

Copper-Catalysed Chemoslective C–OH Bond Activation of N-Benzoyl Cytosine: A Facile Access to 2-(Dimethylamino)pyrimidine

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1. Experimental Section

1.1. General Information

All starting materials and commercial reagent were purchased from Alfa Aesar, Sigma Aldrich, Avra, Spectrochem, TCI. Thin Layer Chromatography plates were visualized by exposure to ultraviolet light (UV) with 254 nm of wavelength and then further analyzed by using iodine chamber. Thin-layer chromatography was performed using pre-coated plates. Column chromatography was performed in 120 to 200 mesh size silica gel. The reactions were carried out in round bottom flask and sealed tube. NMR spectra were recorded by Bruker Advance 400 spectrometer (^1H at 400 MHz and ^{13}C at 100 MHz). Chemical shifts for ^1H NMR spectra have been reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard (CDCl_3 : δ 7.26 ppm). Similarly, ^{13}C NMR spectra have been reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard (CDCl_3 : δ 77.0 ppm). The ^1H NMR and ^{13}C NMR of the known products were compared with literature reports.

1.2. General procedure for the synthesis of *N*-benzoyl cytosine (1):

In a clean dry three-neck round bottom flask purge nitrogen for 2 min and add benzoic acid (249 mg, 1.02 equiv., 2.02 mmol) and 10 ml of DMF. Add 4-Dimethylaminopyridine (50 mg, 20 mol%) *N,N*-Diisopropylethylamine (1043 μl , 6 mmol, 3 equiv.) and HATU (767 mg, 1.01 equiv., 2.02 mmol) in the mixture. During addition, nitrogen purging was monitored and maintained carefully. After 15 min of stirring at room temperature, cytosine (222 mg, 2 mmol) was added gradually to the reaction mass and continued the reactions for 12 hrs at rt. After the completion of the reaction, a milky white precipitate was observed. Then the reaction mixture was poured into 50 ml of ice water to quench the DMF. Finally, filter the mixture and wash out the crude product with chilled methanol and dry the product.

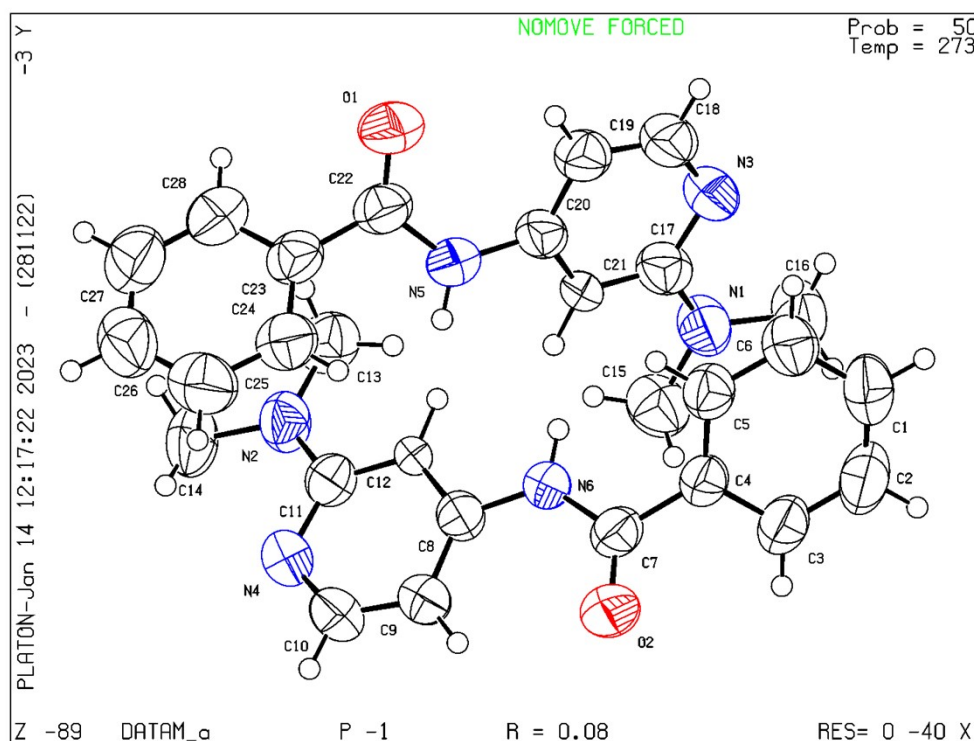
1.2. Synthesis of (dimethylamino)pyrimidin-4-yl)benzamide from *N*-benzoyl cytosine (3a):

In a clean dry round bottom flask *N*-benzoyl cytosine (**1a**, 216 mg, 1.0 mmol) with DMF (**2a**, 773 μL , 10 equiv. 0.730 mg) and 4 ml DMSO. Was taken and then $\text{Cu}(\text{OAc})_2\cdot\text{H}_2\text{O}$ (20 mg, 10 Mol %) was added to the mixture. In continued stirring for 2 min, then add *tert*-butyl hydroperoxide (386 μl , 4 equiv.) was added dropwise and the reaction mixture was stirred at 100 $^\circ\text{C}$ for 12 hr. The

reaction was monitored by TLC, after completion of the reaction, the mixture was poured into the ice water to quench DMF and DMSO after then extracted product crude was washed with ethyl acetate/water and dried over anhydrous Na_2SO_4 followed by concentrating under reduced pressure. Finally, the crude product was purified by column chromatography on silica gel (*n*-Hexane/EtOAc Mobile phase ~ 8:2) to afford the desired amide **3a**.

2. Characterization data

2.1. X-ray crystallographic data for **3a**:



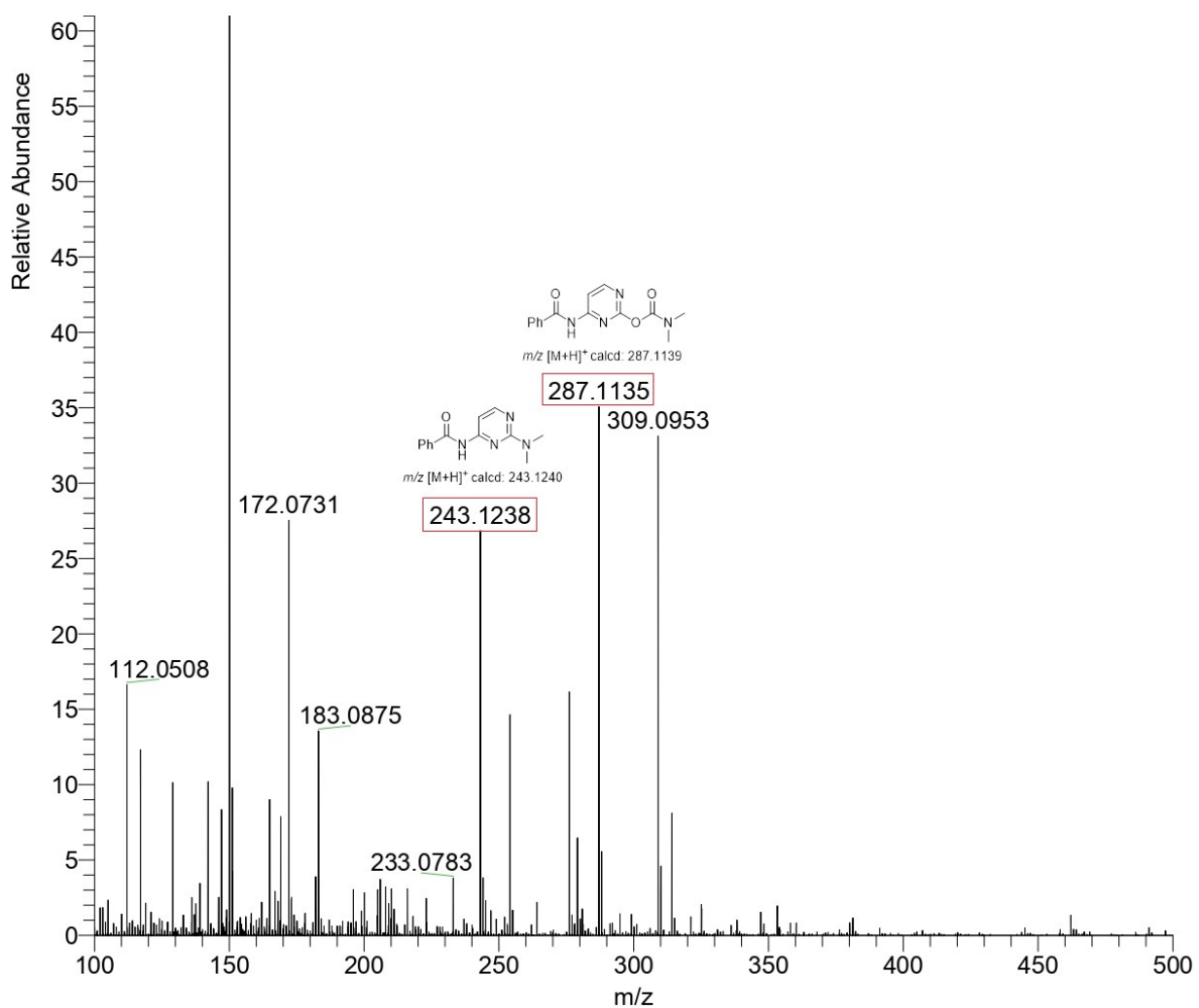
ORTEP diagram for the structure *N*-(2-(dimethylamino)pyrimidin-4-yl)benzamide **3a**

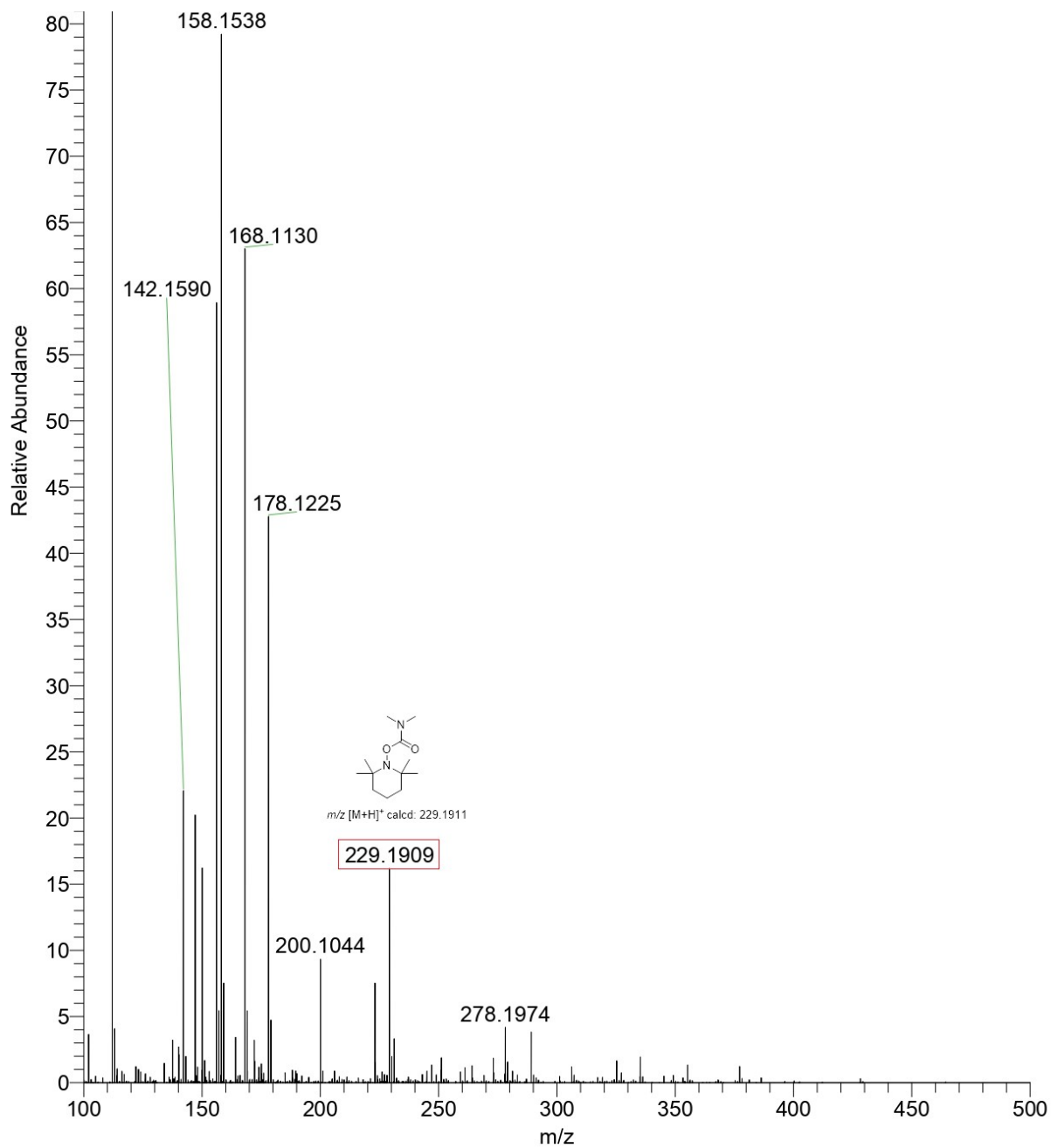
Wavelength	0.71073
Moiety formula	$\text{C}_{14}\text{H}_{14}\text{N}_4\text{O}_3$
Crystal system	Monoclinic
Space group	P 32 2 1
Unit cell dimensions	a=10.073(1) b=11.310(1) c=11.486(1)

	$\alpha=75.83(1)$ $\beta=81.71(1)$ $\gamma=80.98(1)$
Volume	1245.4(2)
Z	4
R-factor (%)	7.97

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication with a CCDC reference number **CCDC 2259305**.

2.2 HRMS spectra of the compounds:





2.3. ¹H and ¹³C data of compounds:

N-(2-(dimethylamino)pyrimidin-4-yl)benzamide (3a): Pale yellow solid, m.p. 147-150 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.24 (d, *J* = 5.4 Hz, 2H), 7.87 – 7.81 (m, 2H), 7.54 – 7.48 (m, 1H), 7.46 – 7.40 (m, 3H), 3.09 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 165.02, 160.85, 158.37, 156.55, 132.93, 131.49, 127.87, 126.25, 97.24, 35.99. HRMS-ESI (m/z): calcd for C₁₃H₁₆N₄O⁺ [M+H]⁺ 243.1240, found 243.1246.

N-(2-(dimethylamino)pyrimidin-4-yl)-2-methylbenzamide (3b): Pale orange solid, m.p. 142-145 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.24 (d, *J* = 4.8 Hz, 1H), 7.92 (s, 1H), 7.42 (dd, *J* = 16.6, 6.4 Hz, 2H), 7.32 (t, *J* = 7.7 Hz, 1H), 7.19 (d, *J* = 4.5 Hz, 2H), 3.07 (s, 6H), 2.44 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.47, 161.50, 158.88, 157.62, 136.93, 135.32, 131.52, 130.91, 126.70, 126.01, 98.14, 37.04, 19.93. HRMS-ESI (m/z): calcd for C₁₄H₁₇N₄O⁺ [M+H]⁺ 257.1397, found 257.1402.

N-(2-(dimethylamino)pyrimidin-4-yl)-3-methylbenzamide (3c): White solid, m.p. 141-143 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.24 (d, *J* = 4.9 Hz, 2H), 7.64 (d, *J* = 15.7 Hz, 2H), 7.45 (t, *J* = 4.2 Hz, 1H), 7.32 (d, *J* = 4.1 Hz, 2H), 3.11 (s, 6H), 2.38 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.19, 160.40, 157.70, 156.78, 137.89, 132.76, 132.38, 127.76, 127.02, 123.25, 97.30, 36.16, 20.37. HRMS-ESI (m/z): calcd for C₁₄H₁₇N₄O⁺ [M+H]⁺ 257.1397, found 257.1401.

N-(2-(dimethylamino)pyrimidin-4-yl)-4-methylbenzamide (3d): White solid, m.p. 151-153 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 – 8.26 (m, 2H), 7.87 – 7.79 (m, 2H), 7.52 (dd, *J* = 5.6, 1.7 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 3.18 (s, 6H), 2.45 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 164.92, 160.76, 158.21, 156.67, 142.22, 130.03, 128.53, 126.30, 97.26, 36.01, 20.54. HRMS-ESI (m/z): calcd for C₁₄H₁₇N₄O⁺ [M+H]⁺ 257.1397, found 257.1402.

N-(2-(dimethylamino)pyrimidin-4-yl)-2-methoxybenzamide (3e): Pale white solid, m.p. 150-152 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.09 (s, 1H), 8.24 – 8.19 (m, 1H), 8.16 (dd, *J* = 7.8, 2.4 Hz, 1H), 7.47 (dq, *J* = 10.6, 6.7, 4.5 Hz, 2H), 7.06 (td, *J* = 7.7, 2.6 Hz, 1H), 6.97 (dd, *J* = 8.5, 2.7 Hz, 1H), 3.99 (s, 3H), 3.11 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 164.12, 158.54, 158.12, 157.54, 134.02, 132.61, 121.67, 121.13, 111.66, 99.09, 56.21, 36.98. HRMS-ESI (m/z): calcd for C₁₄H₁₇N₄O₂⁺ [M+H]⁺ 273.1346, found 273.1352

N-(2-(dimethylamino)pyrimidin-4-yl)-4-methoxybenzamide (3f): Pale white solid, m.p. 153-156 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.09 (s, 1H), 8.22 (dd, *J* = 5.9, 3.0 Hz, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 7.47 (dt, *J* = 12.3, 5.3 Hz, 2H), 7.07 (dt, *J* = 8.1, 4.1 Hz, 1H), 6.97 (dd, *J* = 8.5, 2.7 Hz, 1H), 4.00 (s, 3H), 3.12 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 164.13, 158.24, 157.55, 134.06, 132.63, 121.69, 121.10, 111.67, 99.11, 56.22, 37.04. HRMS-ESI (*m/z*): calcd for C₁₄H₁₇N₄O₂⁺ [M+H]⁺ 273.1346, found 273.1352.

N-(2-(dimethylamino)pyrimidin-4-yl)-4-ethoxybenzamide (3g): Pale white solid, m.p. 156-159 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.29 (t, *J* = 4.5 Hz, 1H), 8.20 (s, 1H), 7.90 – 7.83 (m, 2H), 7.48 (t, *J* = 4.4 Hz, 1H), 7.01 – 6.95 (m, 2H), 4.16 – 4.09 (m, 2H), 3.16 (d, *J* = 3.0 Hz, 6H), 1.46 – 1.43 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.45, 162.46, 161.98, 159.31, 157.72, 129.27, 128.20, 114.54, 98.24, 63.82, 36.98, 14.66. HRMS-ESI (*m/z*): calcd for C₁₅H₁₉N₄O₂⁺ [M+H]⁺ 287.1503, found 287.1508.

N-(2-(dimethylamino)pyrimidin-4-yl)-2-fluorobenzamide (3h): Pale white solid, m.p. 135-138 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.73 (d, *J* = 13.6 Hz, 1H), 8.24 (d, *J* = 5.5 Hz, 1H), 8.05 (t, *J* = 8.0 Hz, 1H), 7.54 – 7.45 (m, 1H), 7.42 (d, *J* = 5.5 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.13 (dd, *J* = 12.1, 8.4 Hz, 1H), 3.09 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 162.10, 162.06, 161.76, 161.69, 159.25, 159.22, 157.45, 134.47, 134.37, 132.19, 132.17, 125.17, 125.14, 120.97, 120.86, 116.50, 116.26, 98.75, 36.97. HRMS-ESI (*m/z*): calcd for C₁₃H₁₄FN₄O⁺ [M+H]⁺ 261.1146, found 261.1152.

N-(2-(dimethylamino)pyrimidin-4-yl)-4-fluorobenzamide (3i): Pale white solid, m.p. 139-141 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.24 (dd, *J* = 5.8, 2.6 Hz, 2H), 7.87 (p, *J* = 3.3 Hz, 2H), 7.40 (dd, *J* = 6.0, 2.6 Hz, 1H), 7.12 (td, *J* = 8.5, 2.6 Hz, 2H), 3.09 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 165.59, 163.88, 163.06, 160.70, 158.35, 156.50, 128.83, 128.74, 115.14, 114.92, 97.21, 36.04. HRMS-ESI (*m/z*): calcd for C₁₃H₁₄FN₄O⁺ [M+H]⁺ 261.1146, found 261.1152.

3-bromo-N-(2-(dimethylamino)pyrimidin-4-yl)benzamide (3j): Brown solid, m.p. 158-160 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.27 (d, *J* = 5.7 Hz, 1H), 8.00 (s, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.44 (d, *J* = 5.9 Hz, 1H), 7.33 (t, *J* = 7.9 Hz, 1H), 3.14 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 164.46, 159.45, 157.34, 135.37, 134.76, 130.59, 130.50, 126.00, 123.27, 98.04, 37.08. HRMS-ESI (*m/z*): calcd for C₁₃H₁₄BrN₄O⁺ [M+H]⁺ 321.0346, found 321.0351.

4-bromo-N-(2-(dimethylamino)pyrimidin-4-yl)benzamide (3k): Pale brown solid, m.p. 157-160 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.28 – 8.23 (m, 1H), 8.19 (s, 1H), 7.75 – 7.68 (m, 2H), 7.61 – 7.54 (m, 2H), 7.40 (t, *J* = 4.1 Hz, 1H), 3.10 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 165.04, 159.28, 157.43, 132.69, 132.20, 128.88, 127.50, 98.25, 37.09. HRMS-ESI (*m/z*): calcd for C₁₃H₁₄BrN₄O⁺ [M+H]⁺ 321.0346, found 321.0351.

N-(2-(dimethylamino)pyrimidin-4-yl)pentanamide (3l): Gummy liquid; ¹H NMR (400 MHz, CDCl₃) δ 8.17 (d, *J* = 2.9 Hz, 1H), 7.64 (s, 1H), 7.26 (d, *J* = 4.0 Hz, 1H), 3.07 (d, *J* = 2.7 Hz, 6H), 2.34 – 2.29 (m, 2H), 1.63 (t, *J* = 7.9 Hz, 2H), 1.34 (t, *J* = 7.7 Hz, 2H), 0.91 – 0.85 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 171.23, 160.37, 157.78, 156.43, 97.07, 36.63, 36.02, 26.16, 21.28, 12.73. HRMS-ESI (*m/z*): calcd for C₁₁H₁₉N₄O⁺ [M+H]⁺ 223.1553, found 223.1559.

N-(2-(dimethylamino)pyrimidin-4-yl)isobutyramide (3m): Gummy liquid; ¹H NMR (400 MHz, CDCl₃) δ 8.21 – 8.14 (m, 1H), 7.62 (s, 1H), 7.32 – 7.25 (m, 1H), 3.08 (s, 6H), 2.47 (p, *J* = 7.3 Hz, 1H), 1.19 (d, *J* = 4.3 Hz, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 176.08, 161.42, 158.84, 157.56, 98.13, 37.03, 36.89, 19.28. HRMS-ESI (*m/z*): calcd for C₁₀H₁₇N₄O⁺ [M+H]⁺ 209.1397, found 209.1402.

N-(2-(diethylamino)pyrimidin-4-yl)benzamide (4a): Pale white solid, m.p. 132-135 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.30 (d, *J* = 5.1 Hz, 1H), 8.19 (s, 1H), 7.91 (d, *J* = 7.2 Hz, 2H), 7.58 (d, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.45 (d, *J* = 4.6 Hz, 1H), 3.60 (q, *J* = 7.3 Hz, 4H), 1.21 – 1.16 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 166.00, 160.81, 159.56, 157.60, 134.14, 132.43, 128.89, 127.25, 98.09, 41.63, 13.13. HRMS-ESI (*m/z*): calcd for C₁₅H₁₈N₄NaO⁺ [M+Na]⁺ 293.1393, found 293.1378.

