

Supporting Information

One pot, Metal-free, Three-component Domino Sequence for the Synthesis of Furans: An Efficient C-O and C-N Bond Formation Approach

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^1H and ^{13}C NMR spectra were recorded at 400 and 100 Hz, respectively. Mass spectra were recorded were obtained on a ESIMS. Elemental analyses were performed with a elemental analyzer. GC-MS was obtained using electron ionization. TLC was performed using commercially prepared 100-400 mesh silica gel plates.

Synthesis of 4a according to the following procedure: A reaction tube was charged with 3-phenylpropionaldehyde (**1a**, 0.5 mmol), cyclohexane-1,3-dione (**2a**, 0.6 mmol) and pyrazin-2-amine (**3a**, 0.6 mmol), TFA (11.4mg, 10 mol%), and DMF (3 mL). The mixture was stirred at 80 °C for 8 h. After reaction completion, as monitored by TLC and GC-MS analysis, water (8 mL) was added and the aqueous solution was extracted with diethyl ether (3×12 mL). The combined extract was dried with anhydrous MgSO_4 . And the solvent was then removed and the crude product was separated by column chromatography (eluted with petroleum ether : ethyl acetate = 3:1) to give a pure sample of **4a**.

Synthesis of 7a according to the following procedure: A reaction tube was charged with 3-phenylpropionaldehyde (**1a**, 65mg, 0.5 mmol), cyclohexane-1,3-dione (**2a**, 67.2mg, 0.5 mmol) and AcOH (120 mg, 2 mmol), and DMF (3 mL). The mixture was stirred at 80 °C for 8 h. After reaction completion, as monitored by TLC and GC-MS analysis, water (8 mL) was added and the aqueous solution was extracted with diethyl ether (3×12 mL). The combined extract was dried with anhydrous MgSO_4 . And the solvent was then removed and the crude product was separated by column chromatography (eluted with petroleum ether : ethyl acetate = 4:1) to give a pure sample of **7a**.

6,7-dihydro-2-(phenyl(pyrazin-2-ylamino)methyl)benzofuran-4(5H)-one (4a): Yield: 129mg, 81%; Brown solid, 193-195 °C. IR(KBr, cm^{-1}): 3378, 2961, 1711, 742, 696. ^1H NMR (400

MHz, CD δ 7.97 (s, 3H), 7.39-7.27 (m, 5H), 6.43 (s, 1H), 6.23 (d, J = 7.2Hz, 1H), 5.66 (d, J = 7.2Hz, 1H), 2.82 (t, J = 6.4Hz, 2H), 2.45 (t, J = 6.4Hz, 2H), 2.16-2.10 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.4, 167.3, 155.0, 142.0, 141.9, 138.9, 133.6, 132.6, 128.9, 128.2, 127.2, 121.8, 104.3, 53.1, 37.5, 23.4, 22.5. ESI-MS m/z (%) 320 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{19}\text{H}_{17}\text{N}_3\text{O}_2$ C, 71.46; H, 5.37; N, 13.16; Found: C, 71.14; H, 5.39; N, 13.23;

6,7-dihydro-6-phenyl-2-(phenyl(pyrazin-2-ylamino)methyl)benzofuran-4(5H)-one (4b):

Yield: 164mg, 83%; Yellow solid, 172-174°C. IR(KBr, cm^{-1}): 3352, 2957, 1701, 744, 692. ^1H NMR (400 MHz, CDCl_3) δ 7.97 (d, J = 5.6Hz, 2H), 7.83 (s, 1H), 7.40-7.23 (m, 10H), 6.48 (s, 1H), 6.24 (d, J = 7.2Hz, 1H), 5.61 (d, J = 7.2Hz, 1H), 3.54-3.45 (m, 1H), 3.13-2.96 (m, 2H), 2.72 (d, J = 8.0Hz, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.0, 166.4, 155.6, 153.3, 142.3, 142.0, 138.9, 133.7, 132.6, 129.0, 128.9, 128.3, 127.4, 127.3, 127.3, 126.8, 121.7, 104.3, 53.2, 44.9, 41.3, 31.3. ESI-MS m/z (%) 396 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{25}\text{H}_{21}\text{N}_3\text{O}_2$ C, 75.93; H, 5.35; N, 10.63; Found: C, 75.58; H, 5.38; N, 10.68;

6,7-dihydro-6,6-dimethyl-2-(phenyl(pyrazin-2-ylamino)methyl)benzofuran-4(5H)-one

(4c): Yield: 146mg, 84%; Brown oil. IR(KBr, cm^{-1}): 3364, 2935, 1704, 688. ^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, J = 14.4Hz, 2H), 7.83 (s, 1H), 7.39-7.31 (m, 5H), 6.41 (s, 1H), 6.21 (d, J = 7.2Hz, 1H), 5.53 (d, J = 7.2Hz, 1H), 2.70 (s, 2H), 2.33 (s, 2H), 1.12 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.9, 166.4, 155.3, 142.0, 138.9, 133.7, 132.4, 128.9, 128.3, 127.2, 120.6, 104.3, 53.2, 51.9, 37.4, 35.3, 28.6. ESI-MS m/z (%) 348 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_2$ C, 72.60; H, 6.09; N, 12.10; Found: C, 72.27; H, 6.12; N, 12.16;

2-((3-methylpyrazin-2-ylamino)(phenyl)methyl)-6,7-dihydrobenzofuran-4(5H)-one (4d):

Yield: 137mg, 82%; Yellow oil. IR(KBr, cm^{-1}): 3356, 2947, 1699, 738, 702. ^1H NMR (400 MHz,

CDCl₃) δ 7.85 (s, 1H), 7.71 (d, J = 2.0 Hz, 1H), 7.38-7.28 (m, 5H), 6.49 (d, J = 7.6 Hz, 1H), 6.41 (s, 1H), 5.19 (d, J = 6.8 Hz, 1H), 2.81 (t, J = 6.0 Hz, 2H), 2.41 (t, J = 6.4 Hz, 5H), 2.13 (q, J = 6.0 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 194.4, 167.2, 155.4, 151.5, 140.1, 139.6, 139.4, 132.4, 128.8, 128.4, 128.0, 127.3, 126.6, 121.7, 104.1, 52.5, 37.5, 23.4, 22.5, 20.0. ESI-MS m/z (%) 334 (100)[M+H]⁺; Anal. Calcd for C₂₀H₁₉N₃O₂ C, 72.05; H, 5.74; N, 12.60; Found: C, 71.70; H, 5.72; N, 12.67;

2-((3-methylpyrazin-2-ylamino)(phenyl)methyl)-6,7-dihydro-6-phenylbenzofuran-4(5H)

-one (4e): Yield:164mg, 80%; Brown solid, 62-64°C. IR(KBr, cm⁻¹): 3372, 2941, 1743, 758, 700. ¹H NMR (400 MHz, CDCl₃) δ 7.86 (s, 1H), 7.73 (d, J = 2.0 Hz, 1H), 7.40-7.21 (m, 10H), 6.52 (t, J = 7.6 Hz, 2H), 3.56-3.41 (m, 1H), 3.10-2.94 (m, 2H), 2.69 (d, J = 7.6 Hz, 2H), 2.41 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 193.0, 166.4, 156.0, 156.0, 151.5, 142.4, 140.1, 139.7, 139.4, 132.6, 128.9, 128.9, 128.5, 128.2, 127.3, 126.8, 126.7, 121.7, 104.1, 52.6, 44.8, 41.3, 31.3, 20.1. ESI-MS m/z (%) 410 (100)[M+H]⁺; Anal. Calcd for C₂₆H₂₃N₃O₂ C, 76.26; H, 5.66; N, 10.26; Found: C, 75.94; H, 5.64; N, 10.31;

2-((3-methylpyrazin-2-ylamino)(phenyl)methyl)-6,7-dihydro-6,6-dimethylbenzofuran-4(

5H)-one(4f):Yield:150mg,83%; Brown solid, 50-52°C. IR(KBr, cm⁻¹): 3365, 2931, 1715,740, 702. ¹H NMR (400 MHz, CDCl₃) δ 7.86 (s, 1H), 7.73 (s, 1H), 7.39-7.28 (m, 5H), 6.53 (d, J = 7.6 Hz, 1H), 6.41 (s, 1H), 5.23 (s, 1H), 2.69 (s, 2H), 2.42 (s, 3H), 2.31 (s, 2H), 1.10 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 193.8, 166.3, 155.8, 151.5, 140.1, 139.6, 139.4, 132.4, 128.7, 128.0, 127.2, 120.5, 104.1, 52.4, 51.9, 37.3, 35.2, 28.6, 28.6, 20.0. ESI-MS m/z (%) 362 (100)[M+H]⁺; Anal. Calcd for C₂₂H₂₃N₃O₂ C, 73.11; H, 6.41; N, 11.63; Found: C, 73.43; H, 6.38; N, 11.57;

6,7-dihydro-2-(phenyl(pyrimidin-2-ylamino)methyl)benzofuran-4(5H)-one (4g): Yield:

128mg, 80%; Brown solid, 60-63°C. IR(KBr, cm^{-1}): 3642, 1678, 740, 700. ^1H NMR (400 MHz, CDCl_3) δ 8.16 (d, $J = 2.0$ Hz, 2H), 7.40-7.29 (m, 5H), 6.77 (d, $J = 8.0$ Hz, 1H), 6.52 (t, $J = 4.8$ Hz, 1H), 6.42 (d, $J = 8.8$ Hz, 2H), 2.80 (t, $J = 6.0$ Hz, 2H), 2.46 (t, $J = 7.2$ Hz, 2H), 2.15-2.09 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.4, 167.2, 161.3, 158.1, 155.5, 139.3, 128.7, 127.9, 127.2, 121.7, 111.4, 104.0, 53.0, 37.5, 23.4, 22.5. ESI-MS m/z (%) 320 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{19}\text{H}_{17}\text{N}_3\text{O}_2$ C, 71.46; H, 5.37; N, 13.16; Found: C, 71.14; H, 5.39; N, 13.22;

6,7-dihydro-6-phenyl-2-(phenyl(pyrimidin-2-ylamino)methyl)benzofuran-4(5H)-one

(4h): Yield: 166mg, 84%; Brown solid, 178-181°C. IR(KBr, cm^{-1}): 3348, 1678, 758, 700. ^1H NMR (400 MHz, CDCl_3) δ 8.19 (d, $J = 4.0$ Hz, 2H), 7.41-7.23 (m, 10H), 6.63-6.42 (m, 4H), 3.56-3.45 (m, 1H), 3.11-2.93 (m, 2H), 2.72 (d, $J = 6.4$ Hz, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.0, 166.3, 161.3, 158.1, 156.1, 156.1, 142.4, 139.3, 128.9, 128.8, 128.0, 127.3, 127.2, 126.8, 121.6, 111.5, 104.0, 53.0, 44.9, 41.3, 41.3, 31.2. ESI-MS m/z (%) 396 (100) [$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{25}\text{H}_{21}\text{N}_3\text{O}_2$ C, 75.93; H, 5.35; N, 10.63; Found: C, 75.58; H, 5.39; N, 10.68;

6,7-dihydro-6,6-dimethyl-2-(phenyl(pyrimidin-2-ylamino)methyl)benzofuran-4(5H)-one

(4i): Yield: 148mg, 85%, White solid, 186-188°C. IR(KBr, cm^{-1}): 3248, 2958, 1681, 734, 700. ^1H NMR (400 MHz, CDCl_3) δ 8.14 (d, $J = 2.8$ Hz, 2H), 7.40-7.28 (m, 5H), 6.91 (d, $J = 8.0$ Hz, 1H), 6.51-6.39 (m, 3H), 2.66 (s, 2H), 2.32 (s, 2H), 1.10 (d, $J = 4.4$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.8, 166.3, 161.3, 158.0, 155.9, 139.4, 128.7, 127.9, 127.2, 120.5, 111.3, 104.0, 52.9, 52.0, 37.4, 35.2, 28.6, 28.6. ESI-MS m/z (%) 348 (100) [$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_2$ C, 72.60; H, 6.09; N, 12.10; Found: C, 72.26; H, 6.12; N, 12.16;

6,7-dihydro-2-(phenyl(pyridin-2-ylamino)methyl)benzofuran-4(5H)-one (4j): Yield:

124mg, 78%; Yellow solid, 162-164°C. IR(KBr, cm^{-1}): 3347, 2950, 1693, 689. ^1H NMR (400

MHz, CDCl₃) δ 7.98 (d, J = 4.0 Hz, 1H), 7.38-7.26 (m, 6H), 6.53 (t, J = 6.0 Hz, 1H), 6.39 (d, J = 9.2 Hz, 2H), 6.11 (d, J = 6.8 Hz, 1H), 5.76 (d, J = 7.2 Hz, 1H), 2.72 (t, J = 6.0 Hz, 2H), 2.39 (t, J = 6.4 Hz, 2H), 2.05 (q, J = 6.4 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 194.5, 167.2, 157.3, 155.8, 148.0, 139.6, 137.5, 128.8, 127.9, 127.3, 121.7, 113.7, 107.7, 104.0, 53.8, 37.5, 23.3, 22.5. ESI-MS m/z (%) 319 (100)[M+H]⁺; Anal. Calcd for C₂₀H₁₈N₂O₂ C, 75.45; H, 5.70; N, 8.80; Found: C, 75.14; H, 5.72; N, 8.85;

6,7-dihydro-6-phenyl-2-(phenyl(pyridin-2-ylamino)methyl)benzofuran-4(5H)-one (4k):

Yield: 146mg, 74%, Brown solid, 173-175°C. IR(KBr, cm⁻¹): 3346, 2937, 1698, 744, 695. ¹H NMR (400 MHz, CDCl₃) δ 8.08 (d, J = 4.4 Hz, 1H), 7.45-7.28 (m, 11H), 6.66 (t, J = 5.6 Hz, 1H), 6.50 (s, 1H), 6.46 (d, J = 8.4 Hz, 1H), 6.06 (d, J = 4.0 Hz, 1H), 5.91 (s, 1H), 3.58 (q, J = 5.6 Hz, 1H), 3.16-2.96 (m, 2H), 2.75 (d, J = 4.0 Hz, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 193.0, 166.4, 157.0, 155.9, 147.2, 142.4, 139.2, 138.2, 128.9, 128.2, 128.2, 127.3, 126.8, 126.8, 121.7, 113.8, 107.7, 104.2, 54.3, 44.9, 41.3, 31.2. ESI-MS m/z (%) 395 (100)[M+H]⁺; Anal. Calcd for C₂₆H₂₂N₂O₂ C, 79.16; H, 5.62; N, 7.10; Found: C, 79.46; H, 5.65; N, 7.14;

6,7-dihydro-6,6-dimethyl-2-(phenyl(pyridin-2-ylamino)methyl)benzofuran-4(5H)-one

(4l): Yield: 138mg, 80%; Brown solid, 166-167°C. IR(KBr, cm⁻¹): 3343, 2938, 1688, 696. ¹H NMR (400 MHz, CDCl₃) δ 8.06 (d, J = 4.0 Hz, 1H), 7.40-7.29 (m, 6H), 6.60 (t, J = 6.4 Hz, 1H), 6.39 (t, J = 4.8 Hz, 2H), 6.08 (d, J = 7.2 Hz, 1H), 5.38 (d, J = 6.8 Hz, 1H), 2.68 (s, 2H), 2.32 (s, 2H), 1.10 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ 193.8, 166.3, 157.2, 155.9, 148.0, 139.5, 137.6, 128.8, 128.0, 127.2, 120.5, 113.9, 107.5, 104.0, 54.0, 52.0, 37.4, 35.2, 28.6. ESI-MS m/z (%) 347 (100)[M+H]⁺; Anal. Calcd for C₂₂H₂₂N₂O₂ C, 76.28; H, 6.40; N, 8.09; Found: C, 75.95; H, 6.43; N, 8.12;

2-((5-chloropyridin-2-ylamino)(phenyl)methyl)-6,7-dihydro-6,6-dimethylbenzofuran-4(5H)-one (4m): Yield: 150mg, 79%, Yellow oil. IR(KBr, cm^{-1}): 3356, 2947, 1680, 738, 702. ^1H NMR (400 MHz, CDCl_3) δ 7.98 (s, 1H), 7.31-7.39 (m, 5H), 6.36 (t, $J = 8.0$ Hz, 2H), 6.04 (d, $J = 5.2$ Hz, 1H), 5.55 (d, $J = 5.6$ Hz, 1H), 5.29 (s, 1H), 2.69 (s, 2H), 2.34 (s, 2H), 1.12 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.8, 166.3, 155.5, 146.3, 139.1, 137.4, 128.9, 128.2, 127.2, 120.7, 120.5, 108.4, 104.2, 54.2, 51.9, 37.4, 35.2, 28.7, 28.6. ESI-MS m/z (%) 381 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{22}\text{H}_{21}\text{ClN}_2\text{O}_2$ C, 69.38; H, 5.56; N, 7.36; Found: C, 69.71; H, 5.53; N, 7.33;

2-((5-iodopyridin-2-ylamino)(phenyl)methyl)-6,7-dihydro-6,6-dimethylbenzofuran-4(5H)-one (4n): Yield: 165mg, 70%, Brown oil. IR(KBr, cm^{-1}): 3348, 2932, 2895, 1686. ^1H NMR (400 MHz, CDCl_3) δ 8.17 (s, 1H), 7.58 (d, $J = 8.8$ Hz, 1H), 7.38-7.29 (m, 5H), 6.36 (s, 1H), 6.27 (d, $J = 8.8$ Hz, 1H), 6.03 (d, $J = 6.4$ Hz, 1H), 5.55 (d, $J = 6.4$ Hz, 1H), 2.68 (s, 2H), 2.33 (s, 2H), 1.11 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.8, 166.4, 156.0, 155.4, 153.6, 145.2, 139.0, 128.9, 128.2, 127.2, 120.5, 109.9, 104.3, 77.7, 54.0, 52.0, 37.4, 35.2, 28.7, 28.6, 28.6. ESI-MS m/z (%) 473 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{22}\text{H}_{21}\text{IN}_2\text{O}_2$ C, 55.94; H, 4.48; N, 5.93; Found: C, 56.19; H, 4.50; N, 5.90;

2-((5-bromopyridin-2-ylamino)(phenyl)methyl)-6,7-dihydro-6,6-dimethylbenzofuran-4(5H)-one (4o): Yield: 161mg, 76%; Yellow oil. IR(KBr, cm^{-1}): 3372, 2985, 2922, 1704. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (s, 1H), 7.44-7.30 (m, 5H), 6.37 (s, 1H), 6.34 (d, $J = 8.8$ Hz, 1H), 6.05 (d, $J = 6.0$ Hz, 1H), 5.72 (d, $J = 6.4$ Hz, 1H), 5.28 (s, 1H), 2.68 (s, 2H), 2.33 (s, 2H), 1.11 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.8, 166.3, 155.9, 155.6, 148.6, 139.9, 139.1, 128.9, 128.1, 127.2, 120.5, 109.1, 108.0, 104.2, 54.1, 51.9, 37.3, 35.2, 28.6, 28.6. ESI-MS m/z (%) 425 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{22}\text{H}_{21}\text{BrN}_2\text{O}_2$ C, 62.13; H, 4.98; N, 6.59; Found: C, 62.43; H, 5.01;

N, 6.56;

1-(2-methyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-yl)ethanone (5a): Yield: 115mg, 75%; Brown solid, 55-57°C. IR(KBr, cm^{-1}): 3325, 2938, 1701. ^1H NMR (400 MHz, CDCl_3) δ 8.03-7.90 (m, 3H), 7.41-7.35 (m, 5H), 6.40 (s, 1H), 6.18 (d, $J = 7.2$ Hz, 1H), 5.41 (d, $J = 7.2$ Hz, 1H), 2.57 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.0, 158.6, 152.1, 142.0, 139.1, 133.8, 132.3, 128.9, 128.2, 127.2, 122.1, 108.3, 53.2, 29.2, 14.5. ESI-MS m/z (%) 308 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_2$ C, 70.34; H, 5.58; N, 13.67; Found: C, 70.01; H, 5.60; N, 13.73;

methyl 2-methyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-carboxylate (5b): Yield: 113mg, 74%; Brown solid, 171-173°C. IR(KBr, cm^{-1}): 3350, 2924, 1716. ^1H NMR (400 MHz, CDCl_3) δ 7.96 (d, $J = 11.6$ Hz, 2H), 7.81 (s, 1H), 7.38-7.30 (m, 5H), 6.38 (s, 1H), 6.16 (d, $J = 7.2$ Hz, 1H), 5.62 (d, $J = 5.6$ Hz, 1H), 3.76 (s, 3H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 164.3, 159.4, 153.4, 152.3, 142.0, 139.2, 133.6, 132.4, 131.7, 128.8, 128.3, 128.1, 127.2, 113.9, 108.6, 53.0, 51.4, 13.8. ESI-MS m/z (%) 324 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_3$ C, 66.86; H, 5.30; N, 13.00; Found: C, 66.54; H, 5.33; N, 13.06;

ethyl 2-phenyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-carboxylate (5c): Yield: 140mg, 70%, Black brown solid, 93-95°C. IR(KBr, cm^{-1}): 3321, 2973, 2856, 1712, 1463, 1391, 1369. ^1H NMR (400 MHz, CDCl_3) δ 7.99-7.83 (m, 5H), 7.44-7.33 (m, 8H), 6.61 (s, 1H), 6.26 (d, $J = 6.8$ Hz, 1H), 5.74 (d, $J = 7.2$ Hz, 1H), 4.28 (q, $J = 6.9$ Hz, 2H), 1.30 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 171.2, 163.4, 157.4, 153.4, 153.0, 142.0, 139.0, 133.5, 132.3, 129.5, 129.4, 128.9, 128.4, 128.2, 128.1, 127.3, 114.5, 110.8, 53.2, 14.2. ESI-MS m/z (%) 400 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}_3$ C, 72.16; H, 5.30; N, 10.52; Found: C, 71.84; H,

