

Supporting information

Synthesis and Structural Features of Indium(III) furan-2-thiocarboxylates: Efficient Catalytic Activity Toward Multicomponent Reactions *via* Knoevenagel Condensation

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NMR study of complexes

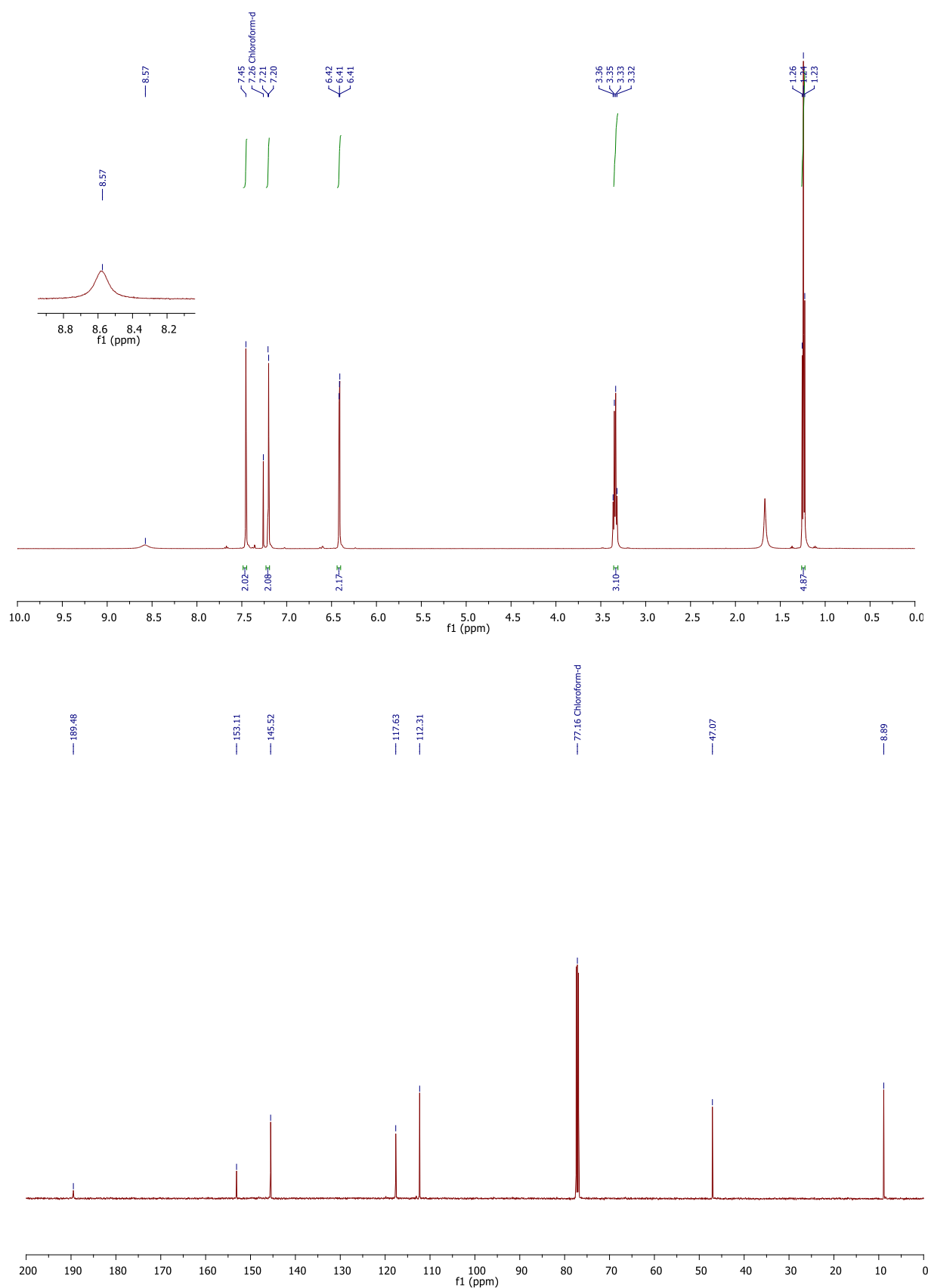


Figure S1(a): ^1H , ^{13}C NMR spectra of Complex 1

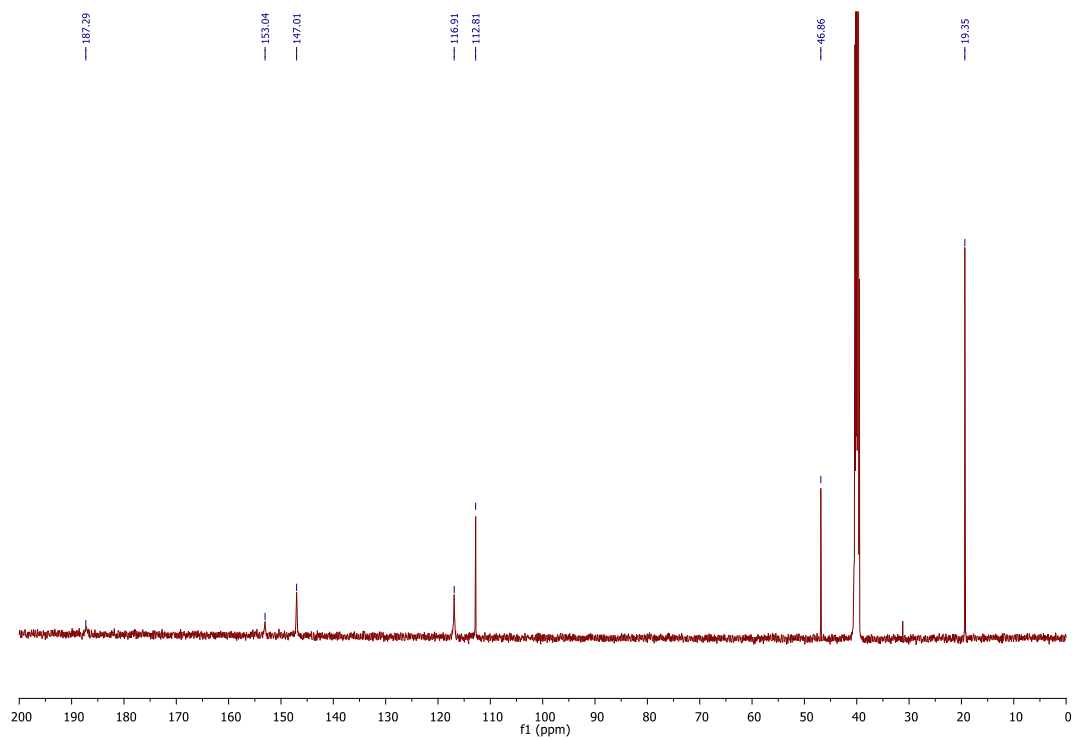
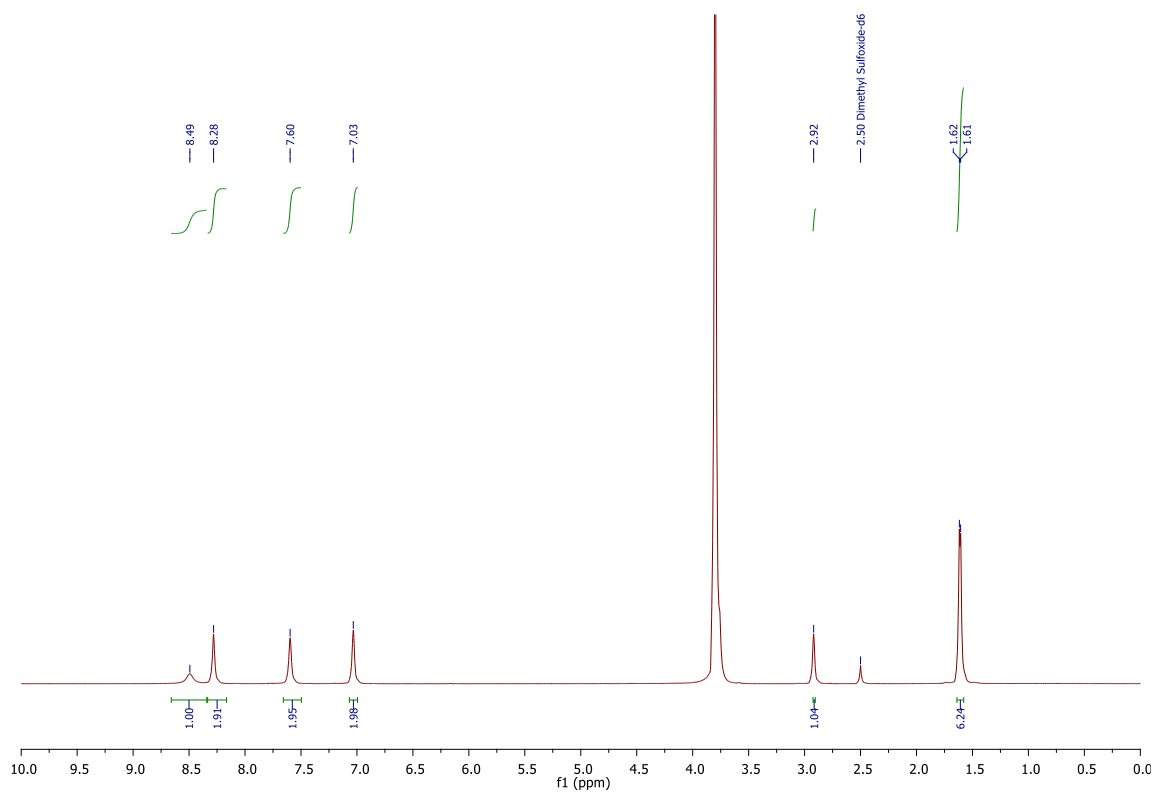
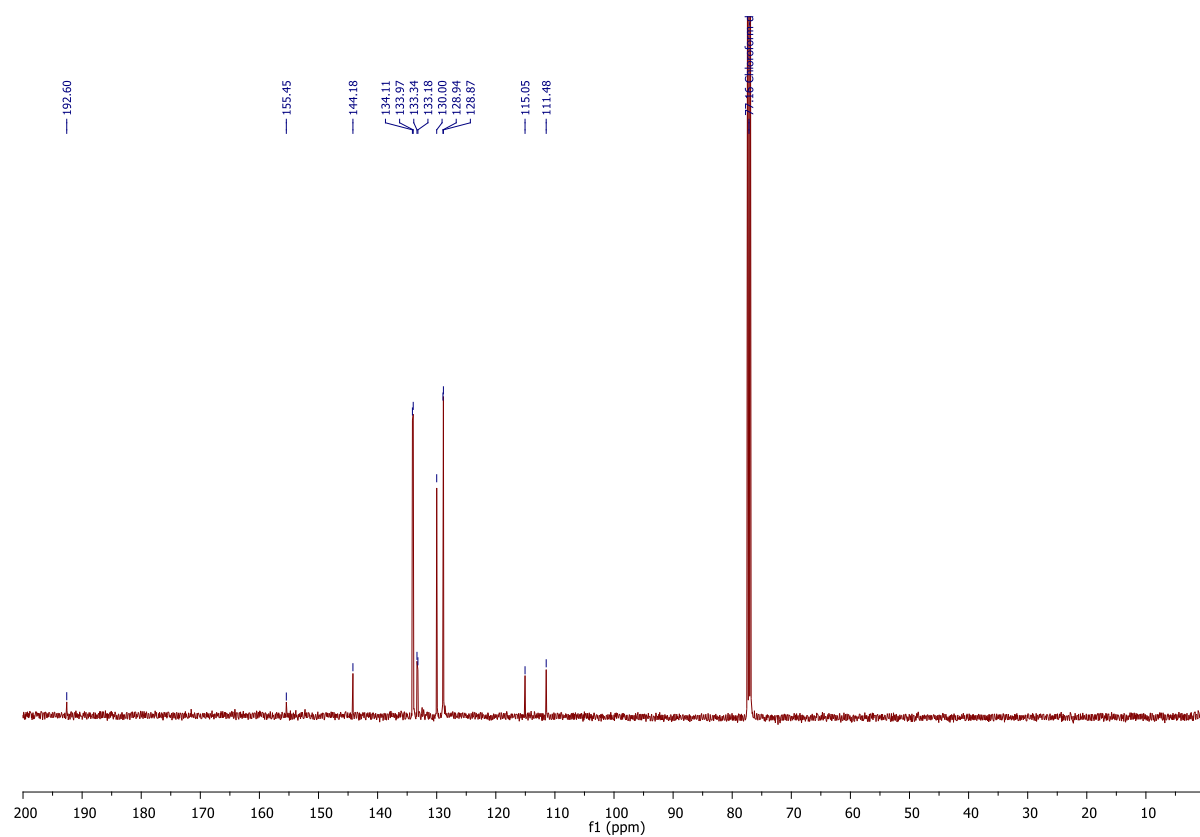
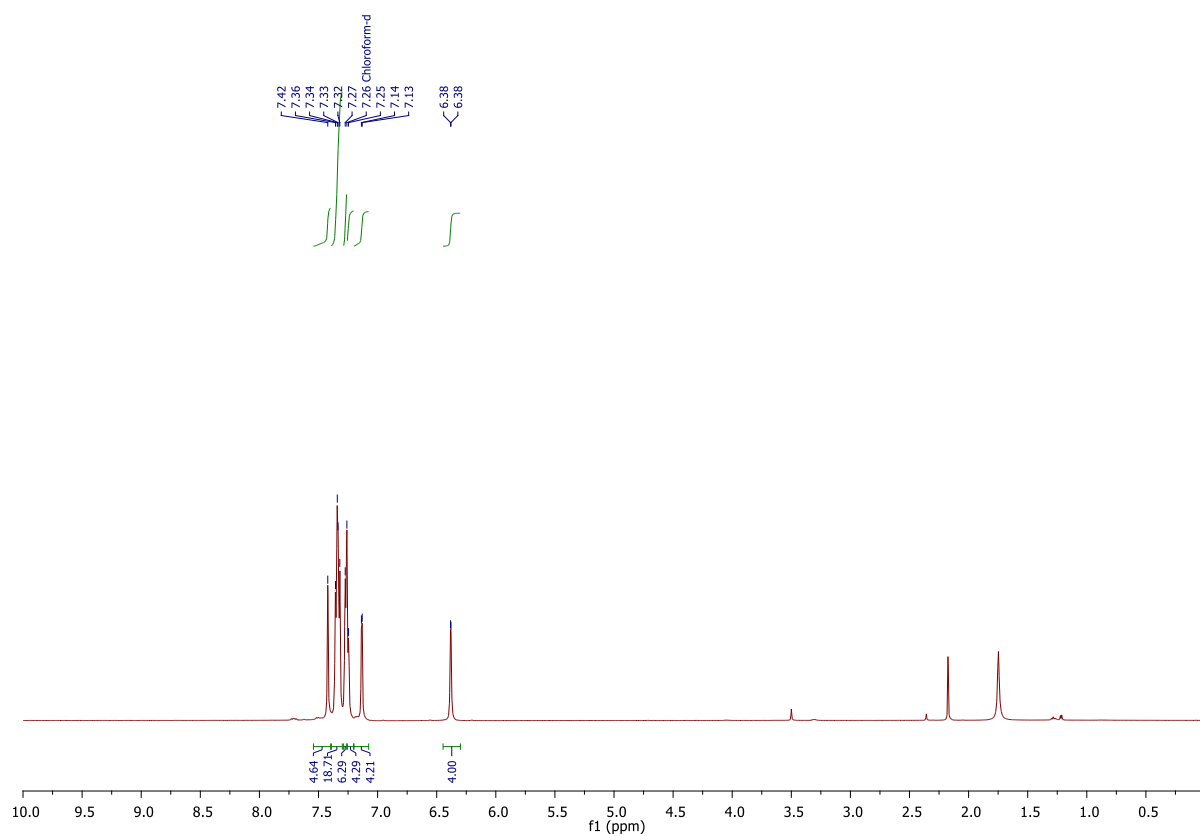


Figure S1(b): ^1H , ^{13}C NMR spectra of Complex 2



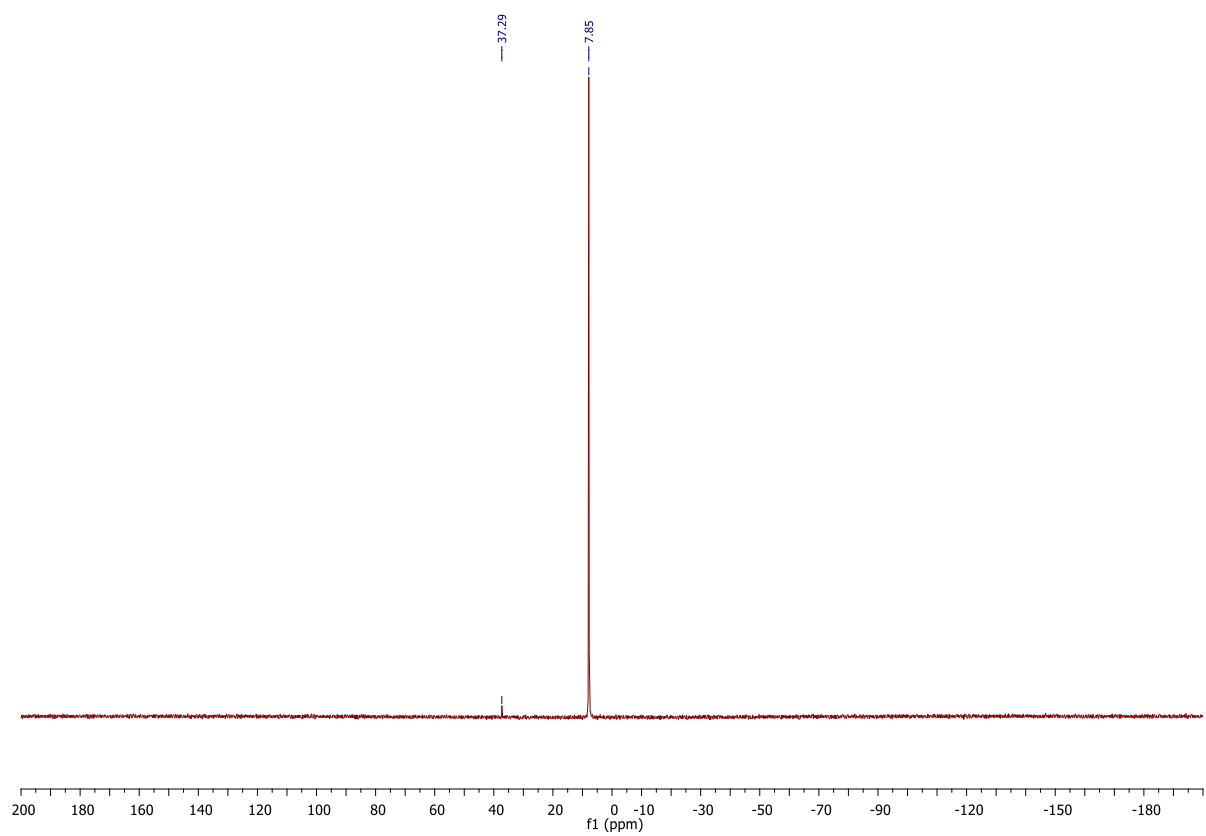


Figure S1(c): ^1H , ^{13}C , ^{31}P NMR spectra of Complex **6**.