N-(2-(diethylamino)pyrimidin-4-yl)-3-methylbenzamide (4b): White solid, m.p. 131-134 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.29 (d, *J* = 4.5 Hz, 1H), 8.19 (s, 1H), 7.75 – 7.66 (m, 2H), 7.44 (d, *J* = 5.1 Hz, 1H), 7.39 (d, *J* = 4.2 Hz, 2H), 3.60 (q, *J* = 7.3 Hz, 4H), 2.45 (d, *J* = 3.0 Hz, 3H), 1.18 (t, *J* = 7.3 Hz, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 166.24, 160.79, 159.52, 157.64, 138.86, 134.11, 133.20, 128.73, 128.01, 124.18, 98.12, 41.61, 21.39, 13.13. HRMS-ESI (*m/z*): calcd for C₁₆H₂₀N₄NaO⁺ [M+H]⁺ 307.1529, found 307.1535.

N-(2-(diethylamino)pyrimidin-4-yl)-4-methylbenzamide (4c): Pale white solid, m.p. 133-136 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.28 (d, *J* = 4.6 Hz, 1H), 8.16 (s, 1H), 7.80 (d, *J* = 7.7 Hz, 2H),

7.45 (d, $J = 2.7$ Hz, 1H), 7.31 (d, $J = 7.8$ Hz, 2H), 3.60 (q, $J = 7.2, 5.0$ Hz, 4H), 2.43 (s, 3H), 1.21 – 1.16 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 165.91, 160.80, 159.49, 157.68, 143.13, 131.25, 129.54, 127.29, 98.10, 41.61, 21.55, 13.14. HRMS-ESI (m/z): calcd for $\text{C}_{16}\text{H}_{20}\text{N}_4\text{NaO}^+$ $[\text{M}+\text{H}]^+$ 307.1529, found 307.1535.

N-(2-(diethylamino)pyrimidin-4-yl)-4-methoxybenzamide (4d): Pale white solid, m.p. 141-144 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.28 (s, 1H), 8.14 (s, 1H), 7.92 – 7.86 (m, 2H), 7.43 (d, $J = 5.1$ Hz, 1H), 6.99 (d, $J = 6.1$ Hz, 2H), 3.88 (s, 3H), 3.64 – 3.56 (m, 4H), 1.21 – 1.16 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 165.42, 163.00, 160.79, 159.43, 157.77, 129.26, 126.26, 114.09, 98.08, 55.51, 41.61, 13.14. HRMS-ESI (m/z): calcd for $\text{C}_{16}\text{H}_{21}\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 301.1659, found 301.1664.

N-(2-(diethylamino)pyrimidin-4-yl)-4-ethoxybenzamide (4e): Pale white solid, m.p. 149-152 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.27 (d, $J = 4.7$ Hz, 1H), 8.12 (s, 1H), 7.90 – 7.83 (m, 2H), 7.43 (d, $J = 4.8$ Hz, 1H), 7.02 – 6.94 (m, 2H), 4.11 (q, $J = 7.3, 5.0$ Hz, 2H), 3.60 (q, $J = 7.6, 7.0$ Hz, 4H), 1.48 – 1.43 (m, 3H), 1.21 – 1.16 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 165.44, 162.42, 160.80, 159.42, 157.78, 129.25, 126.03, 114.54, 98.08, 63.82, 41.60, 14.67, 13.14. HRMS-ESI (m/z): calcd for $\text{C}_{17}\text{H}_{23}\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 315.1816, found 315.1821.

N-(2-(diethylamino)pyrimidin-4-yl)-3-fluorobenzamide (4f): Pale white solid, m.p. 143-146 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.30 (d, $J = 4.5$ Hz, 1H), 8.15 (s, 1H), 7.65 (dd, $J = 19.0, 8.4$ Hz, 2H), 7.49 (td, $J = 8.4, 7.5, 4.6$ Hz, 1H), 7.42 (d, $J = 4.9$ Hz, 1H), 7.30 (d, $J = 8.1$ Hz, 1H), 3.60 (d, $J = 7.2$ Hz, 4H), 1.18 (d, $J = 6.4$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.65, 164.14, 161.67, 160.78, 159.68, 157.37, 136.40, 136.34, 130.64, 130.56, 122.69, 122.66, 119.59, 119.38, 114.85, 114.62, 98.08, 41.65, 13.11. HRMS-ESI (m/z): calcd for $\text{C}_{15}\text{H}_{18}\text{FN}_4\text{O}^+$ $[\text{M}+\text{H}]^+$ 289.1459, found 289.1465.

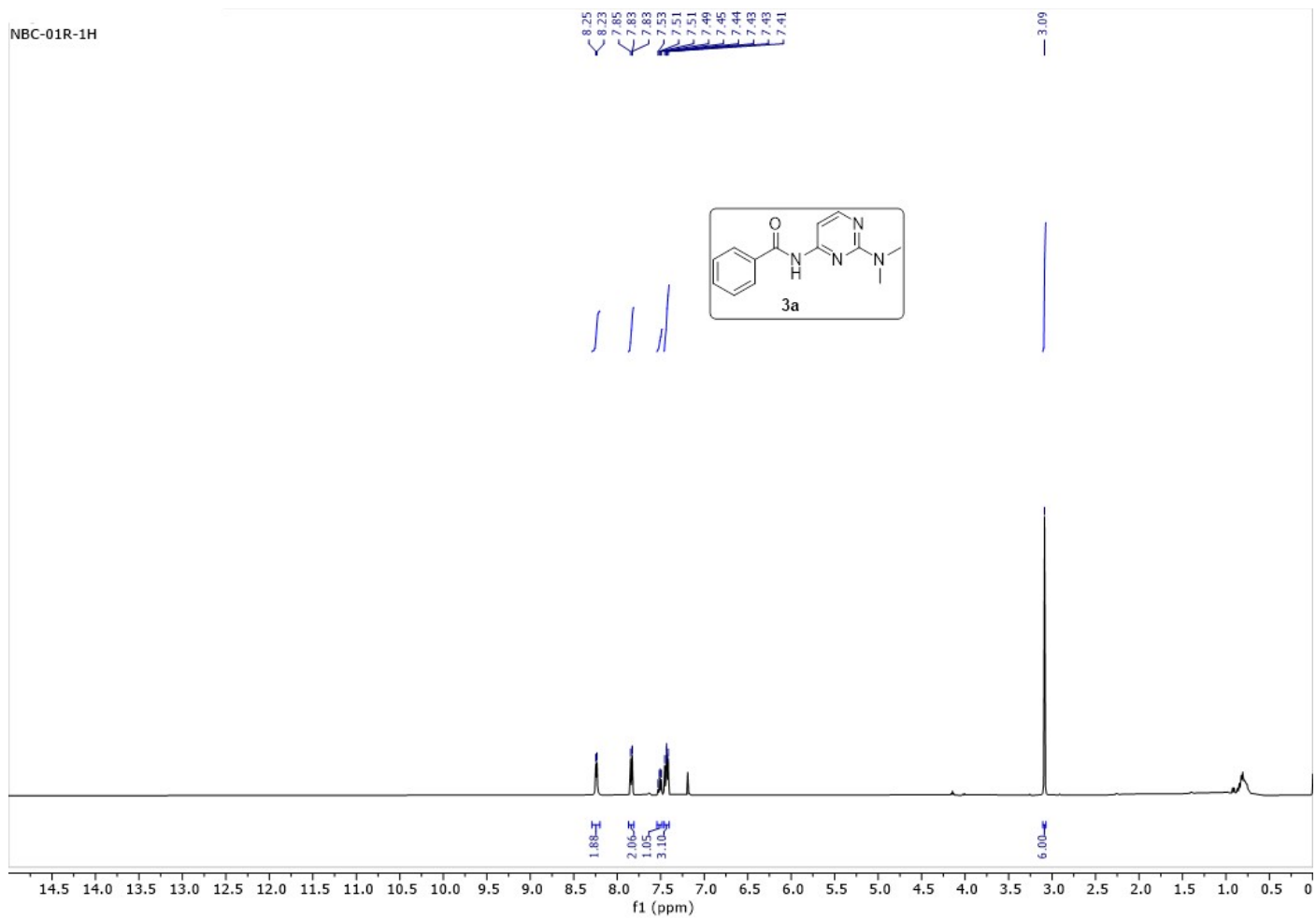
3-chloro-N-(2-(diethylamino)pyrimidin-4-yl)benzamide (4g): White solid, m.p. 152-155 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.30 (d, $J = 3.7$ Hz, 1H), 8.14 (s, 1H), 7.89 (s, 1H), 7.78 (d, $J = 7.7$ Hz, 1H), 7.56 (d, $J = 7.6$ Hz, 1H), 7.50 – 7.39 (m, 2H), 3.60 (q, $J = 7.3$ Hz, 4H), 1.19 (t, $J = 7.2$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.63, 160.77, 159.69, 157.36, 135.90, 135.16, 132.45, 130.20, 127.61, 125.31, 98.08, 41.65, 13.12. HRMS-ESI (m/z): calcd for $\text{C}_{15}\text{H}_{18}\text{ClN}_4\text{O}^+$ $[\text{M}+\text{H}]^+$ 305.1164, found 305.1169.

N-(2-(diethylamino)pyrimidin-4-yl)pentanamide (4h): Gummy liquid; ^1H NMR (400 MHz, CDCl_3) δ 8.22 (t, $J = 4.3$ Hz, 1H), 7.55 (s, 1H), 3.60 – 3.53 (m, 4H), 2.39 (t, $J = 7.8$ Hz, 2H), 1.69 (d, $J = 7.8$ Hz, 2H), 1.40 (q, $J = 7.5$ Hz, 2H), 1.17 (d, $J = 7.5$ Hz, 6H), 0.97 – 0.92 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 172.17, 160.71, 159.37, 157.35, 97.87, 41.61, 37.66, 27.21, 22.31, 13.76, 13.10. HRMS-ESI (m/z): calcd for $\text{C}_{13}\text{H}_{23}\text{N}_4\text{O}^+$ $[\text{M}+\text{H}]^+$ 251.1866, found 251.1872.

4-benzamidopyrimidin-2-yl dimethylcarbamate (C): ^1H NMR (400 MHz, CDCl_3) δ 8.73 (s, 1H), 8.55 (d, $J = 4.0$ Hz, 1H), 8.16 (d, $J = 4.3$ Hz, 1H), 7.84 (d, $J = 7.2$ Hz, 2H), 7.53 (d, $J = 7.2$ Hz, 1H), 7.44 (t, $J = 7.2$ Hz, 2H), 3.05 (s, 3H), 2.98 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 165.97, 161.17, 160.78, 159.75, 152.75, 133.07, 132.96, 129.04, 127.41, 107.55, 36.81, 36.78. HRMS-ESI (m/z): calcd for $\text{C}_{14}\text{H}_{15}\text{N}_4\text{O}_3^+$ $[\text{M}+\text{H}]^+$ 287.1139, found 287.1144.

3. ^1H and ^{13}C NMR Spectra of Compounds

NBC-01R-1H



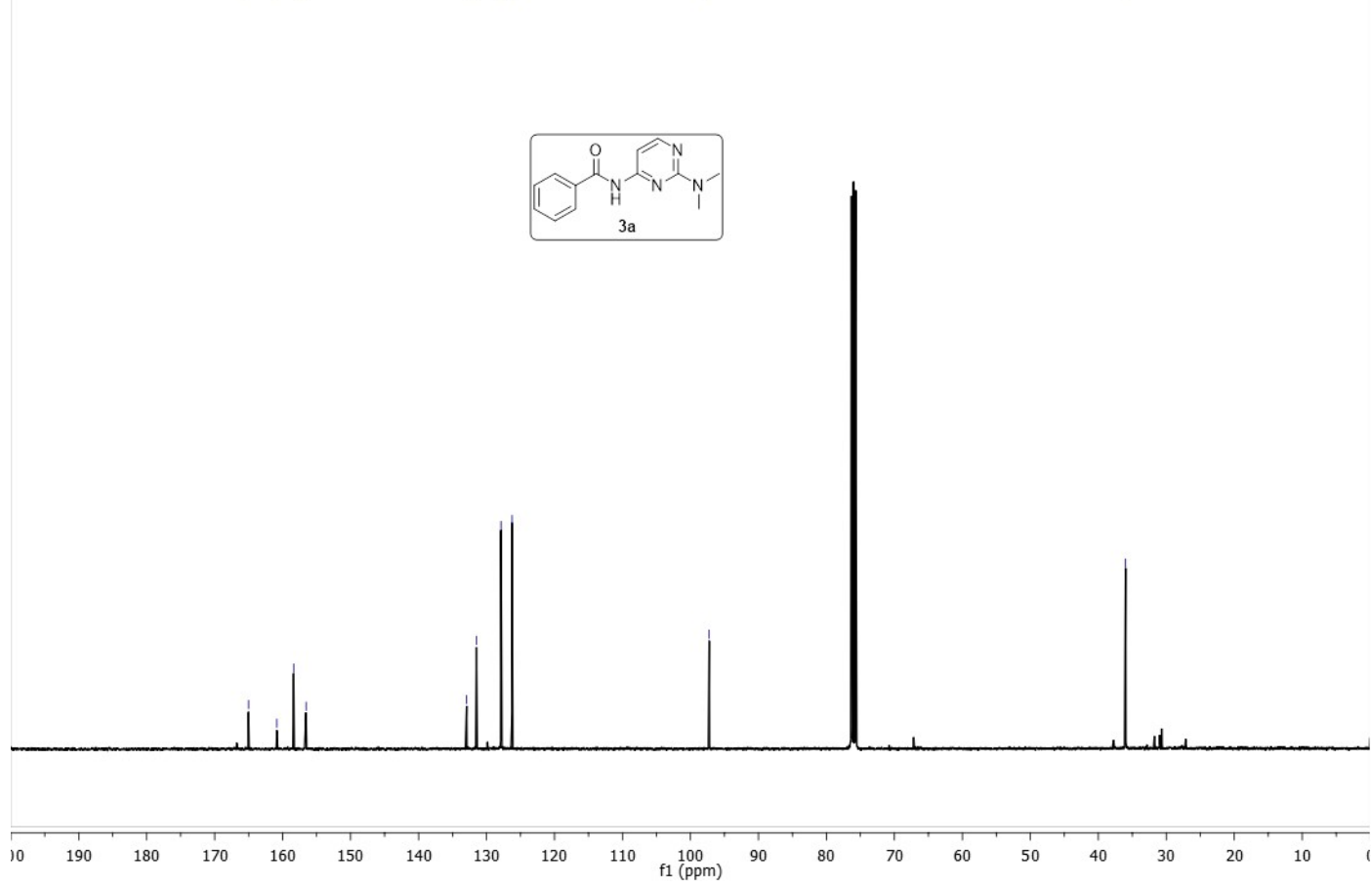
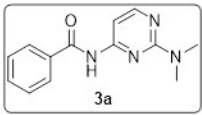
NBC-01R-13C