5.32; N, 10.57;

tert-butyl 2-methyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-carboxylate (5d):

Yield: 133mg, 73%, Brown solid, 52-55°C. IR(KBr, cm^{-1}): 3289, 2978, 1708, 1382, 1365, 740, 700. ^1H NMR (400 MHz, CDCl_3) δ 7.96 (q, $J = 2.4$ Hz, 3H), 7.38-7.29 (m, 5H), 6.37 (s, 1H), 6.15 (d, $J = 7.2$ Hz, 1H), 5.55 (d, $J = 6.8$ Hz, 1H), 2.49 (s, 3H), 1.51 (s, 9H). ^{13}C NMR (100 MHz, CDCl_3) δ 163.3, 158.5, 153.4, 151.8, 142.0, 139.3, 133.6, 132.3, 128.0, 127.2, 115.7, 108.8, 80.7, 53.1, 28.3, 13.9. ESI-MS m/z (%) 366 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{21}\text{H}_{23}\text{N}_3\text{O}_3$ C, 69.02; H, 6.34; N, 11.50; Found: C, 68.72; H, 6.37; N, 11.56;

benzyl 2-methyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-carboxylate (5e): Yield:

144mg, 72%; Yellow oil. IR(KBr, cm^{-1}): 3362, 2958, 1668, 742, 700. ^1H NMR (400 MHz, CDCl_3) δ 7.97 (t, $J = 22$ Hz, 3H), 7.41-7.29 (m, 10H), 6.43 (s, 1H), 6.15 (d, $J = 7.2$ Hz, 1H), 5.40 (d, $J = 7.2$ Hz, 1H), 5.23 (s, 2H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 163.7, 159.6, 153.3, 142.1, 142.0, 139.2, 136.1, 133.7, 132.4, 128.9, 128.6, 128.3, 128.2, 128.2, 127.2, 114.0, 108.6, 66.0, 53.1, 14.0. ESI-MS m/z (%) 400 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}_3$ C, 72.16; H, 5.30; N, 10.52; Found: C, 72.31; H, 5.27; N, 10.47;

phenyl(2-phenyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-yl)methanone (5f): Yield:

164mg, 76%; Brown solid, 57-60°C. IR(KBr, cm^{-1}): 3321, 1654, 727, 694. ^1H NMR (400 MHz, CDCl_3) δ 7.97 (d, $J = 10.0$ Hz, 2H), 7.81-7.75 (m, 3H), 7.46 (d, $J = 7.2$ Hz, 2H), 7.45-7.21 (m, 11H), 6.46 (s, 1H), 6.34 (d, $J = 8.0$ Hz, 1H), 5.89 (d, $J = 7.2$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.7, 155.8, 153.4, 142.0, 139.2, 137.8, 133.5, 133.0, 132.6, 129.7, 129.5, 129.1, 129.0, 128.9, 128.7, 128.4, 128.3, 128.2, 127.5, 127.3, 121.5, 111.6, 53.2. ESI-MS m/z (%) 432 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{28}\text{H}_{21}\text{N}_3\text{O}_2$ C, 77.94; H, 4.91; N, 9.74; Found: C, 77.59; H, 4.93; N, 9.79;

tert-butyl5-((3-methylpyrazin-2-ylamino)(phenyl)methyl)-2-methylfuran-3-carboxylate

(5g): Yield: 137mg, 72%; Brown oil. IR(KBr, cm^{-1}): 3380, 2976, 2929, 1708, 1392, 1362, 779, 700. ^1H NMR (400 MHz, CDCl_3) δ 7.88 (s, 1H), 7.75 (s, 1H), 7.36-7.29 (m, 5H), 6.45 (d, J = 7.6 Hz, 1H), 6.37 (s, 1H), 4.96 (d, J = 7.2 Hz, 1H), 2.51 (s, 3H), 2.42 (s, 3H), 1.52 (s, 9H). ^{13}C NMR (100 MHz, CDCl_3) δ 163.3, 158.3, 152.2, 151.6, 140.0, 139.9, 139.8, 132.4, 128.7, 127.9, 127.2, 115.7, 108.6, 80.6, 52.3, 28.3, 20.0, 13.9. ESI-MS m/z (%) 380 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{22}\text{H}_{25}\text{N}_3\text{O}_3$ C, 69.64; H, 6.64; N, 11.07; Found: C, 69.93; H, 6.61; N, 11.01;

methyl5-((3-methylpyrazin-2-ylamino)(phenyl)methyl)-2-methylfuran-3-carboxylate

(5h):Yield: 118mg, 70%; Brown oil. IR(KBr, cm^{-1}): 3389, 2951, 1714, 777, 700. ^1H NMR (400 MHz, CDCl_3) δ 7.88 (s, 1H), 7.75 (s, 1H), 7.36-7.30 (m, 5H), 6.45 (d, J = 7.6 Hz, 1H), 6.39 (s, 1H), 5.00 (d, J = 7.2 Hz, 1H), 3.77 (s, 3H), 2.54 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 164.3, 159.3, 152.7, 151.5, 139.9, 139.8, 139.7, 132.4, 128.7, 127.9, 127.2, 113.9, 108.4, 52.4, 51.3, 20.0, 13.9. ESI-MS m/z (%) 338 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3$ C, 67.64; H, 5.68; N, 12.46; Found: C, 67.36; H, 5.70; N, 12.52;

methyl 2-methyl-5-(phenyl(pyrimidin-2-ylamino)methyl)furan-3-carboxylate (5i): Yield:

120mg, 74%; Yellow oil. IR(KBr, cm^{-1}): 3331, 2966, 1709. ^1H NMR (400 MHz, CDCl_3) δ 8.27 (d, J = 3.6 Hz, 2H), 7.39-7.30 (m, 5H), 6.58 (d, J = 4.0 Hz, 1H), 6.40 (t, J = 8.0 Hz, 2H), 6.05 (d, J = 0.8 Hz, 1H), 3.78 (s, 3H), 2.52 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 164.4, 161.2, 159.3, 158.2, 158.1, 152.7, 139.6, 128.7, 127.8, 127.1, 113.8, 111.5, 108.2, 52.9, 51.3, 13.8. ESI-MS m/z (%) 324 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_3$ C, 66.86; H, 5.30; N, 13.00; Found: C, 67.15; H, 5.33; N, 13.06;

1-(2-methyl-5-(phenyl(pyridin-2-ylamino)methyl)furan-3-yl)ethanone (5j): Yield: 109mg,

71%; Yellow oil. IR(KBr, cm^{-1}): 3346, 2939, 1712. ^1H NMR (400 MHz, CDCl_3) δ 8.08 (d, $J = 3.6$ Hz, 2H), 7.42-7.28 (m, 6H), 6.63 (t, $J = 5.6$ Hz, 1H), 6.40 (t, $J = 8.4$ Hz, 2H), 6.02 (d, $J = 6.4$ Hz, 1H), 5.38 (d, $J = 4.4$ Hz, 1H), 2.53 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.1, 158.4, 157.2, 152.8, 147.8, 139.7, 137.8, 128.8, 128.0, 127.2, 122.1, 113.9, 108.0, 107.5, 54.1, 29.1, 14.5. ESI-MS m/z (%) 307 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_2$ C, 74.49; H, 5.92; N, 9.14; Found: C, 74.15; H, 5.94; N, 9.19;

phenyl(2-phenyl-5-(phenyl(pyridin-2-ylamino)methyl)furan-3-yl)methanone (5k): Yield: 157mg, 73%; Brown oil. IR(KBr, cm^{-1}): 3342, 3052, 3031, 1685, 1583, 745, 701. ^1H NMR (400 MHz, CDCl_3) δ 8.07 (d, $J = 5.2$ Hz, 1H), 7.79 (d, $J = 7.6$ Hz, 2H), 7.62 (t, $J = 2.4$ Hz, 2H), 7.49-7.25 (m, 12H), 6.63 (t, $J = 6.0$ Hz, 1H), 6.48 (d, $J = 18$ Hz 2H), 6.15 (d, $J = 4.8$ Hz, 1H), 5.84 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.6, 157.2, 155.7, 153.8, 147.5, 139.6, 138.0, 137.9, 132.8, 129.7, 129.6, 129.0, 128.9, 128.3, 128.3, 128.1, 127.5, 127.3, 121.4, 113.8, 111.3, 107.7, 54.3. ESI-MS m/z (%) 431 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{29}\text{H}_{22}\text{N}_2\text{O}_2$ C, 80.91; H, 5.15; N, 6.51; Found: C, 80.52; H, 5.17; N, 6.54;

1-(5-((5-chloropyridin-2-ylamino)(phenyl)methyl)-2-methylfuran-3-yl)ethanone (5l): Yield: 119mg, 70%; Brown oil. IR(KBr, cm^{-1}): 3348, 3023, 2955, 1703. ^1H NMR (400 MHz, CDCl_3) δ 7.97 (d, $J = 2.4$ Hz, 1H), 7.40-7.30 (m, 6H), 6.35 (t, $J = 5.2$ Hz, 2H), 5.98 (d, $J = 6.4$ Hz, 1H), 5.49 (d, $J = 6.4$ Hz, 1H), 2.53 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.0, 158.4, 155.6, 152.5, 146.4, 139.4, 137.4, 129.2, 128.9, 128.6, 128.1, 127.2, 122.1, 120.7, 108.3, 108.1, 54.2, 29.1, 14.5. ESI-MS m/z (%) 341 (100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{19}\text{H}_{17}\text{ClN}_2\text{O}_2$ C, 66.96; H, 5.03; N, 8.22; Found: C, 66.65; H, 5.05; N, 8.26;

1-(2-phenyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-yl)ethan-1-one (6a): Yield:

70mg, 38%; Yellow oil. IR(KBr, cm^{-1}): 3052, 3022, 2849, 1703. ^1H NMR (400 MHz, CDCl_3) δ 7.98-7.77 (m, 5H), 7.43-7.31 (m, 8H), 6.55 (s, 1H), 6.28 (d, $J = 6.8$ Hz, 1H), 5.71 (d, $J = 6.8$ Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.0, 156.5, 153.5, 142.0, 139.1, 133.7, 132.5, 129.8, 129.7, 129.0, 128.6, 128.3, 127.3, 122.9, 110.1. ESI-MS m/z (%) 370(100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_2$ C, 74.78; H, 5.18; N, 11.37; Found: C, 74.45; H, 5.21; N, 11.43;

(2-methyl-5-(phenyl(pyrazin-2-ylamino)methyl)furan-3-yl)(phenyl)methanone (6b): IR(KBr, cm^{-1}): 3043, 3022, 2960, 1681. ^1H NMR (400 MHz, CDCl_3) δ 7.20 – 7.45 (m, 11H), 6.46 (s, 1H), 6.33 (d, $J = 7.2$ Hz, 1H), 5.88 (d, $J = 7.2$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 191.7, 155.8, 153.4, 141.9, 139.1, 137.7, 132.9, 128.7, 121.4, 111.5, 53.1. ESI-MS m/z (%) 245(100)[$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_2$ C, 74.78; H, 5.18; N, 11.37; Found: C, 74.48; H, 5.20; N, 11.45;

(4,5,6,7-tetrahydro-4-oxobenzofuran-2-yl)(phenyl)methyl acetate (7a): Yield: 107mg, 75%; Yellow oil. IR(KBr, cm^{-1}): 3026, 2957, 2849, 1696, 1465. ^1H NMR (400 MHz, CDCl_3): δ 7.43-7.35 (m, 5H), 6.84 (s, 1H), 6.42 (s, 1H), 2.87 (t, $J = 6.4$ Hz, 2H), 2.48 (t, $J = 6.4$ Hz, 2H), 2.19-2.11 (m, 5H). ^{13}C NMR (100 MHz, CDCl_3): δ 194.3, 169.7, 167.6, 153.1, 136.6, 128.7, 128.7, 127.2, 121.7, 106.1, 100.0, 70.3, 37.5, 23.4, 22.5, 21.1. ESI-MS m/z (%) 285 (100) [$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{17}\text{H}_{16}\text{O}_4$ C, 71.82; H, 5.67; Found: C, 71.58; H, 5.62;

(4,5,6,7-tetrahydro-4-oxo-6-phenylbenzofuran-2-yl)(phenyl)methyl acetate (7b): Yield: 130mg, 72%; Brown oil. IR(KBr, cm^{-1}): 3056, 3038, 2941, 2887, 1702. ^1H NMR (400 MHz, CDCl_3): δ 7.44-7.25 (m, 10H), 6.85 (s, 1H), 6.47 (s, 1H), 3.57-3.49 (m, 1H), 3.18-3.00 (m, 2H), 2.74 (d, $J = 8.4$ Hz, 2H), 2.15 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 192.8, 169.7, 166.8, 153.6, 142.3, 136.6, 128.9, 128.8, 128.7, 127.3, 127.2, 126.8, 121.6, 106.1, 70.3, 44.9, 41.2, 31.3, 21.1.

ESI-MS m/z (%) 361 (100) $[M+H]^+$; Anal. Calcd for $C_{23}H_{20}O_4$ C, 76.65; H, 5.59; Found: C, 76.37; H, 5.62;

(4,5,6,7-tetrahydro-6,6-dimethyl-4-oxobenzofuran-2-yl)(phenyl)methyl acetate (7c):

Yield: 122mg, 78%; Yellow oil. IR(KBr, cm^{-1}): 3045, 2960, 2877, 1694, 1462. 1H NMR (400 MHz, $CDCl_3$): δ 7.43-7.32 (m, 5H), 6.85 (s, 1H), 6.40 (s, 1H), 2.72 (s, 2H), 2.33 (s, 2H), 2.14 (s, 3H), 1.12 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.7, 169.7, 166.8, 153.4, 136.6, 128.7, 128.7, 127.2, 120.5, 106.1, 70.3, 51.9, 37.4, 35.2, 28.7, 28.6, 21.1 ESI-MS m/z (%) 361 (100) $[M+H]^+$; Anal. Calcd for $C_{19}H_{20}O_4$ C, 73.06; H, 6.45; Found: C, 72.86; H, 6.48;

(4,5,6,7-tetrahydro-4-oxobenzofuran-2-yl)(phenyl)methyl propionate (7d): Yield: 109mg,

73%; Brown solid, 68-70°C. IR(KBr, cm^{-1}): 3035, 2963, 2876, 1703, 1462, 1374. 1H NMR (400 MHz, $CDCl_3$): δ 7.42-7.32 (m, 5H), 6.85 (s, 1H), 6.41 (s, 1H), 2.87 (t, $J = 6.4$ Hz, 2H), 2.48-2.40 (m, 4H), 2.19-2.12 (m, 2H), 1.18 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.3, 173.1, 167.6, 153.2, 136.8, 128.7, 128.7, 127.1, 121.8, 106.0, 70.1, 37.5, 27.7, 23.4, 22.5, 9.0. ESI-MS m/z (%) 299 (100) $[M+H]^+$; Anal. Calcd for $C_{18}H_{18}O_4$ C, 72.47; H, 6.08; Found: C, 72.18; H, 6.11;

(4,5,6,7-tetrahydro-4-oxo-6-phenylbenzofuran-2-yl)(phenyl)methyl propionate (7e):

Yield: 138mg, 74%; Yellow oil. IR(KBr, cm^{-1}): 3058, 3022, 2974, 2862, 1706, 1459, 1373. 1H NMR (400 MHz, $CDCl_3$): δ 7.44-7.33 (m, 7H), 7.27 (d, $J = 7.2$ Hz, 3H), 6.86 (s, 1H), 6.46 (s, 1H), 3.57-3.49 (m, 1H), 3.18-3.00 (m, 2H), 2.74 (d, $J = 8.0$ Hz, 2H), 2.51-2.38 (m, 2H), 1.19 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.8, 173.1, 166.7, 153.8, 142.3, 136.7, 128.9, 128.8, 128.7, 127.3, 127.2, 126.8, 121.6, 106.0, 105.9, 70.1, 44.9, 41.2, 31.3, 27.7, 9.0. ESI-MS m/z (%) 375 (100) $[M+H]^+$; Anal. Calcd for $C_{24}H_{22}O_4$ C, 76.99; H, 5.92; Found: C, 76.68; H, 5.95;

(4,5,6,7-tetrahydro-6,6-dimethyl-4-oxobenzofuran-2-yl)(phenyl)methyl propionate (7f):

Yield: 126mg, 77%; Brown oil. IR(KBr, cm^{-1}): 3036, 2966, 2935, 1698, 1464, 1370. ^1H NMR (400 MHz, CDCl_3): δ 7.43-7.34 (m, 5H), 6.86 (s, 1H), 6.39 (s, 1H), 2.72 (s, 2H), 2.48-2.37 (m, 2H), 2.34 (s, 2H), 1.18 (q, $J = 7.6$ Hz, 9H). ^{13}C NMR (100 MHz, CDCl_3): δ 193.7, 173.1, 166.7, 153.5, 136.8, 128.7, 128.6, 127.2, 120.5, 105.9, 70.1, 51.9, 37.4, 35.2, 28.7, 28.6, 27.7, 9.0. ESI-MS m/z (%) 327 (100) $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{20}\text{H}_{22}\text{O}_4$ C, 73.60; H, 6.79; Found: C, 73.29; H, 6.82;

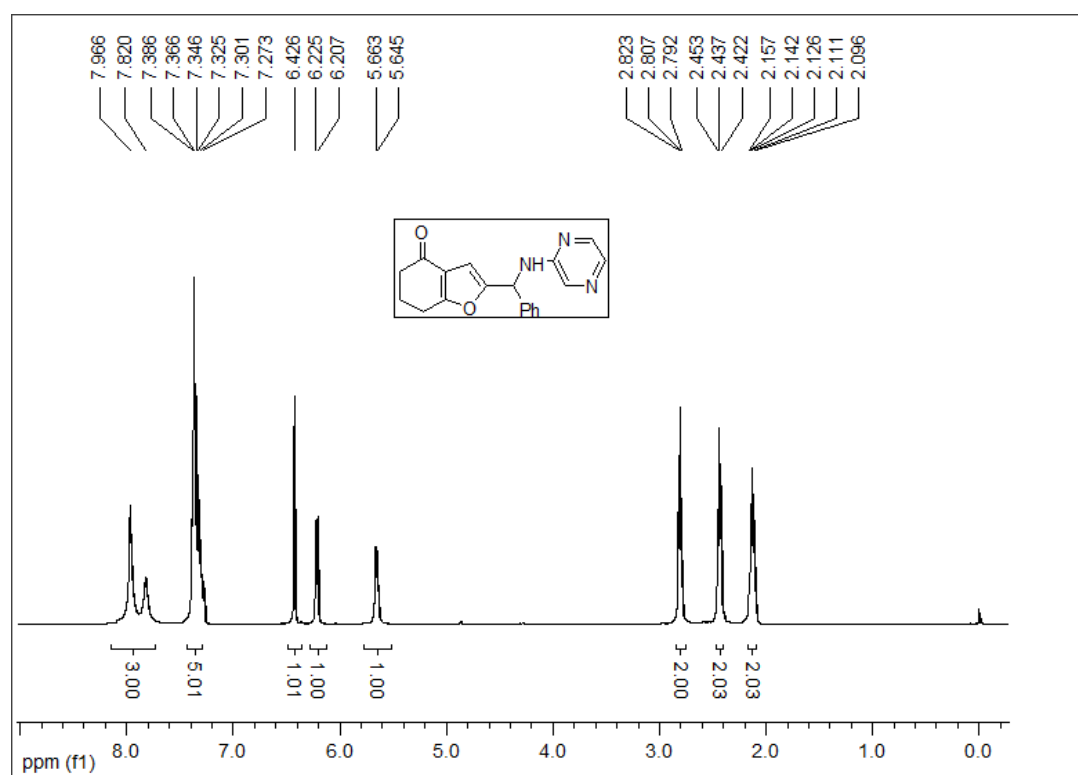
(4,5,6,7-tetrahydro-4-oxobenzofuran-2-yl)(phenyl)methyl butyrate (7g): Yield: 109mg, 70%; Yellow oil. IR(KBr, cm^{-1}): 3024, 2965, 1703, 1465, 1381. ^1H NMR (400 MHz, CDCl_3): δ 7.42-7.32 (m, 5H), 6.85 (s, 1H), 6.41 (s, 1H), 2.87 (t, $J = 6.4$ Hz, 2H), 2.48-2.37 (m, 4H), 2.18-2.12 (m, 2H), 1.73-1.64 (m, 2H), 0.95 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 194.3, 172.4, 167.6, 153.2, 136.8, 128.7, 128.6, 127.1, 121.7, 105.9, 70.0, 37.5, 36.2, 23.4, 22.5, 18.4, 13.6. ESI-MS m/z (%) 313 (100) $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{19}\text{H}_{20}\text{O}_4$ C, 73.06; H, 6.45; Found: C, 72.79; H, 6.48;