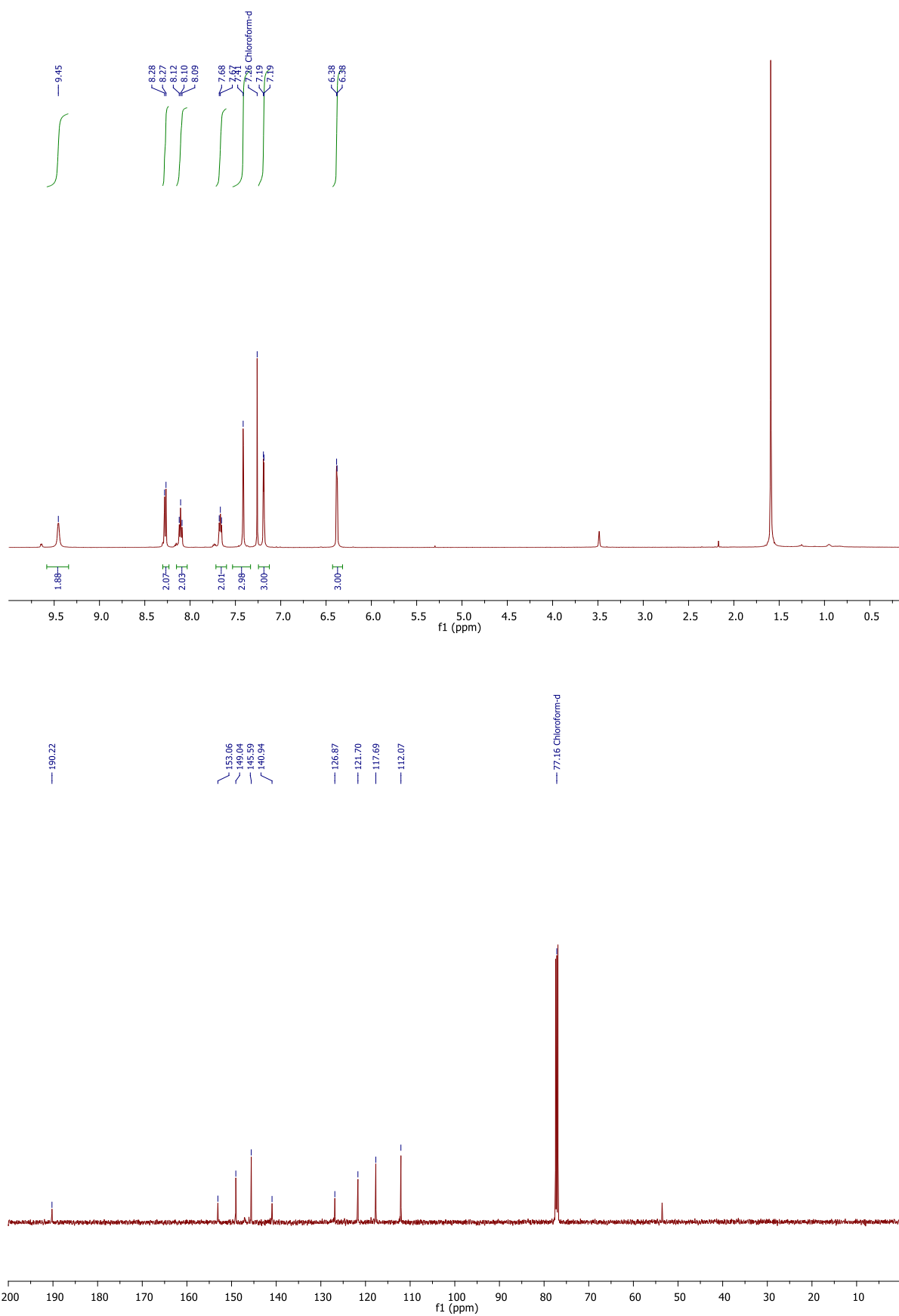


Figure S1(e): ^1H , ^{13}C , ^{31}P NMR spectra of Complex **3a**

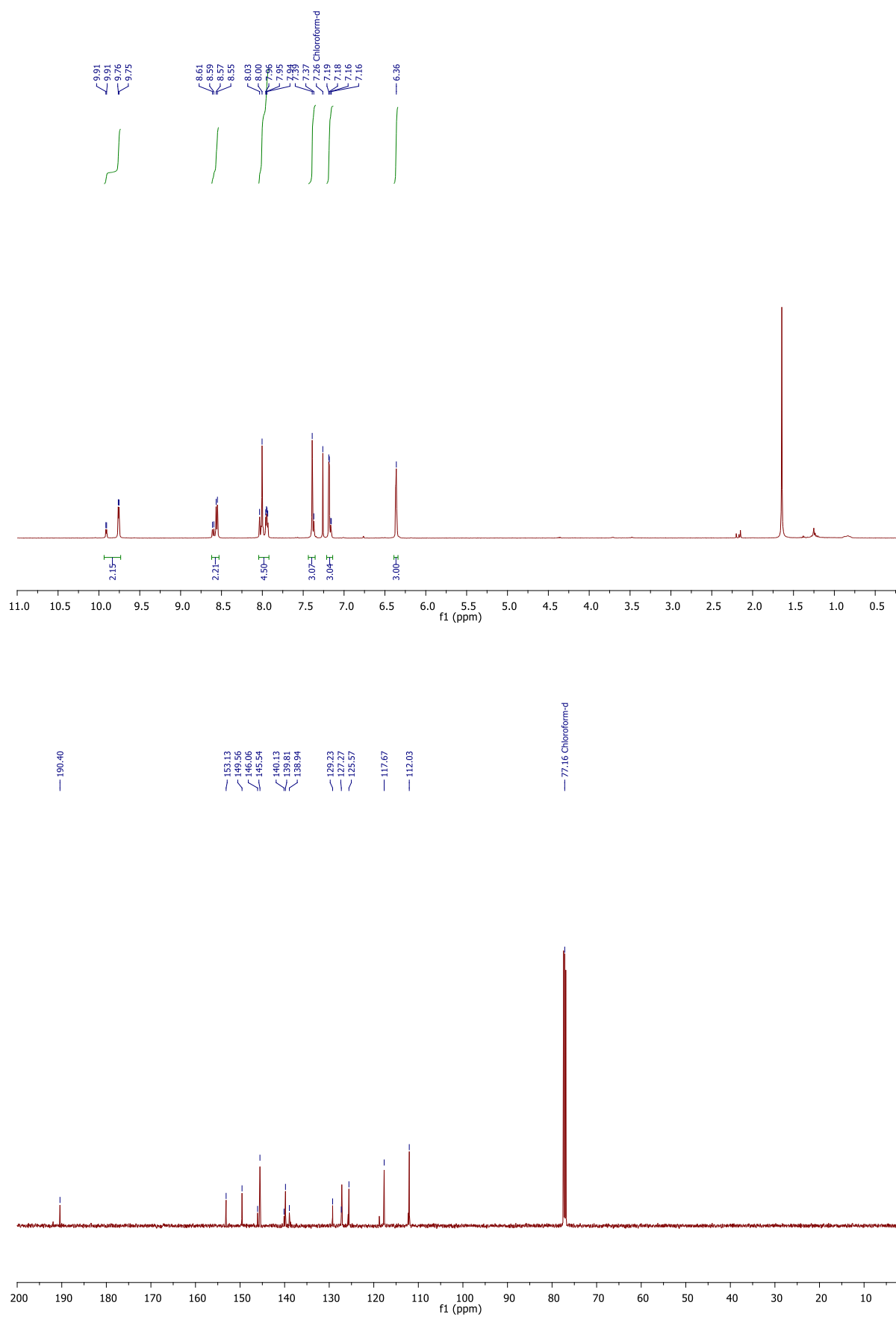


Figure S1(f): ^1H , ^{13}C , ^{31}P NMR spectra of Complex **3b**

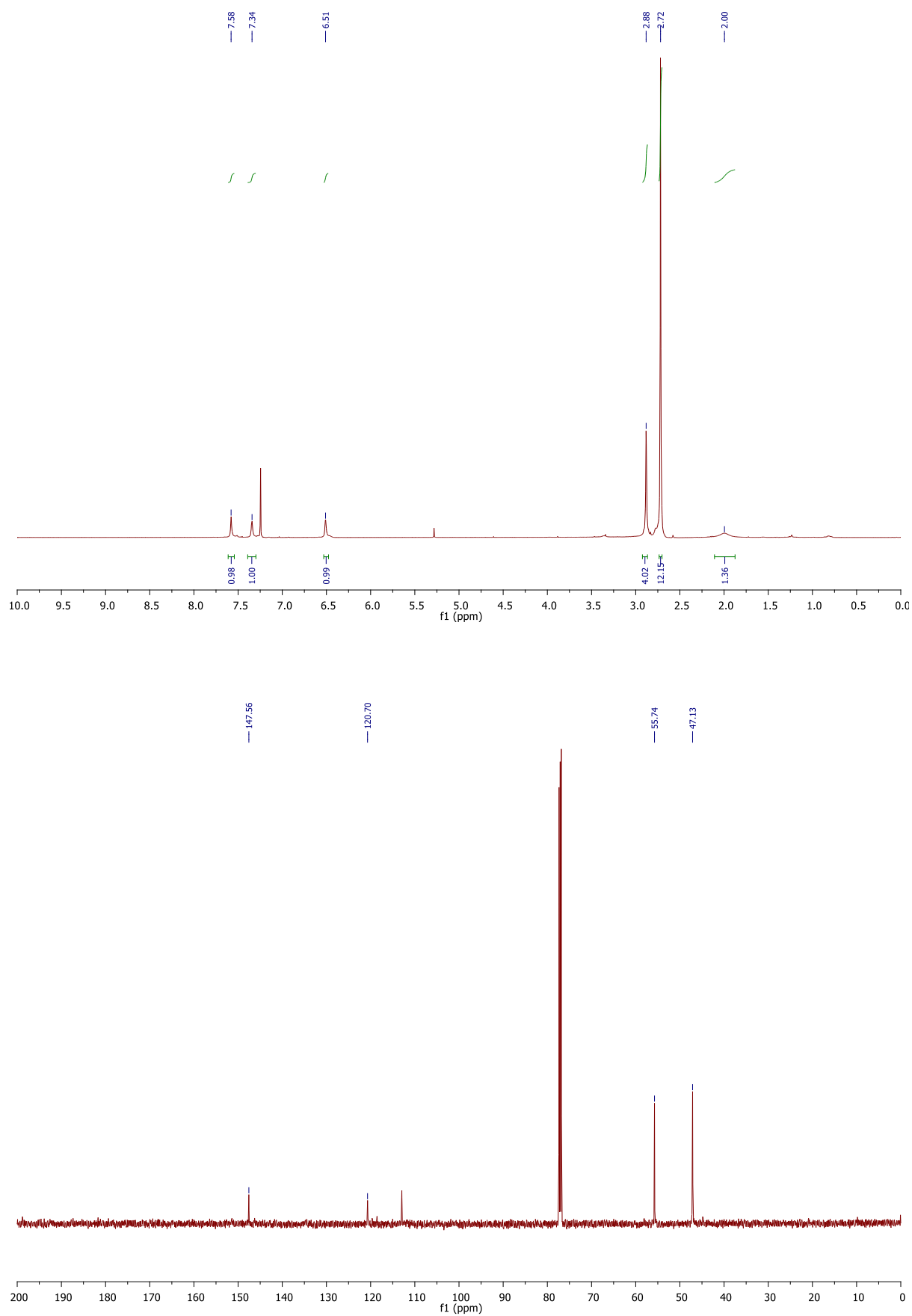


Figure S1(g): ^1H , ^{13}C NMR spectra of Complex 4

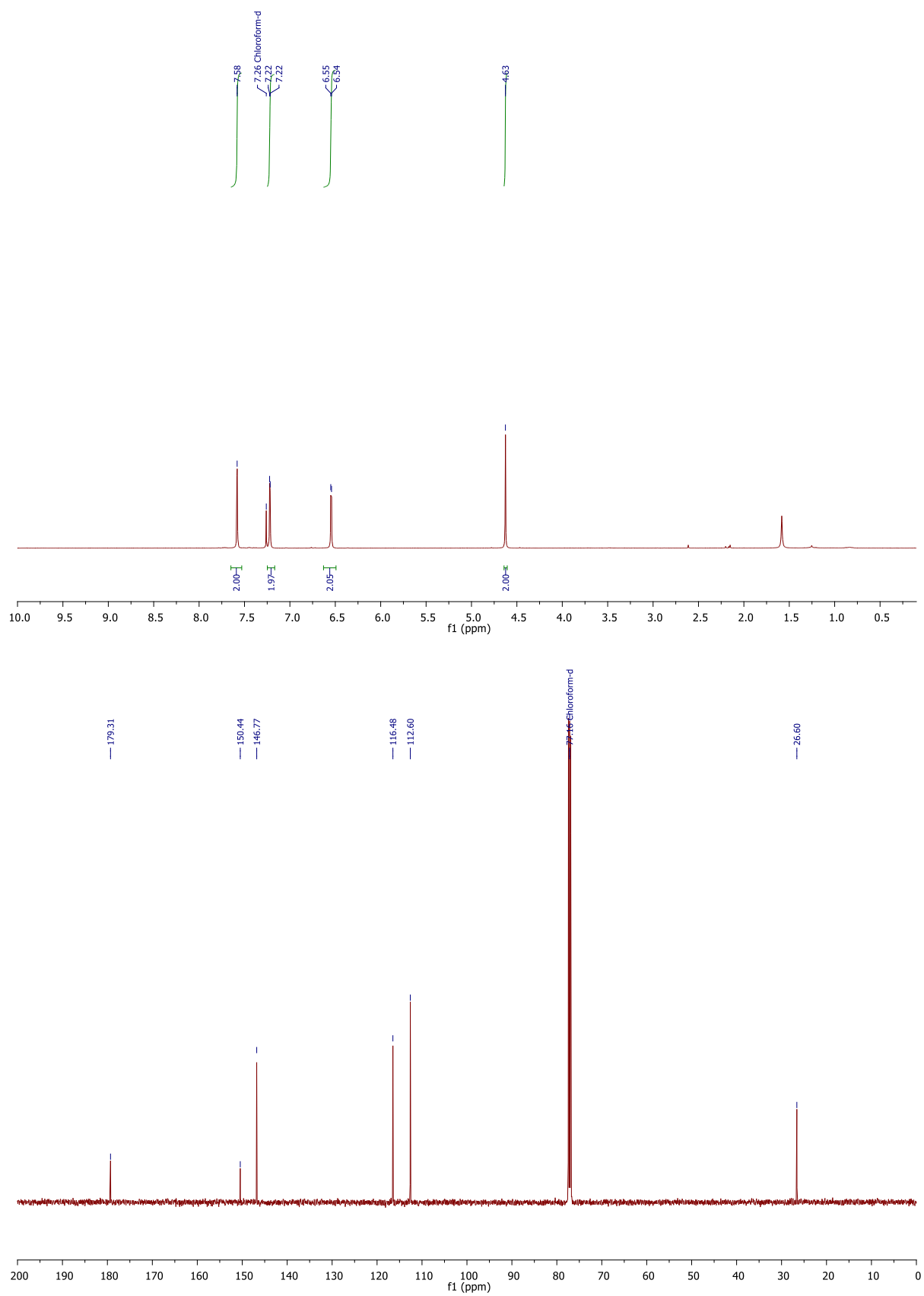
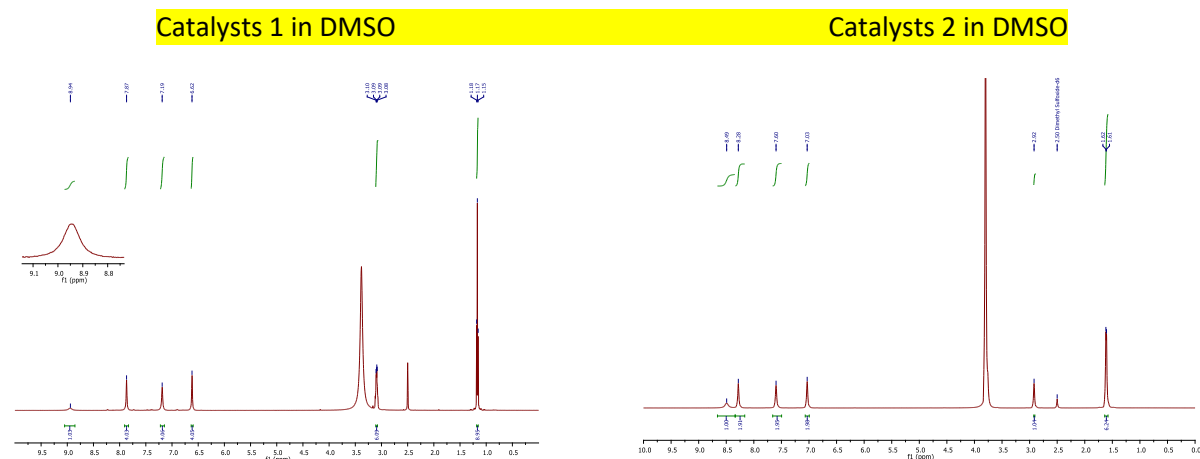


Figure S1(h): ^1H , ^{13}C NMR spectra of Complex **8**.

Comparative ^1H NMR studies for catalysts 1 and 2



IR spectra of catalyst 2

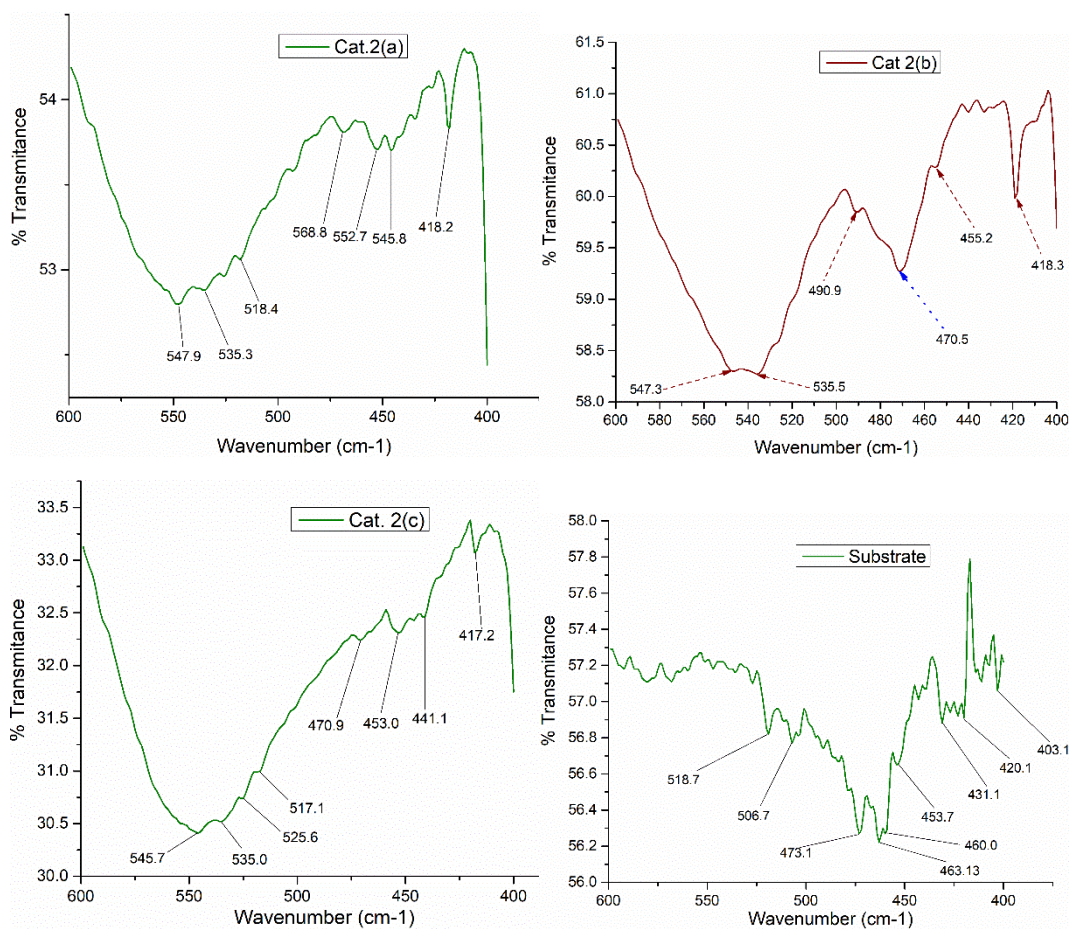


Figure S2(b): IR spectra of catalysts 2, (a) before reaction, (b) during reaction (c) end of the reaction and the substrates (without catalyst).

Table S1 Important Crystallographic data and refinement parameter for catalytic product 9a, 10e, 10i.

| | 9a | 10e | 10i |
|------------------------------|--|---|---|
| CCDC number | 2211085 | 2211083 | 2211964 |
| Formula | C ₁₀ H ₅ FN ₂ | C ₃₈ H ₃₁ N ₆ O ₄ | C ₁₆ H ₁₃ N ₃ O ₄ |
| Fw | 172.16 | 635.69 | 311.29 |
| Crystal system | triclinic | Monoclinic | Monoclinic |
| Space group | <i>P</i> -1 | <i>P</i> 2 ₁ / <i>n</i> | <i>C</i> 2/ <i>c</i> |
| <i>a</i> (Å) | 6.96810(10) | 11.8236(3) | 13.8640(3) |
| <i>b</i> (Å) | 7.37580(10) | 16.9993(4) | 11.0917(3) |
| <i>c</i> (Å) | 9.1552(2) | 17.1930(5) | 20.7199(5) |
| α (°) | 107.203(2) | 90 | 90 |
| β (°) | 98.978(2) | 102.291(3) | 110.751(3) |
| γ (°) | 102.864(2) | 90 | 90 |
| Measured Reflections | 6919 | 79938 | 8750 |
| Independent Reflections | 1526 | 7227 | 2633 |
| <i>V</i> (Å ³) | 425.581(14) | 3376.46(15) | 2979.52(14) |
| <i>Z</i> | 2 | 4 | 8 |
| F(000) | 176.0 | 1332.0 | 1296.0 |
| μ (mm ⁻¹) | 0.821 | 0.083 | 0.854 |
| ρ (g cm ⁻³) | 1.343 | 1.251 | 1.388 |
| Final R | 0.0343 | 0.0543 | 0.0576 |
| wR(F ²) | 0.0945 | 0.1908 | 0.1783 |
| GoF | 1.075 | 1.087 | 1.070 |

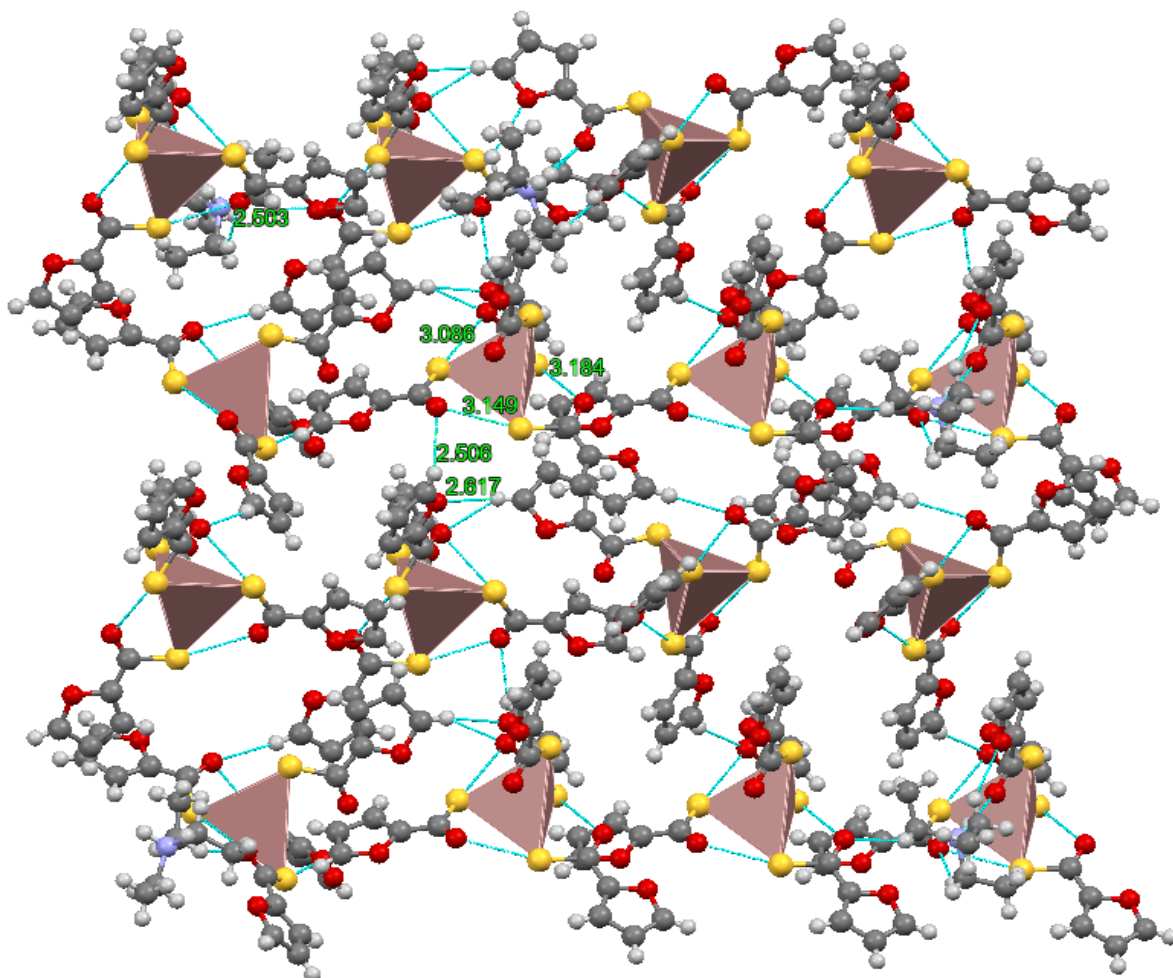


Figure S3: Weak interactions as well as polyhedral are shown by crystal structure **1**

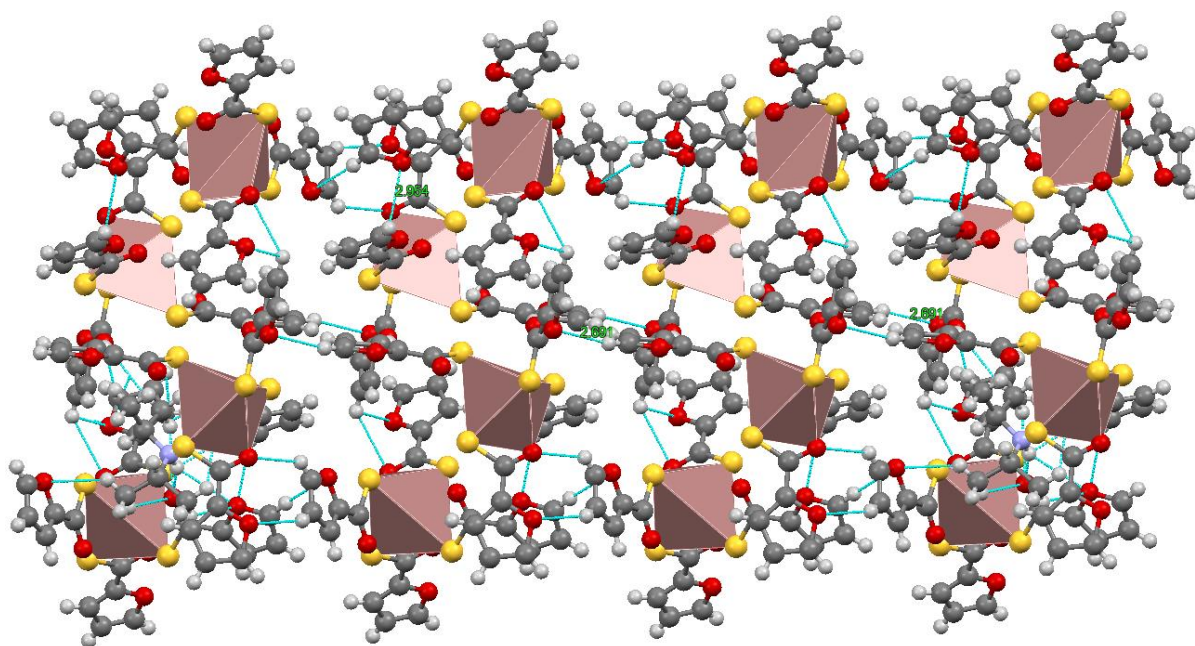


Figure S4: Weak interactions as well as polyhedral are shown by crystal structure **2**

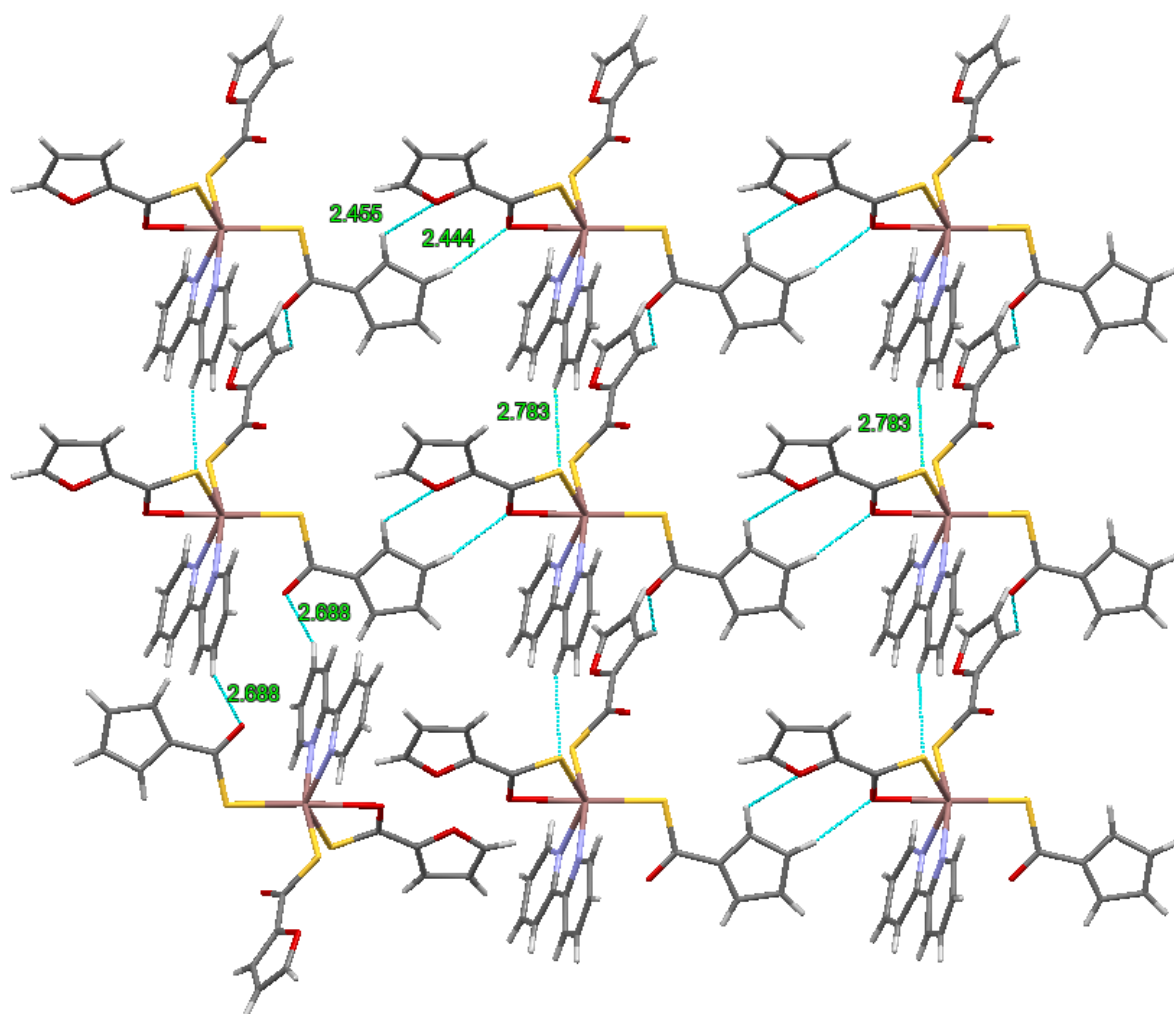


Figure S5: Weak interactions as well as polyhedral are shown by crystal structure **3a**

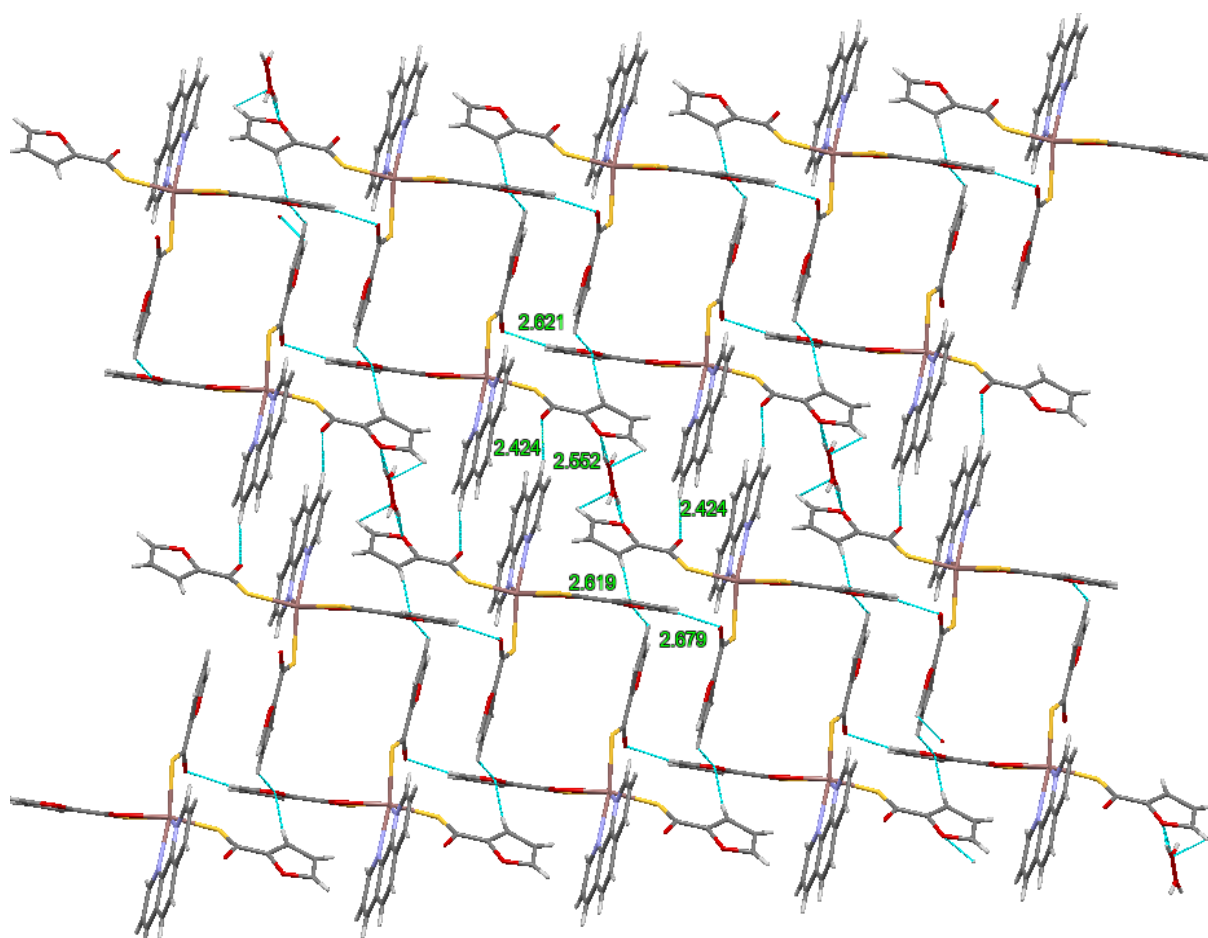


Figure S6: Weak interactions as well as polyhedral are shown by crystal structure **3b**

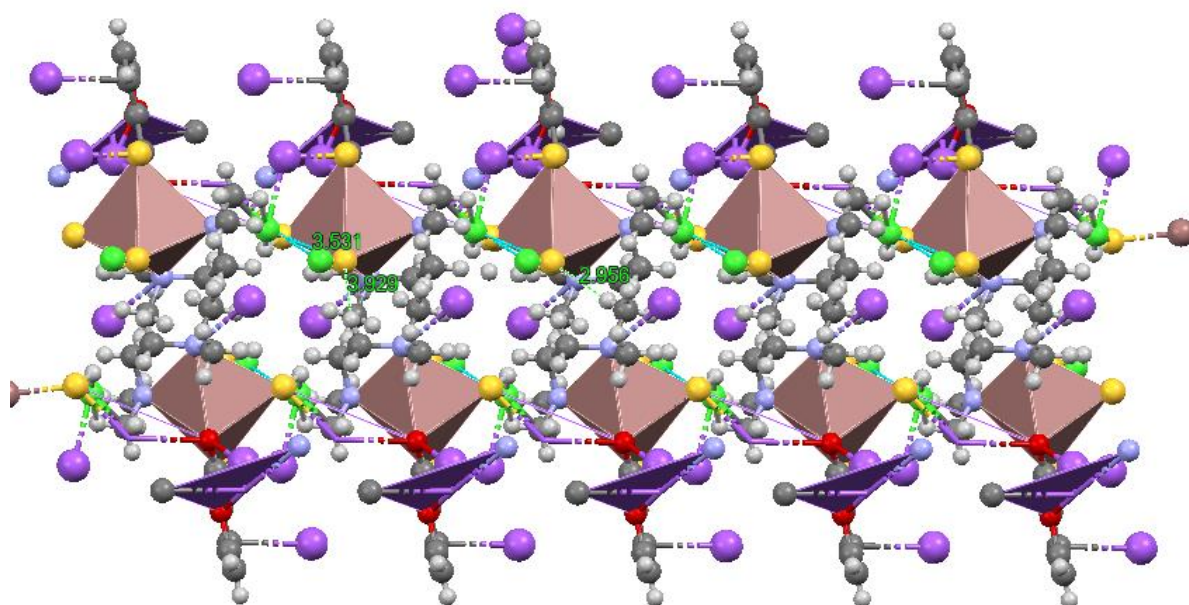


Figure S7: Weak interactions as well as polyhedral are shown by crystal structure **4**