165.02
160.85
158.37
156.55

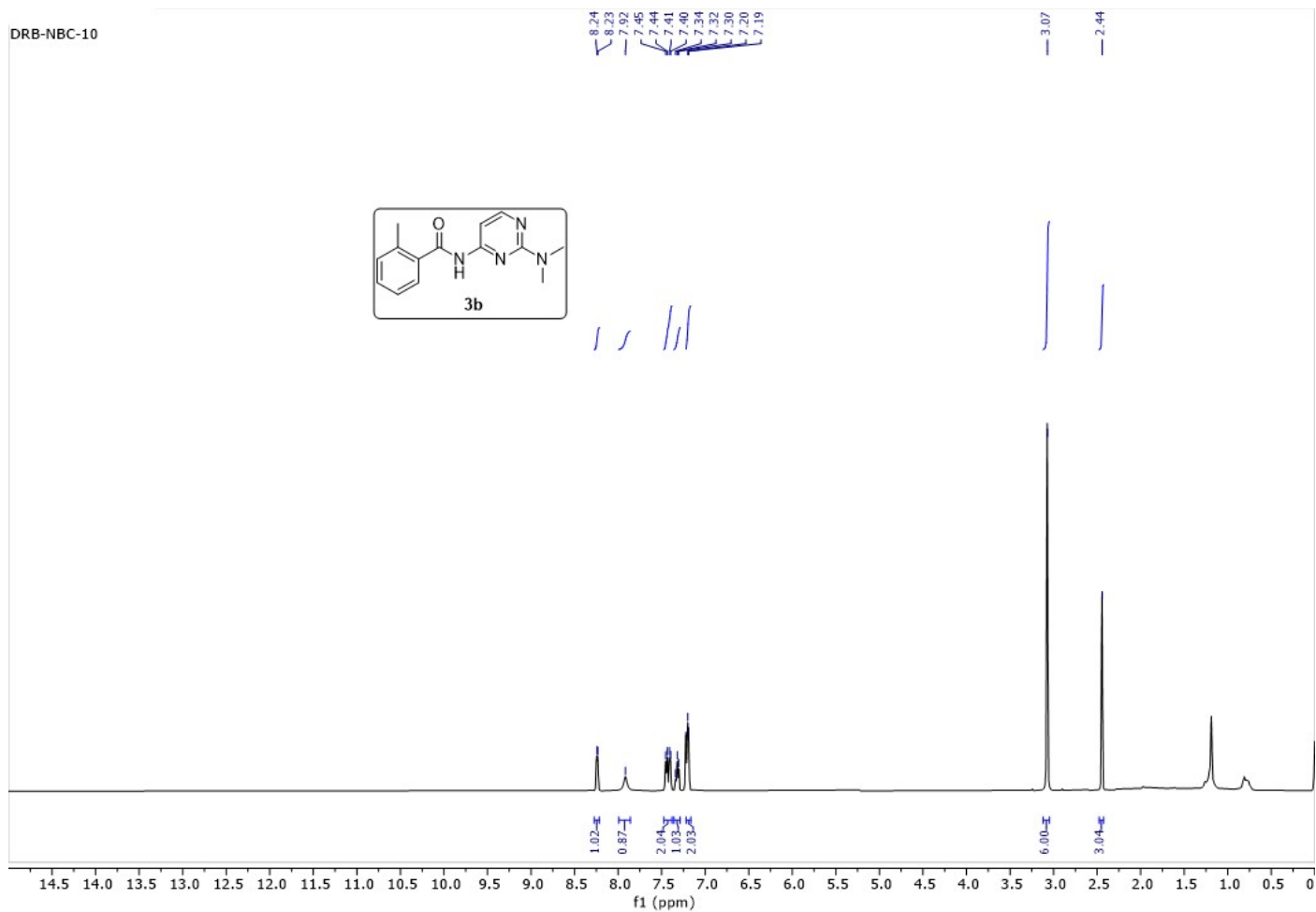
132.93
131.49
127.87
126.25

97.24

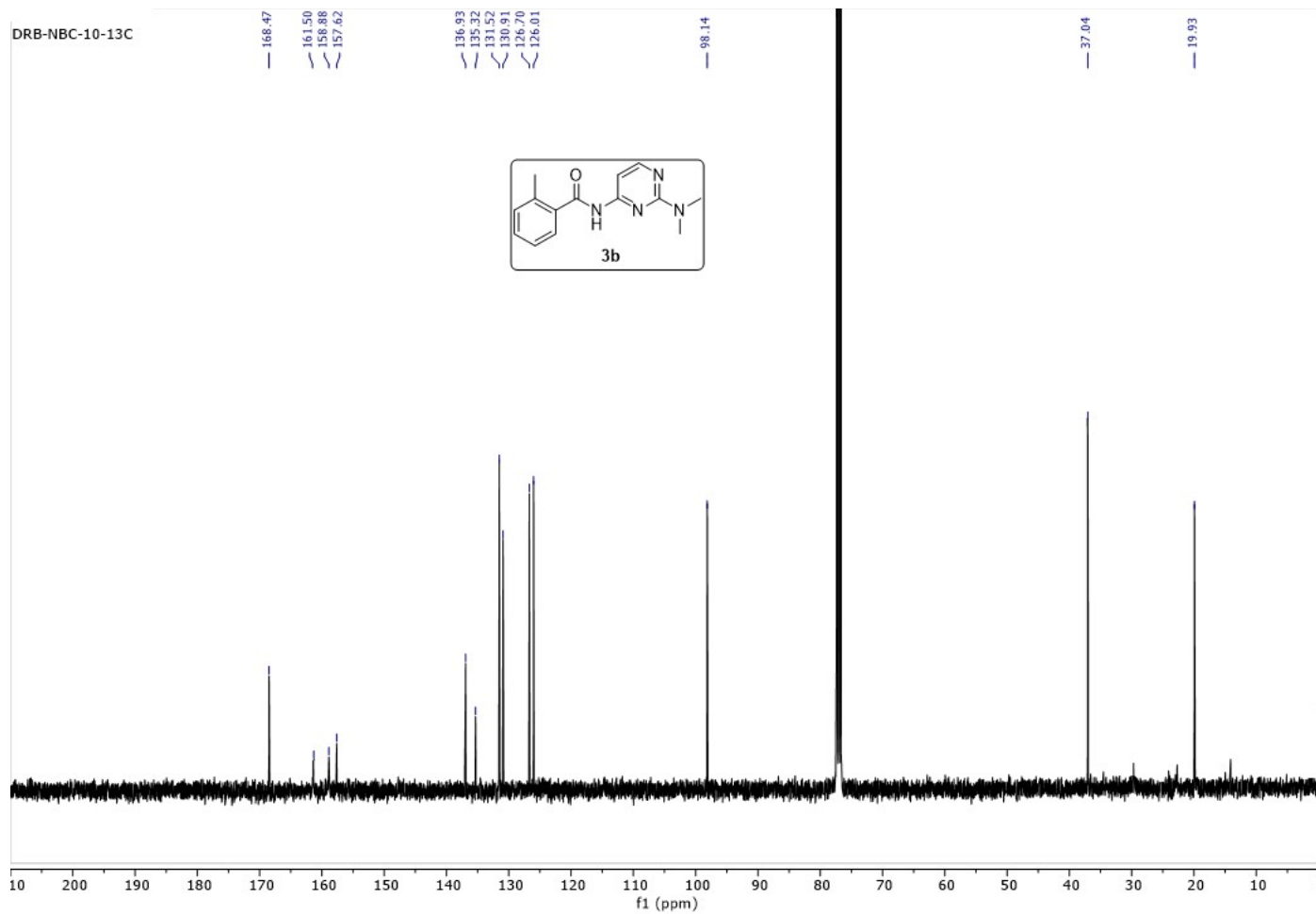
35.99



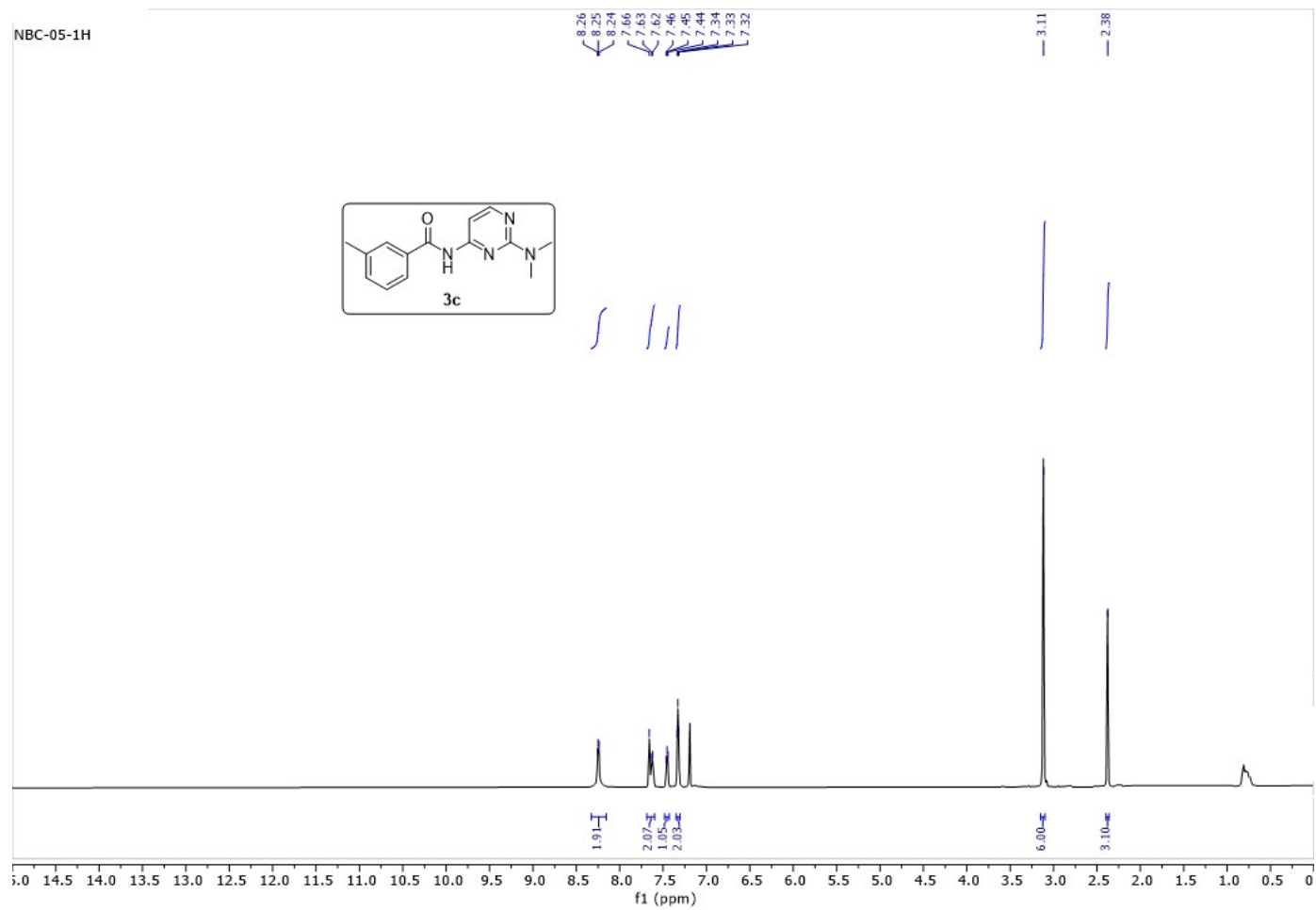
DRB-NBC-10



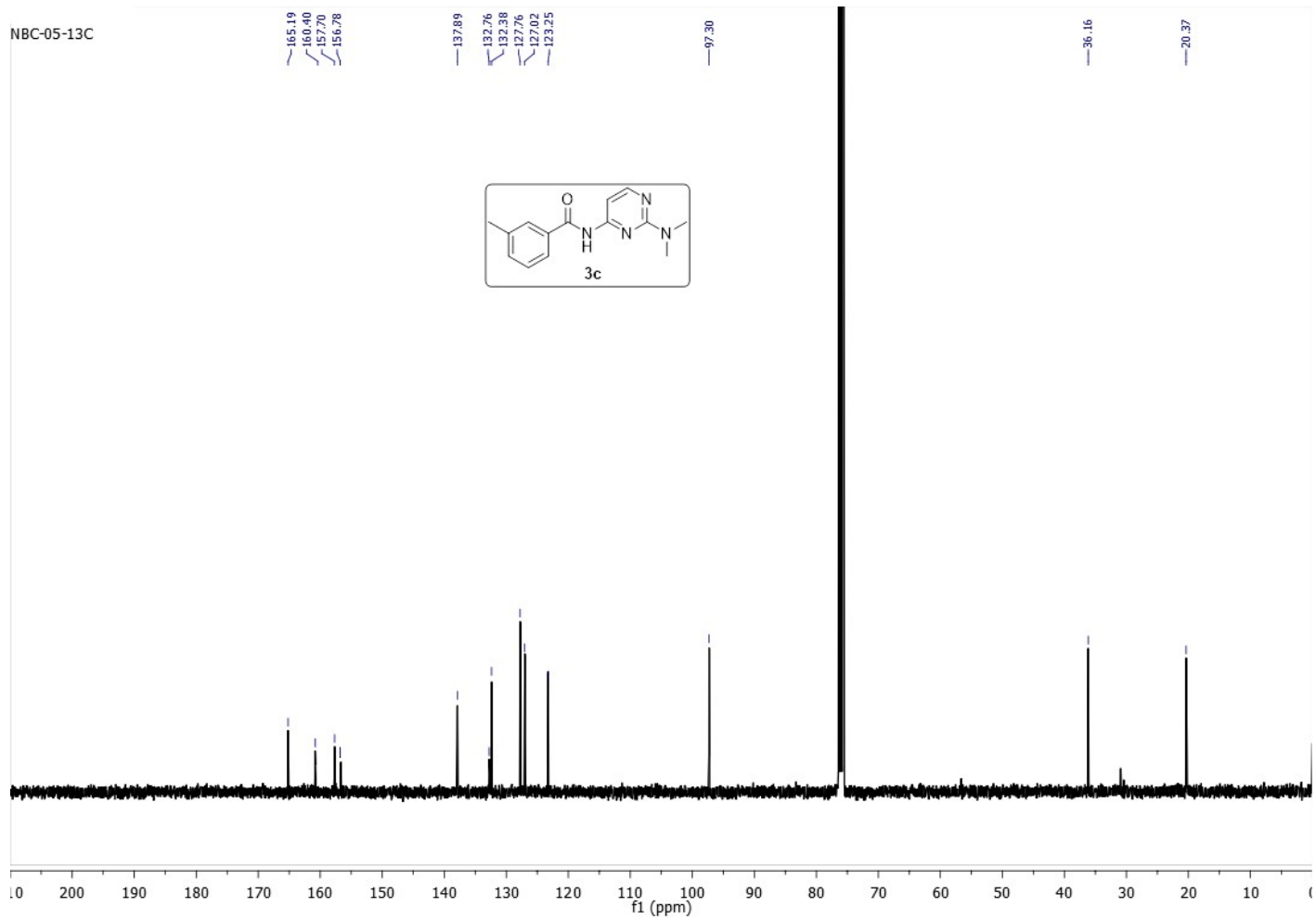
DRB-NBC-10-13C



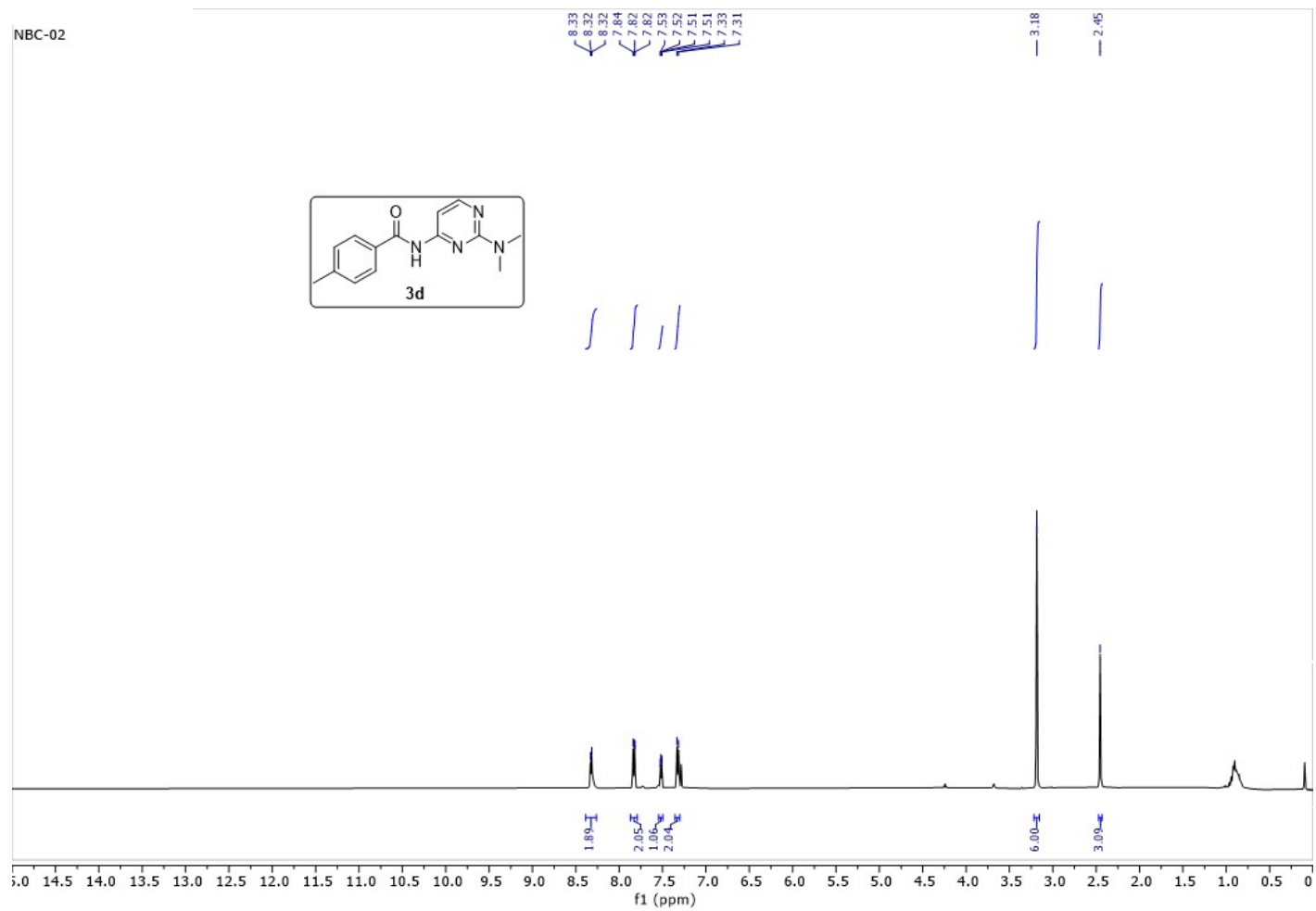
NBC-05-1H



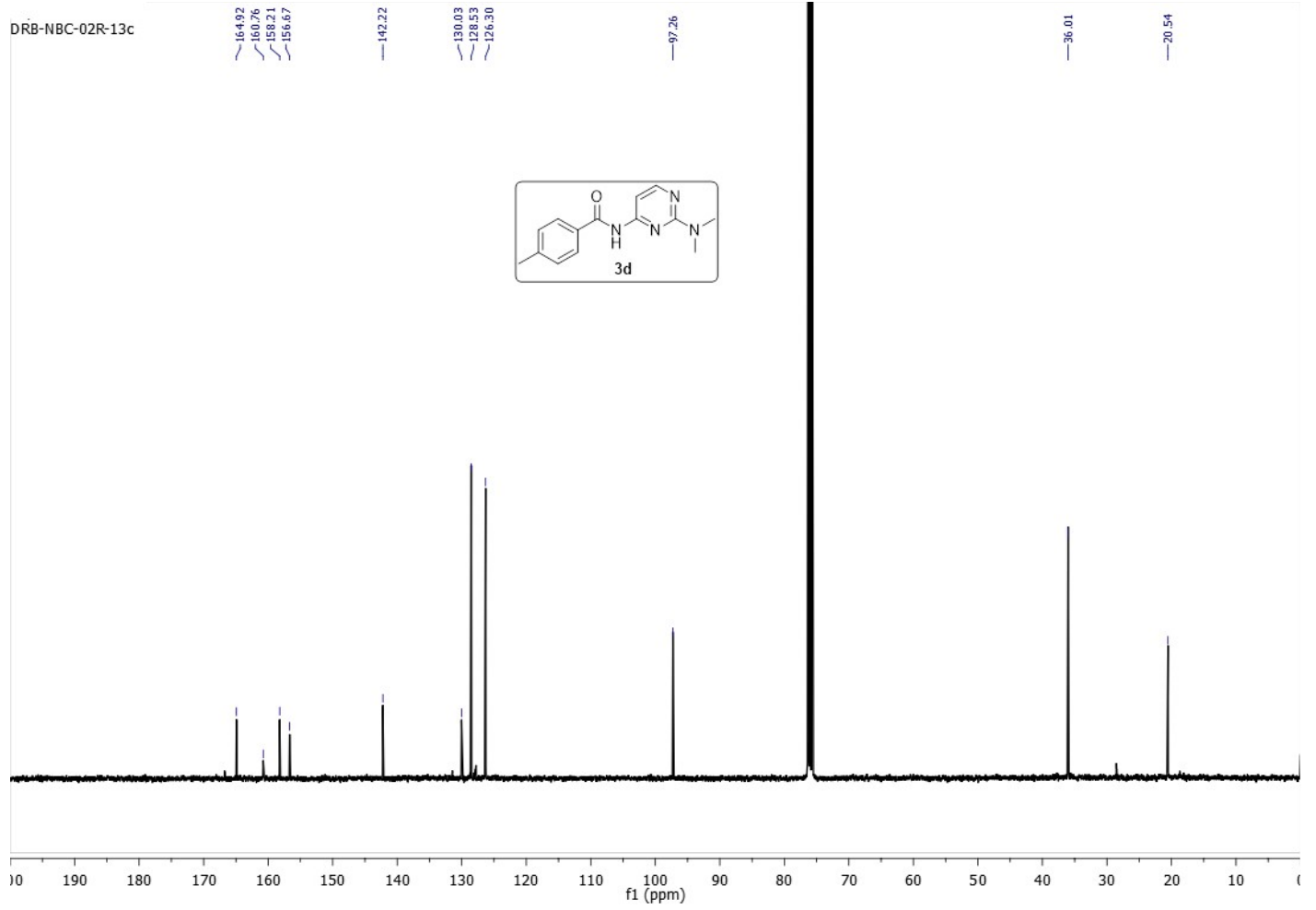
NBC-05-13C



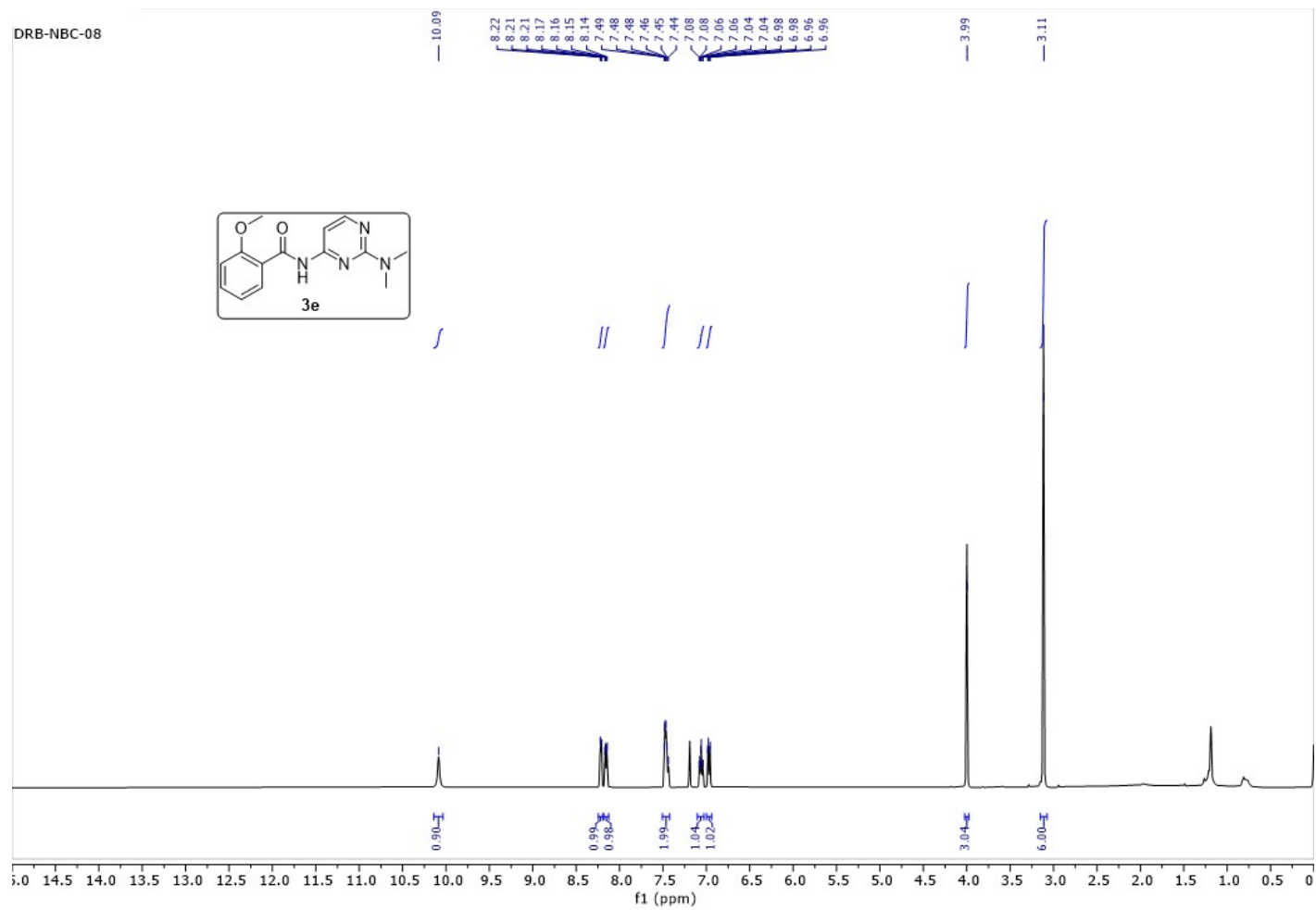