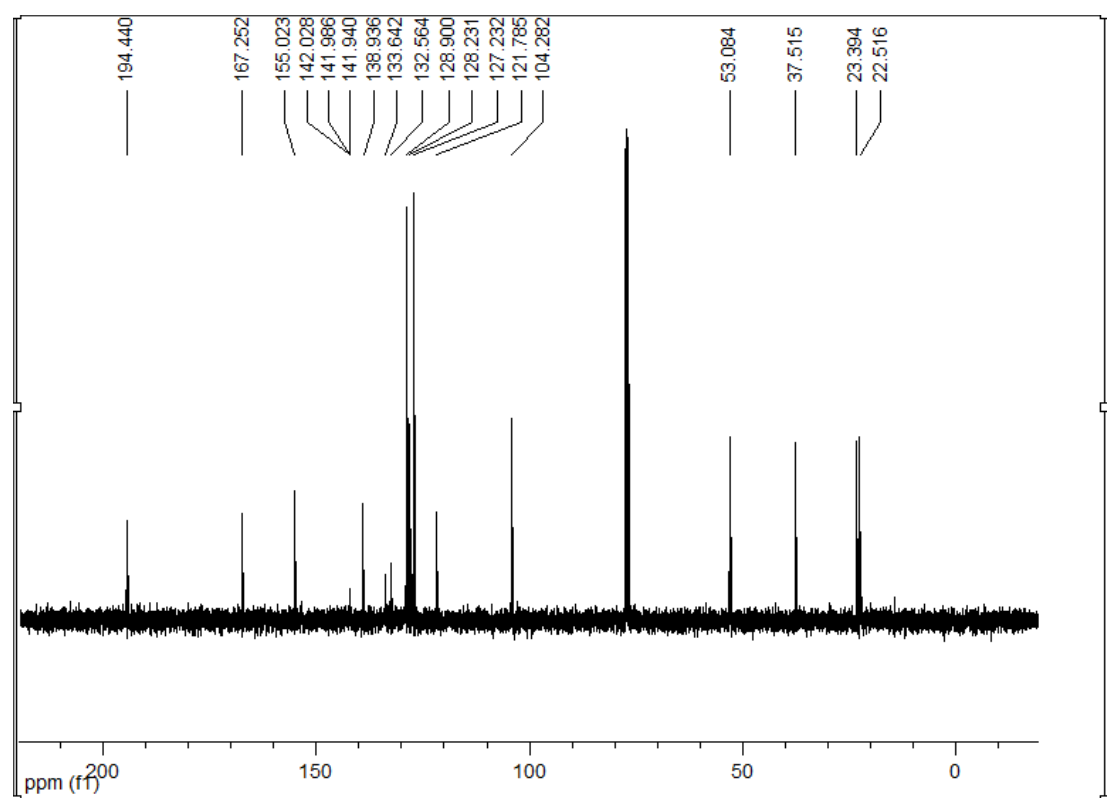
(4,5,6,7-tetrahydro-4-oxo-6-phenylbenzofuran-2-yl)(phenyl)methyl butyrate (7h): Yield: 142mg, 73%; Yellow oil. IR(KBr, cm^{-1}): 3038, 2865, 1704, 1468, 1377. ^1H NMR (400 MHz, CDCl_3): δ 7.44-7.25 (m, 10H), 6.87 (s, 1H), 6.46 (s, 1H), 3.59-3.49 (m, 1H), 3.18-3.00 (m, 2H), 2.74 (d, $J = 8.4$ Hz, 2H), 2.41 (t, $J = 7.6$ Hz, 2H), 1.73-1.64 (m, 2H), 0.95 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 192.8, 172.3, 166.7, 153.8, 142.3, 136.7, 128.9, 128.8, 128.7, 127.3, 127.2, 126.8, 121.6, 105.9, 105.9, 70.0, 44.9, 41.2, 36.2, 31.3, 18.4, 13.6. ESI-MS m/z (%) 389 (100) $[\text{M}+\text{H}]^+$; Anal. Calcd for $\text{C}_{25}\text{H}_{24}\text{O}_4$ C, 77.30; H, 6.23; Found: C, 76.99; H, 6.27;

(4,5,6,7-tetrahydro-6,6-dimethyl-4-oxobenzofuran-2-yl)(phenyl)methyl butyrate (7i): Yield: 128mg, 75%; Brown oil. IR(KBr, cm^{-1}): 3041, 2953, 1689, 1466, 1380. ^1H NMR (400 MHz,

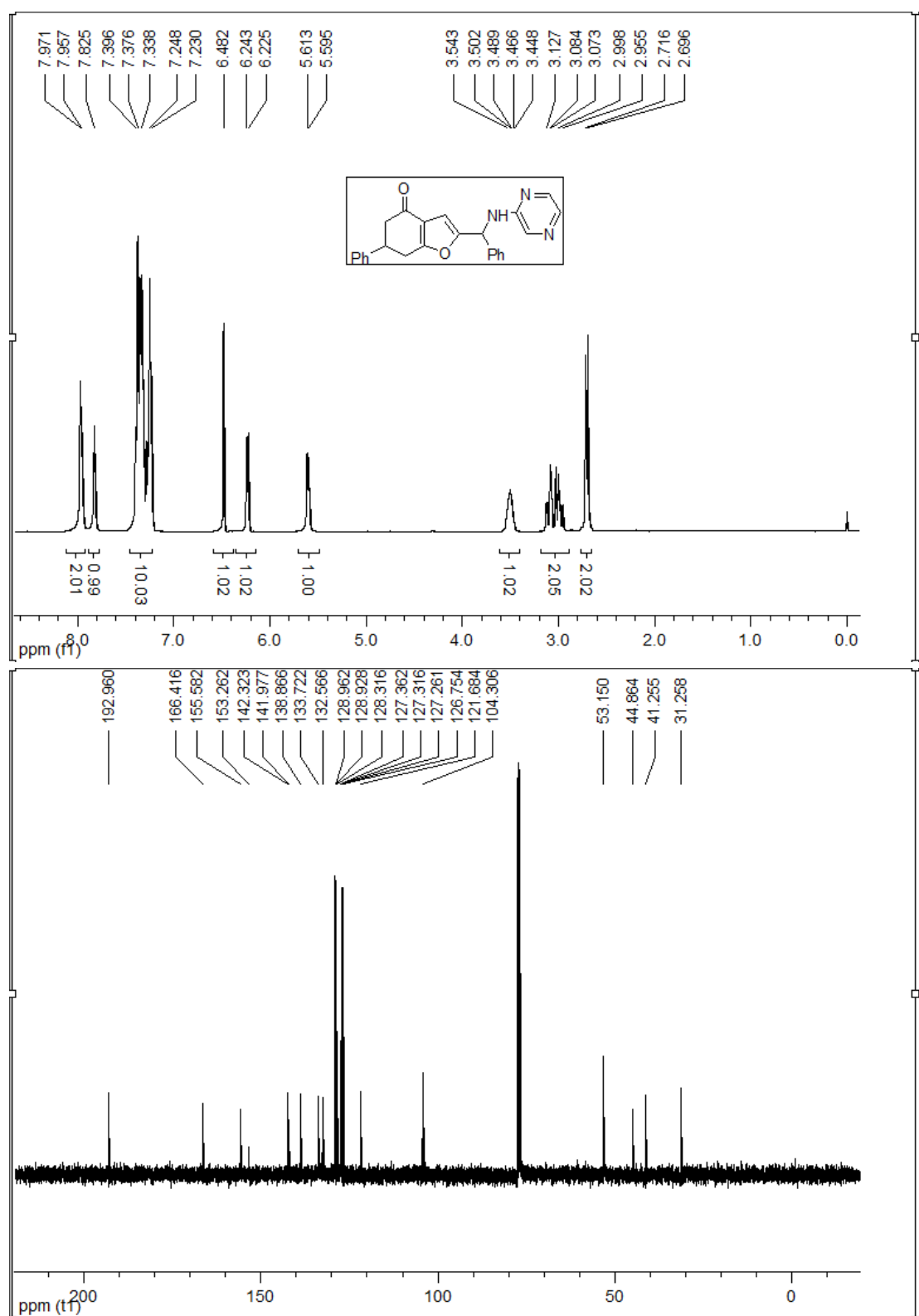
CDCl₃): δ 7.42-7.33 (m, 5H), 6.86 (s, 1H), 6.39 (s, 1H), 2.72 (s, 2H), 2.40 (q, J = 7.6 Hz, 4H), 1.71 (t, J = 7.6 Hz, 2H), 1.13 (d, J = 7.6 Hz, 3H), 0.95 (t, J = 7.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 193.8, 172.4, 166.8, 153.6, 136.8, 128.7, 128.6, 127.2, 120.5, 105.9, 70.0, 51.9, 37.4, 36.2, 35.2, 28.7, 28.6, 18.4, 13.6. ESI-MS m/z (%) 340.17 (100) [M+H]⁺; Anal. Calcd for C₂₁H₂₄O₄: C, 74.09; H, 7.11; Found: C, 74.72; H, 7.15;

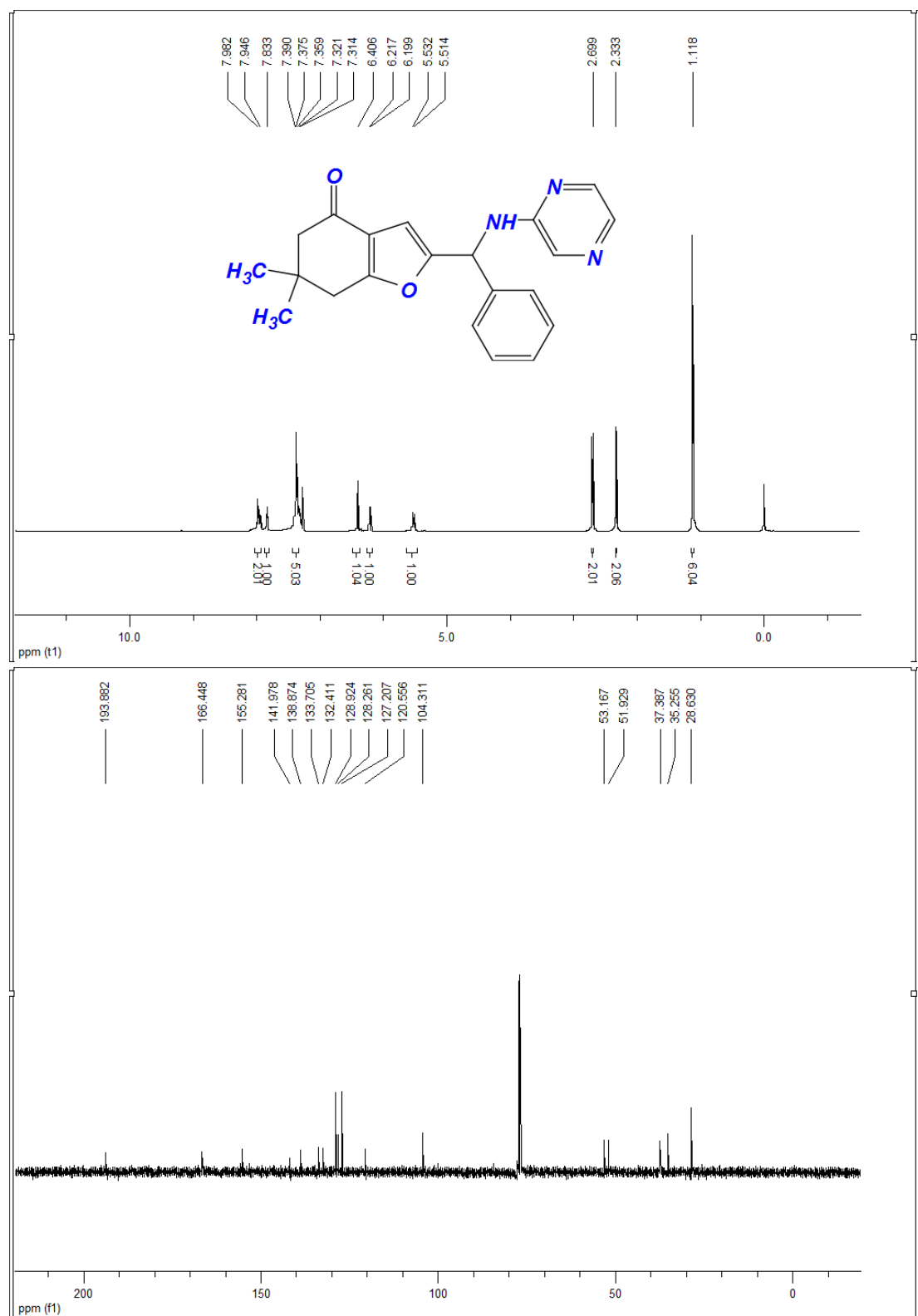
4a



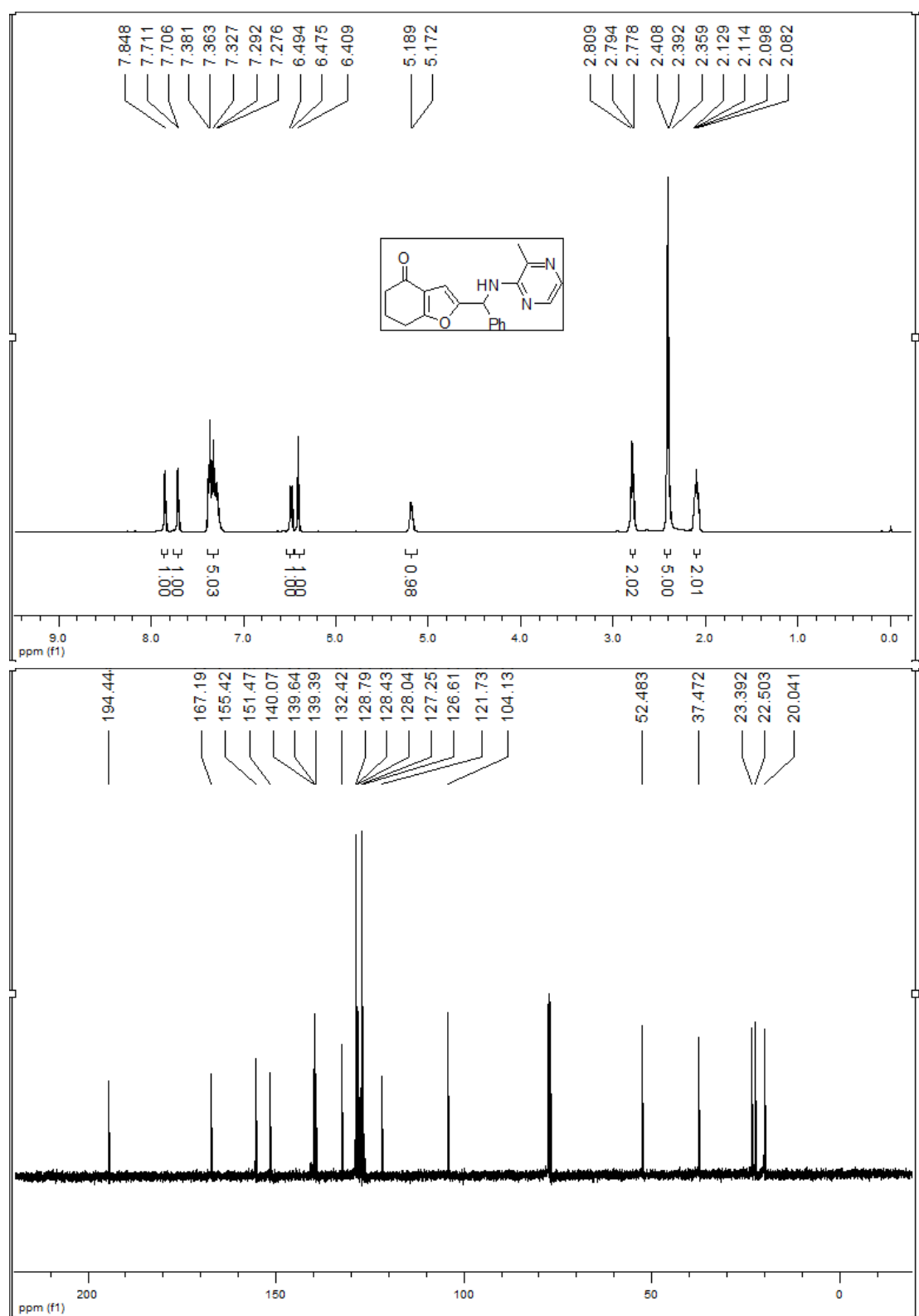


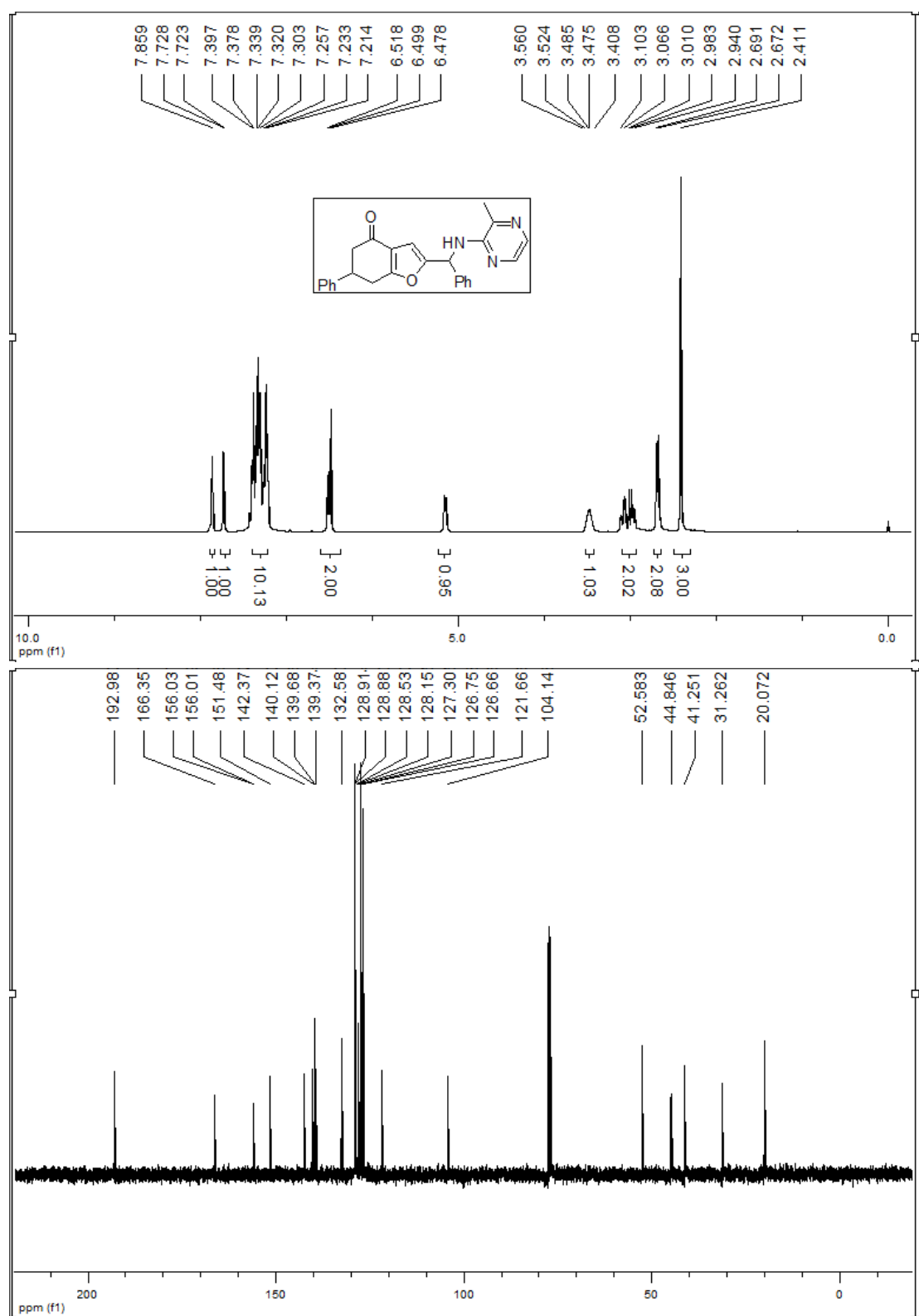
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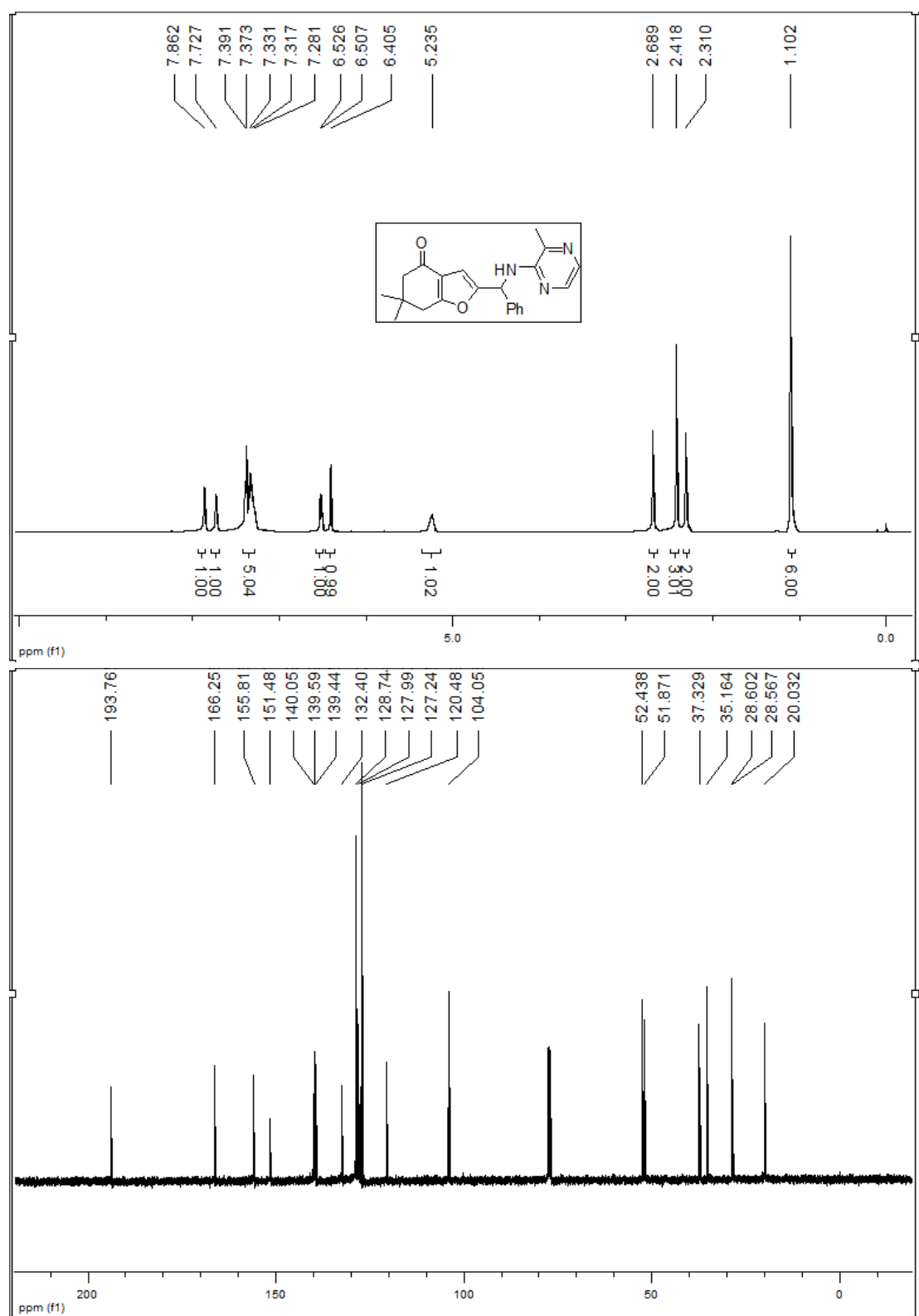


