 4.13 (m, 2H), 1.97 (s, 3H), 1.48 (t, *J* = 7.0 Hz, 3H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 187.84, 172.04, 156.55, 142.59, 139.51, 136.28, 130.65,

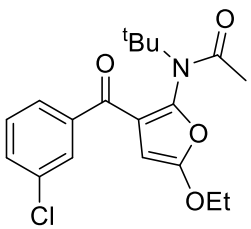
129.07, 120.63, 82.49, 67.33, 60.80, 28.36, 24.75, 14.57. HRMS (ESI): Calcd. for $C_{19}H_{22}ClNNaO_4$ $[M+Na]^+$ 386.1130, Found: 386.1123.



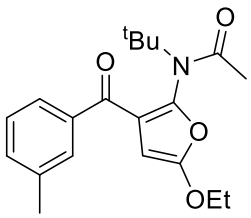
(**3e**): 126 mg, 62% yield, white solid: m. p. 103 - 104 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.6 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 2H), 5.35 (s, 1H), 4.18 - 4.12 (m, 2H), 1.96 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.37 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 187.97, 171.94, 156.54, 142.60, 136.68, 132.02, 130.73, 128.12, 120.57, 82.43, 67.30, 60.75, 28.33, 24.73, 14.55. HRMS (ESI): Calcd. for $C_{19}H_{22}BrNNaO_4$ $[M+Na]^+$ 430.0624, Found: 430.0613.



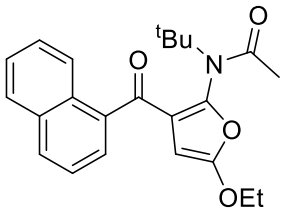
(**3f**): 102 mg, 59% yield, white solid: m. p. 92 - 93 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.95 - 7.88 (m, 2H), 7.21 - 7.16 (m, 2H), 5.37 (s, 1H), 4.19 - 4.13 (m, 2H), 1.97 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 187.57, 172.06, 166.74, 164.71, 156.52, 142.45, 134.29, 131.91, 131.84, 120.73, 115.99, 115.82, 82.59, 67.32, 60.75, 28.35, 24.77, 14.57. HRMS (ESI): Calcd. for $C_{19}H_{22}FNNaO_4$ $[M+Na]^+$ 370.1425, Found: 370.1422.



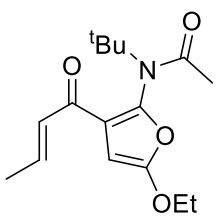
(**3g**): 74 mg, 41% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.83 (t, *J* = 1.8 Hz, 1H), 7.77 - 7.71 (m, 1H), 7.61 - 7.55 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 5.37 (s, 1H), 4.20 - 4.14 (m, 2H), 1.97 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 187.70, 171.91, 156.61, 142.86, 139.61, 135.01, 132.93, 130.06, 129.20, 127.28, 120.53, 82.42, 67.37, 60.83, 28.37, 24.75, 14.56. HRMS (ESI): Calcd. for $C_{19}H_{22}ClNNaO_4$ $[M+Na]^+$ 386.1130, Found: 386.1119.



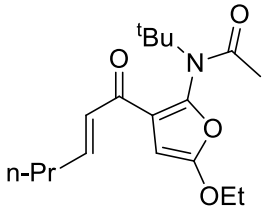
(**3h**): 91 mg, 53% yield, white solid: m. p. 83 - 84 °C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.69 - 7.65 (m, 1H), 7.66 - 7.62 (m, 1H), 7.42 - 7.36 (m, 2H), 5.39 (s, 1H), 4.18 - 4.12 (m, 2H), 2.43 (s, 3H), 1.98 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H), 1.37 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.36, 172.06, 156.37, 142.31, 138.61, 138.03, 133.76, 129.59, 128.46, 126.51, 121.09, 82.83, 67.24, 60.66, 28.31, 24.76, 21.46, 14.54. HRMS (ESI): Calcd. for $C_{20}H_{25}NNaO_4$ $[M+Na]^+$ 366.1676, Found: 366.1670.



(**3i**): 91 mg, 48% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.33 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.95 - 7.91 (m, 1H), 7.70 (dd, *J* = 7.1, 1.2 Hz, 1H), 7.62 - 7.55 (m, 2H), 7.53 (dd, *J* = 8.3, 7.1 Hz, 1H), 5.26 (s, 1H), 4.12 - 4.06 (m, 2H), 2.05 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H), 1.38 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 190.90, 171.84, 156.49, 143.05, 136.08, 134.04, 132.23, 130.54, 128.62, 127.83, 126.76, 125.52, 124.34, 122.55, 82.67, 67.22, 60.91, 28.40, 24.81, 14.51. HRMS (ESI): Calcd. for $C_{23}H_{26}NO_4$ $[M+H]^+$ 380.1856, Found: 380.1854.

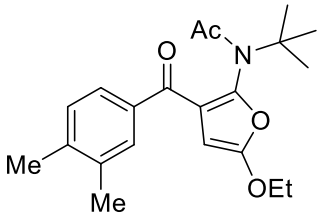


(**3j**): 69 mg, 47% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.14 - 7.08 (m, 1H), 6.76 - 6.70 (m, 1H), 5.57 (s, 1H), 4.14 (q, *J* = 7.1 Hz, 2H), 1.96 (dd, *J* = 6.9, 1.8 Hz, 3H), 1.91 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H), 1.43 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 183.90, 172.15, 157.16, 144.66, 142.07, 127.76, 123.29, 67.14, 61.00, 28.40, 24.83, 18.56, 14.52. HRMS (ESI): Calcd. for $C_{16}H_{23}NNaO_4$ $[M+Na]^+$ 316.1519, Found: 316.1518.

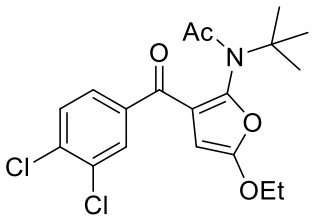


(**3k**): 61 mg, 30% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.15 - 7.09 (m, 1H), 6.75 - 6.69 (m, 1H), 5.57 (s, 1H), 4.14 (q, *J* = 7.1 Hz, 2H), 2.29 - 2.23 (m, 2H), 1.91 (s, 3H), 1.57 - 1.53 (m, 2H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.43 (s, 9H), 0.97 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 184.01,

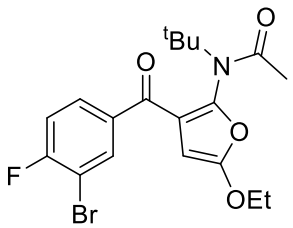
172.10, 157.16, 149.53, 142.05, 126.16, 123.44, 80.54, 67.13, 61.01, 53.57, 34.82, 28.43, 24.83, 21.51, 18.59, 14.52, 13.89. HRMS (ESI): Calcd. for $C_{18}H_{27}NNaO_4$ $[M+Na]^+$ 344.1832, Found: 344.1831.



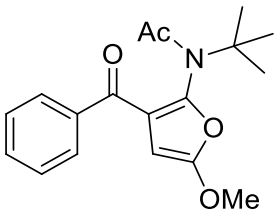
(3l): 103 mg, 58% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 2.0 Hz, 1H), 7.60 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.24 (d, *J* = 7.7 Hz, 1H), 5.38 (s, 1H), 4.18 - 4.12 (m, 2H), 2.35 (s, 3H), 2.34 (s, 3H), 1.97 (s, 3H), 1.46 (t, *J* = 7.0 Hz, 3H), 1.37 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.04, 172.21, 156.30, 142.67, 142.03, 137.21, 135.75, 130.28, 129.80, 127.14, 121.18, 82.92, 67.21, 60.63, 28.30, 24.77, 20.15, 19.90, 14.54. HRMS (ESI): Calcd. for $C_{21}H_{27}NO_4$ $[M+Na]^+$ 380.1832, Found: 380.1845.



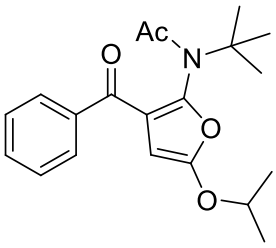
(3m): 123 mg, 62% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 2.0 Hz, 1H), 7.70 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.59 (d, *J* = 8.2 Hz, 1H), 5.35 (s, 1H), 4.19 - 4.13 (m, 2H), 1.95 (s, 3H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.37 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 186.59, 171.85, 156.69, 142.95, 137.63, 137.51, 133.42, 131.08, 130.87, 128.23, 120.21, 82.16, 67.39, 60.85, 28.35, 24.72, 14.54. HRMS (ESI): Calcd. for C19H21Cl$_2$NO4 $[M+Na]^+$ 420.0740, Found: 420.0733.



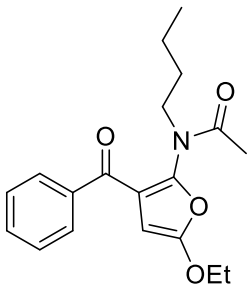
(**3n**): 130 mg, 61% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 6.6, 2.1 Hz, 1H), 7.86 - 7.80 (m, 1H), 7.24 (t, *J* = 8.3 Hz, 1H), 5.35 (s, 1H), 4.20 - 4.14 (m, 2H), 1.96 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.37 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 186.24, 171.88, 162.99, 160.95, 156.66, 142.85, 135.42, 135.39, 134.97, 130.43, 130.36, 120.25, 116.92, 116.73, 110.00, 82.25, 67.39, 60.82, 28.36, 24.73, 14.54. HRMS (ESI): Calcd. for $C_{19}H_{21}BrFNNaO_4$ $[M+Na]^+$ 448.0530, Found: 448.0509.



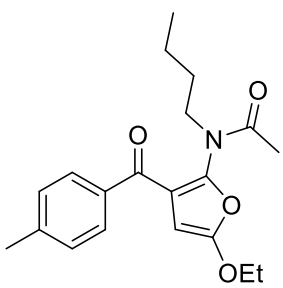
(**3o**): 99 mg, 63% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.86 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.63 - 7.57 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 5.38 (s, 1H), 3.90 (s, 3H), 1.97 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.11, 172.07, 157.35, 142.43, 137.90, 133.01, 129.18, 128.67, 121.02, 81.68, 60.69, 57.82, 28.28, 24.72. HRMS (ESI): Calcd. for $C_{18}H_{21}NO_4$ $[M+H]^+$ 316.1543, Found: 316.1566.



(**3p**): 113 mg, 66% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.87 - 7.81 (m, 2H), 7.61 - 7.56 (m, 1H), 7.48 (dd, *J* = 8.4, 7.1 Hz, 2H), 5.43 (s, 1H), 4.53 - 4.49 (m, 1H), 1.95 (s, 3H), 1.39 (dd, *J* = 6.2, 3.1 Hz, 6H), 1.36 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 172.05, 155.37, 142.59, 138.04, 133.00, 129.25, 128.69, 120.91, 85.54, 75.95, 60.67, 28.35, 24.78, 21.93. HRMS (ESI): Calcd. for $C_{20}H_{25}NO_4$ $[M+H]^+$ 344.1856, Found: 344.1876.

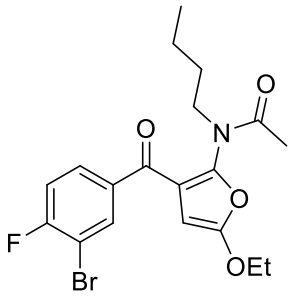


(**4a**): 110 mg, 67% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.84 - 7.79 (m, 2H), 7.62 - 7.57 (m, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 5.46 (s, 1H), 4.16 (q, *J* = 7.0 Hz, 2H), 3.53 (t, *J* = 7.7 Hz, 2H), 2.03 (s, 3H), 1.49 - 1.43 (m, 5H), 1.30 - 1.23 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.24, 171.37, 156.84, 142.55, 138.06, 132.93, 128.93, 128.61, 119.26, 82.67, 67.30, 48.33, 30.21, 22.33, 20.03, 14.56, 13.86. HRMS (ESI): Calcd. for $C_{19}H_{23}NNaO_4$ $[M+Na]^+$ 352.1519, Found: 352.1526.

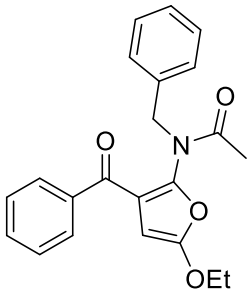


(**4b**): 94 mg, 55% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 - 7.70 (m, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 5.45 (s, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.53 (t, *J* = 7.6 Hz, 2H), 2.44 (s, 3H), 2.02 (s, 3H), 1.48 - 1.42 (m, 5H), 1.30 - 1.23 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 188.89, 171.48, 156.77, 143.85, 142.15, 135.37, 129.30, 129.16, 119.42, 82.77, 67.25,

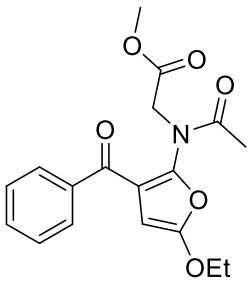
48.32, 30.19, 22.32, 21.78, 20.02, 14.55, 13.85. HRMS (ESI): Calcd. for $C_{20}H_{25}NNaO_4$ $[M+Na]^+$ 366.1676, Found: 366.1681.



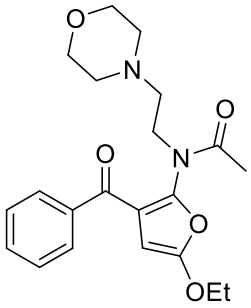
(**4c**): 166 mg, 78% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.05 (dd, *J* = 6.6, 2.2 Hz, 1H), 7.82 - 7.76 (m, 1H), 7.23 (t, *J* = 8.3 Hz, 1H), 5.42 (s, 1H), 4.17 (q, *J* = 7.0 Hz, 2H), 3.53 (t, *J* = 7.5 Hz, 2H), 2.01 (s, 3H), 1.49 - 1.43 (m, 5H), 1.27 (d, *J* = 8.0 Hz, 2H), 0.85 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 186.25, 171.17, 162.90, 160.87, 157.06, 142.89, 135.40, 134.76, 130.13, 130.07, 118.56, 116.90, 116.72, 109.65, 82.24, 67.43, 48.38, 30.23, 22.28, 19.99, 14.53, 13.84. HRMS (ESI): Calcd. for $C_{19}H_{21}BrFNNaO_4$ $[M+Na]^+$ 448.0530, Found: 448.0518.



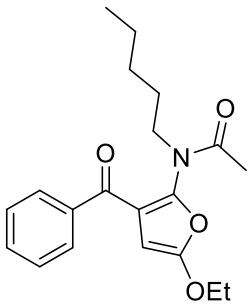
(**4d**): 105 mg, 58% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.20 - 7.04 (m, 5H), 5.30 (s, 1H), 4.79 (s, 2H), 4.07 (q, *J* = 7.1 Hz, 2H), 2.16 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.00, 171.64, 156.68, 141.34, 137.72, 136.20, 132.79, 129.00, 128.97, 128.36, 128.33, 127.51, 120.06, 83.04, 67.35, 51.46, 22.44, 14.49. HRMS (ESI): Calcd. for $C_{22}H_{21}NNaO_4$ $[M+Na]^+$ 386.1363, Found: 386.1352.



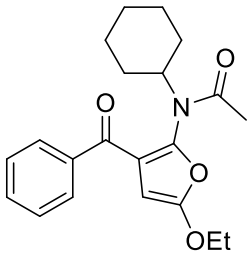
(**4e**): 78 mg, 45% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.83 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.63 - 7.59 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 5.46 (s, 1H), 4.33 (s, 2H), 4.17 (q, *J* = 7.0 Hz, 2H), 3.67 (s, 3H), 2.12 (s, 3H), 1.47 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.17, 171.56, 169.04, 157.03, 141.42, 137.90, 133.11, 129.06, 128.71, 119.18, 82.94, 67.44, 52.31, 49.95, 21.80, 14.59. HRMS (ESI): Calcd. for $C_{18}H_{19}NNaO_6$ $[M+Na]^+$ 368.1105, Found: 368.1101.



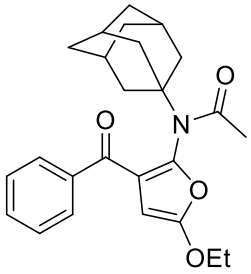
(**4f**): 87 mg, 45% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.85 - 7.77 (m, 2H), 7.63 - 7.55 (m, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 5.44 (s, 1H), 4.14 (q, *J* = 7.0 Hz, 2H), 3.69 (t, *J* = 6.8 Hz, 2H), 3.55 (t, *J* = 4.5 Hz, 4H), 2.47 (t, *J* = 6.9 Hz, 2H), 2.36 (t, *J* = 4.6 Hz, 4H), 2.03 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 188.95, 171.42, 156.74, 142.51, 138.00, 132.94, 128.90, 128.60, 118.81, 82.58, 67.25, 66.91, 56.43, 53.58, 45.12, 22.15, 14.53. HRMS (ESI): Calcd. for $C_{21}H_{27}N_2O_5$ $[M+H]^+$ 387.1914, Found: 387.1919.



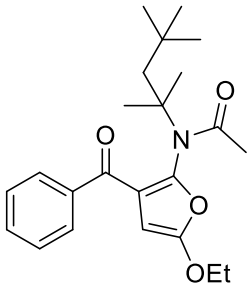
(**4g**): 101 mg, 59% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.86 - 7.78 (m, 2H), 7.64 - 7.56 (m, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 5.46 (s, 1H), 4.17 (q, *J* = 7.0 Hz, 2H), 3.52 (t, *J* = 7.7 Hz, 2H), 2.04 (s, 3H), 1.48 (t, *J* = 7.0 Hz, 5H), 1.28 - 1.22 (m, 4H), 0.83 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.26, 171.39, 156.85, 142.58, 138.08, 132.96, 128.95, 128.63, 119.29, 82.72, 67.33, 48.61, 28.96, 27.83, 22.46, 22.37, 14.59, 14.03. HRMS (ESI): Calcd. for $C_{20}H_{25}NNaO_4$ $[M+Na]^+$ 366.1676, Found: 366.1672.



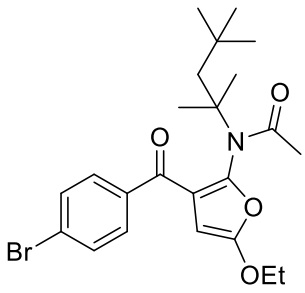
(**4h**): 85 mg, 48% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.93 - 7.84 (m, 2H), 7.64 - 7.58 (m, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 5.40 (s, 1H), 4.39 - 4.33 (m, 1H), 4.16 (t, *J* = 6.7 Hz, 2H), 2.07 (s, 3H), 2.05 - 1.92 (m, 1H), 1.74 (s, 1H), 1.67 - 1.52 (m, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.38 - 1.29 (m, 2H), 1.16 (m, 1H), 1.03 - 0.81 (m, 2H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.09, 171.51, 156.74, 140.14, 137.85, 132.90, 128.54, 128.54, 121.22, 82.76, 67.09, 55.56, 25.45, 22.76, 14.47. HRMS (ESI): Calcd. for $C_{21}H_{25}NNaO_4$ $[M+Na]^+$ 378.1676, Found: 378.1675.



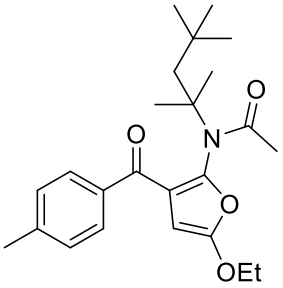
(**4i**): 106 mg, 52% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.89 - 7.84 (m, 2H), 7.63 - 7.57 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 5.38 (s, 1H), 4.18 - 4.12 (m, 2H), 2.14 - 2.02 (m, 9H), 1.96 (s, 3H), 1.67 - 1.58 (m, 6H), 1.47 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.22, 172.05, 156.39, 142.03, 138.10, 132.92, 129.22, 128.64, 121.28, 82.64, 67.18, 61.95, 39.87, 36.38, 30.19, 25.15, 14.54. HRMS (ESI): Calcd. for $C_{25}H_{30}NO_4$ $[M+H]^+$ 408.2169, Found: 408.2155.



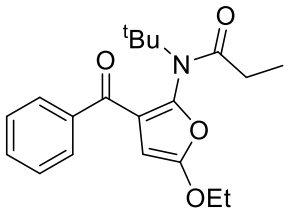
(**4j**): 79 mg, 41% yield, white solid: m. p. 102 - 105 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.95 - 7.81 (m, 2H), 7.68 - 7.56 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 5.37 (s, 1H), 4.19 - 4.13 (m, 2H), 2.45 (d, *J* = 14.7 Hz, 1H), 1.98 (s, 3H), 1.70 (d, *J* = 14.8 Hz, 1H), 1.47 (t, *J* = 7.0 Hz, 3H), 1.44 (s, 3H), 1.25 (s, 3H), 1.02 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.25, 172.39, 156.29, 142.41, 137.95, 133.04, 129.32, 128.68, 121.36, 82.90, 67.25, 65.07, 50.56, 31.83, 31.49, 29.03, 28.45, 25.12, 14.58. HRMS (ESI): Calcd. for $C_{23}H_{31}NNaO_4$ $[M+Na]^+$ 408.2415, Found: 408.2410.



(**4k**): 108 mg, 47% yield, white solid: m. p. 142 - 148 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 8.6 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 5.34 (s, 1H), 4.19 - 4.13 (m, 2H), 2.45 (d, *J* = 14.6 Hz, 1H), 1.97 (s, 3H), 1.68 (d, *J* = 14.9 Hz, 1H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.43 (s, 3H), 1.23 (s, 3H), 1.02 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 188.11, 172.32, 156.43, 142.65, 136.65, 132.05, 130.82, 128.21, 120.98, 82.57, 67.32, 65.15, 50.55, 31.84, 31.49, 29.10, 28.46, 25.10, 14.59. HRMS (ESI): Calcd. for $C_{23}H_{30}BrNNaO_4$ $[M+Na]^+$ 486.1250, Found: 486.1248.



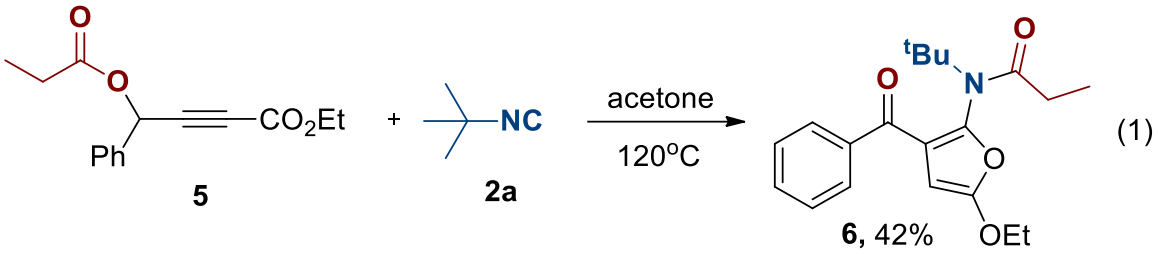
(**4l**): 72 mg, 36% yield, white solid: m. p. 160 - 161 ^{o}C. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.37 (s, 1H), 4.19 - 4.13 (m, 2H), 2.44 (d, *J* = 11.0 Hz, 4H), 1.99 (s, 3H), 1.67 (s, 1H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.43 (s, 3H), 1.24 (s, 3H), 1.02 (s, 9H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 188.95, 172.52, 156.23, 143.97, 142.12, 135.35, 129.53, 129.38, 121.51, 82.99, 67.22, 65.02, 50.53, 31.83, 31.49, 29.03, 28.45, 25.15, 21.82, 14.59. HRMS (ESI): Calcd. for $C_{24}H_{33}NNaO_4$ $[M+Na]^+$ 422.2302, Found: 422.2303.