NBC-02



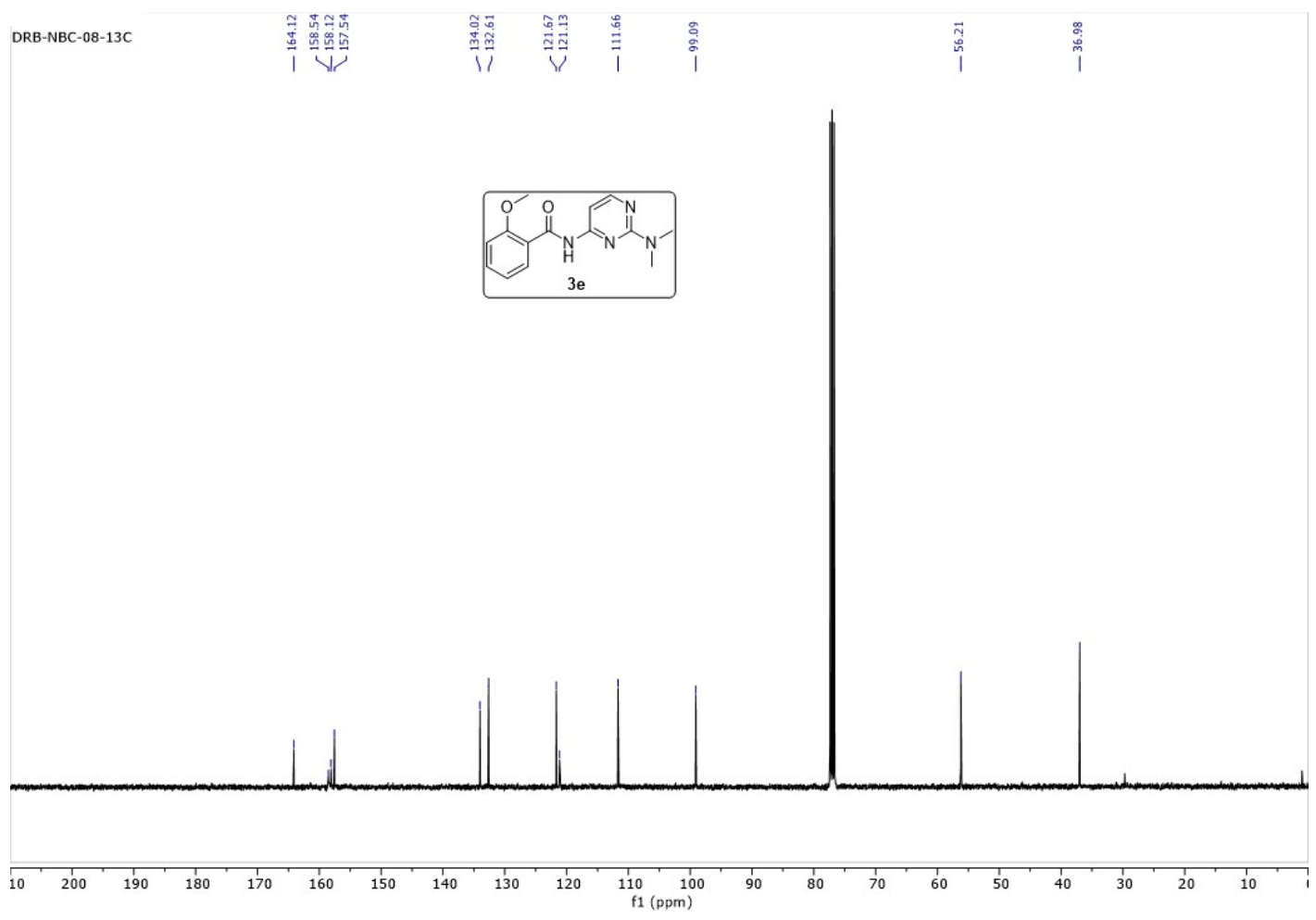
DRB-NBC-02R-13c



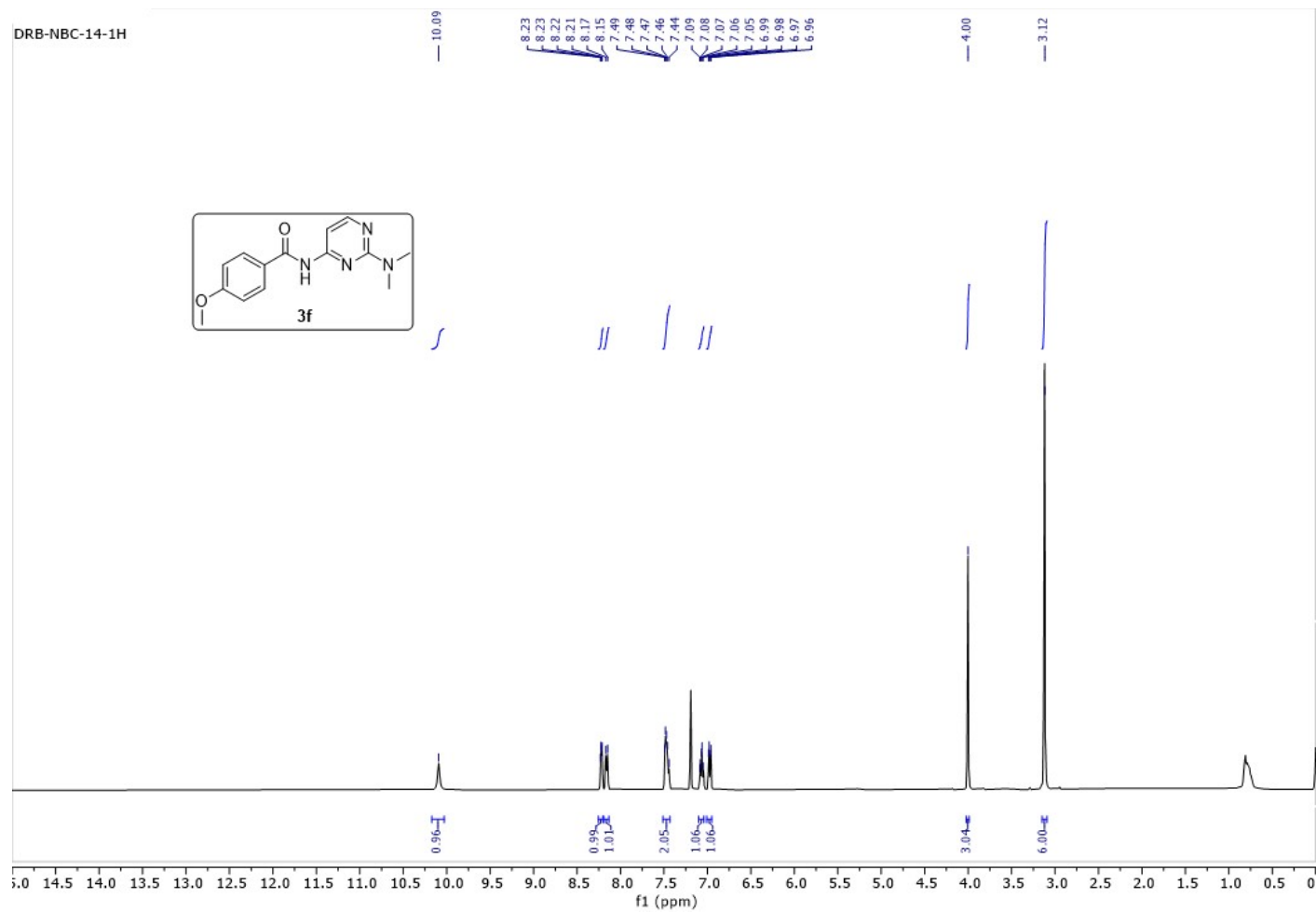
DRB-NBC-08



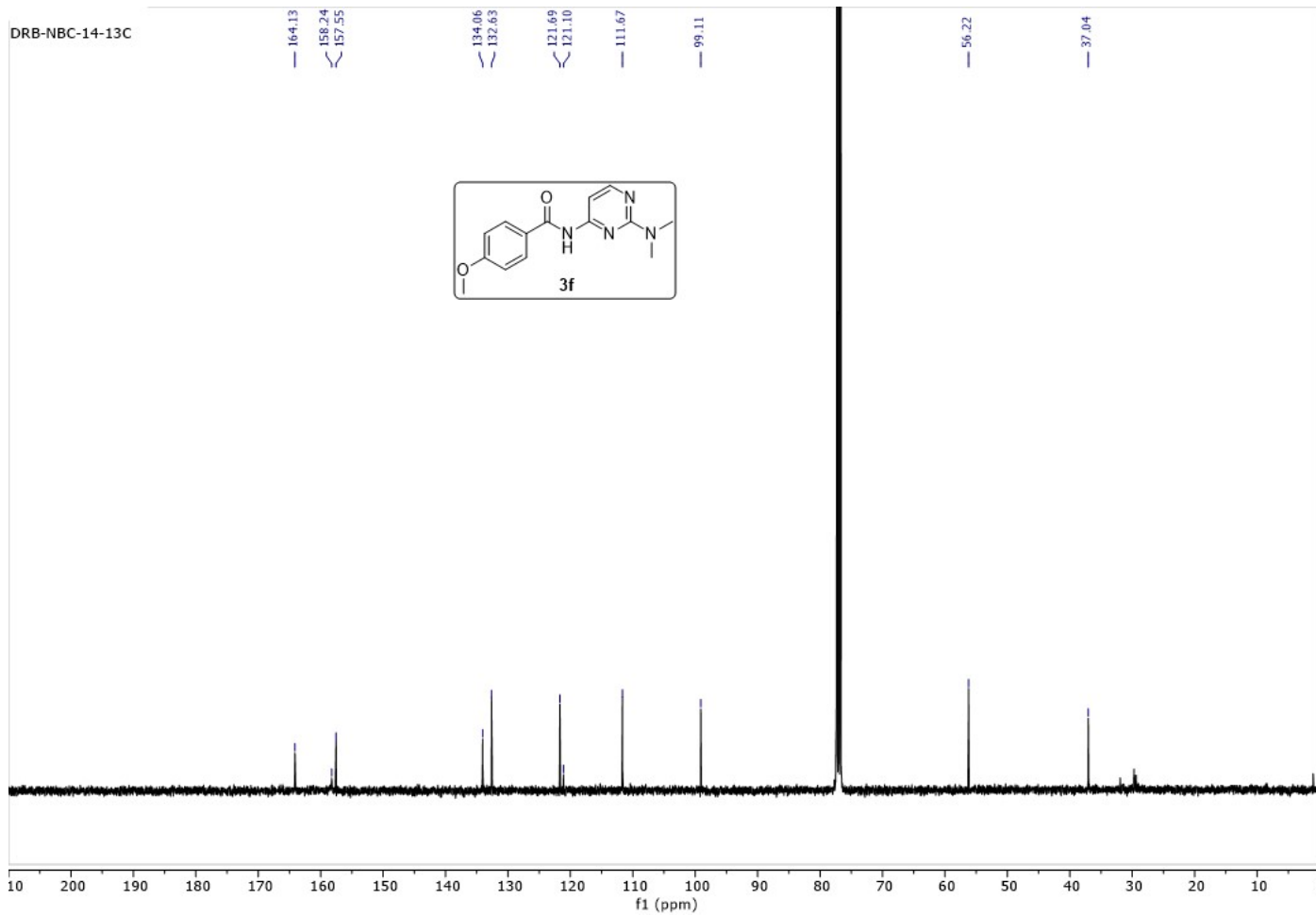
DRB-NBC-08-13C



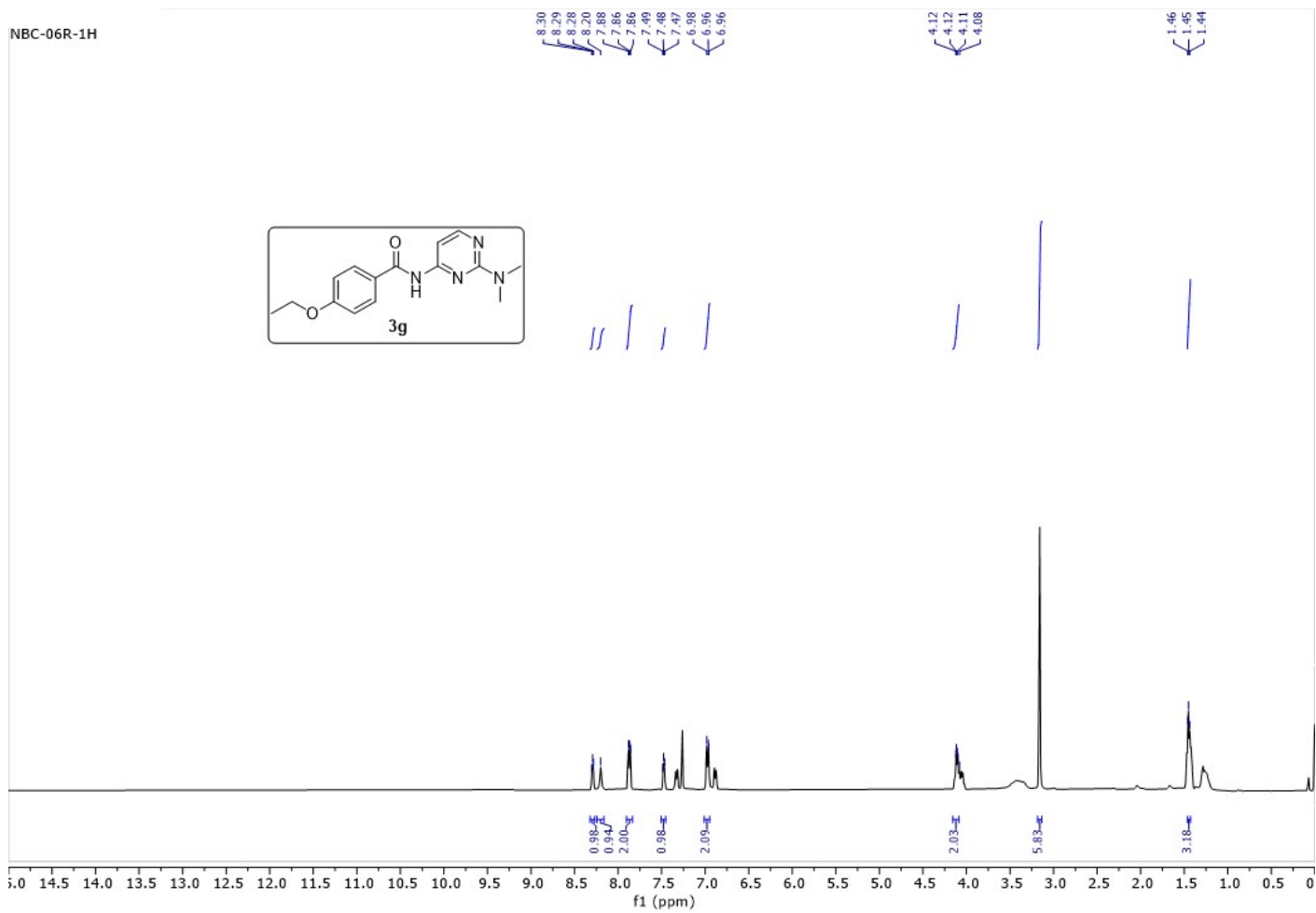
DRB-NBC-14-1H



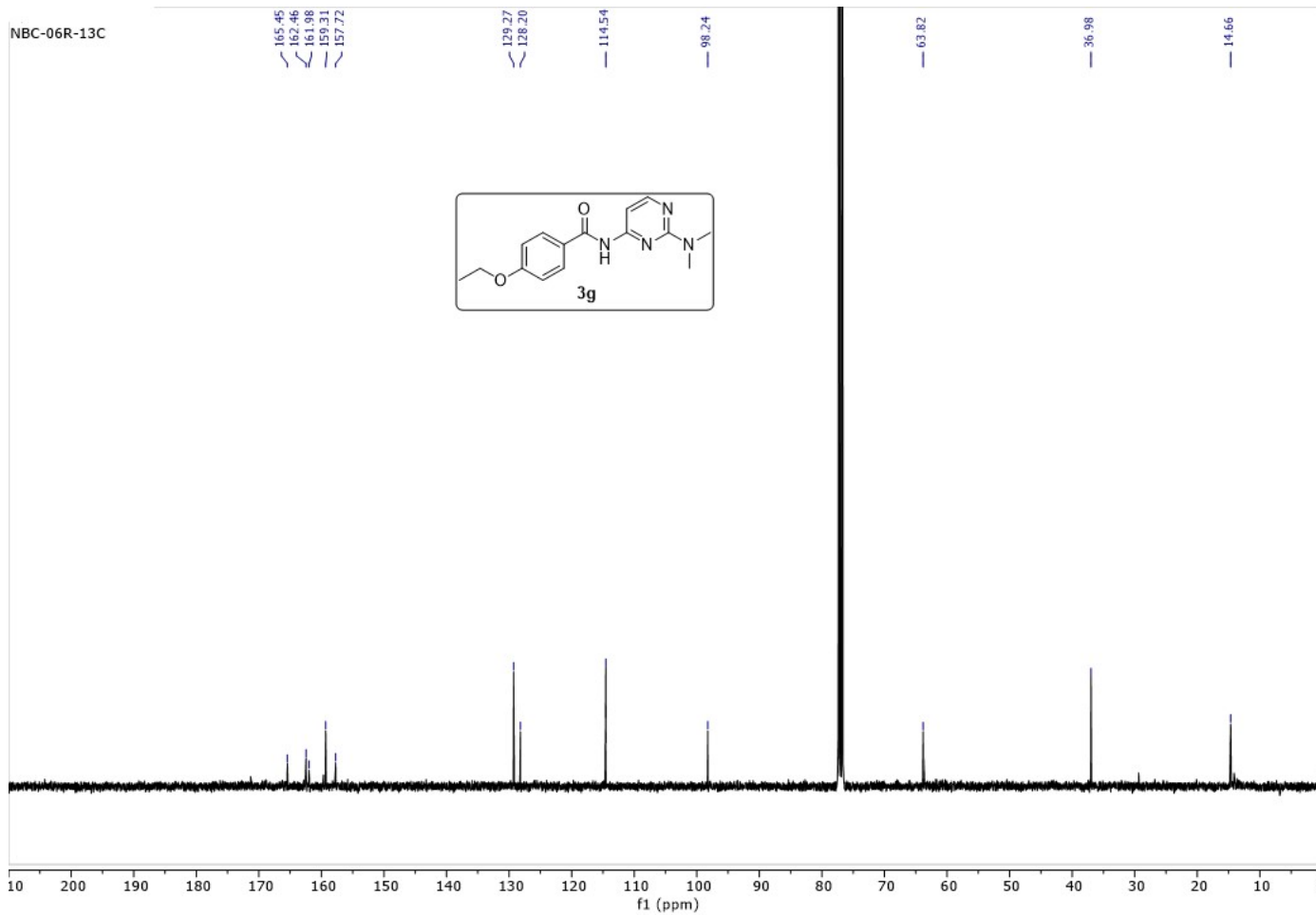
DRB-NBC-14-13C



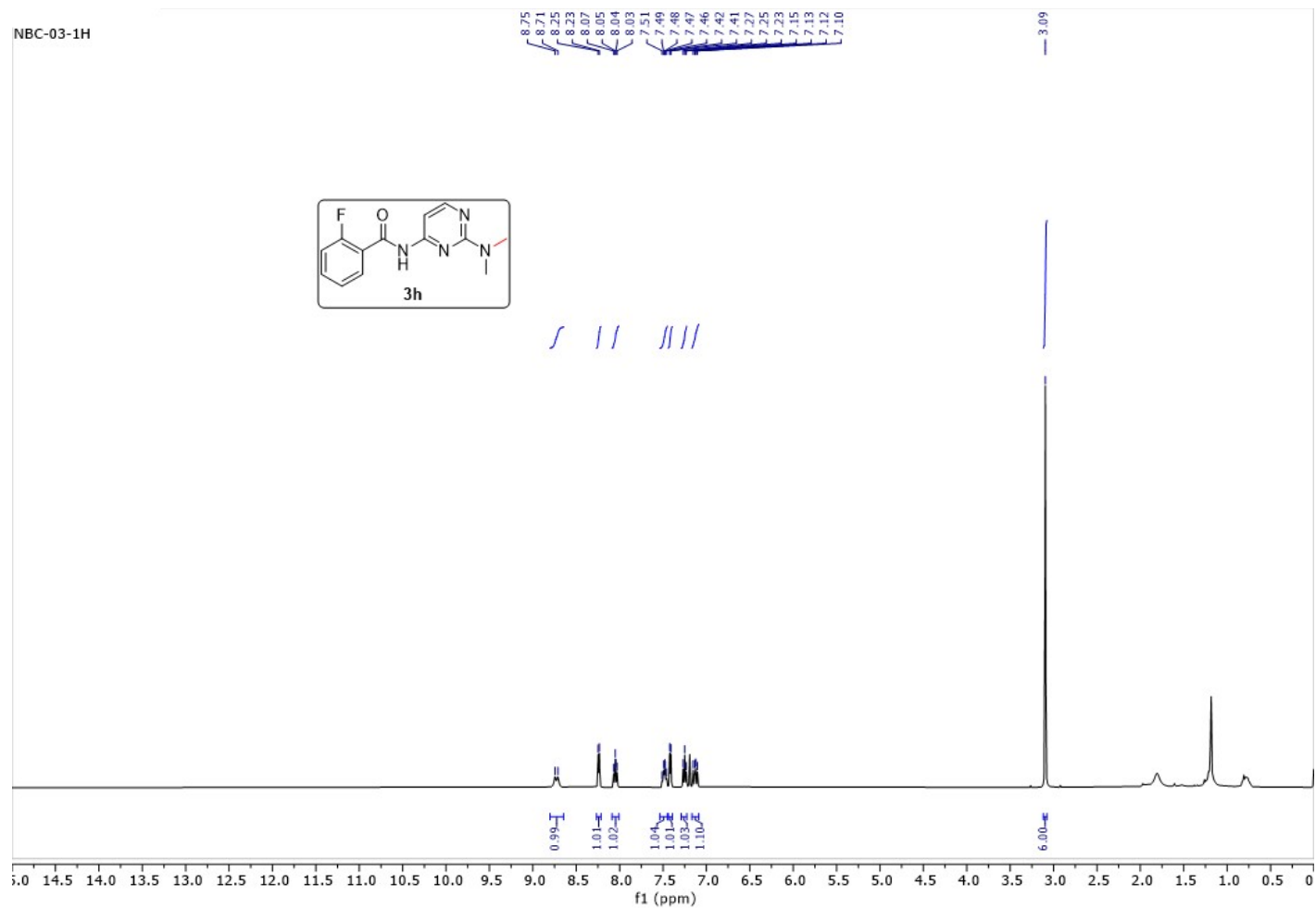
NBC-06R-1H



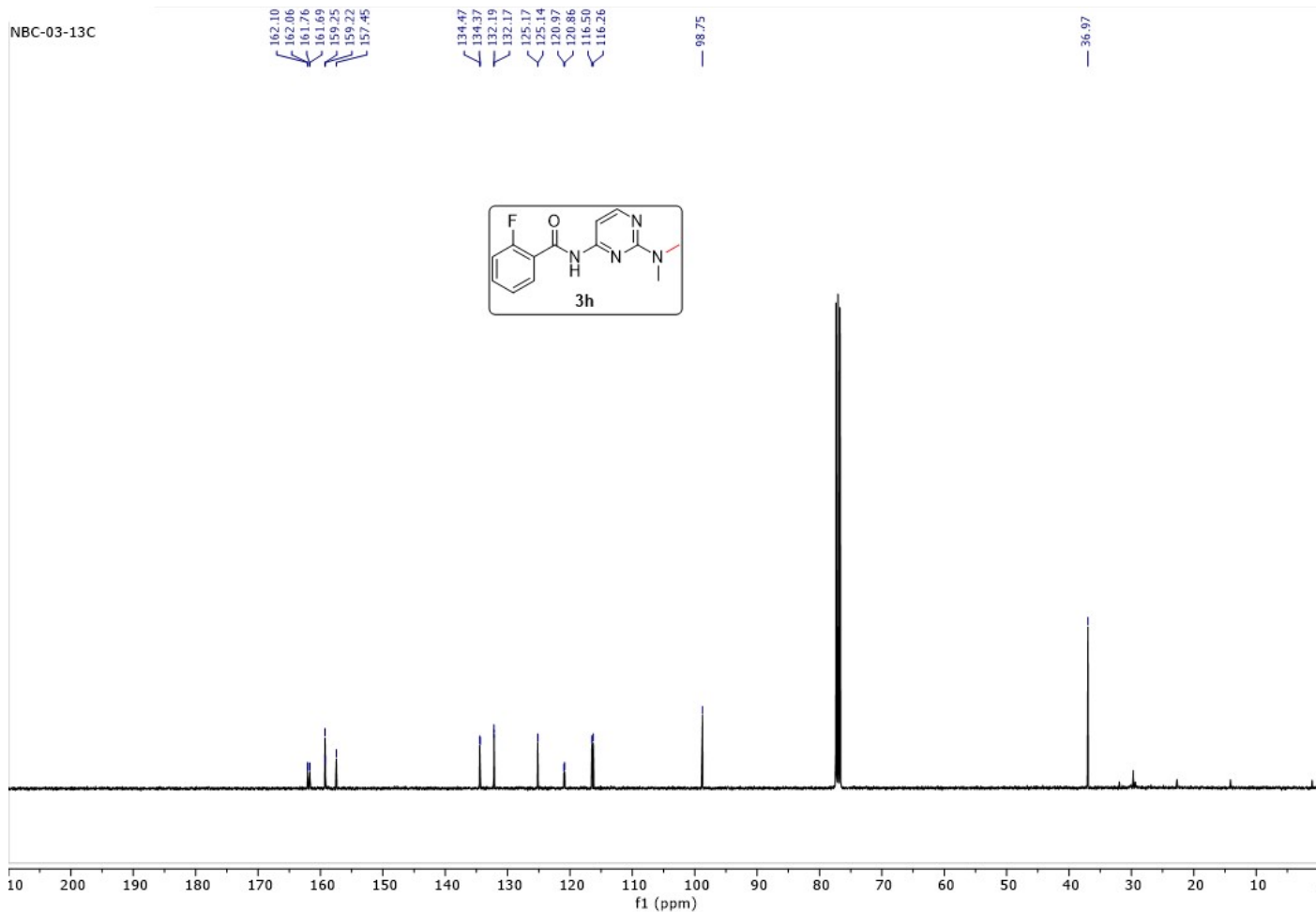