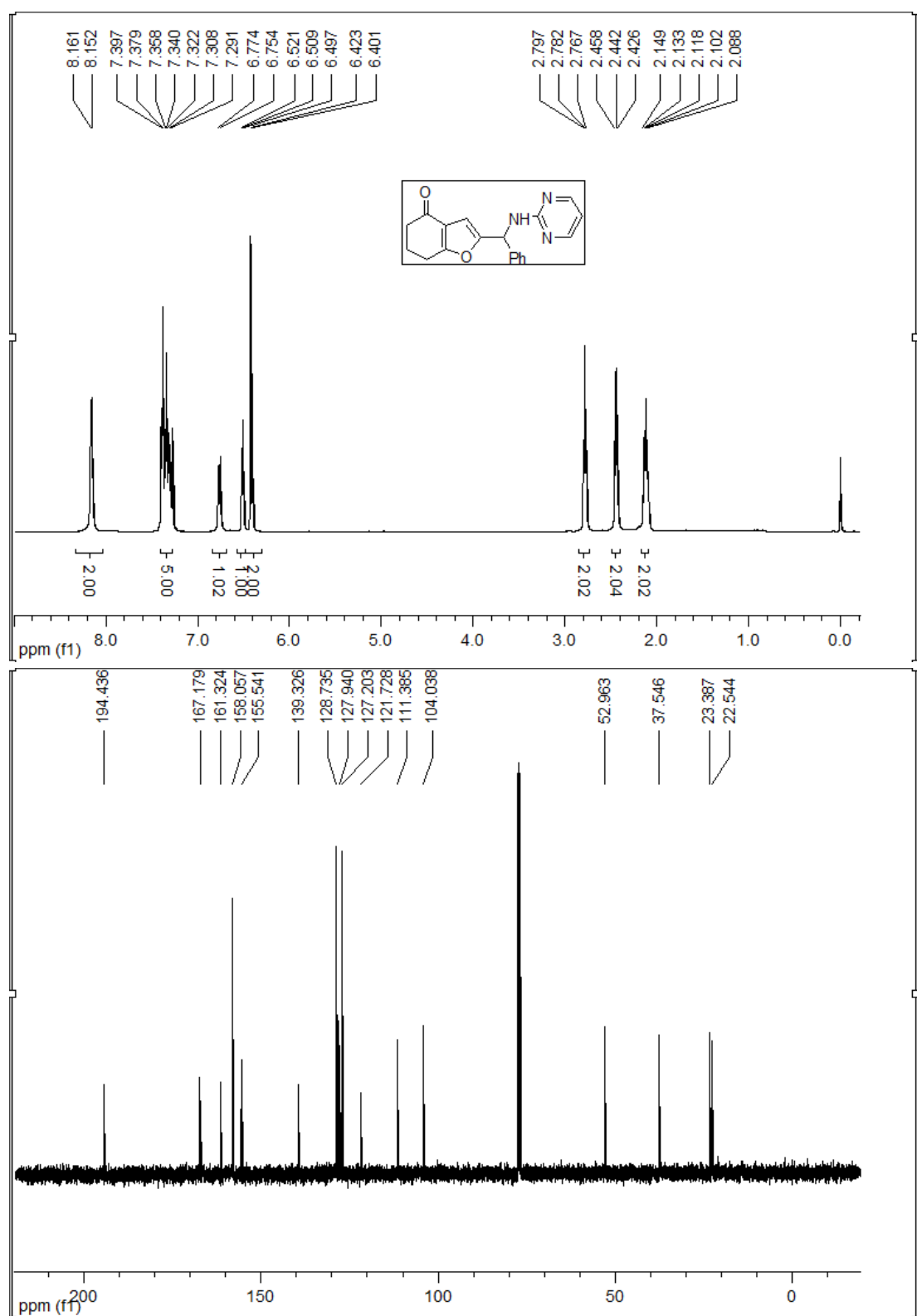


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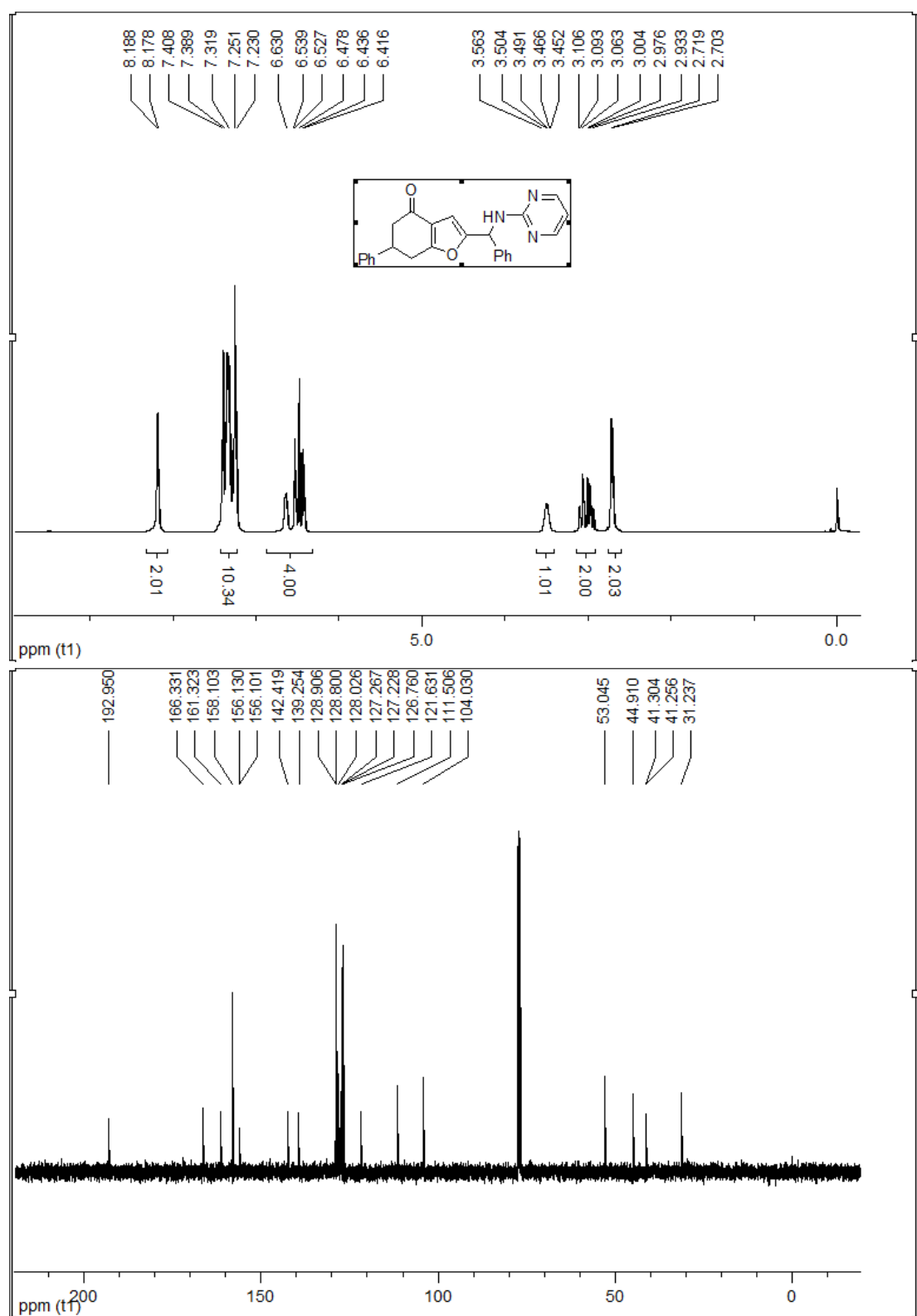


