

SUPPORTING INFORMATION

Organocatalytic domino Knöevenagel-Michael reaction in water for the regioselective synthesis of benzimidazo[1,2-*a*]pyrimidines and pyrido[2,3-*d*]pyrimidin-2-amines

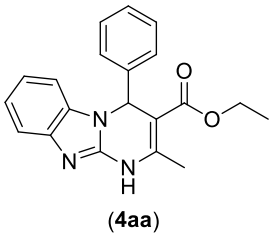
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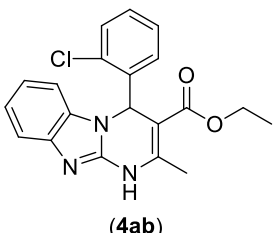
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1. Compound characterization data from (4aa-4bn) and (6aa-6bh)

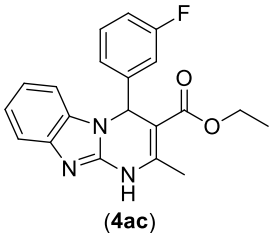
Ethyl 2-methyl-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (4aa)

 <p>(4aa)</p>	Yield, 0.303 g (91%). White solid, mp 287-288 °C. ¹ H NMR (300 MHz, DMSO- <i>d</i> ₆): δ(ppm) 1.09-1.14 (t, 3H, <i>J</i> = 7.2 Hz), 2.44 (s, 3H), 3.95-4.04 (m, 2H), 6.40 (s, 1H), 6.90-6.95 (t, 1H, <i>J</i> = 7.5 Hz), 6.99-7.04 (t, 1H, <i>J</i> = 7.5 MHz), 7.13-7.35 (m, 7H), 10.81 (s, 1H); ¹³ C (100 MHz, DMSO- <i>d</i> ₆) δ(ppm) 13.9, 18.5, 55.8, 59.3, 97.8, 109.7, 116.7, 120.1, 121.7, 127.0, 127.7, 128.3, 131.4, 141.9, 142.2, 145.5, 146.4, 165.1; IR (KBr) (ν_{\max} / cm ⁻¹) 3028, 2972, 2942, 2856, 1697, 1616, 1570, 1257; MS (ESI) <i>m/z</i> calcd for C ₂₀ H ₁₉ N ₃ O ₂ : 333.15; found 334.0 [M + H] ⁺ , 356.0 [M + Na] ⁺ ; anal. calcd for C ₂₀ H ₁₉ N ₃ O ₂ : C, 72.05; H, 5.74; N, 12.60. Found C, 72.18; H, 5.91; N, 12.42%.
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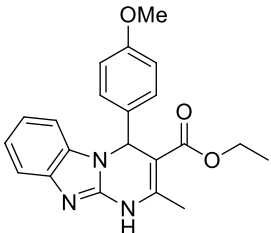
Ethyl 4-(2-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (4ab)

 <p>(4ab)</p>	Yield, 0.337 g (92%). White solid, mp 192-193 °C. ¹ H NMR (300 MHz, DMSO- <i>d</i> ₆): δ(ppm) 1.03-1.08 (t, 3H, <i>J</i> = 7.2 Hz), 2.44 (s, 3H), 3.95-3.98 (m, 2H), 6.72 (s, 1H), 6.91-6.96 (t, 1H, <i>J</i> = 7.2 Hz), 7.00-7.06 (t, 1H, <i>J</i> = 7.8 Hz), 7.16-7.44 (m, 6H), 10.93 (s, 1H); ¹³ C (100 MHz, DMSO- <i>d</i> ₆) δ(ppm) 13.9, 18.6, 53.6, 59.2, 96.2, 109.1, 116.8, 120.2, 121.8, 127.7, 129.4, 129.6, 130.5, 131.5, 138.7, 142.0, 145.1, 147.2, 164.9; IR (KBr) (ν_{\max} / cm ⁻¹) 3026, 2976, 2926, 2856, 1699, 1620, 1775, 1253; MS (ESI) <i>m/z</i> calcd for C ₂₀ H ₁₈ ClN ₃ O ₂ : 367.11; found 368.0 [M + H] ⁺ , 390.1 [M + Na] ⁺ ; anal. calcd for C ₂₀ H ₁₈ ClN ₃ O ₂ : C, 65.31; H, 4.93; N, 11.42. Found C, 65.13; H, 4.81; N, 11.58%.
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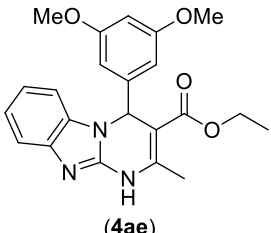
Ethyl 4-(3-fluorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4ac**)

 <p style="text-align: center;">(4ac)</p>	<p>Yield, 0.315 g (90%). White solid, mp 287-288 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.10-1.15 (t, 3H, <i>J</i> = 7.2 Hz), 2.44 (s, 3H), 3.97-4.05 (m, 2H), 6.45 (s, 1H), 6.92-7.06 (m, 3H), 7.11 (d, 1H, <i>J</i> = 7.8 Hz), 7.22-7.35 (m, 4H), 10.89 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 13.9, 18.6, 55.2, 59.3, 97.2, 109.8, 116.7, 120.2, 121.8, 122.9, 130.4, 130.5, 131.3, 142.1, 144.6, 144.7, 145.3, 146.9, 163.0, 165.0; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3051, 2976, 2927, 2862, 1697, 1616, 1571, 1259; MS (ESI) <i>m/z</i> calcd for C₂₀H₁₈FN₃O₂: 351.14; found 352.1 [M + H]⁺; anal. calcd for C₂₀H₁₈FN₃O₂: C, 68.36; H, 5.16; N, 11.96. Found C, 68.19; H, 5.28; N, 12.09%.</p>
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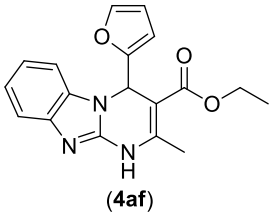
Ethyl 4-(4-methoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4ad**)

 <p style="text-align: center;">(4ad)</p>	<p>Yield, 0.319 g (88%). White solid, mp 273-274 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.11-1.15 (t, 3H, <i>J</i> = 7.2 Hz), 2.43 (s, 3H), 3.64 (s, 3H), 3.97-4.00 (m, 2H), 6.36 (s, 1H), 6.77 (d, 2H, <i>J</i> = 8.7 Hz), 6.92-6.95 (m, 1H), 6.99-7.01 (m, 1H), 7.22-7.33 (m, 4H), 10.76 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.0, 18.5, 54.8, 55.2, 59.2, 98.0, 109.8, 113.5, 116.6, 120.0, 121.6, 128.2, 131.4, 134.1, 142.2, 145.5, 146.0, 158.5, 165.1; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3049, 2977, 2926, 2856, 1694, 1613, 1570, 1253; MS (ESI) <i>m/z</i> calcd for C₂₁H₂₁N₃O₃: 363.16; found 364.1 [M + H]⁺, 386.0 [M + Na]⁺; anal. calcd for C₂₁H₂₁N₃O₃: C, 69.41; H, 5.82; N, 11.56. Found C, 69.22; H, 5.99; N, 11.67%.</p>
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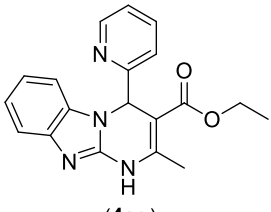
Ethyl 4-(3,5-dimethoxyphenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4ae**)

 <p style="text-align: center;">(4ae)</p>	<p>Yield, 0.334 g (85%). White Solid, mp > 300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.14-1.18 (t, 3H, <i>J</i> = 6.9 Hz), 2.42 (s, 3H), 3.64 (s, 6H), 3.99-4.05 (m, 2H), 6.32-6.34 (m, 2H), 6.43-6.44 (m, 2H), 6.93-7.06 (m, 2H), 7.30-7.34 (m, 2H), 10.79 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.0, 18.5, 55.0, 55.6, 59.3, 97.6, 98.5, 105.3, 109.9, 116.7, 120.1, 121.7, 131.5, 142.2, 144.2, 145.5, 146.5, 160.2, 165.1; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3047, 2971, 2922, 2846, 1695, 1600, 1581, 1246; MS (ESI) <i>m/z</i> calcd for C₂₂H₂₃N₃O₄: 393.17; found 394.0 [M + H]⁺, 416.1 [M + Na]⁺; anal. calcd for C₂₂H₂₃N₃O₄: C, 67.16; H, 5.89; N, 10.68. Found C, 67.30; H, 5.78; N, 10.55%.</p>
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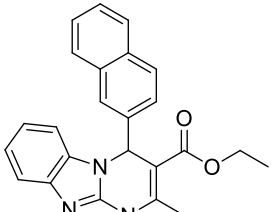
Ethyl 4-(furan-2-yl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4af**)

 <p style="text-align: center;">(4af)</p>	<p>Yield, 0.258 g (80%). Yellow solid, mp > 300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.11-1.16 (t, 3H, <i>J</i> = 6.9 Hz), 2.44 (s, 3H), 4.01-4.08 (m, 2H), 6.30 (d, 1H, <i>J</i> = 2.1 Hz), 6.44 (d, 1H, <i>J</i> = 3.0 Hz), 6.55 (s, 1H), 7.01-7.09 (m, 2H), 7.33-7.35 (m, 1H), 7.40-7.43 (m, 2H), 10.84 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.0, 18.6, 49.0, 59.3, 94.2, 107.7, 109.7, 110.3, 116.7, 120.2, 121.8, 131.4, 142.0, 142.5, 145.5, 147.7, 152.6, 165.0; IR (KBr) (ν_{\max}/cm⁻¹) 3044, 2973, 2921, 2845, 1693, 1605, 1571, 1241; MS (ESI) <i>m/z</i> calcd for C₁₈H₁₇N₃O₃: 323.13; found 324.0 [M + H]⁺, 346.1 [M + Na]⁺; anal. calcd for C₁₈H₁₇N₃O₃: C, 66.86; H, 5.30; N, 13.00. Found C, 67.05; H, 5.19; N, 12.84%</p>
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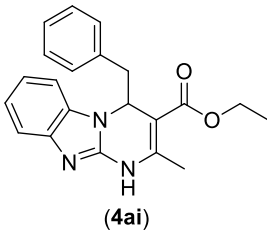
Ethyl 2-methyl-4-(pyridin-2-yl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4ag**)

 <p style="text-align: center;">(4ag)</p>	<p>Yield, 0.310 g (93%). White solid, mp > 300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm): 1.07-1.12 (t, 3H, <i>J</i> = 7.2 Hz), 2.42 (s, 3H), 3.96-4.01 (m, 2H), 6.49 (s, 1H), 6.88-6.93 (m, 1H), 6.98-7.03 (m, 1H), 7.14-7.18 (m, 1H), 7.25-7.32 (m, 2H), 7.62-7.64 (m, 1H), 7.70-7.75 (m, 1H), 8.34-8.35 (m, 1H), 10.77 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.0, 18.7, 57.0, 59.2, 96.0, 109.5, 116.6, 120.0, 121.6, 122.4, 122.9, 131.6, 136.3, 142.1, 145.9, 147.6, 149.4, 159.2, 165.1; IR (KBr) (ν_{\max}/cm⁻¹) 3035, 2974, 2918, 2850, 1695, 1612, 1569, 1251; MS (ESI) <i>m/z</i> calcd for C₁₉H₁₈N₄O₂: 334.14; found 335.0 [M + H]⁺, 357.1 [M + Na]⁺; anal. calcd for C₁₉H₁₈N₄O₂: C, 68.25; H, 5.43; N, 16.76. Found C, 68.38; H, 5.62; N, 16.59%</p>
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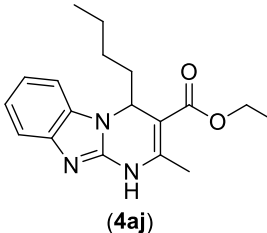
Ethyl 2-methyl-4-(naphthalen-2-yl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4ah**)