NBC-06R-13C



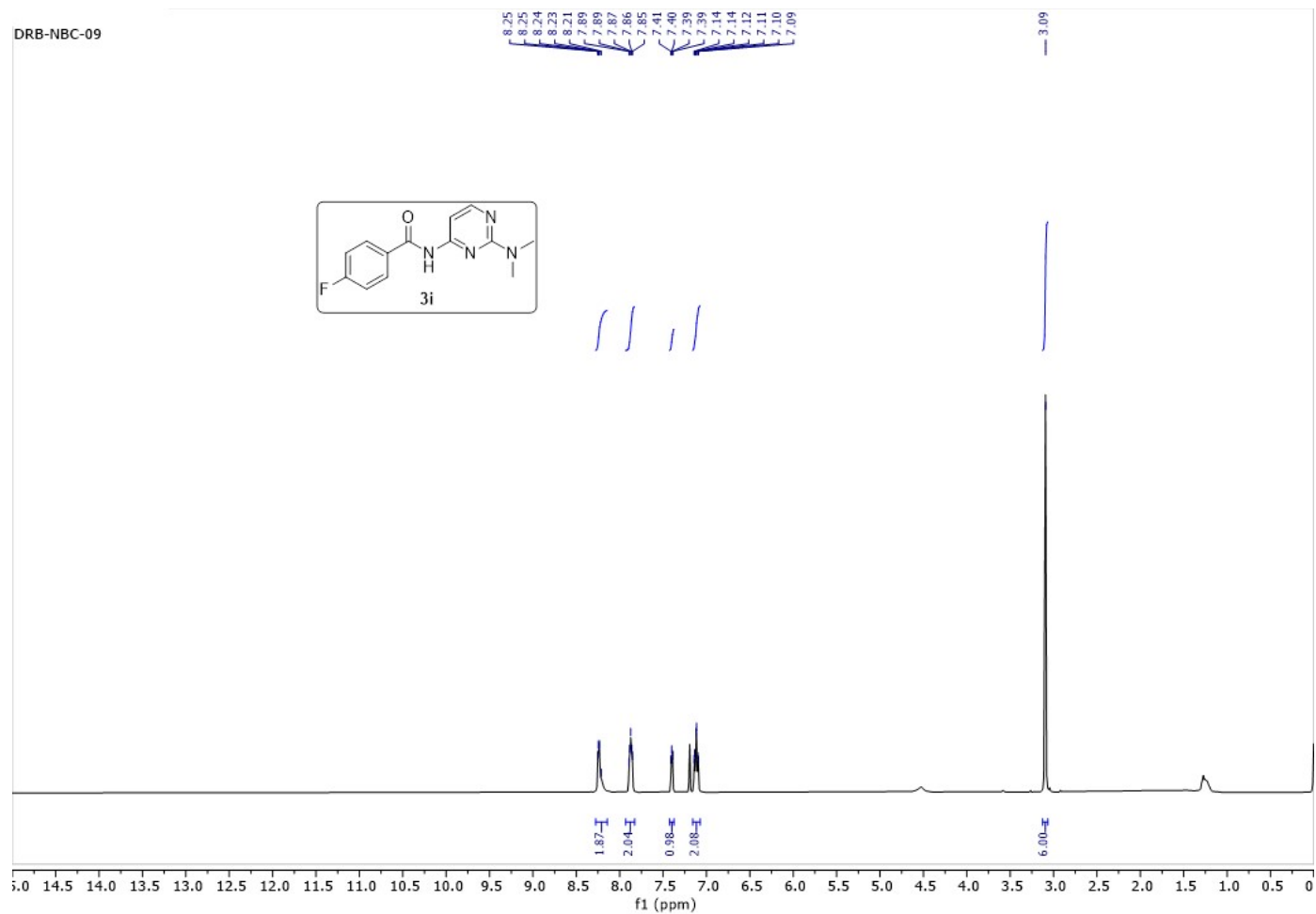
NBC-03-1H



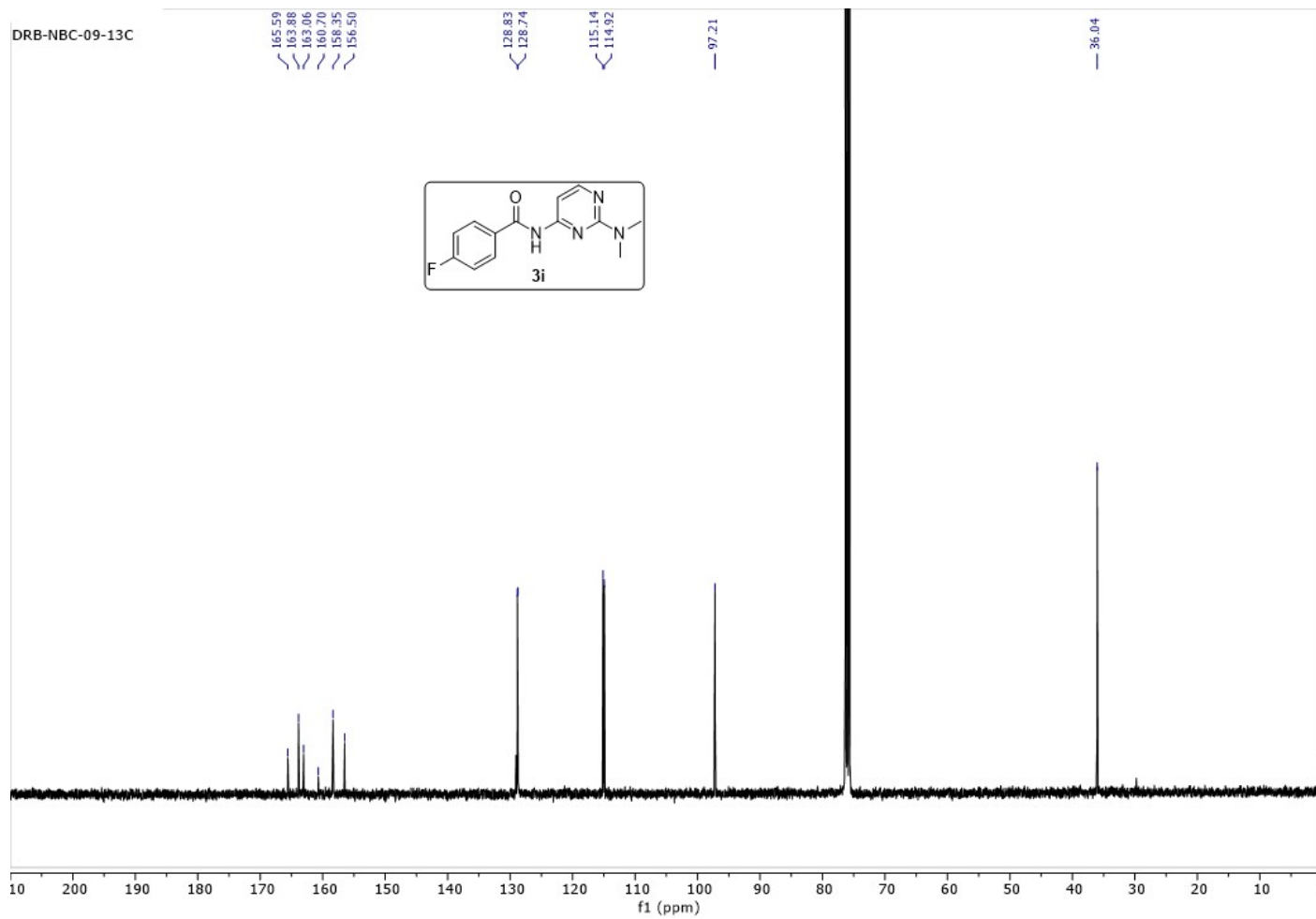
NBC-03-13C



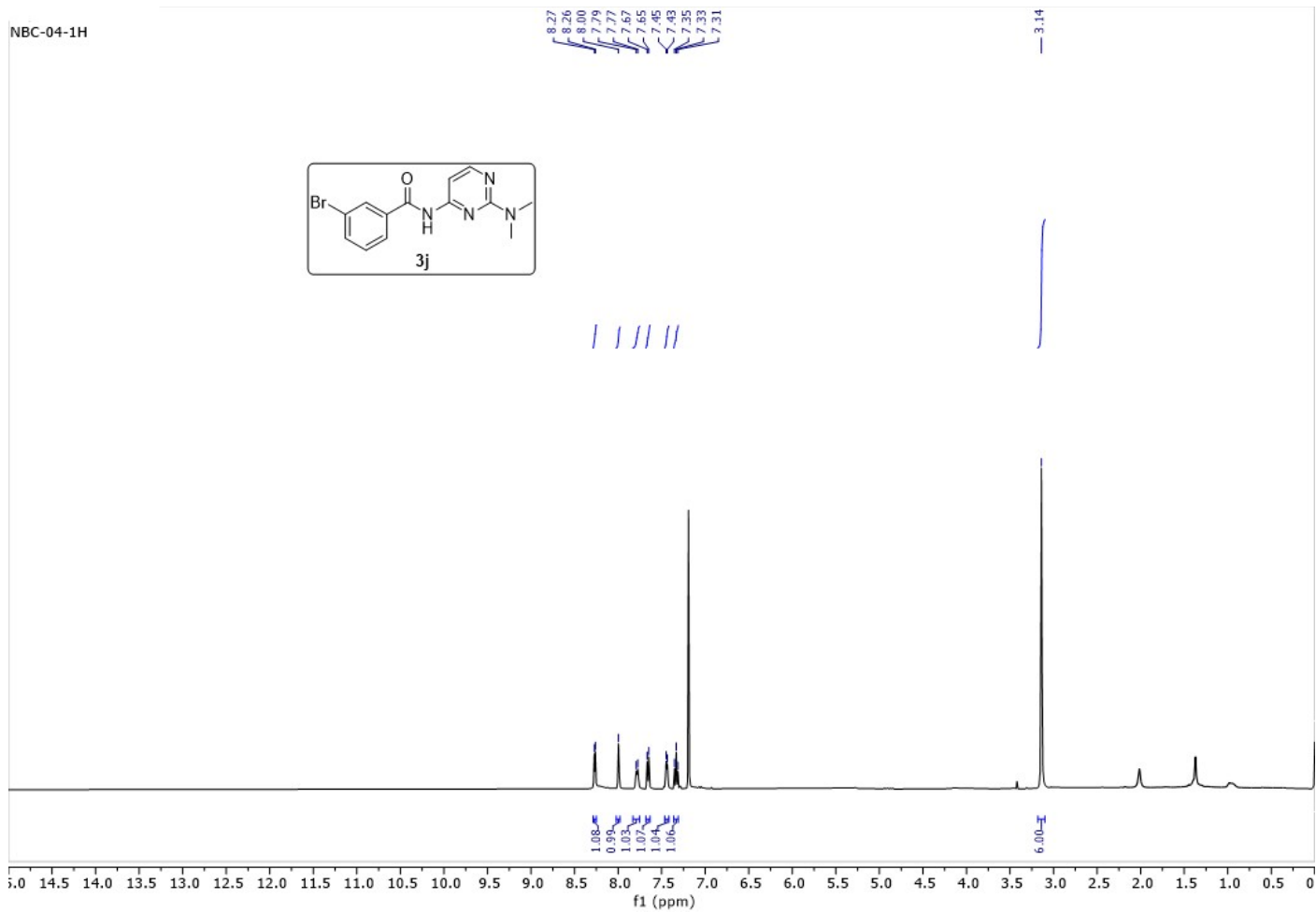
DRB-NBC-09



DRB-NBC-09-13C



NBC-04-1H



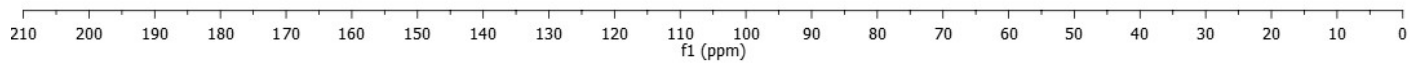
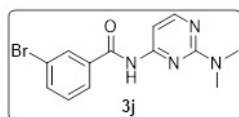
NBC-04-13c

164.46
159.45
157.34

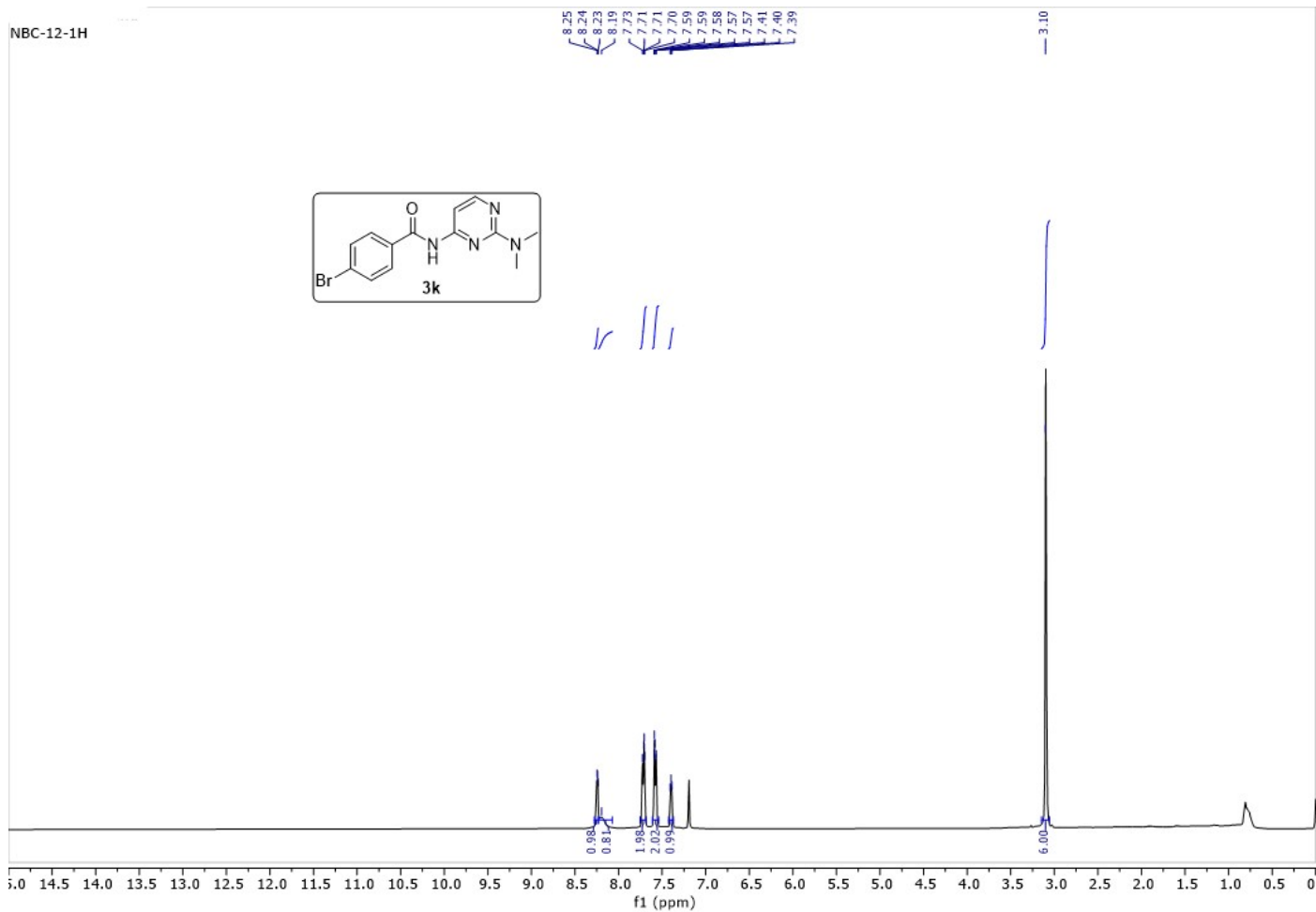
135.37
134.76
130.59
130.50
126.00
123.27