(**6**): 72 mg, 42% yield, yellow oil. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.90 - 7.83 (m, 2H), 7.64 - 7.58 (m, 1H), 7.51 (dd, *J* = 8.4, 7.0 Hz, 2H), 5.39 (s, 1H), 4.18 - 4.12 (m, 2H), 2.40 - 2.34 (m, 1H), 2.09 - 2.03 (m, 1H), 1.47 (t, *J* = 7.1 Hz, 3H), 1.38 (s, 9H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, Chloroform-*d*) δ 189.21, 175.26, 156.47, 142.04, 138.09, 132.97, 129.25, 128.68, 121.18, 82.82, 67.24, 60.71, 29.30, 28.39, 14.59, 9.22. HRMS (ESI): Calcd. for $C_{20}H_{25}NNaO_4$ $[M+Na]^+$ 366.1676, Found: 366.1674.

4 Control Experiment and Mechanistic Study

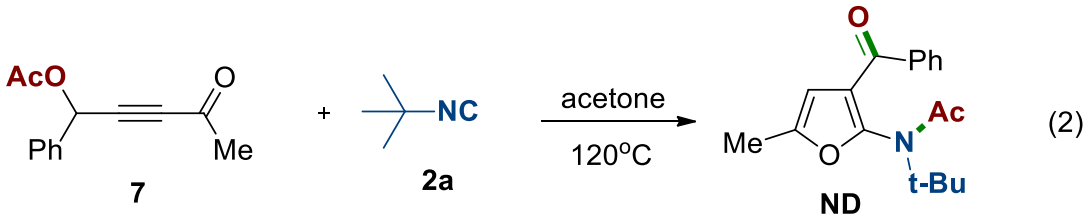
1) Experiment with propargylic ester with propionyl group



(1)

Under air atmosphere, a solution of the propargylic ester **5** (0.5 mmol) in 3 mL acetone was added *tert*-butyl isocyanide **2a** (0.5 mmol). The stirred mixture was heated at 120 °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 = 40:1] to afford the desired product.

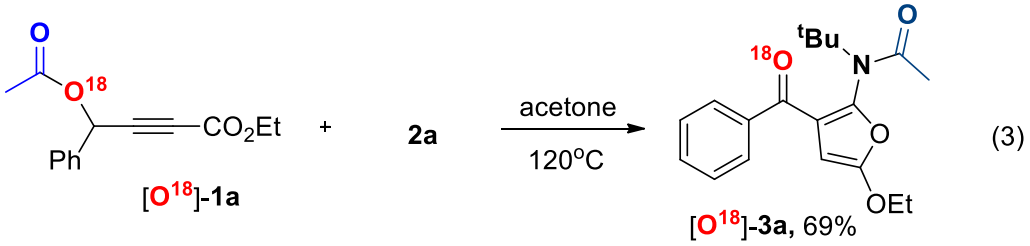
2) Experiment under nitrogen atmosphere



(2)

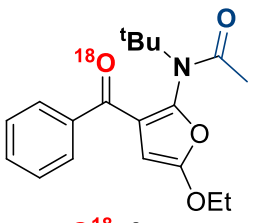
Under air atmosphere, a solution of the acetylenic ketone **7** (0.5 mmol) in 3 mL acetone was added *tert*-butyl isocyanide **2a** (0.5 mmol). The stirred mixture was heated at 120 °C for 12 hours and the progress was monitored using TLC detection. After completion of present reaction, no desired product was detected.

3) Isotope-labeling experiment



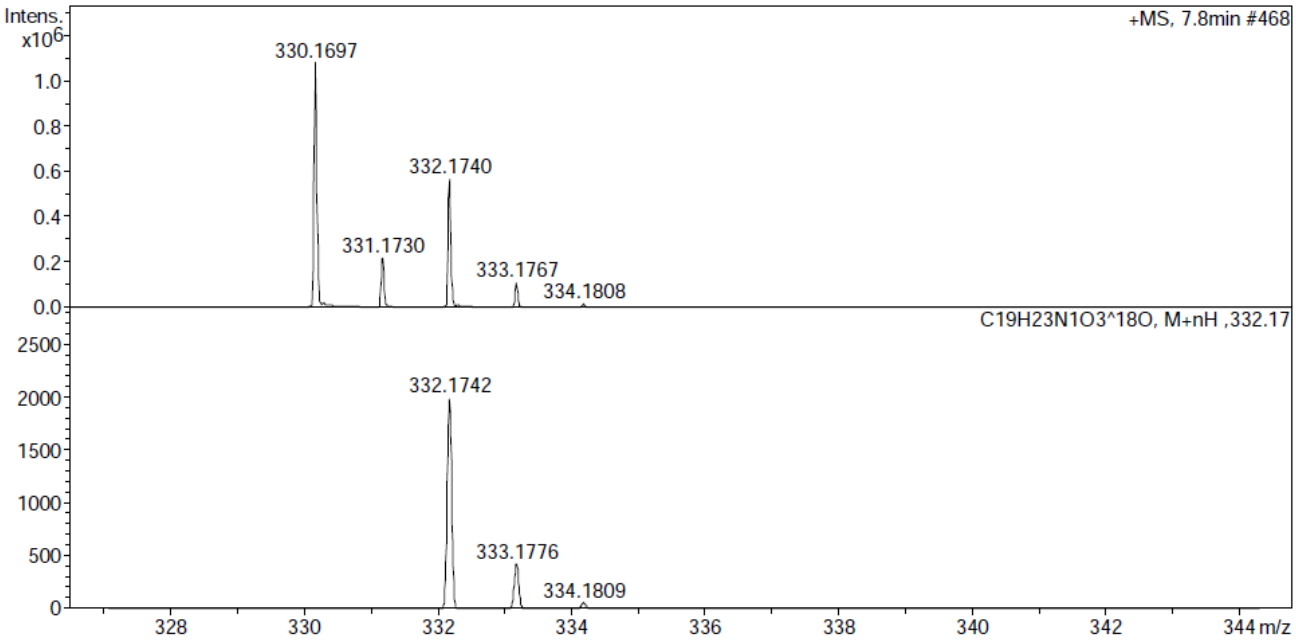
(3)

Under air atmosphere, an O^{18}-labeled propargylic ester [O^{18}]-**1a** (0.5 mmol) in 3 mL acetone was added *tert*-butyl isocyanide **2a** (0.5 mmol). The stirred mixture was heated at 120 ^{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 = 40:1] to afford the desired product [O^{18}]-**3a**.



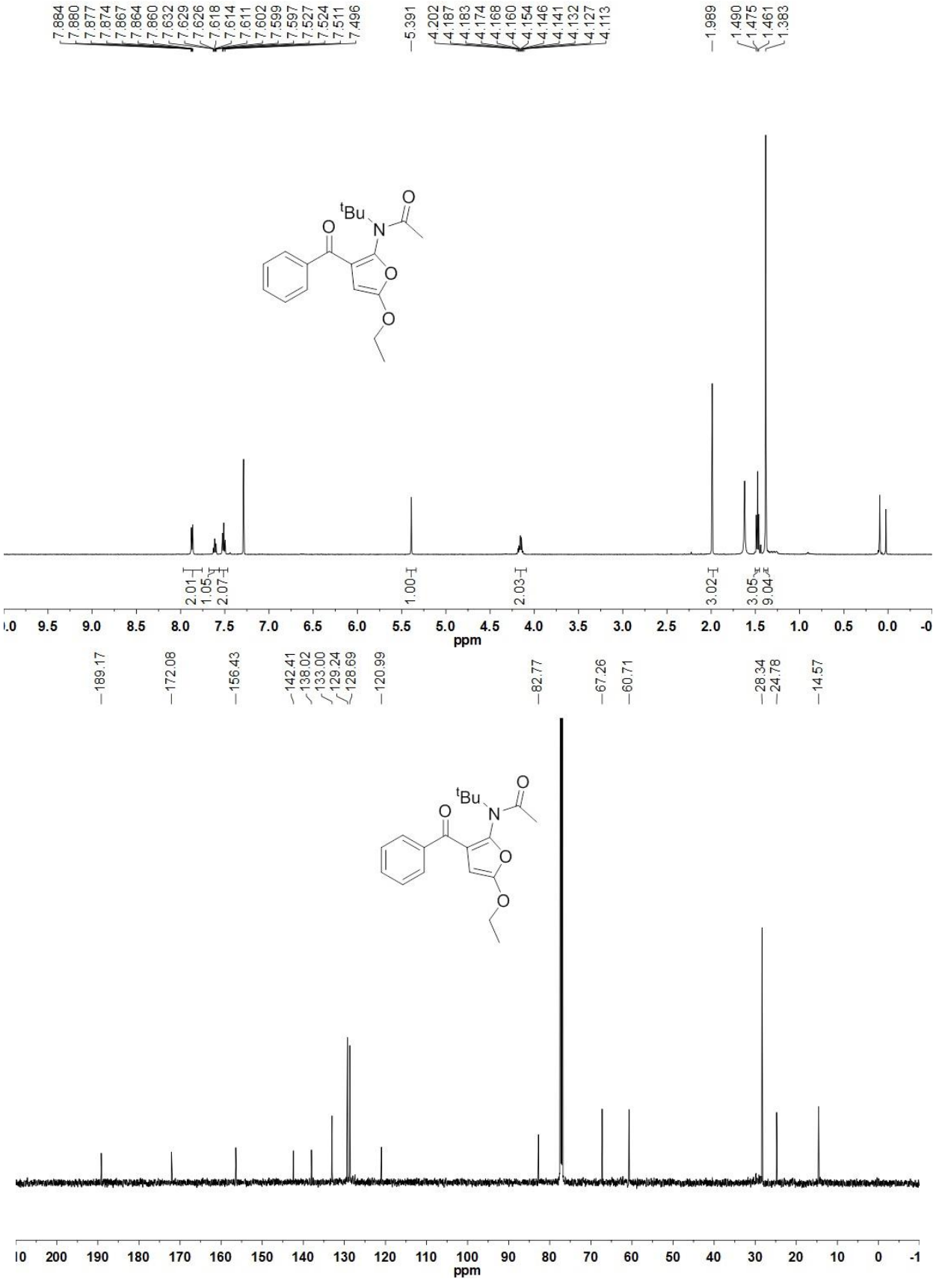
[O^{18}]-**3a**

Chemical Formula: $C_{19}H_{242}O_3{}^{18}O$
Calcd: 332.1742
Found: 332.1740

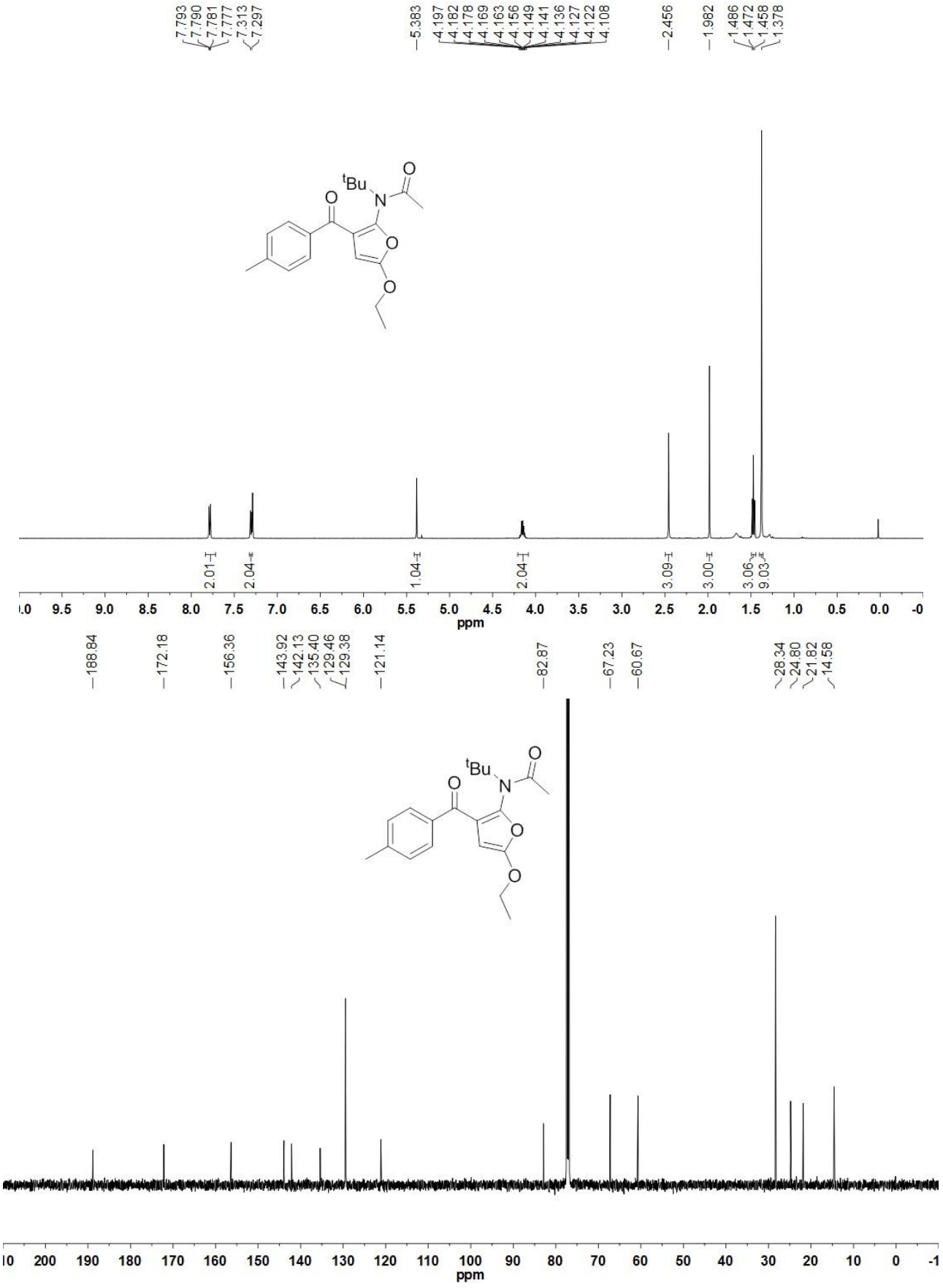


5 ^{1}H NMR and ^{13}C NMR Spectra of All Compounds

Compound 3a



Compound 3b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4.178
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4.156
4.149
4.141
4.136
4.127
4.122
4.108
2.456
1.982
1.486
1.472
1.458
1.378
tBu
N
O
O
O
O
2.01
2.04
1.04
2.04
3.09
3.00
3.06
9.03
ppm
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172.18
156.36
143.92
142.13
135.40
129.46
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121.14
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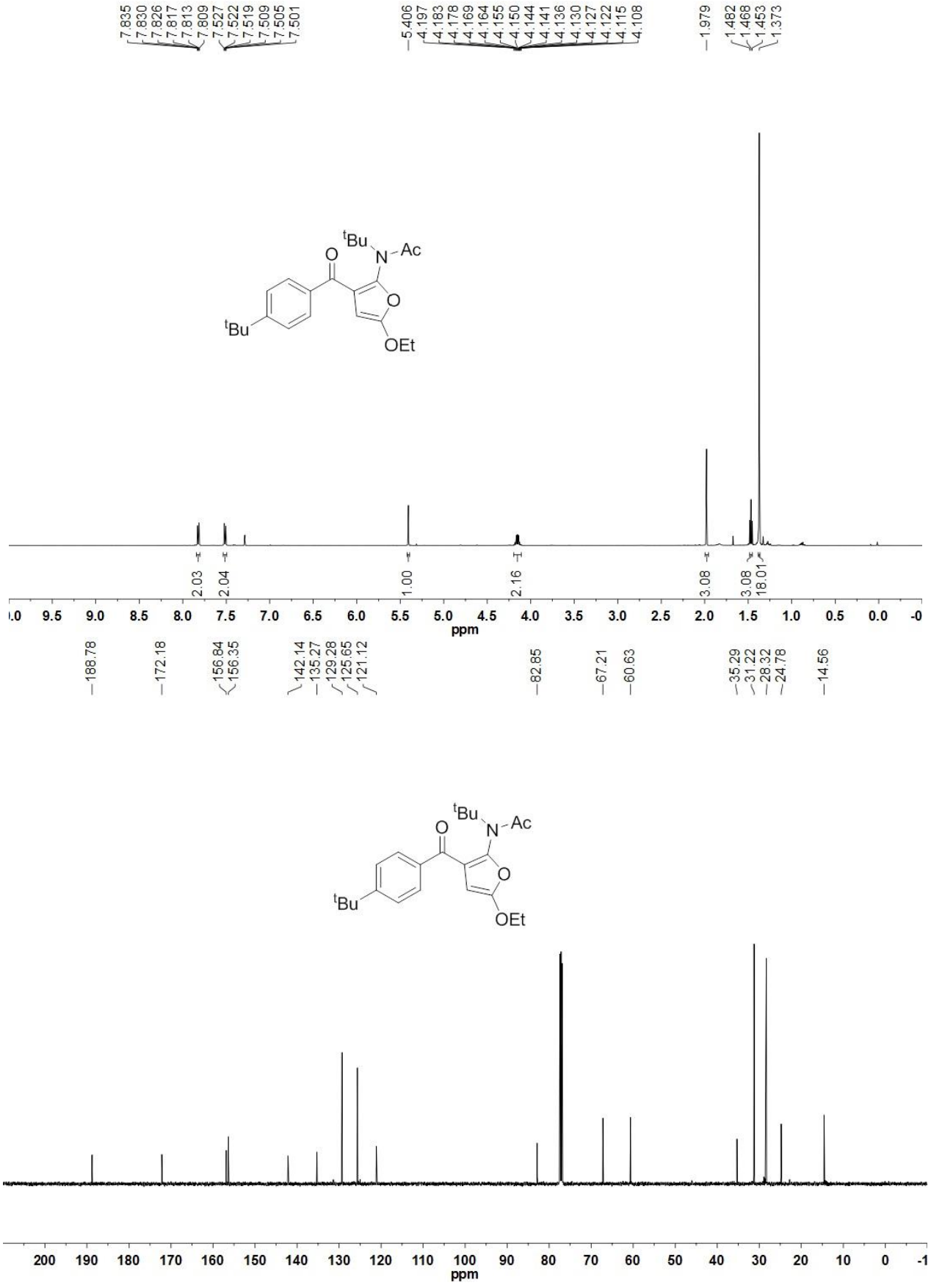
24.80
21.82
14.58
ppm

Compound 3c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7.826
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7.522
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7.509
7.505
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5.406
4.197
4.183
4.178
4.169
4.164
4.155
4.150
4.144
4.141
4.136
4.130
4.127
4.122
4.115
4.108
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Ac
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OEt
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2.04
1.00
2.16
3.08
3.08
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ppm
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172.18
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156.35
142.14
135.27
129.28
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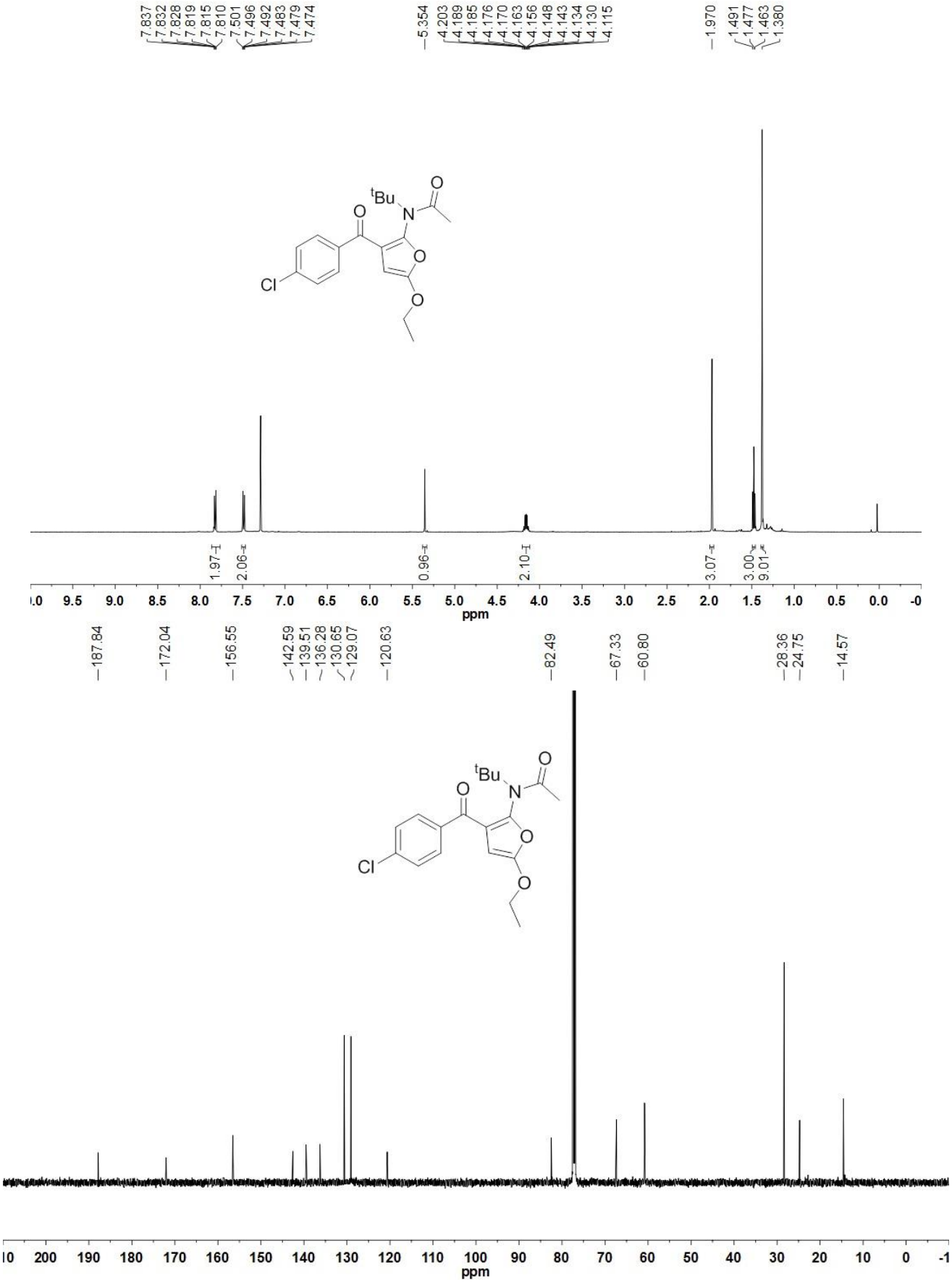
ppm