 <p style="text-align: center;">(4ah)</p>	<p>Yield, 0.306 g (80%). White solid, mp 148-149 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.08-1.13 (t, 3H, <i>J</i> = 6.9 Hz), 2.47 (s, 3H), 3.95-3.98 (m, 2H), 6.58 (s, 1H), 6.88 (m, 1H), 6.99 (m, 1H), 7.25-7.37 (m, 3H), 7.44-7.49 (m, 2H), 7.76-7.80 (m, 2H), 7.88-7.90 (m, 1H), 7.99 (s, 1H), 10.87 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.0, 18.6, 56.1, 59.3, 97.5, 109.7, 116.7, 120.1, 121.7, 124.6, 126.2, 126.3, 127.4, 127.8, 128.3, 131.5, 132.3, 139.0, 142.2, 145.4, 146.5, 165.1; IR (KBr) (ν_{\max}/cm⁻¹) 3036, 2972, 2920, 2851, 1693, 1615, 1566, 1253; MS (ESI) <i>m/z</i> calcd for C₂₄H₂₁N₃O₂: 383.16; found 383.9 [M + H]⁺, 405.9 [M + Na]⁺; anal. calcd for C₂₄H₂₁N₃O₂: C, 75.18; H, 5.52; N, 10.96. Found C, 75.31; H, 5.36; N, 11.13%.</p>
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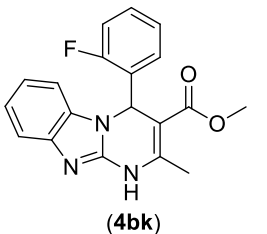
Ethyl 4-benzyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4ai**)

 <p style="text-align: center;">(4ai)</p>	<p>Yield, 0.277 g (80%). White solid, mp 129-130 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm): 1.26-1.31 (t, 3H, <i>J</i> = 6.9 Hz), 2.14 (s, 3H), 2.84-2.90 (m, 1H), 3.19-3.25 (m, 1H), 4.14-4.23 (m, 2H), 5.78 (m, 1H), 6.38 (d, 2H, <i>J</i> = 7.2 Hz), 7.01-7.14 (m, 5H), 7.35 (d, 1H, <i>J</i> = 7.2 Hz), 7.45 (d, 1H, <i>J</i> = 7.2 Hz), 10.00 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.3, 18.3, 38.3, 52.8, 59.3, 93.9, 109.4, 116.9, 120.1, 121.6, 124.4, 126.4, 127.5, 129.3, 131.3, 135.8, 142.1, 146.2, 148.3, 165.3; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3057, 2974, 2926, 2858, 1697, 1620, 1570, 1263; MS (ESI) <i>m/z</i> calcd for C₂₁H₂₁N₃O₂: 347.16; found 348.0 [M + H]⁺, 370.1 [M + Na]⁺; anal. calcd for C₂₁H₂₁N₃O₂: C, 72.60; H, 6.09; N, 12.10. Found C, 72.74; H, 6.21; N, 11.97%.</p>
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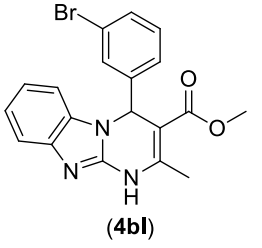
Ethyl 4-butyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4aj**)

 <p style="text-align: center;">(4aj)</p>	<p>Yield, 0.234 g (75%). White solid, mp 196-197 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 0.63-0.68 (m, 4H), 0.81-0.86 (m, 2H), 1.21-1.26 (m, 4H), 1.45 (m, 1H), 2.15-2.19 (m, 1H), 2.37 (s, 3H), 4.11-4.18 (m, 2H), 5.57 (m, 1H), 6.81-6.84 (m, 1H), 7.05-7.09 (m, 3H), 10.47 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 13.7, 14.2, 18.6, 21.8, 24.8, 33.3, 51.5, 59.3, 95.6, 109.2, 116.8, 120.1, 121.5, 131.3, 142.4, 146.8, 148.0, 165.4; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3055, 2973, 2921, 2853, 1696, 1623, 1572, 1265; MS (ESI) <i>m/z</i> calcd for C₁₈H₂₃N₃O₂: 313.18; found 313.9 [M + H]⁺, 335.9 [M + Na]⁺; anal. Calcd for C₁₈H₂₃N₃O₂: C, 68.98; H, 7.40; N, 13.41. Found C, 68.86; H, 7.56; N, 13.59%.</p>
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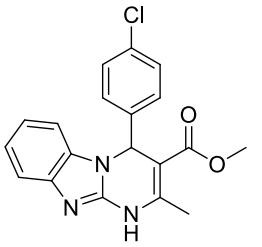
Methyl 4-(2-fluorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4bk**)

 <p style="text-align: center;">(4bk)</p>	<p>Yield, 0.293 g (87%). White solid, mp 254-255 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm): 2.44 (s, 3H), 3.52 (s, 3H), 6.62 (s, 1H), 6.94-7.13 (m, 5H), 7.21-7.28 (m, 1H), 7.32-7.34 (m, 1H), 7.41-7.46 (m, 1H), 10.98 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 18.6, 50.5, 50.7, 95.7, 108.8, 116.8, 120.3, 121.8, 124.6, 128.1, 128.3, 129.8, 129.9, 130.0, 131.3, 142.0, 145.3, 147.4, 158.1, 160.6, 165.4; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3053, 2924, 2852, 1710, 1622, 1577, 1255; MS (ESI) <i>m/z</i> calcd for C₁₉H₁₆FN₃O₂: 337.12; found 338.1 [M + H]⁺; anal. Calcd for C₁₉H₁₆FN₃O₂: C, 67.65; H, 4.78; N, 12.46. Found C, 67.83; H, 4.61; N, 12.58%.</p>
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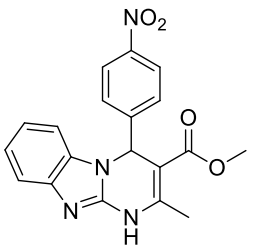
Methyl 4-(3-bromophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4bl**)

 <p style="text-align: center;">(4bl)</p>	<p>Yield, 0.317 g (80%). Yellow solid mp 258-259 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 2.44 (s, 3H), 3.56 (s, 3H), 6.45 (s, 1H), 6.96-7.06 (m, 2H), 7.19-7.24 (m, 1H), 7.28-7.39 (m, 4H), 7.53 (s, 1H), 10.93 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 18.7, 50.8, 55.0, 97.2, 109.8, 116.8, 120.3, 121.5, 121.9, 125.9, 129.5, 130.7, 131.2, 142.1, 144.5, 145.3, 147.1, 165.5; IR (KBr) (ν_{\max}/ cm⁻¹) 3055, 2941, 2839, 1678, 1618, 1570, 1263; MS (ESI) <i>m/z</i> calcd for C₁₉H₁₆BrN₃O₂: 397.04; found 398.0 [M + H]⁺, 420.0 [M + Na]⁺; anal. calcd for C₁₉H₁₆BrN₃O₂: C, 57.30; H, 4.05; N, 10.55. Found C, 57.47; H, 4.18; N, 10.62.</p>
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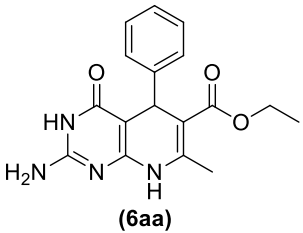
Methyl 4-(4-chlorophenyl)-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4bm**)

 <p style="text-align: center;">(4bm)</p>	<p>Yield, 0.285 g (81%). White solid mp 267-268 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 2.43 (s, 3H), 3.55 (s, 3H), 6.45 (s, 1H), 6.91-7.10 (m, 2H), 7.23-7.37 (m, 6H), 10.90 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 18.6, 50.8, 55.0, 97.3, 109.7, 116.8, 120.2, 121.8, 128.4, 128.8, 131.0, 131.3, 132.2, 140.9, 142.1, 145.3, 146.9, 165.5; IR (KBr) (ν_{\max}/ cm⁻¹) 3051, 2934, 2837, 1671, 1619, 1571, 1267; MS (ESI) <i>m/z</i> calcd for C₁₉H₁₆ClN₃O₂: 353.09; found 353.9 [M + H]⁺, 375.9 [M + Na]⁺; anal. calcd for C₁₉H₁₆ClN₃O₂: C, 64.50; H, 4.56; N, 11.88. Found C, 64.38; H, 4.41; N, 12.06%.</p>
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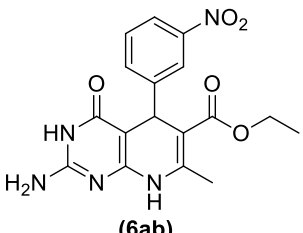
Methyl 2-methyl-4-(4-nitrophenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**4bn**)

 <p style="text-align: center;">(4bn)</p>	<p>Yield, 0.309 g (85%). Yellow solid mp 276-278 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 2.45 (s, 3H), 3.56 (s, 3H), 6.60 (m, 1H), 6.94-7.06 (m, 2H), 7.23 (d, 1H, <i>J</i> = 7.8 Hz), 7.33 (d, 1H, <i>J</i> = 7.8 Hz), 7.60 (d, 2H, <i>J</i> = 8.4 Hz), 8.10 (d, 2H, <i>J</i> = 8.4 Hz), 11.01 (s, 1H); ¹³C (75 MHz, DMSO-<i>d</i>₆): δ(ppm) 18.7, 50.8, 55.0, 96.6, 109.6, 116.9, 120.4, 122.0, 123.7, 128.3, 131.2, 142.1, 145.1, 146.8, 147.5, 148.8, 165.4; IR (KBr) (ν_{\max}/ cm⁻¹) 3053, 2938, 2835, 1670, 1615, 1565, 1259; MS (ESI) <i>m/z</i> calcd for C₁₉H₁₆N₄O₄: 364.12; found 364.9 [M + H]⁺, 386.9 [M + Na]⁺; anal. calcd for C₁₉H₁₆N₄O₄: C, 62.63; H, 4.43; N, 15.38. Found C, 62.80; H, 4.54; N, 15.55%.</p>
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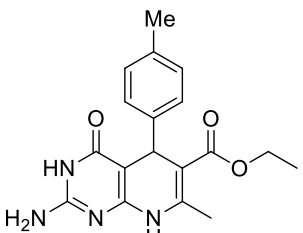
Ethyl 2-amino-7-methyl-4-oxo-5-phenyl-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6aa**)

 <p style="text-align: center;">(6aa)</p>	<p>Yield, 0.267 g (82%). White solid mp >300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.05-1.10 (t, 3H, <i>J</i> = 6.9 Hz), 2.28 (s, 3H), 3.88-3.95 (m, 2H), 4.82 (s, 1H), 6.37 (s, 2H), 7.02-7.08 (m, 1H), 7.15-7.16 (m, 4H), 9.05 (s, 1H), 10.60 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.0, 18.3, 58.7, 90.9, 101.1, 125.5, 127.1, 127.6, 147.0, 148.0, 153.9, 161.5, 166.8; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3334, 3231, 3115, 2980, 2926, 1649, 1602, 1560, 1282; MS (ESI) <i>m/z</i> calcd for C₁₇H₁₈N₄O₃: 326.14; found 327.0 [M + H]⁺, 349.1 [M + Na]⁺; anal. calcd for C₁₇H₁₈N₄O₃: C, 62.57; H, 5.56; N, 17.17. Found C, 62.76; H, 5.71; N, 17.01%.</p>
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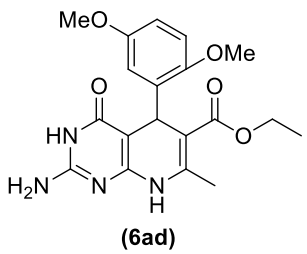
Ethyl 2-amino-7-methyl-5-(3-nitrophenyl)-4-oxo-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6ab**)