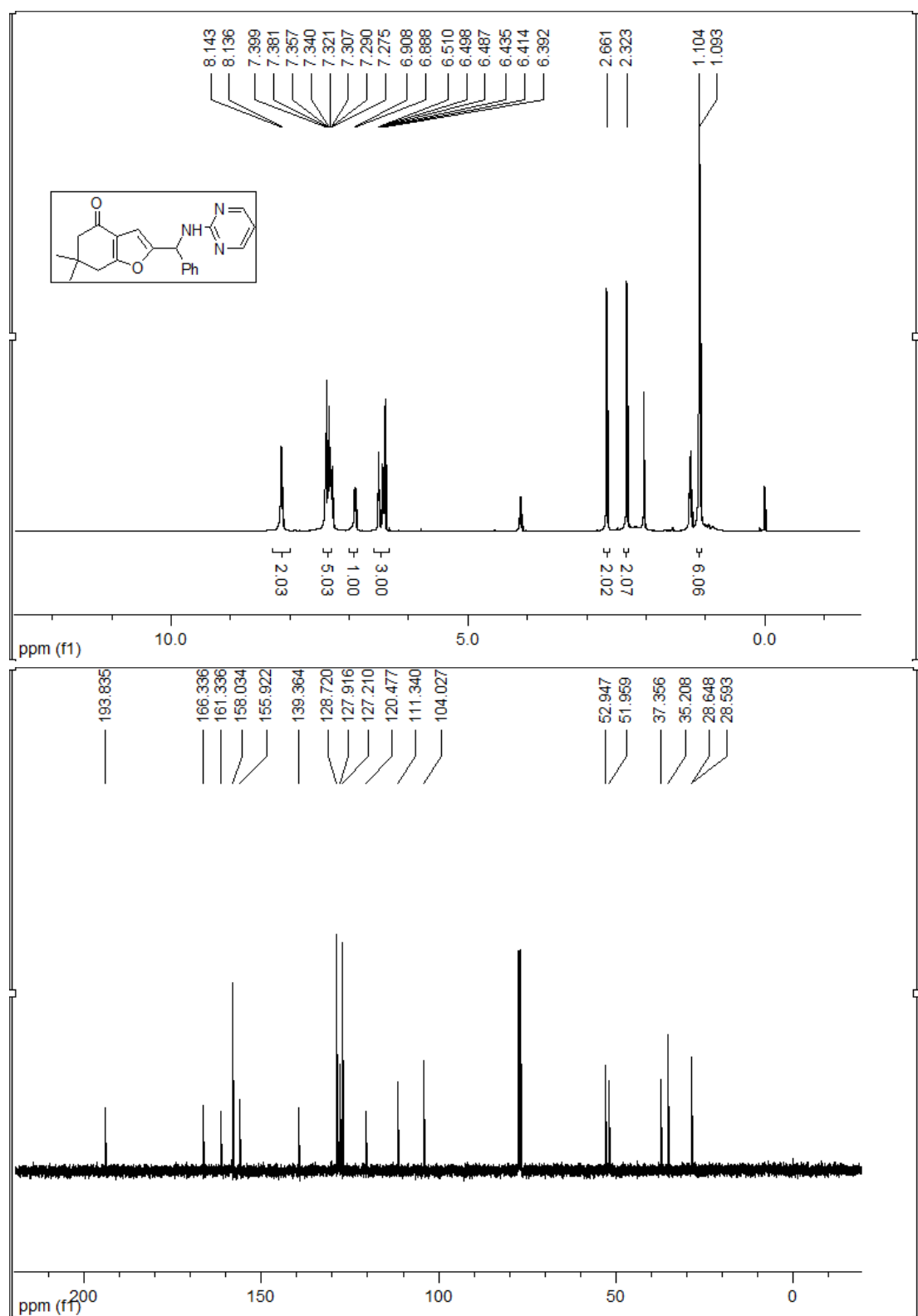


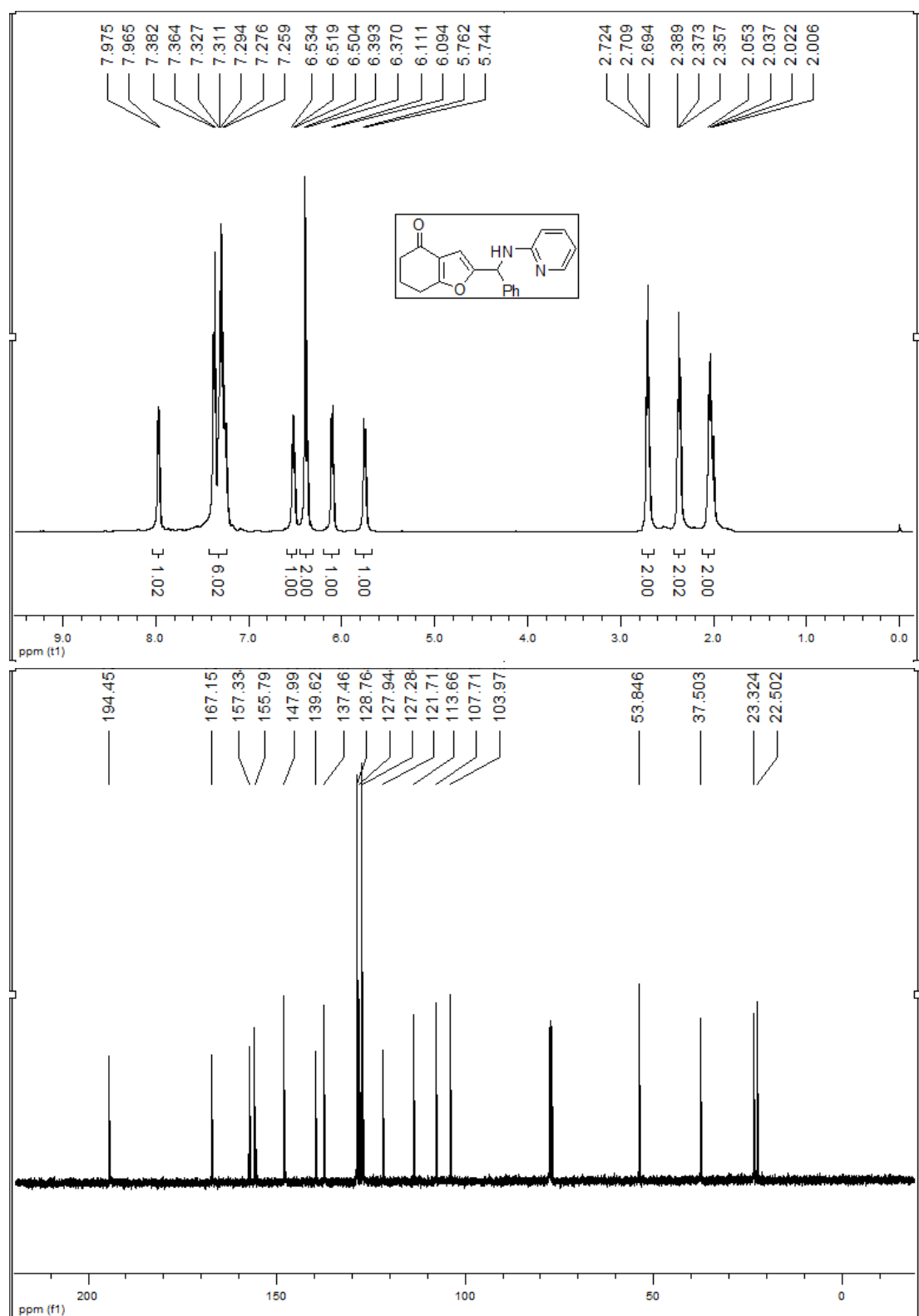


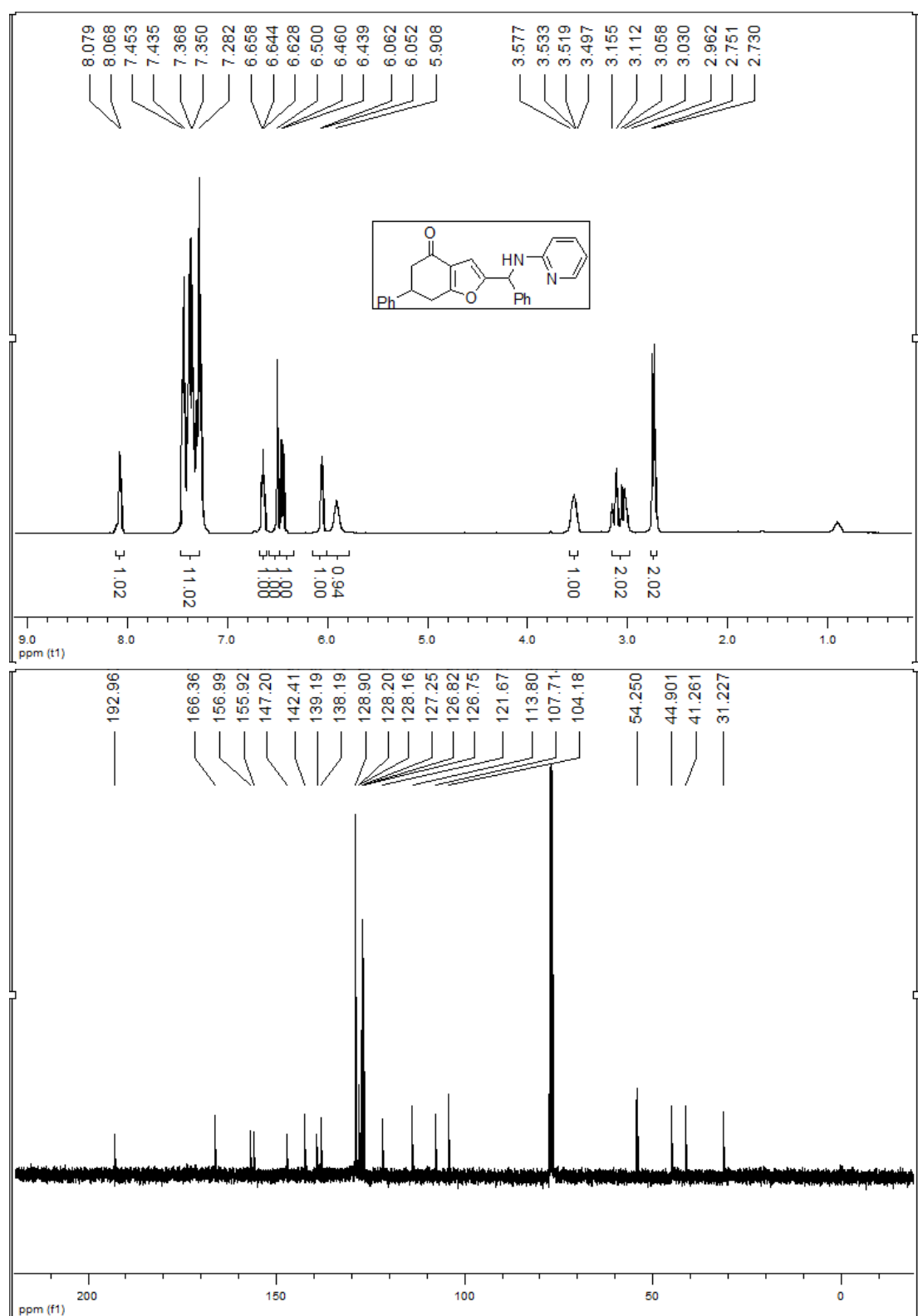


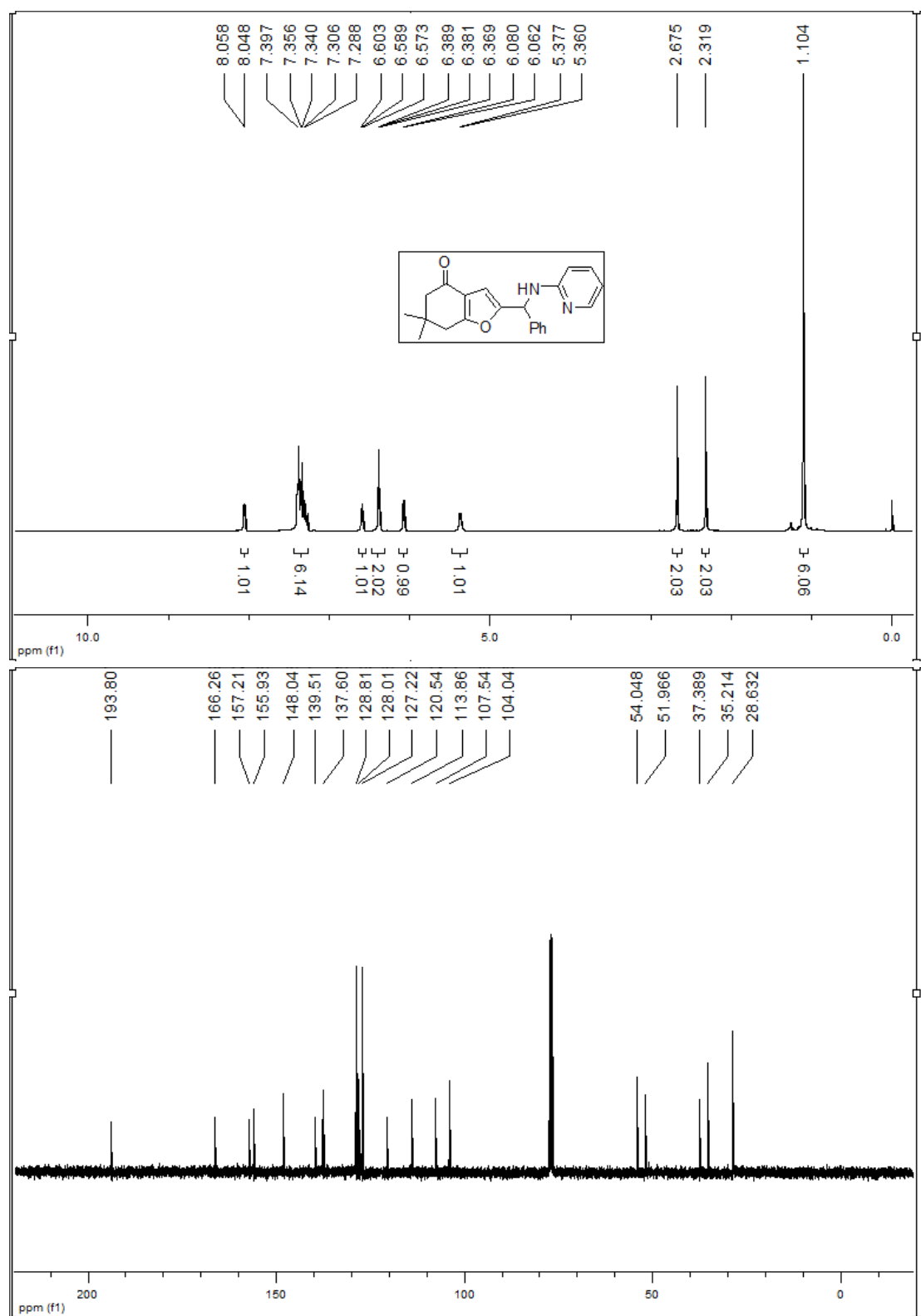
4h



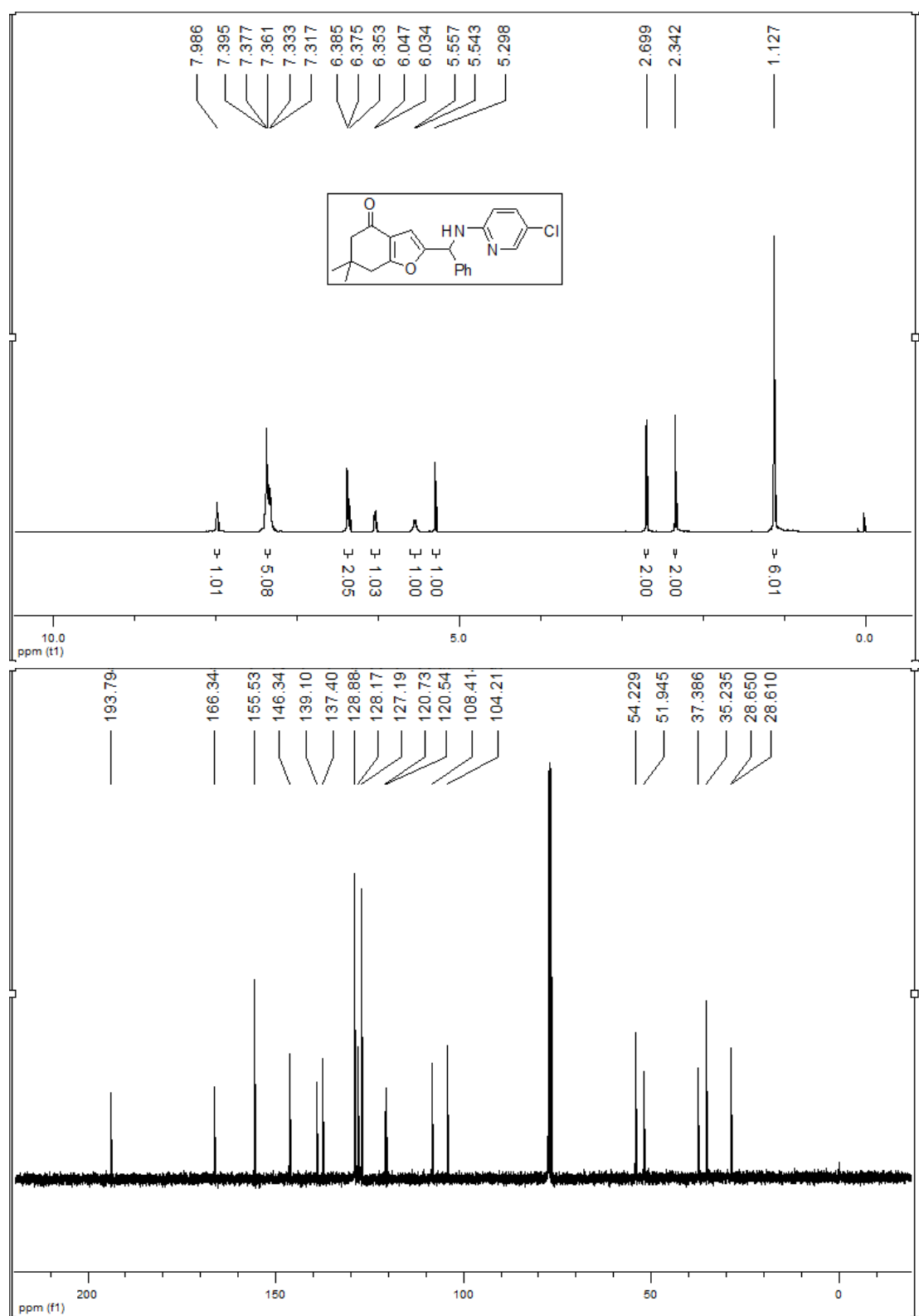




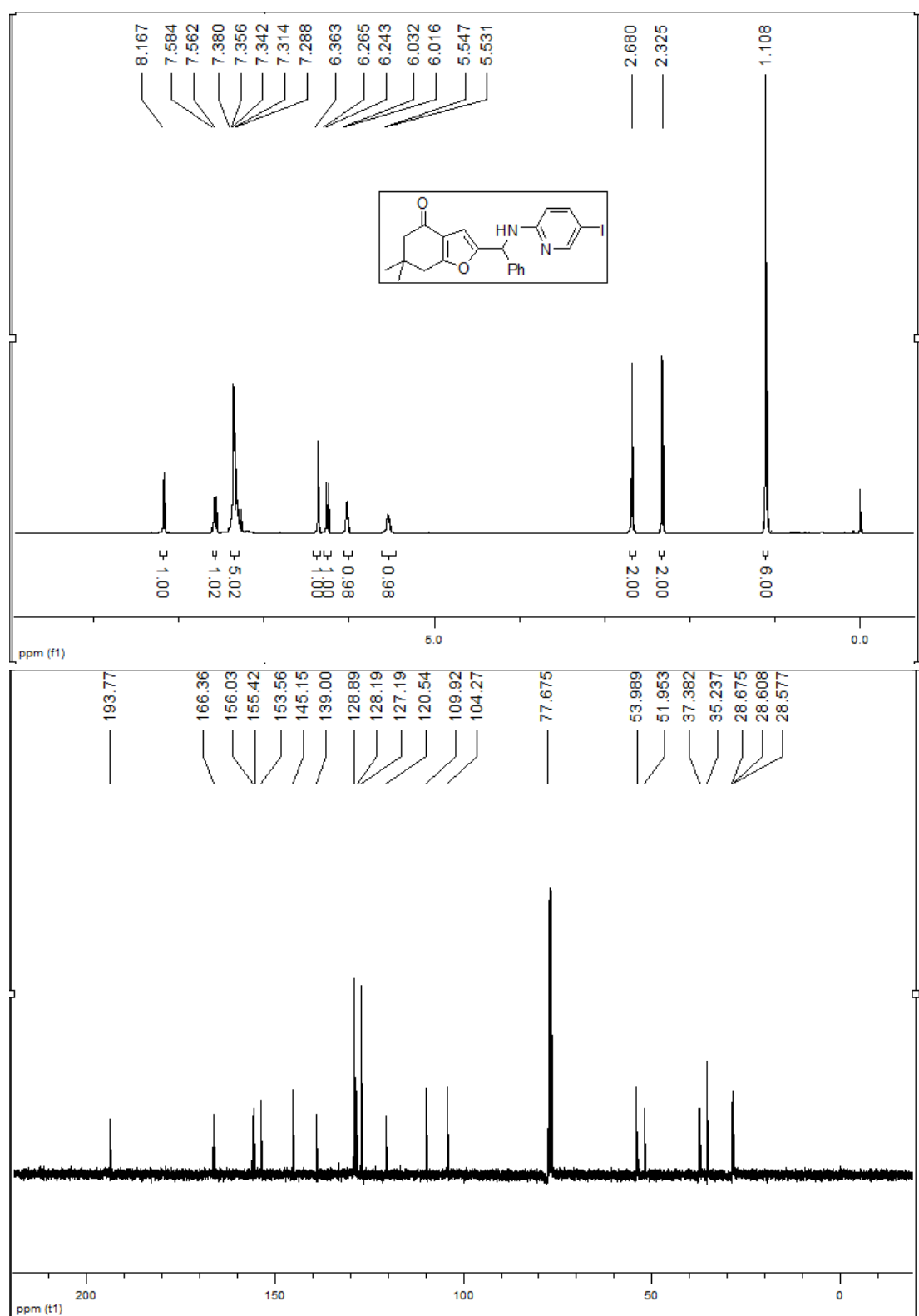


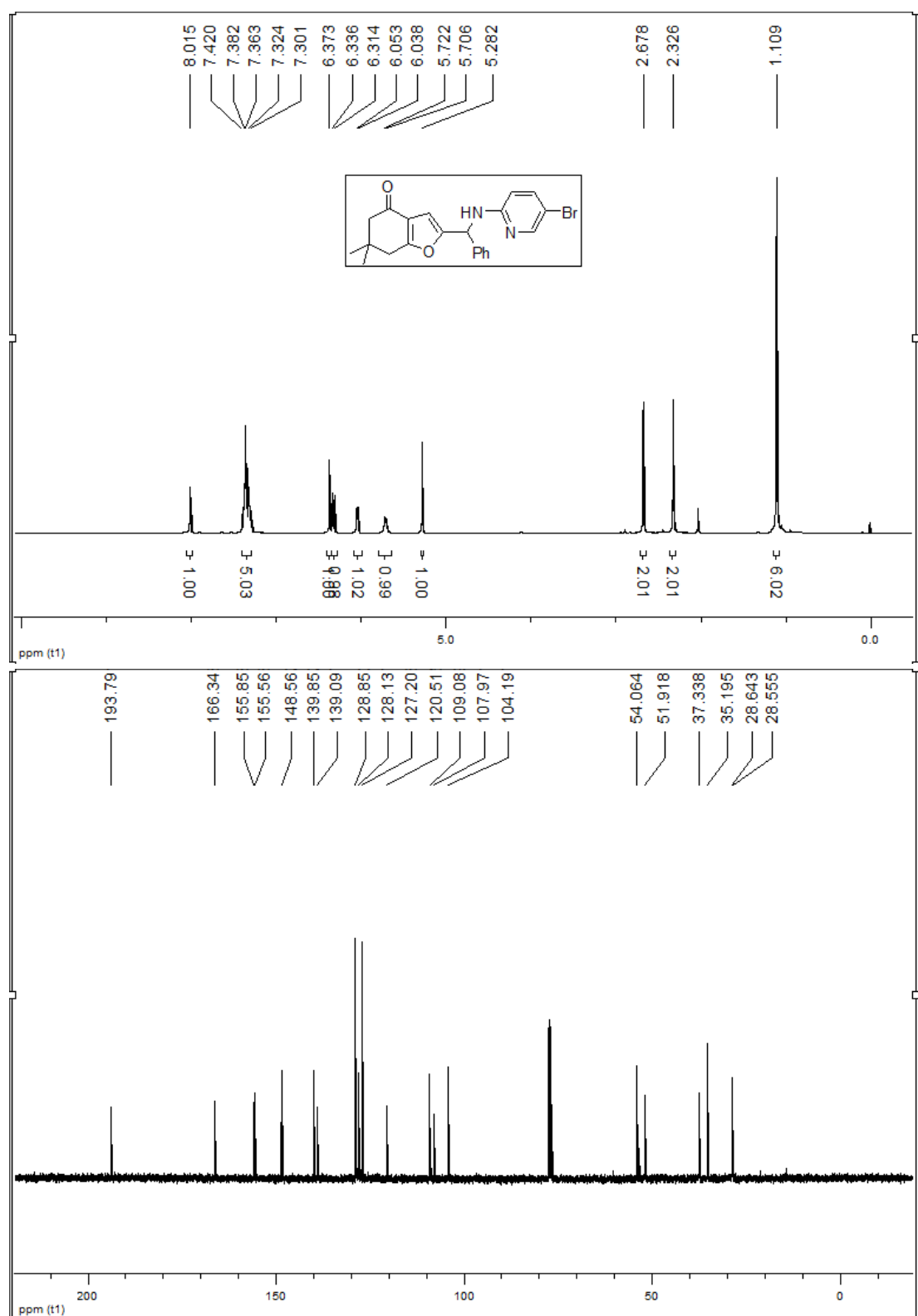


4m

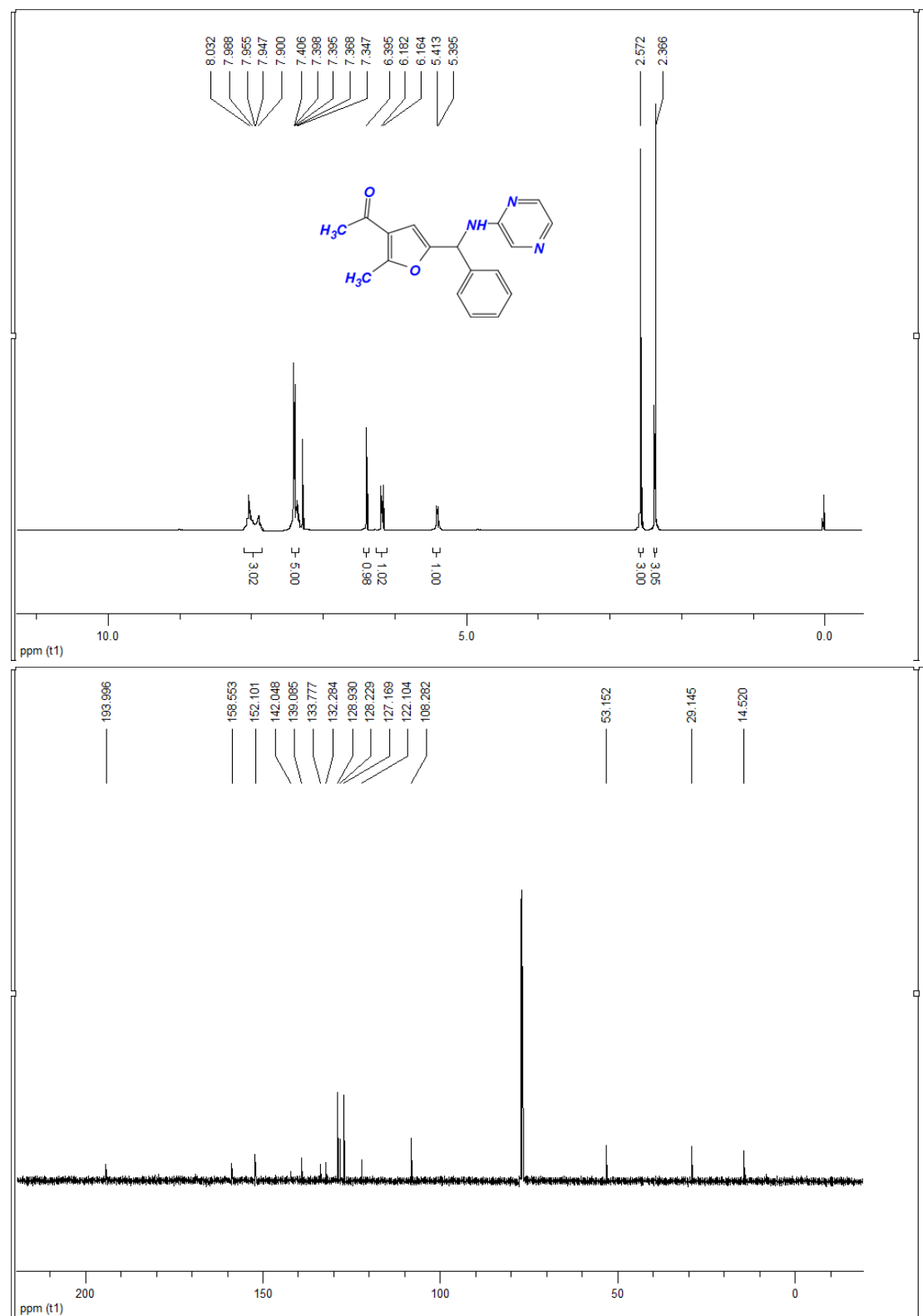


4n

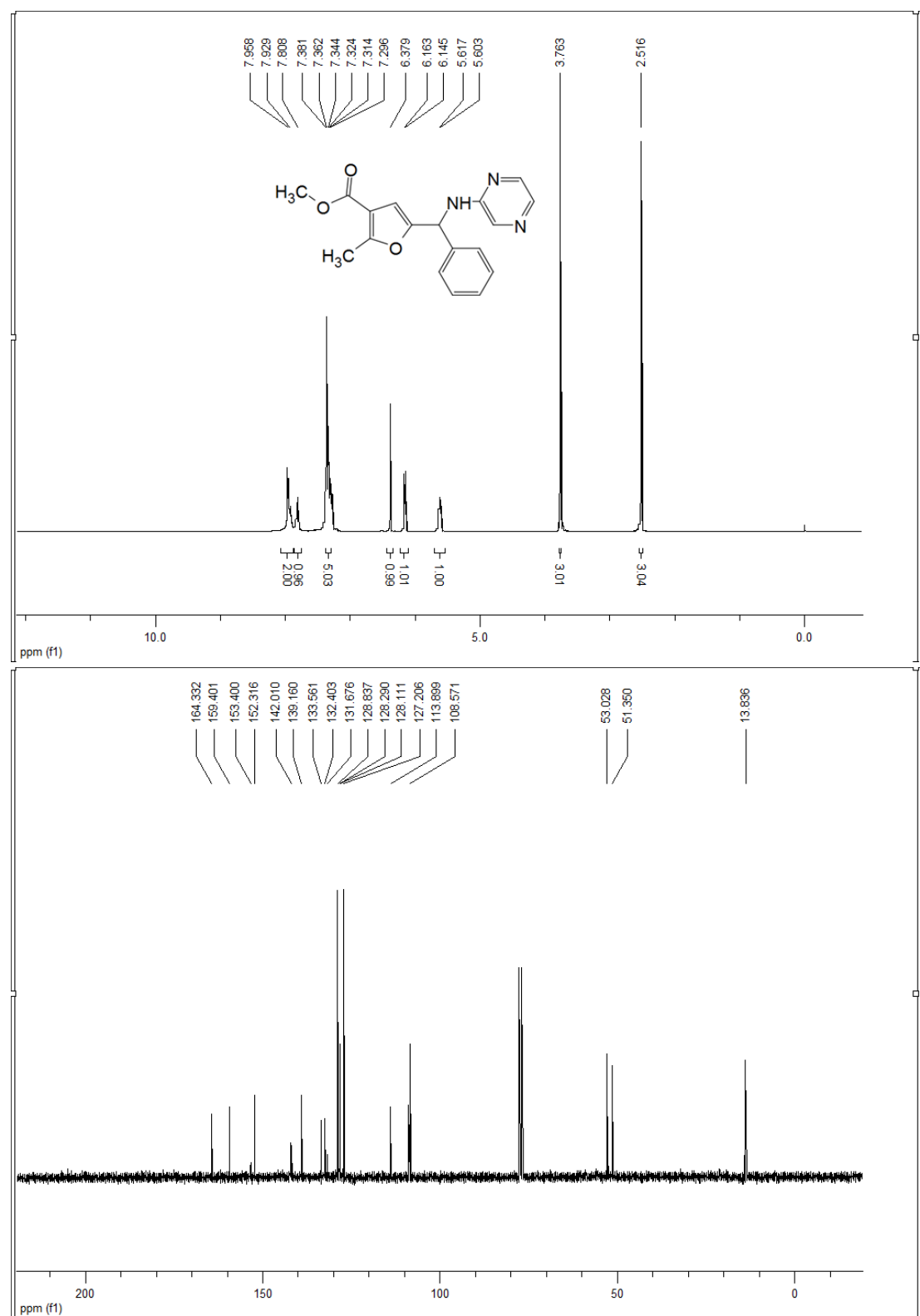