Compound 3d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7.474
5.354
4.203
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4.185
4.176
4.170
4.163
4.156
4.148
4.143
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4.130
4.115
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1.477
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Cl
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0.96
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ppm
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156.55
142.59
139.51
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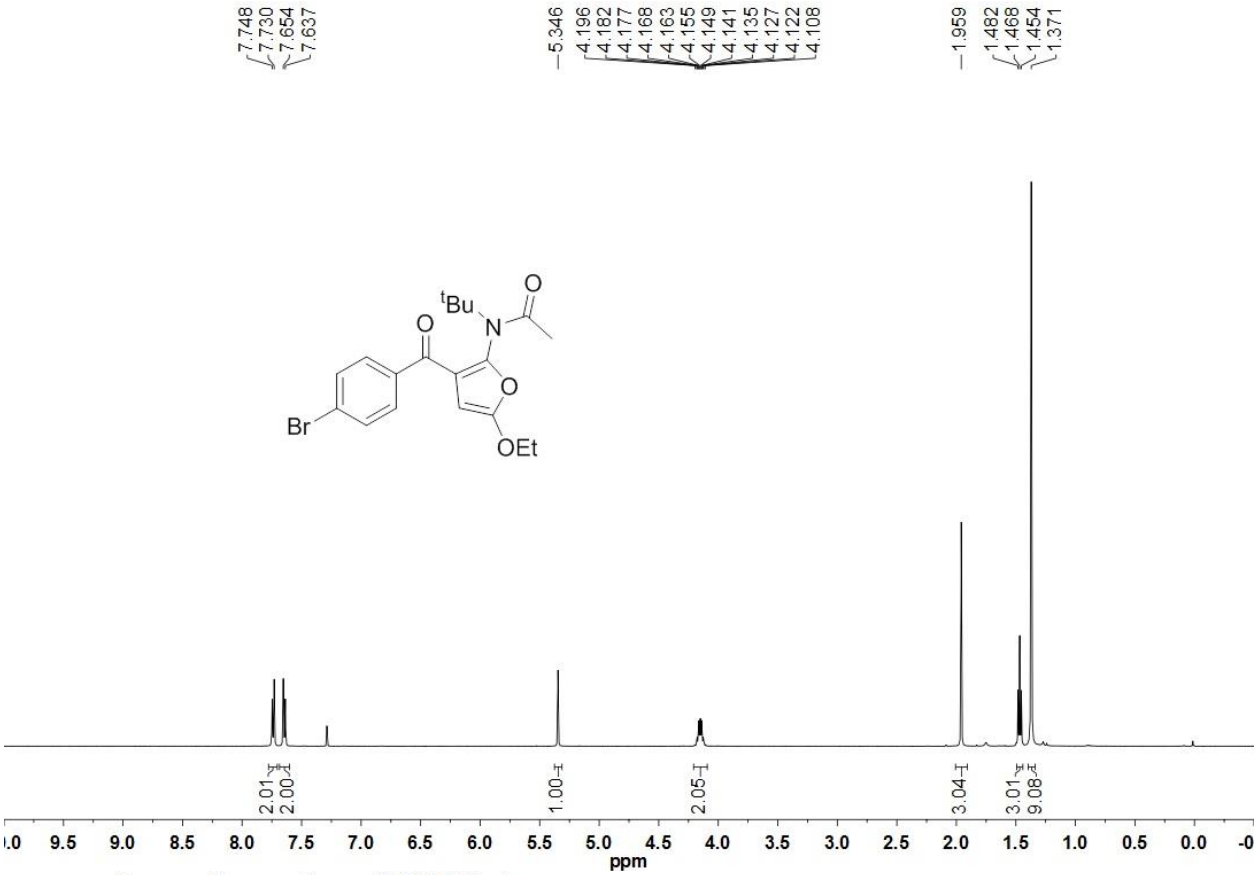
ppm

Compound 3e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Br
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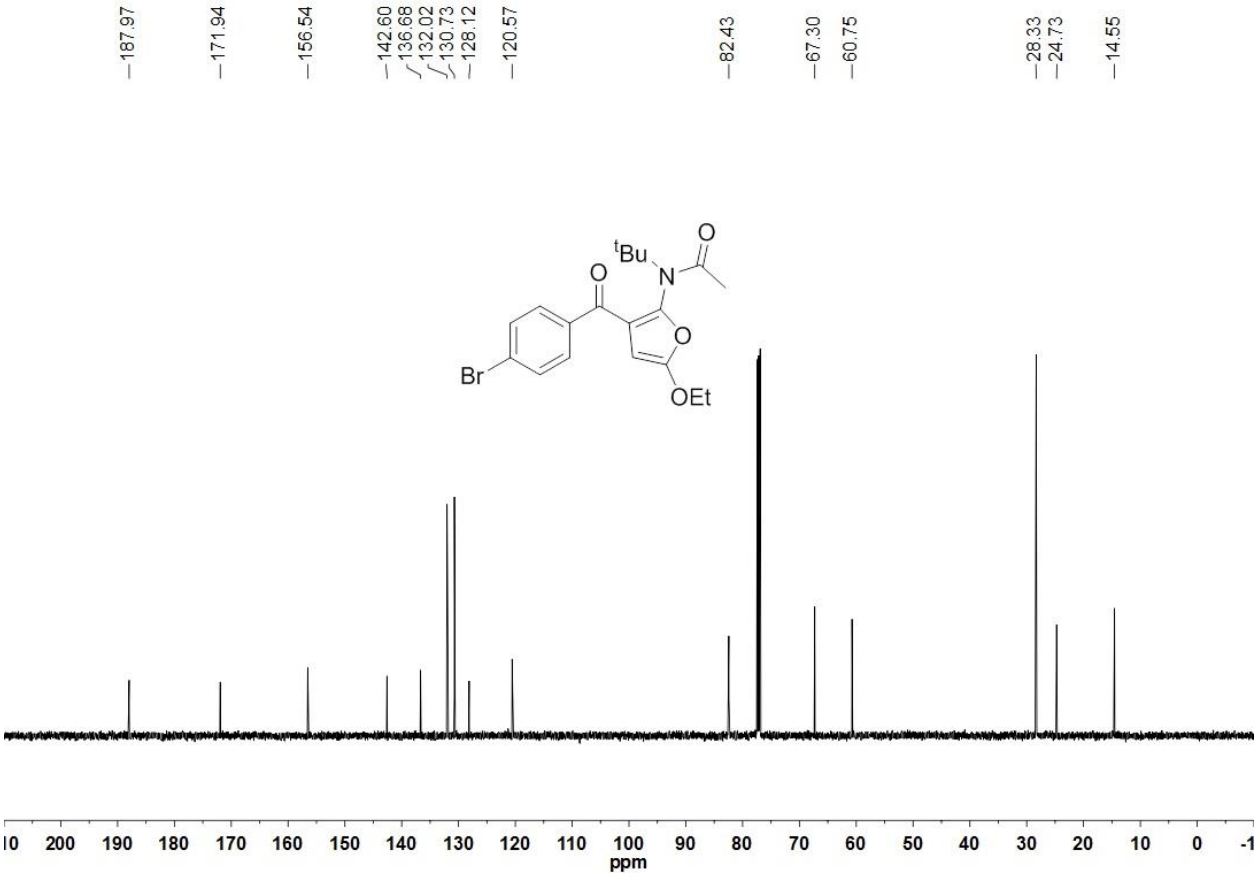
9.08
ppm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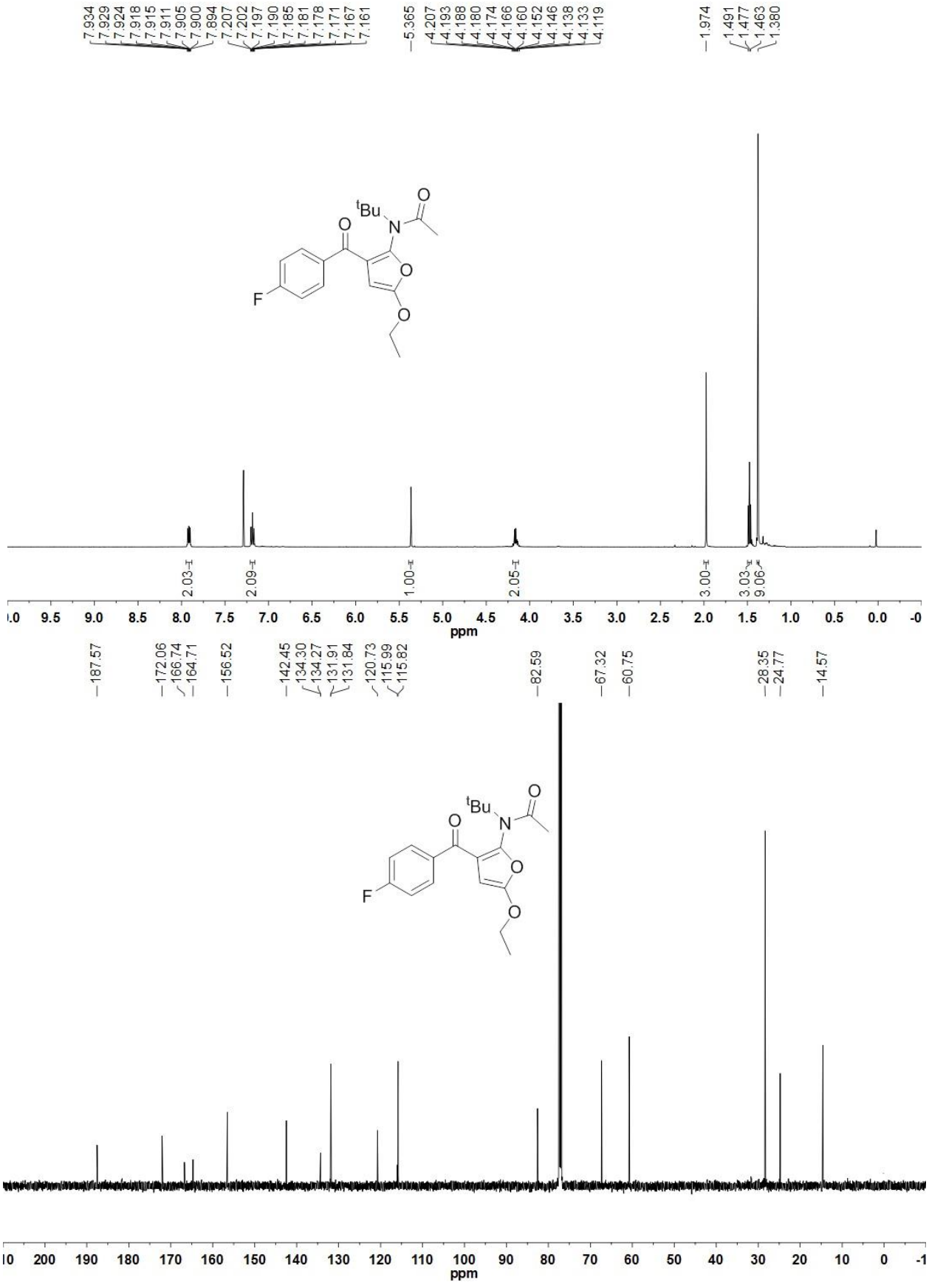
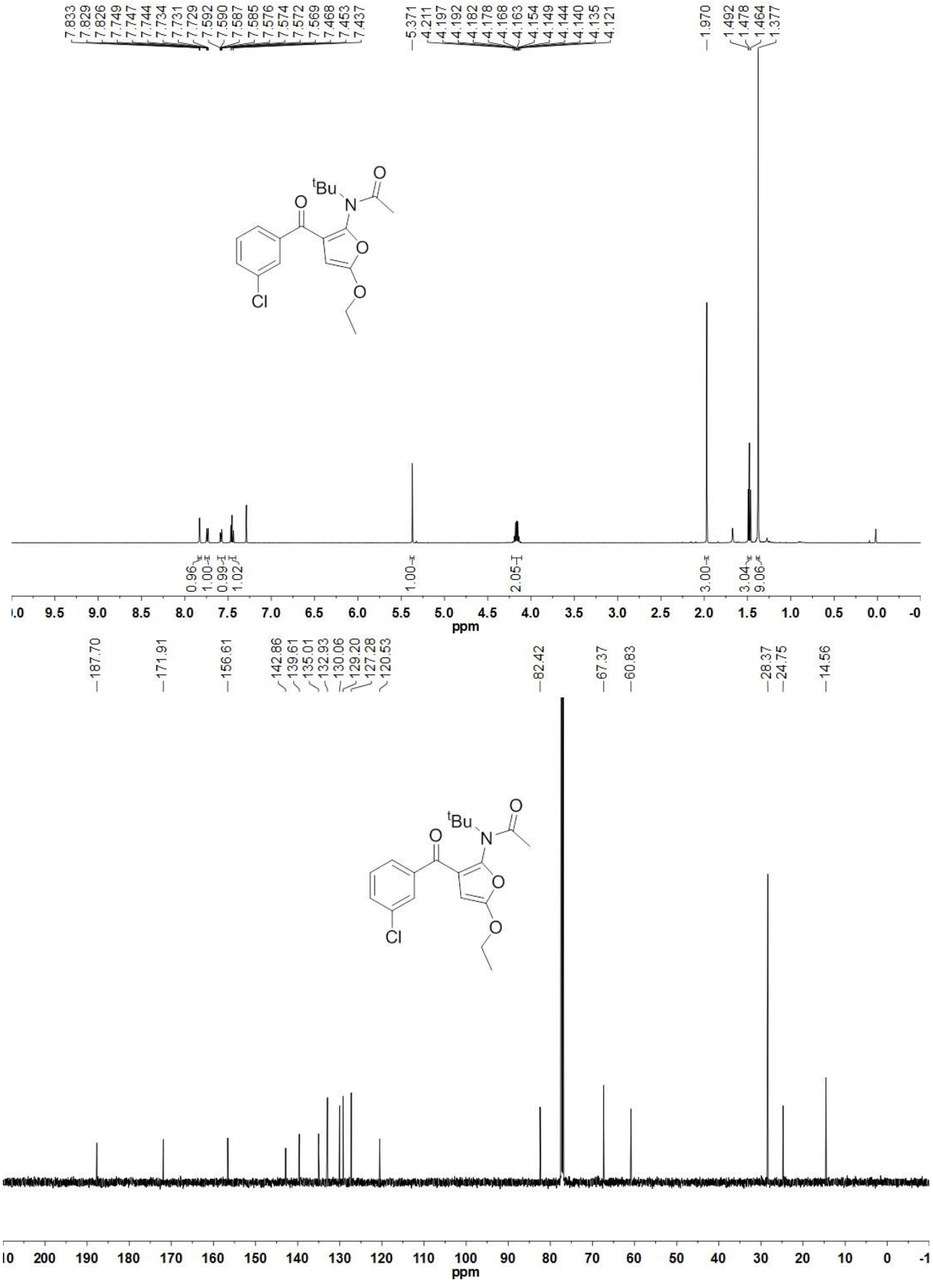
24.73
14.55
tBu
N
O
O
O
Br
OEt
ppm

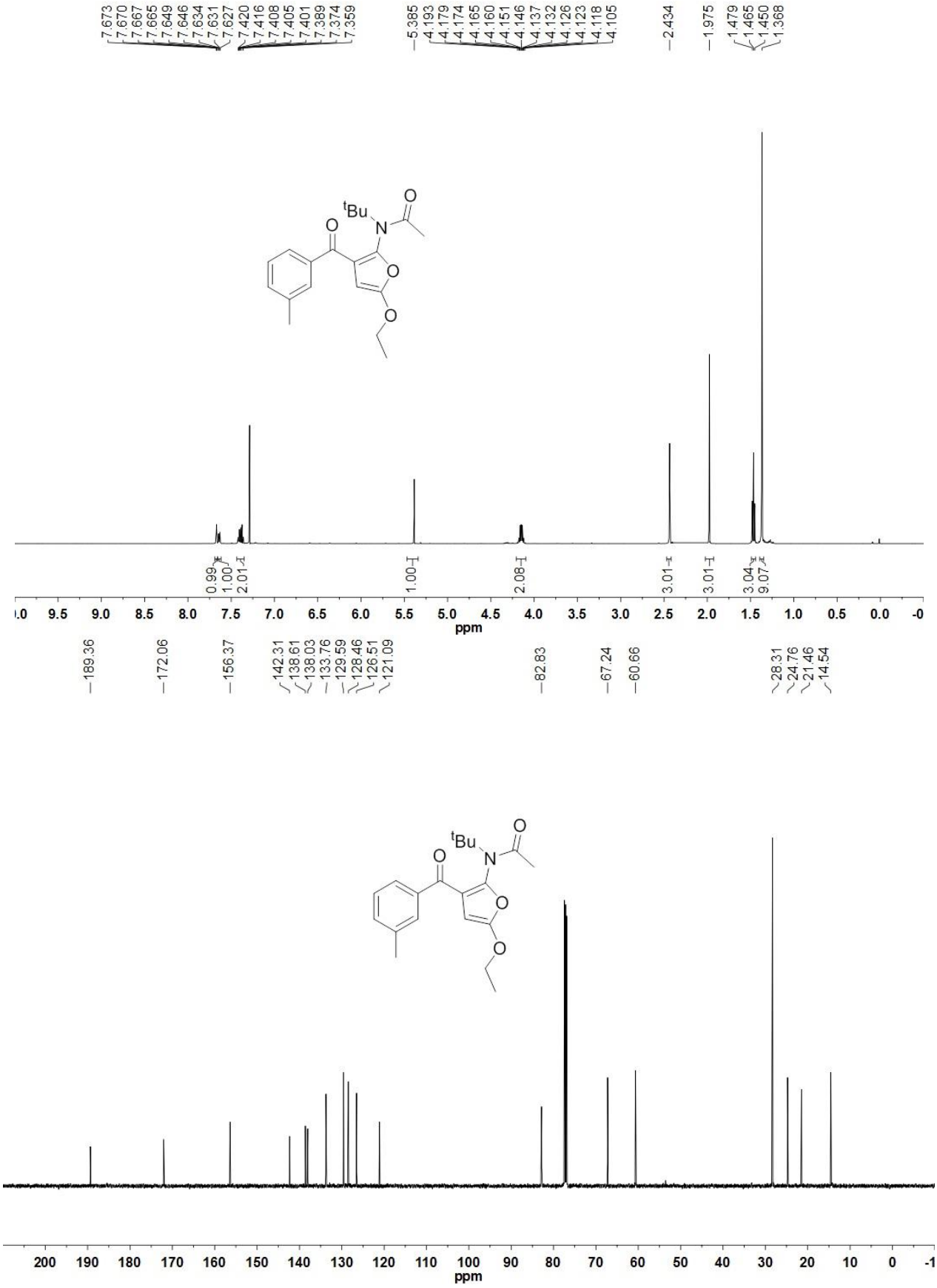
Compound 3f


7.934
7.929
7.924
7.918
7.915
7.911
7.905
7.900
7.894
7.207
7.202
7.197
7.190
7.185
7.181
7.178
7.171
7.167
7.161
5.365
4.207
4.193
4.188
4.180
4.174
4.166
4.160
4.152
4.146
4.138
4.133
4.119
1.974
1.491
1.477
1.463
1.380
tBu
N
O
O
O
F
O
2.03
2.09
1.00
2.05
3.00
3.03
9.06
ppm
187.57
172.06
166.74
164.71
156.52
142.45
134.30
134.27
131.91
131.84
120.73
115.99
115.82
82.59
67.32
60.75
28.35
24.77
14.57
ppm

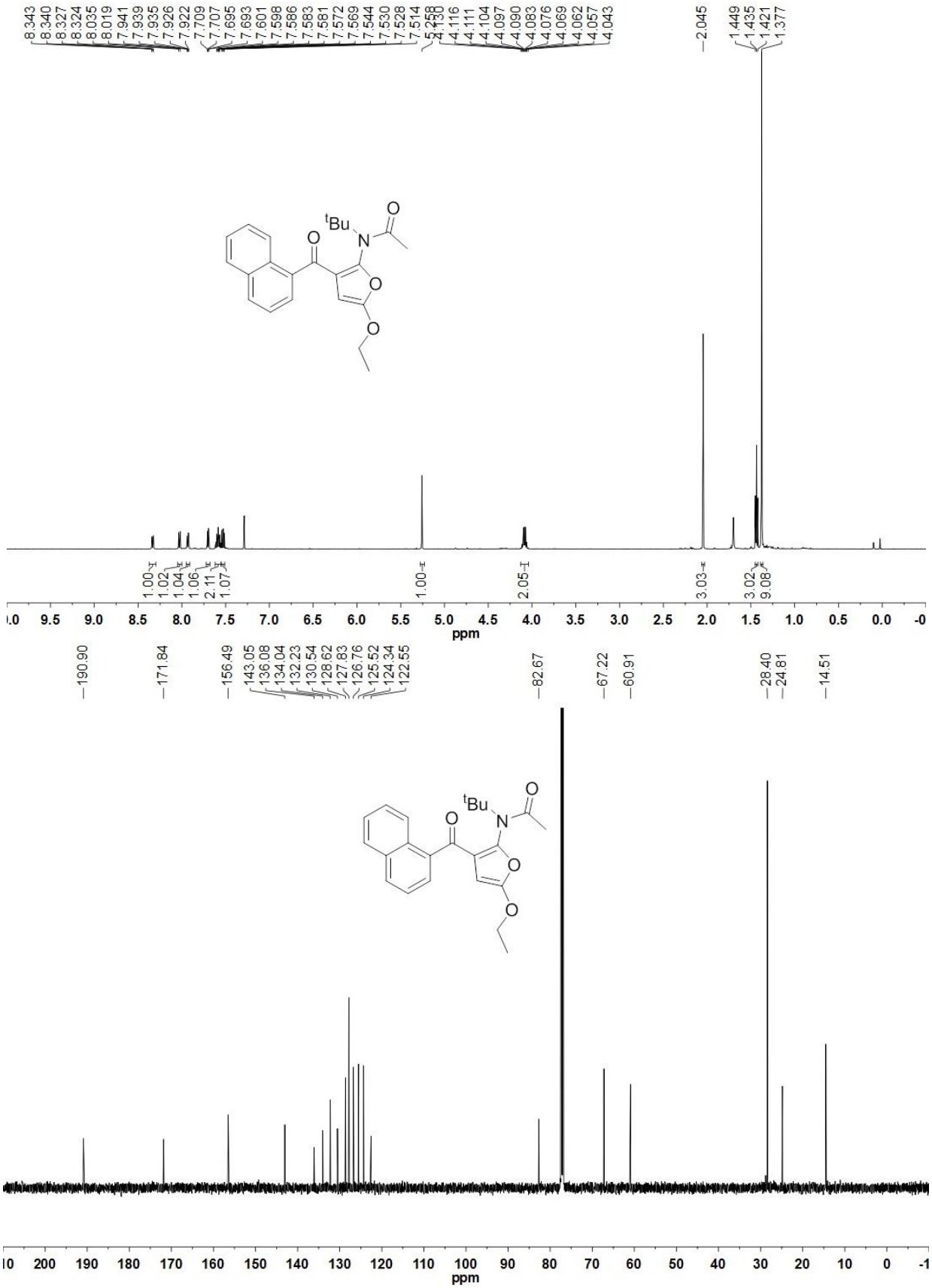
Compound 3g


7.833
7.829
7.826
7.749
7.747
7.744
7.734
7.731
7.729
7.592
7.590
7.587
7.585
7.576
7.574
7.572
7.569
7.468
7.453
7.437
5.371
4.211
4.197
4.192
4.182
4.178
4.168
4.163
4.154
4.149
4.144
4.140
4.135
4.121
1.970
1.492
1.478
1.464
1.377
tBu
N
O
O
O
O
Cl
0.96
1.00
0.99
1.02
1.00
2.05
3.00
3.04
9.06
ppm
187.70
171.91
156.61
142.86
139.61
135.01
132.93
130.06
129.20
127.28
120.53
82.42
67.37
60.83
28.37
24.75
14.56
ppm