 <p style="text-align: center;">(6ab)</p>	<p>Yield 0.326 g (88%). Yellow solid mp >300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.04-1.08 (t, 3H, <i>J</i> = 7.2 Hz), 2.31 (s, 3H), 3.87-3.94 (m, 2H), 4.93 (s, 1H), 6.56 (s, 2H), 7.47-7.52 (m, 1H), 7.59 (d, 1H, <i>J</i> = 7.5 Hz), 7.95-7.99 (m, 2H), 9.22 (s, 1H), 10.87 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 13.9, 18.4, 58.9, 90.0, 99.9, 120.7, 121.7, 129.3, 134.1, 147.2, 148.3, 150.2, 153.9, 154.6, 161.8, 166.4; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3321, 3235, 3112, 2985, 2923, 1644, 1631, 1564, 1280; MS (ESI) <i>m/z</i> calcd for C₁₇H₁₇N₅O₅: 371.12; found 371.9 [M + H]⁺, 393.9 [M + Na]⁺; anal. calcd for C₁₇H₁₇N₅O₅: C, 54.98; H, 4.61; N, 18.86. Found C, 55.09; H, 4.74; N, 18.52%.</p>
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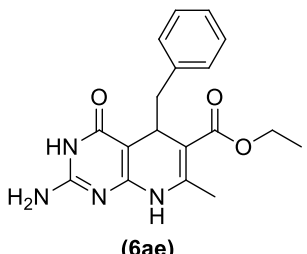
Ethyl 2-amino-7-methyl-4-oxo-5-(*p*-tolyl)-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6ac**)

 <p style="text-align: center;">(6ac)</p>	<p>Yield 0.275 g (81%). White solid mp >300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.07-1.11 (t, 3H, <i>J</i> = 7.2 Hz), 2.17 (s, 3H), 2.26 (s, 3H), 3.87-3.97 (m, 2H), 4.78 (s, 1H), 6.46 (s, 2H), 6.93 (d, 2H, <i>J</i> = 7.8 Hz), 7.02 (d, 2H, <i>J</i> = 7.02), 8.99 (s, 1H), 10.79 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆): δ(ppm) 14.1, 18.3, 20.5, 58.7, 91.0, 101.1, 127.0, 128.1, 134.3, 145.2, 146.9, 153.8, 154.2, 161.7, 166.8; IR (KBr) (<i>v</i>_{max}/ cm⁻¹) 3302, 3119, 3103, 2981, 2922, 1660, 1622, 1597, 1284; MS (ESI) <i>m/z</i> calcd for C₁₈H₂₀N₄O₃: 340.15; found 341.0 [M + H]⁺; anal. calcd for C₁₈H₂₀N₄O₃: C, 63.52; H, 5.92; N, 16.46. Found C, 63.39; H, 6.07; N, 16.28%.</p>
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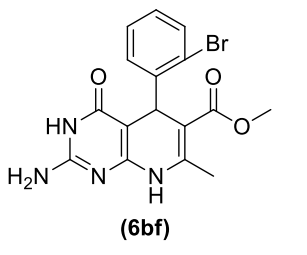
Ethyl 2-amino-5-(2,5-dimethoxyphenyl)-7-methyl-4-oxo-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6ad**)

 <p style="text-align: center;">(6ad)</p>	<p>Yield 0.294 g (80%). White solid mp 175-176 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.06-1.11 (t, 3H, <i>J</i> = 7.2 Hz), 2.17 (s, 3H), 3.59 (s, 3H), 3.60 (s, 3H), 3.85-3.89 (m, 2H), 4.95 (s, 1H), 6.56 (s, 2H), 6.58-6.62 (m, 2H), 6.72-6.75 (m, 1H), 8.89 (s, 1H), 10.96 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆) δ(ppm) 14.1, 18.2, 33.5, 55.1, 56.3, 58.6, 90.0, 100.5, 110.4, 112.6, 116.9, 137.2, 146.2, 151.6, 152.6, 154.0, 154.5, 161.4, 167.2; IR (KBr) (ν_{\max}/ cm⁻¹) 3371, 3319, 3137, 2985, 2933, 1647, 1631, 1519, 1215; MS (ESI) <i>m/z</i> calcd for C₁₉H₂₂N₄O₅: 386.16; found 387.0 [M + H]⁺; anal. calcd for C₁₉H₂₂N₄O₅: C, 59.06; H, 5.74; N, 14.50. Found C, 59.19; H, 5.92; N, 14.34%</p>
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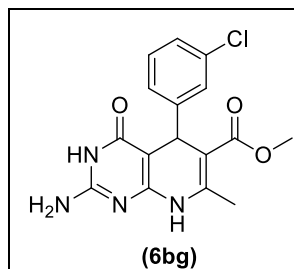
Ethyl 2-amino-5-benzyl-7-methyl-4-oxo-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6ae**)

 <p style="text-align: center;">(6ae)</p>	<p>Yield, 0.278 g (82%). White solid mp >300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 1.09-1.14 (t, 3H, <i>J</i> = 6.9 Hz), 2.02 (s, 3H), 2.54-2.55 (m, 2H), 3.82-3.97 (m, 2H), 4.07-4.10 (m, 1H), 6.60 (s, 2H), 6.77-6.80 (m, 2H), 7.07-7.10 (m, 3H); 8.36 (s, 1H), 11.21 (s, 1H); ¹³C (100 MHz, DMSO-<i>d</i>₆) δ(ppm) 14.2, 18.1, 32.5, 40.5, 58.5, 88.5, 98.5, 125.3, 127.0, 129.6, 139.0, 148.1, 154.2, 155.0, 162.0, 167.0; IR (KBr) (ν_{\max}/ cm⁻¹) 3381, 3315, 3186, 2980, 2924, 2750, 1656, 1598, 1523, 1234; MS (ESI) <i>m/z</i> calcd for C₁₈H₂₀N₄O₃: 340.15; found 341.0 [M + H]⁺, 363.1 [M + Na]⁺; anal. calcd for C₁₈H₂₀N₄O₃: C, 63.52; H, 5.92; N, 16.46. Found C, 63.34; H, 5.79; N, 16.63%.</p>
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Methyl 2-amino-5-(2-bromophenyl)-7-methyl-4-oxo-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6bf**)

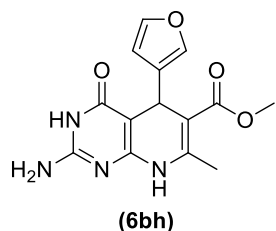
 <p style="text-align: center;">(6bf)</p>	<p>Yield, 0.323 g (83%). White solid mp > 300 °C. ¹H NMR (300 MHz, DMSO-<i>d</i>₆): δ(ppm) 2.23 (s, 3H), 3.42 (s, 3H), 5.13 (s, 1H), 6.80 (s, 2H), 6.93-6.98 (m, 1H), 7.16-7.24 (m, 2H), 7.34-7.37 (m, 1H), 9.05 (s, 1H), 11.37 (s, 1H); ¹³C (150 MHz, DMSO-<i>d</i>₆) δ(ppm) 18.3, 37.3, 50.2, 91.2, 101.0, 122.4, 127.2, 127.5, 131.1, 132.0, 147.2, 148.0, 153.8, 167.3, 175.1; IR (KBr) (ν_{\max}/ cm⁻¹) 3378, 3317, 3176, 2978, 2932, 1644, 1632, 1528, 1219; MS (ESI) <i>m/z</i> calcd for C₁₆H₁₅BrN₄O₃: 390.03; found 390.9 [M + H]⁺; 412.9 [M + Na]⁺; anal. calcd for C₁₆H₁₅BrN₄O₃: C, 49.12; H, 3.86; N, 14.32. Found C, 49.30; H, 3.71; N, 14.18%.</p>
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Methyl 2-amino-5-(3-chlorophenyl)-7-methyl-4-oxo-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6bg**)



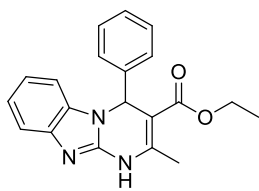
Yield 0.262 g (76%). White solid mp > 300 °C. ¹H NMR (300 MHz, DMSO-*d*₆): δ(ppm) 2.30 (s, 3H), 3.48 (s, 3H), 4.83 (s, 1H), 6.82 (s, 2H), 7.09-7.23 (m, 4H), 9.11 (s, 1H), 11.54 (s, 1H); ¹³C (150 MHz, DMSO-*d*₆): δ(ppm) 18.6, 24.9, 36.3, 50.6, 90.3, 99.8, 125.5, 125.7, 126.8, 129.7, 132.3, 148.3, 150.6, 154.0, 167.2, 175.5; IR (KBr) (ν_{max}/ cm⁻¹) 3365, 3315, 3177, 2968, 2930, 1641, 1635, 1519, 1224; MS (ESI) *m/z* calcd for C₁₆H₁₅ClN₄O₃: 346.08; found 347.0 [M + H]⁺, 369.0 [M + Na]⁺; anal. calcd for C₁₆H₁₅ClN₄O₃: C, 55.42; H, 4.36; N, 16.16. Found C, 55.54; H, 4.20; N, 16.01%.

Methyl 2-amino-5-(furan-3-yl)-7-methyl-4-oxo-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carboxylate (**6bh**)

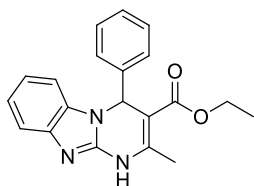
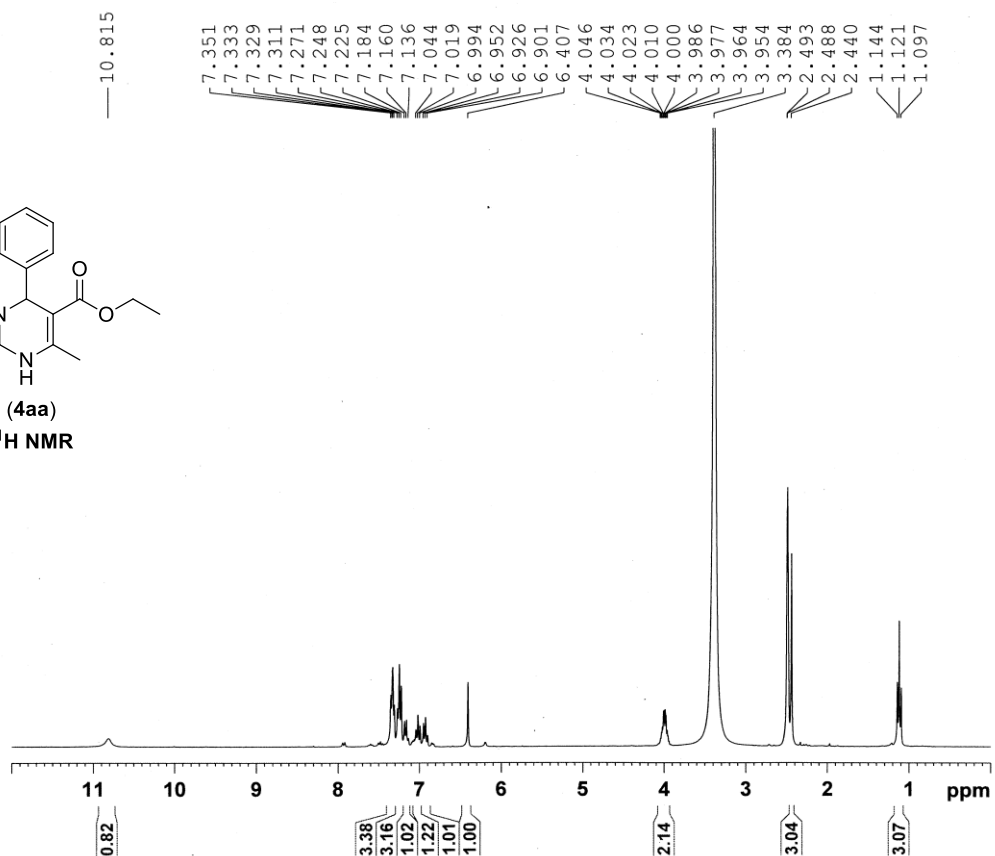