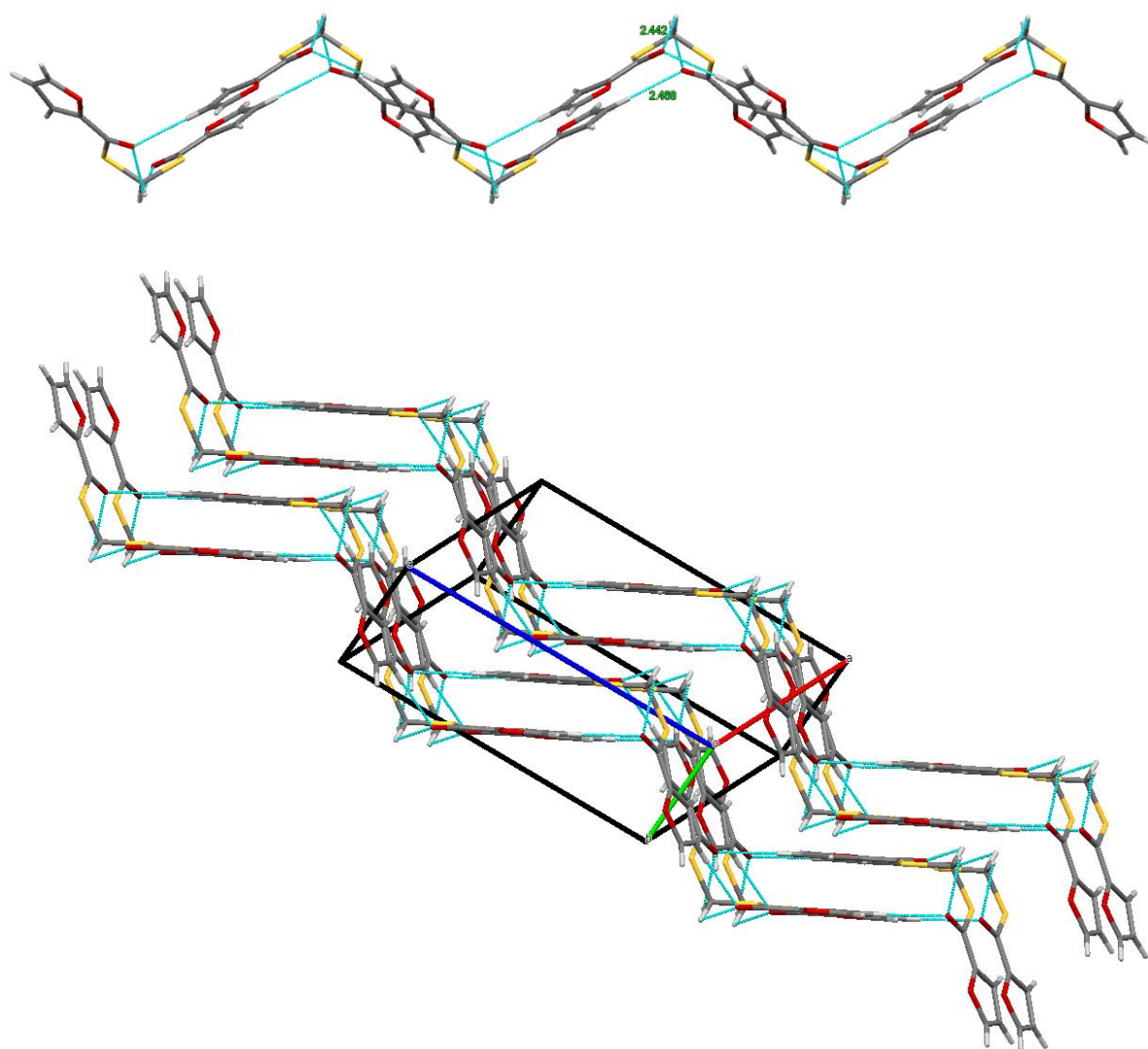
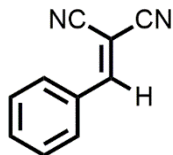


Figure S8: Weak interactions as well as polyhedral are shown by crystal structure **8**

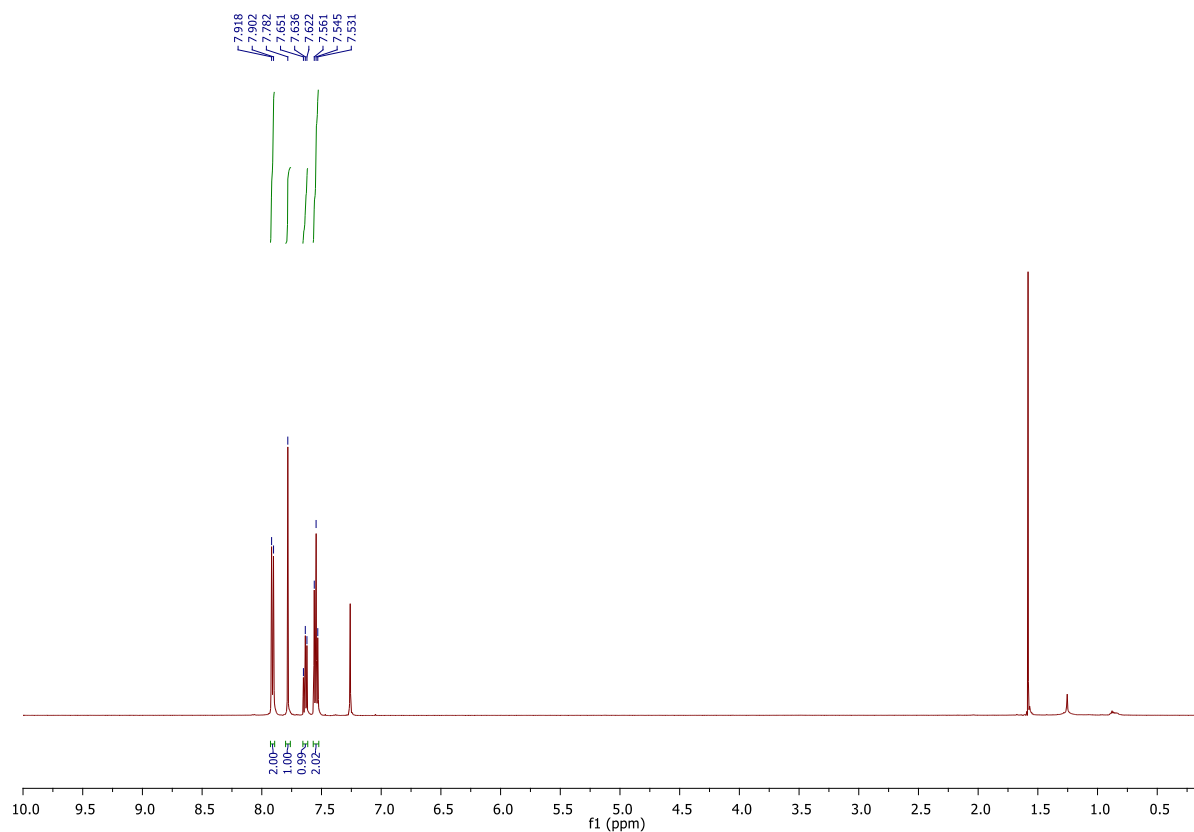
NMR spectra of 2 component Knoevenagel Condensation Products (^1H and ^{13}C)

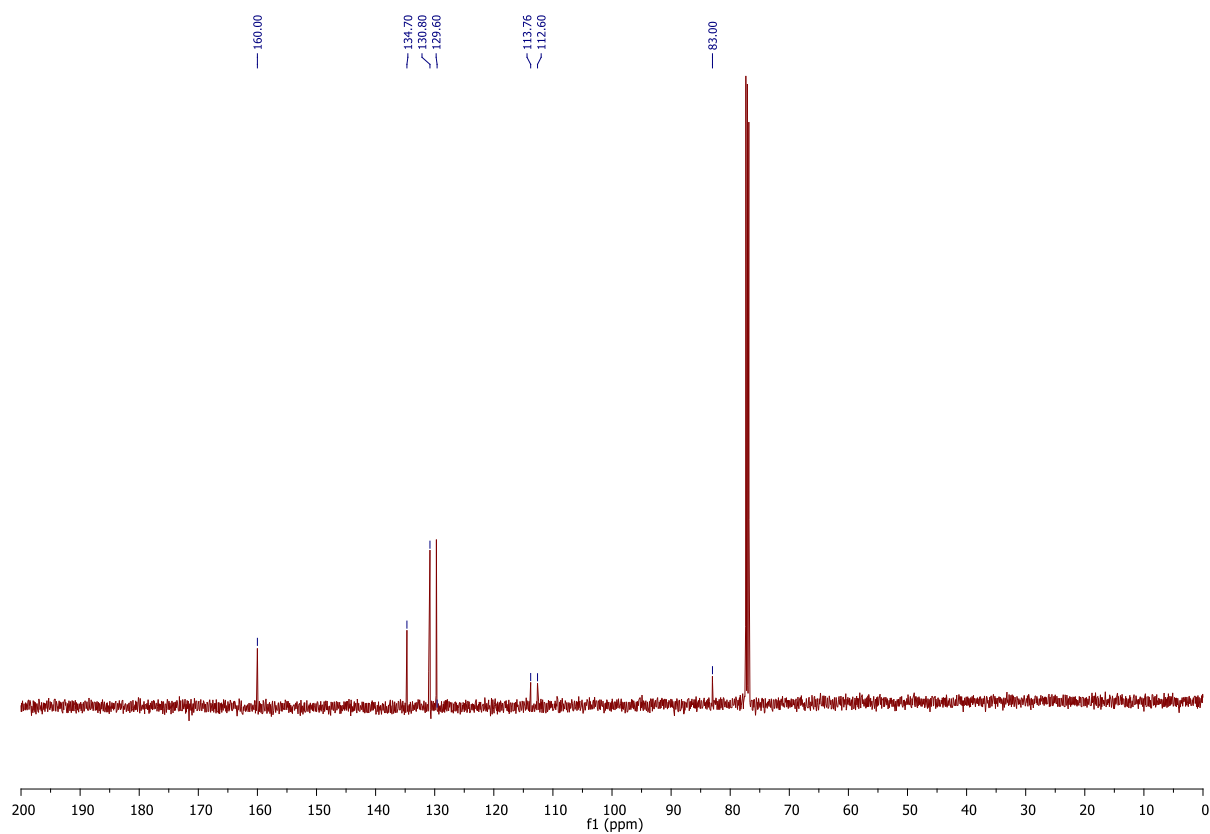
Characterization data and figure (spectra ^1H , ^{13}C) of Knoevenagel Condensation Products (9a-9j)

2-Benzylidenemalononitrile (9a)

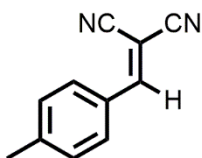


M. F. $\text{C}_{10}\text{H}_6\text{N}_2$ (154.17). Yield: (0.152 g, 97%). White powder. ^1H NMR (500 MHz, CDCl_3 , ppm) δ 7.90 (d, $J = 8.0$ Hz, 2H), 7.77 (s, 1H), 7.66 (t, $J = 7.0$ Hz, 1H), 7.55 (t, $J = 7.0$ Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3 , ppm) δ 160.0, 134.7, 130.8, 129.6, 113.7, 112.6, 83.0.

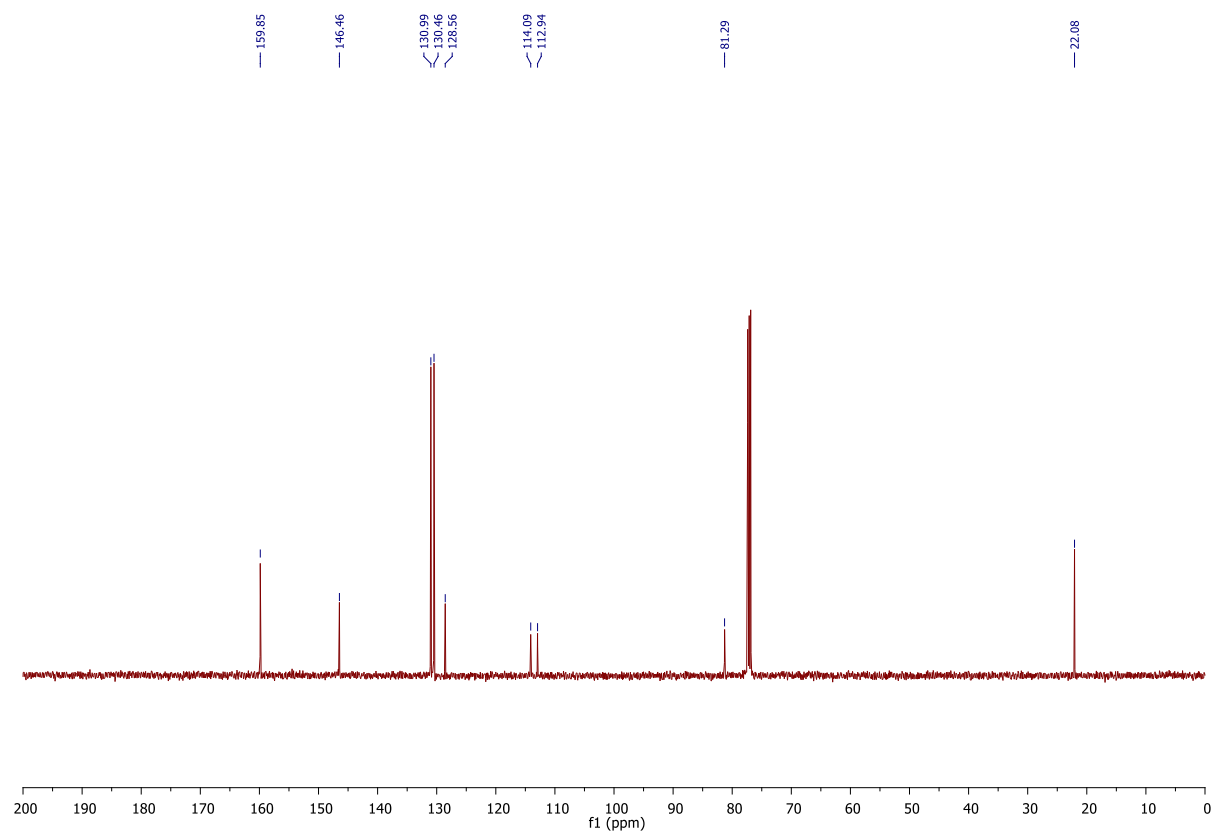
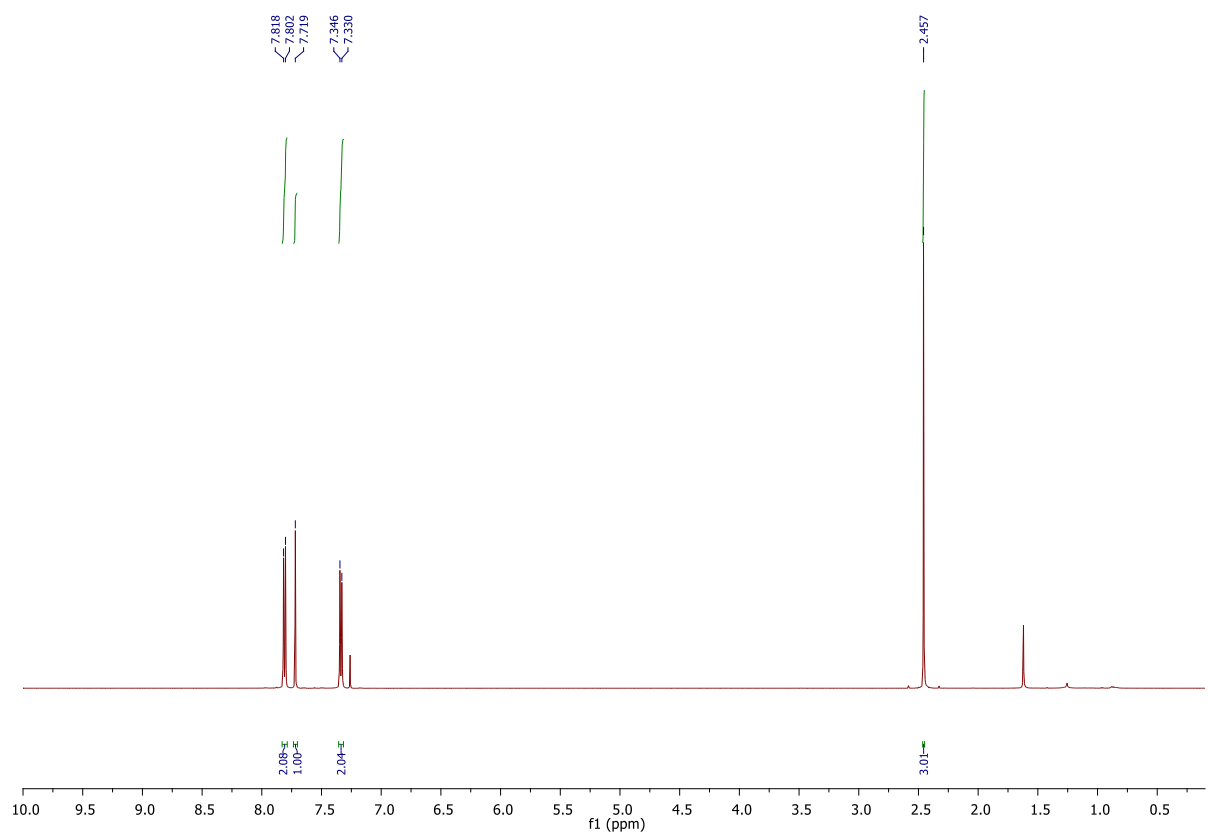




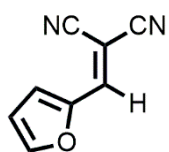
2-(4-Methylbenzylidene) malononitrile (9b)



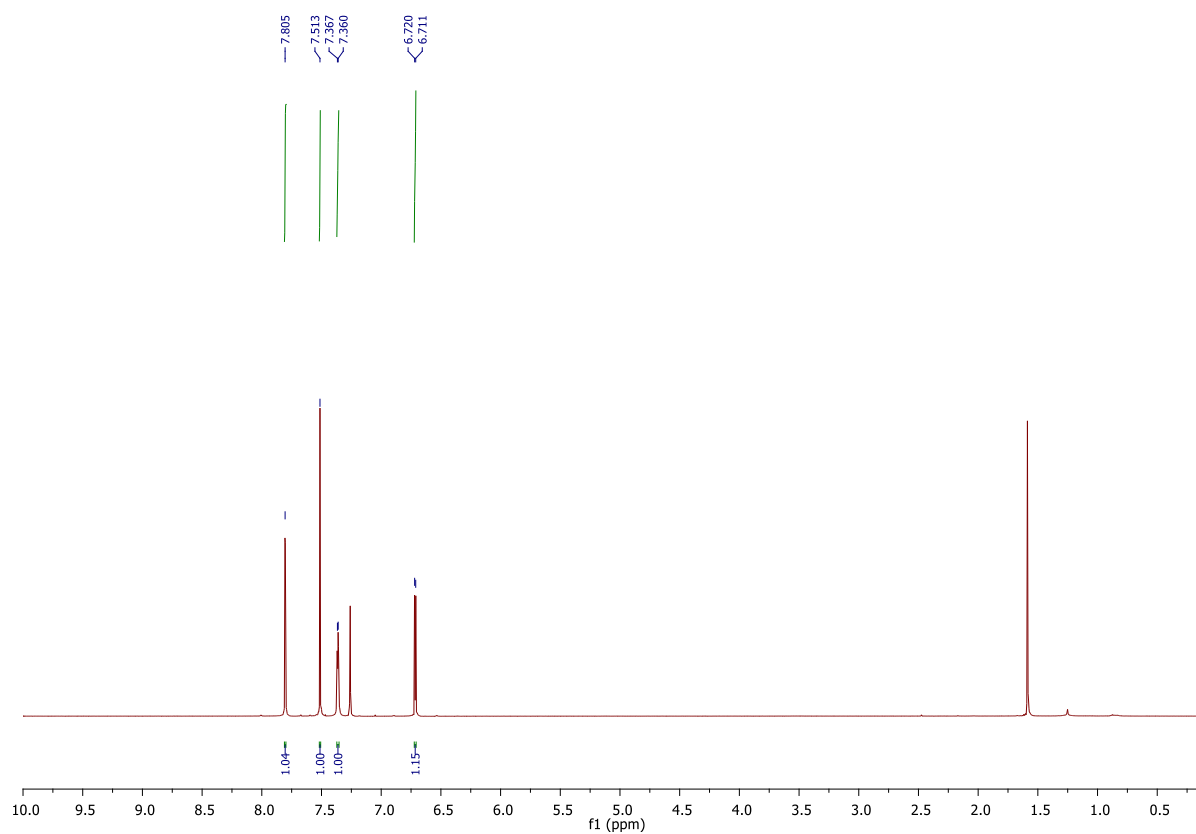
M. F. $C_{11}H_8N_2$ (168.19). Yield: (0.159 g, 95%). White powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.8 (d, J = 8.1 Hz, 2H), 7.71 (s, 1H), 7.34 (d, J = 8.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 159.8, 146.4, 131.6, 130.9, 130.4, 128.56, 114.0, 112.9, 81.2, 22.0.

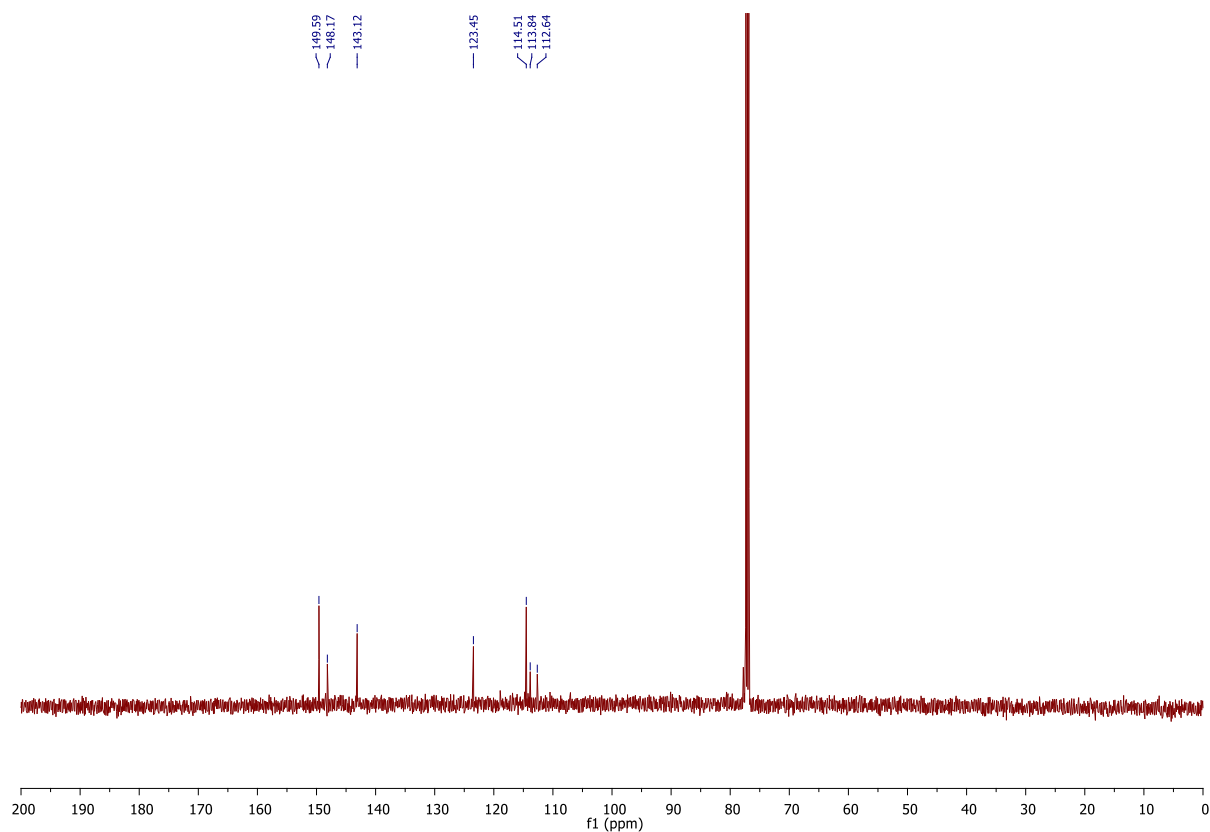


2-(Furan-2-ylmethylene) malononitrile (9c)

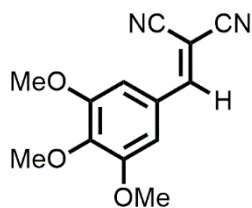


M. F. C₈H₄N₂S (144.13). Yield: (0.134.0 g, 93%). pale yellow powder. ¹H NMR (500 MHz, CDCl₃, ppm) δ 7.80 (s, 1H), 7.51 (s, 1H), 7.36 (d, J = 3.5 Hz, 1H), 6.7 (d, J = 4.5 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃, ppm) δ 149.5, 148.1, 143.1, 123.4, 114.5, 113.9, 112.6.

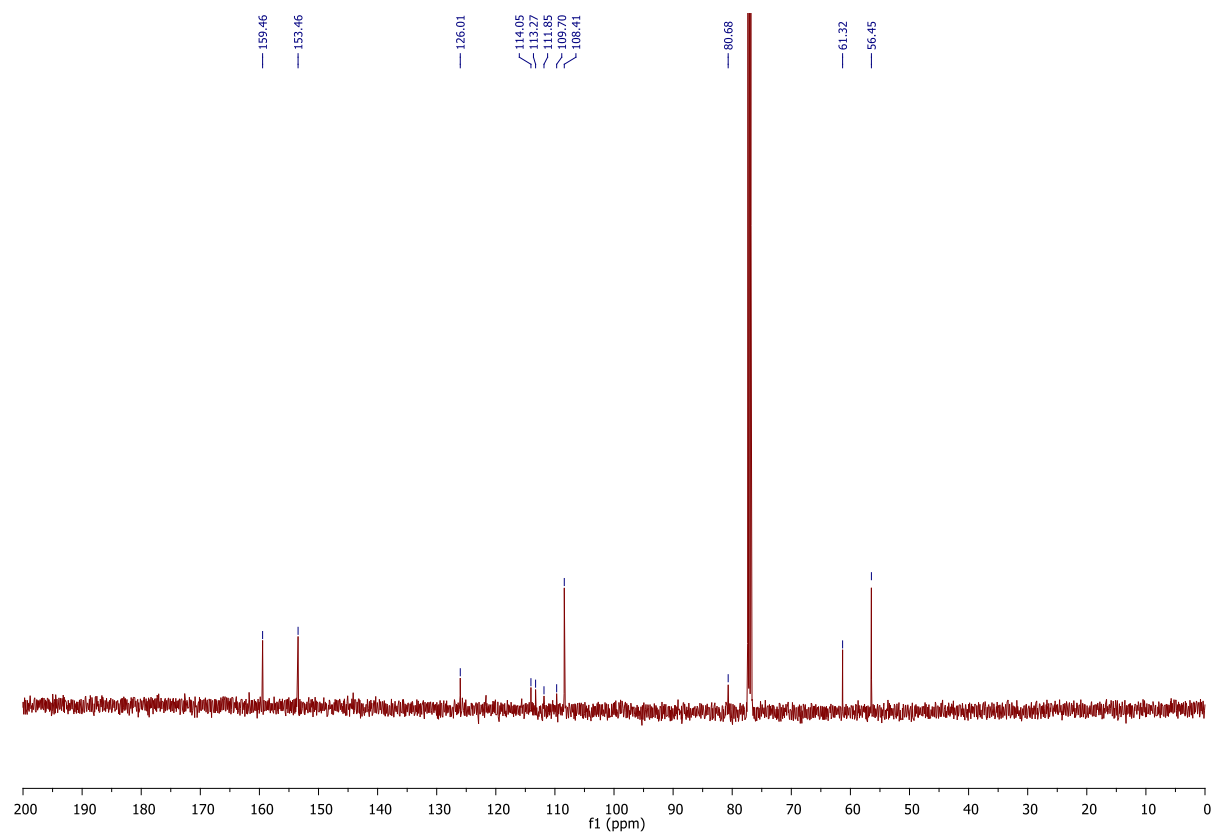
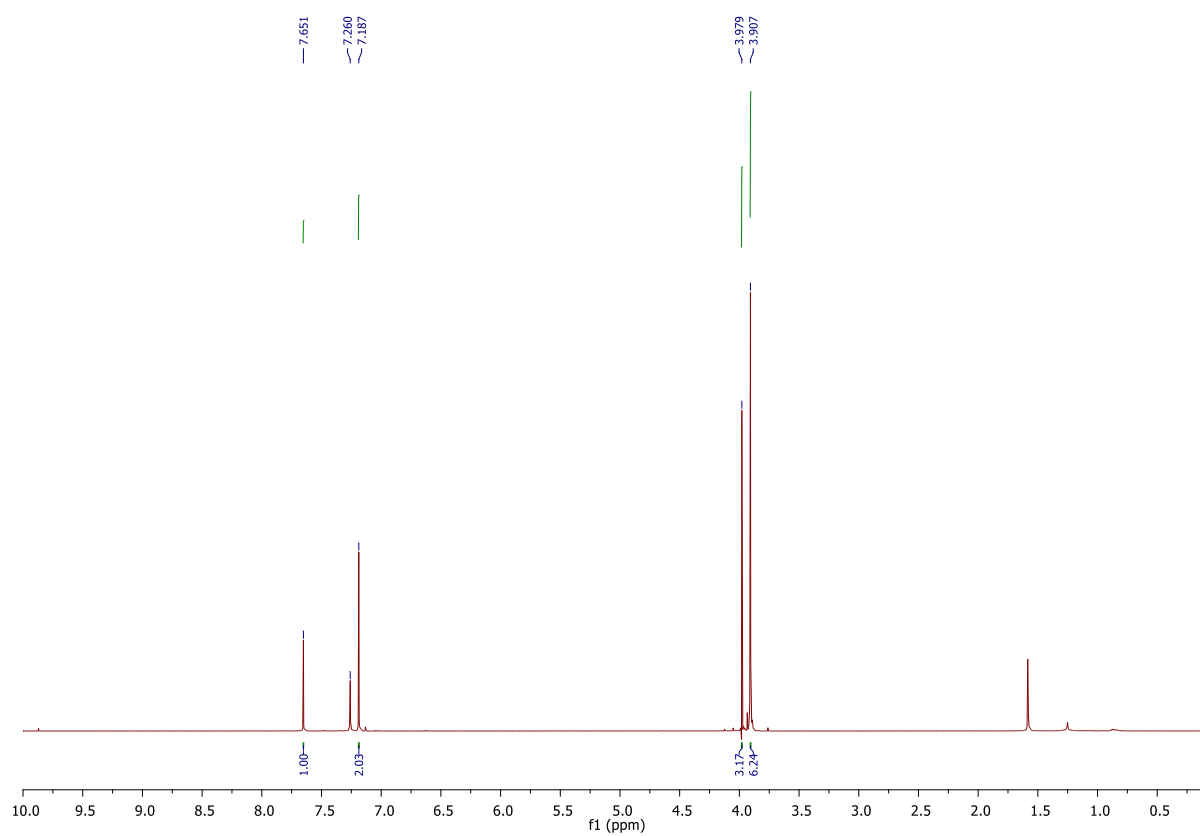