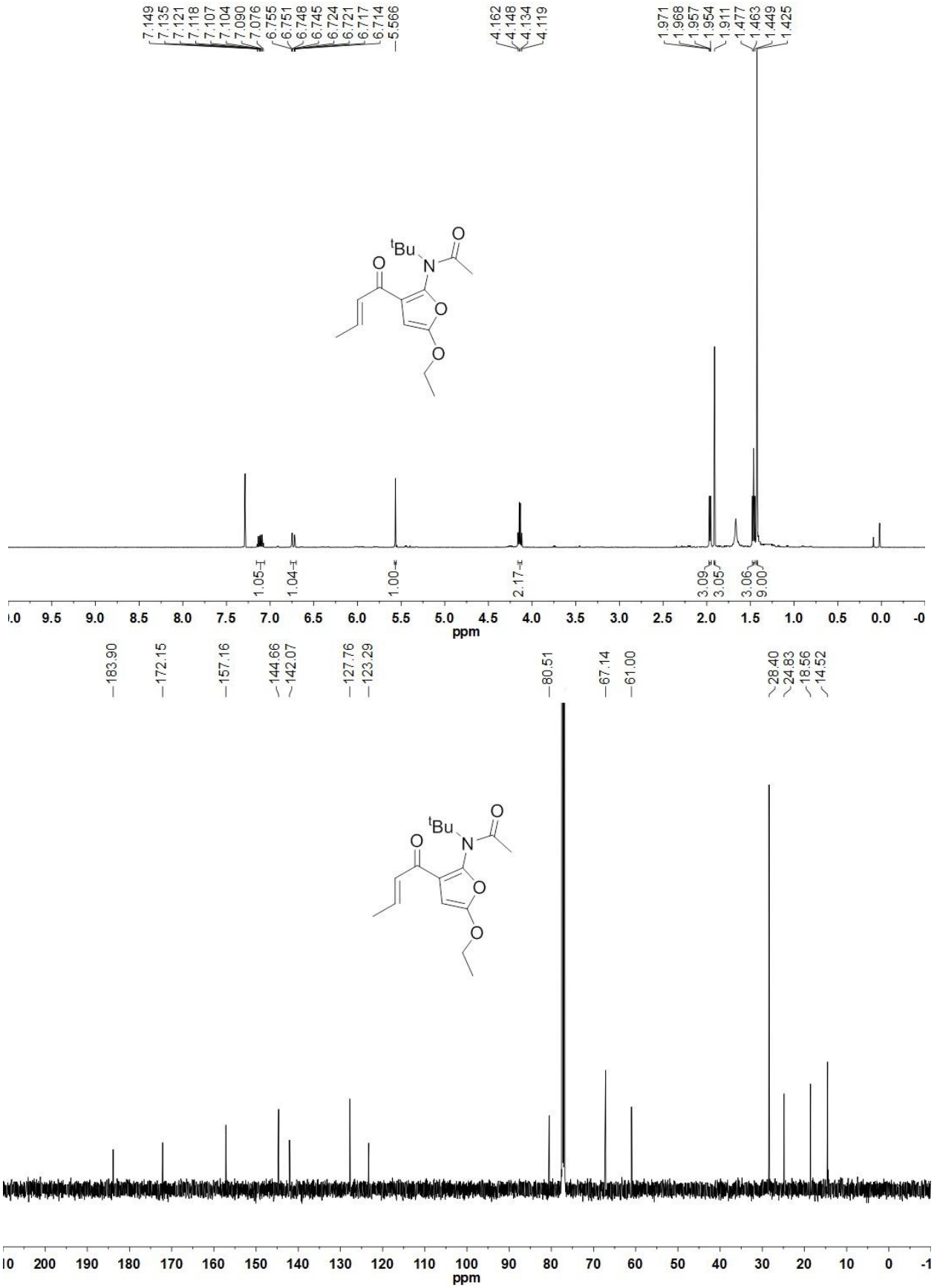
Compound 3h


7.673
7.670
7.667
7.665
7.649
7.646
7.634
7.631
7.627
7.420
7.416
7.408
7.405
7.401
7.389
7.374
7.359
5.385
4.193
4.179
4.174
4.165
4.160
4.151
4.146
4.137
4.132
4.126
4.123
4.118
4.105
2.434
1.975
1.479
1.465
1.450
1.368
tBu
N
O
O
O
O
0.99
1.00
2.01
1.00
2.08
3.01
3.01
3.04
9.07
ppm
189.36
172.06
156.37
142.31
138.61
138.03
133.76
129.59
128.46
126.51
121.09
82.83
67.24
60.66
28.31
24.76
21.46
14.54
ppm

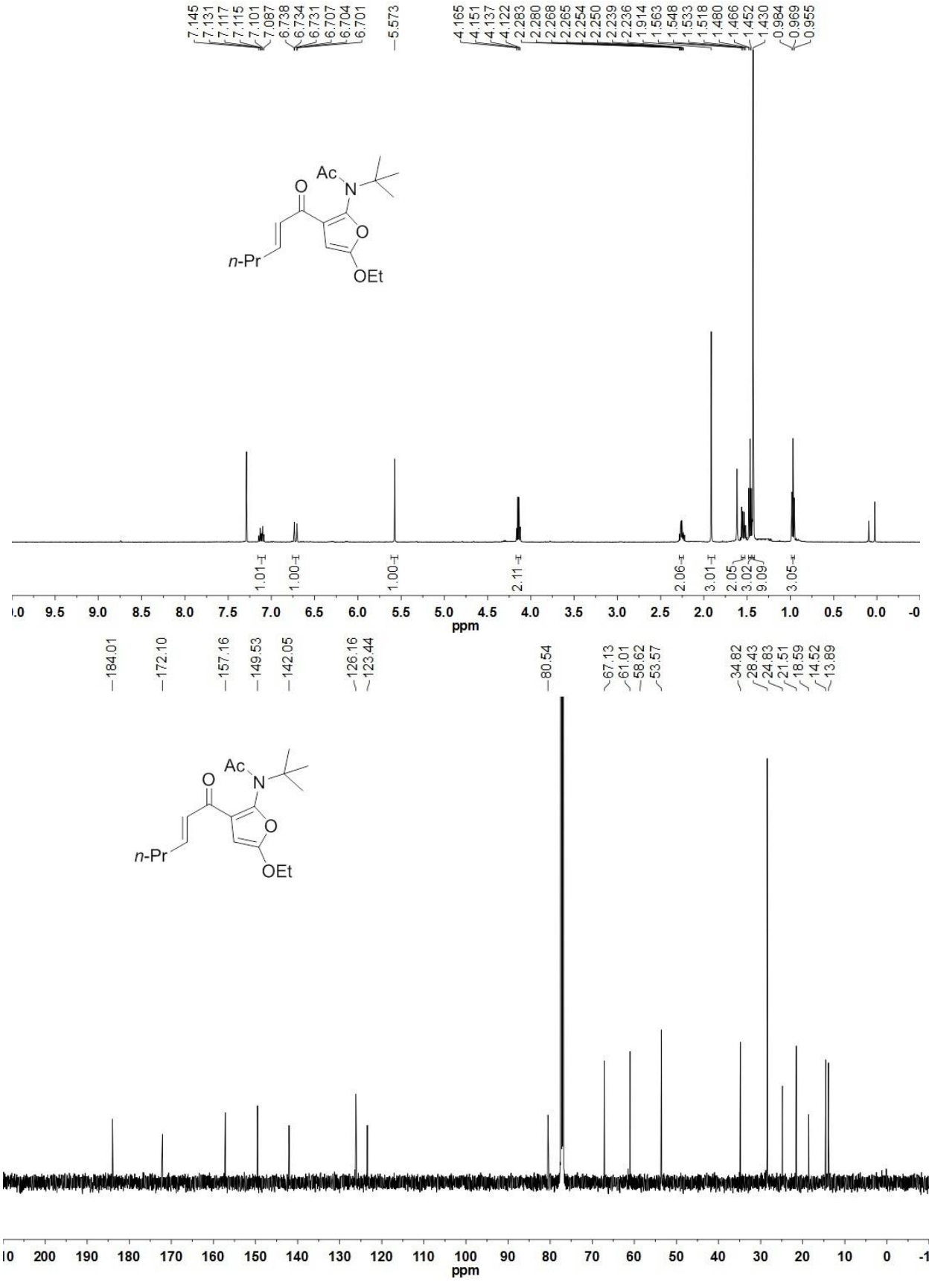
Compound 3i


8.343
8.340
8.327
8.324
8.035
8.019
7.941
7.939
7.935
7.926
7.922
7.709
7.707
7.695
7.693
7.601
7.598
7.586
7.583
7.581
7.572
7.569
7.544
7.530
7.528
7.514
5.158
5.130
4.116
4.111
4.104
4.097
4.090
4.083
4.076
4.069
4.062
4.057
4.043
2.045
1.449
1.435
1.421
1.377
tBu
N
O
O
O
O
1.00
1.02
1.04
1.06
2.11
1.07
1.00
2.05
3.03
3.02
9.08
ppm
190.90
171.84
156.49
143.05
136.08
134.04
132.23
130.54
128.62
127.83
126.76
125.52
124.34
122.55
82.67
67.22
60.91
28.40
24.81
14.51
ppm

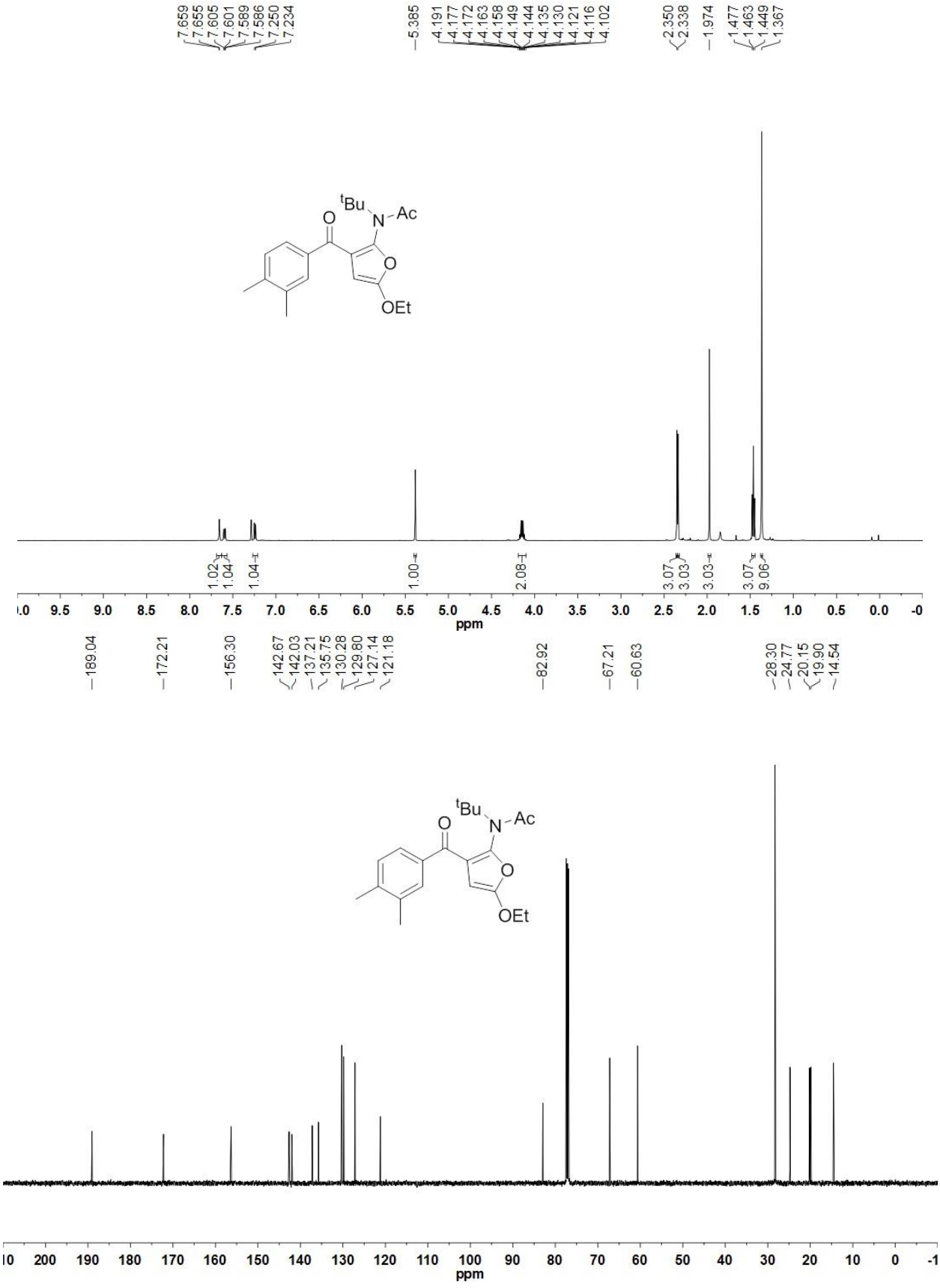
Compound 3j


7.149
7.135
7.121
7.118
7.107
7.104
7.090
7.076
6.755
6.751
6.748
6.745
6.724
6.721
6.717
6.714
5.566
4.162
4.148
4.134
4.119
1.971
1.968
1.957
1.954
1.911
1.477
1.463
1.449
1.425
tBu
N
O
1.05
1.04
1.00
2.17
3.09
3.05
3.06
9.00
ppm
183.90
172.15
157.16
144.66
142.07
127.76
123.29
80.51
67.14
61.00
28.40
24.83
18.56
14.52
ppm

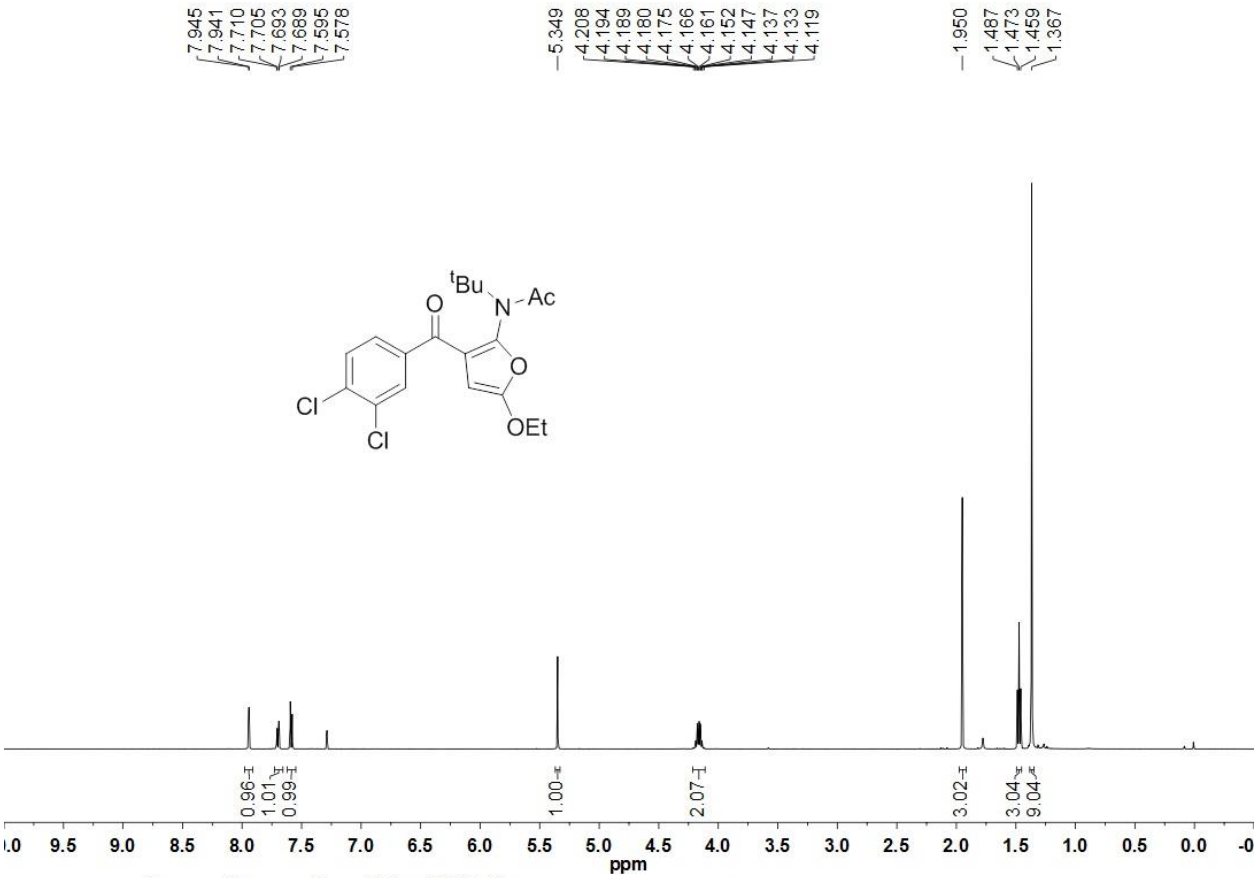
Compound 3k

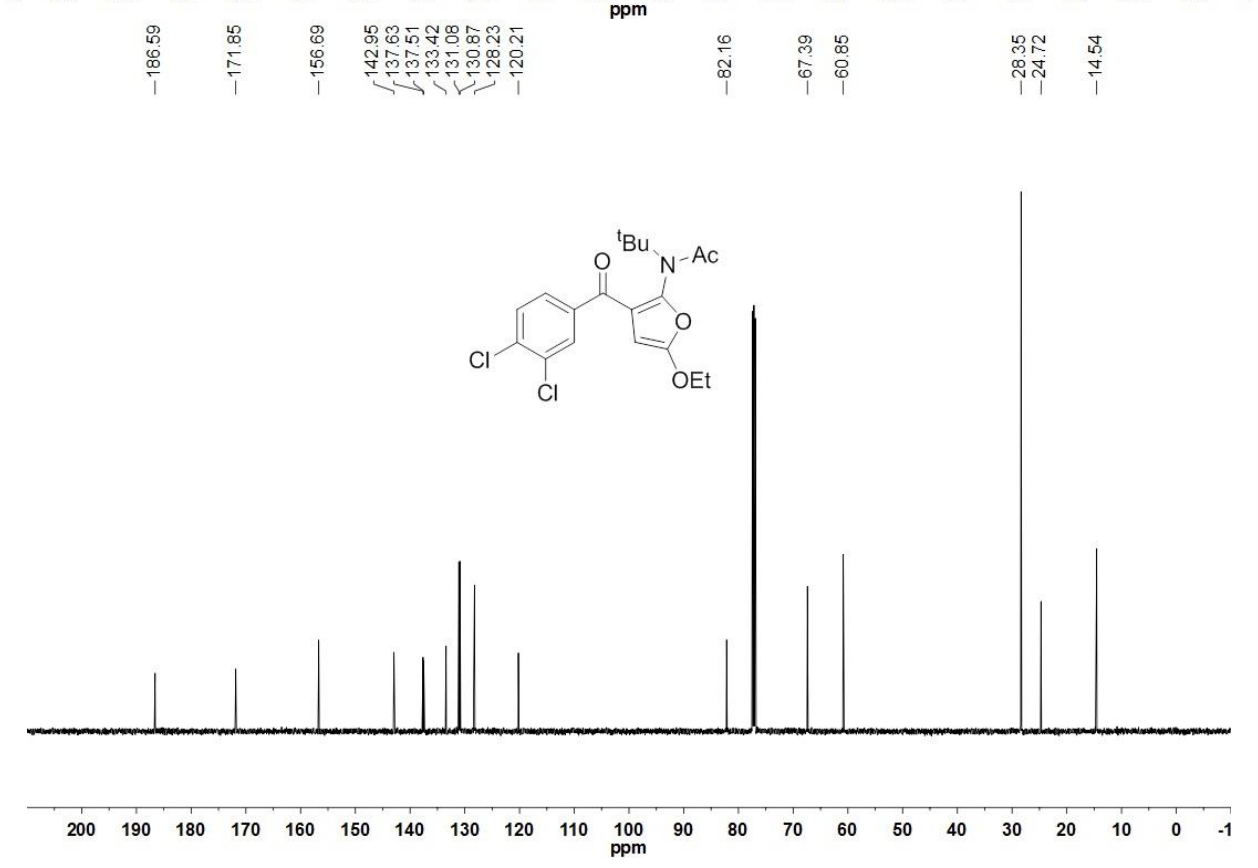

7.145
7.131
7.117
7.115
7.101
7.087
6.738
6.734
6.731
6.707
6.704
6.701
5.573
4.165
4.151
4.137
4.122
2.283
2.280
2.268
2.265
2.254
2.250
2.239
2.236
1.914
1.563
1.548
1.533
1.518
1.480
1.466
1.452
1.430
0.984
0.969
0.955
Ac
N
O
O
n-Pr
OEt
1.01
1.00
1.00
2.11
2.06
3.01
2.05
3.02
9.09
3.05
ppm
184.01
172.10
157.16
149.53
142.05
126.16
123.44
80.54
67.13
61.01
58.62
53.57
34.82
28.43
24.83
21.51
18.59
14.52
13.89
ppm

Compound 3l

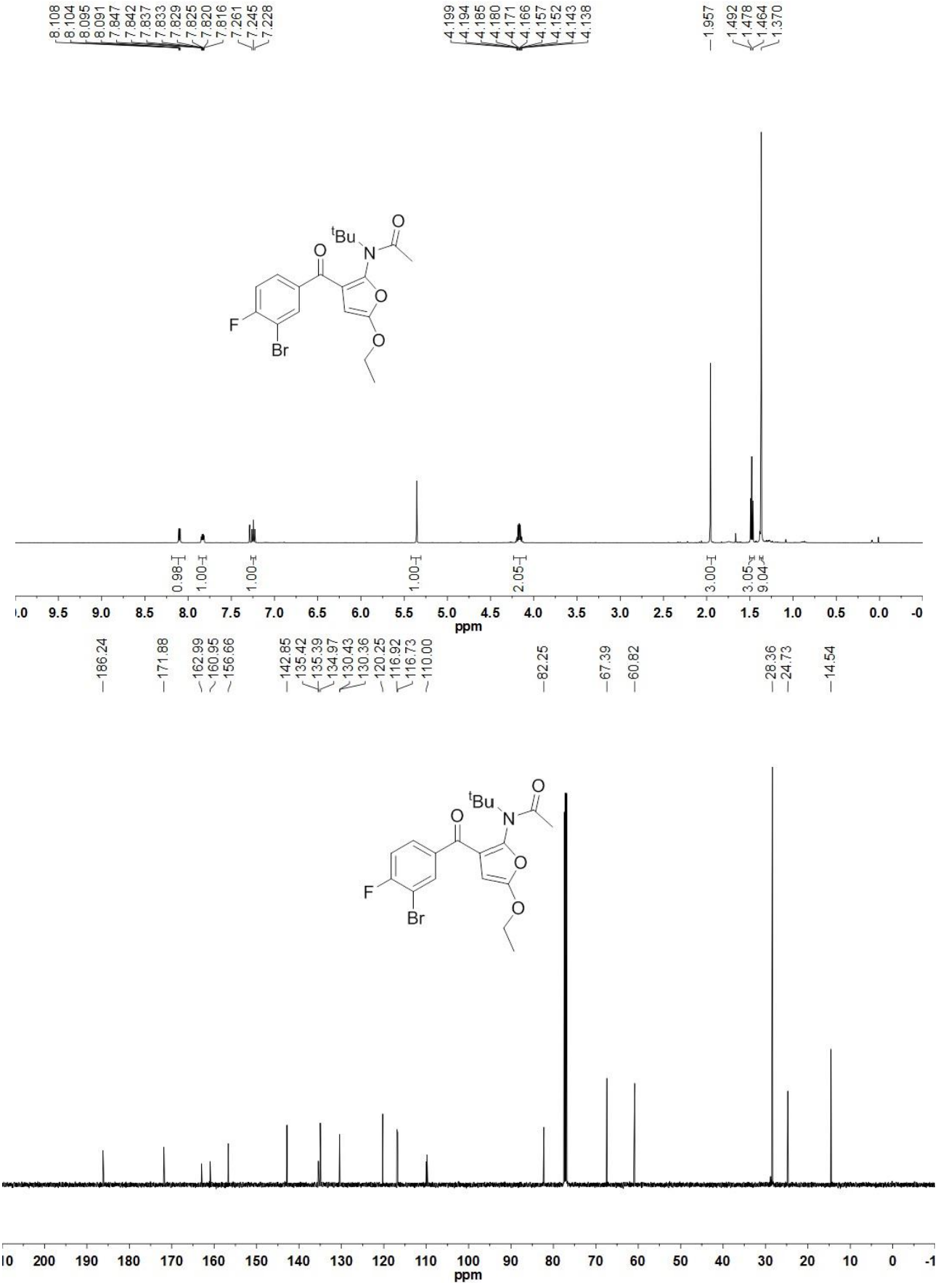

7.659
7.655
7.605
7.601
7.589
7.586
7.250
7.234
5.385
4.191
4.177
4.172
4.163
4.158
4.149
4.144
4.135
4.130
4.121
4.116
4.102
2.350
2.338
1.974
1.477
1.463
1.449
1.367
tBu
N
Ac
O
O
OEt
1.02
1.04
1.04
1.00
2.08
3.07
3.03
3.03
3.07
9.06
ppm
189.04
172.21
156.30
142.67
142.03
137.21
135.75
130.28
129.80
127.14
121.18
82.92
67.21
60.63
28.30
24.77
20.15
19.90
14.54
ppm