Yield 0.241g (80%). White solid mp > 300 °C. ¹H NMR (300 MHz, DMSO-*d*₆): δ(ppm) 2.24 (s, 3H), 3.55 (s, 3H), 4.77 (s, 1H), 6.18 (s, 1H), 6.63 (s, 2H), 7.10 (s, 1H), 7.39 (s, 1H), 9.03 (s, 1H), 11.23 (s, 1H); ¹³C (150 MHz, DMSO-*d*₆): δ(ppm) 18.4, 27.0, 50.6, 89.9, 99.6, 110.2, 131.1, 138.0, 142.5, 147.9, 154.2, 154.3, 161.7, 167.3; IR (KBr) (ν_{max}/ cm⁻¹) 3471, 3431, 3305, 2947, 2924, 1660, 1637, 1516, 1226; MS (ESI) *m/z* calcd for C₁₄H₁₄N₄O₄: 302.10; found 303.0 [M + H]⁺, 325.0 [M + Na]⁺; anal. calcd for C₁₄H₁₄N₄O₄: C, 55.63; H, 4.67; N, 18.53. Found C, 55.50; H, 4.51; N, 18.66%.

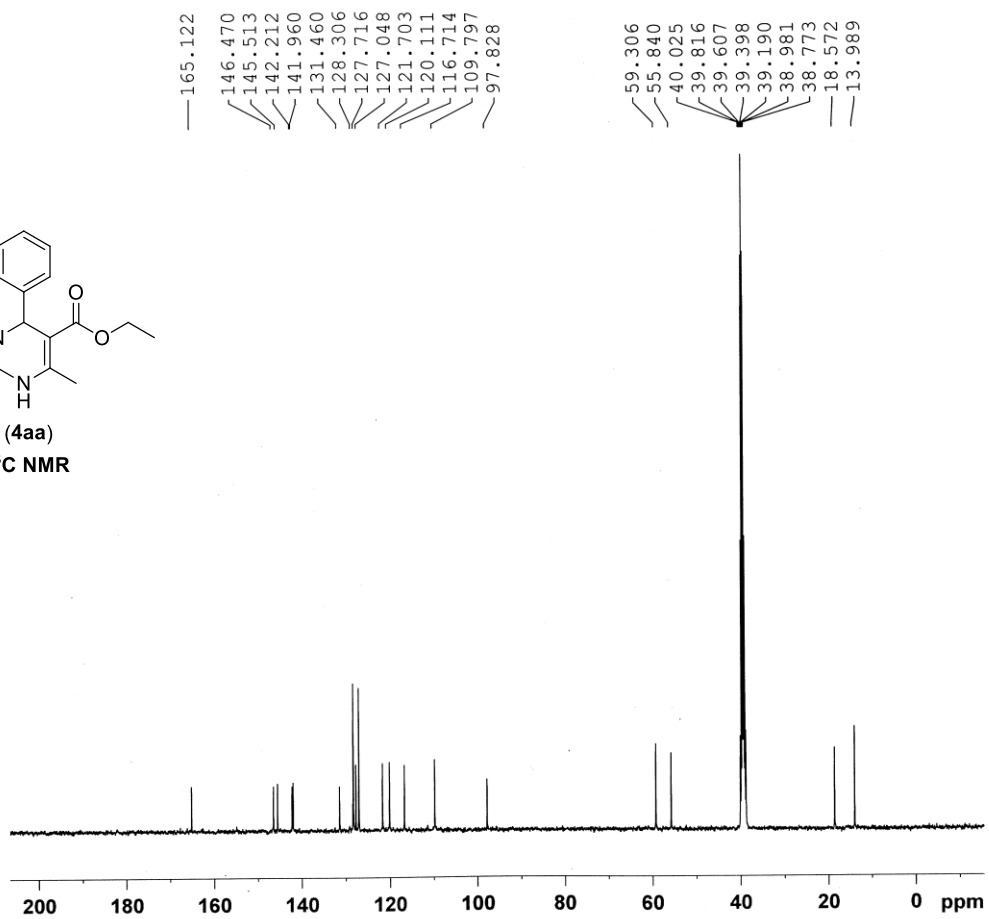
^1H and ^{13}C NMR spectra

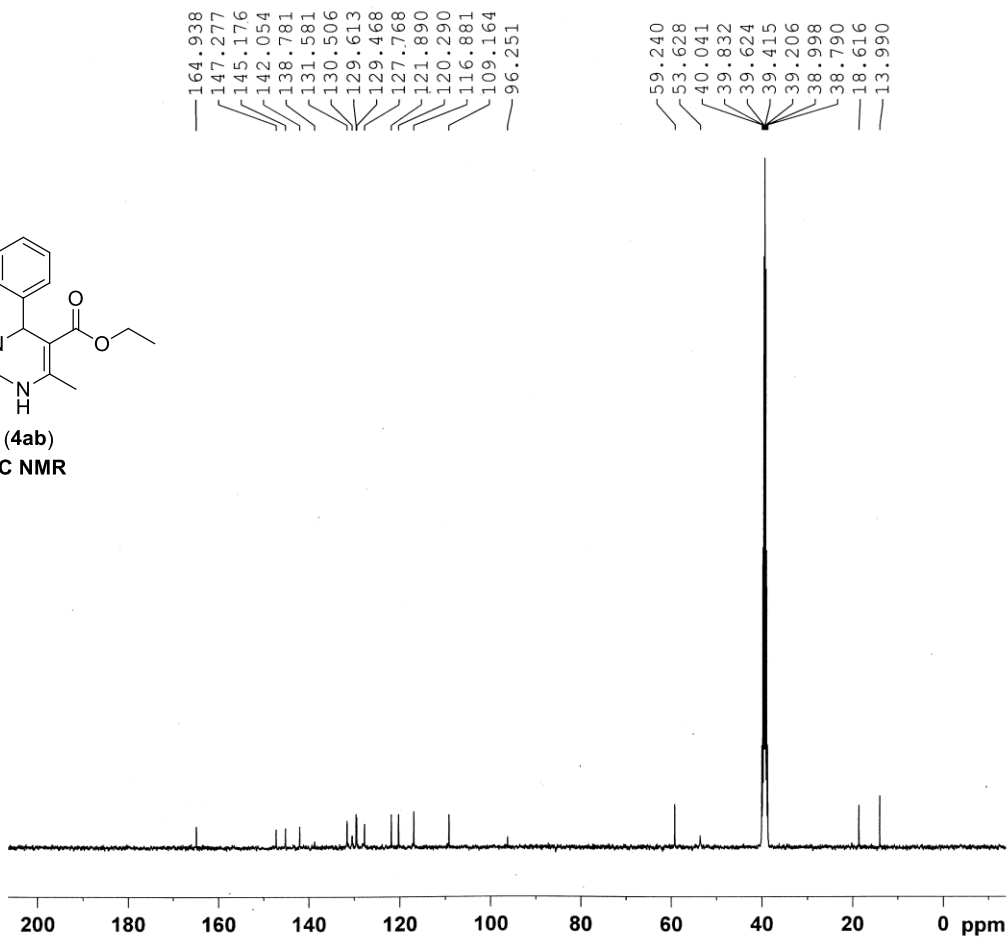
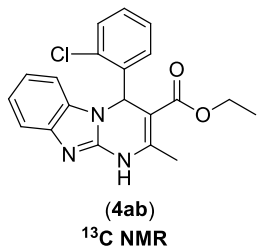
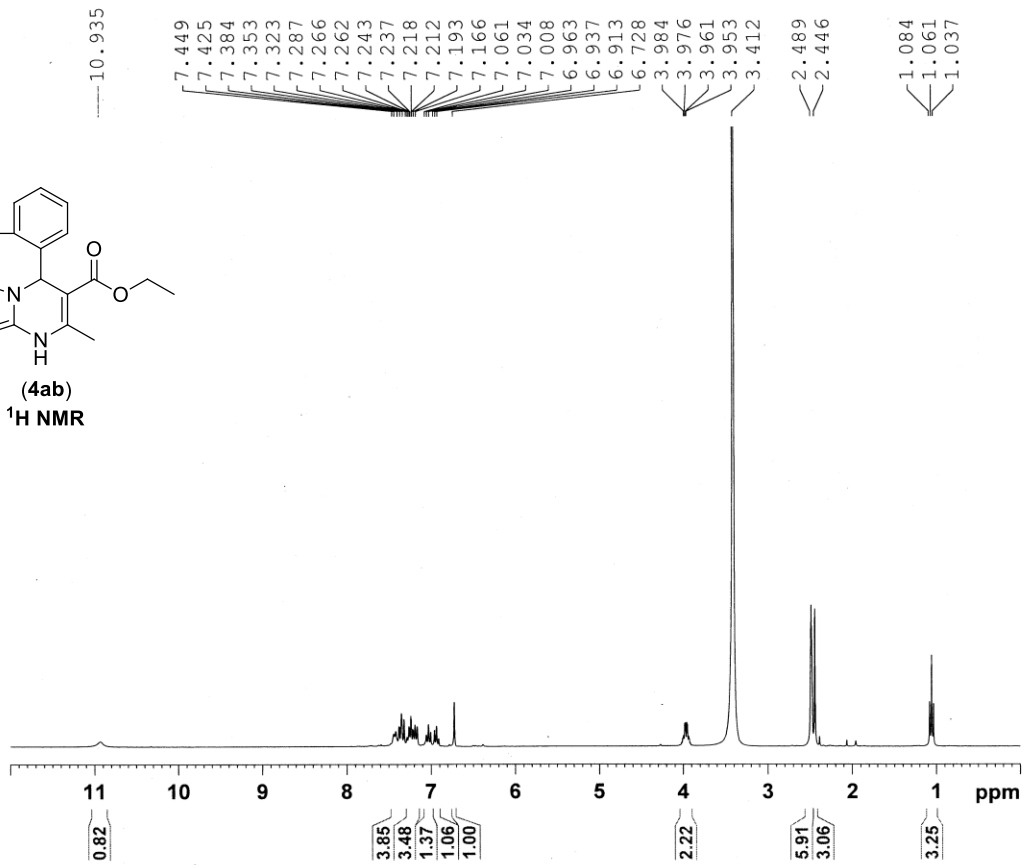
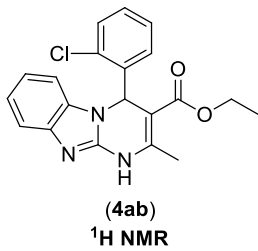