98.04

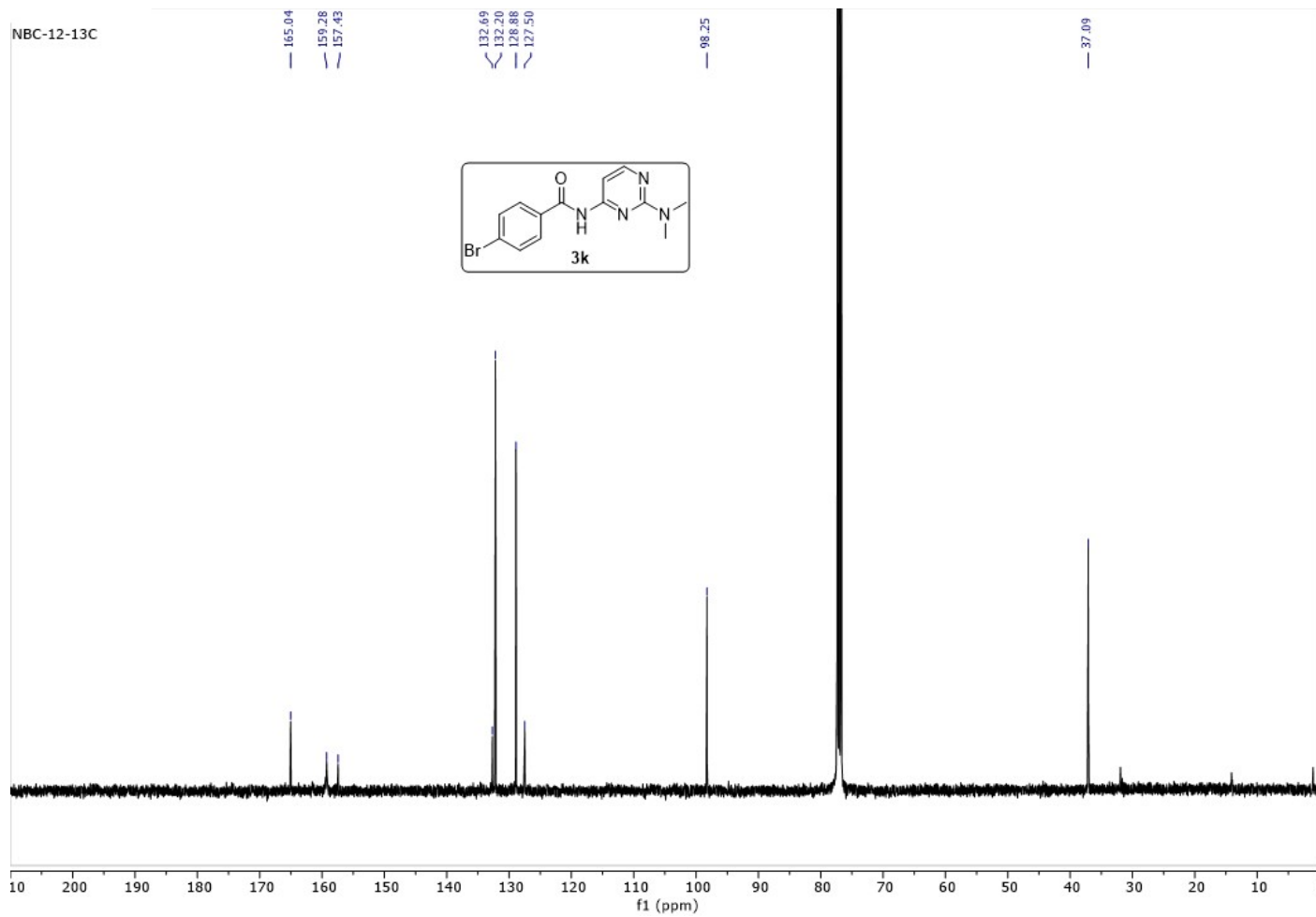
37.08



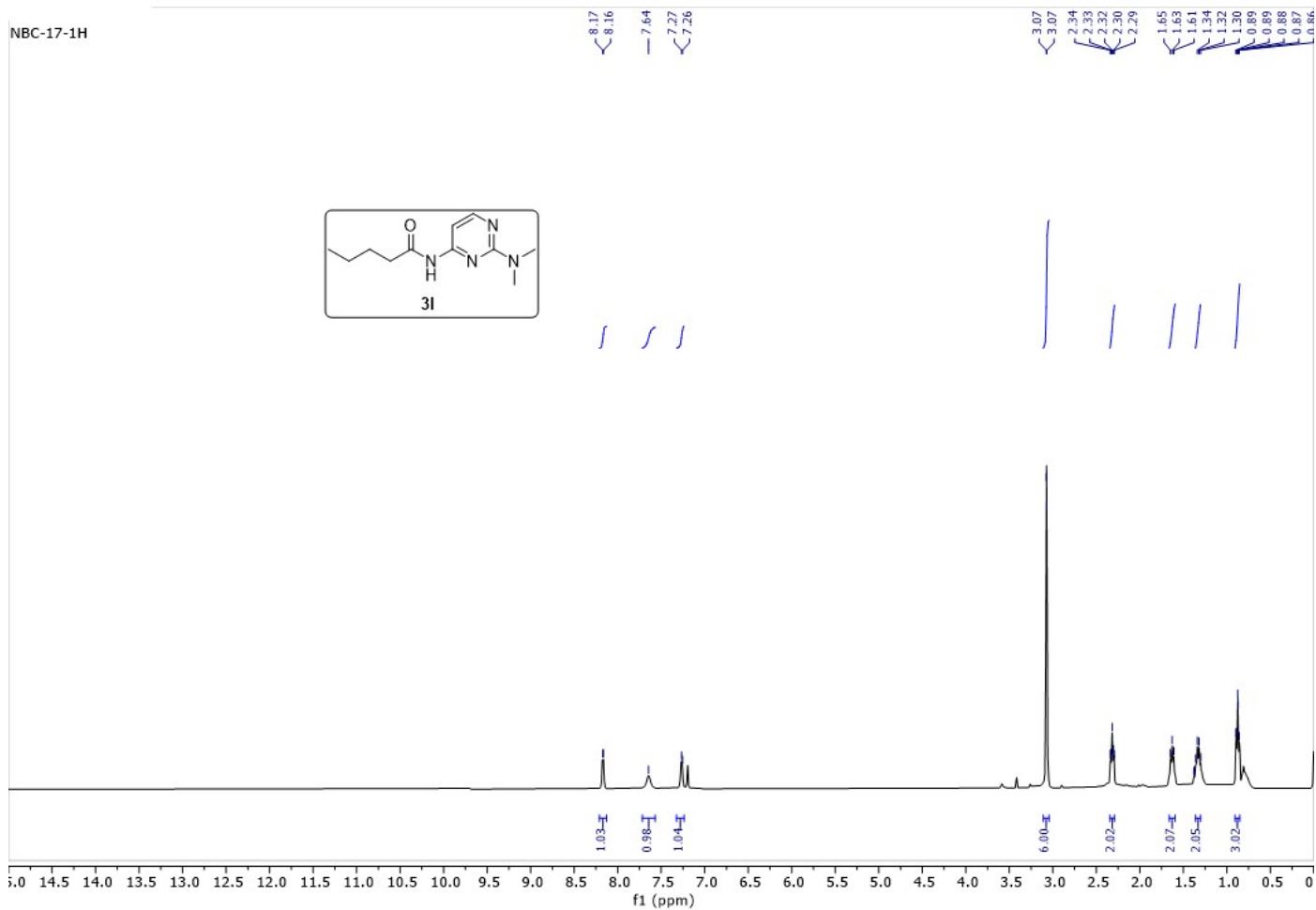
NBC-12-1H



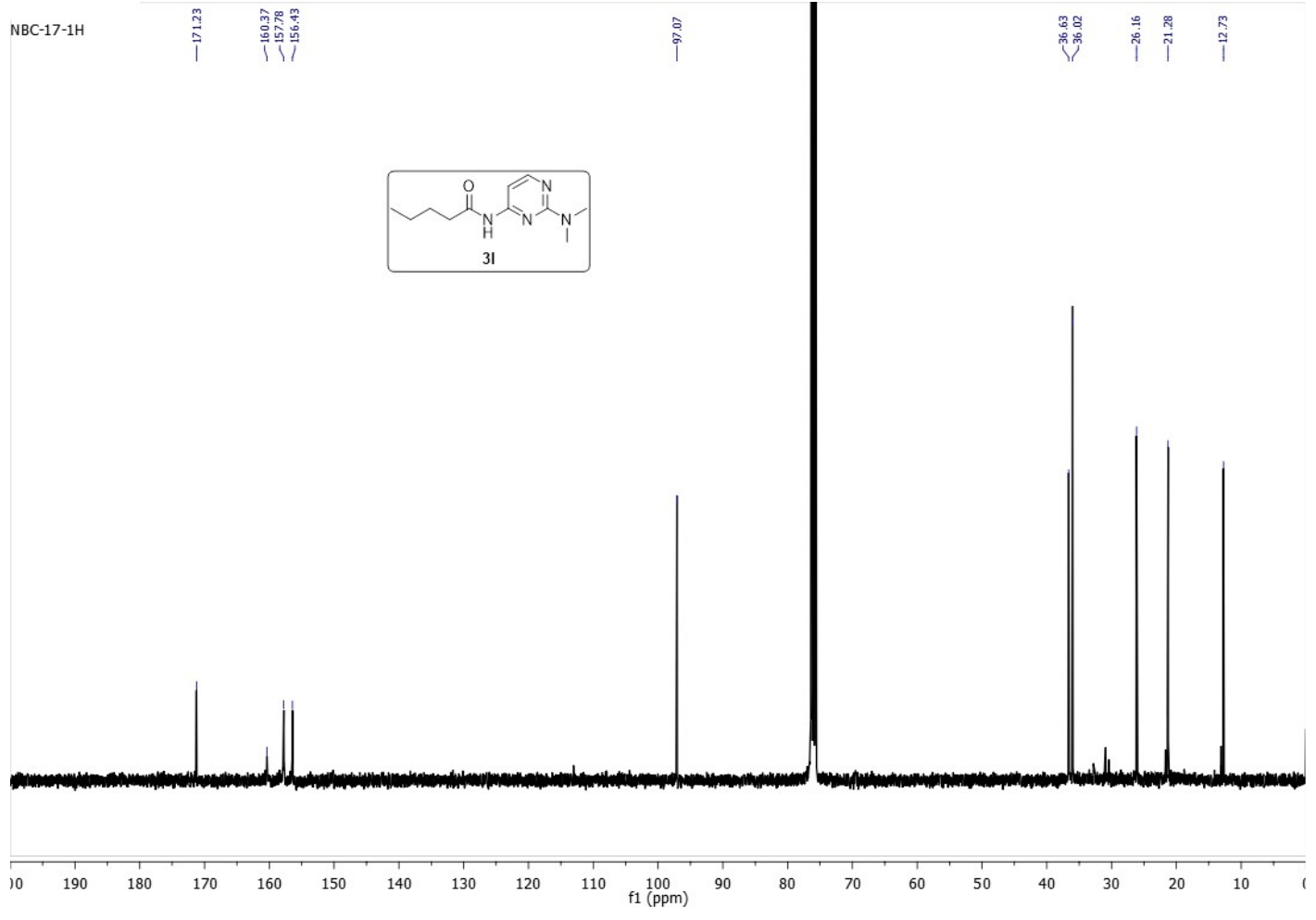
NBC-12-13C



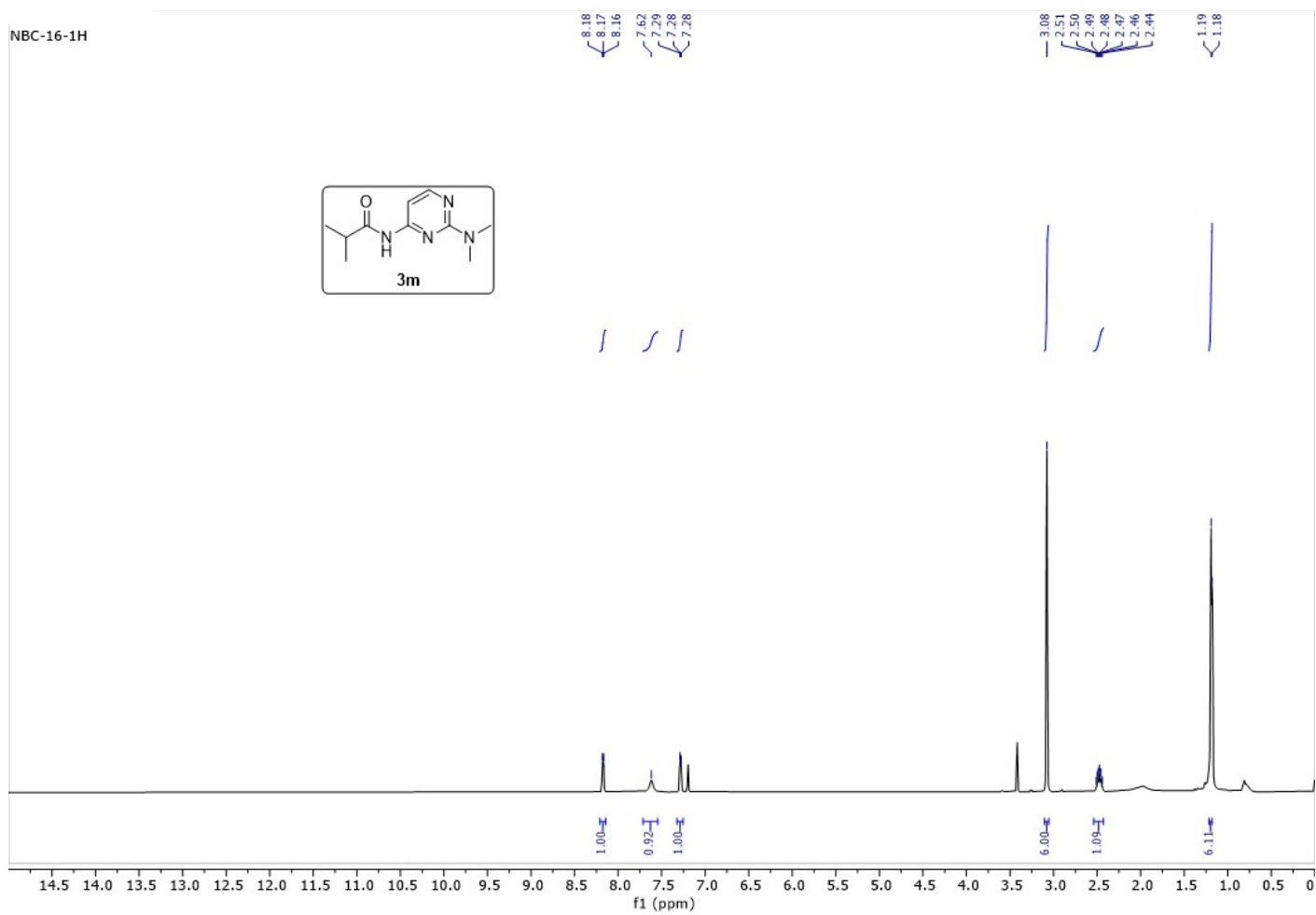
NBC-17-1H



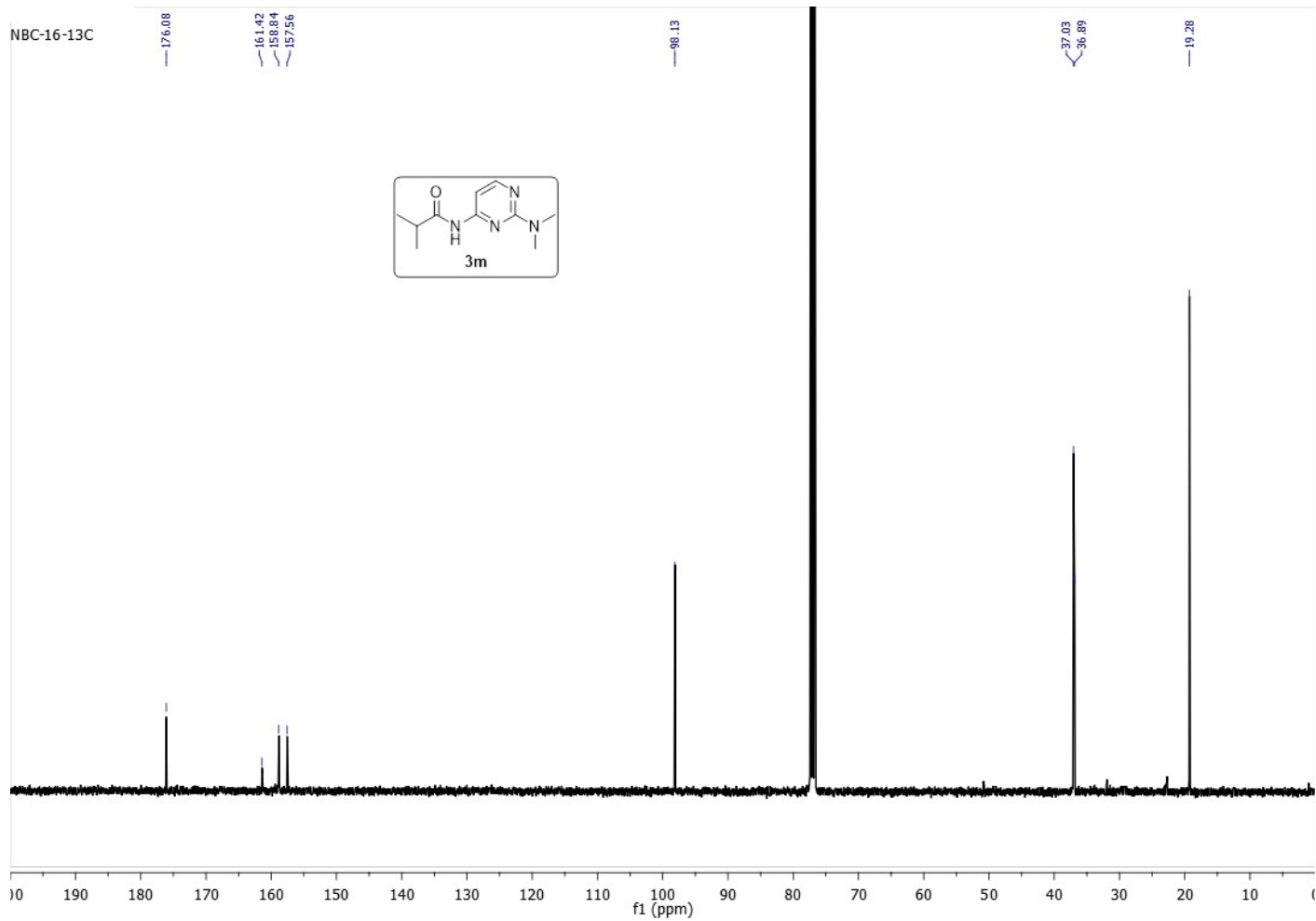
NBC-17-1H



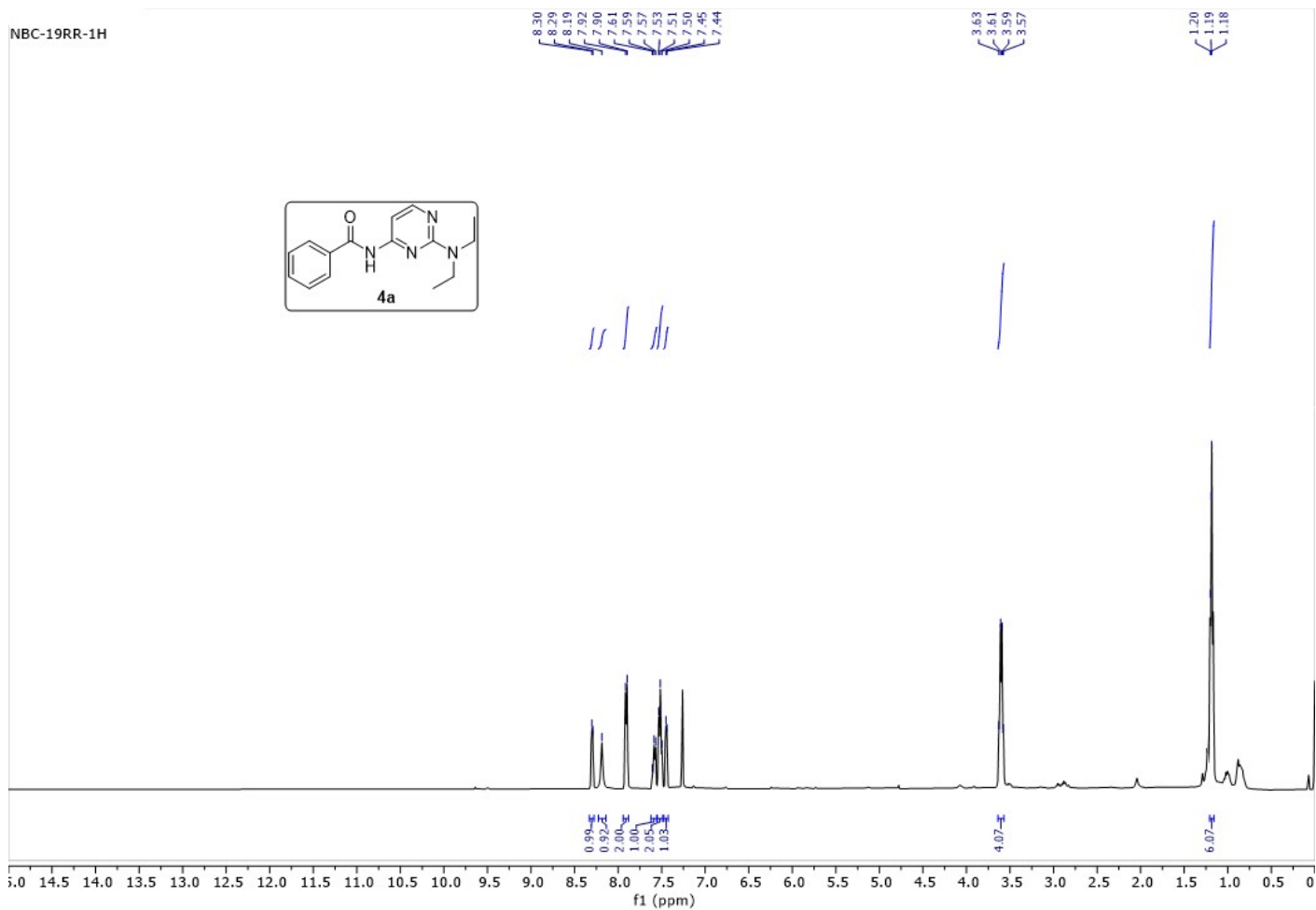
NBC-16-1H



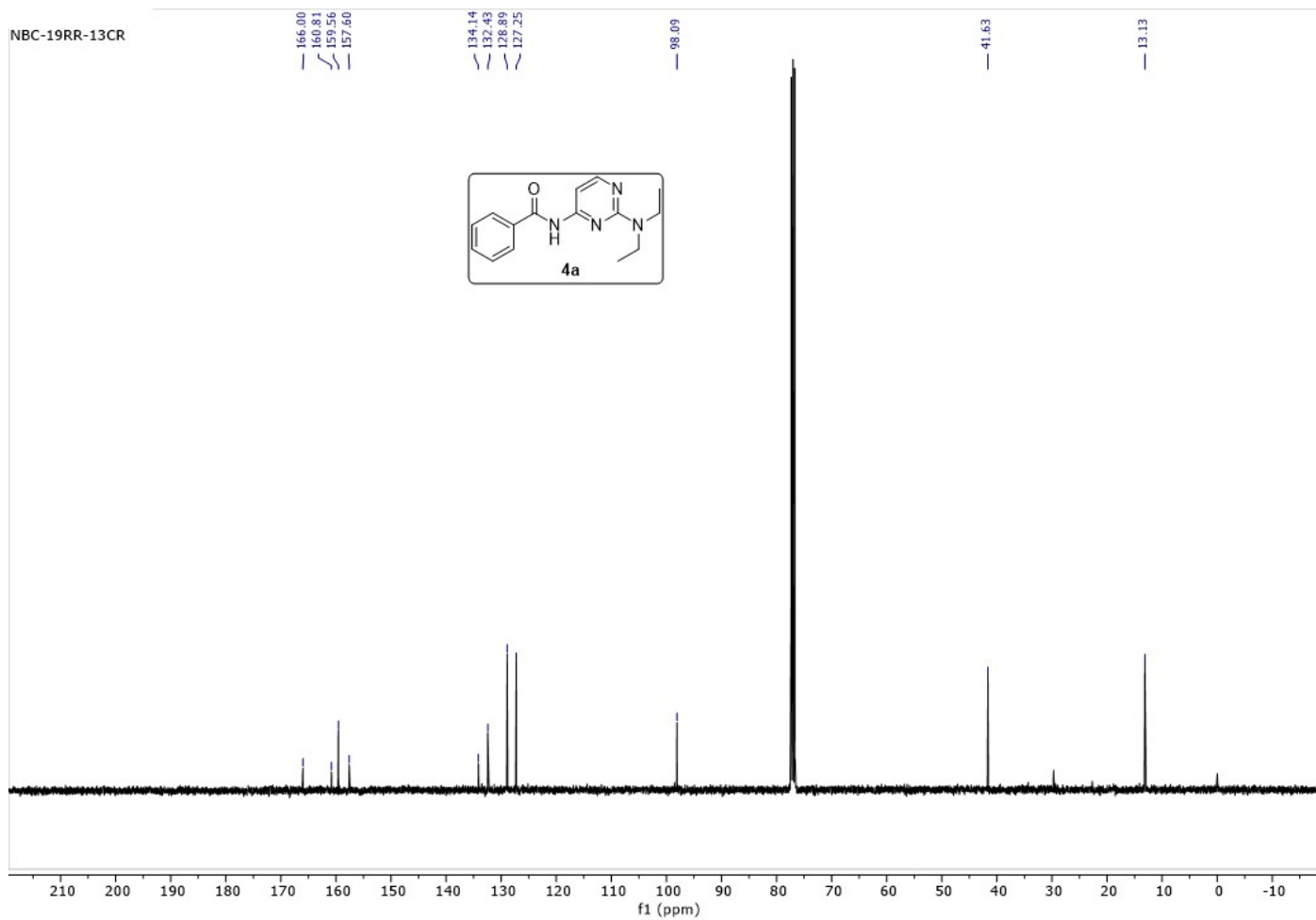
NBC-16-13C



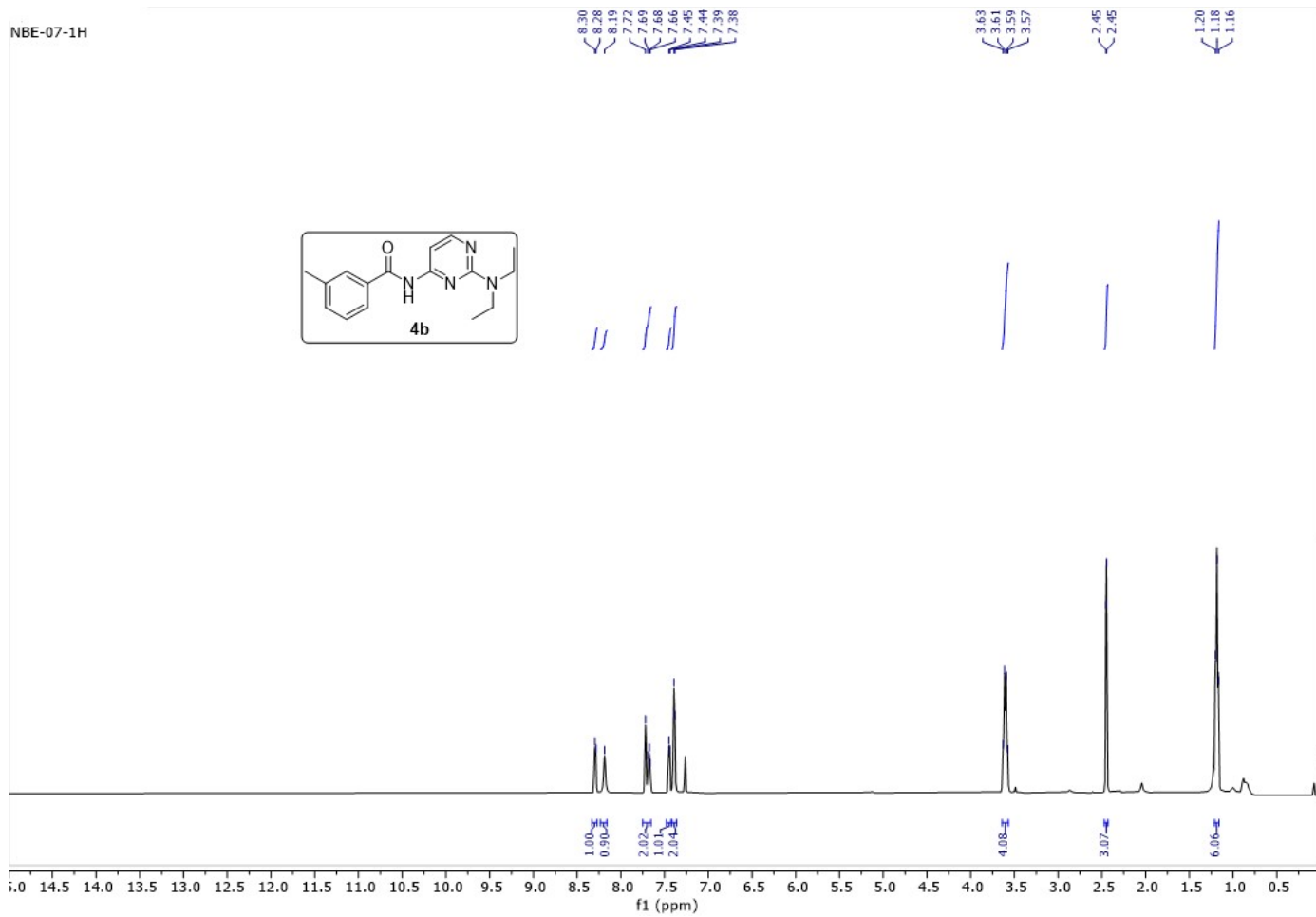