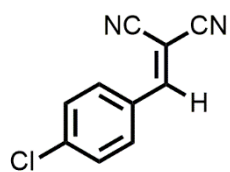
2-(3,4,5-Trimethoxybenzylidene) malononitrile (9d)



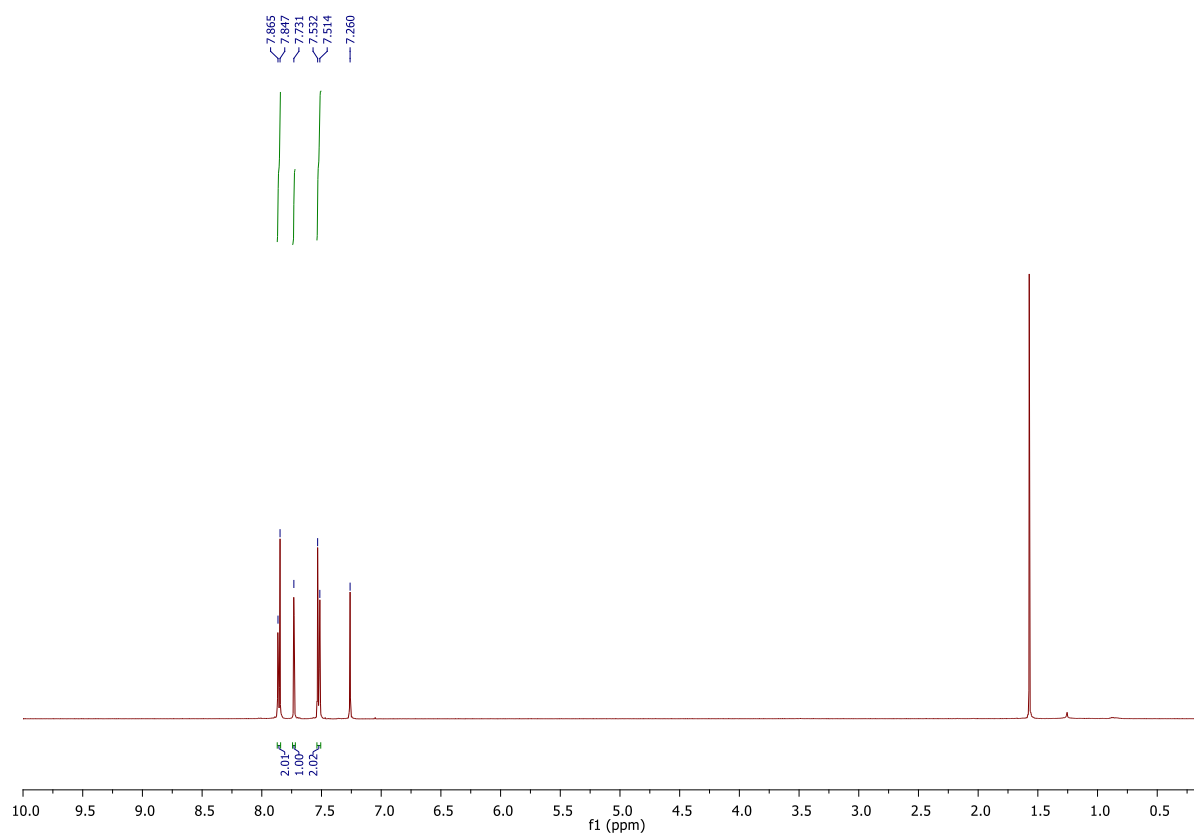
M. F. $C_{13}H_{12}N_2O_3$ (244.25). Yield: (0.238 g, 95%). Light yellow powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.6 (s, 1H), 7.18 (s, 2H), 3.97 (s, 3H), 3.90 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 159.4, 153.4, 126.0, 114.0, 113.2, 111.8, 109.7, 108.4, 80.6, 61.3, 56.4.

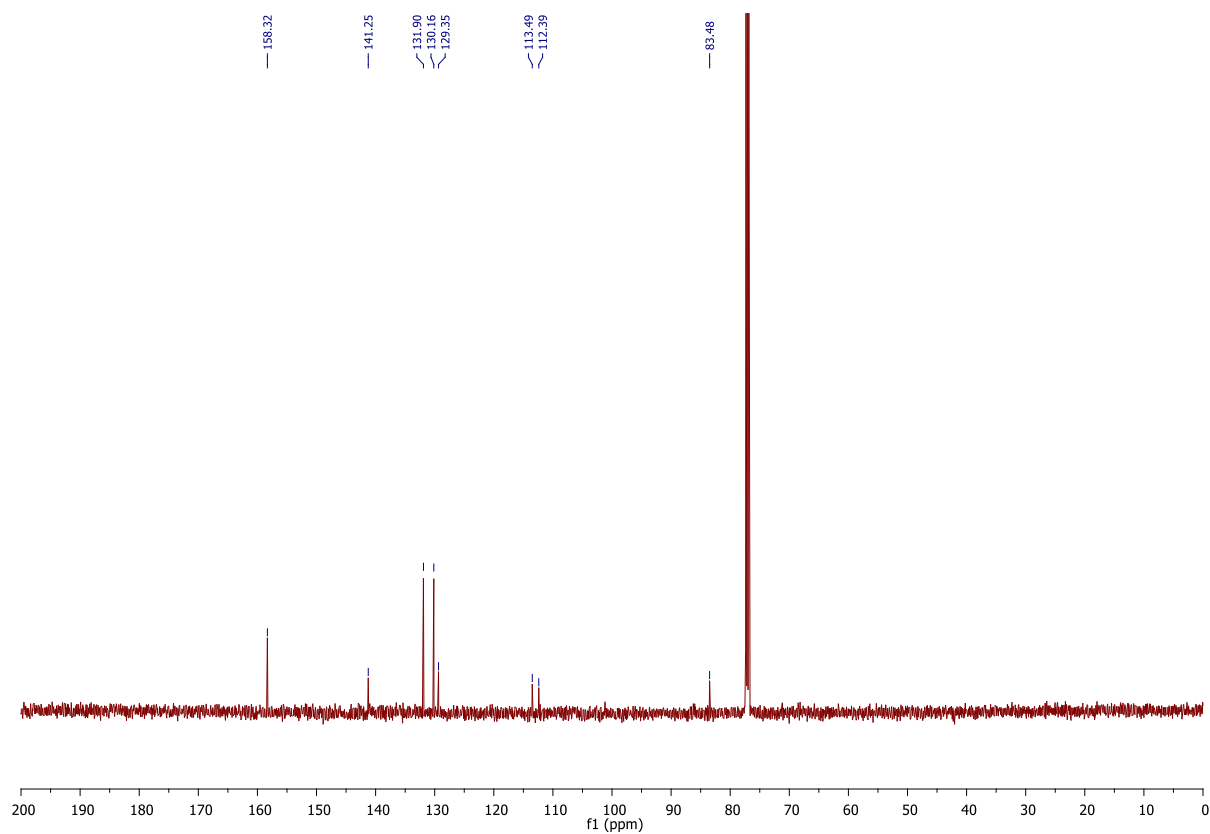


2-(4-chlorobenzylidene) malononitrile (9e)

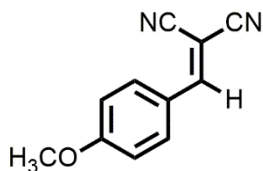


M.F. $C_{10}H_5ClN_2$ (188.61). Yield: (0.162 g, 86%). White powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.85 (d, $J = 9$ Hz, 2H), 7.73 (s, 1H), 7.52 (d, $J = 9$ Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 158.4, 141.3, 132.0, 130.3, 129.4, 113.9, 112.5, 83.5

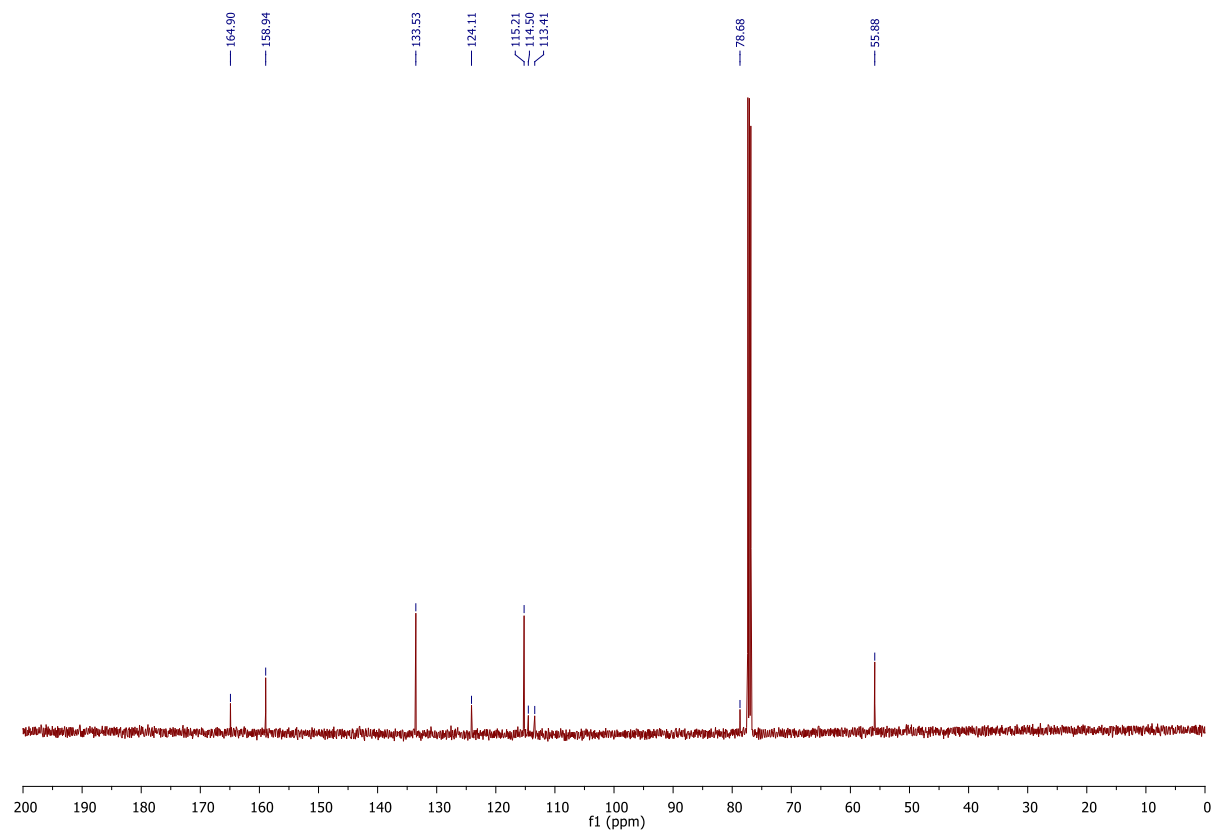
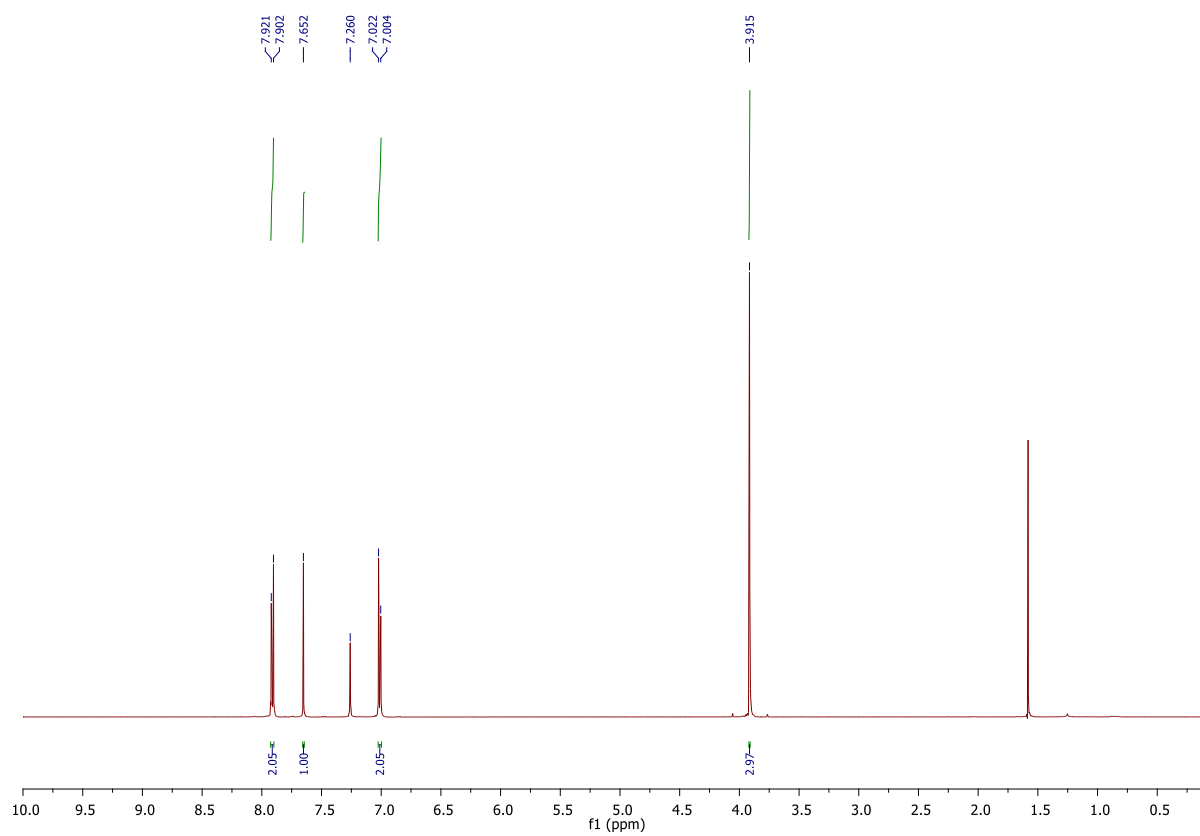




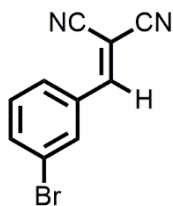
2-(4-Methoxybenzylidene) malononitrile (9f)



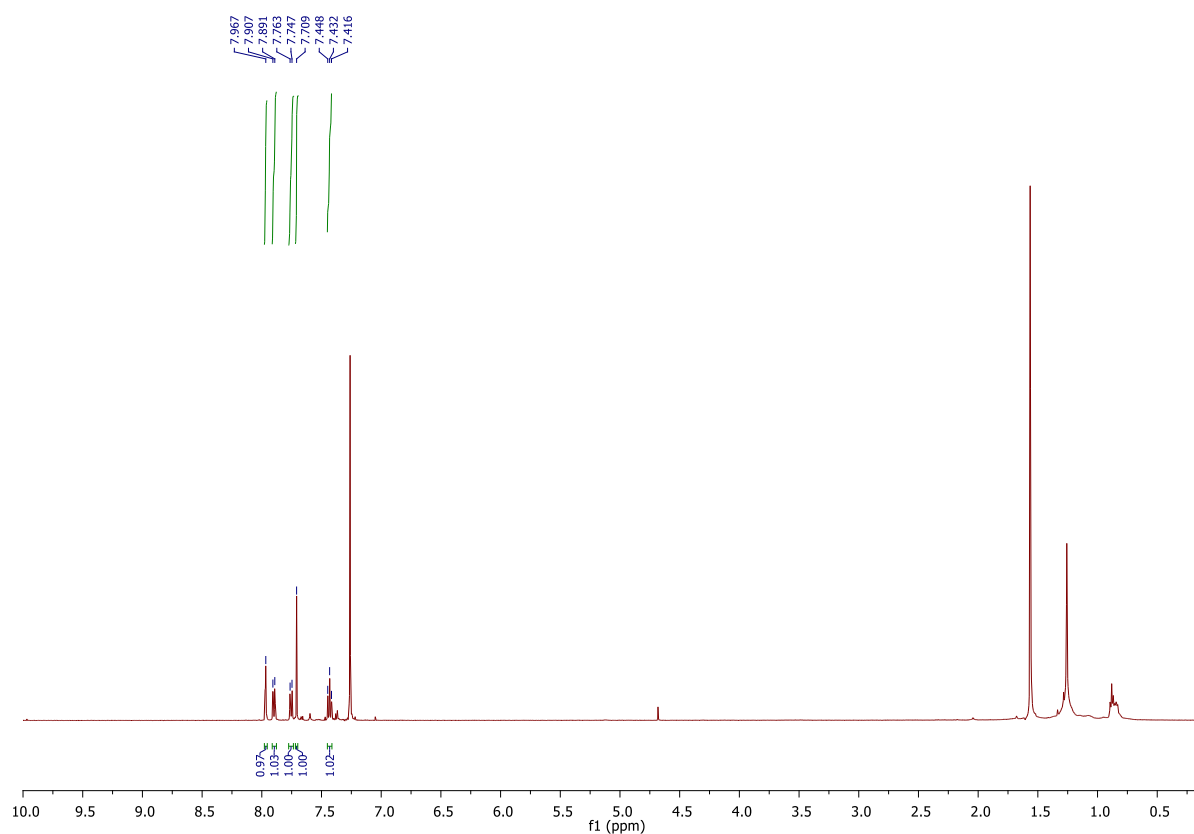
M.F. $C_{11}H_8N_2O$ (184.19). Yield: (0.176 g, 96%). Yellow powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.91 (d, $J = 9.5$ Hz, 2H), 7.65 (s, 1H), 7.01 (d, $J = 9.0$ Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.9, 158.9, 133.5, 124.1, 115.2, 114.5, 113.4, 78.6 55.8.

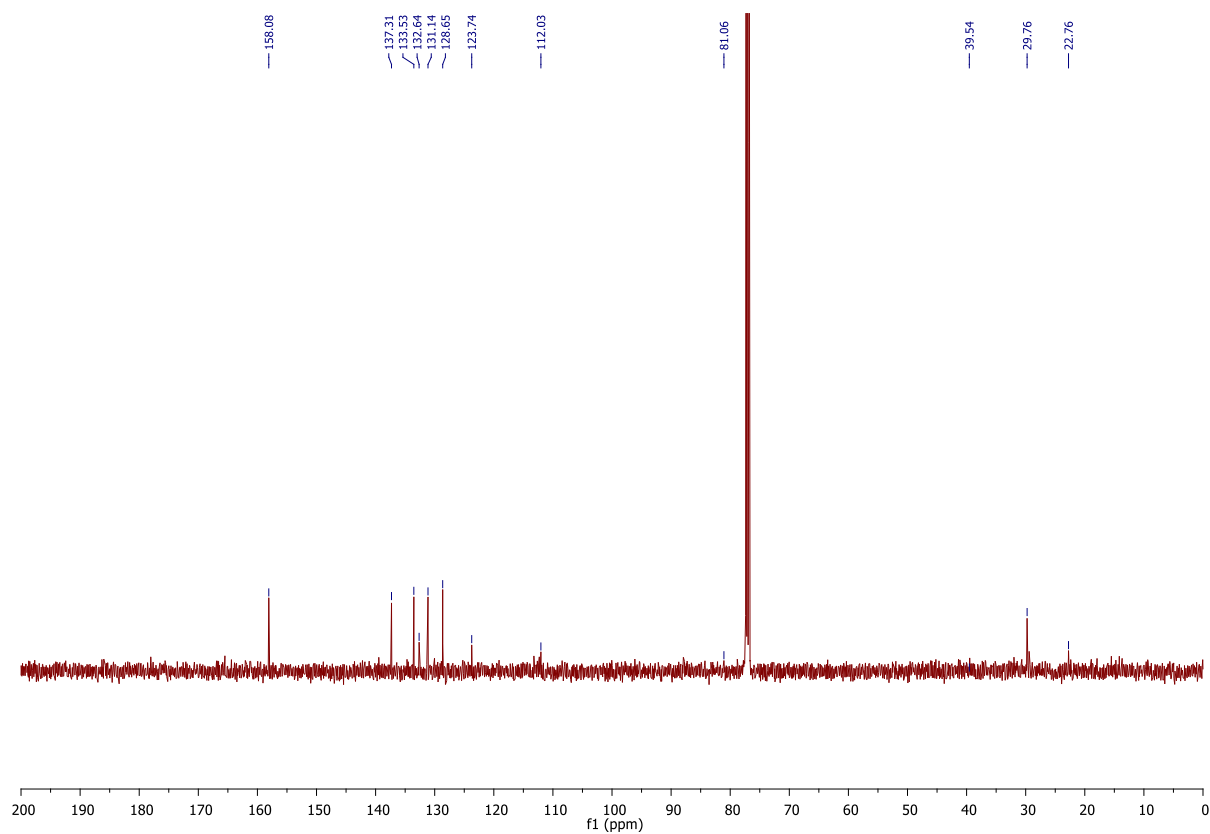


2-(3-Bromobenzylidene) malononitrile (**9g**)

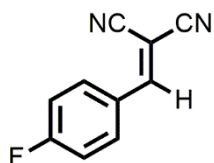


M.F. $C_{10}H_5BrN_2$ (233.06). Yield: (0.205g, 88%). White powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.96 (s, 1H), 7.90 (d, $J = 8.0$ Hz, 1H), 7.75 (d, $J = 8.0$ Hz, 1H), 7.70 (s, 1H), 7.43 (t, $J = 8.0$ Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 158.0, 137.3, 133.5, 132.6, 131.1, 128.6, 123.7, 112.0, 81.0.

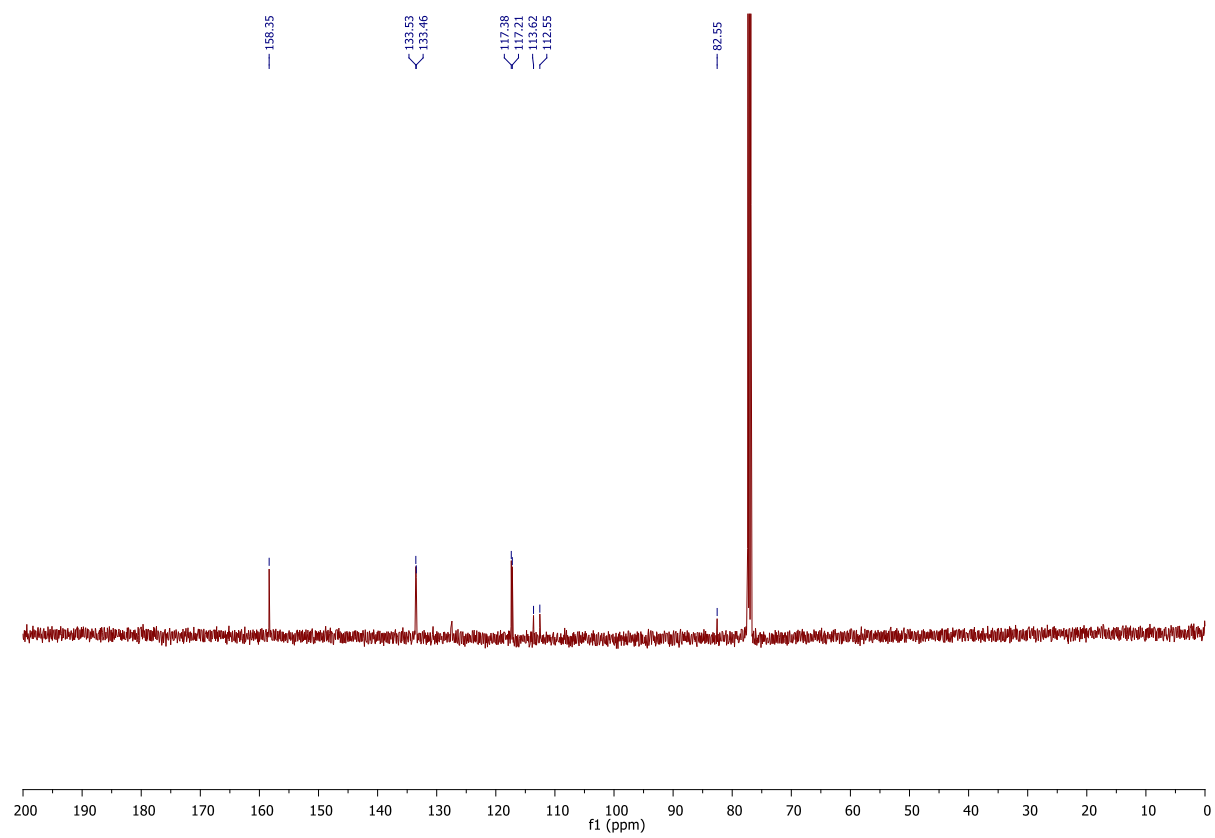
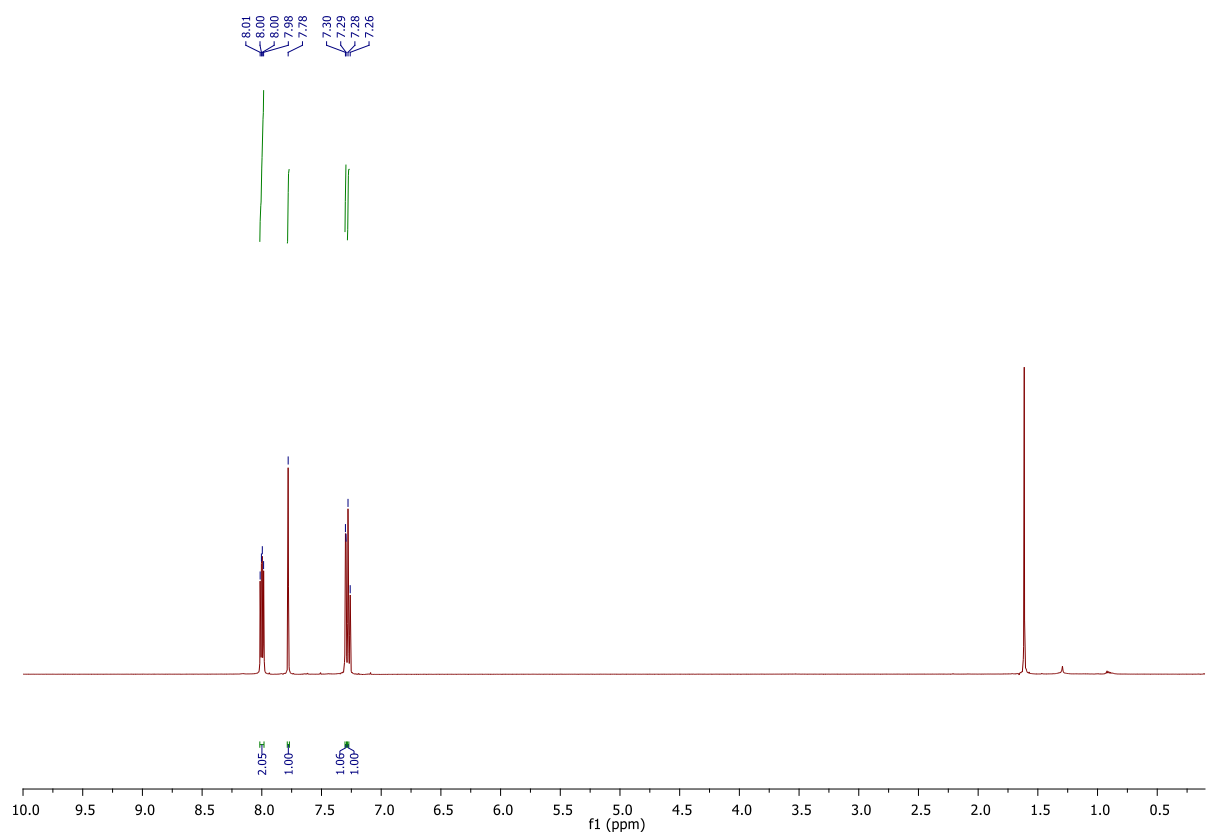




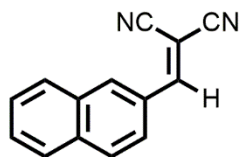
2-(4-fluorobenzylidene) malononitrile (9h)



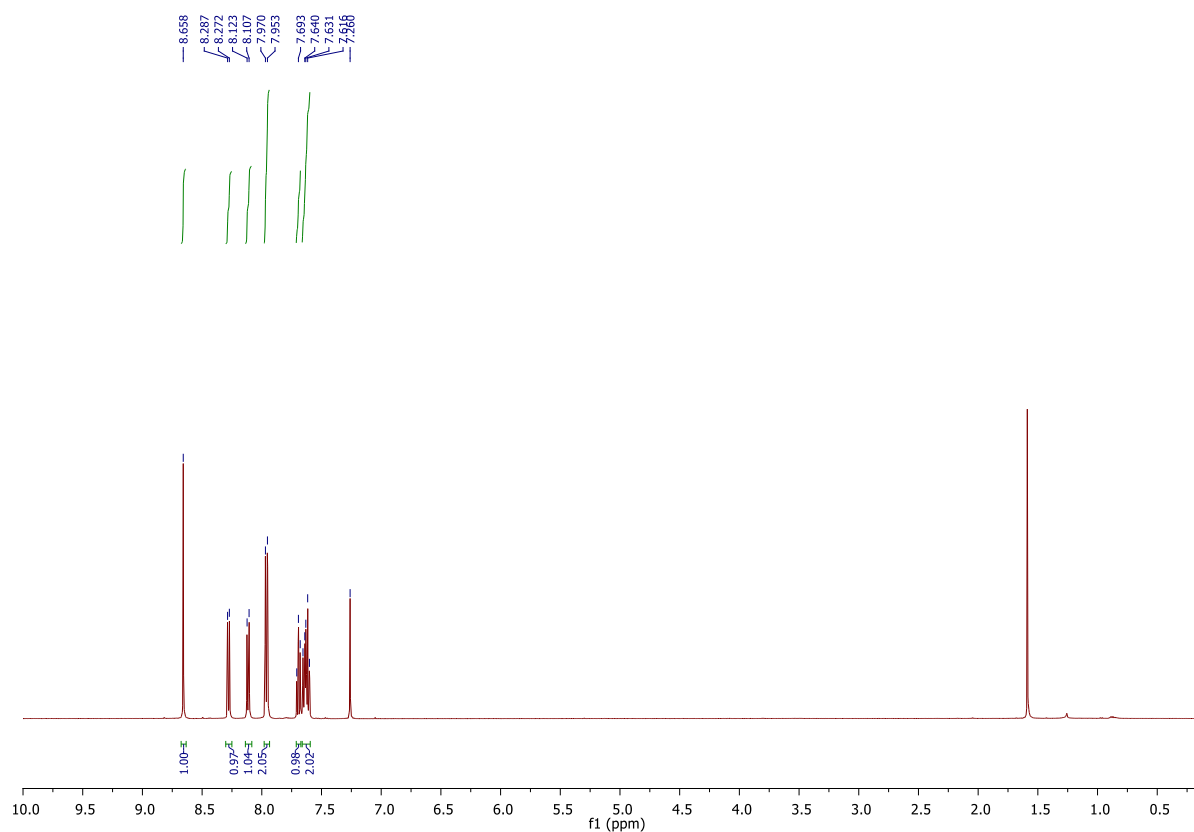
M.F. $C_{10}H_5FN_2$ (172.15). Yield: (0.158 g, 92%). White powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.01 – 7.98 (m, 2H), 7.78 (s, 1H), 7.30 – 7.26 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 158.3, 133.5, 133.4, 117.3, 117.2, 113.6, 112.5, 82.5.