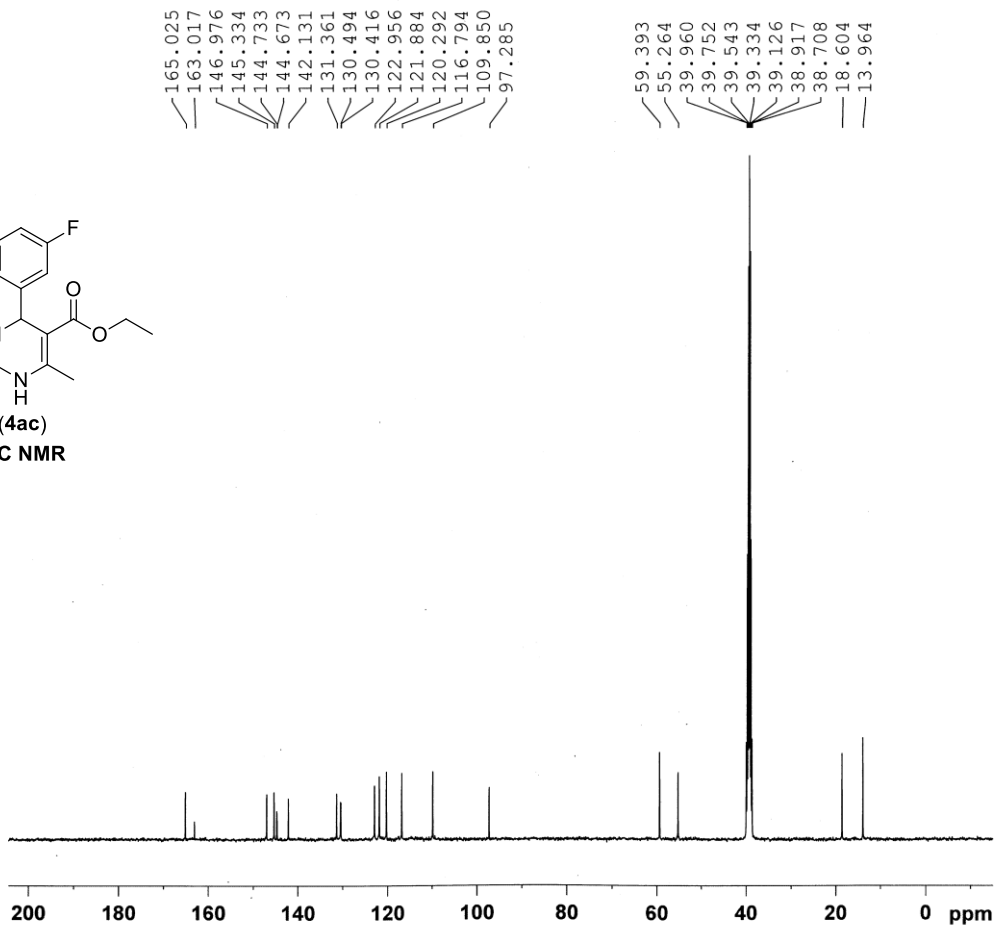
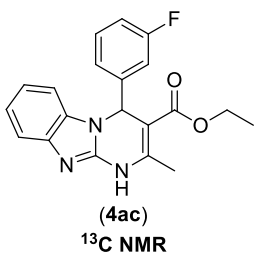
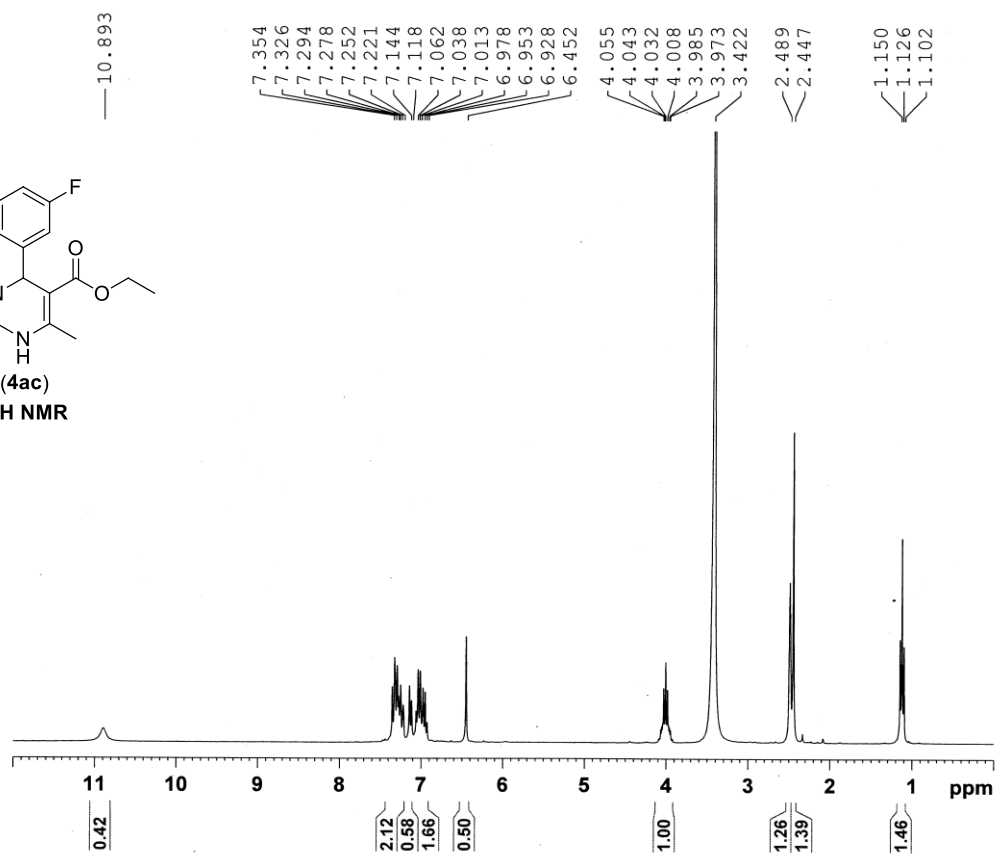
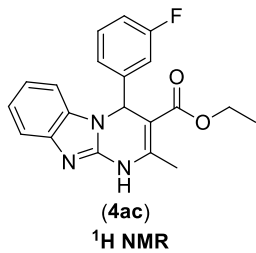
(4aa)
 ^1H NMR

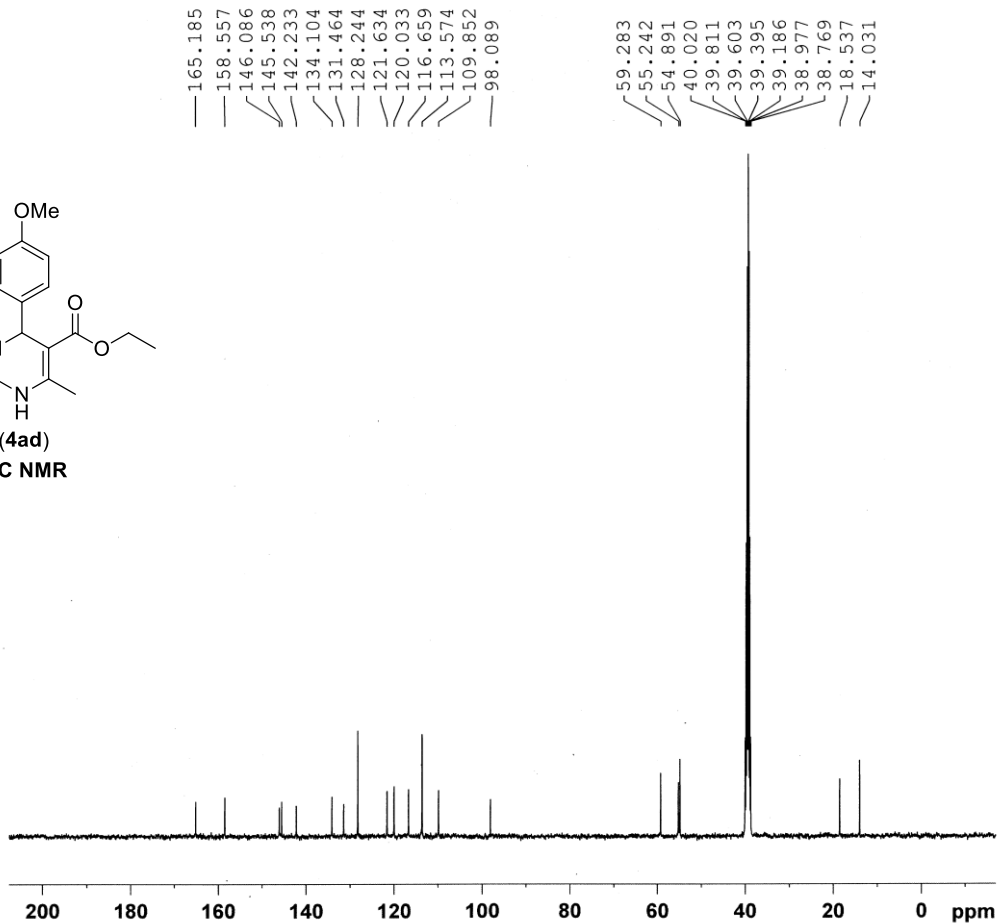
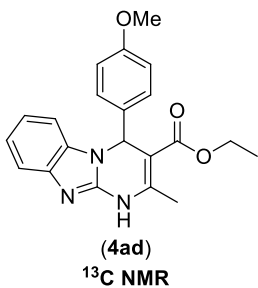
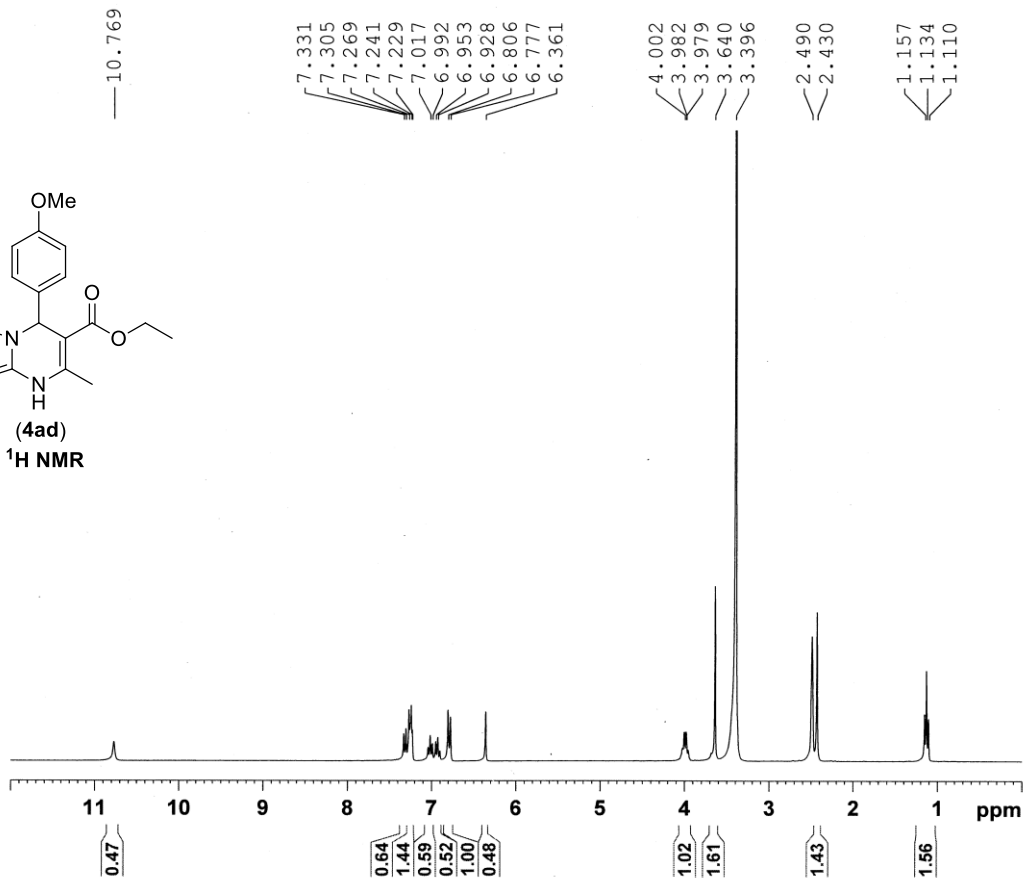
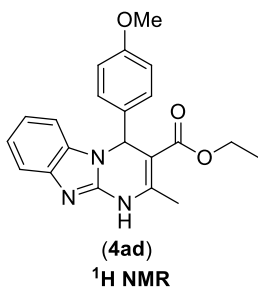