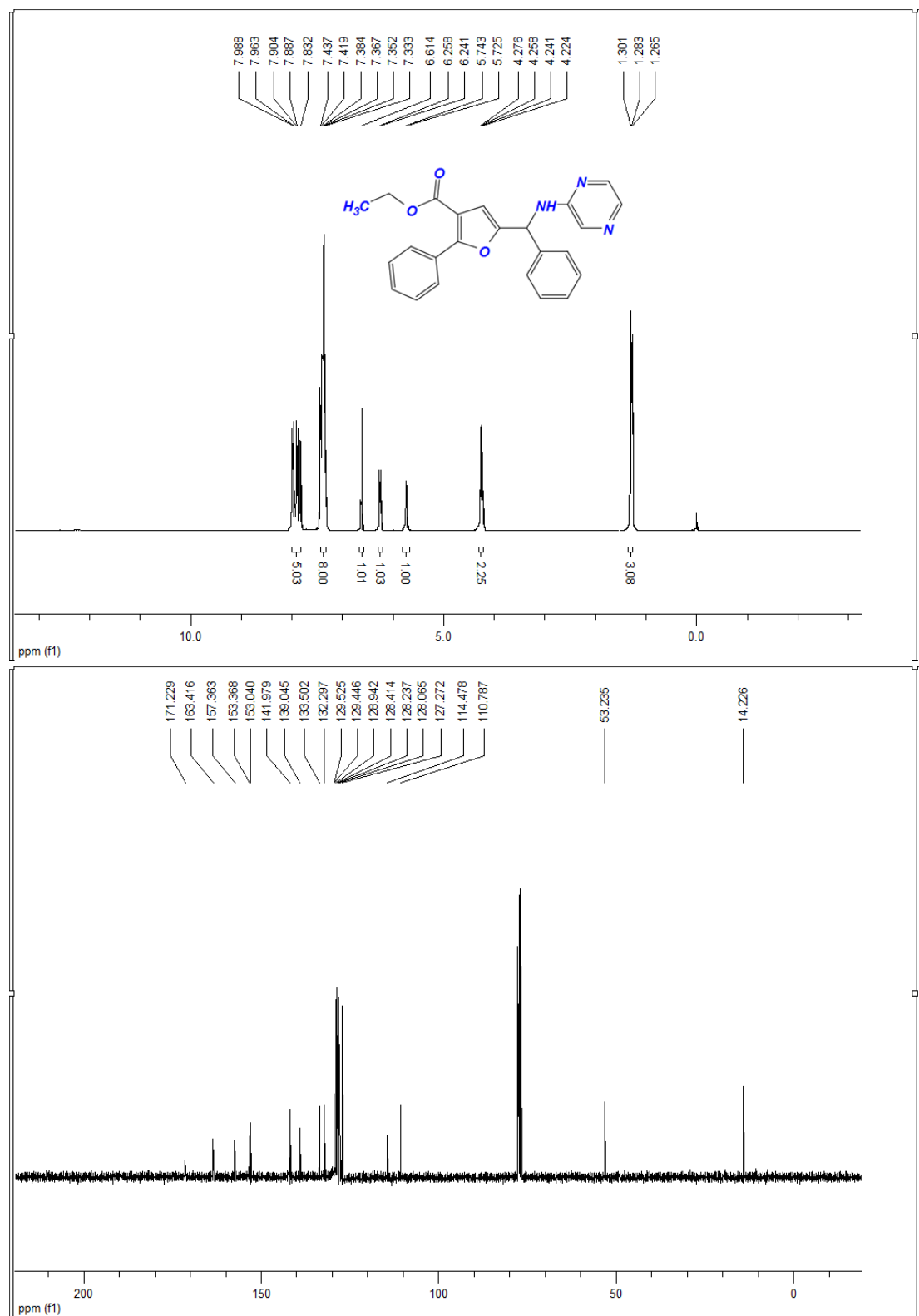
5a



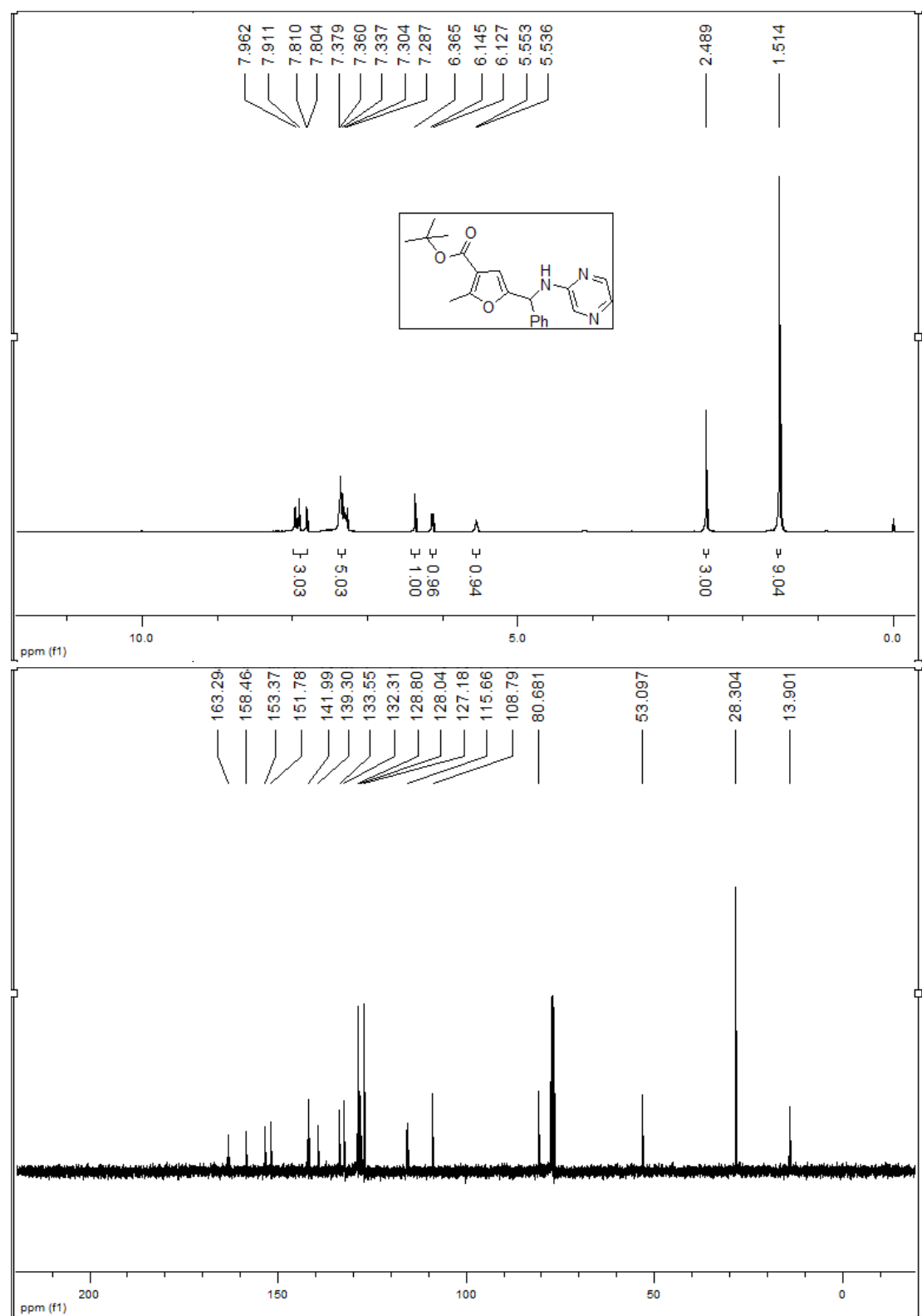
5b



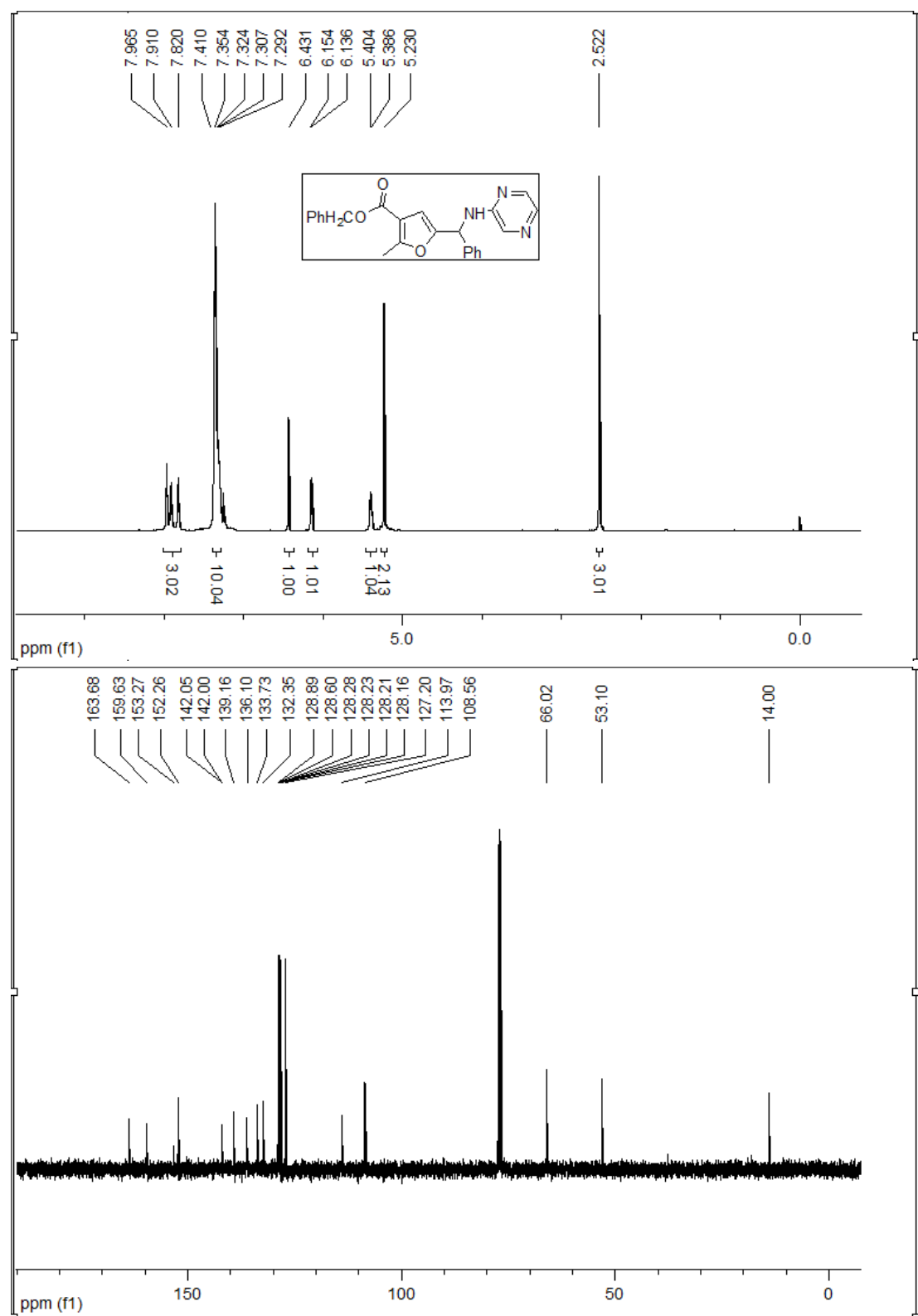
5c



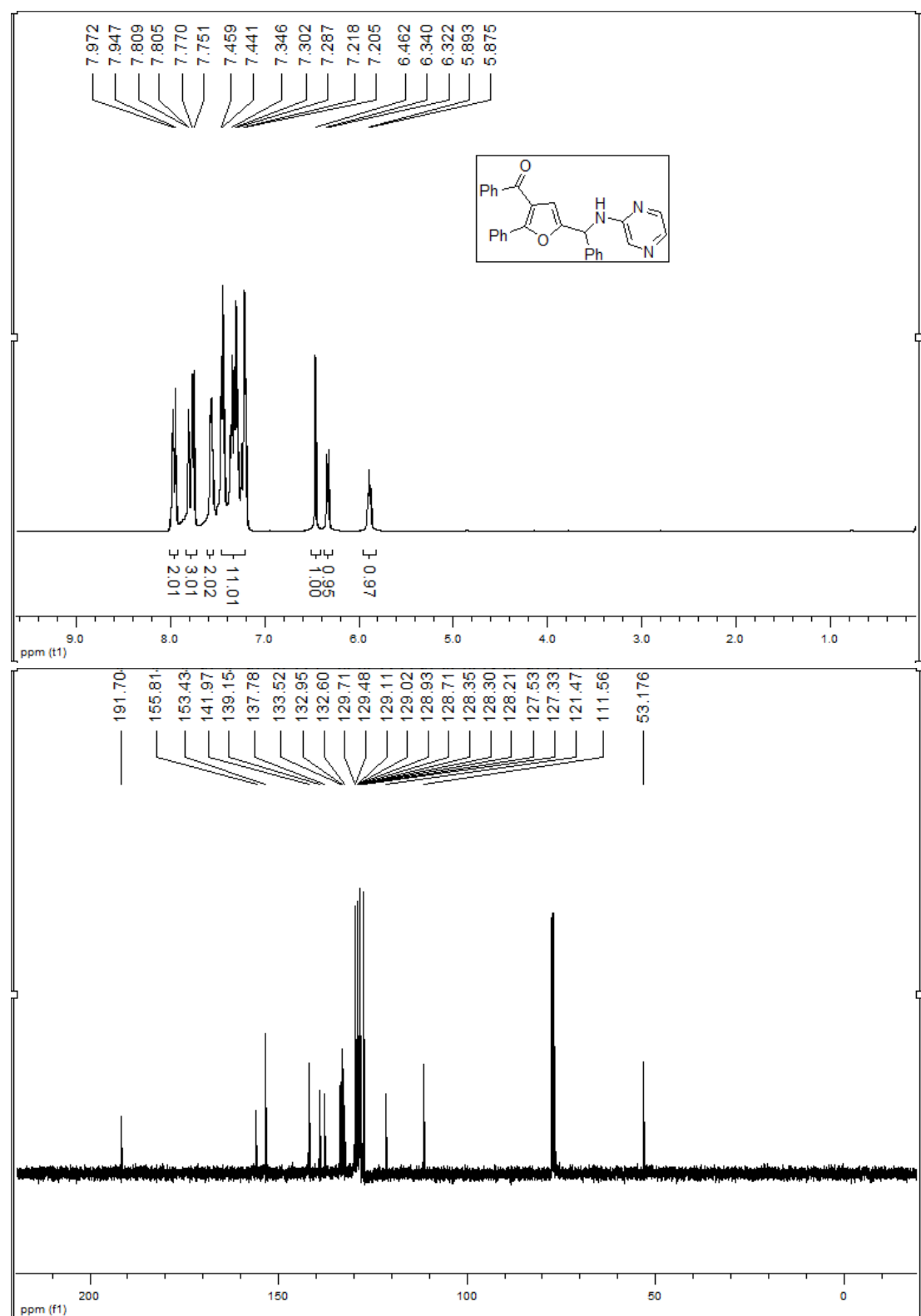
5d



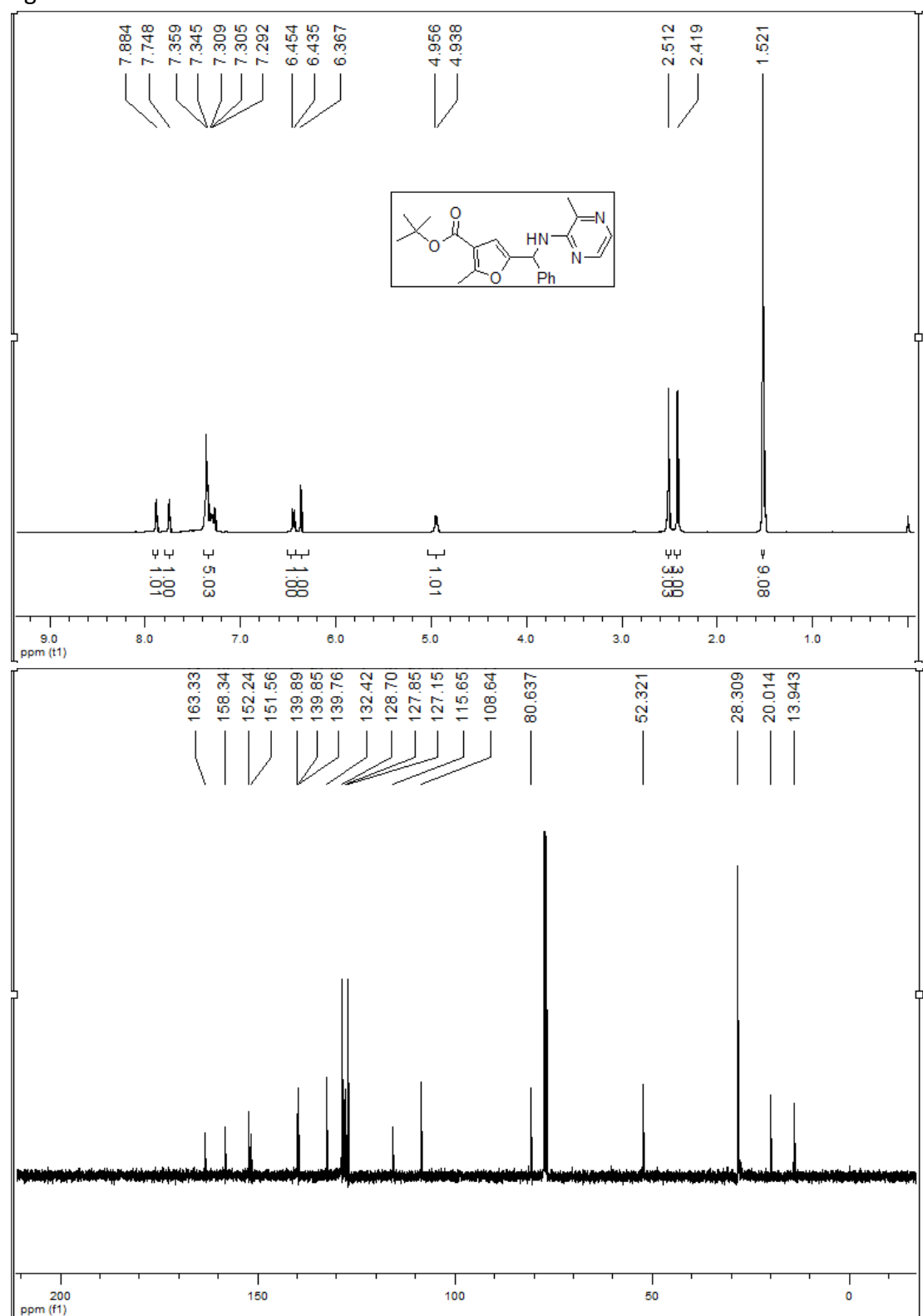
5e



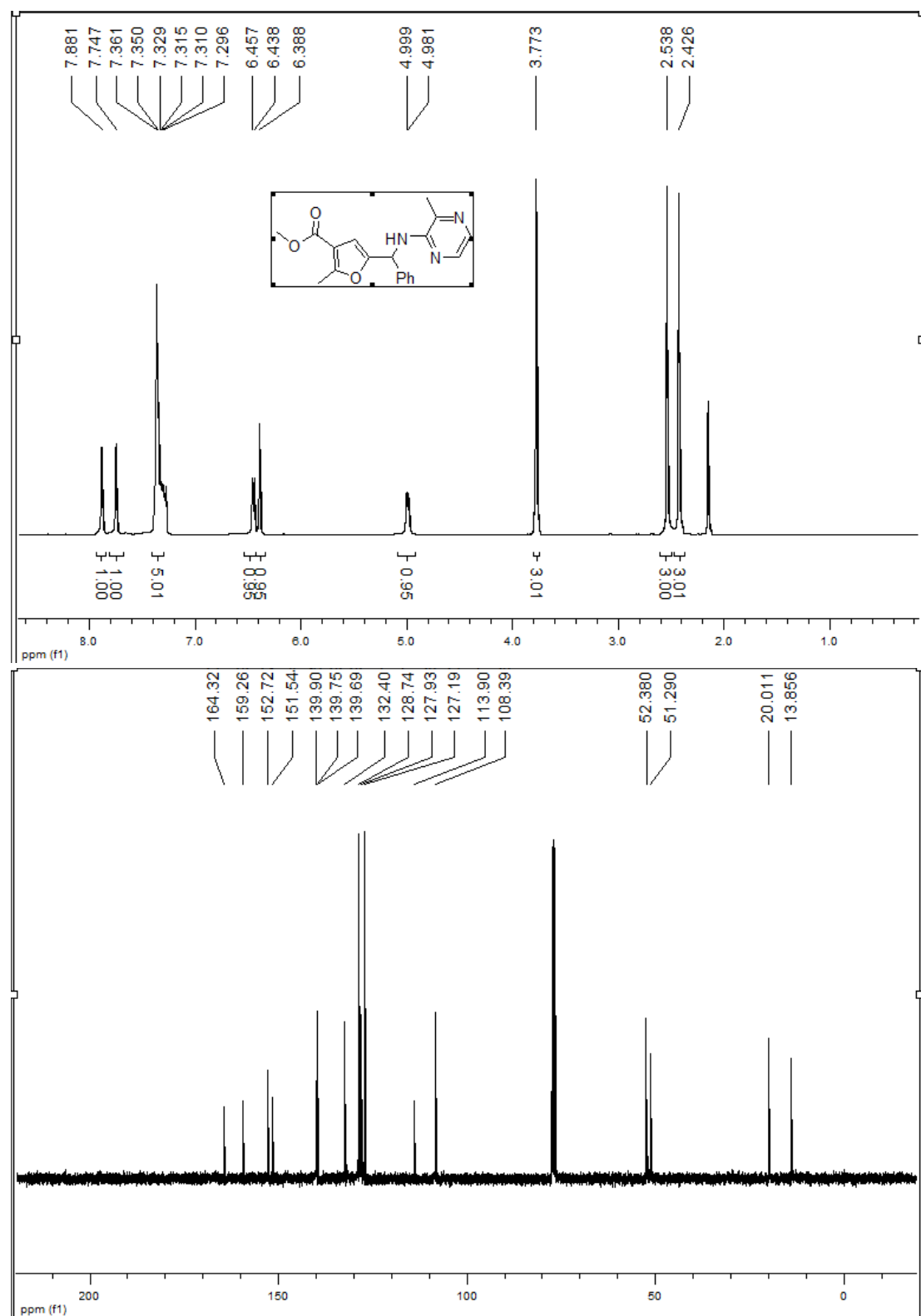
5f



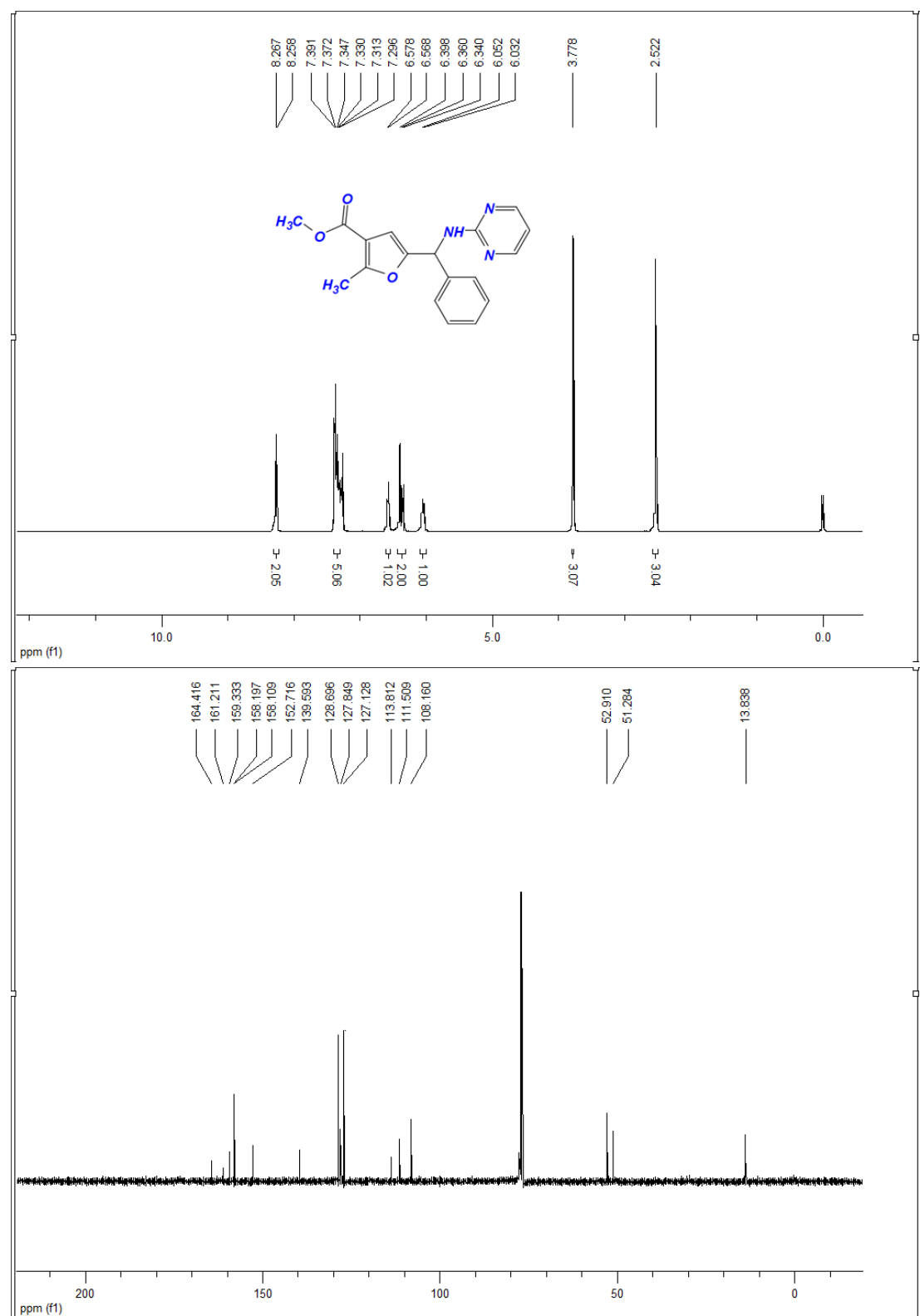
5g



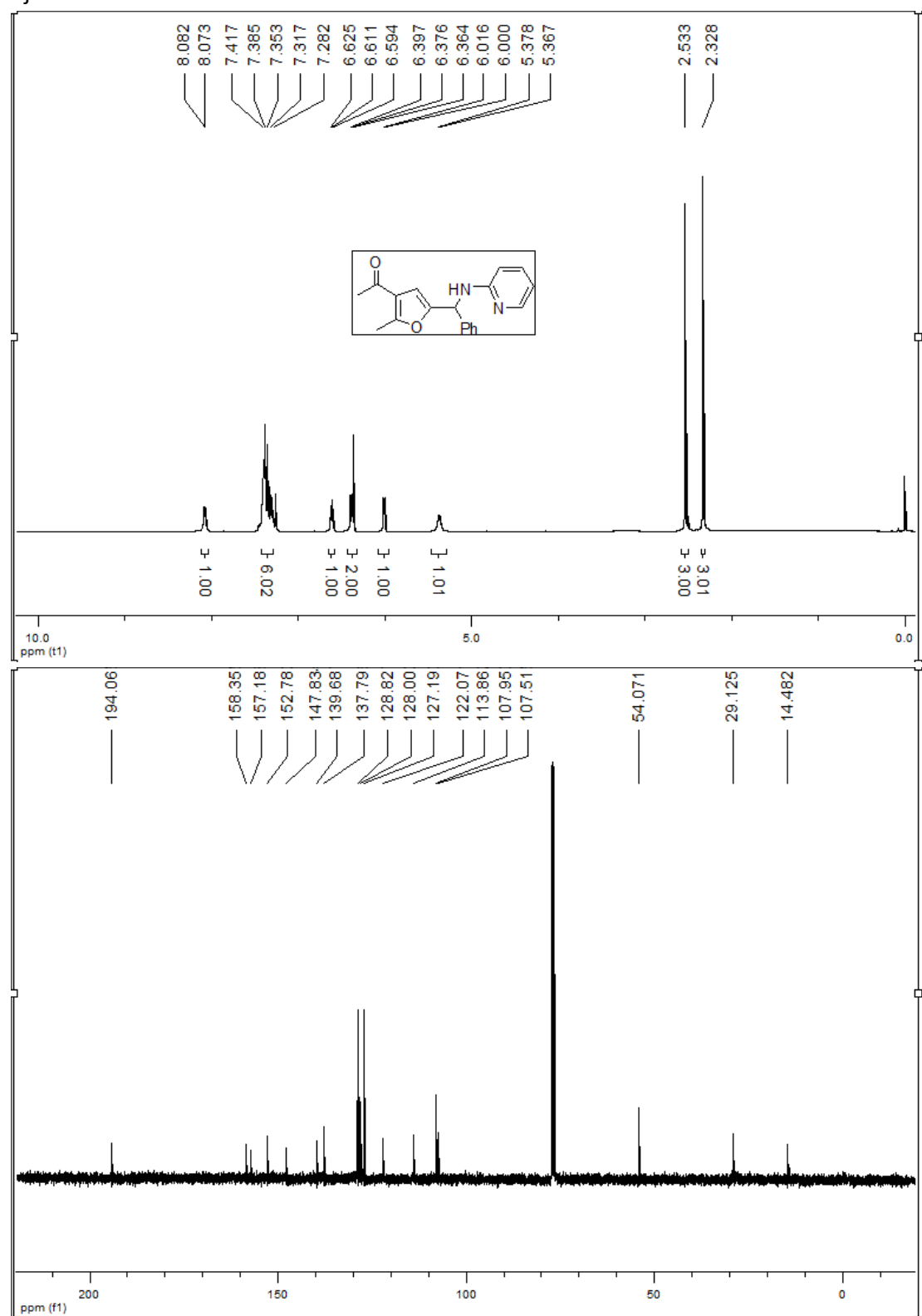