Compound 3m

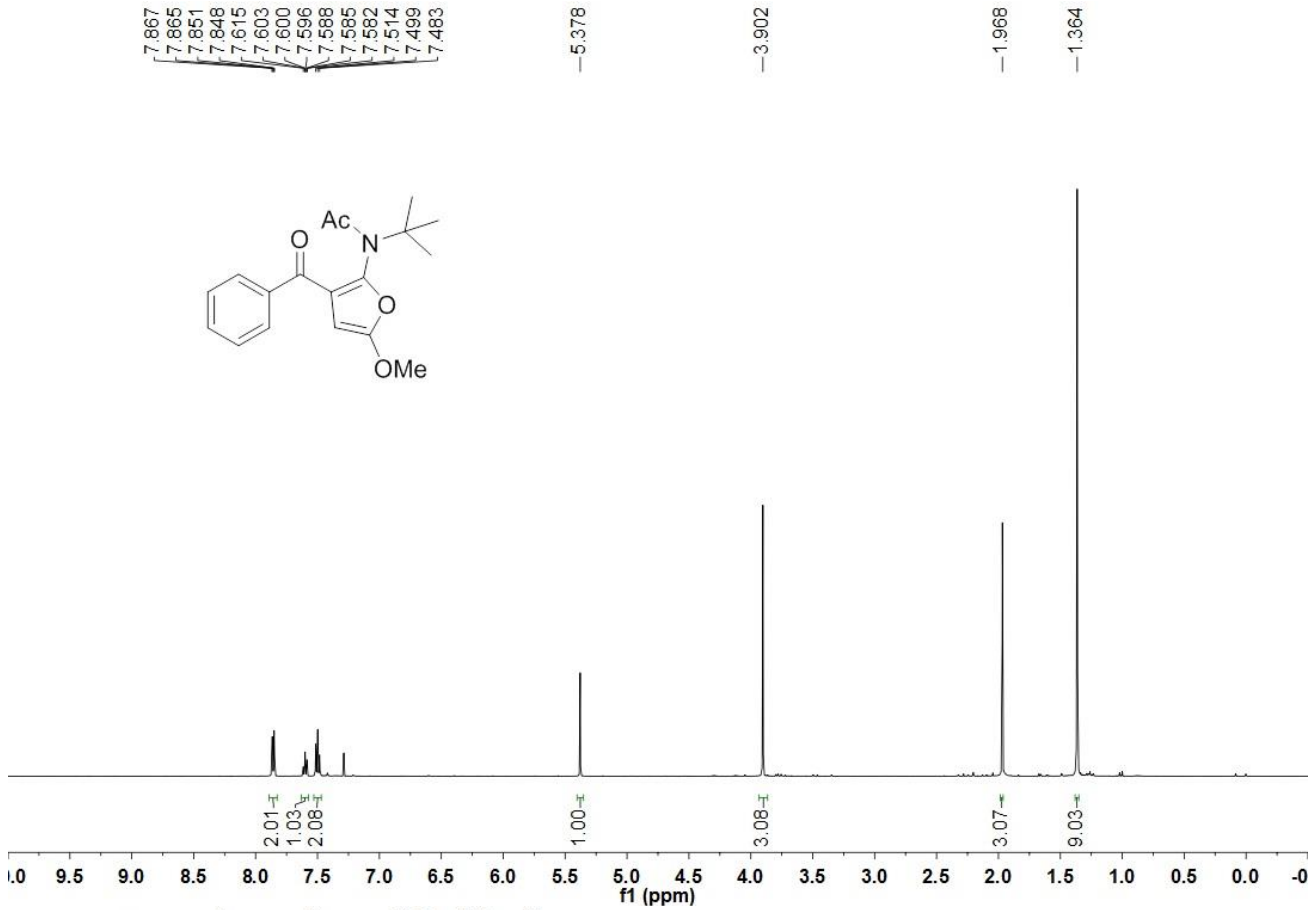

7.945
7.941
7.710
7.705
7.693
7.689
7.595
7.578
5.349
4.208
4.194
4.189
4.180
4.175
4.166
4.161
4.152
4.147
4.137
4.133
4.119
1.950
1.487
1.473
1.459
1.367
tBu
N
Ac
O
O
Cl
Cl
OEt
0.96
1.01
0.99
1.00
2.07
3.02
3.04
9.04
ppm

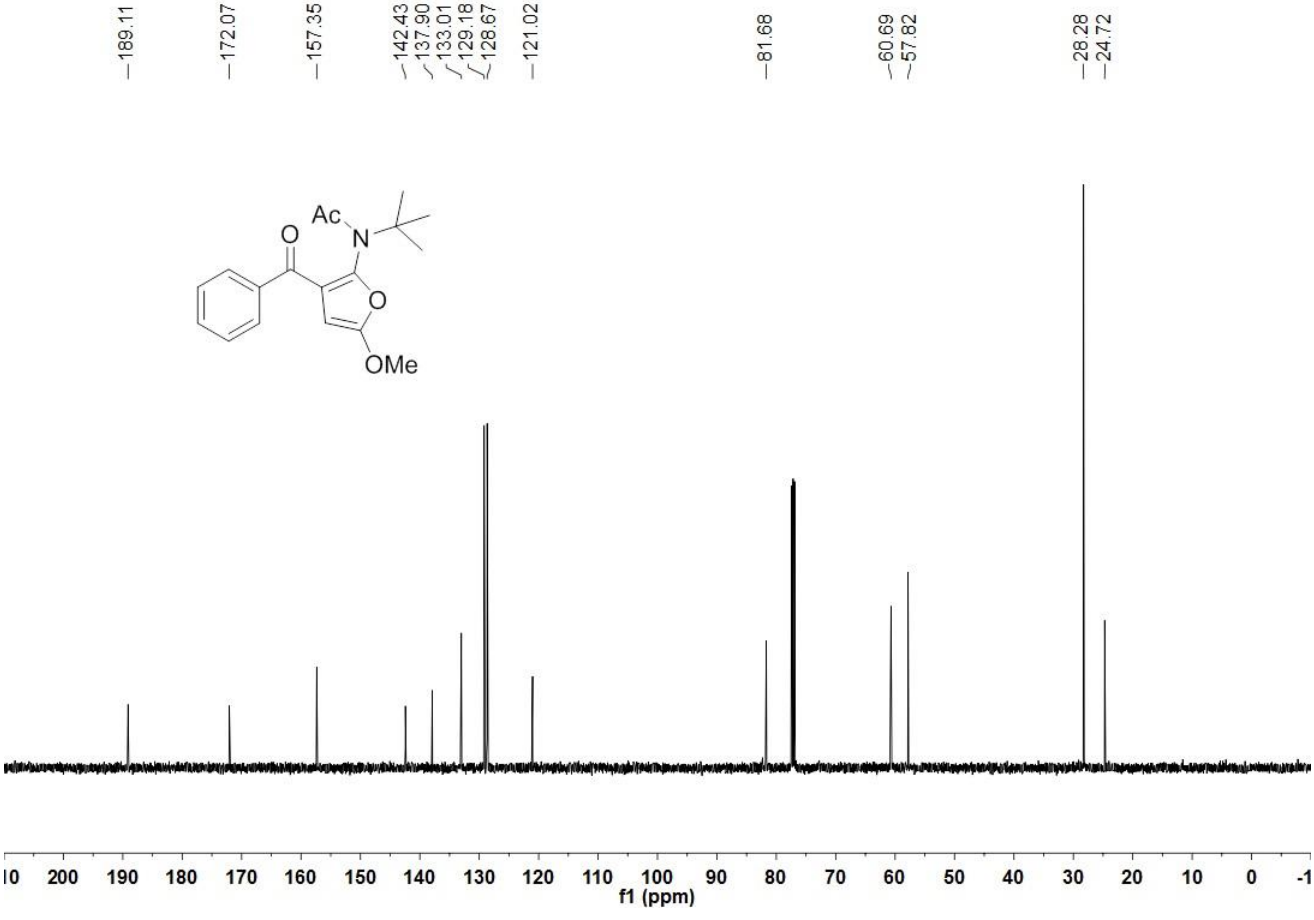

186.59
171.85
156.69
142.95
137.63
137.51
133.42
131.08
130.87
128.23
120.21
82.16
67.39
60.85
28.35
24.72
14.54
tBu
N
Ac
O
O
Cl
Cl
OEt
ppm

Compound 3n

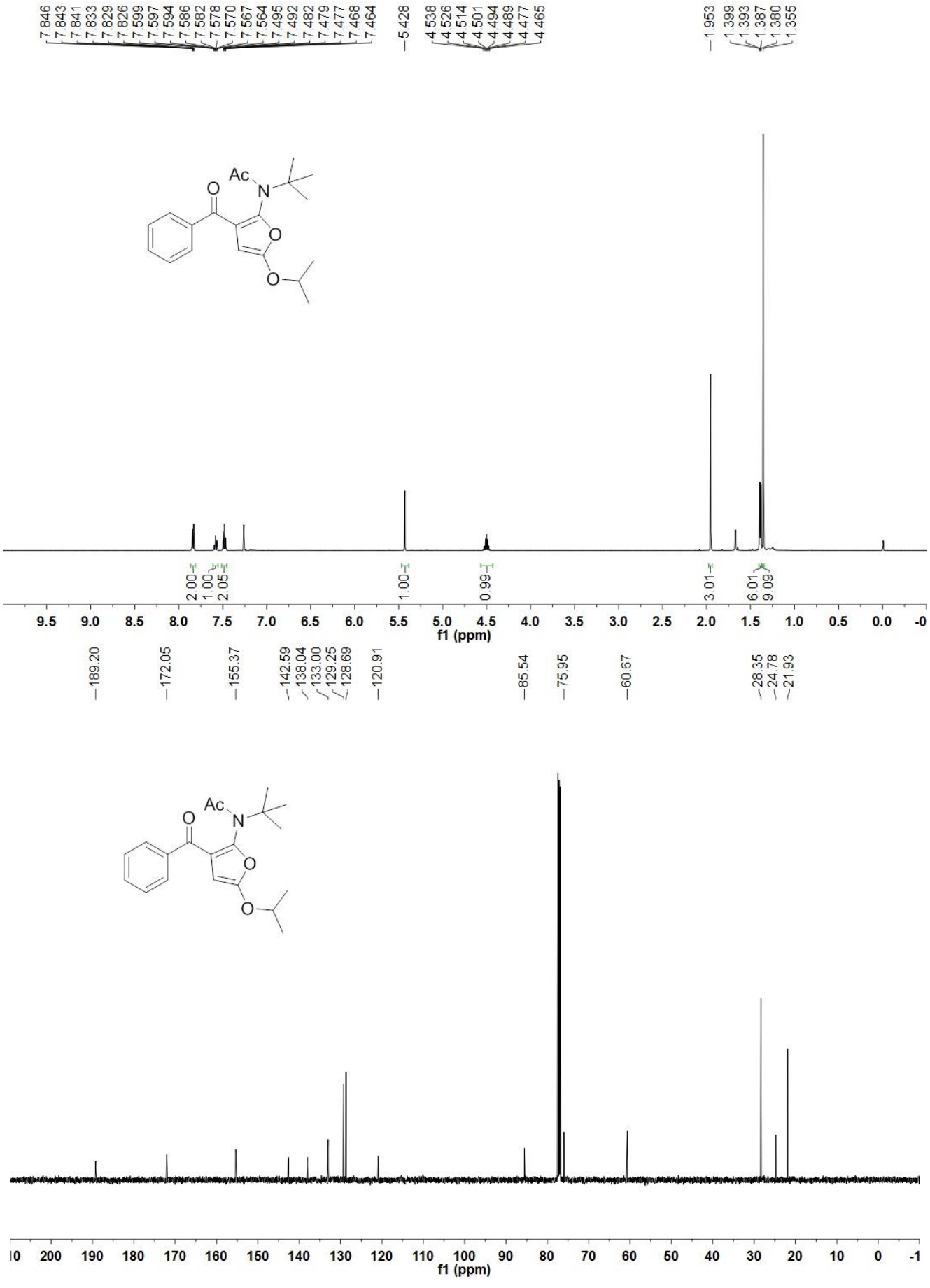

8.108
8.104
8.095
8.091
7.847
7.842
7.837
7.833
7.829
7.825
7.820
7.816
7.261
7.245
7.228
4.199
4.194
4.185
4.180
4.171
4.166
4.157
4.152
4.143
4.138
1.957
1.492
1.478
1.464
1.370
tBu
N
O
O
O
O
F
Br
0.98
1.00
1.00
1.00
2.05
3.00
3.05
9.04
ppm
186.24
171.88
162.99
160.95
156.66
142.85
135.42
135.39
134.97
130.43
130.36
120.25
116.92
116.73
110.00
82.25
67.39
60.82
28.36
24.73
14.54
ppm

Compound 3o

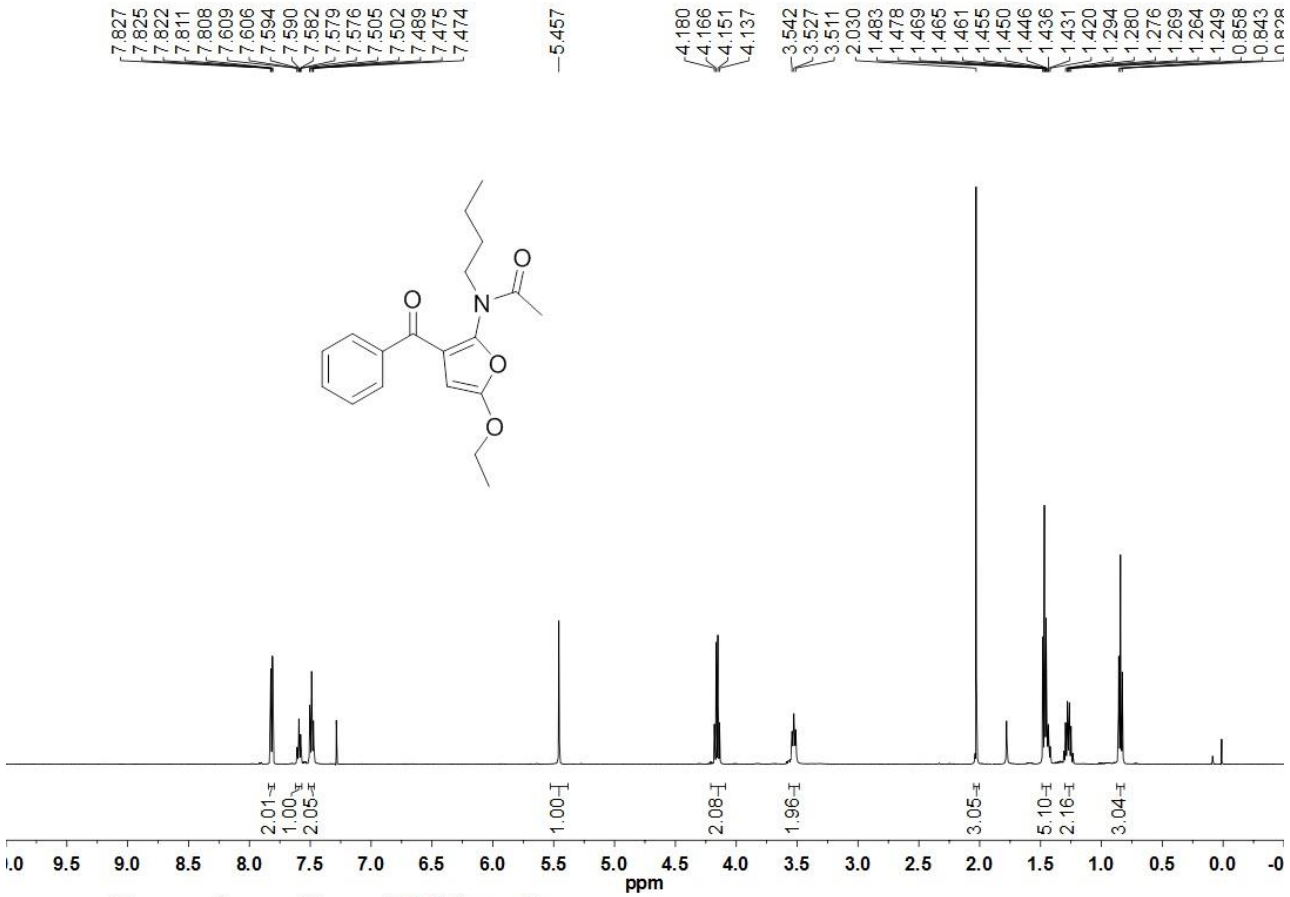

7.867
7.865
7.851
7.848
7.615
7.603
7.600
7.596
7.588
7.585
7.582
7.514
7.499
7.483
5.378
3.902
1.968
1.364
Ac
N
O
O
OMe
2.01
1.03
2.08
1.00
3.08
3.07
9.03
f1 (ppm)

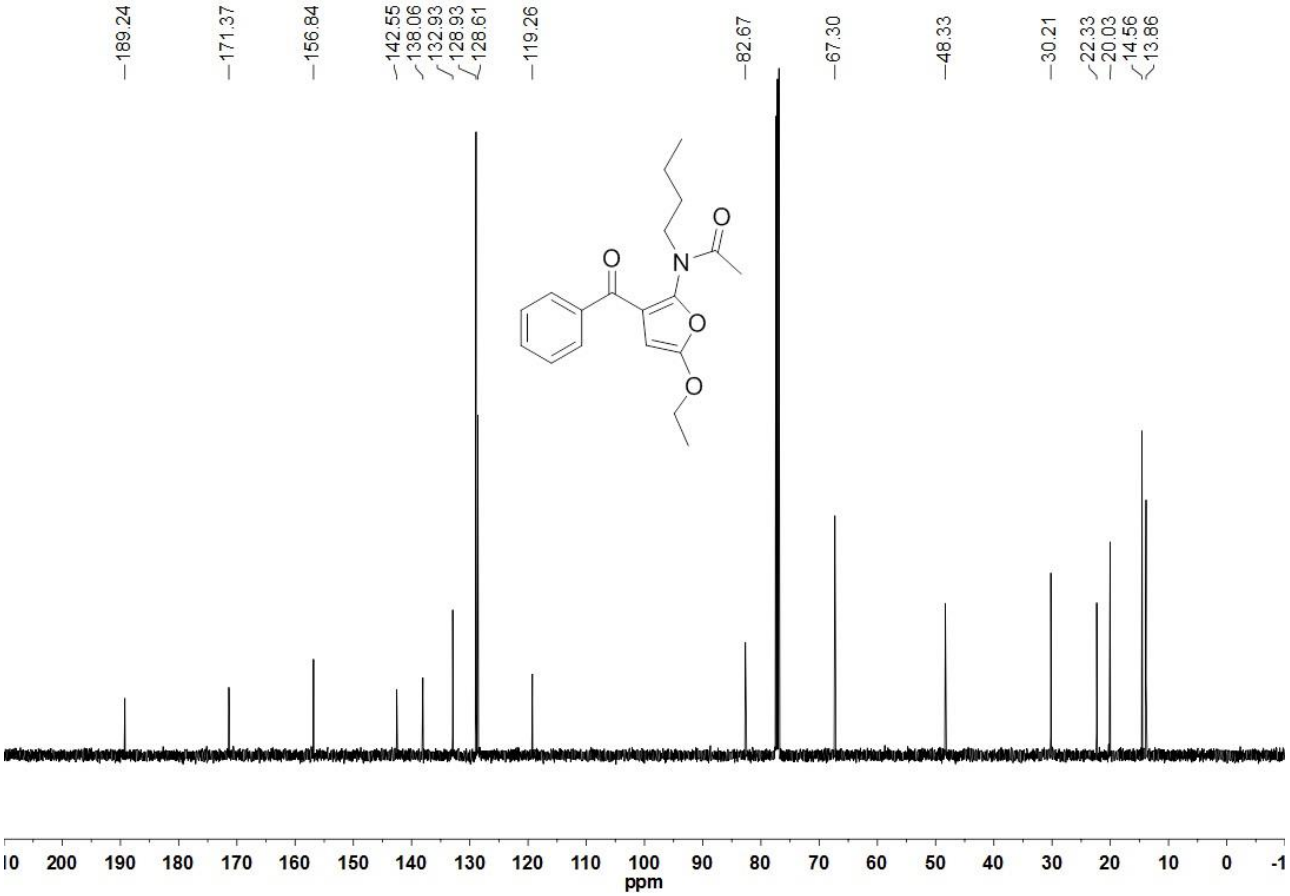

189.11
172.07
157.35
142.43
137.90
133.01
129.18
128.67
121.02
81.68
60.69
57.82
28.28
24.72
Ac
N
O
O
OMe
f1 (ppm)