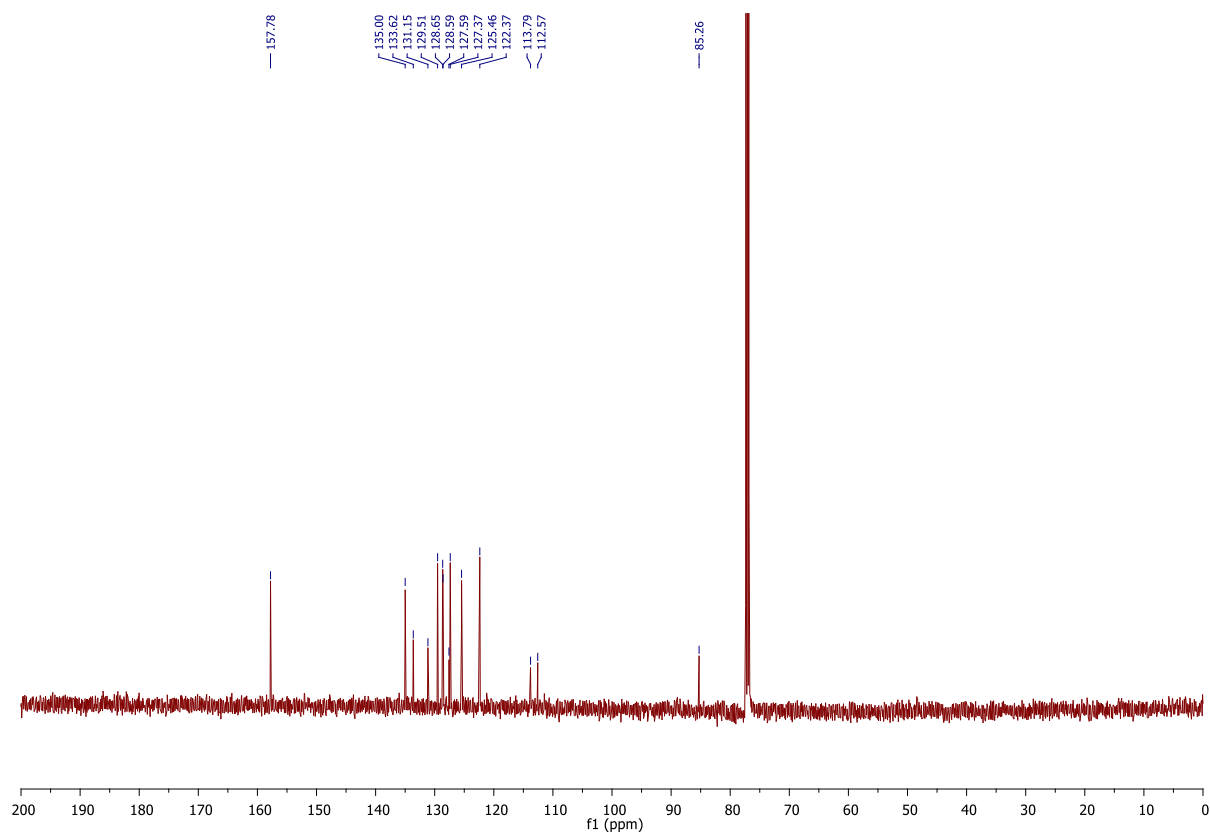


2-((Naphthalen-1-yl)methylene)malononitrile (9i)

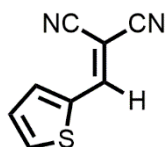


M.F. $C_{14}H_8N_2$ (204.23). Yield: (0.195 g, 96%). Pale yellow powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.66 (s, 1H), 8.28 (d, $J = 7.5$ Hz, 1H), 8.11 (d, $J = 8.0$ Hz, 1H), 7.96 (d, $J = 8.5$ Hz, 2H), 7.60 – 7.70 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 157.7, 135.0, 133.6, 131.2, 129.5, 128.7, 128.6, 127.6, 127.4, 125.5, 122.4, 113.8, 112.6, 85.3.

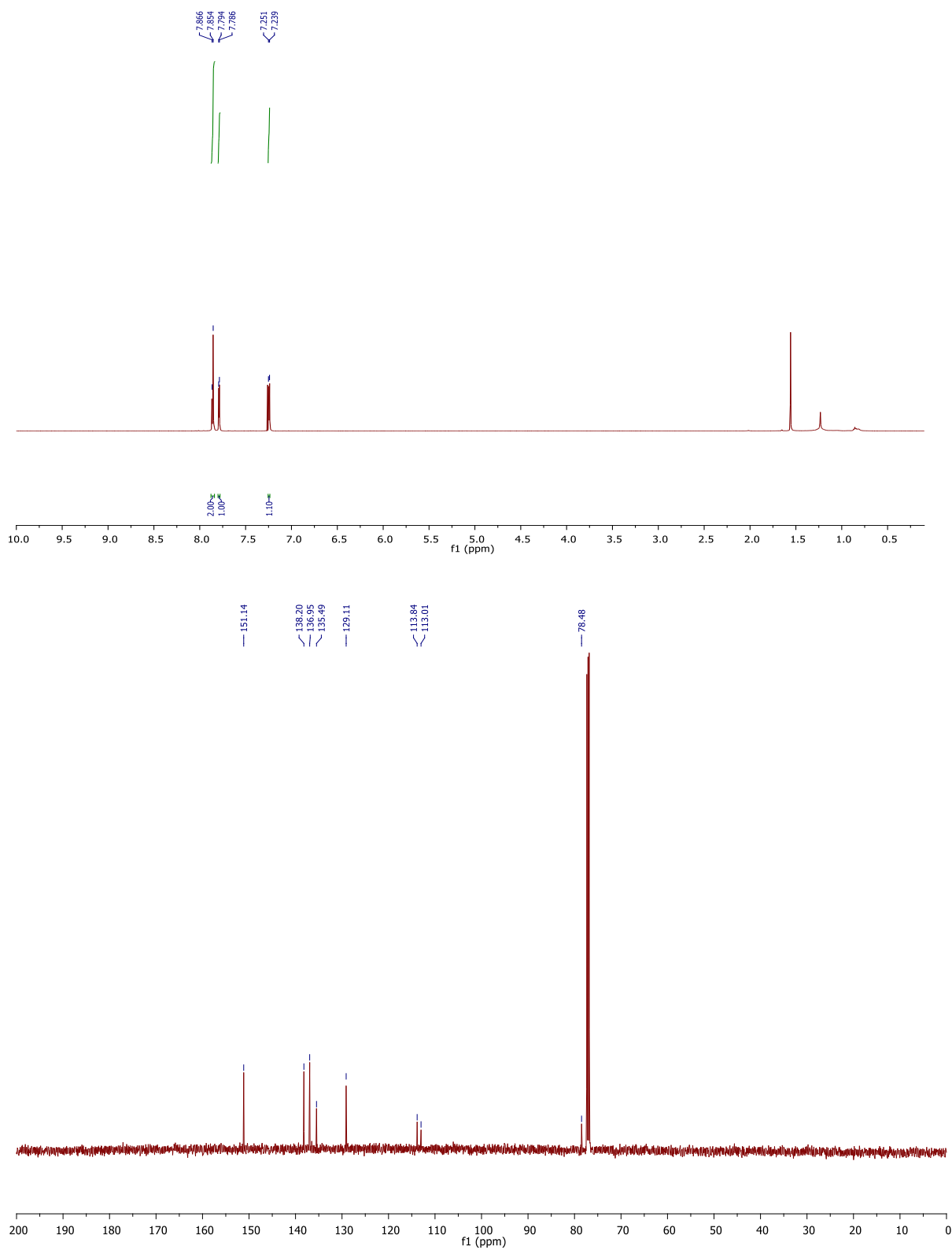




2-(Thiophen-2-ylmethylene) malononitrile (9j)

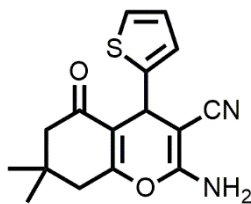


M.F. C₈H₄N₂S (160.20). Yield: (0.129 g, 81%). Light yellow powder. ¹H NMR (500 MHz, CDCl₃, ppm) δ 7.85 (d, J = 6.0 Hz, 2H), 7.78 (d, J = 4.0 Hz, 1H), 7.24 (d, J = 6.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃, ppm) δ 151.1, 138.2, 137.0, 135.5, 129.1, 113.8, 113.0, 78.5.

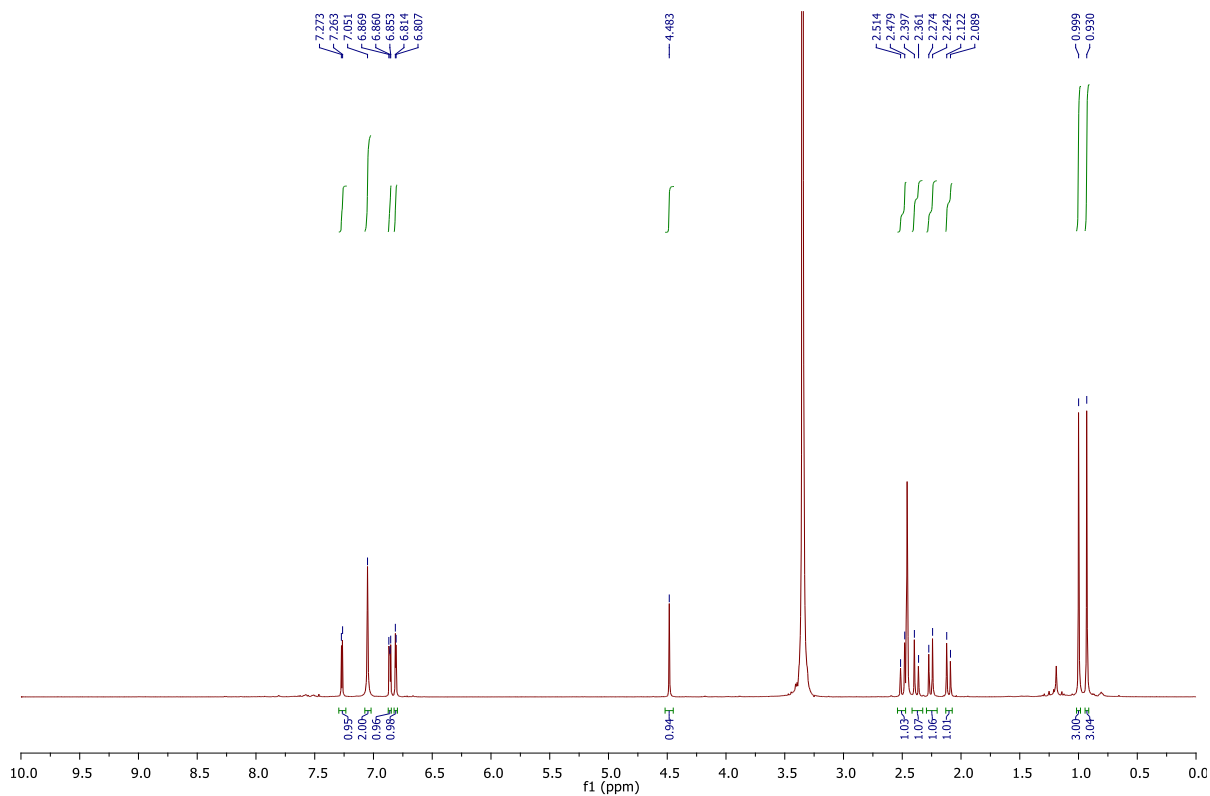


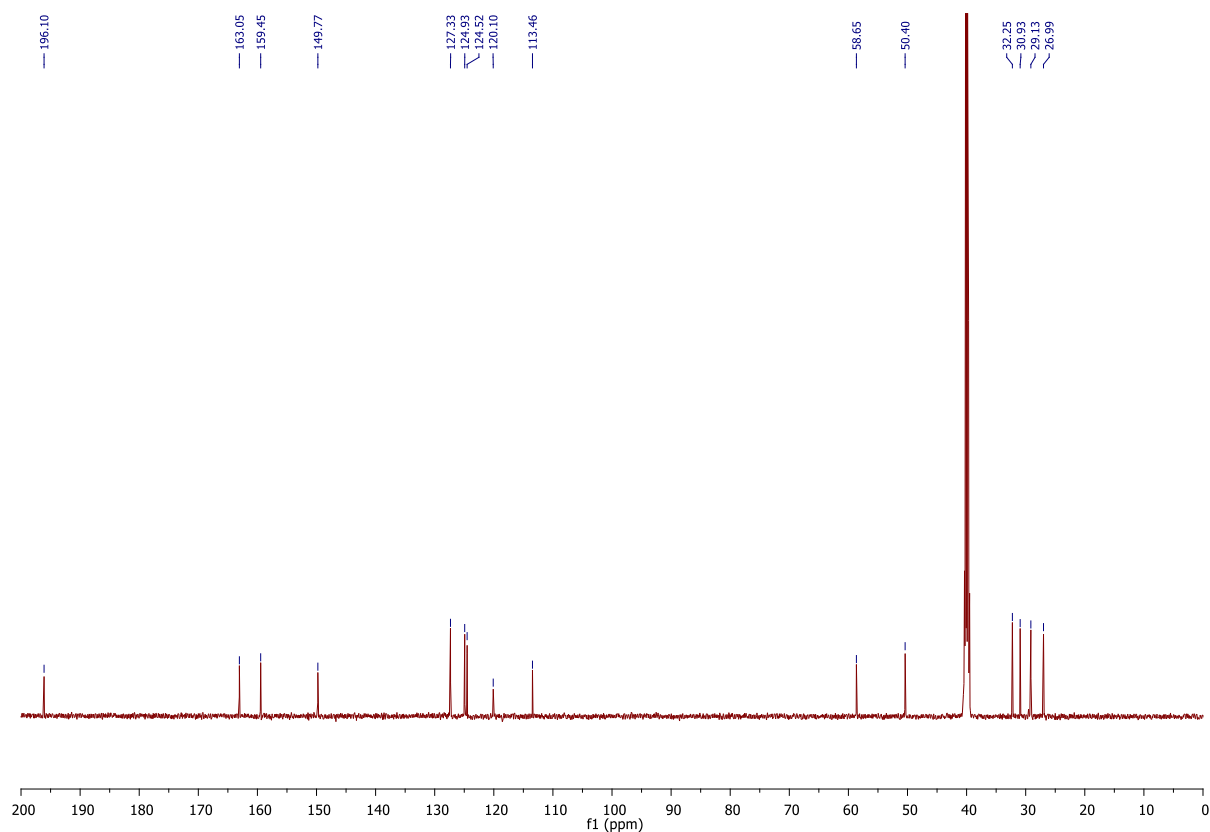
Characterization data and spectra (¹H and ¹³C) of the Multicomponent reaction Products {2-amino-4*H*-chromene derivatives} (10a-10o)

2-amino-7,7-dimethyl-5-oxo-4-(thiophen-2-yl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10a)

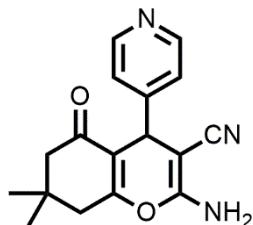


M.F. C₁₆H₁₆N₂O₂S (300.4). Yield: (0.282g, 96%). Yellow powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 7.26 (d, J = 5.0 Hz, 1H), 7.05 (s, 2H), 6.86 (t, J = 3.5 Hz, 1H), 6.81 (t, J = 3.5 Hz, 1H), 4.48 (s, 1H), 2.50 (d, J = 17.5 Hz, 1H), 2.38 (d, J = 18.0 Hz, 1H), 2.25 (d, J = 16.0 Hz, 1H), 2.10 (d, J = 16.5 Hz, 1H), 0.99 (s, 3H), 0.93 (s, 3H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 196.1, 163.1, 159.5, 148.9, 149.8, 127.3, 124.9, 124.5, 120.1, 113.5, 58.6, 50.4, 32.3, 30.9, 29.1, 26.9.

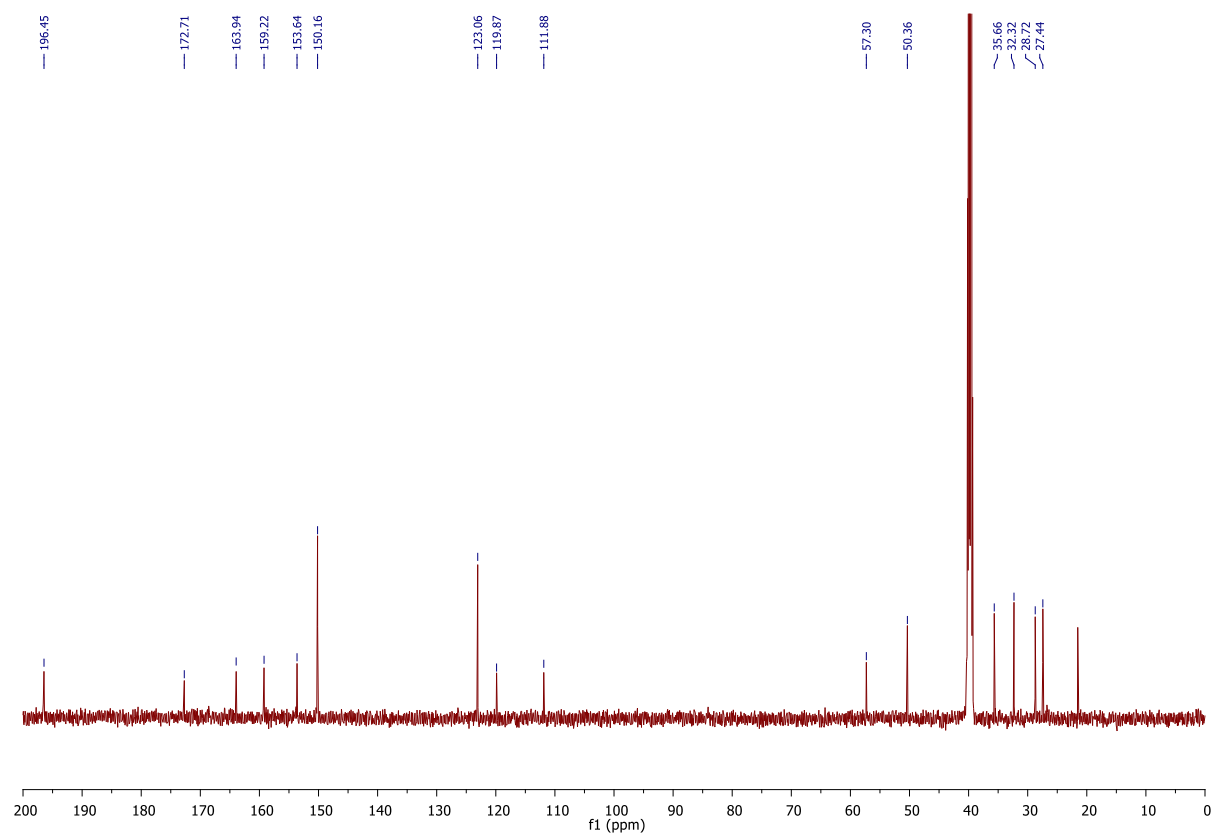
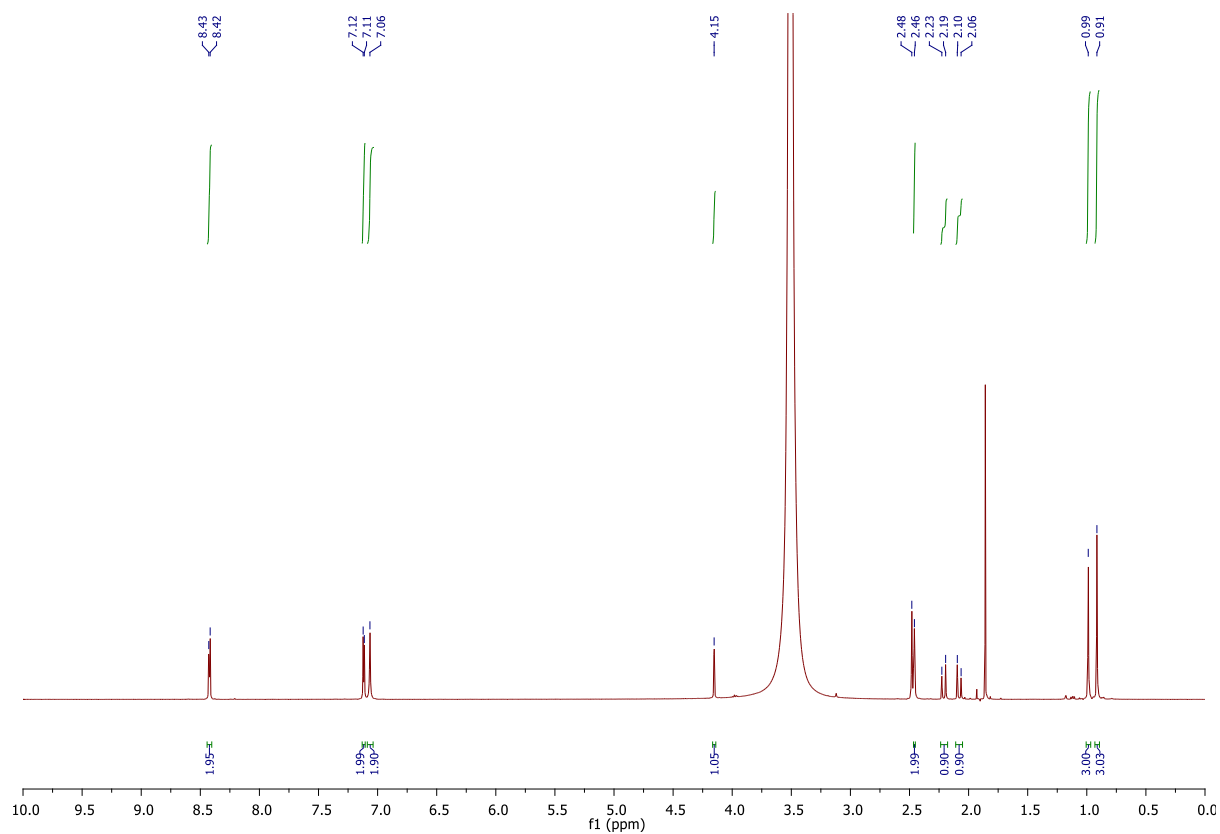




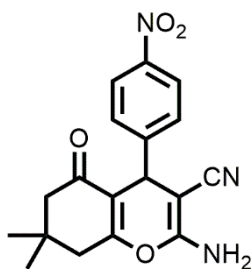
2-amino-7,7-dimethyl-5-oxo-4-(pyridin-4-yl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10b)



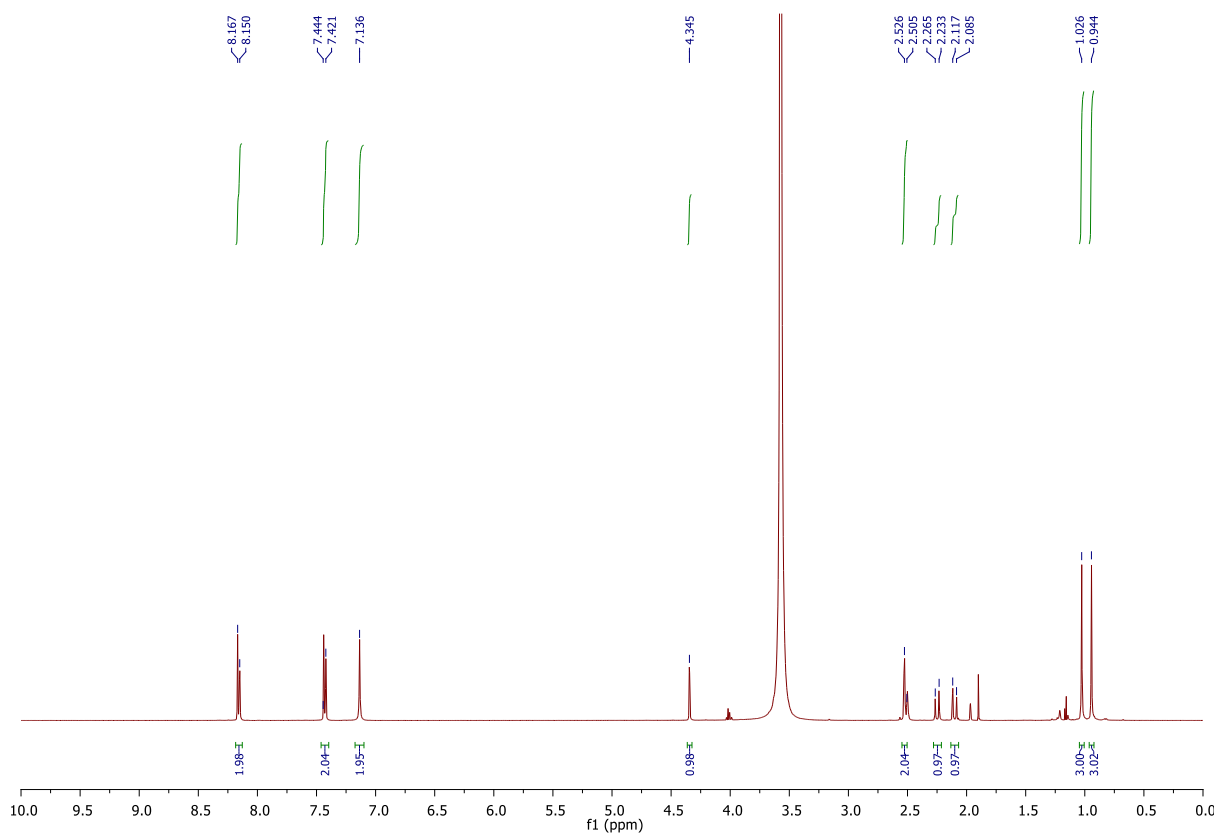
M.F. C₁₇H₁₇N₃O₂ (295.34). Yield: (0.260g, 88%). Yellow powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 8.42 (d, J = 5.5 Hz, 2H), 7.11 (d, J = 5.5 Hz, 2H), 7.06 (s, 2H), 4.15 (s, 1H), 2.45-2.49 (m, 2H), 2.20 (d, J = 16.0 Hz, 1H), 2.08 (d, J = 16.0 Hz, 1H), 0.99(s, 3H), 0.91(s, 3H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 196.5, 172.7, 163.9, 159.2, 153.6, 150.2, 123.1, 119.9, 111.9, 57.3, 50.4, 35.7, 32.3, 28.7, 27.4.