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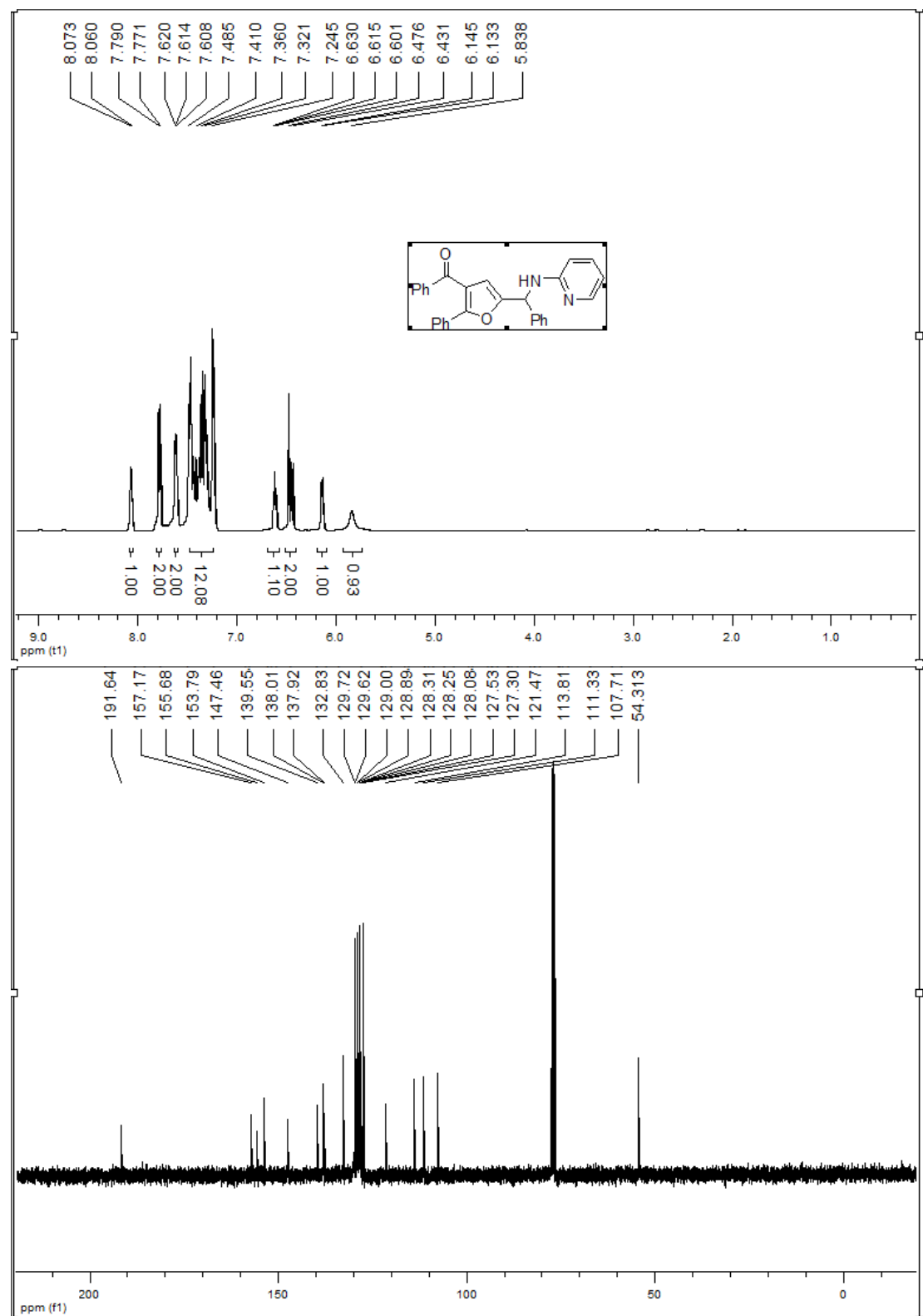
5i

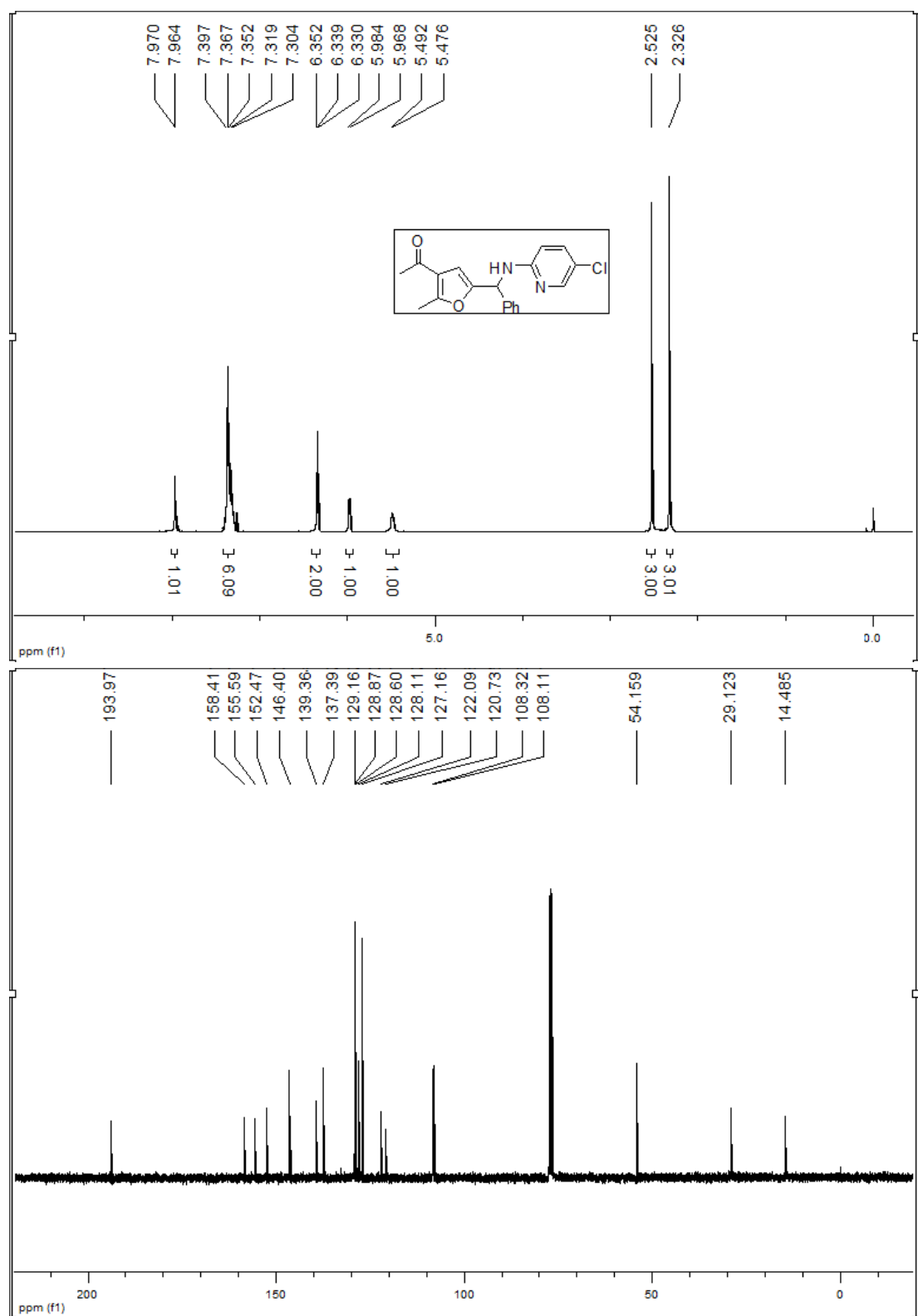


5j

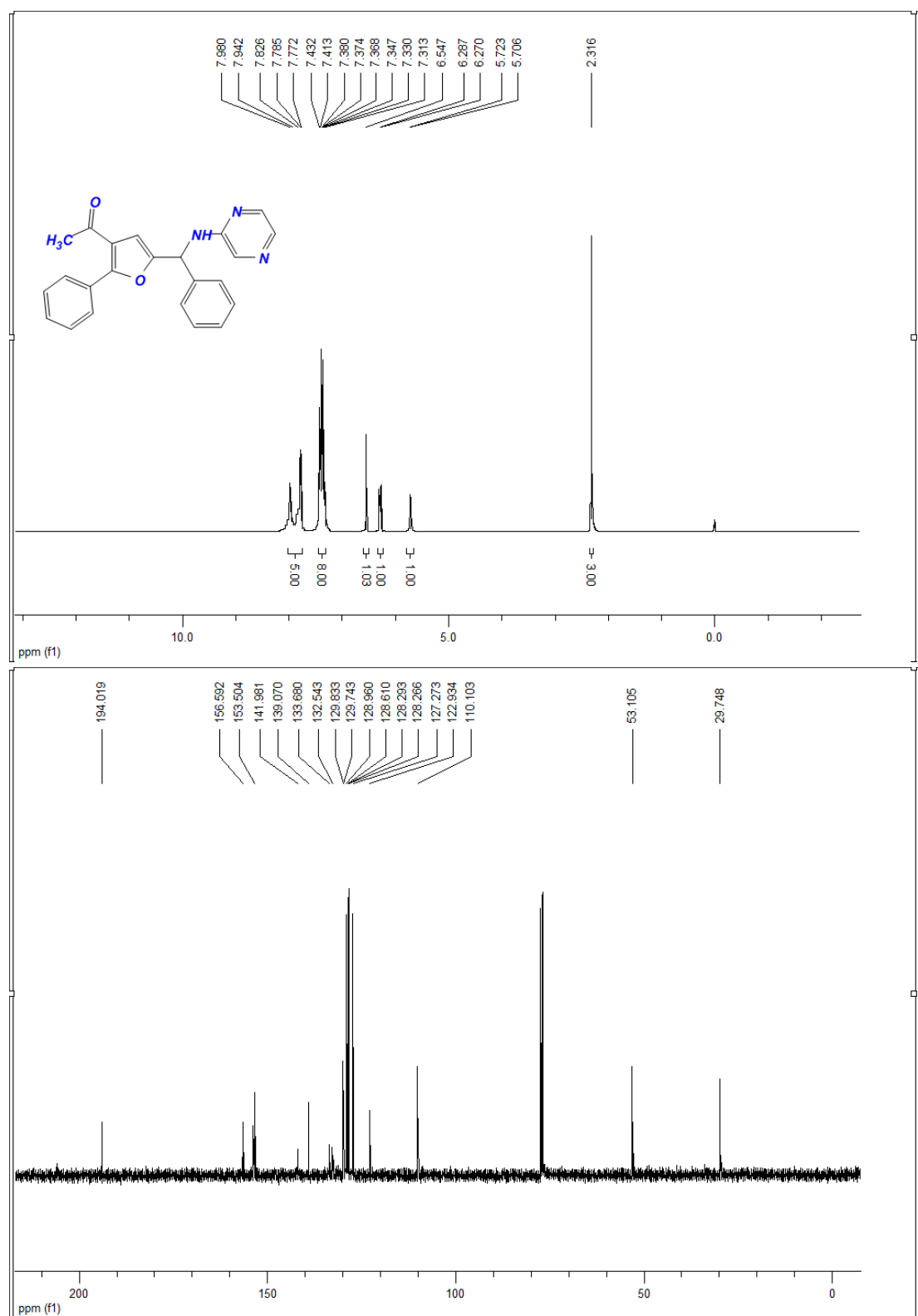


5k





6a



The figure displays the chemical structure of 2-(2-(2-phenyl-2H-pyridin-5-yl)-5-methyl-1,3-benzoxazol-4-yl)benzoic acid and its corresponding ¹H and ¹³C NMR spectra.