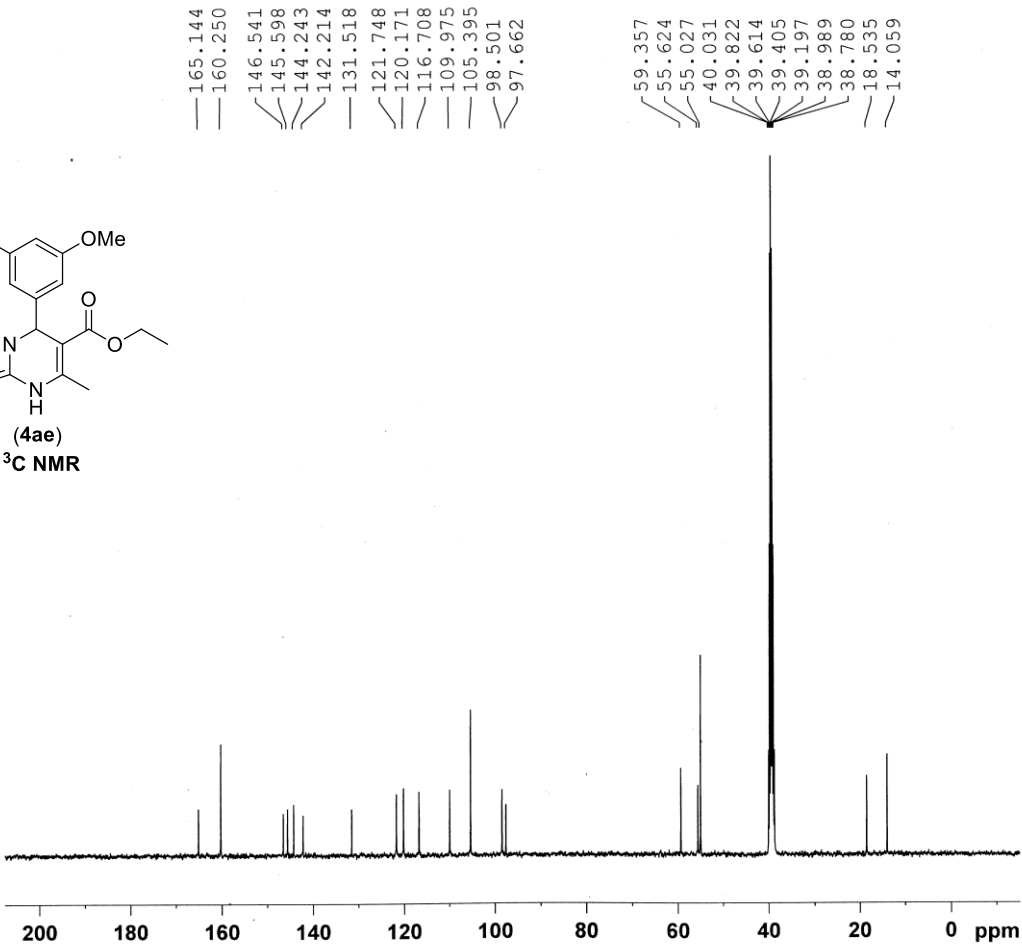
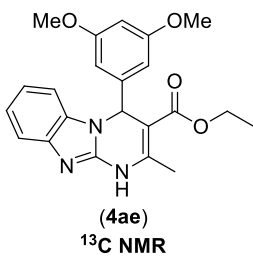
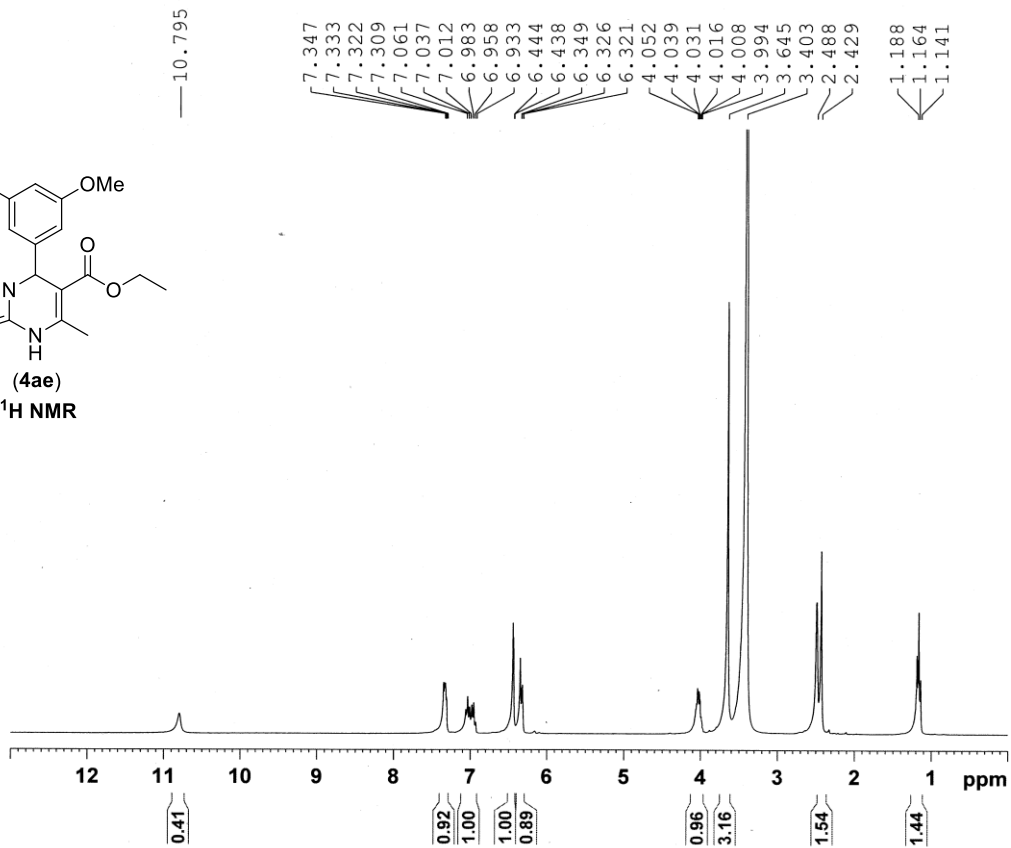
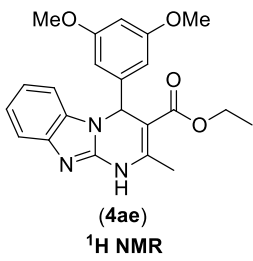
(4aa)
 ^{13}C NMR

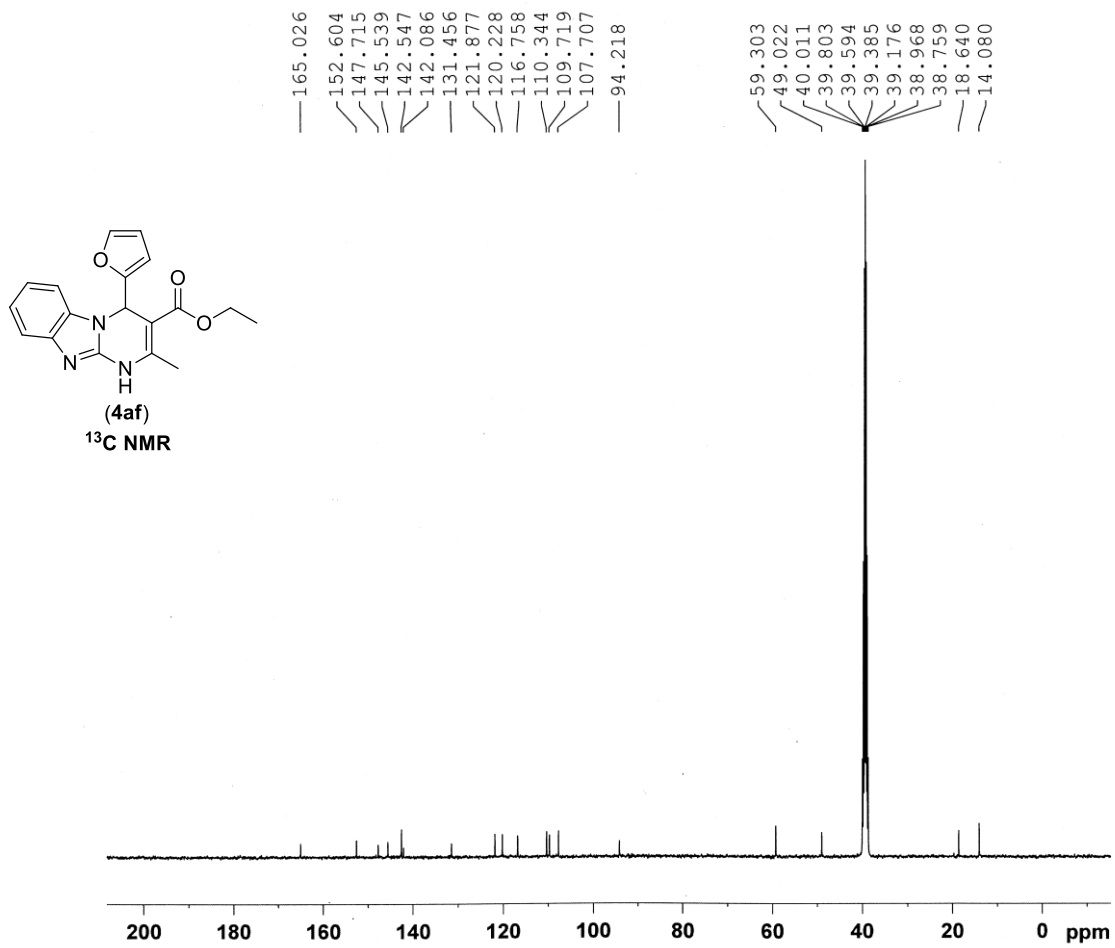
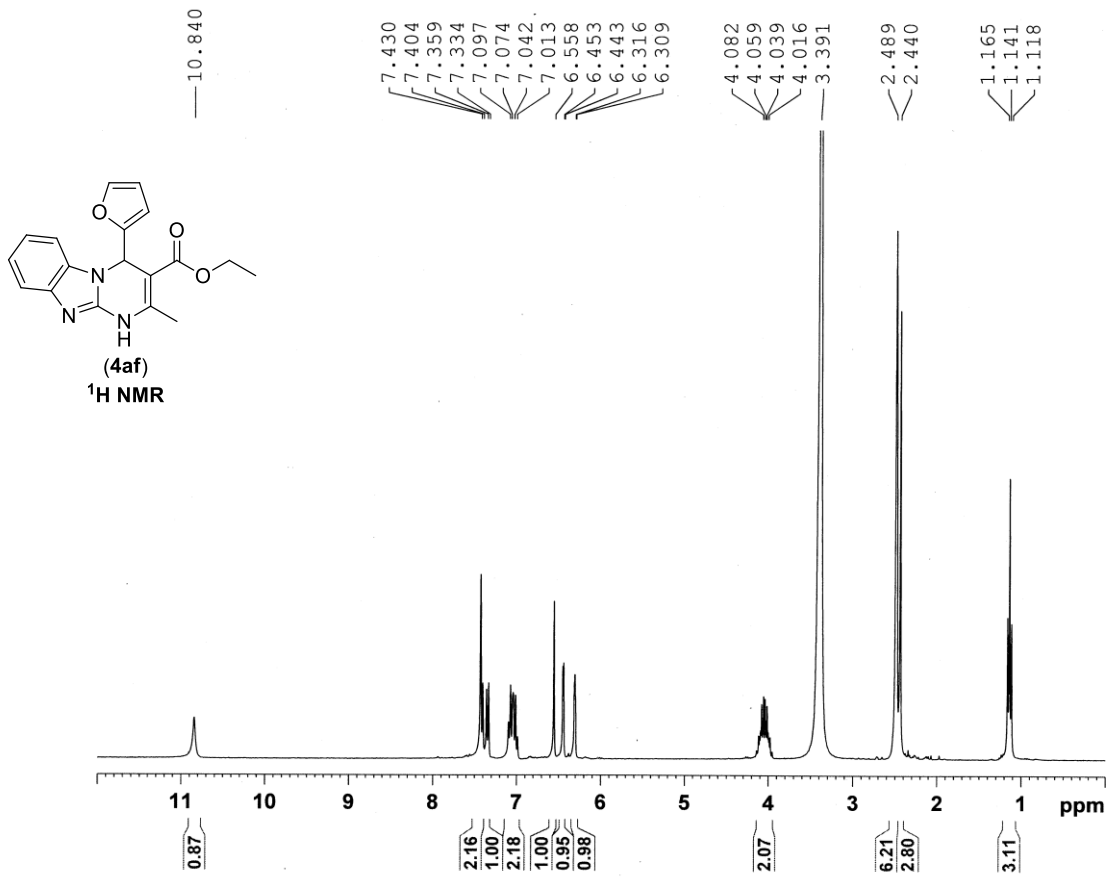