NBC-19RR-1H



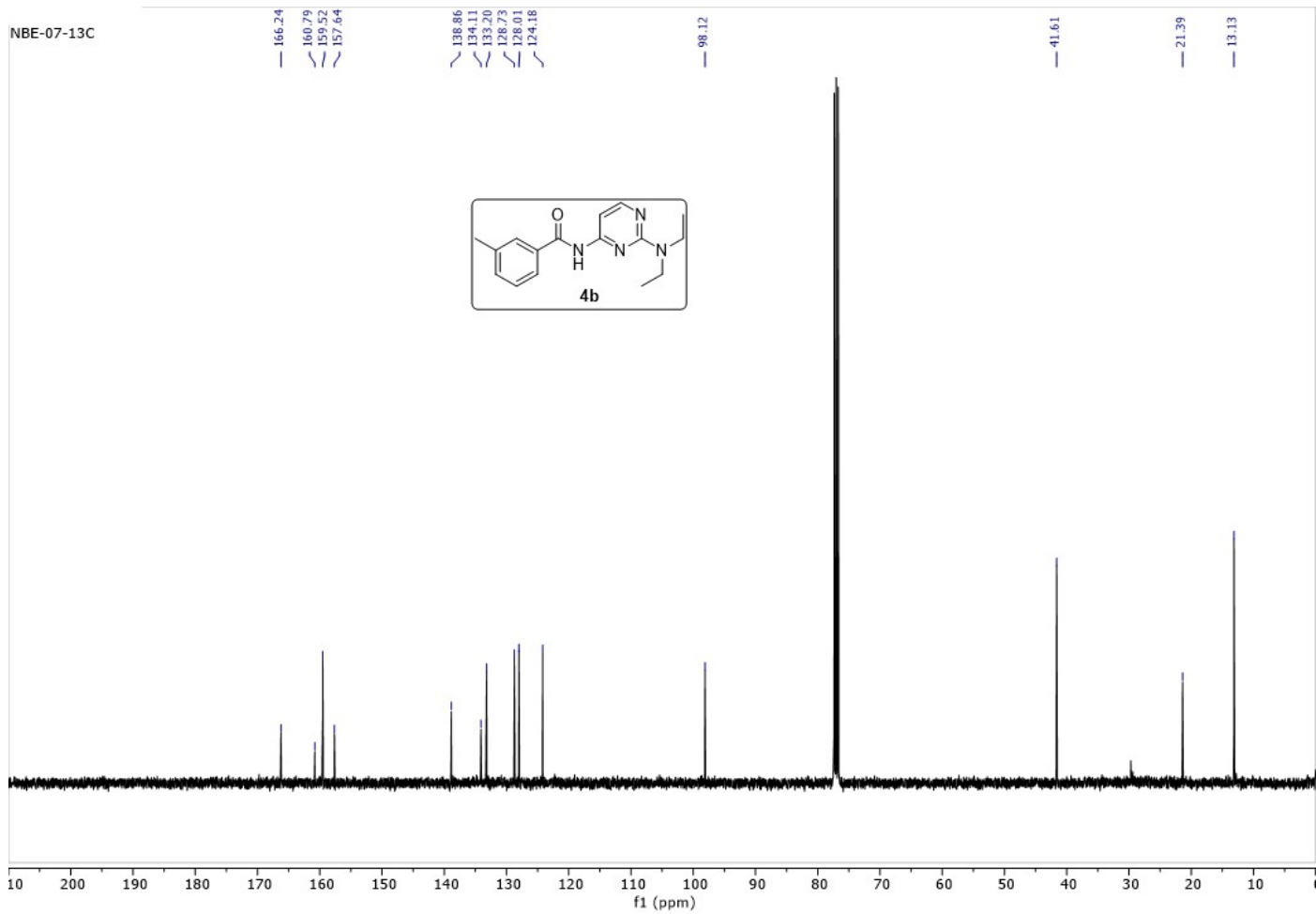
NBC-19RR-13CR



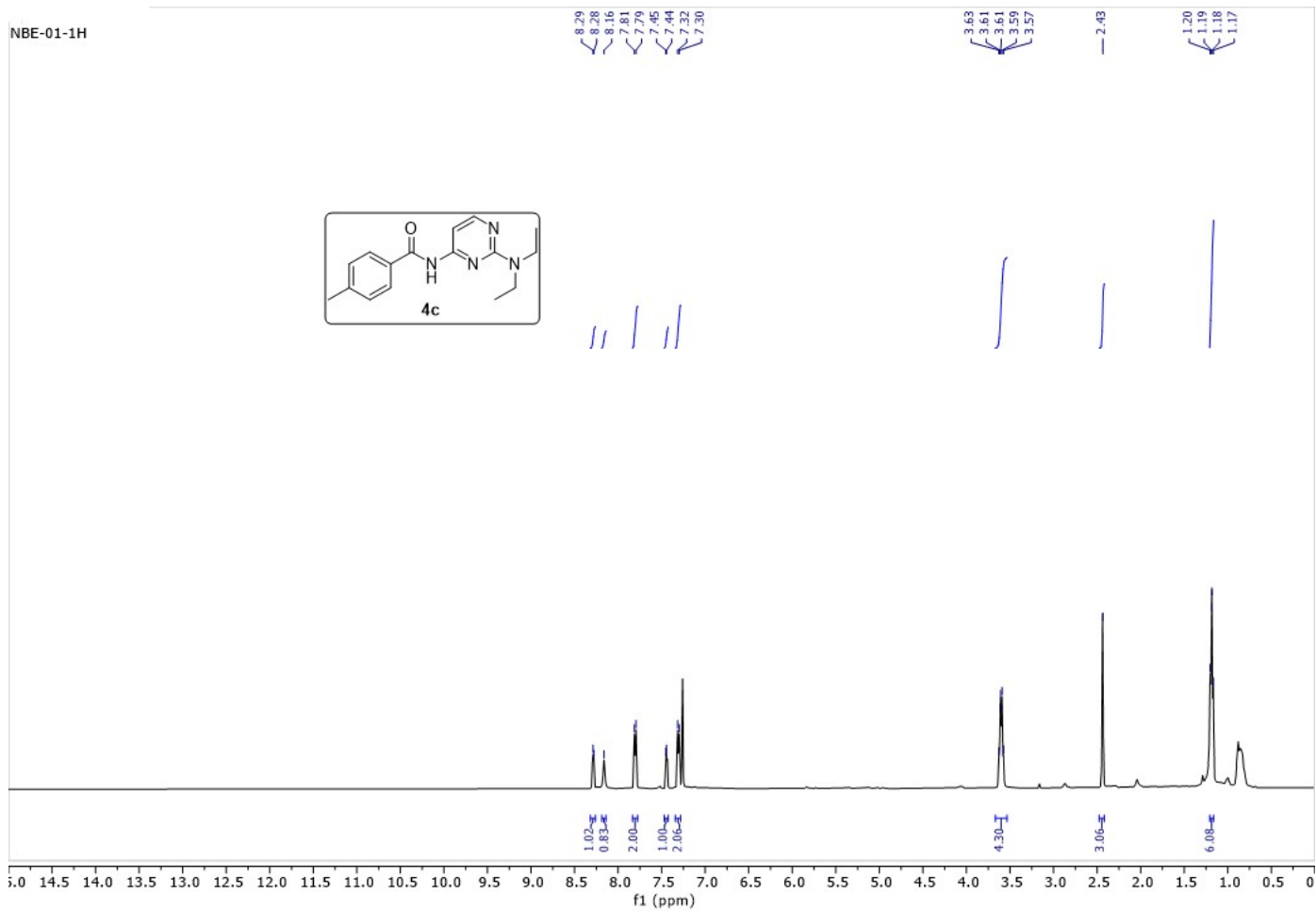
NBE-07-1H



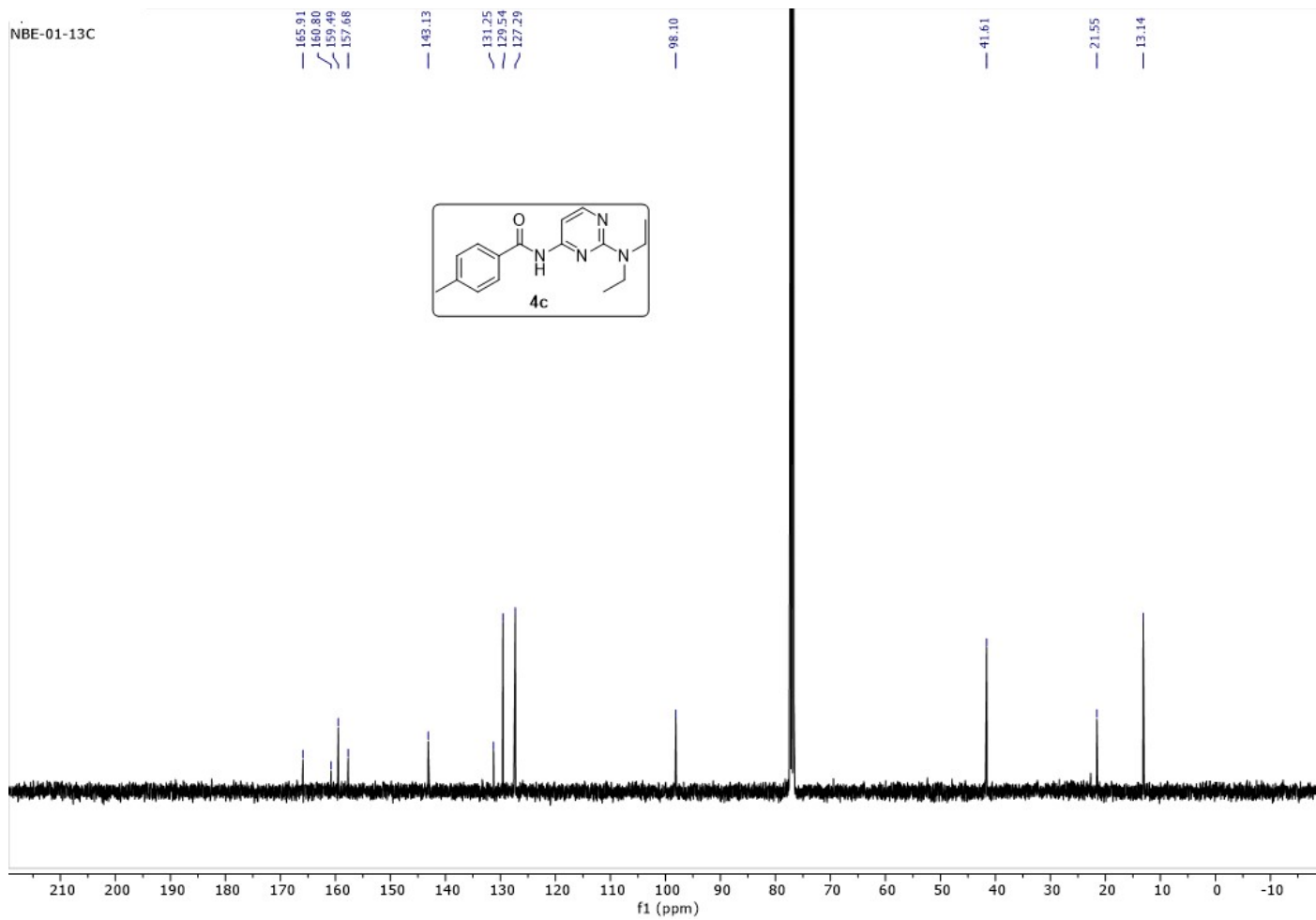
NBE-07-13C



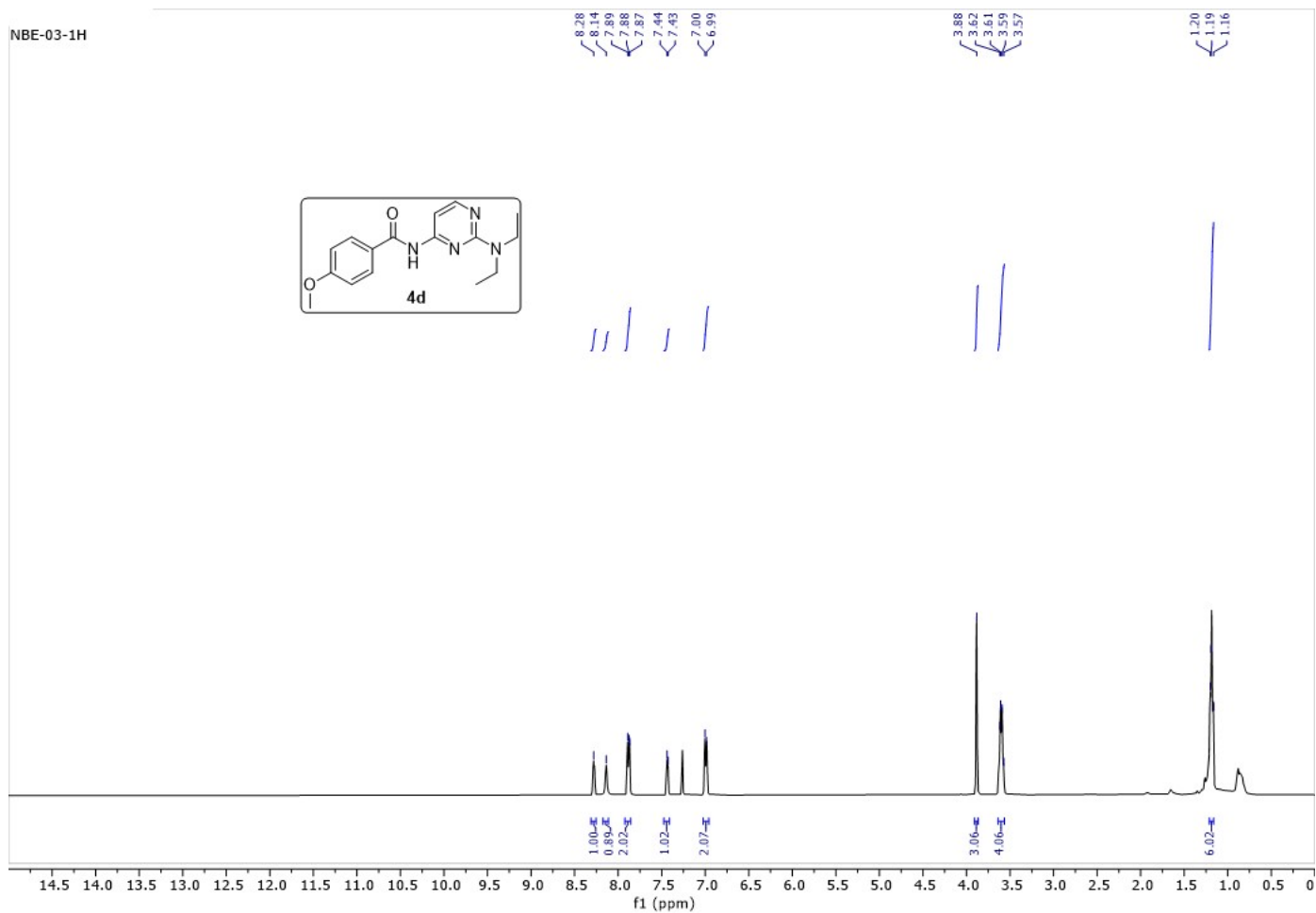
NBE-01-1H



NBE-01-13C



NBE-03-1H



NBE-03-13C

165.42
163.00
160.79
159.43
157.77

129.26
126.26

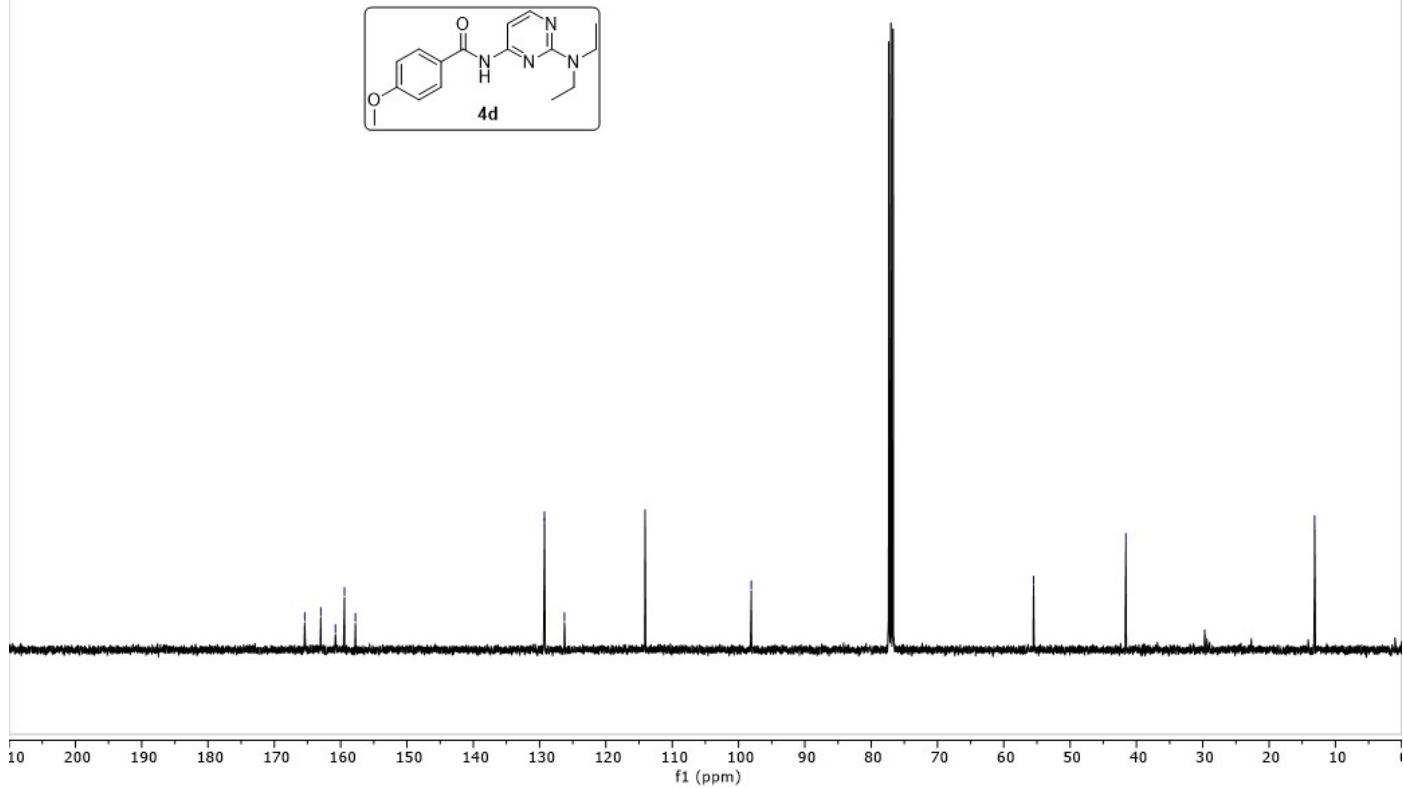
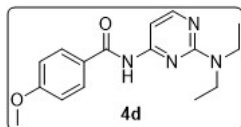
114.09