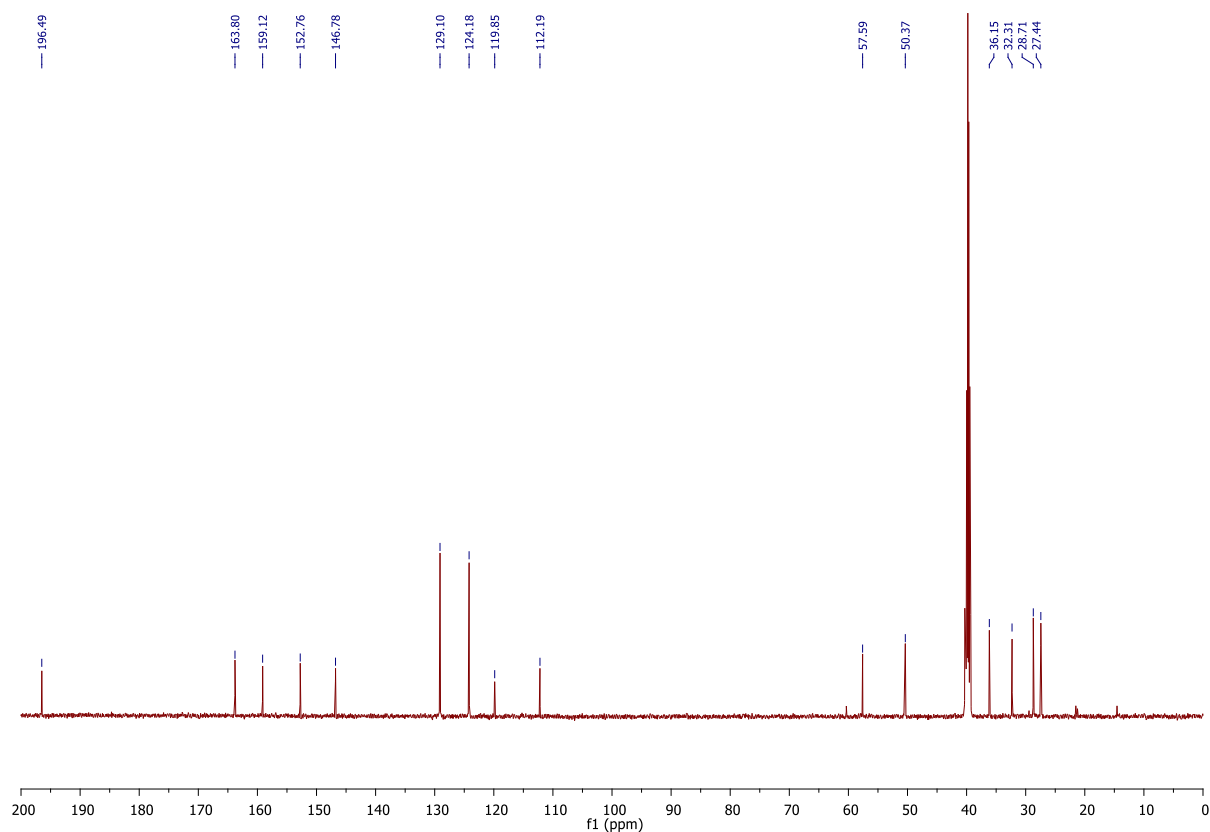


2-amino-7,7-dimethyl-4-(4-nitrophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10c)

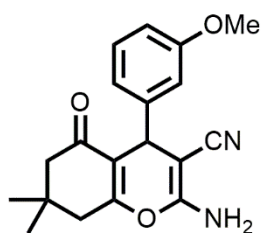


M.F. C₁₈H₁₇N₃O₄ (339.35). Yield: (0.294 g, 87%). Off white powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.16 (d, J = 8.5 Hz, 2H), 7.43 (d, J = 11.5 Hz, 2H), 7.13 (s, 2H), 4.35 (s, 1H), 2.51 (d, J = 10.5 Hz, 2H), 2.25 (d, J = 16.0 Hz, 1H), 2.10 (d, J = 16.0 Hz, 1H), 1.02 (s, 3H), 0.94 (s, 3H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 196.5, 163.8, 159.1, 152.8, 146.8, 129.1, 124.2, 119.9, 112.2, 57.6, 50.4, 36.2, 32.3, 28.7, 27.4.

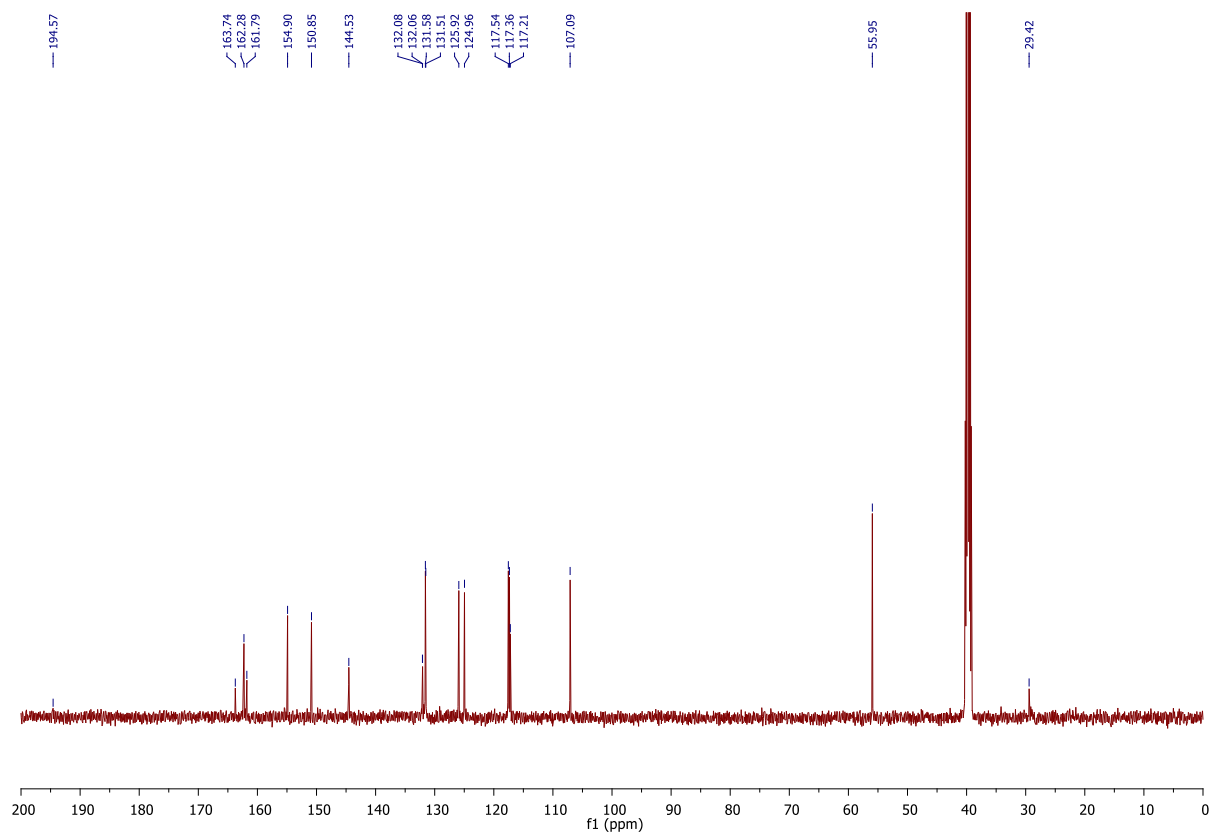
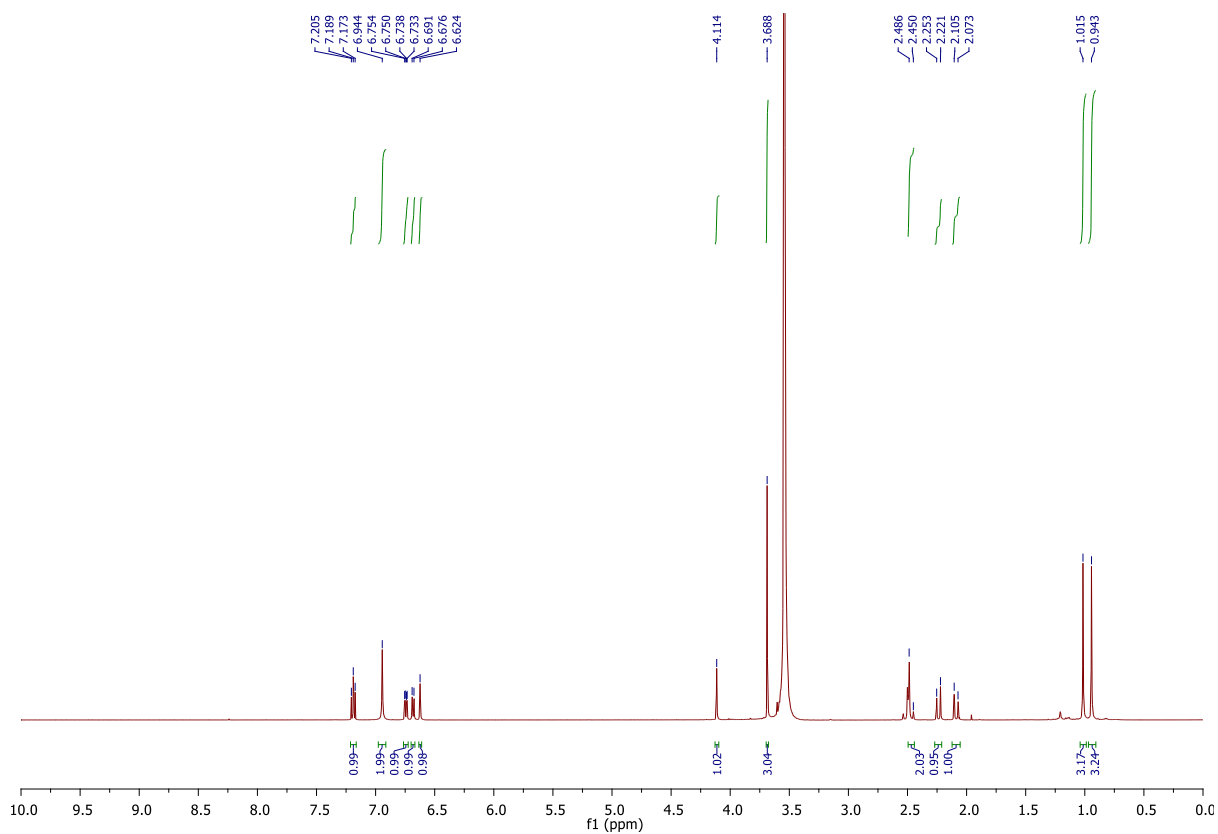




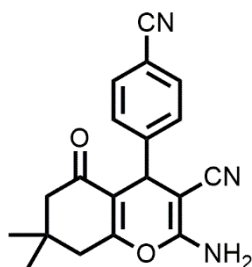
2-amino-4-(3-methoxyphenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10d)



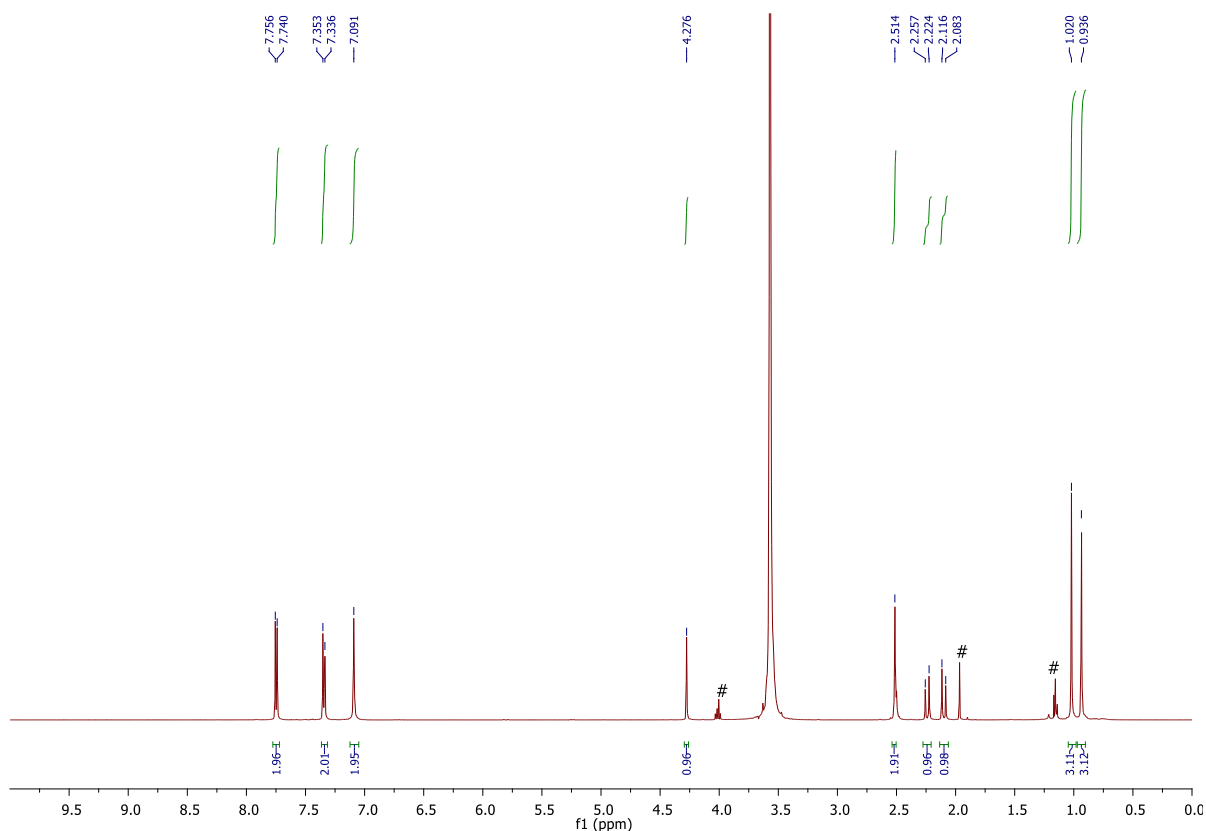
M.F. C₁₉H₂₀N₂O₃ (324.37). Yield: (0.301 g, 93%). Off white powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 7.19 (t, J = 8.0 Hz, 1H), 6.94(s, 2H), 6.75, 6.73 (d,d, J = 2.0, 2.5 Hz, 1H), 6.68 (d, J = 7.5 Hz, 1H), 4.11 (s, 1H), 3.69 (s, 3H), 2.47 (d, J = 16.0 Hz, 1H), 2.10 (d, J = 16.0 Hz, 1H), 1.01 (s, 3H), 0.94 (s, 3H); ¹³C NMR (125 MHz, DMSO d₆, ppm) δ 194.5, 163.7, 162.2, 161.7, 154.9, 150.8, 144.5, 132.0, 131.5, 125.9, 124.9, 117.5, 117.3, 117.2, 107.0, 55.9, 29.4

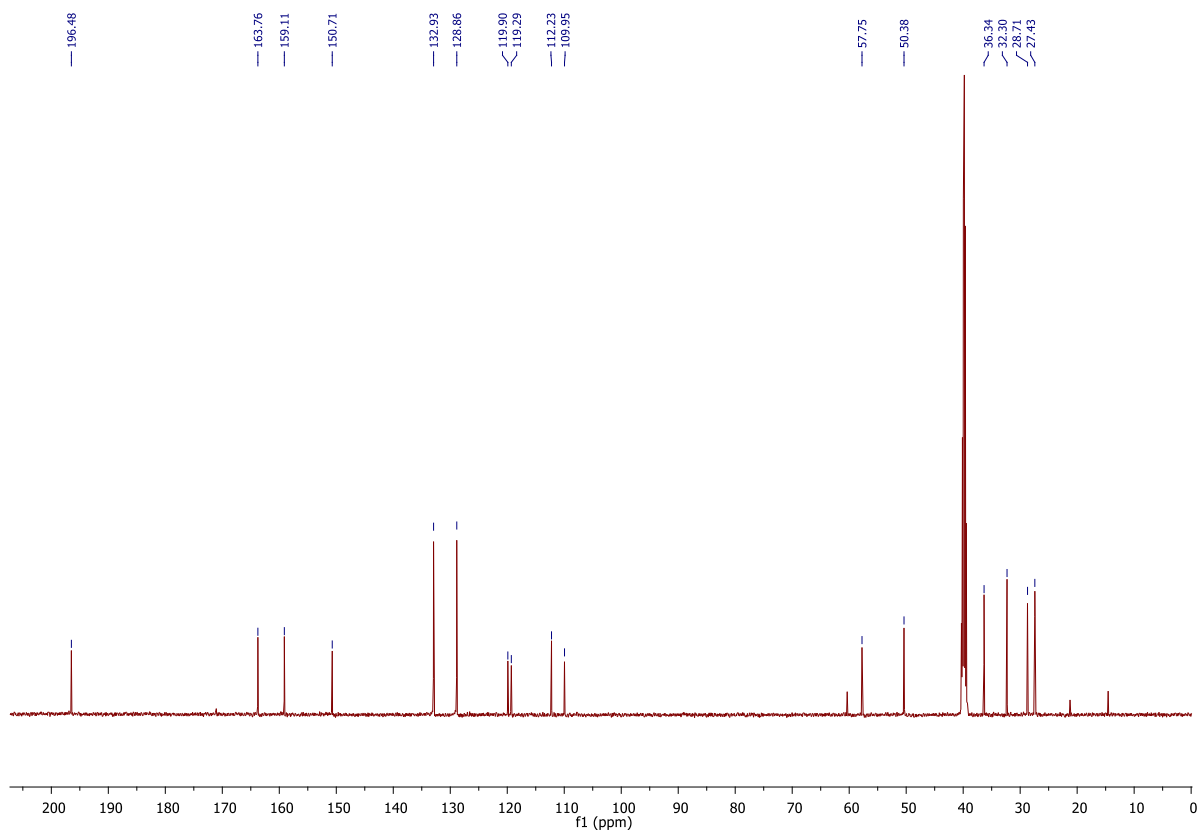


2-amino-4-(4-cyanophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10e)

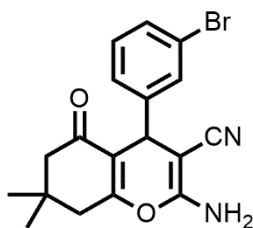


M.F. C₁₉H₁₇N₃O₂ (319.36). Yield: (0.280 g, 88%). White powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 7.75 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.5 Hz, 2H), 7.09 (s, 2H), 4.27 (s, 1H), 2.51 (s, 2H), 2.24 (d, J = 16.5 Hz, 1H), 2.10 (d, J = 16.5 Hz, 1H), 1.02 (s, 3H), 0.94 (s, 3H); ¹³C NMR (125 MHz, DMSO d₆, ppm) δ 196.5, 163.7, 159.1, 150.7, 132.9, 128.8, 119.9, 119.2, 112.2, 109.9, 57.7, 50.3, 36.3, 32.3, 28.7, 27.43.

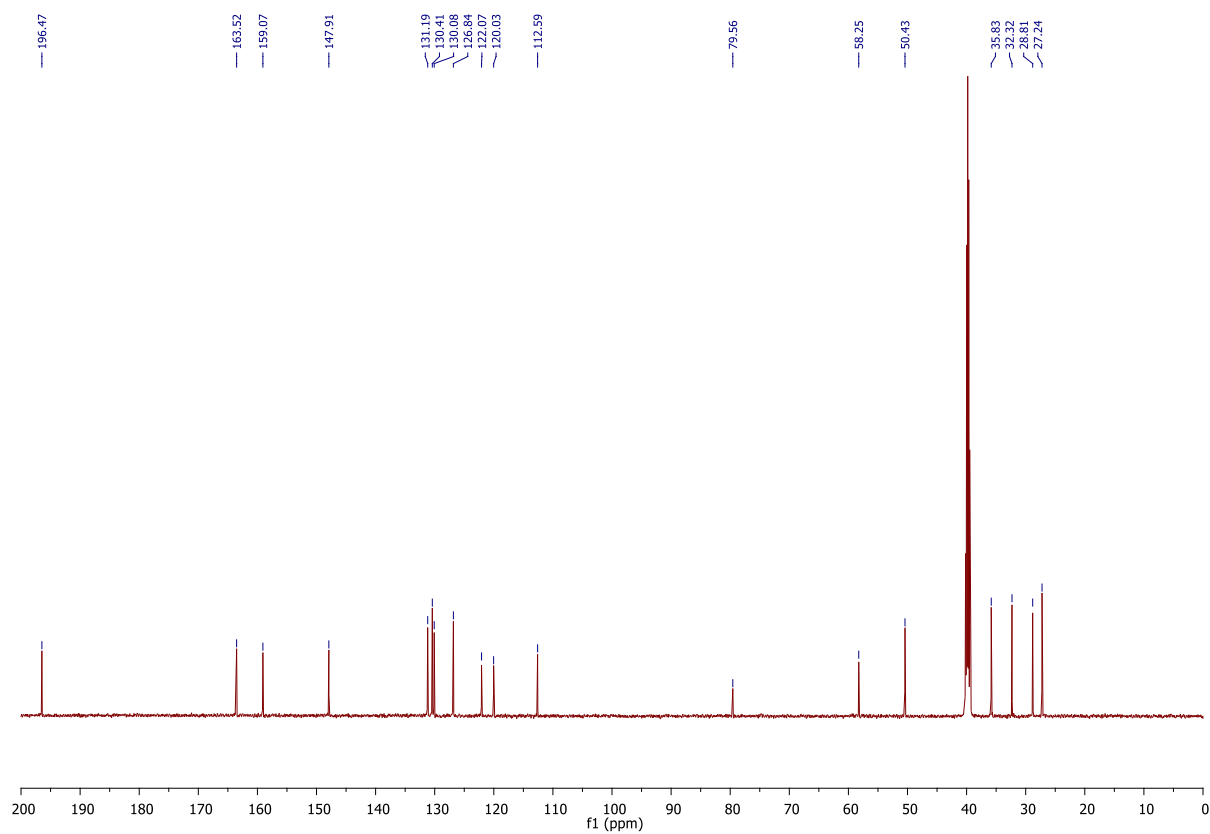
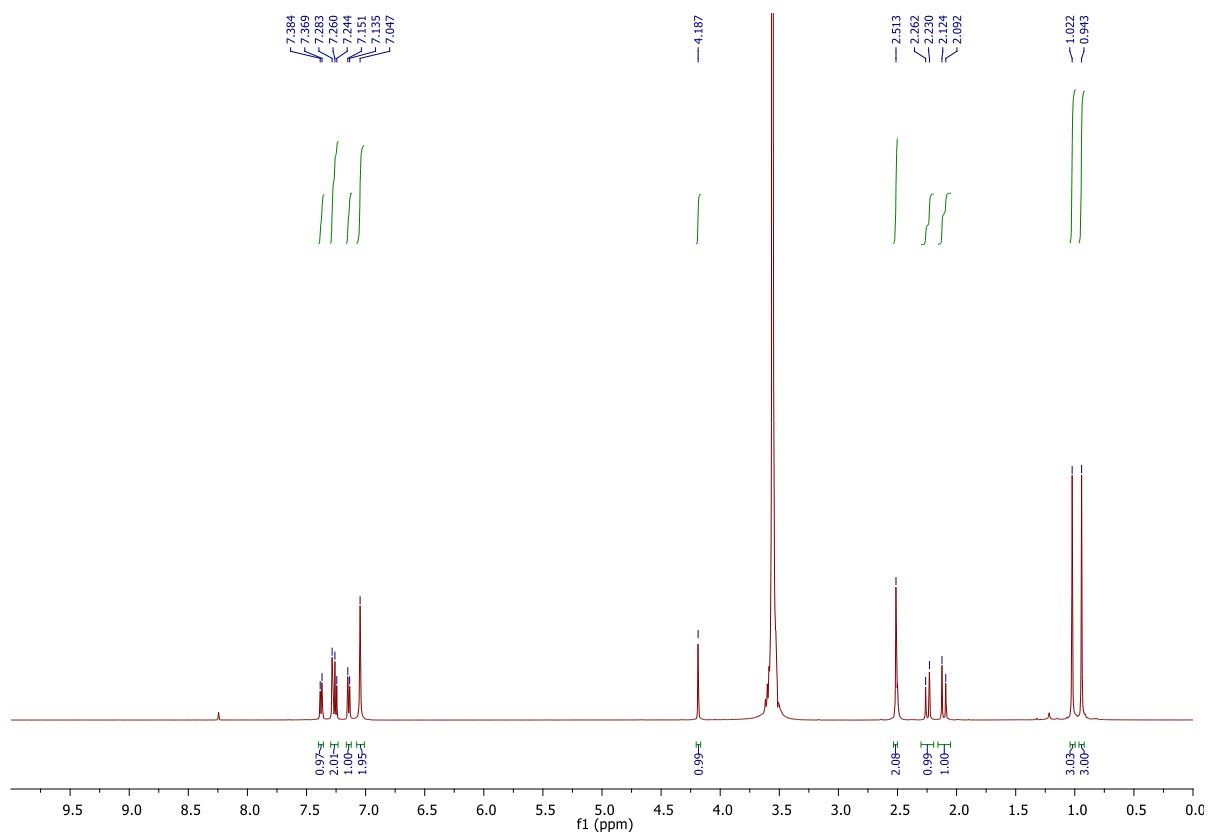




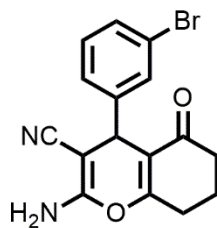
2-amino-4-(3-bromophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10f)



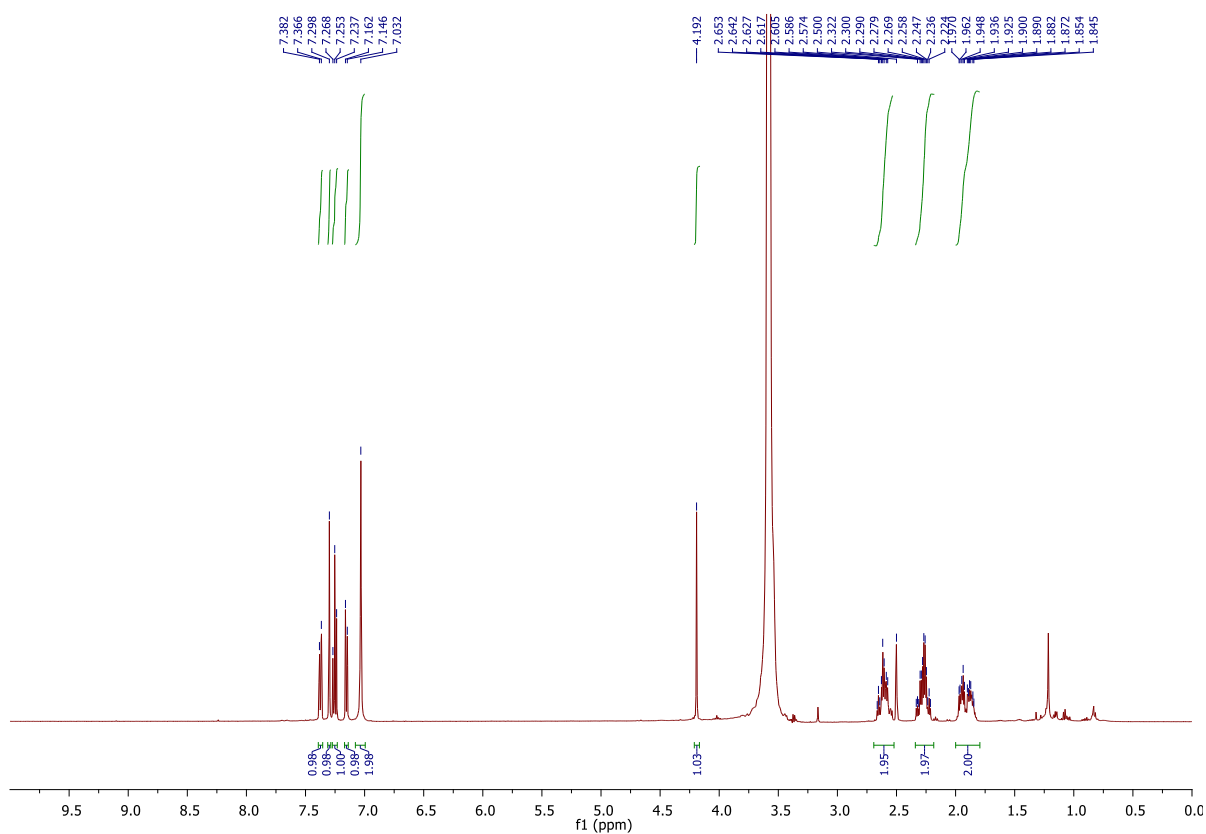
M.F. $C_{18}H_{17}BrN_2O_2$ (358.21). Yield: (0.335 g, 90%). White powder. 1H NMR (500 MHz, DMSO d_6 , ppm) δ 7.37 (d, $J = 7.5$ Hz, 2H), 7.26 (t, $J = 8.0$ Hz, 2H), 7.14 (d, $J = 7.5$ Hz, 1H), 7.04 (s, 2H), 4.19 (s, 1H), 2.51 (s, 2H), 2.25 (d, $J = 16.0$ Hz, 1H), 2.10 (d, $J = 15.0$ Hz, 1H), 1.02 (s, 3H), 0.93 (s, 3H); ^{13}C NMR (125 MHz, DMSO d_6 , ppm) δ 196.5, 163.5, 159.0, 147.9, 131.2, 130.4, 130.0, 126.8, 122.0, 120.0, 79.5, 58.2, 50.4, 35.8, 32.3, 28.8, 27.24.