Compound 3p

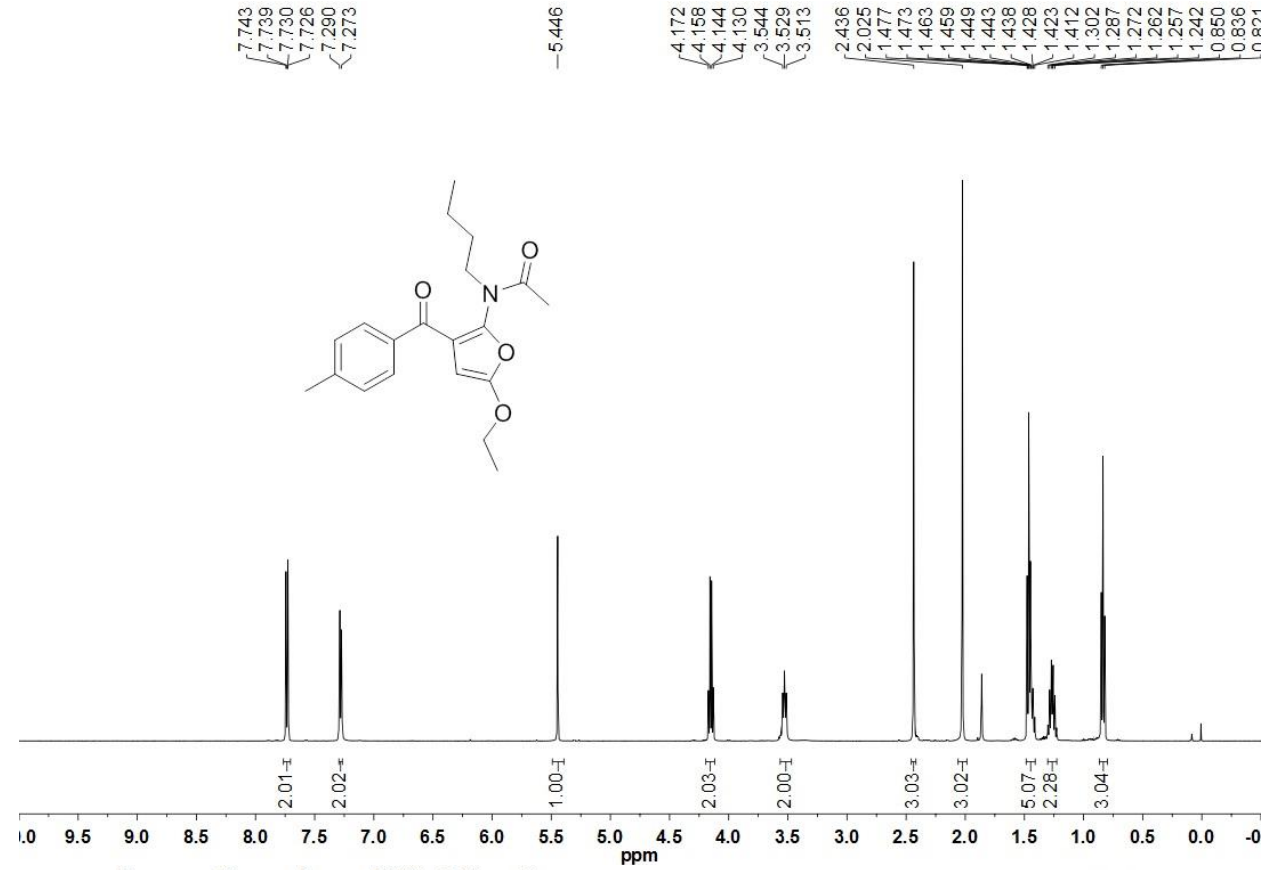

7.846
7.843
7.841
7.833
7.829
7.826
7.599
7.597
7.594
7.586
7.582
7.578
7.570
7.567
7.564
7.495
7.492
7.482
7.479
7.477
7.468
7.464
5.428
4.538
4.526
4.514
4.501
4.494
4.489
4.477
4.465
1.953
1.399
1.393
1.387
1.380
1.355
Ac
N
O
O
O
2.00
1.00
2.05
1.00
0.99
3.01
6.01
9.09
f1 (ppm)
189.20
172.05
155.37
142.59
138.04
133.00
129.25
128.69
120.91
85.54
75.95
60.67
28.35
24.78
21.93
f1 (ppm)

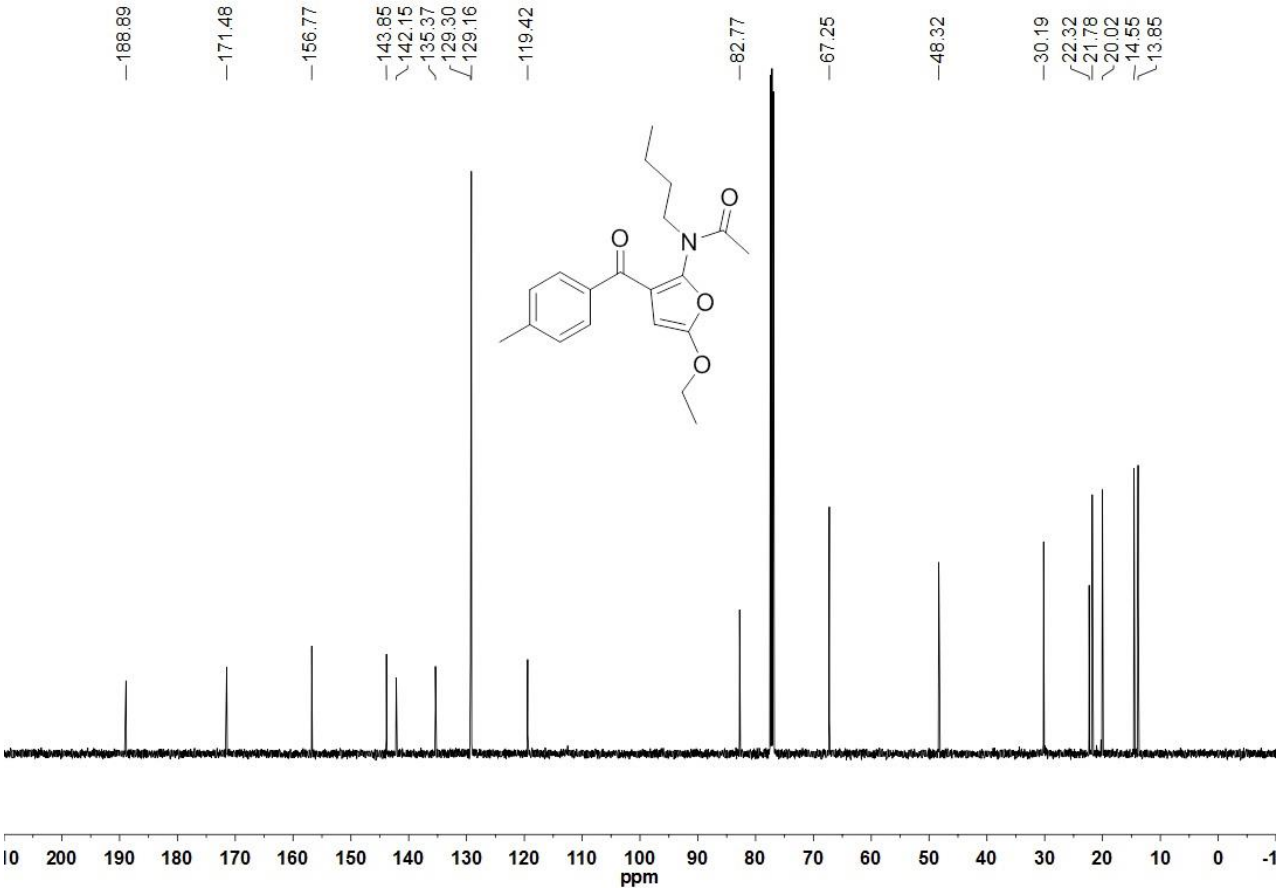
Compound 4a


7.827
7.825
7.822
7.811
7.808
7.609
7.606
7.594
7.590
7.582
7.579
7.576
7.505
7.502
7.489
7.475
7.474
5.457
4.180
4.166
4.151
4.137
3.542
3.527
3.511
2.030
1.483
1.478
1.469
1.465
1.461
1.455
1.450
1.446
1.436
1.431
1.420
1.294
1.280
1.276
1.269
1.264
1.249
0.858
0.843
2.01
1.00
2.05
1.00
2.08
1.96
3.05
5.10
2.16
3.04
ppm

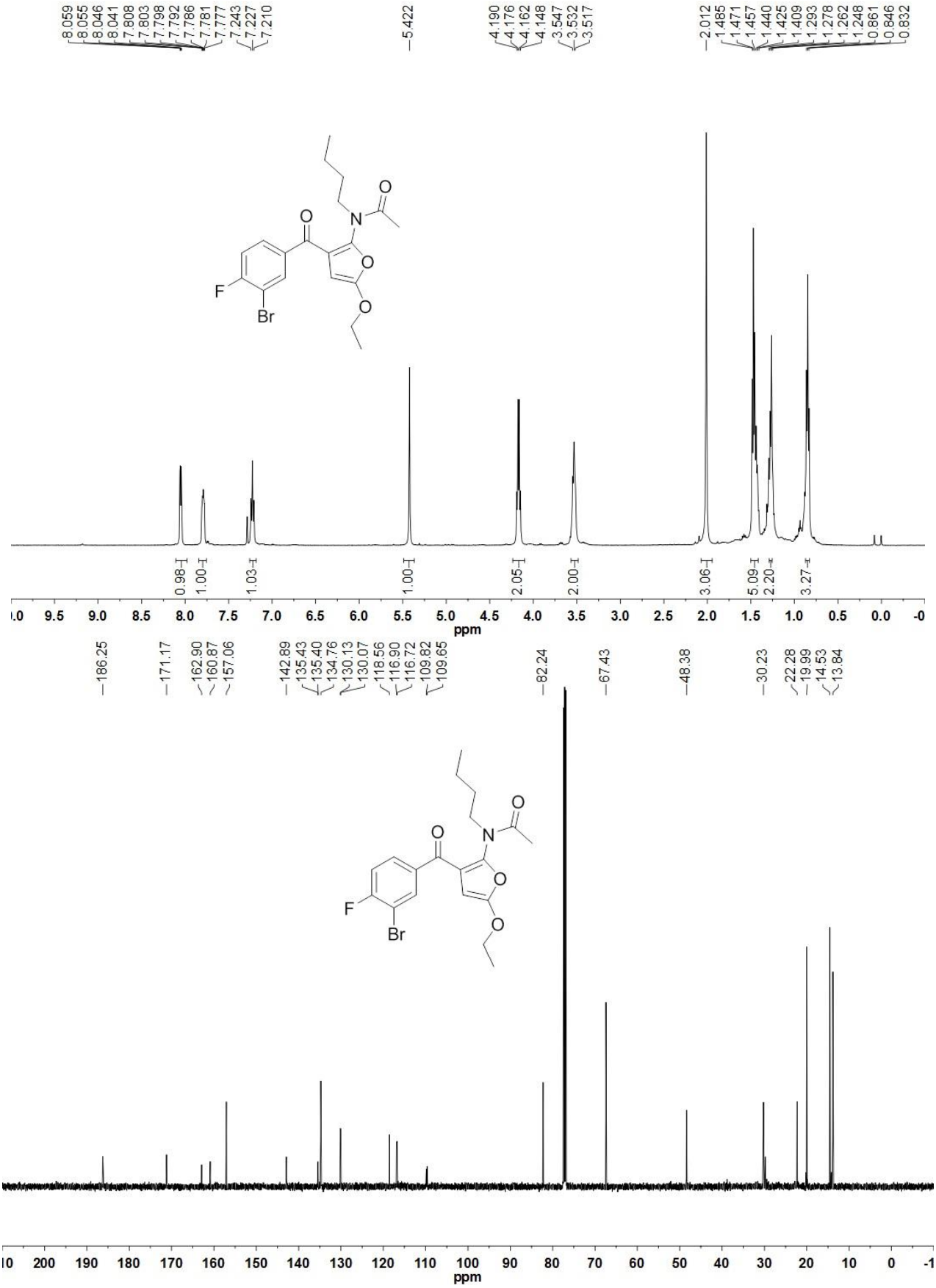

189.24
171.37
156.84
142.55
138.06
132.93
128.93
128.61
119.26
82.67
67.30
48.33
30.21
22.33
20.03
14.56
13.86
ppm

Compound 4b

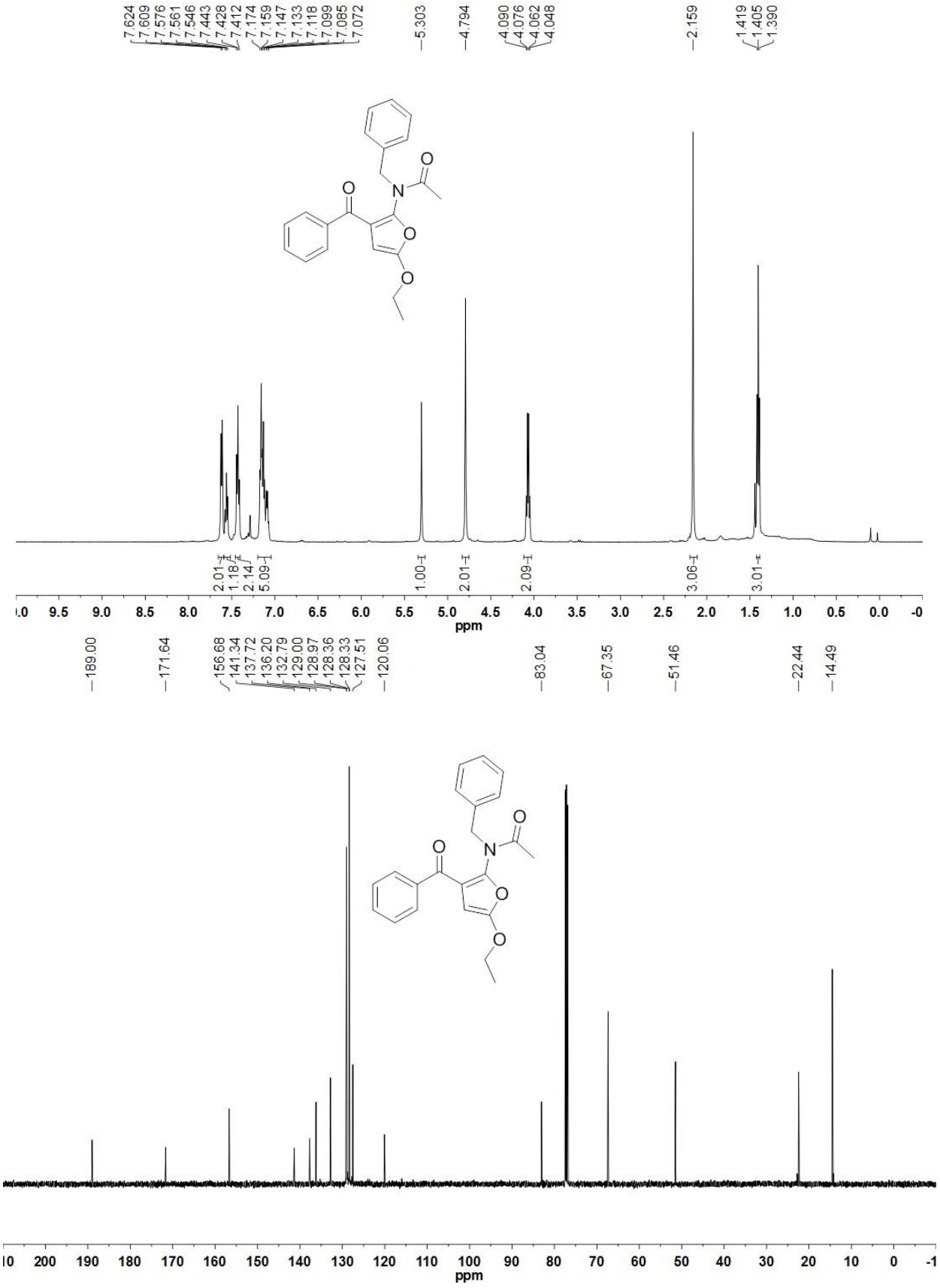

7.743
7.739
7.730
7.726
7.290
7.273
5.446
4.172
4.158
4.144
4.130
3.544
3.529
3.513
2.436
2.025
1.477
1.473
1.463
1.459
1.449
1.443
1.438
1.428
1.423
1.412
1.302
1.287
1.272
1.262
1.257
1.242
0.850
0.836
2.01
2.02
1.00
2.03
2.00
3.03
3.02
5.07
2.28
3.04
ppm


188.89
171.48
156.77
143.85
142.15
135.37
129.30
129.16
119.42
82.77
67.25
48.32
30.19
22.32
21.78
20.02
14.55
13.85
ppm

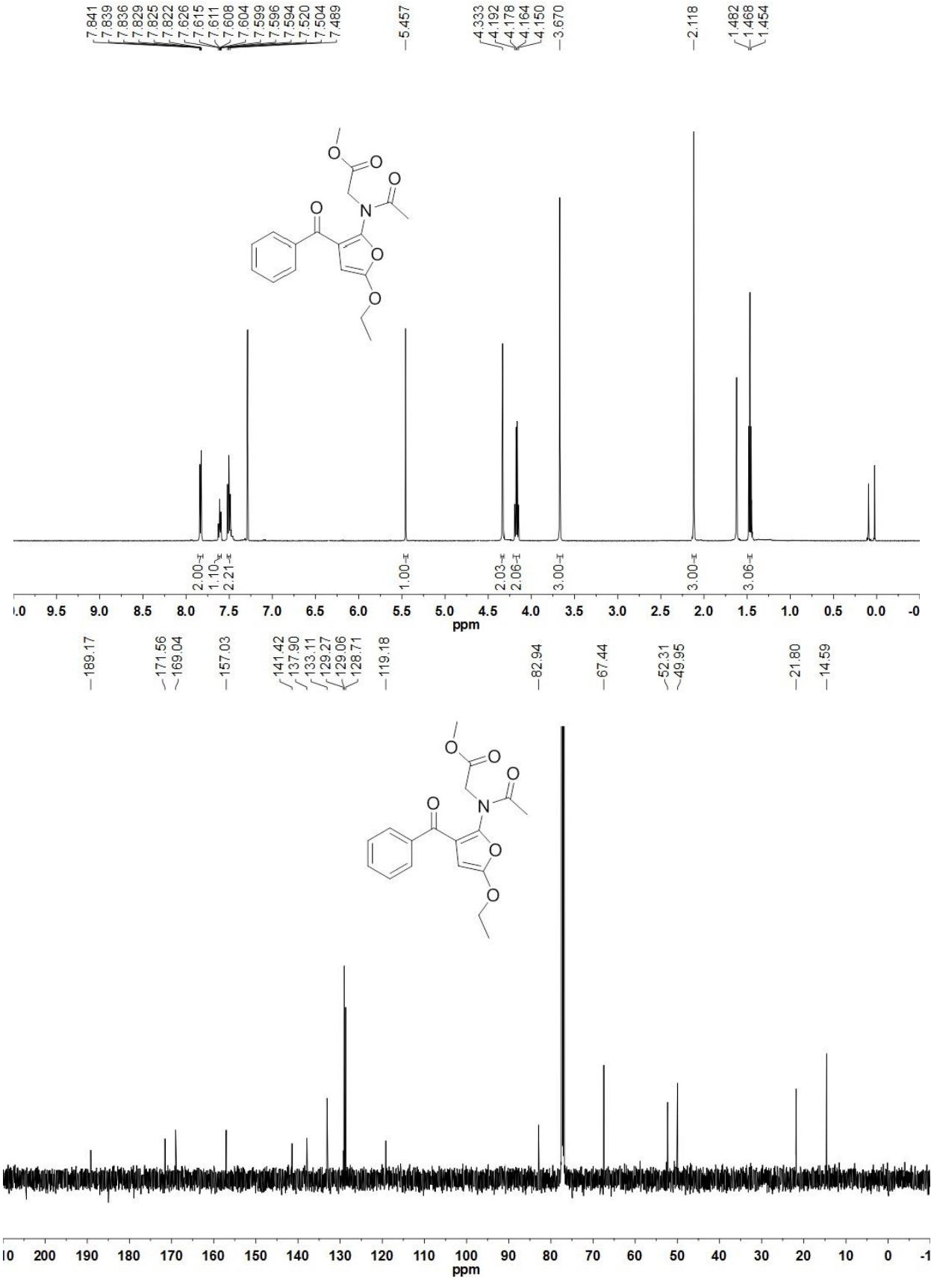
Compound 4c


8.059
8.055
8.046
8.041
7.808
7.803
7.798
7.792
7.786
7.781
7.777
7.243
7.227
7.210
5.422
4.190
4.176
4.162
4.148
3.547
3.532
3.517
2.012
1.485
1.471
1.457
1.440
1.425
1.409
1.293
1.278
1.262
1.248
0.861
0.846
0.832
O
N
O
O
O
F
Br
0.98
1.00
1.03
1.00
2.05
2.00
3.06
5.09
2.20
3.27
ppm
186.25
171.17
162.90
160.87
157.06
142.89
135.43
135.40
134.76
130.13
130.07
118.56
116.90
116.72
109.82
109.65
82.24
67.43
48.38
30.23
22.28
19.99
14.53
13.84
ppm