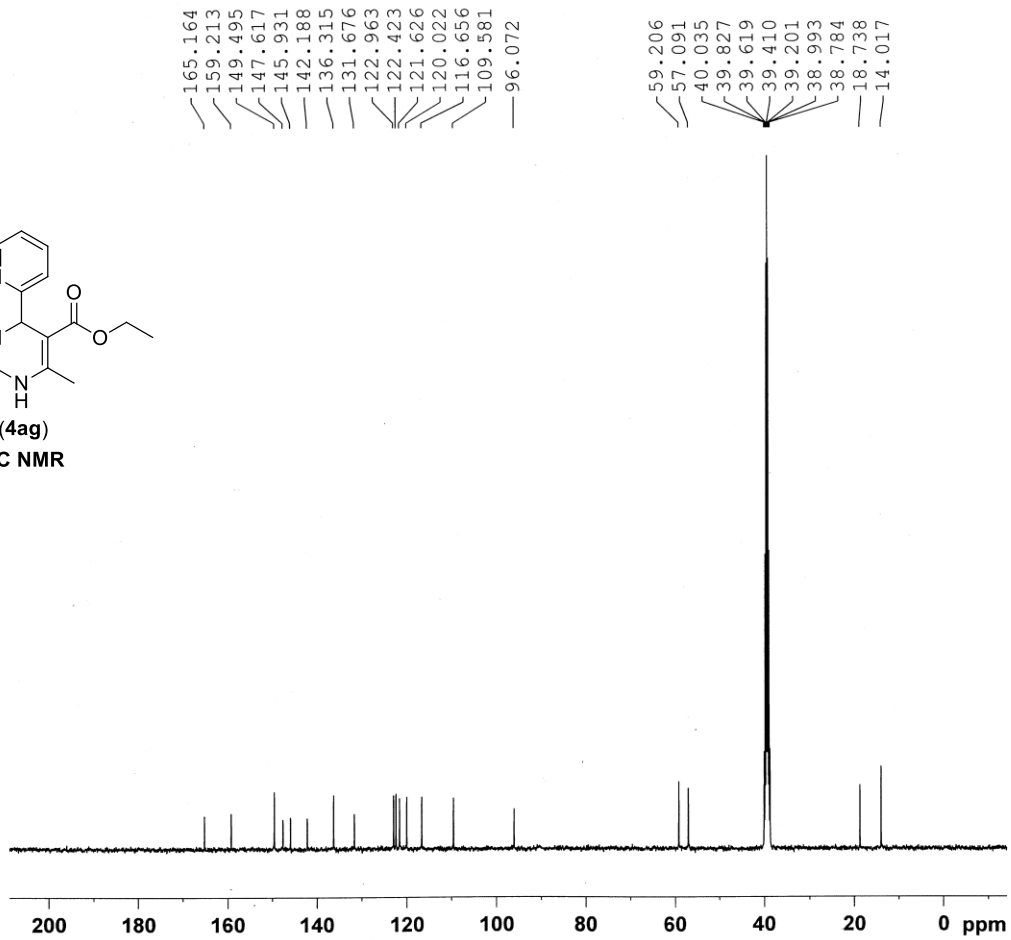
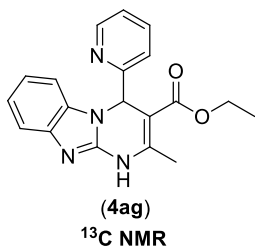
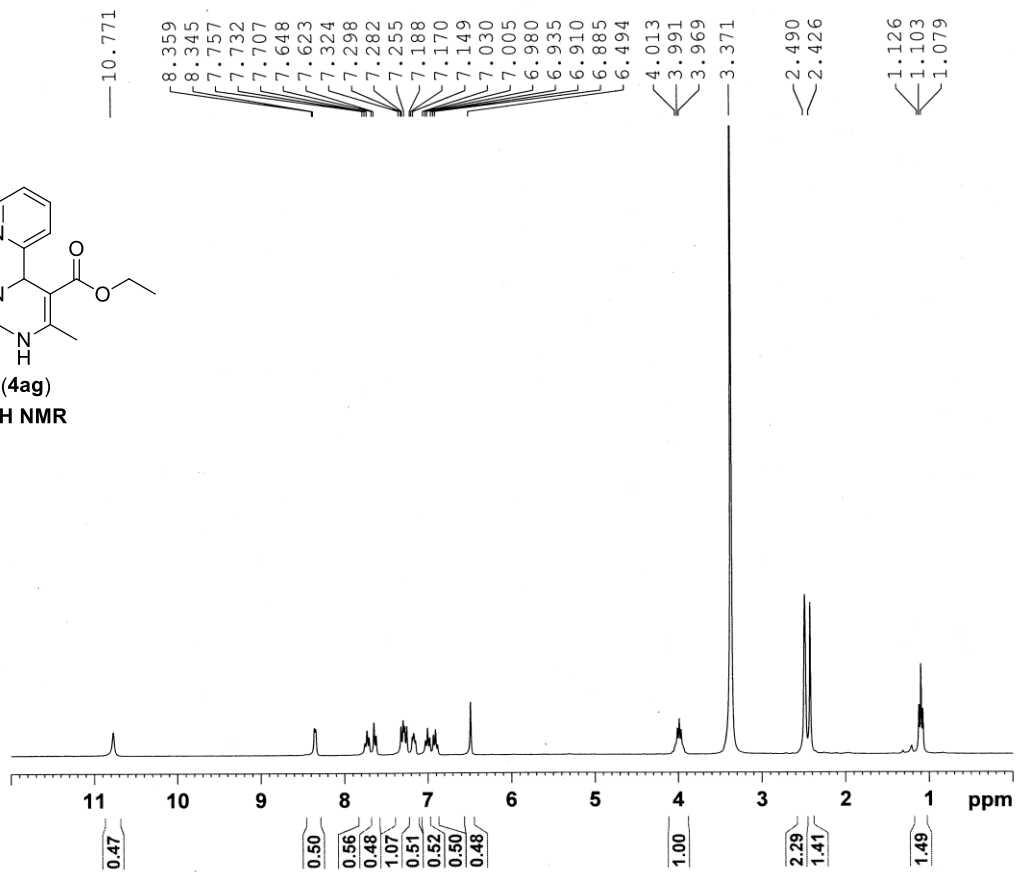
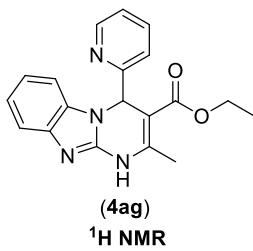