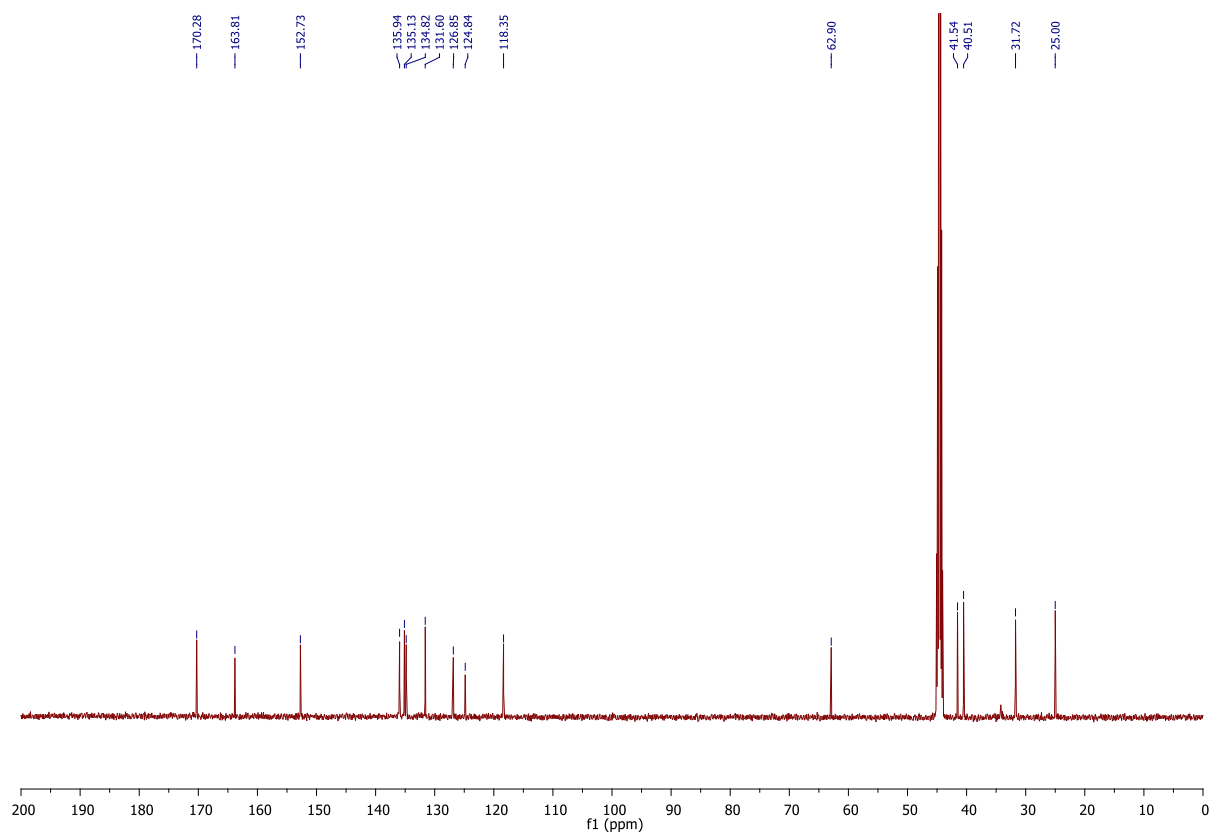


2-amino-4-(3-bromophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10g)

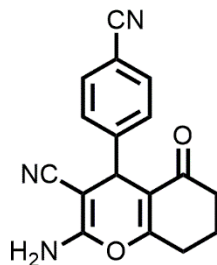


M.F. C₁₆H₁₃BrN₂O₂ (345.19). Yield: (0.327 g, 95%). White powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 7.37 (d, J = 8.0 Hz, 1H), 7.29 (s, 1H), 7.25 (t, J = 8.0 Hz, 1H), 7.15 (d, J = 8.0 Hz, 1H), 7.03 (s, 2H), 4.19 (s, 1H), 2.57-2.66 (m, 2H), 2.21-2.33 (m, 2H), 1.84-1.97 (m, 2H), ¹³C NMR (125 MHz, DMSO d₆, ppm) δ 170.3, 163.8, 152.7, 135.9, 135.1, 134.8, 131.6, 126.8, 124.8, 118.3, 62.9, 41.5, 40.5, 31.7, 25.0.

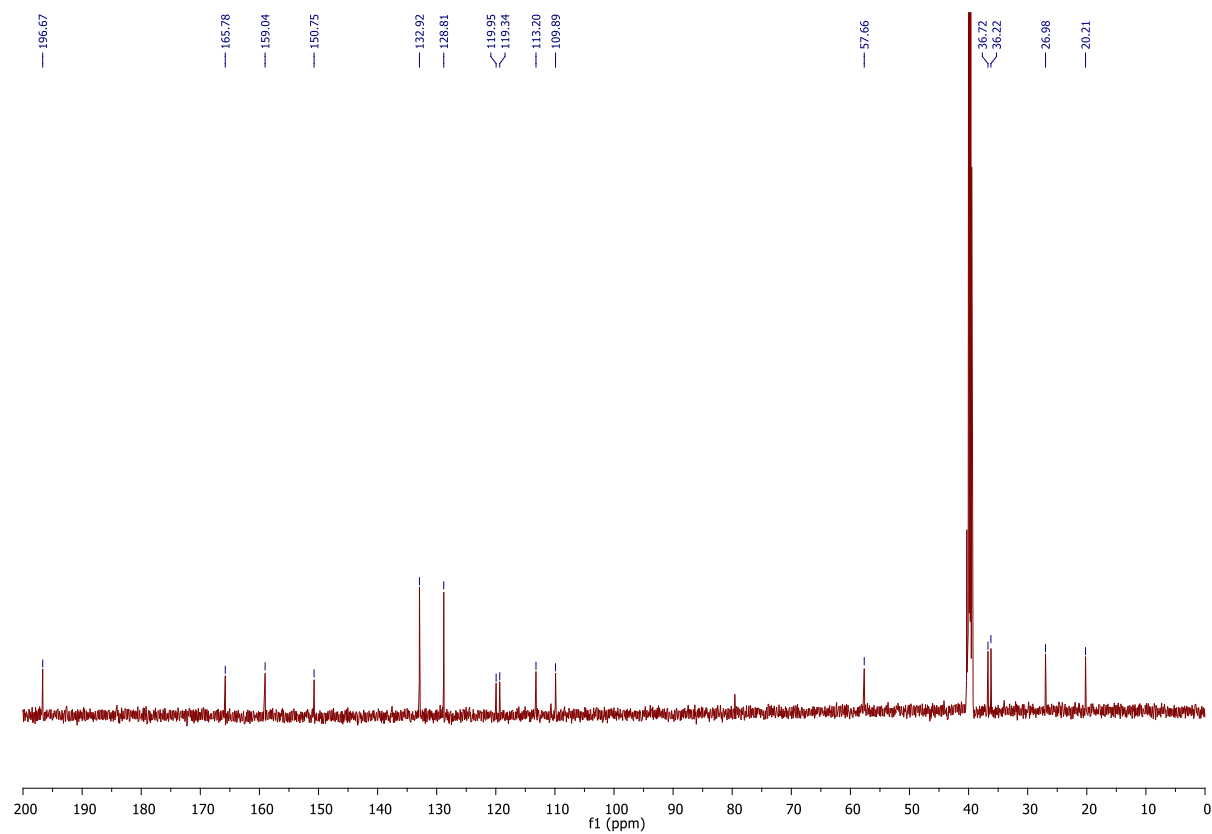
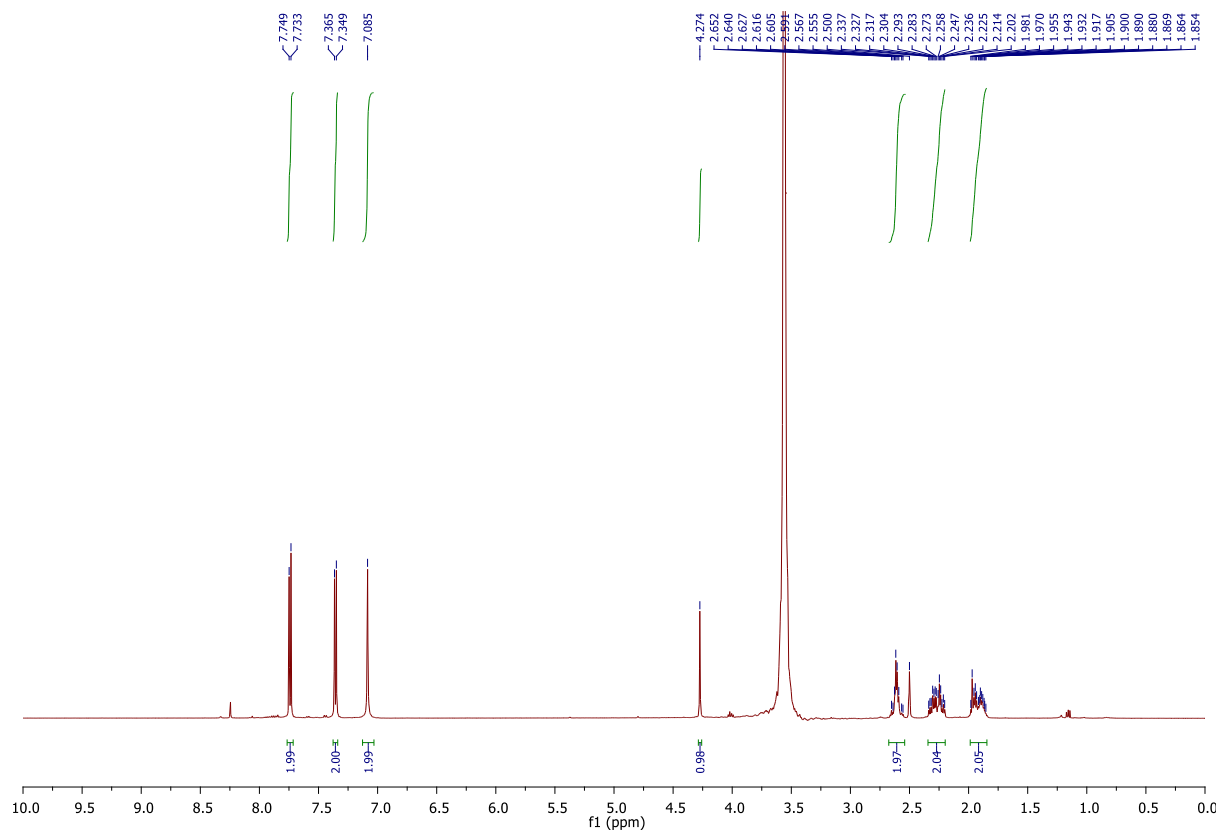




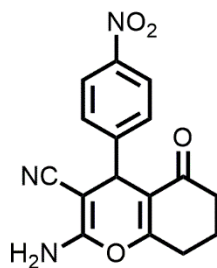
2-amino-4-(4-cyanophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10h)



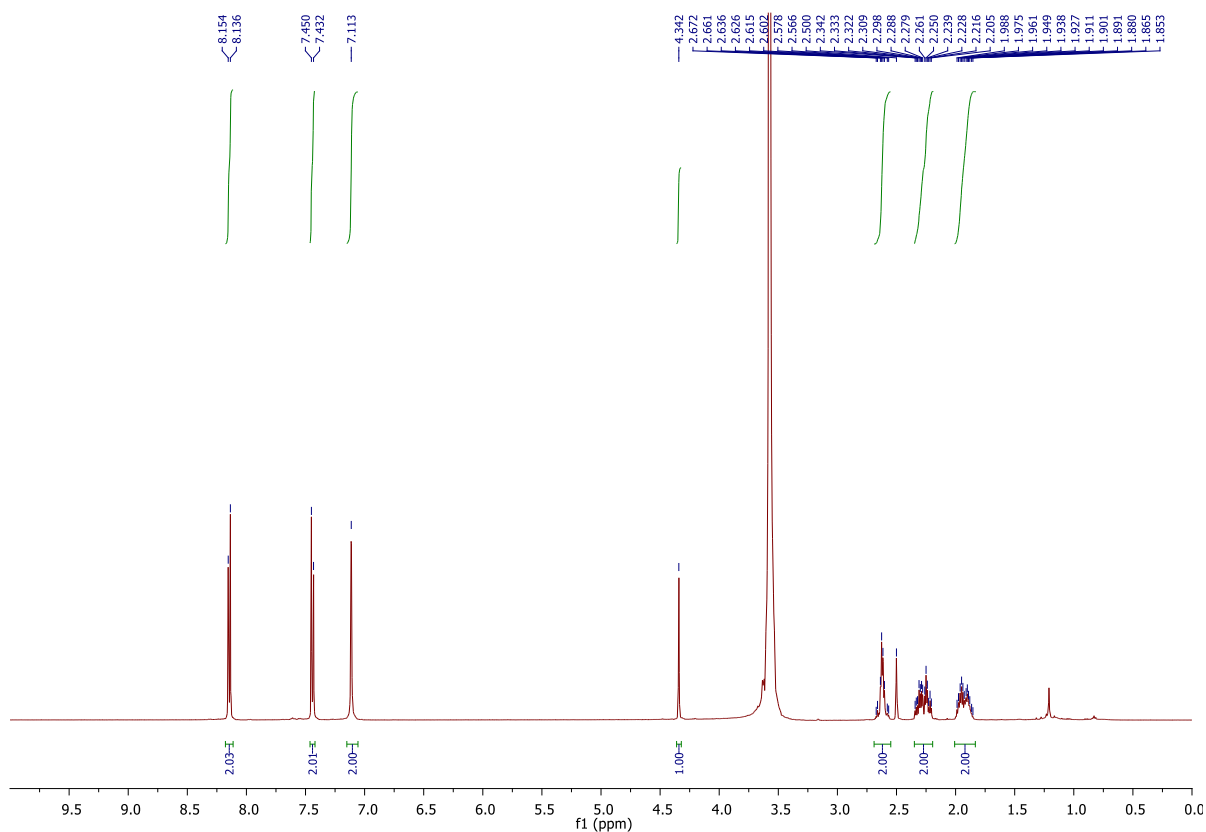
M.F. $C_{17}H_{13}N_3O_2$ (291.30). Yield: (0.270 g, 93%). White powder. 1H NMR (500 MHz, DMSO d_6 , ppm) δ 7.74 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.08 (s, 2H), 4.27 (s, 1H), 2.50-2.65 (m, 2H), 2.23-2.30 (m, 2H), 1.85-1.98 (m, 2H), ^{13}C NMR (125 MHz, DMSO d_6 , ppm) δ 196.6, 165.7, 159.1, 150.7, 135.9, 132.9, 128.8, 126.8, 119.9, 119.3, 57.6, 36.7, 36.2, 26.9, 20.2.

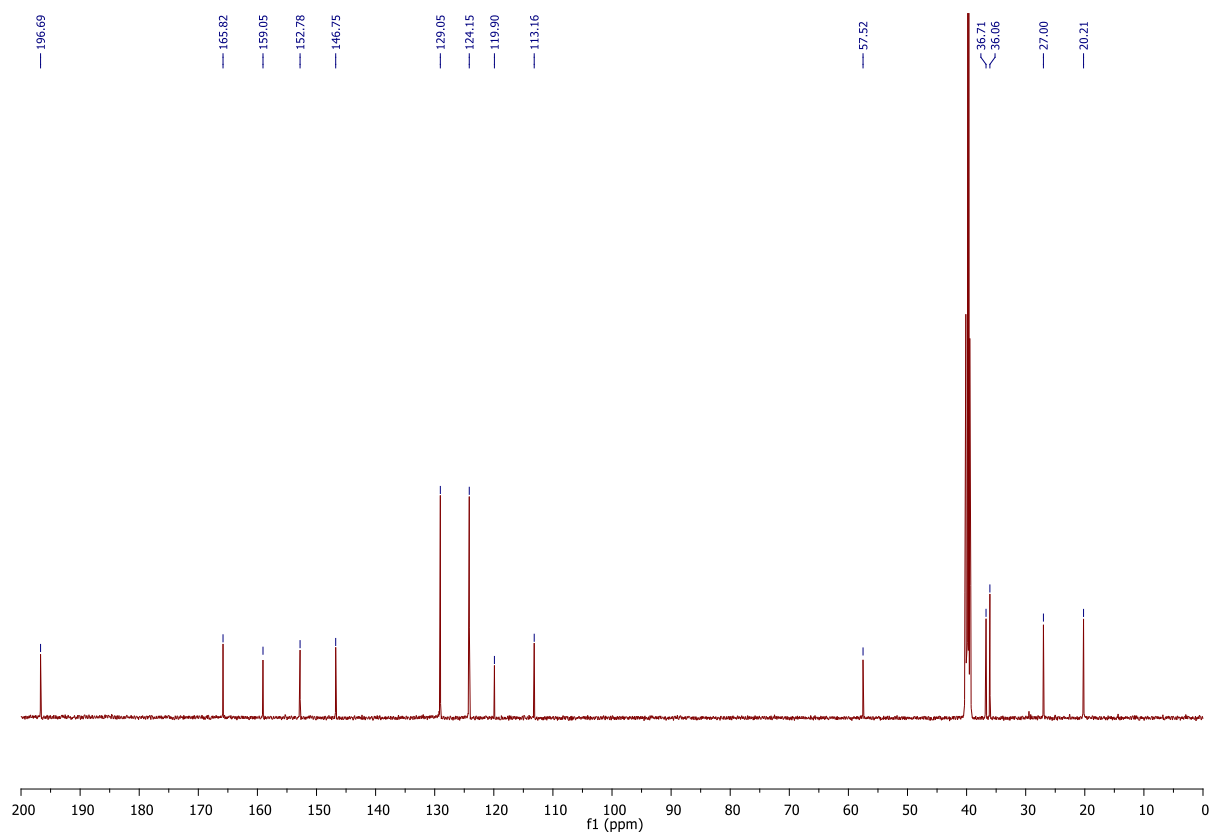


2-amino-4-(4-nitrophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10i)

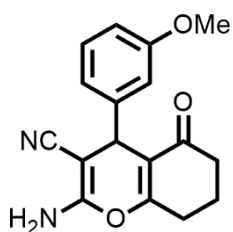


M.F. C₁₆H₁₃N₃O₄ (311.29). Yield: (0.267 g, 86%). White powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 8.14 (d, J = 9.0 Hz, 2H), 7.44 (d, J = 9.0 Hz, 2H), 7.11 (s, 2H), 4.34 (s, 1H), 2.50-2.67 (m, 2H), 2.24-2.30 (m, 2H), 1.85-1.98 (m, 2H), ¹³C NMR (125 MHz, DMSO d₆, ppm) δ 196.7, 165.8, 159.0, 152.7, 146.7, 129.0, 124.2, 119.9, 113.2, 57.5, 36.7, 36.0, 27.0, 20.2.

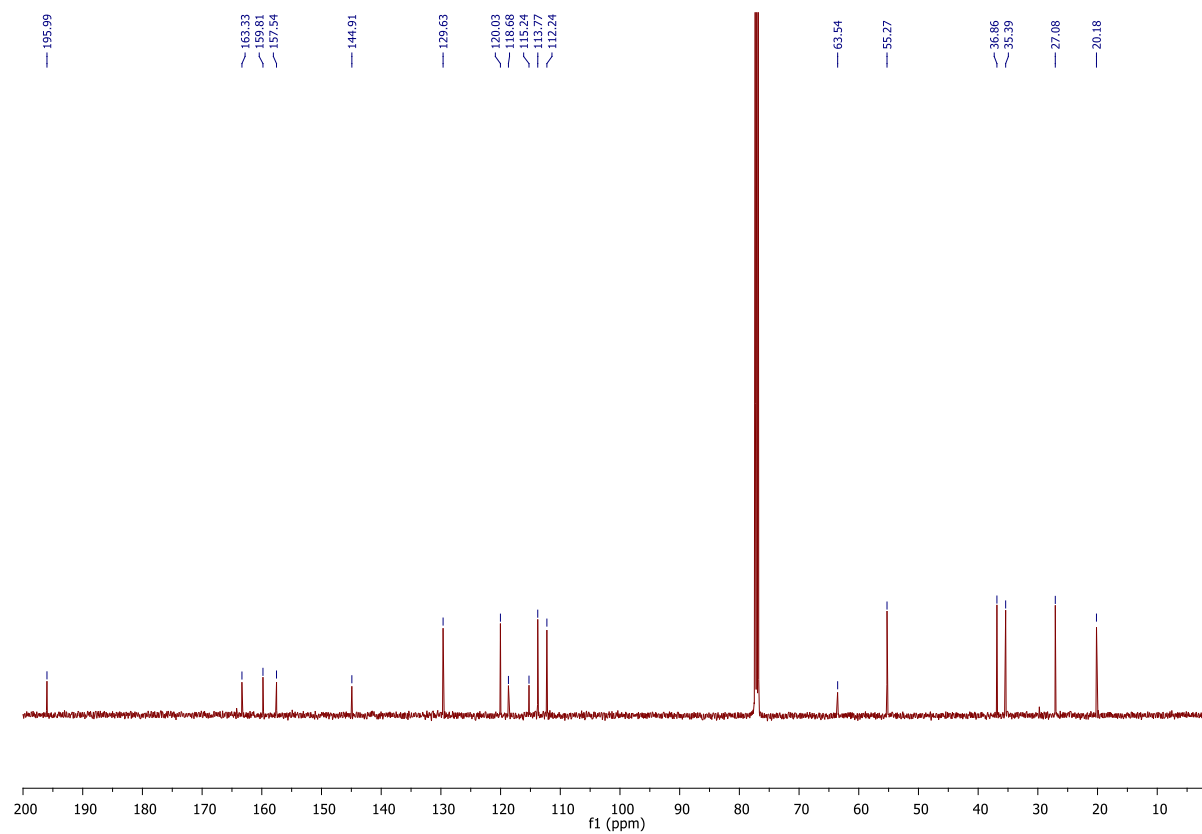
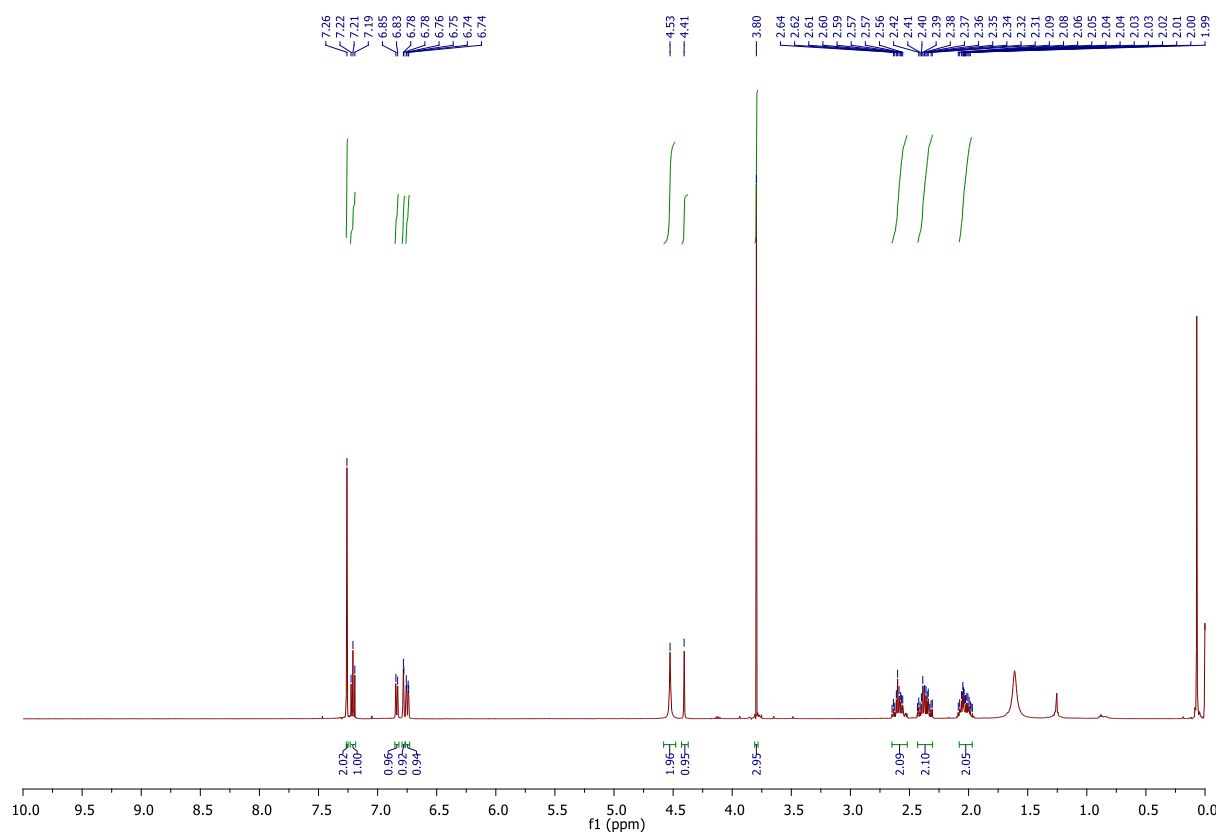




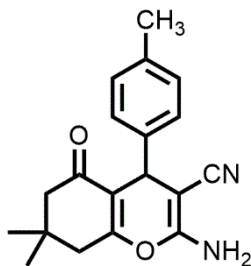
**2-amino-4-(3-methoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile
(10j)**



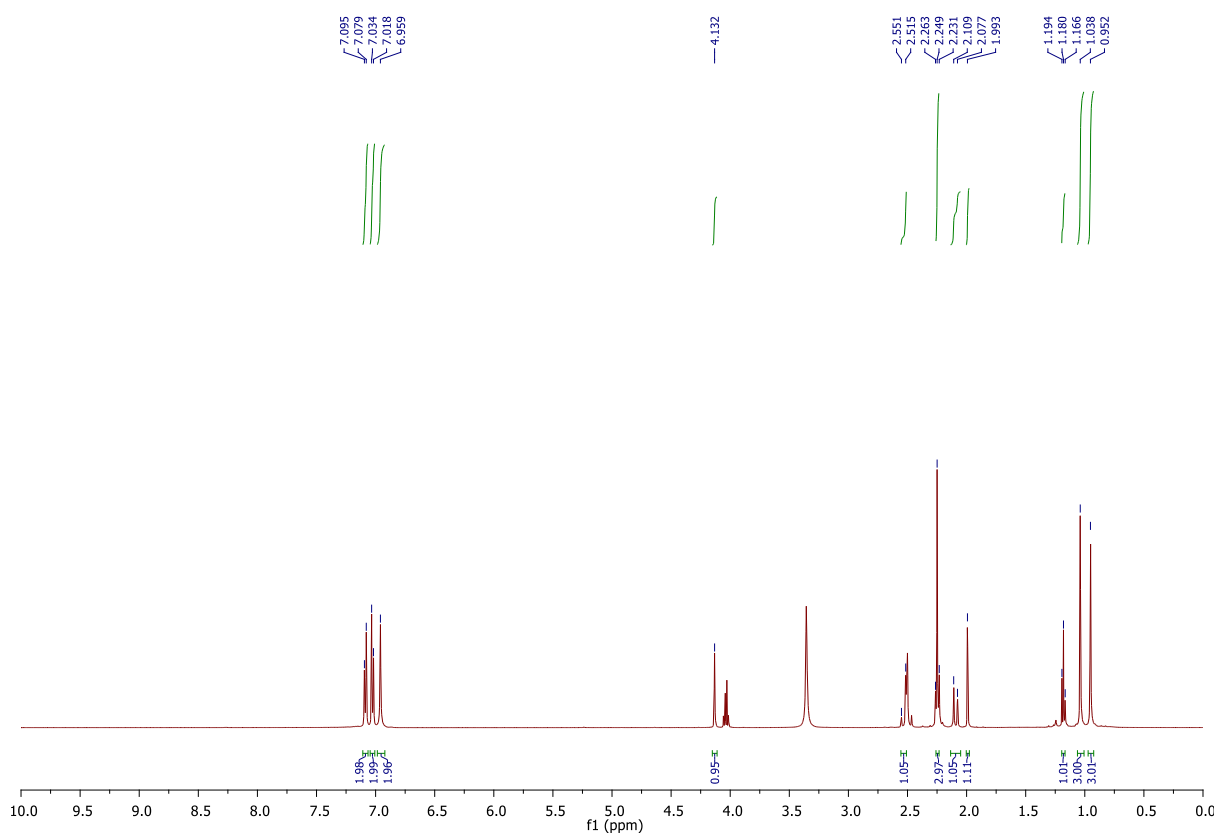
M.F. $C_{17}H_{16}N_2O_3$ (296.31). Yield: (0.272 g, 92%). White powder. 1H NMR (500 MHz, $CDCl_3$, ppm) δ 7.26 (s, 2H), 7.21 (t, $J = 8.0$ Hz, 1H), 6.84 (d, $J = 8.0$ Hz, 1H), 6.78 (d, $J = 2.0$ Hz, 1H), 6.75, 6.74 (d, d, $J = 2.5, 2.0$ Hz, 1H), 4.52 (s, 2H), 4.40 (s, 1H), 2.55-2.64 (m, 2H), 2.34-2.39 (m, 2H), 1.96-2.08 (m, 2H), ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 195.9, 163.3, 159.8, 157.5, 144.9, 129.6, 120.0, 118.7, 115.2, 113.7, 112.2, 63.5, 55.2, 36.8, 35.3, 27.1, 20.2.