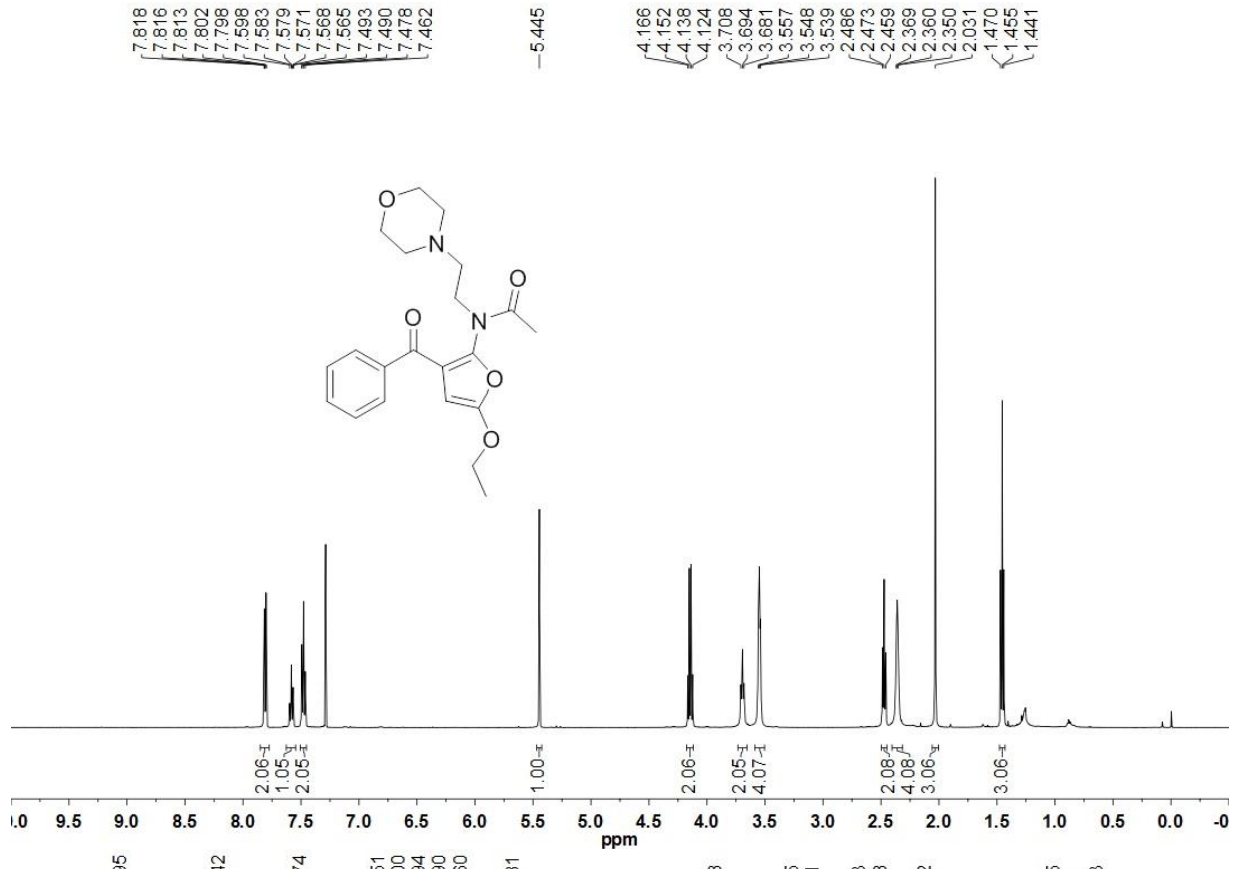
Compound 4d

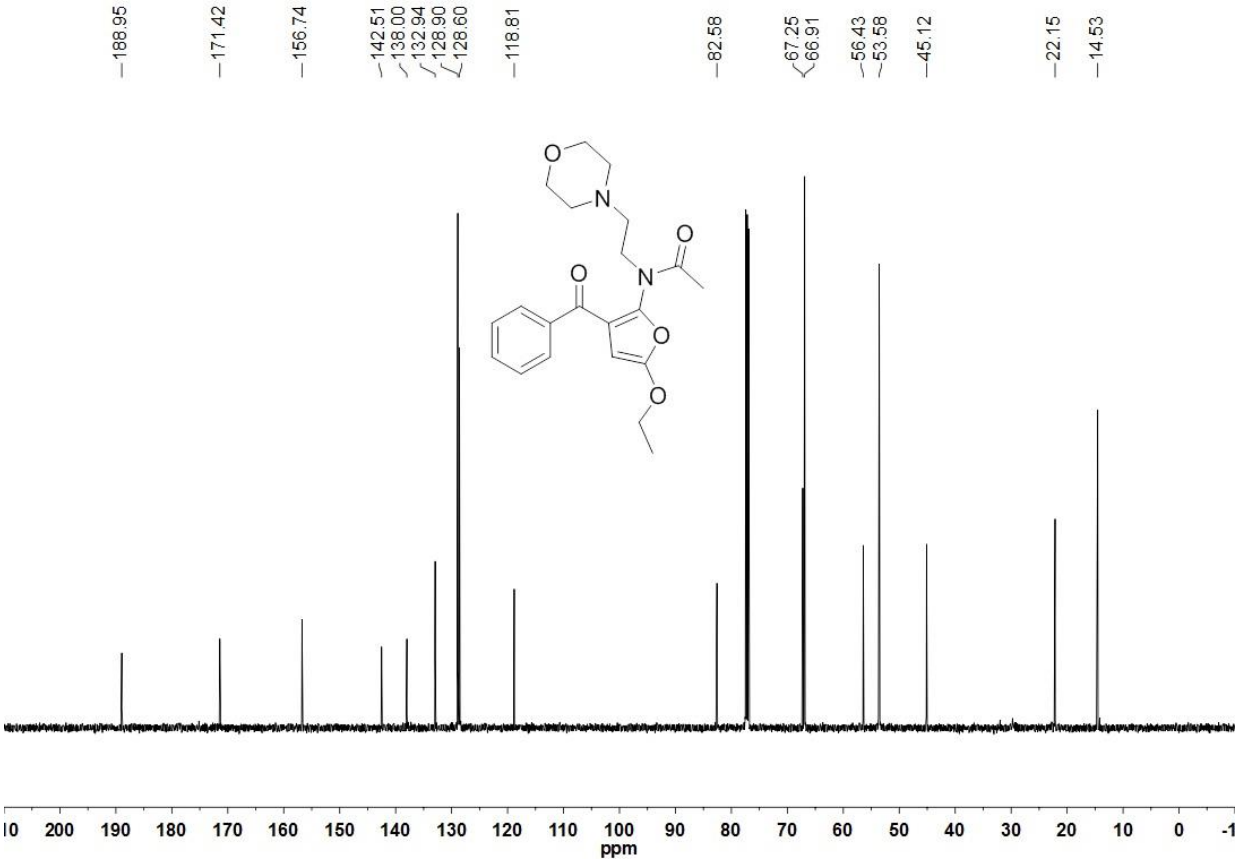

7.624
7.609
7.576
7.561
7.546
7.443
7.428
7.412
7.174
7.159
7.147
7.133
7.118
7.099
7.085
7.072
5.303
4.794
4.090
4.076
4.062
4.048
2.159
1.419
1.405
1.390
2.01
1.18
2.14
5.09
1.00
2.01
2.09
3.06
3.01
ppm
189.00
171.64
156.68
141.34
137.72
136.20
132.79
129.00
128.97
128.36
128.33
127.51
120.06
83.04
67.35
51.46
22.44
14.49
ppm

Compound 4e

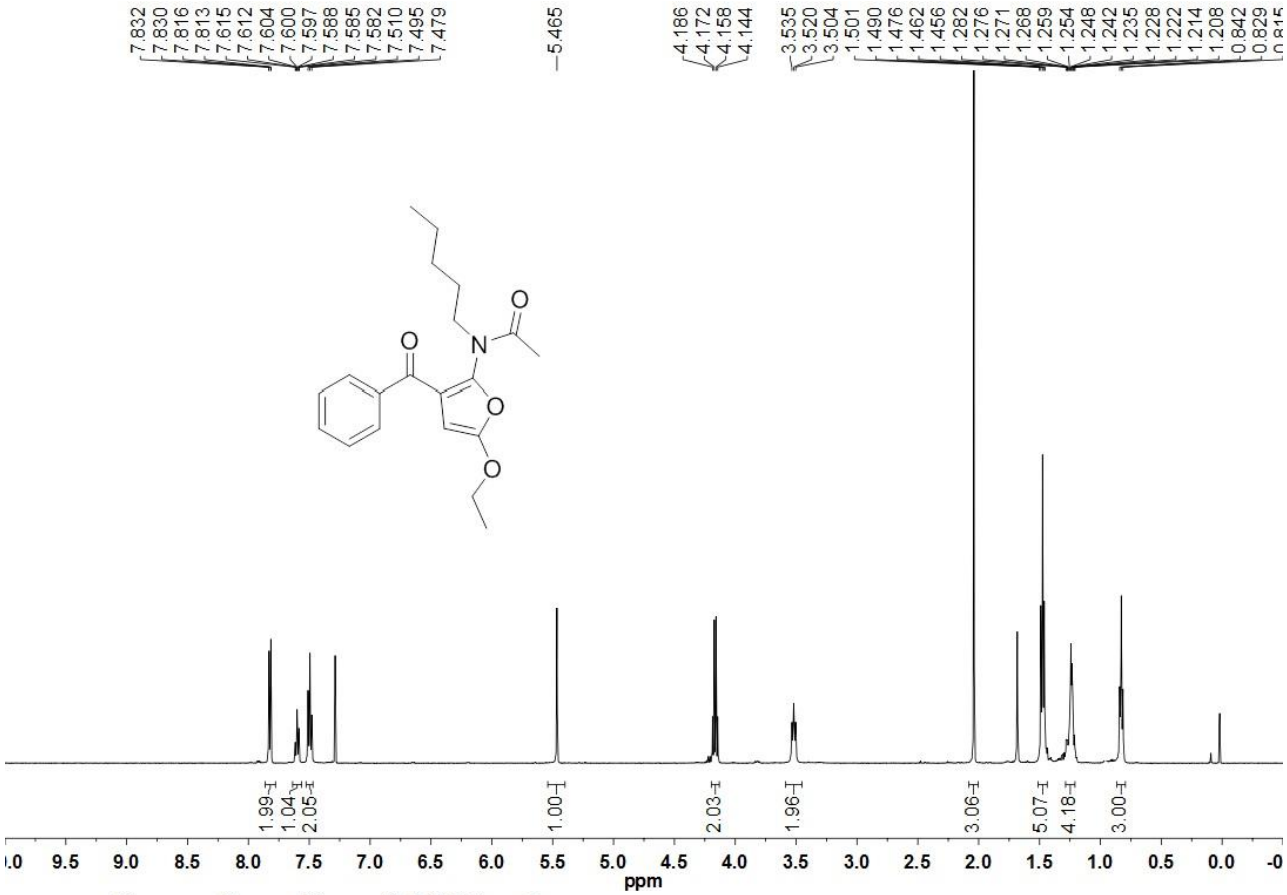

7.841
7.839
7.836
7.829
7.825
7.822
7.626
7.615
7.611
7.608
7.604
7.599
7.596
7.594
7.520
7.504
7.489
5.457
4.333
4.192
4.178
4.164
4.150
3.670
2.118
1.482
1.468
1.454
2.00
1.10
2.21
1.00
2.03
2.06
3.00
3.00
3.06
ppm
189.17
171.56
169.04
157.03
141.42
137.90
133.11
129.27
129.06
128.71
119.18
82.94
67.44
52.31
49.95
21.80
14.59
ppm

Compound 4f


7.818
7.816
7.813
7.802
7.798
7.598
7.583
7.579
7.571
7.568
7.565
7.493
7.490
7.478
7.462
5.445
4.166
4.152
4.138
4.124
3.708
3.694
3.681
3.557
3.548
3.539
2.486
2.473
2.459
2.369
2.360
2.350
2.031
1.470
1.455
1.441
2.06
1.05
2.05
1.00
2.06
2.05
4.07
2.08
4.08
3.06
3.06
ppm


188.95
171.42
156.74
142.51
138.00
132.94
128.90
128.60
118.81
82.58
67.25
66.91
56.43
53.58
45.12
22.15
14.53
ppm

Compound 4g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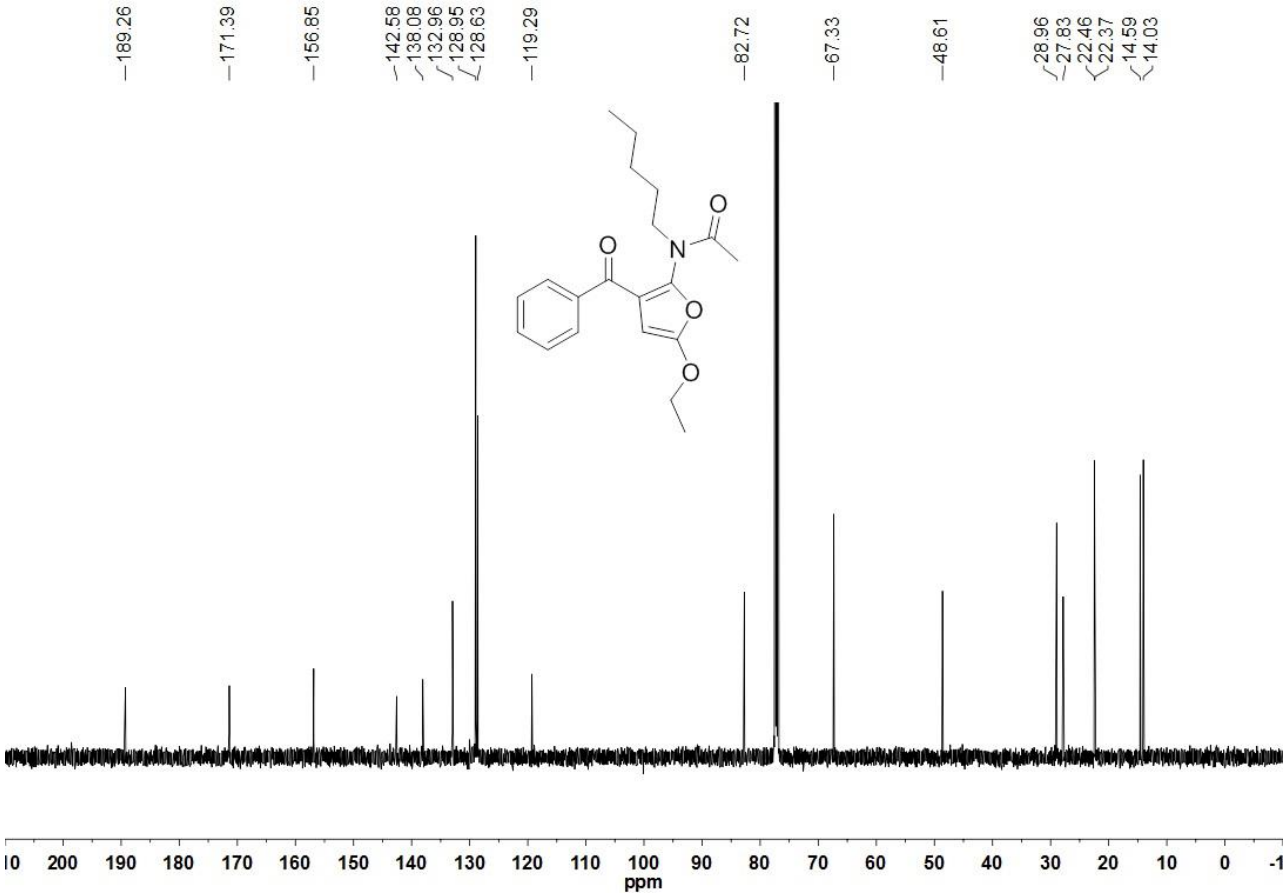
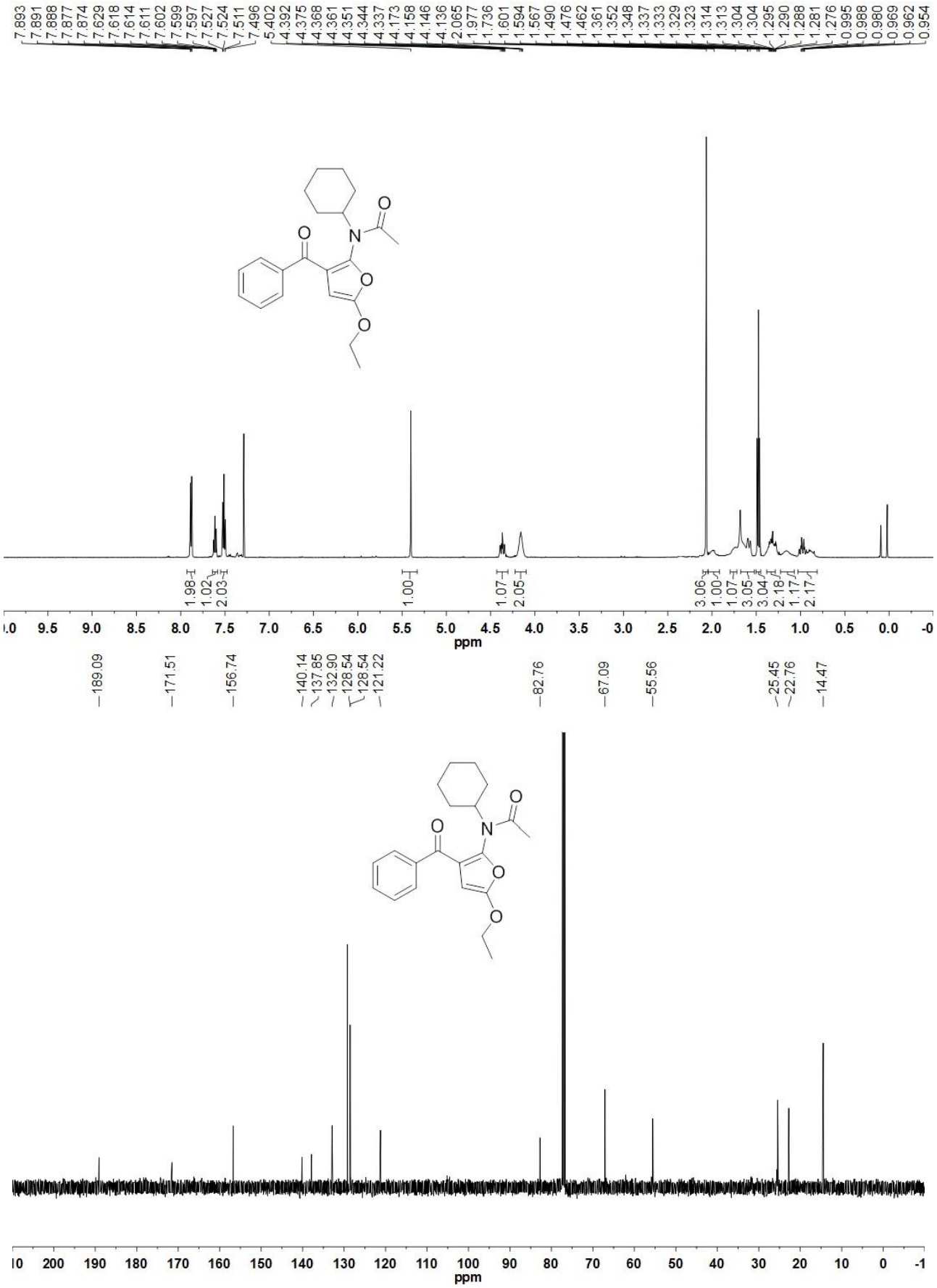
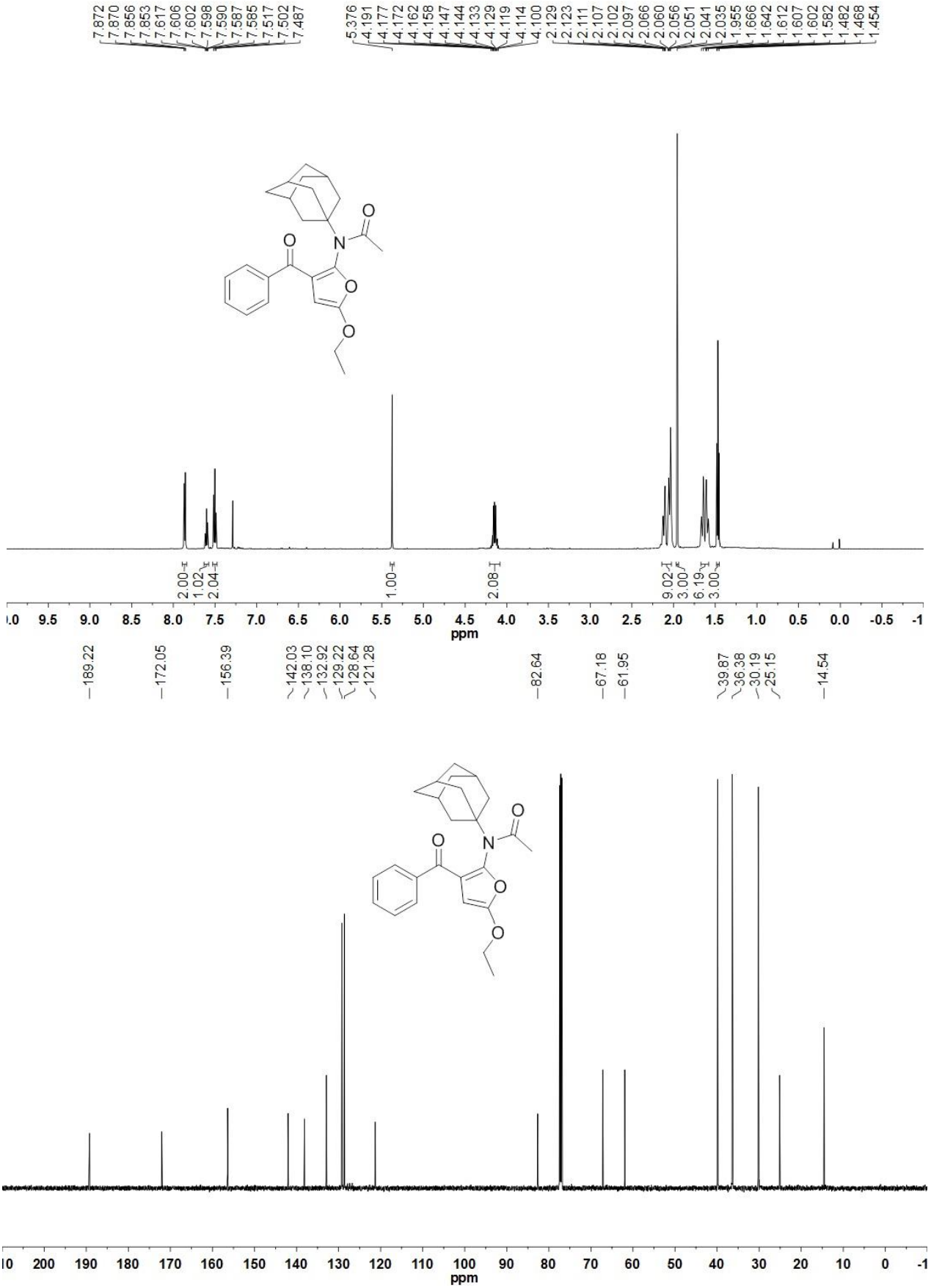
7.830
7.816
7.813
7.615
7.612
7.604
7.600
7.597
7.588
7.585
7.582
7.510
7.495
7.479
5.465
4.186
4.172
4.158
4.144
3.535
3.520
3.504
1.501
1.490
1.476
1.462
1.456
1.282
1.276
1.271
1.268
1.259
1.254
1.248
1.242
1.235
1.228
1.222
1.214
1.208
0.842
0.829
1.99
1.04
2.05
1.00
2.03
1.96
3.06
5.07
4.18
3.00
ppm


189.26
171.39
156.85
142.58
138.08
132.96
128.95
128.63
119.29
82.72
67.33
48.61
28.96
27.83
22.46
22.37
14.59
14.03
ppm

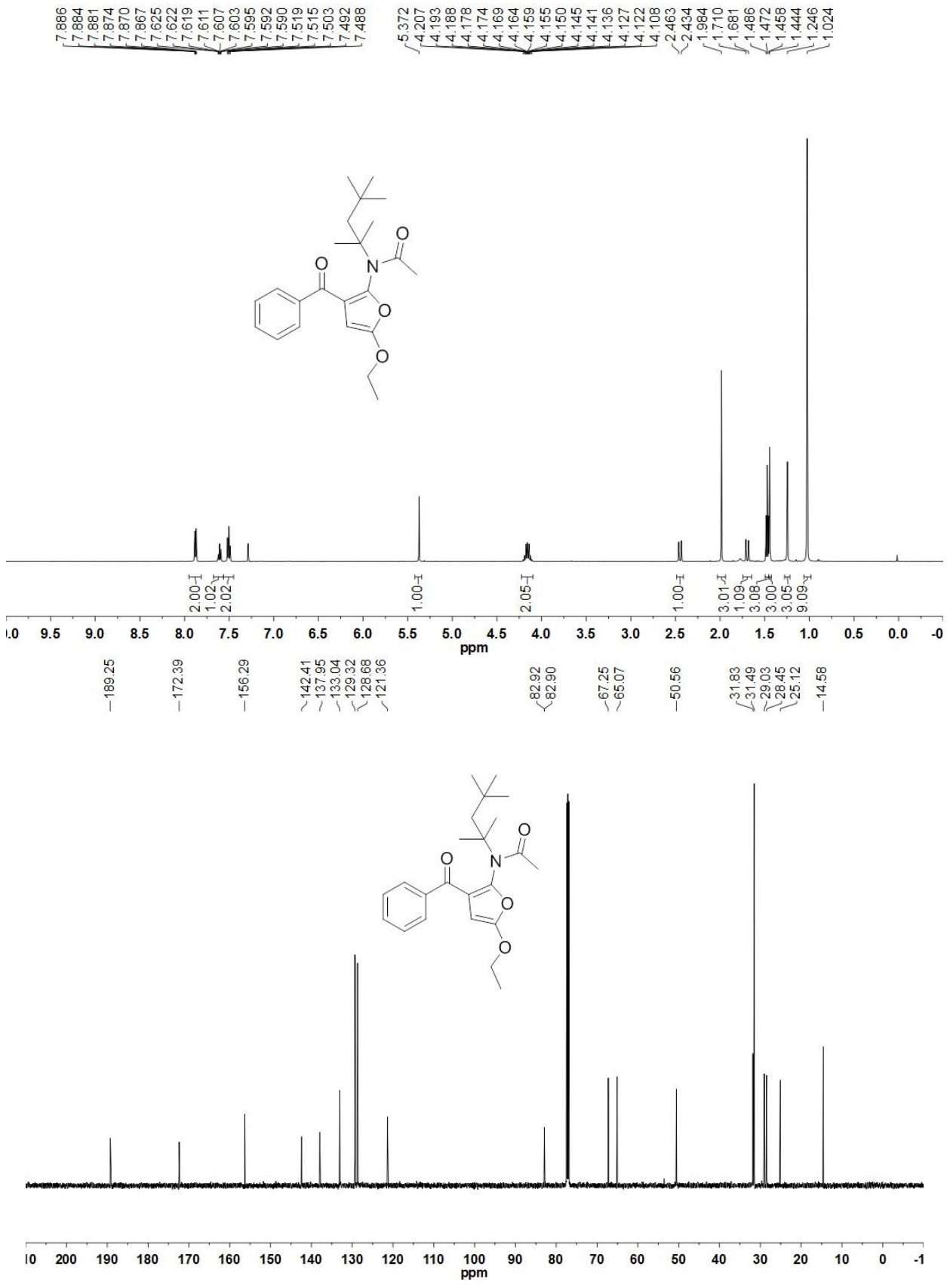
Compound 4h


7.893
7.891
7.888
7.877
7.874
7.629
7.618
7.614
7.611
7.602
7.599
7.597
7.527
7.524
7.511
7.496
5.402
4.392
4.375
4.368
4.361
4.351
4.344
4.337
4.173
4.158
4.146
4.136
2.065
1.977
1.736
1.601
1.594
1.567
1.490
1.476
1.462
1.361
1.352
1.348
1.337
1.333
1.329
1.323
1.314
1.313
1.304
1.304
1.295
1.290
1.288
1.281
1.276
0.995
0.988
0.980
0.969
0.962
0.954
O
N
O
O
O
1.98
1.02
2.03
1.00
1.07
2.05
3.06
1.00
1.07
3.05
3.04
2.18
1.17
2.17
ppm
189.09
171.51
156.74
140.14
137.85
132.90
128.54
128.54
121.22
82.76
67.09
55.56
25.45
22.76
14.47
O
N
O
O
O
ppm