Chemical Structure: Cc1cc2c(c1C(=O)c3ccccc3)oc(Cc4ccccc4Nc5ccncc5)c2

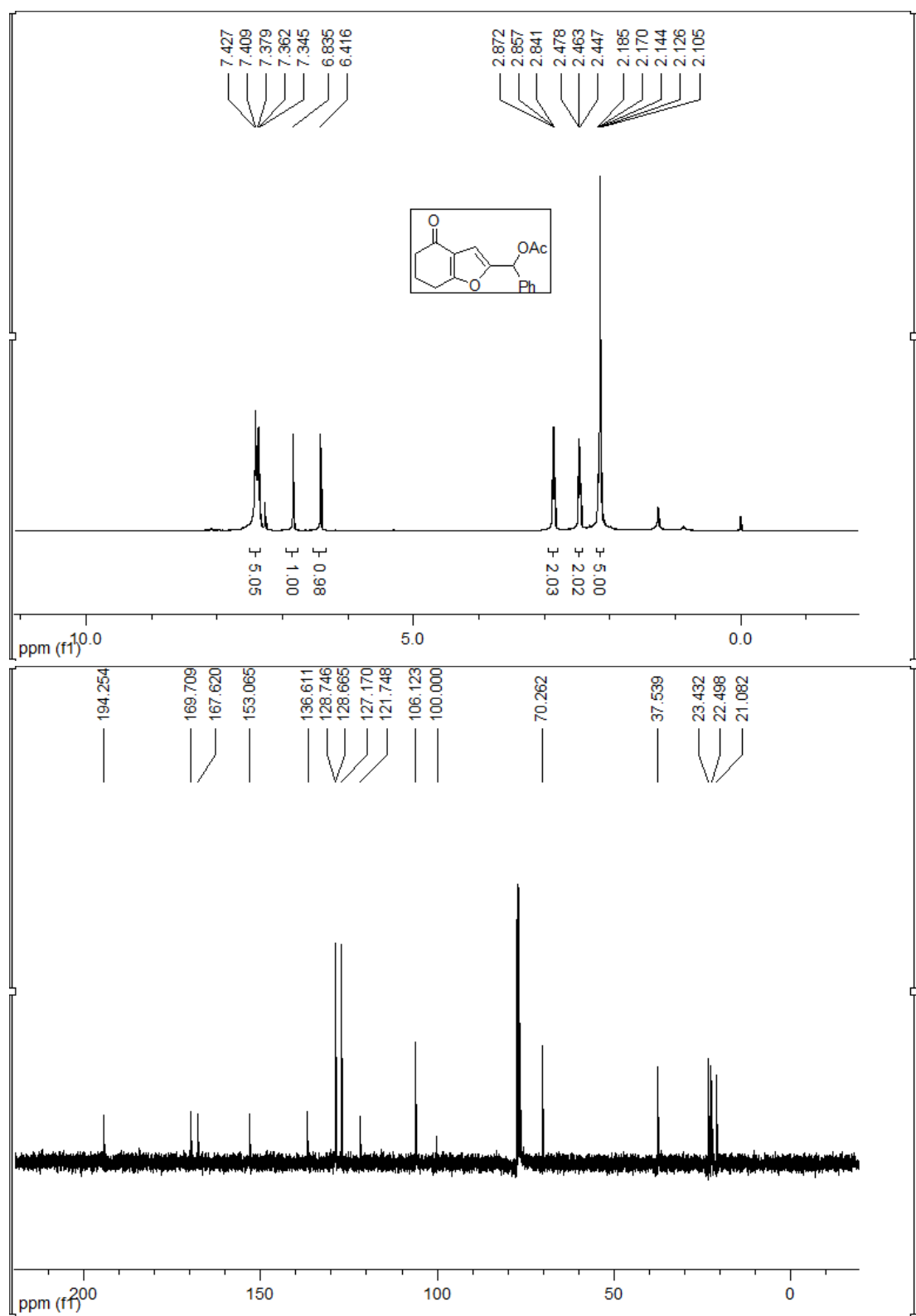
¹H NMR Spectrum (ppm):

- 7.969, 7.946, 7.812, 7.727, 7.708, 7.529, 7.510, 7.492, 7.427, 7.408, 7.390, 7.358, 7.340, 7.305, 7.288, 6.369, 6.234, 6.216, 5.755, 5.737
- 2.438

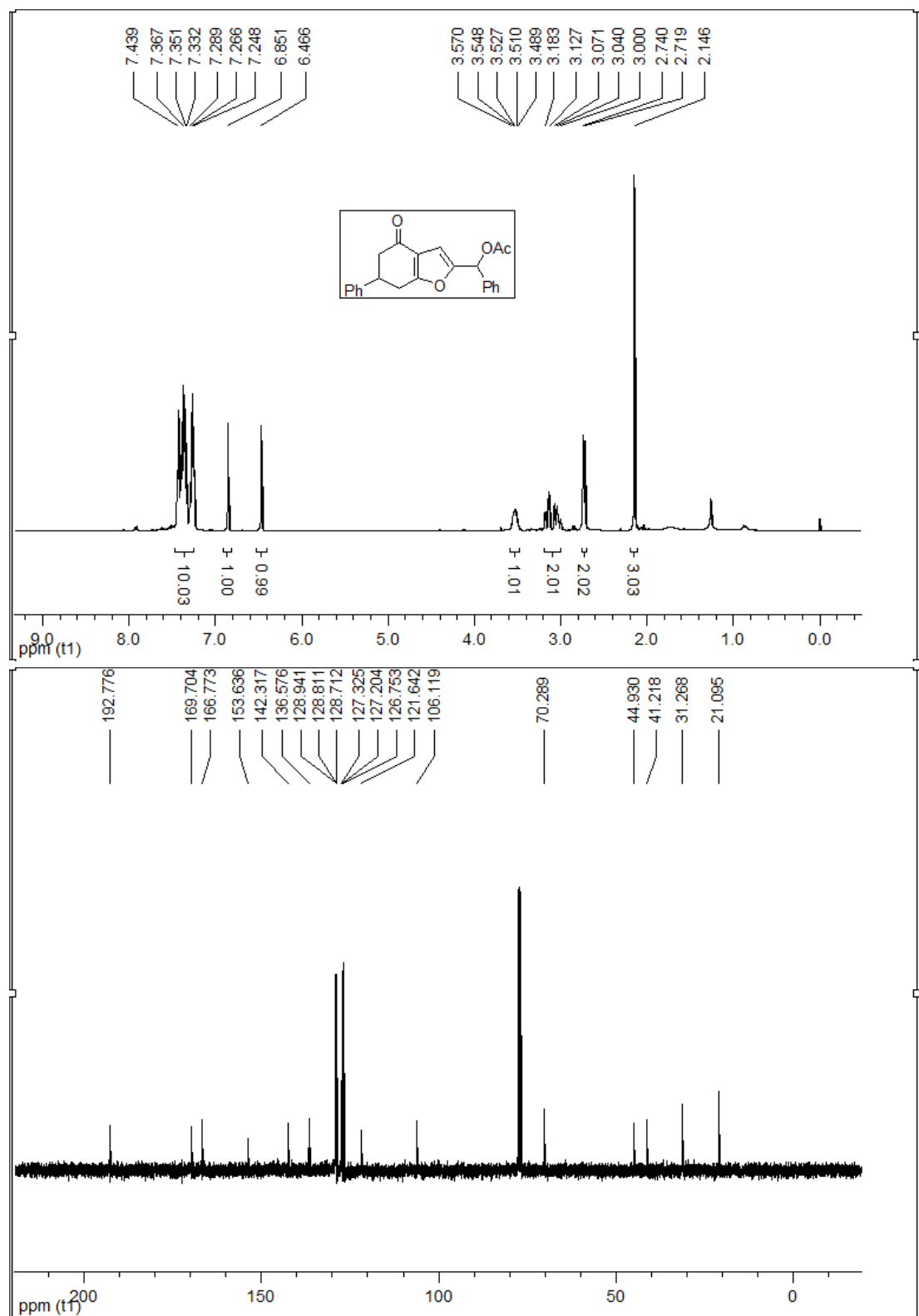
¹³C NMR Spectrum (ppm):

- 191.174
- 159.414, 153.434, 152.224, 141.931, 139.261, 138.934, 133.442, 132.604, 132.263, 128.892, 128.840, 128.390, 128.098, 127.229, 121.207, 109.494
- 52.946
- 14.353

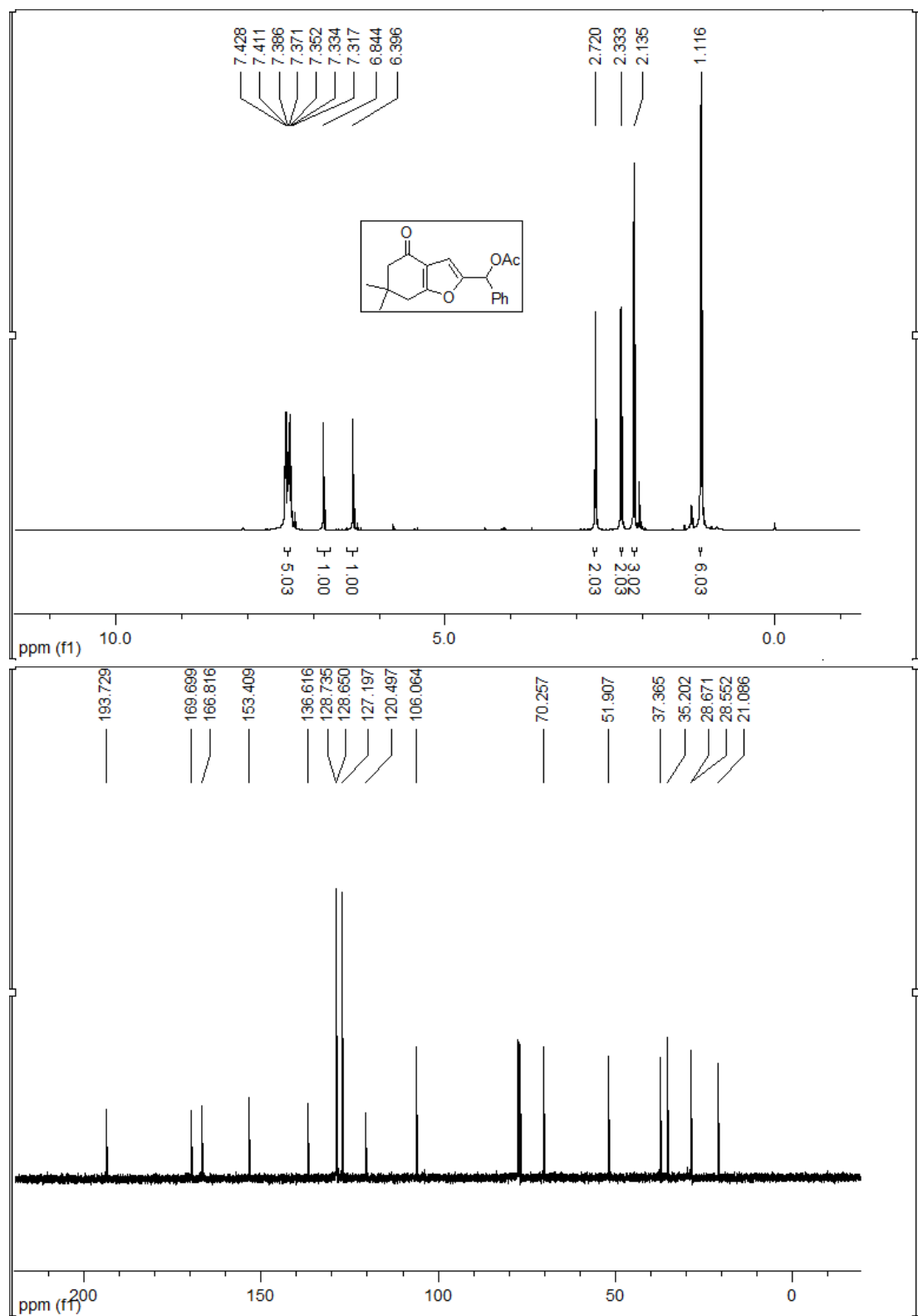
7a



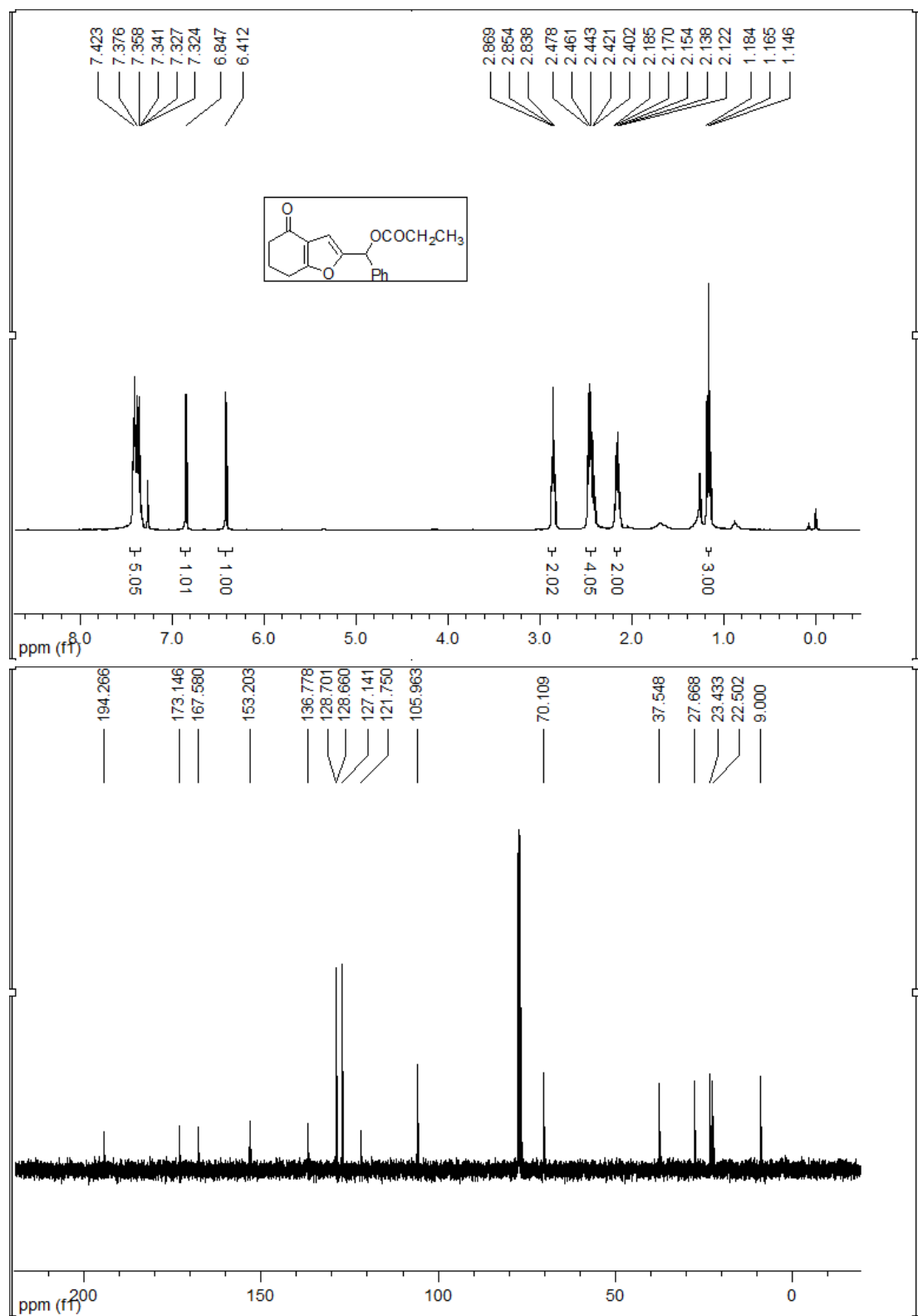
7b



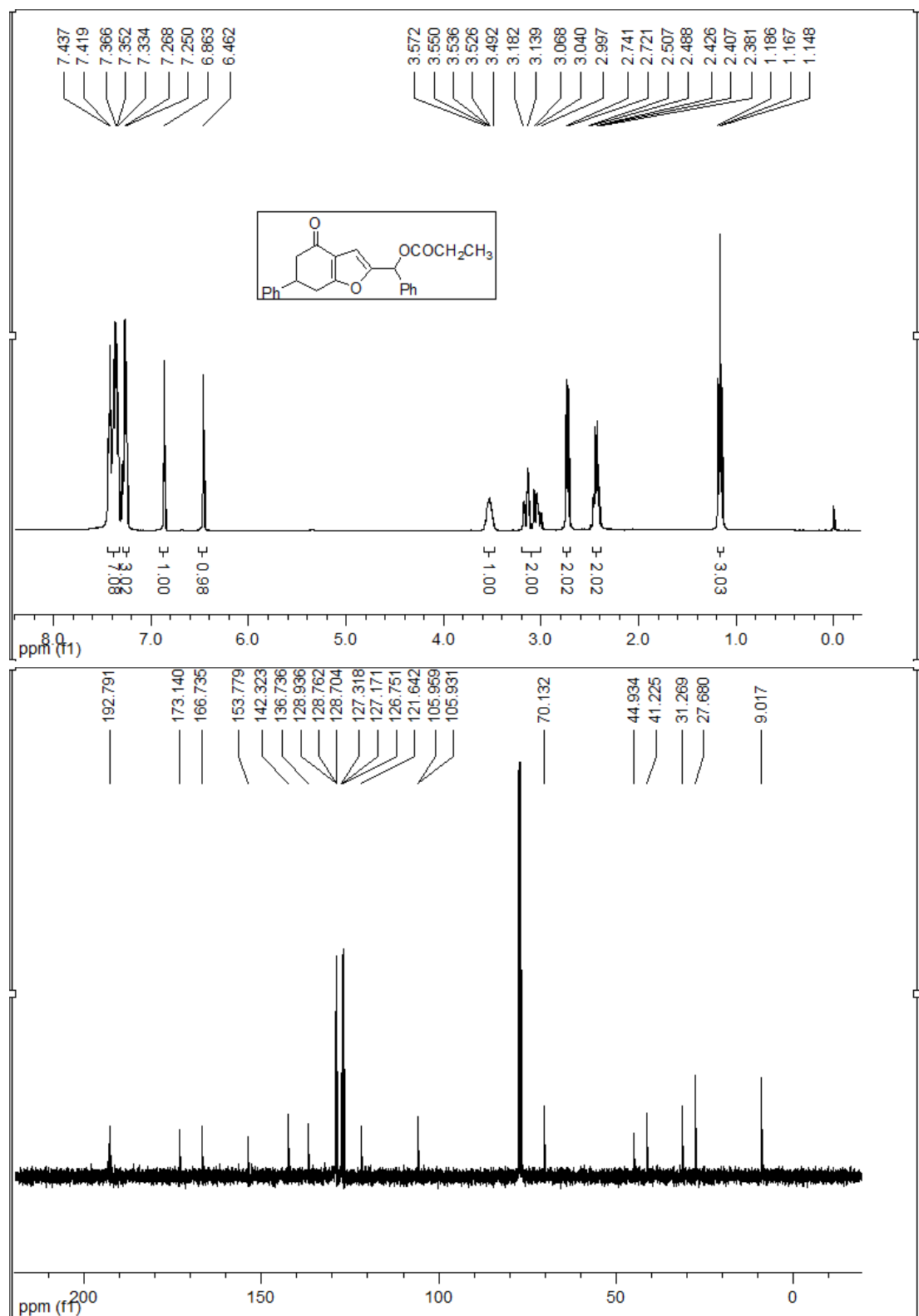
7c



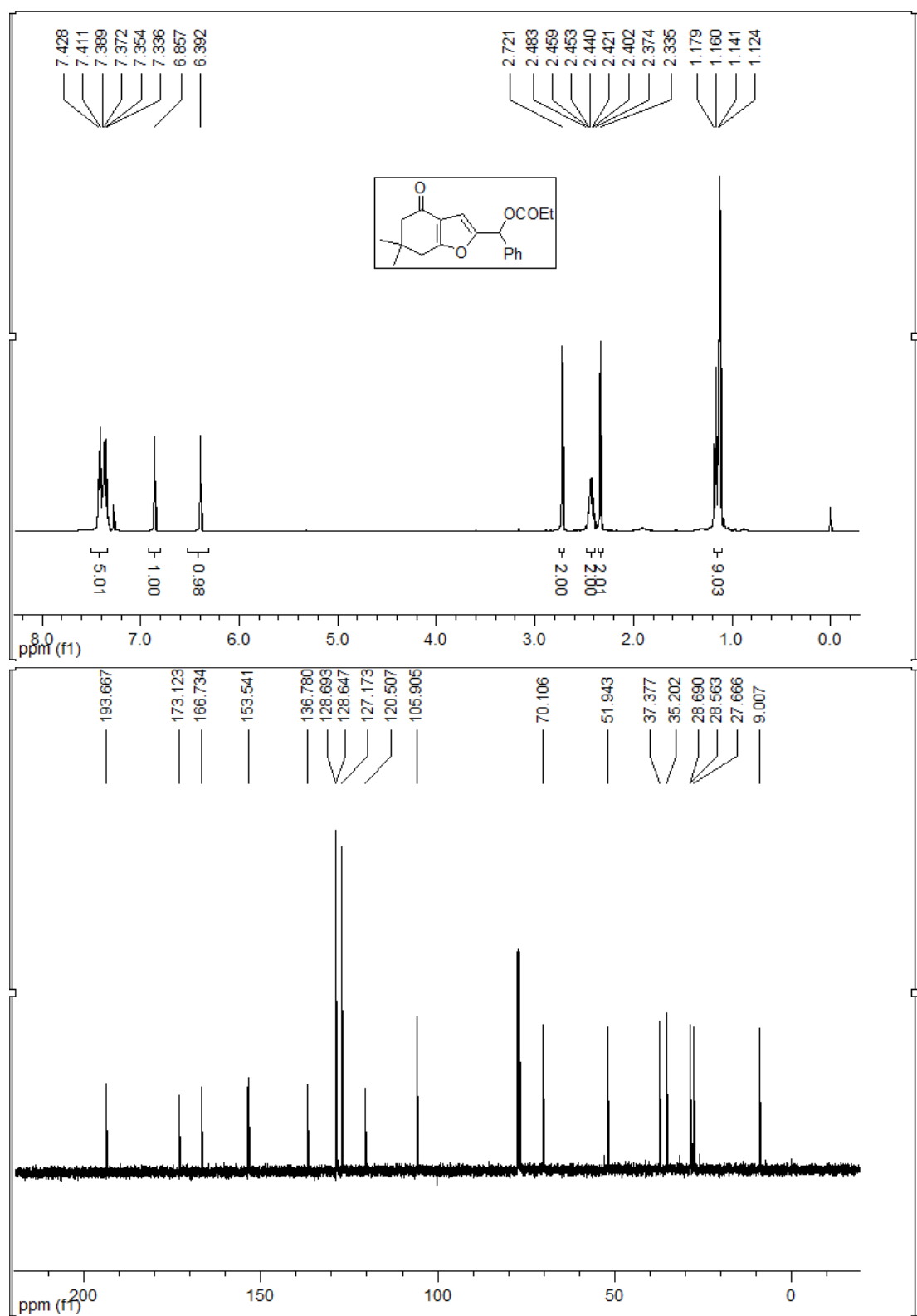
7d



7e



7f



7g