98.08

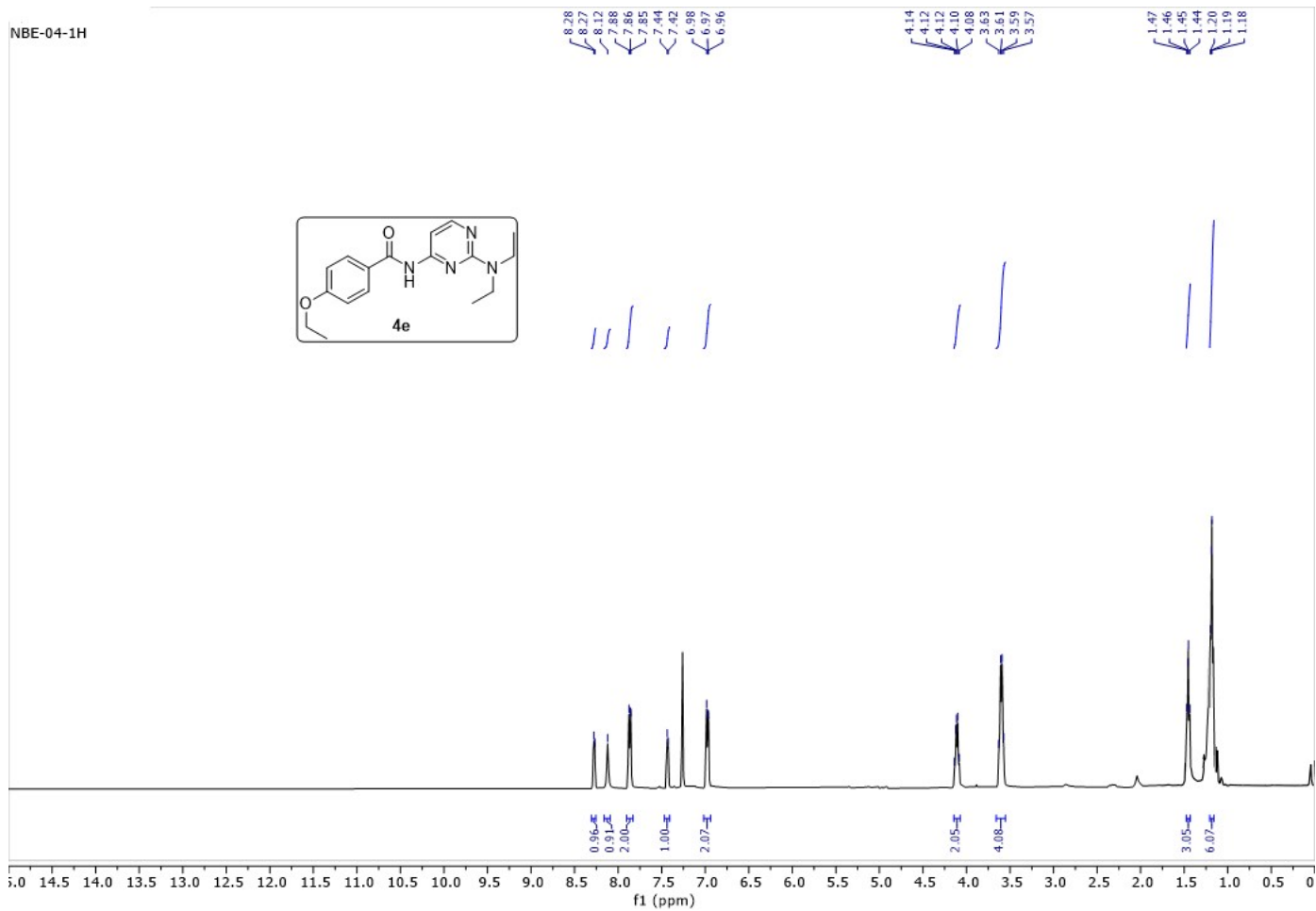
55.51

41.61

13.14



NBE-04-1H



NBE-04-13C

165.44
162.42
160.80
159.42
157.78

129.25
126.03

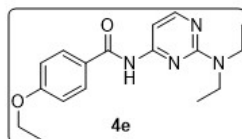
114.54

98.08

63.82

41.60

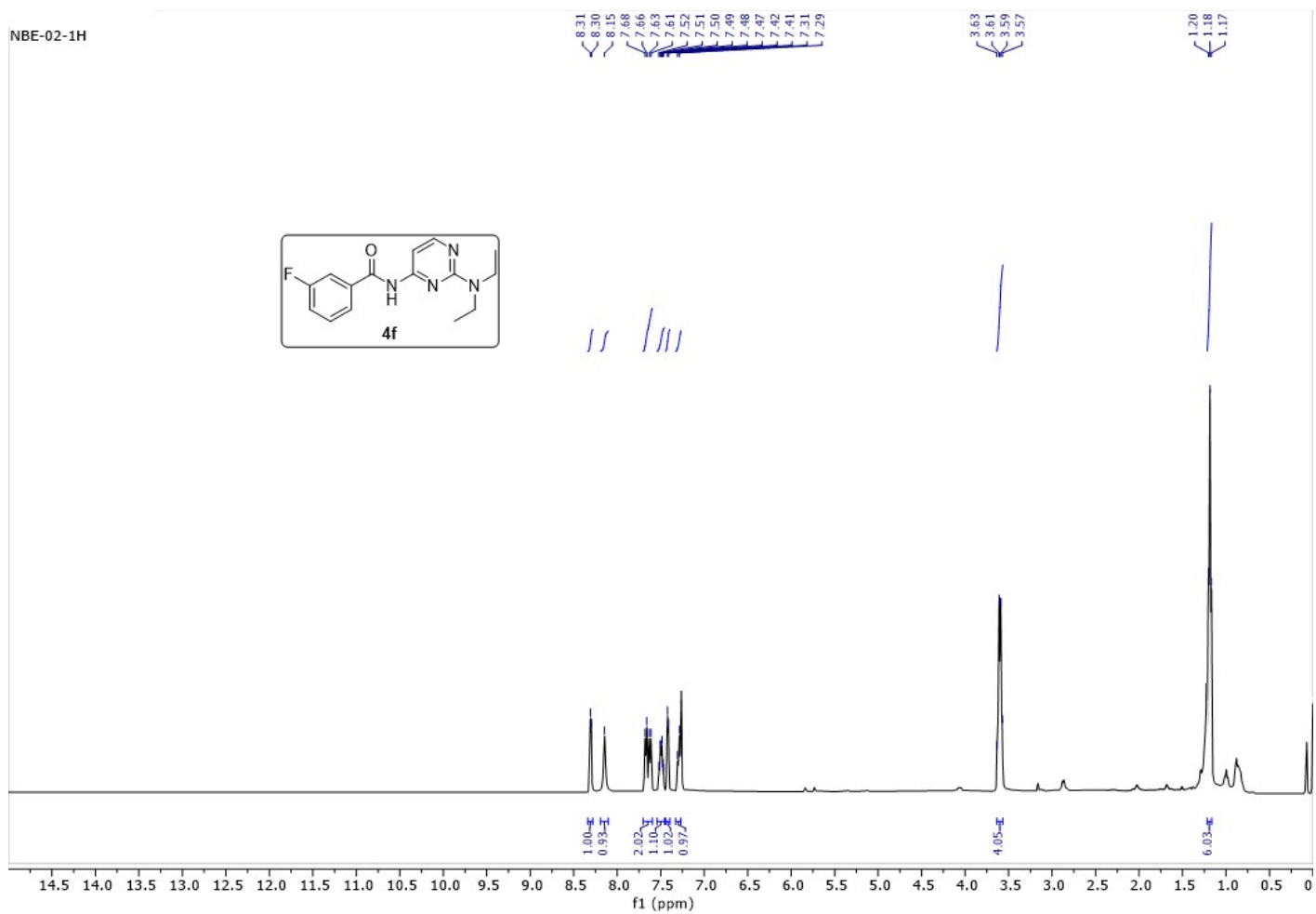
14.67
13.14



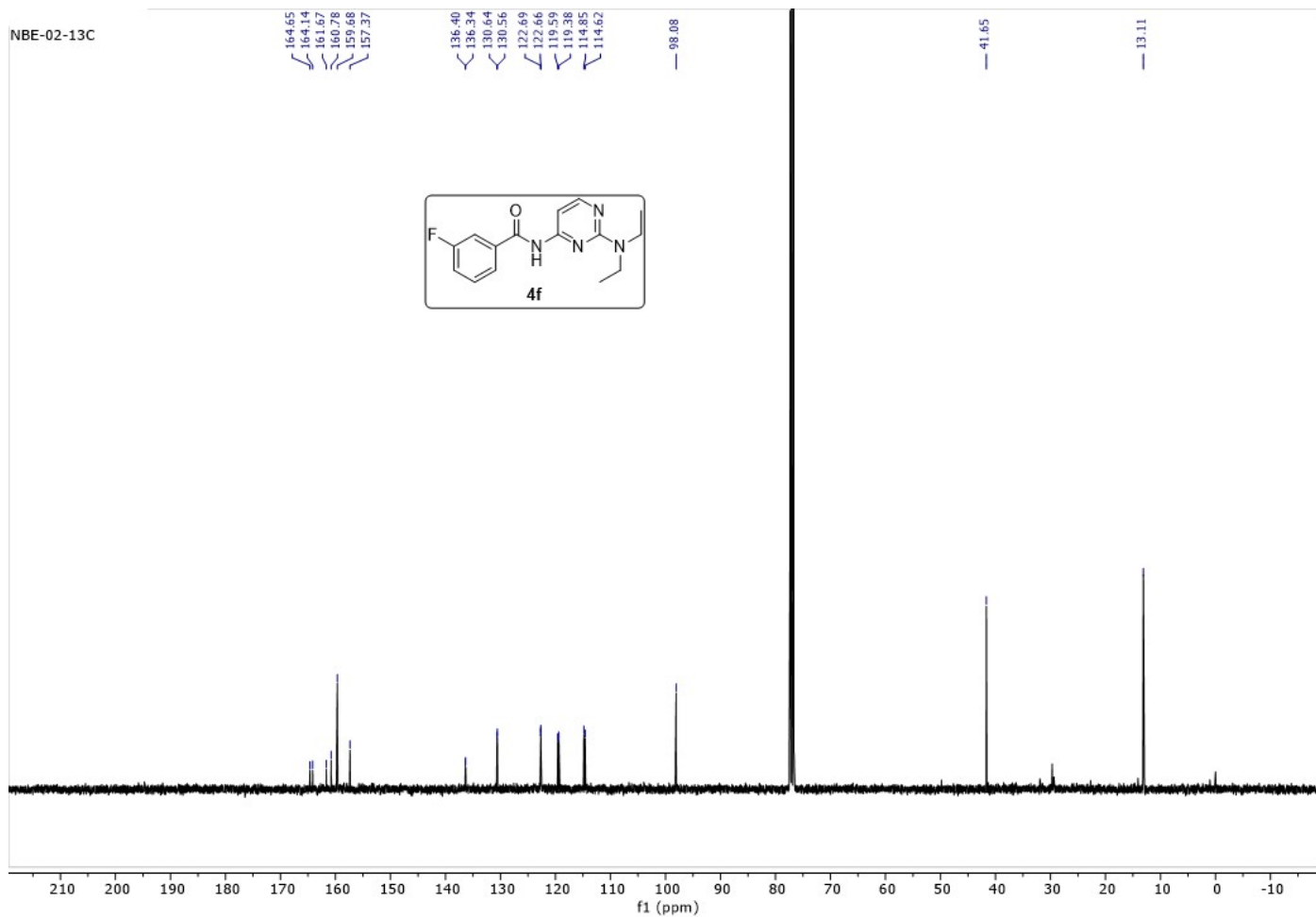
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)

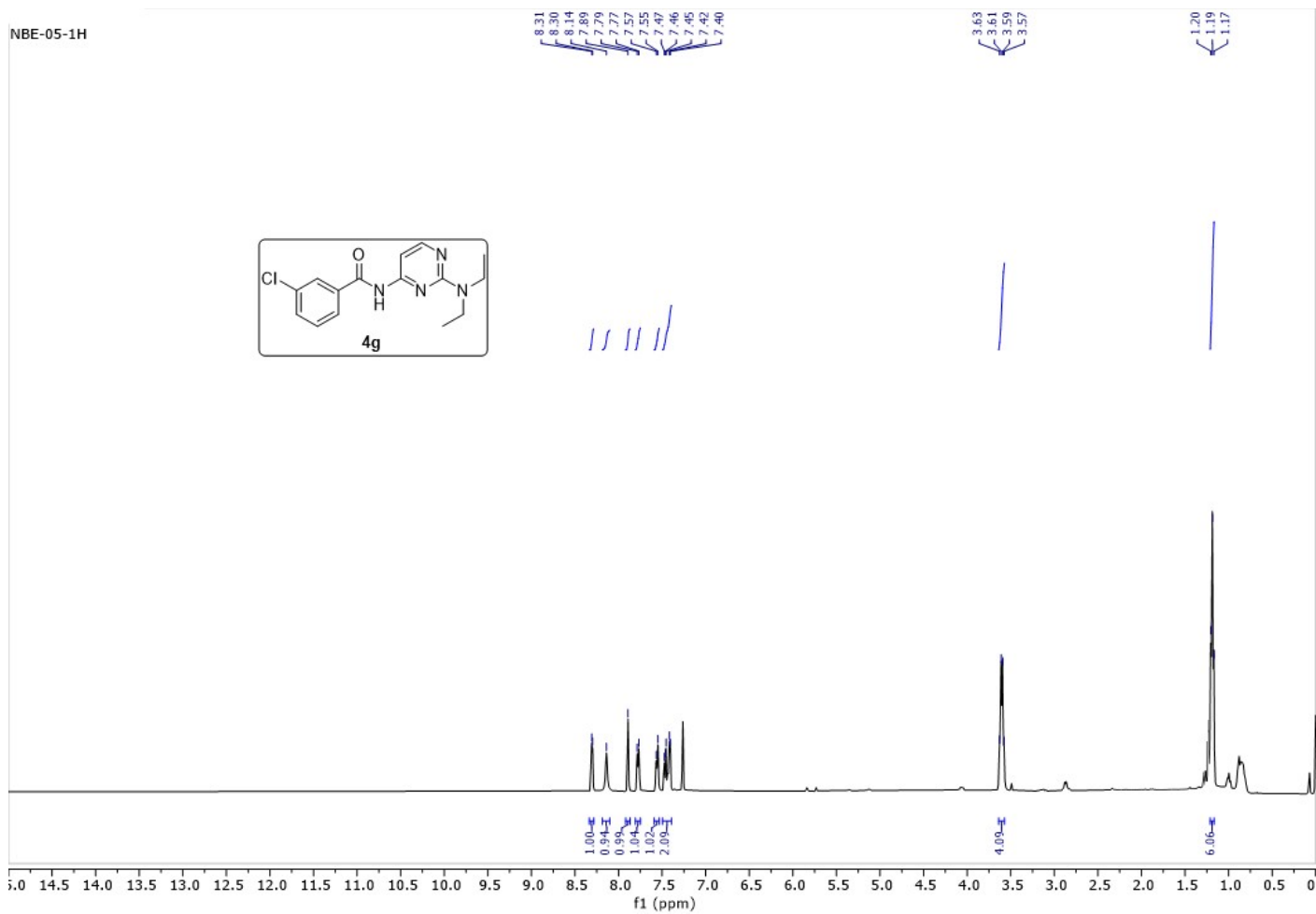
NBE-02-1H



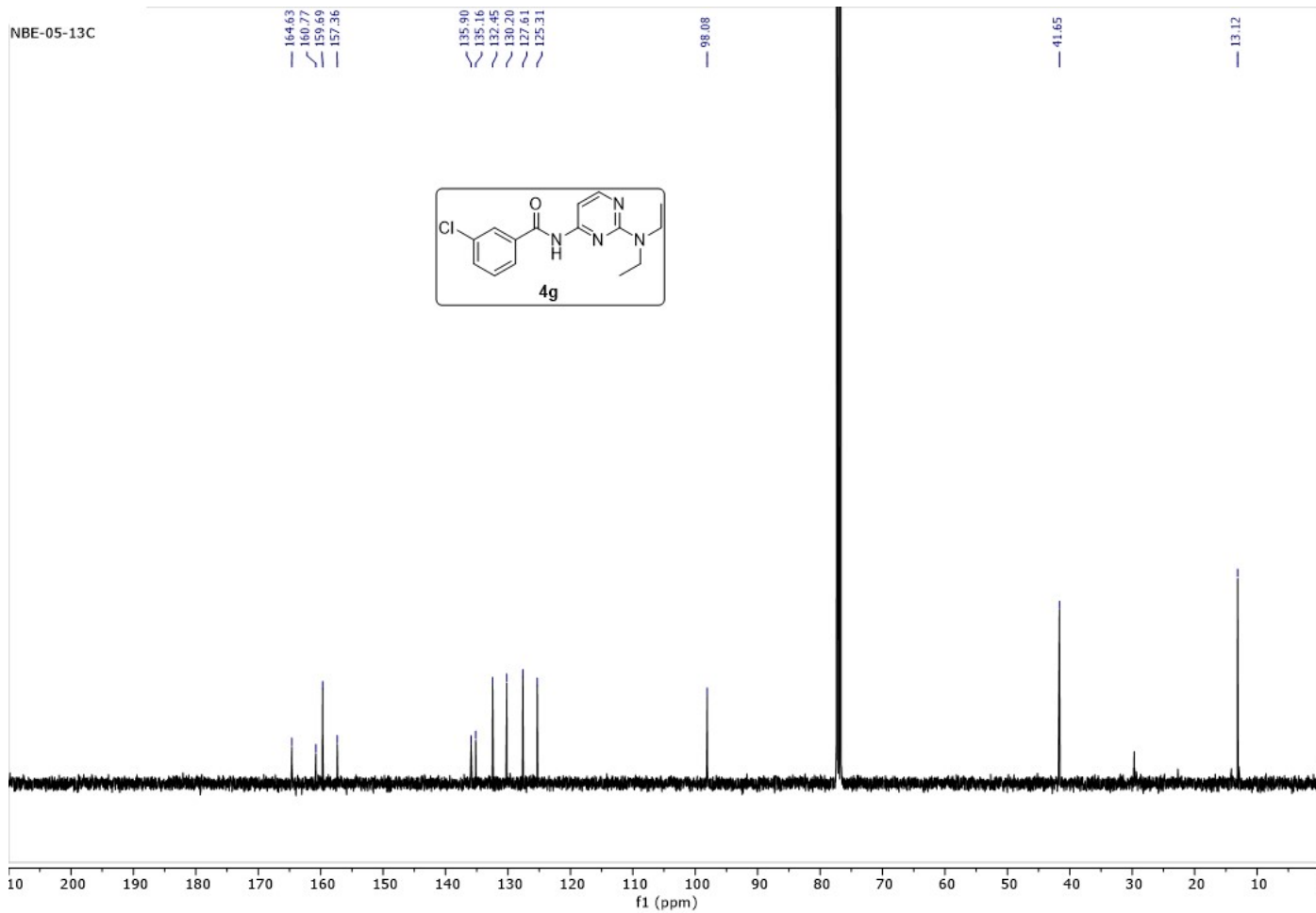
NBE-02-13C



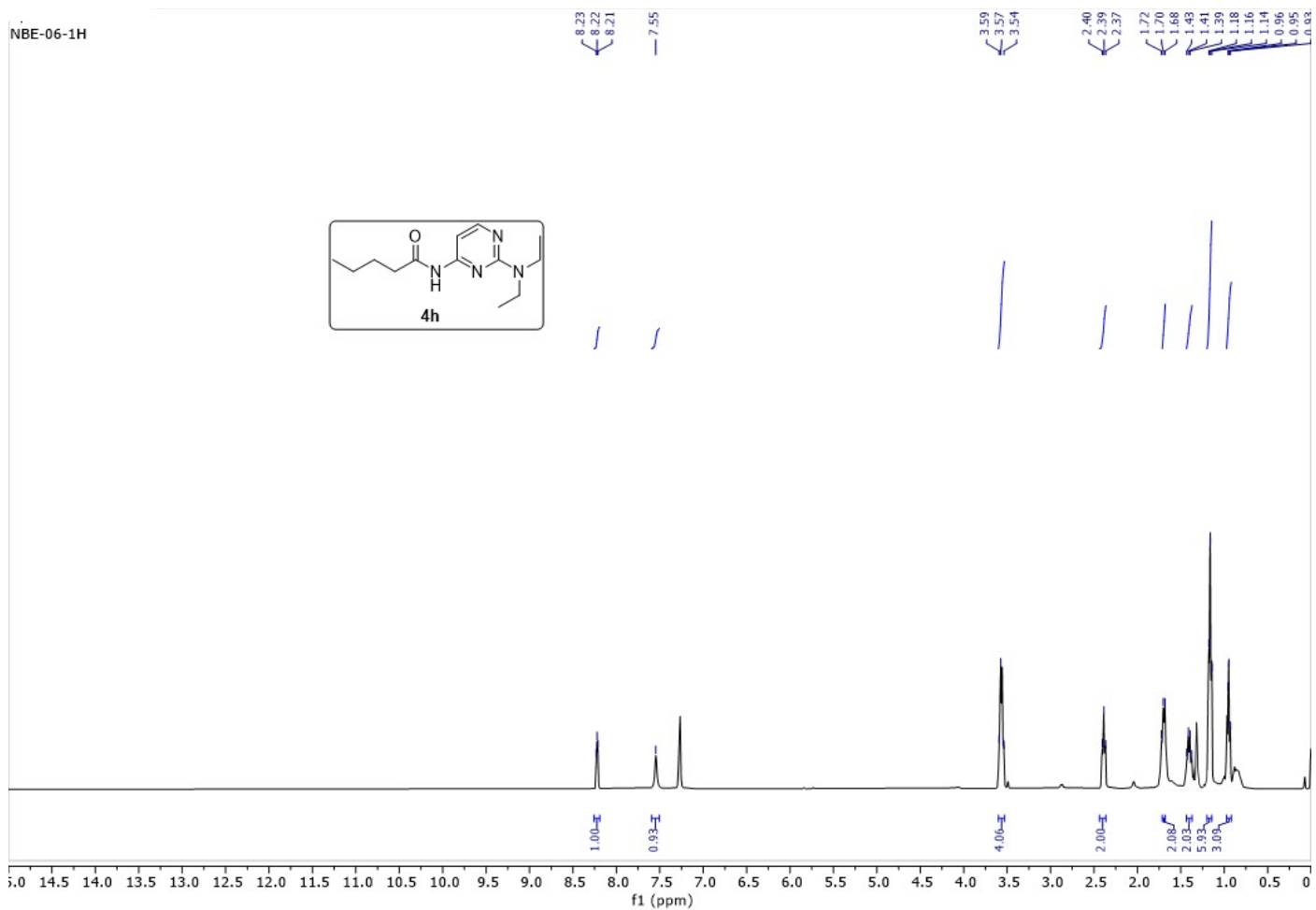
NBE-05-1H



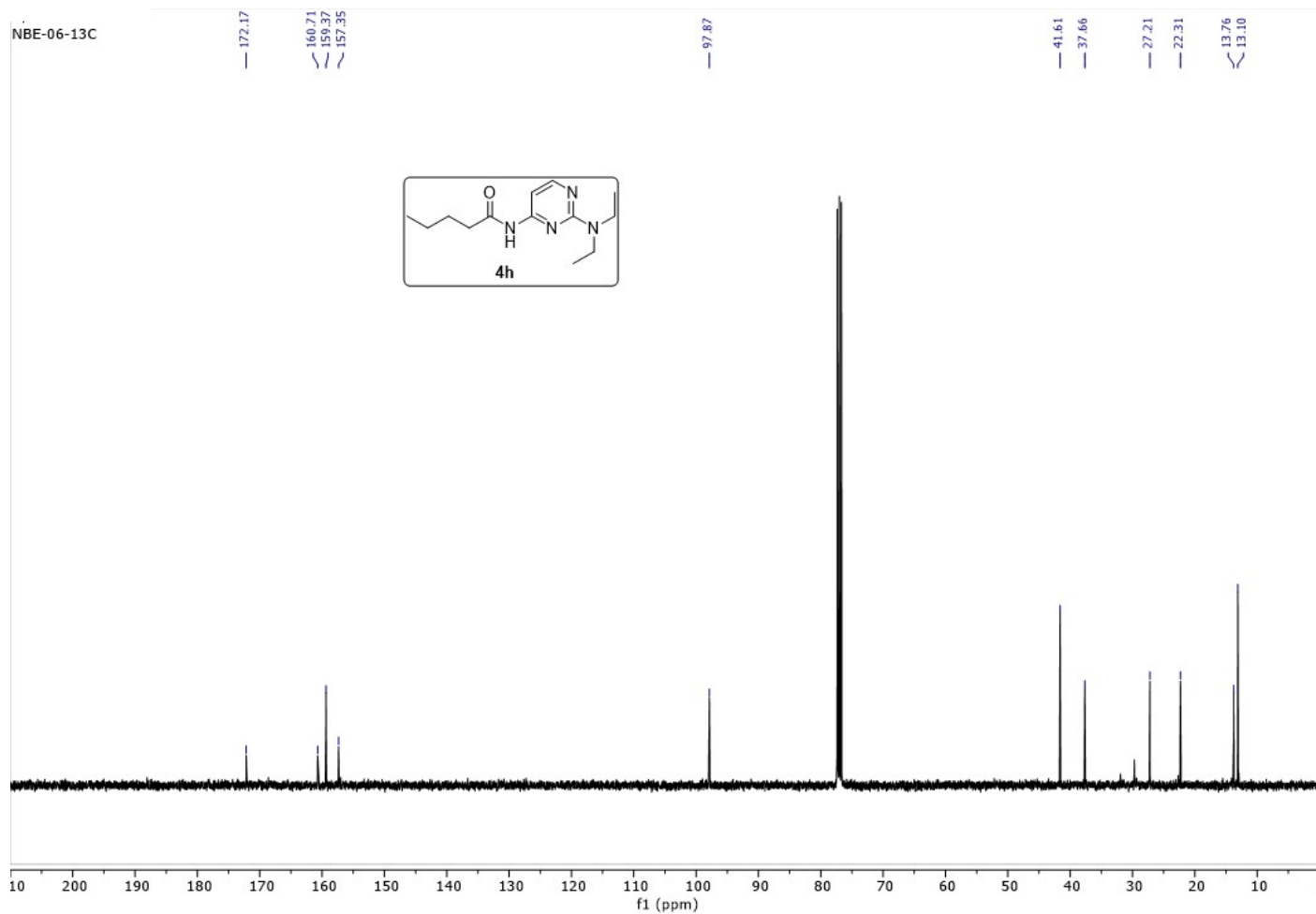
NBE-05-13C



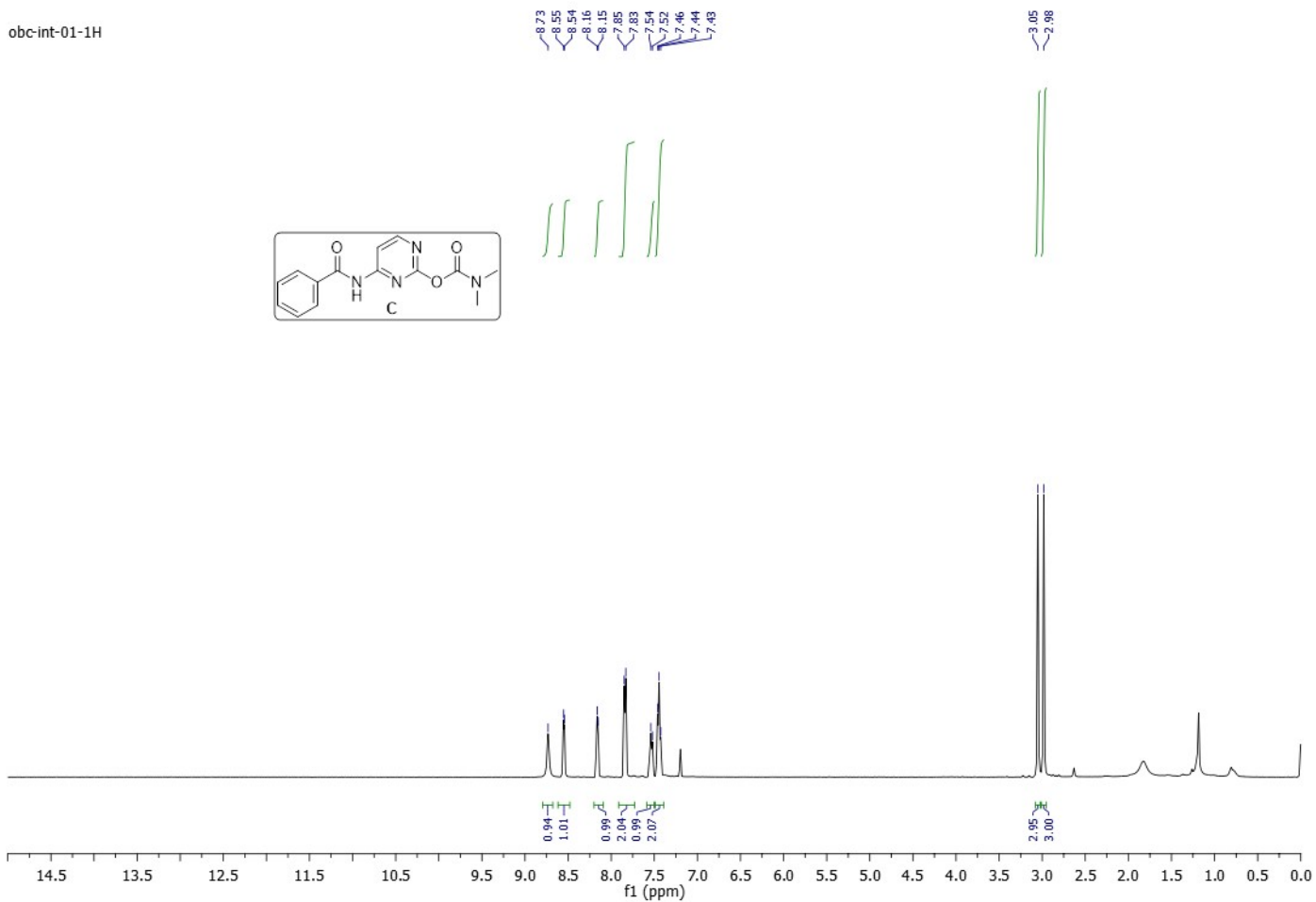
NBE-06-1H



NBE-06-13C



obc-int-01-1H



obc-int-01-13c

165.97
161.17
160.78
159.75
152.75

133.07
132.96
129.04
127.41

107.55

77.95
77.03
76.72

36.81
36.78