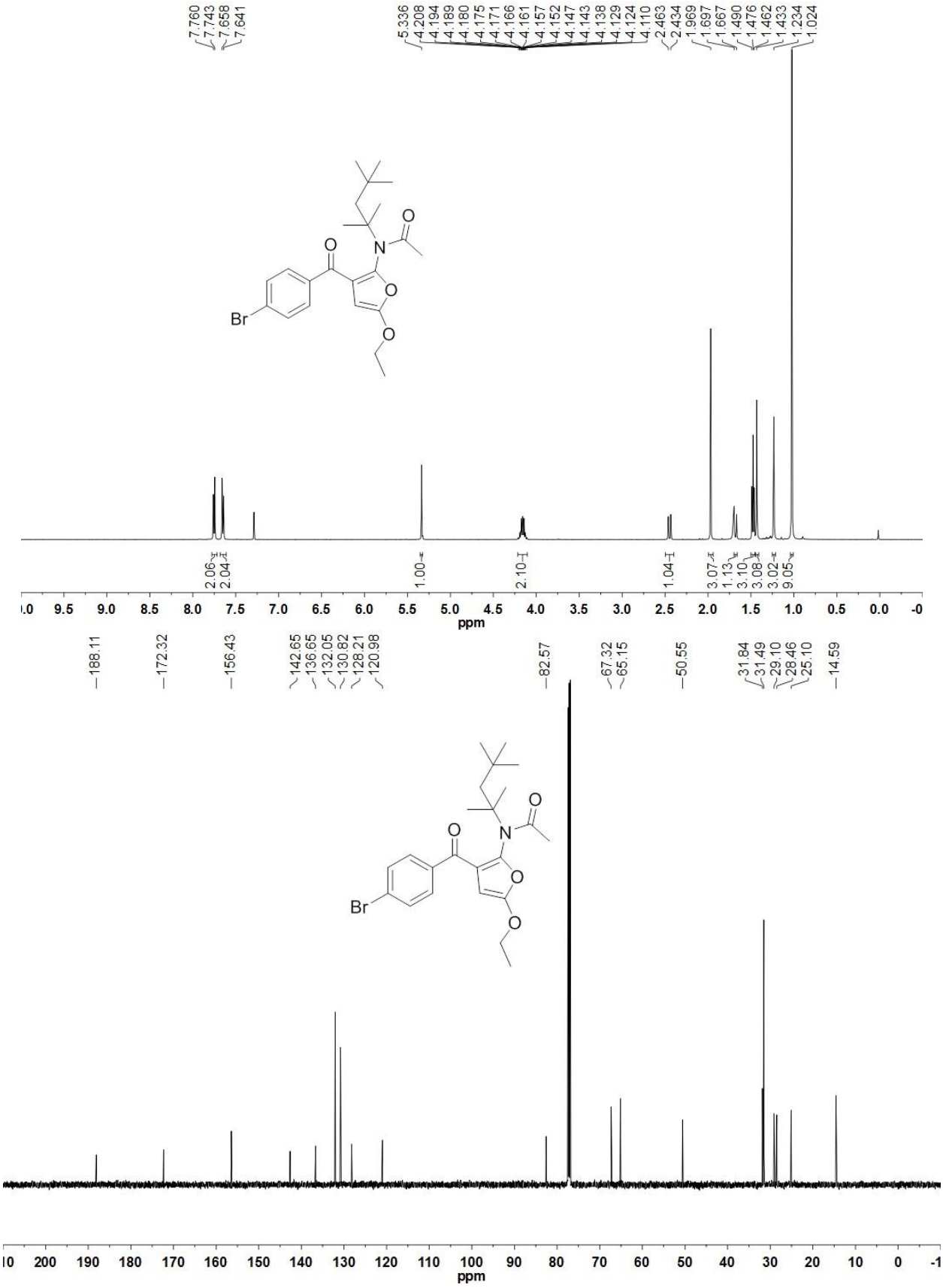
Compound 4i


7.872
7.870
7.856
7.853
7.617
7.606
7.602
7.598
7.590
7.587
7.585
7.517
7.502
7.487
5.376
4.191
4.177
4.172
4.162
4.158
4.147
4.144
4.133
4.129
4.119
4.114
4.100
2.129
2.123
2.111
2.107
2.102
2.097
2.066
2.060
2.056
2.051
2.041
2.035
1.955
1.666
1.642
1.612
1.607
1.602
1.582
1.482
1.468
1.454
2.00
1.02
2.04
1.00
2.08
9.02
3.00
6.19
3.00
ppm
189.22
172.05
156.39
142.03
138.10
132.92
129.22
128.64
121.28
82.64
67.18
61.95
39.87
36.38
30.19
25.15
14.54
ppm

Compound 4j


7.886
7.884
7.881
7.874
7.870
7.867
7.625
7.622
7.619
7.611
7.607
7.603
7.595
7.592
7.590
7.519
7.515
7.503
7.492
7.488
5.372
4.207
4.193
4.188
4.178
4.174
4.169
4.164
4.159
4.155
4.150
4.145
4.141
4.136
4.127
4.122
4.108
2.463
2.434
1.984
1.710
1.681
1.486
1.472
1.458
1.444
1.246
1.024
2.00
1.02
2.02
1.00
2.05
1.00
3.01
1.09
3.08
3.00
3.05
9.09
ppm
189.25
172.39
156.29
142.41
137.95
133.04
129.32
128.68
121.36
82.92
82.90
67.25
65.07
50.56
31.83
31.49
29.03
28.45
25.12
14.58
ppm

Compound 4k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7.658
7.641
5.336
4.208
4.194
4.189
4.180
4.175
4.171
4.166
4.161
4.157
4.152
4.147
4.143
4.138
4.129
4.124
4.110
2.463
2.434
1.969
1.697
1.667
1.490
1.476
1.462
1.433
1.234
1.024
Br
O
N
O
O
O
2.06
2.04
1.00
2.10
1.04
3.07
1.13
3.10
3.08
3.02
9.05
ppm
188.11
172.32
156.43
142.65
136.65
132.05
130.82
128.21
120.98
82.57
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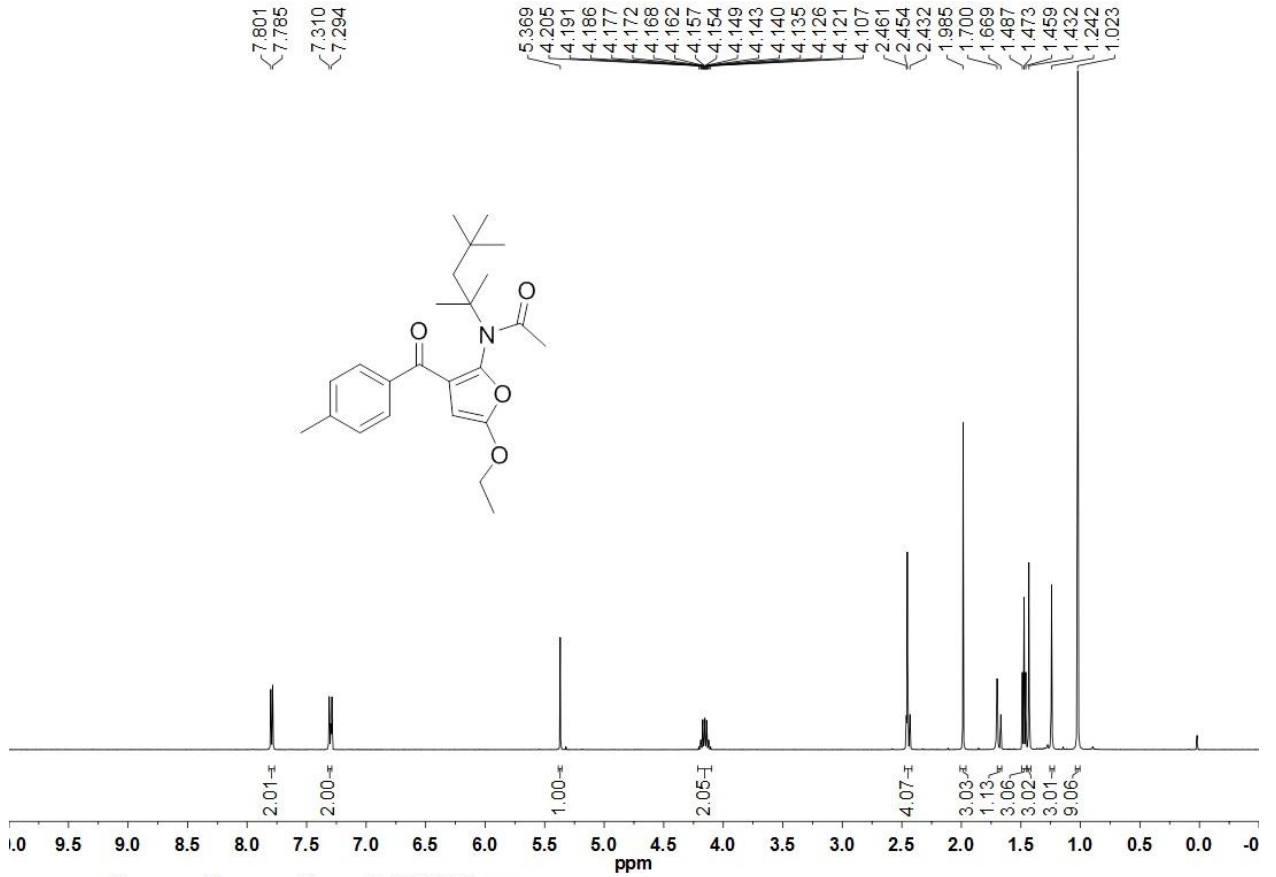
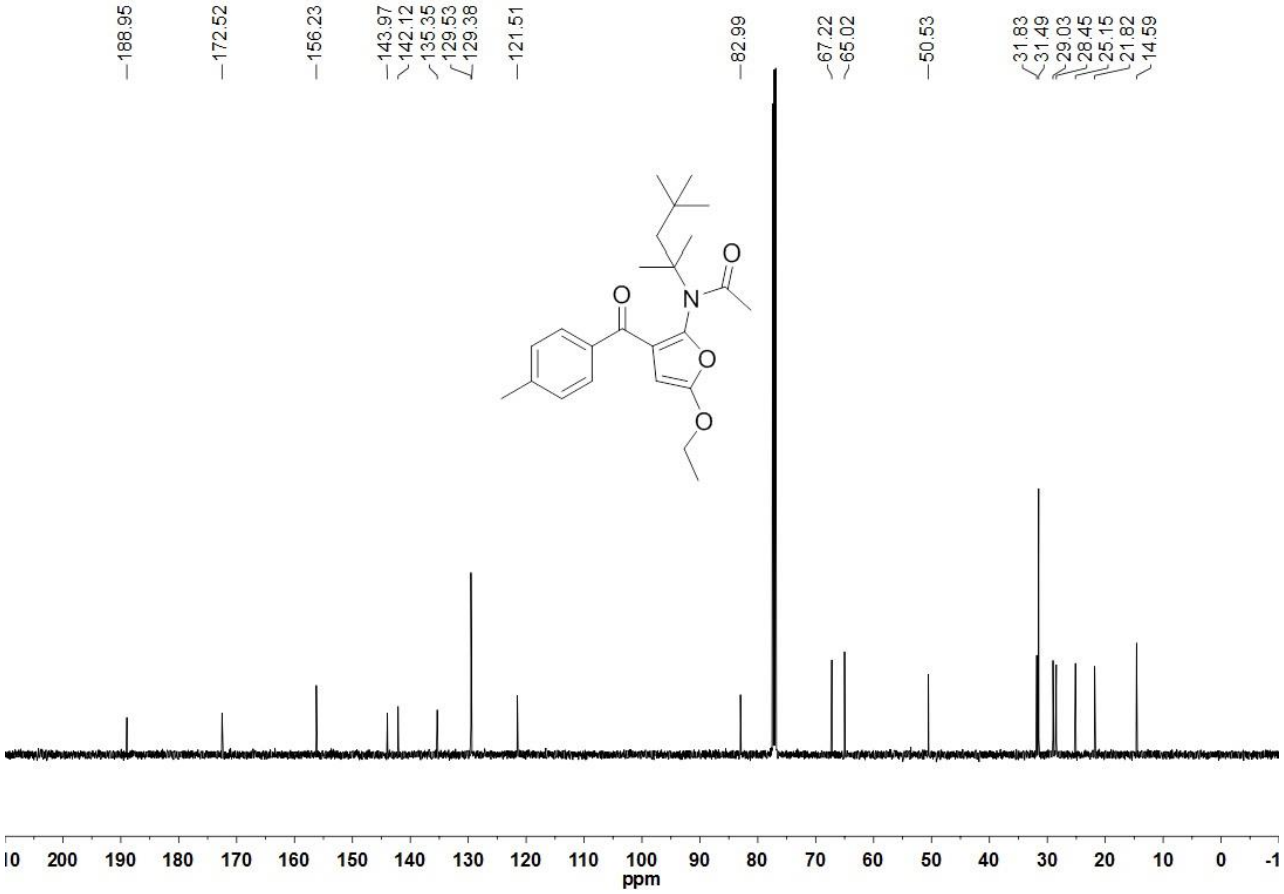
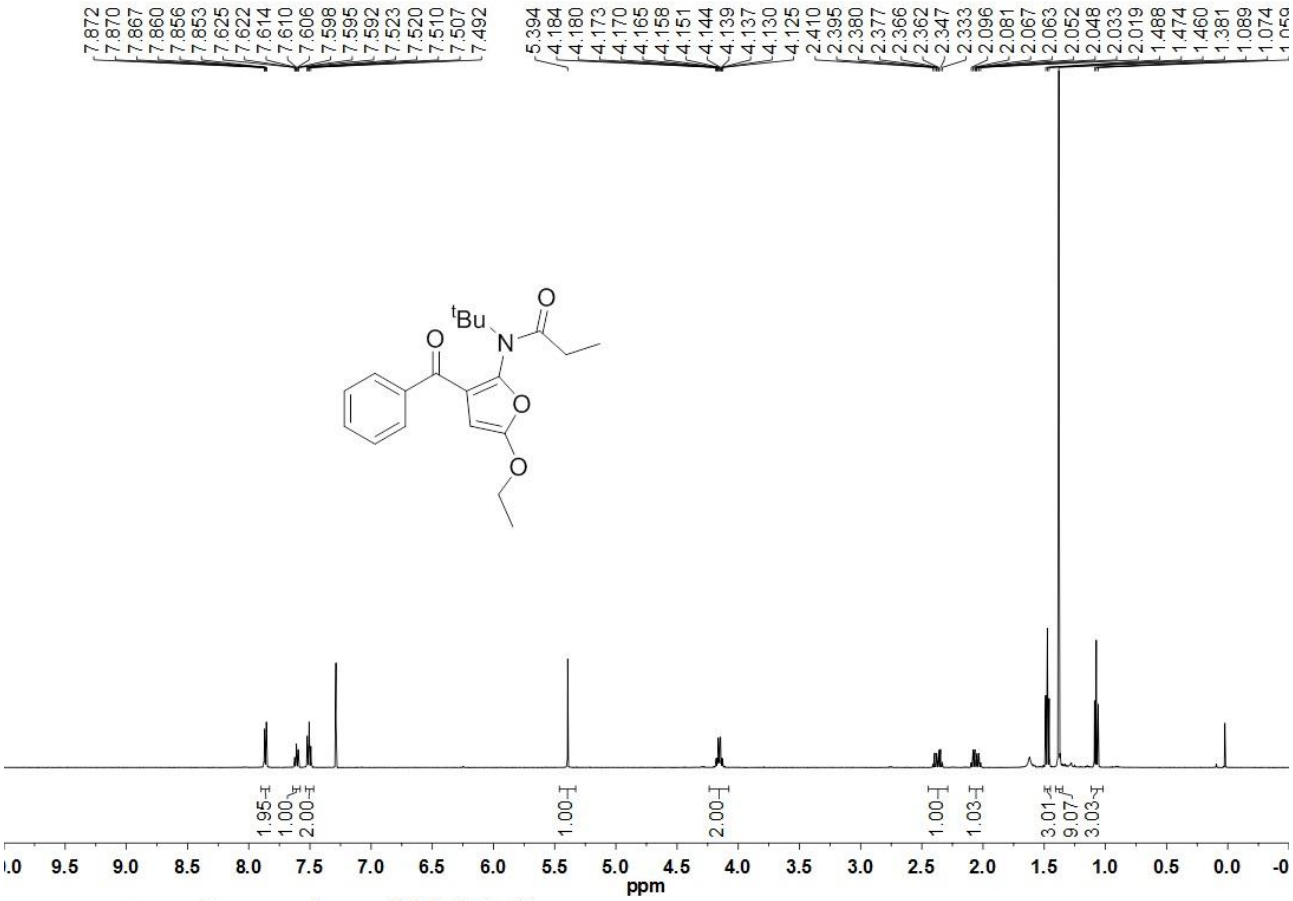
65.15
50.55
31.84
31.49
29.10
28.46
25.10
14.59
ppm

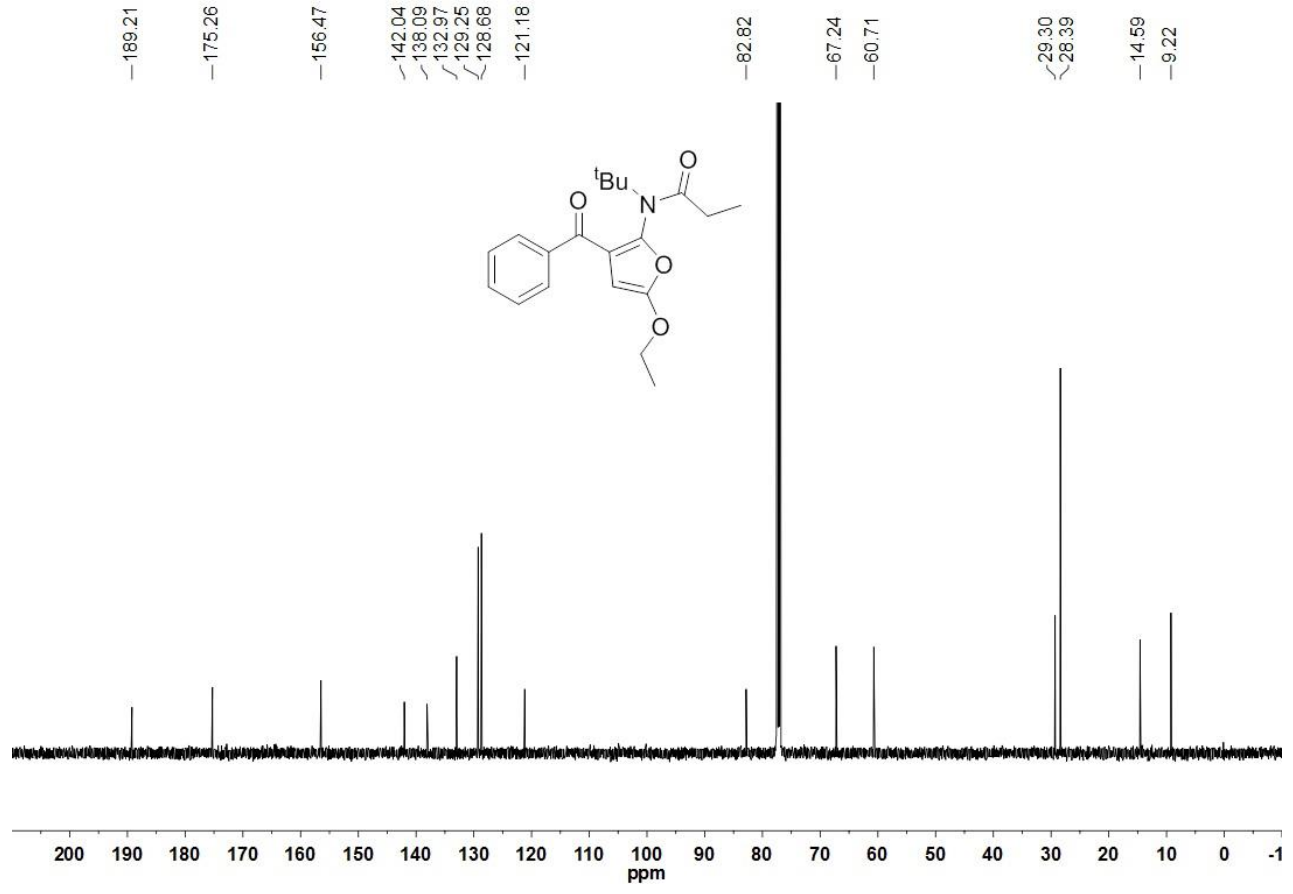
Compound 4l


7.801
7.785
7.310
7.294
5.369
4.205
4.191
4.186
4.177
4.172
4.168
4.162
4.157
4.154
4.149
4.143
4.140
4.135
4.126
4.121
4.107
2.461
2.454
2.432
1.985
1.700
1.669
1.487
1.473
1.459
1.432
1.242
1.023
2.01
2.00
1.00
2.05
4.07
3.03
1.13
3.06
3.02
3.01
9.06
ppm


188.95
172.52
156.23
143.97
142.12
135.35
129.53
129.38
121.51
82.99
67.22
65.02
50.53
31.83
31.49
29.03
28.45
25.15
21.82
14.59
ppm

Compound 6


7.872
7.870
7.867
7.860
7.856
7.853
7.625
7.622
7.614
7.610
7.606
7.598
7.595
7.592
7.523
7.520
7.510
7.507
7.492
5.394
4.184
4.180
4.173
4.170
4.165
4.158
4.151
4.144
4.139
4.137
4.130
4.125
2.410
2.395
2.380
2.377
2.366
2.362
2.347
2.333
2.096
2.081
2.067
2.063
2.052
2.048
2.033
2.019
1.488
1.474
1.460
1.381
1.089
1.074
tBu
N
O
O
O
O
1.95
1.00
2.00
1.00
2.00
1.00
1.03
3.01
9.07
3.03
ppm


189.21
175.26
156.47
142.04
138.09
132.97
129.25
128.68
121.18
82.82
67.24
60.71
29.30
28.39
14.59
9.22
tBu
N
O
O
O
O
ppm