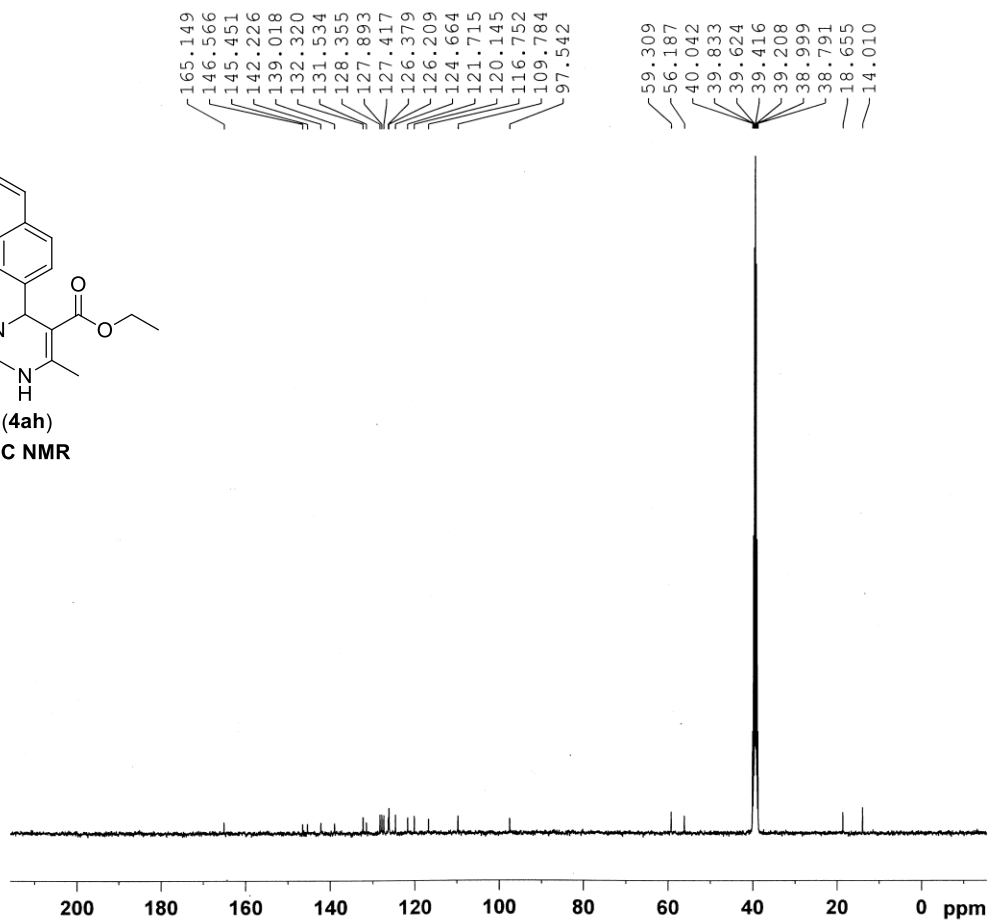
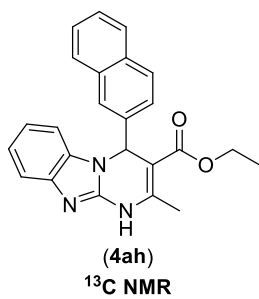
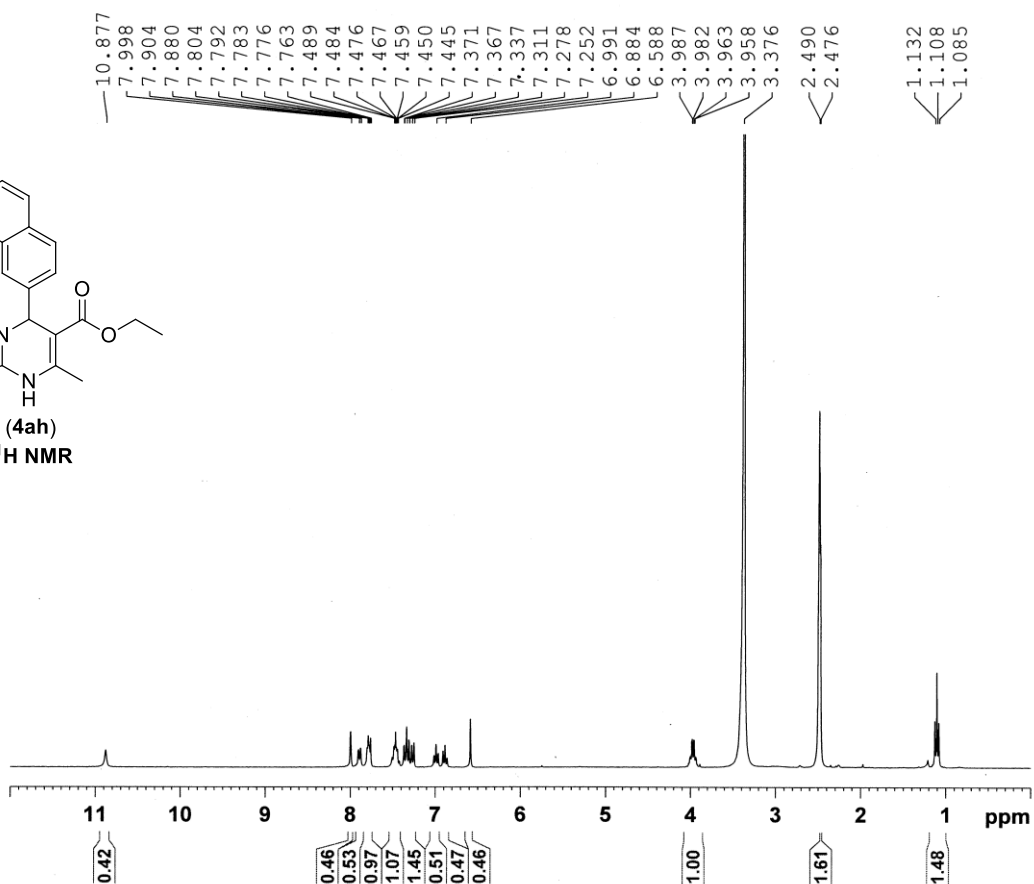
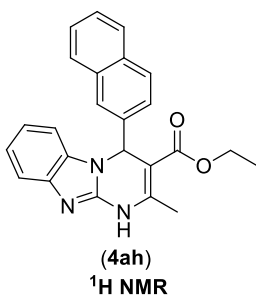


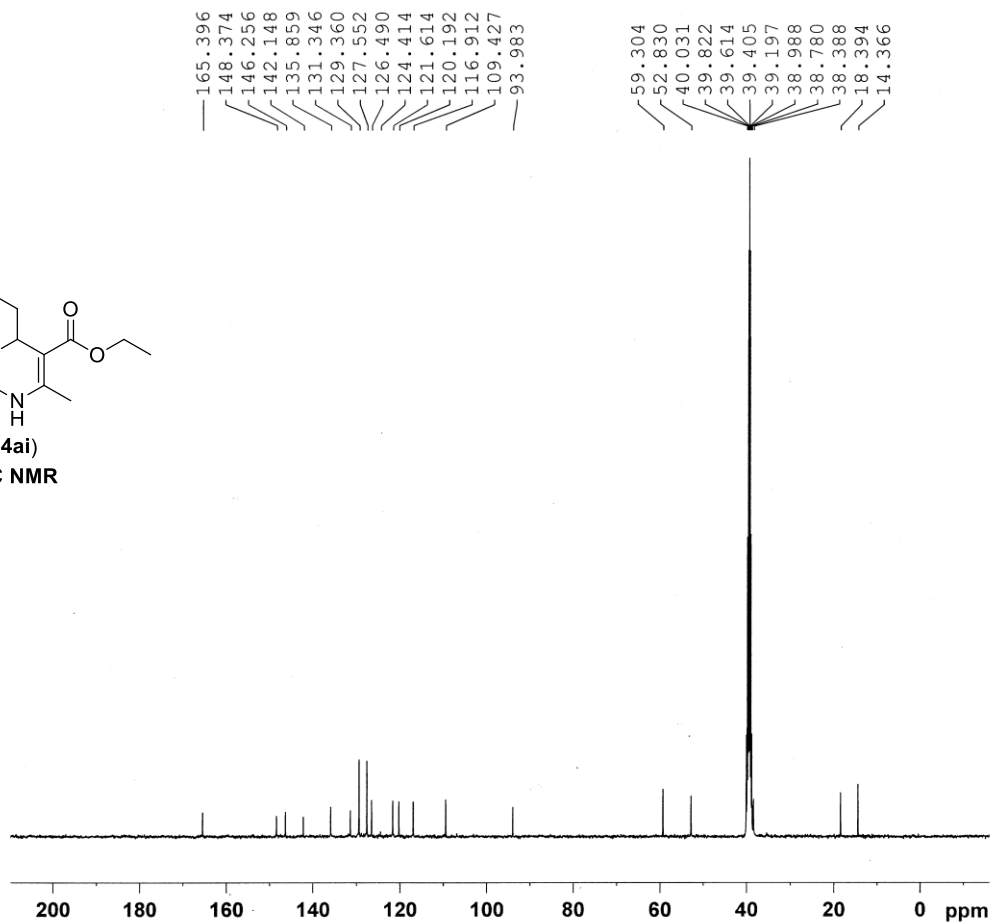
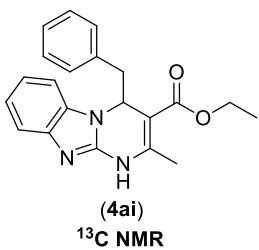
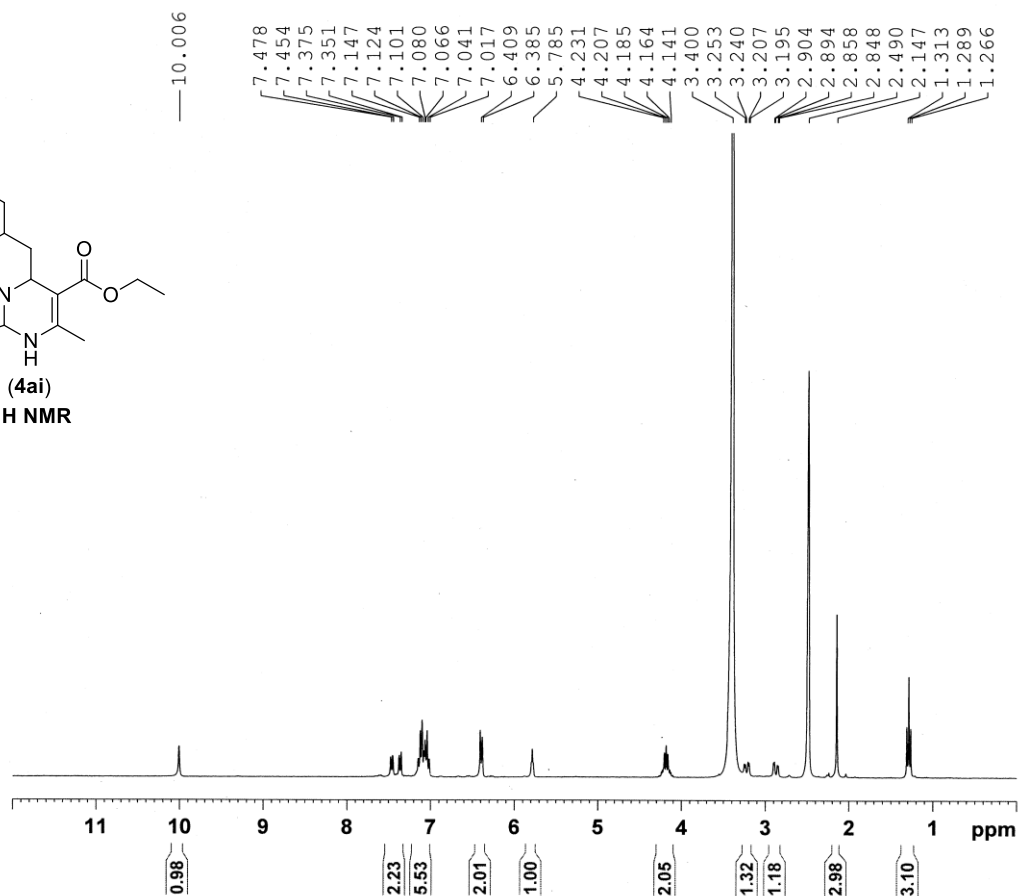
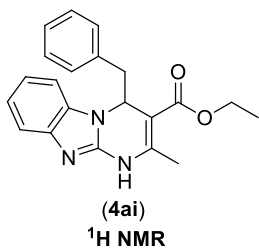


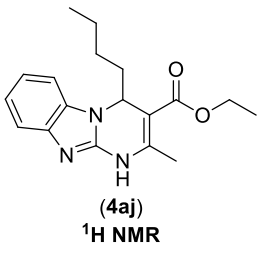




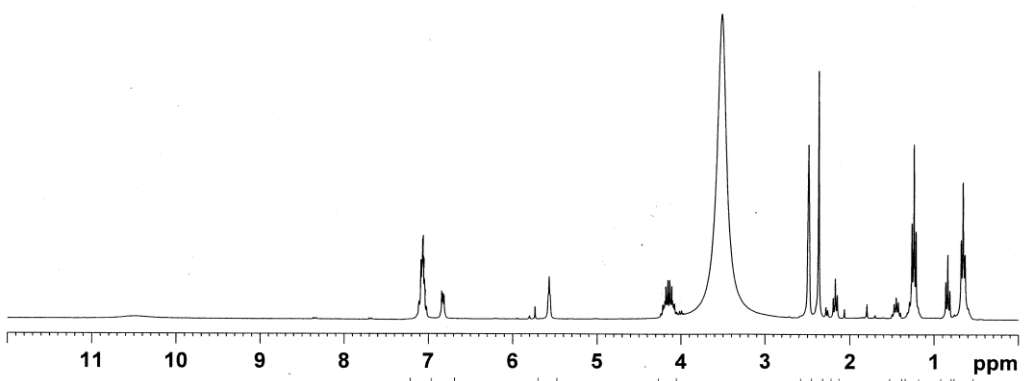








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