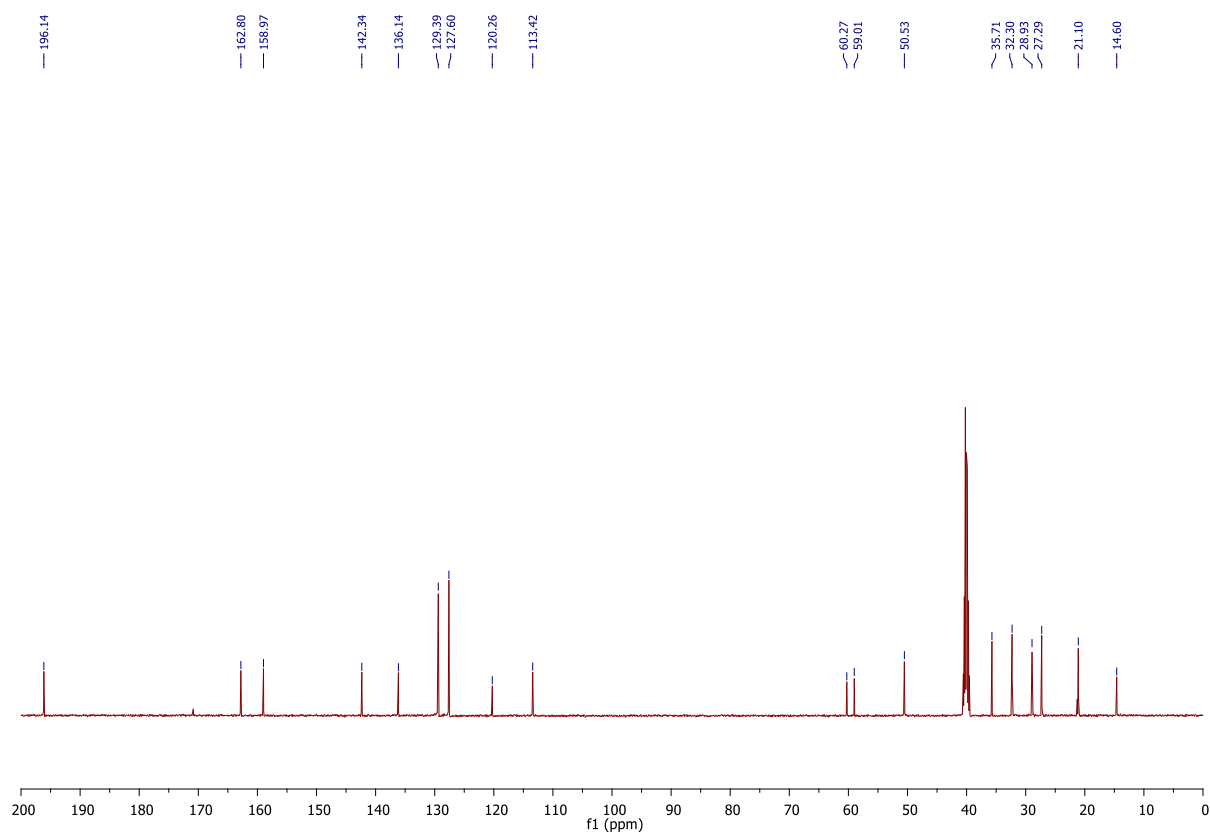


2-amino-7,7-dimethyl-5-oxo-4-(p-tolyl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10k)

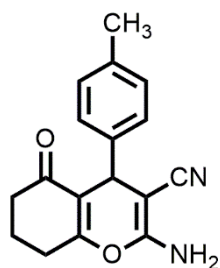


M.F. C₁₉H₂₀N₂O₂ (308.37). Yield: (0.289 g, 94%). White powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 7.08 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 2H), 6.95 (s, 1H), 4.13 (s, 1H), 2.53 (d, J = 8.0 Hz, 1H), 2.55 (t, J = 9.0 Hz, 3H), 2.10 (d, J = 18.0 Hz, 1H), 1.99 (s, 1H), 1.18 (t, J = 7.0 Hz, 1H), 1.03 (s, 3H), 0.95 (s, 3H). ¹³C NMR (125 MHz, DMSO d₆, ppm) δ 196.1, 162.8, 158.9, 142.3, 136.1, 129.3, 127.6, 120.2, 113.4, 60.3, 59.0, 50.5, 35.7, 32.3, 28.9, 27.3, 21.1, 14.6.

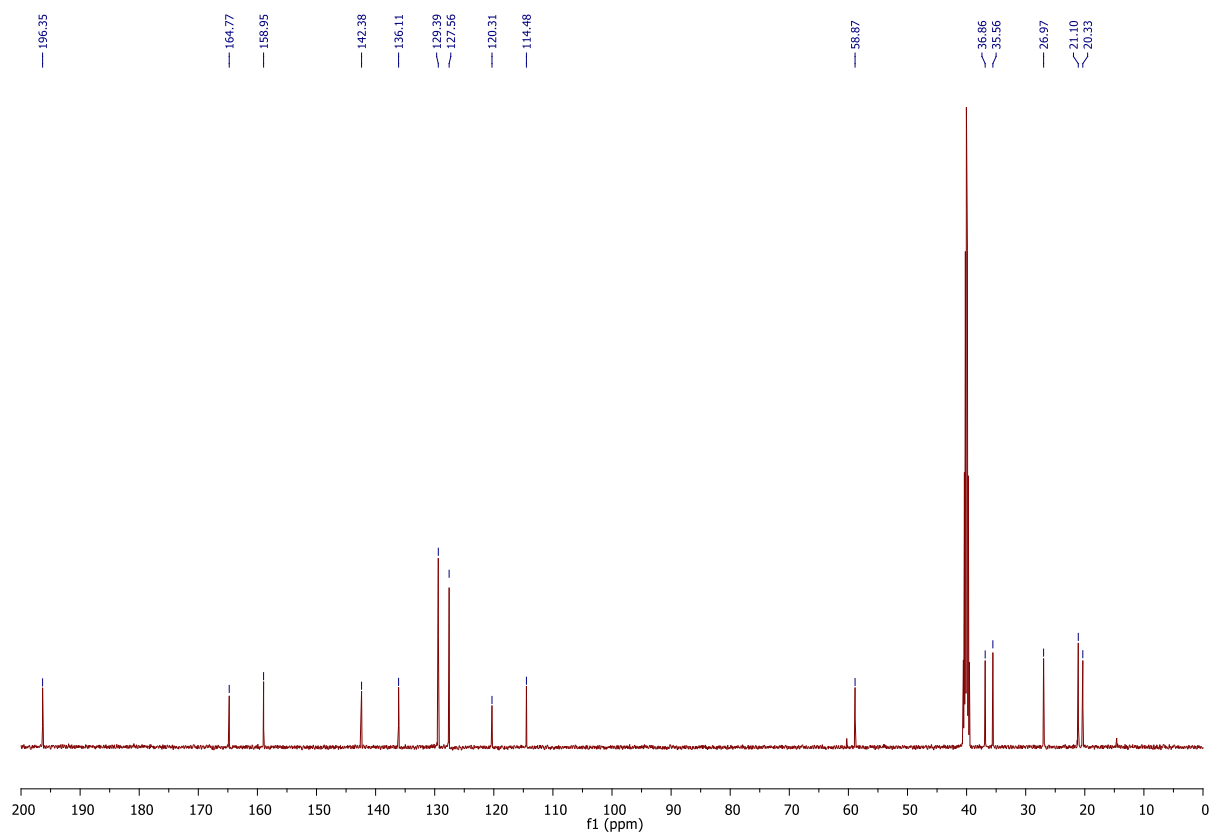
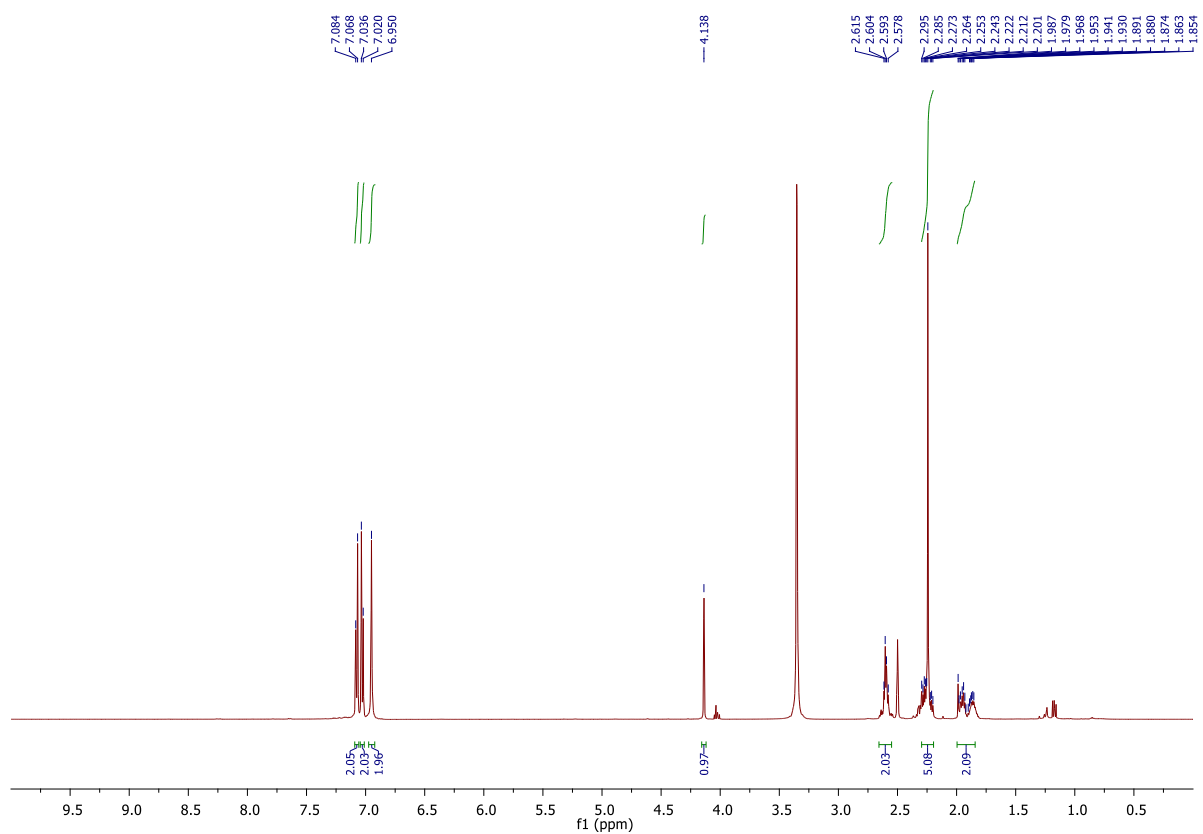




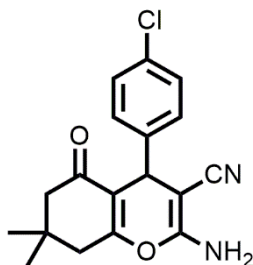
2-amino-5-oxo-4-(p-tolyl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10l)



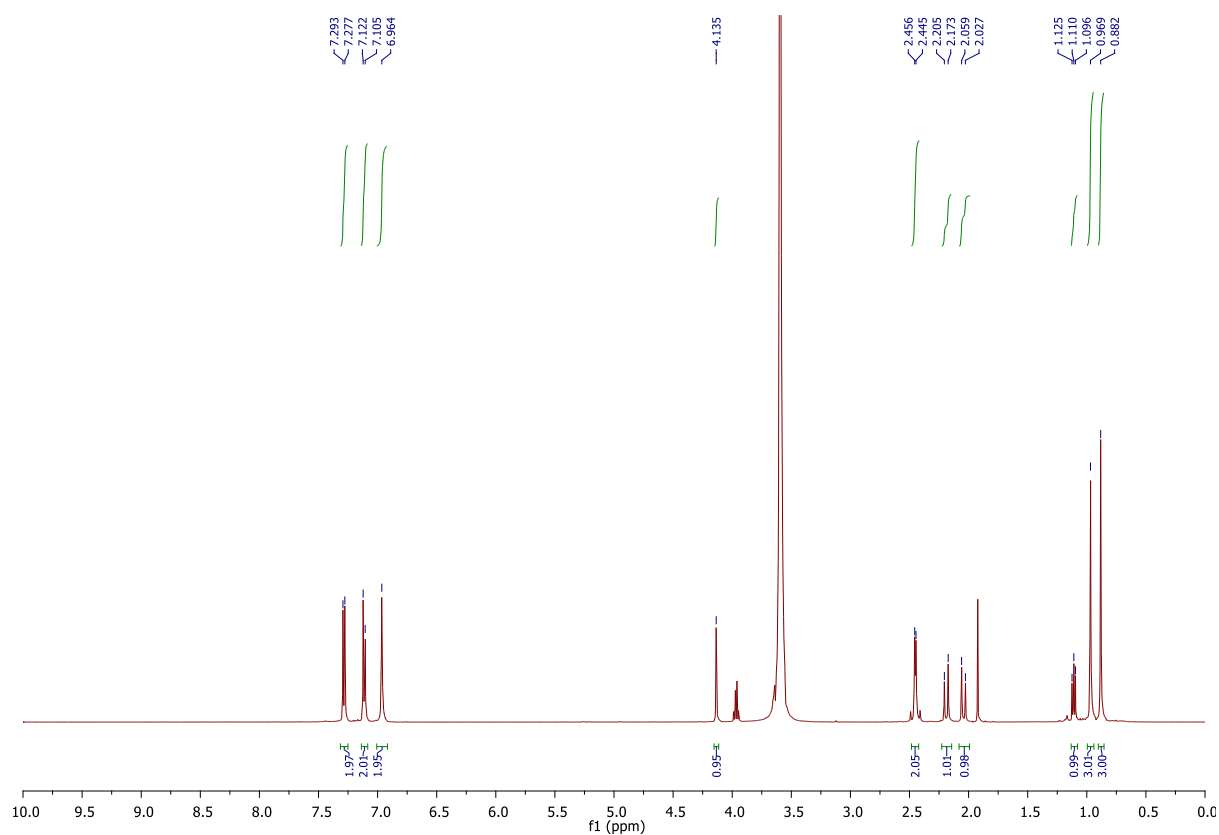
M.F. $C_{17}H_{16}N_2O_2$ (280.32). Yield: (0.260 g, 93%). White powder. 1H NMR (500 MHz, DMSO d_6 , ppm) δ 7.07 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.0 Hz, 2H), 6.95 (s, 1H), 4.14 (s, 1H), 2.57-2.61 (m, 2H), 2.20-2.29 (m, 5H), 1.85-1.995 (m, 2H), ^{13}C NMR (125 MHz, DMSO d_6 , ppm) δ 196.3, 164.7, 158.9, 142.3, 136.1, 129.3, 127.6, 120.3, 114.4, 58.8, 36.8, 35.6, 26.9, 21.1, 20.3

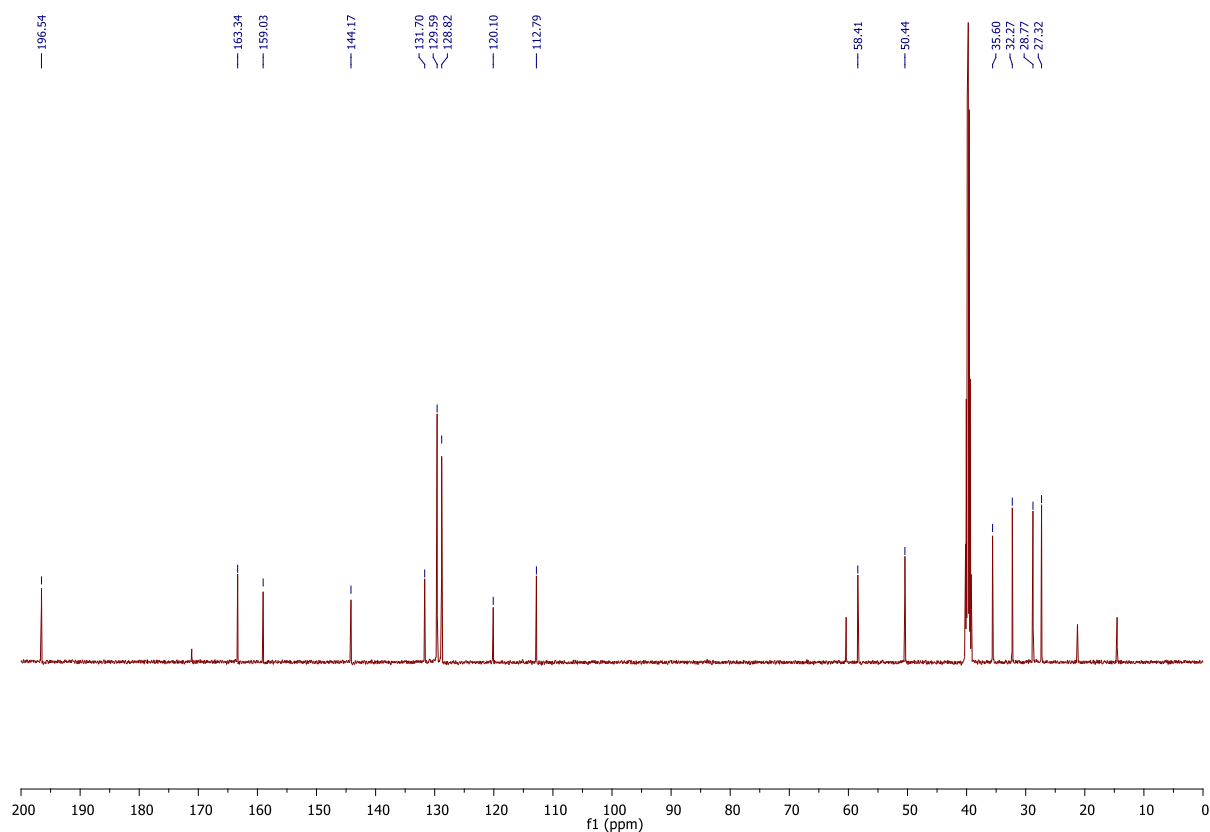


2-amino-4-(4-chlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10m)

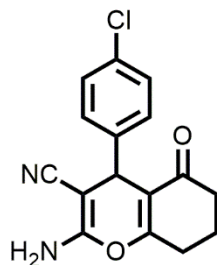


M.F. $C_{18}H_{17}ClN_2O_2$ (328.79). Yield: (0.285 g, 87%). White powder. 1H NMR (500 MHz, DMSO d_6 , ppm) δ 7.28 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.5 Hz, 2H), 6.96 (s, 2H), 4.13 (s, 1H), 2.55 (d, J = 5.5 Hz, 2H), 2.20 (d, J = 16 Hz, 1H), 2.04 (d, J = 16.0 Hz, 1H), 1.11 (t, J = 7.0 Hz, 1H), 0.97 (s, 3H), 0.88 (s, 3H) ^{13}C NMR (125 MHz, DMSO d_6 , ppm) δ 196.5, 163.3, 159.0, 144.2, 131.7, 129.6, 128.8, 120.1, 112.8, 58.4, 50.4, 35.6, 32.3, 28.8, 27.3.

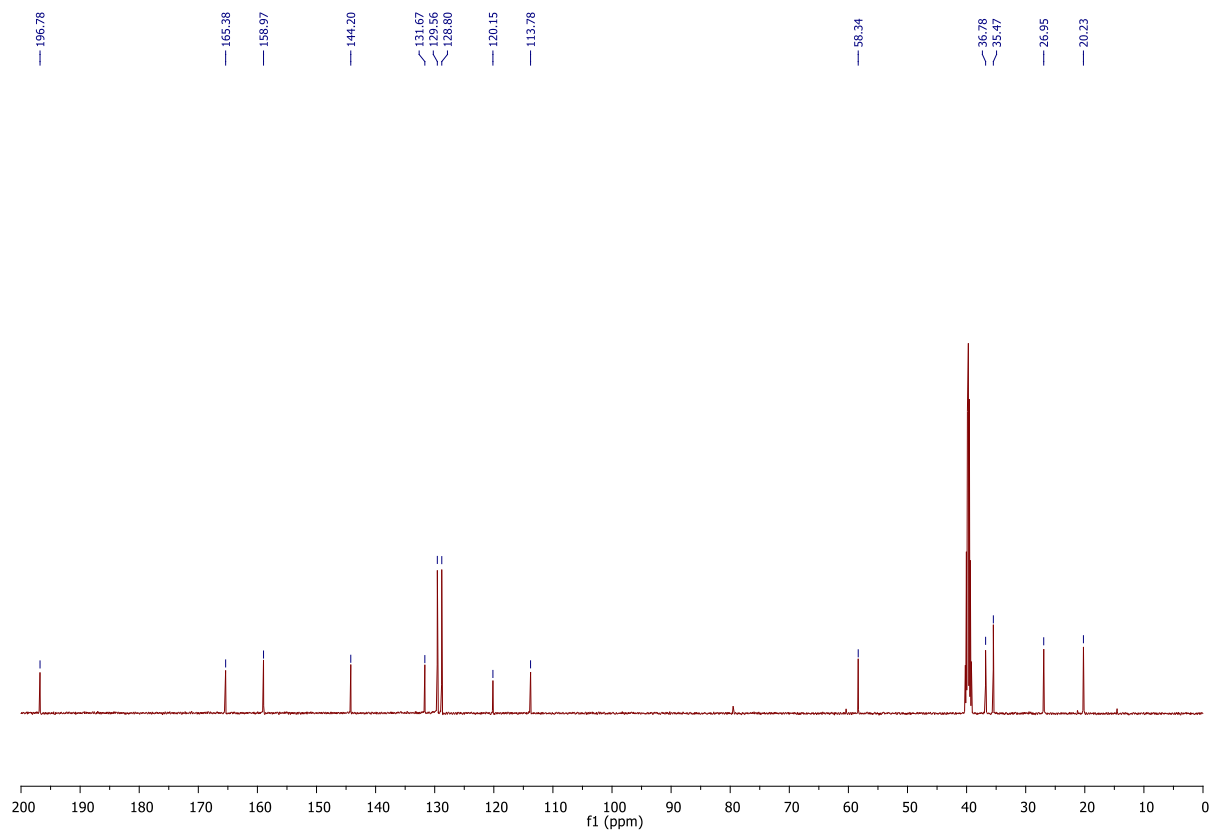
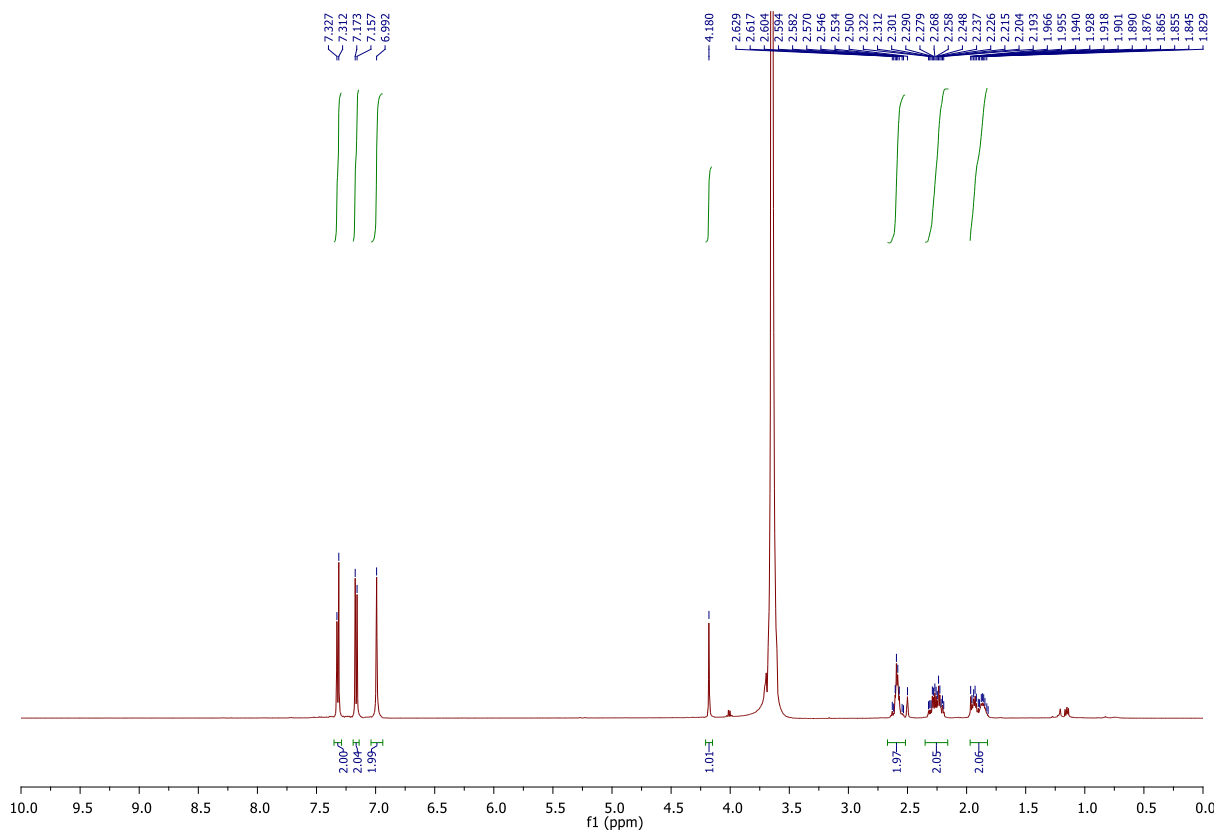




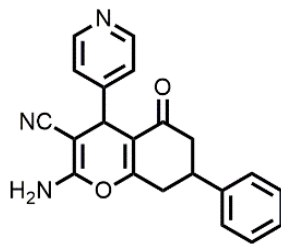
2-amino-4-(4-chlorophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10n)



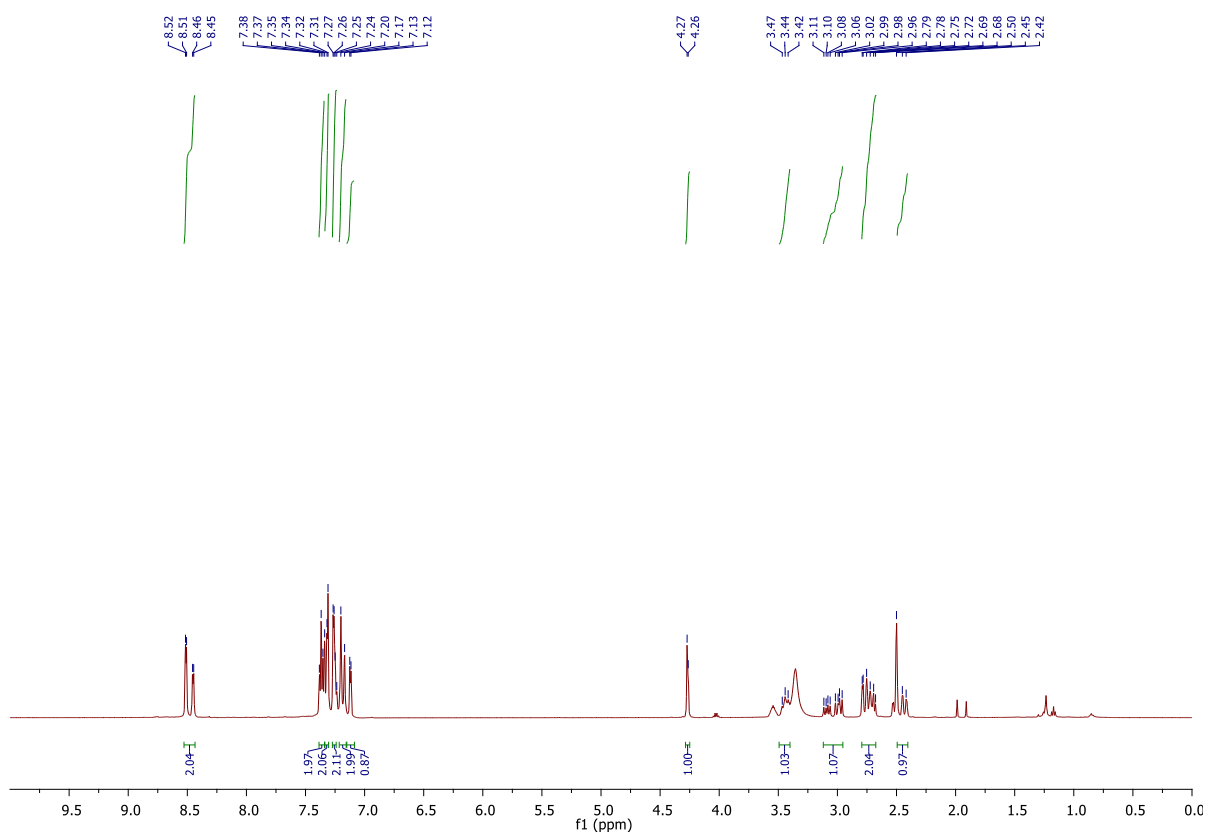
M.F. $C_{16}H_{13}ClN_2O_2$ (300.74). Yield: (0.276 g, 92%). White powder. 1H NMR (500 MHz, DMSO d_6 , ppm) δ 7.32 (d, $J = 7.5$ Hz, 2H), 7.16 (d, $J = 8.0$ Hz, 2H), 6.99 (s, 2H), 4.18 (s, 1H), 2.50-2.63 (m, 2H), 2.20-2.29 (m, 2H), 1.82-1.96 (m, 2H), ^{13}C NMR (125 MHz, DMSO d_6 , ppm) δ 196.8, 165.4, 158.9, 144.2, 131.7, 129.6, 128.8, 120.1, 113.8, 58.4, 36.8, 34.5, 26.9, 20.2.

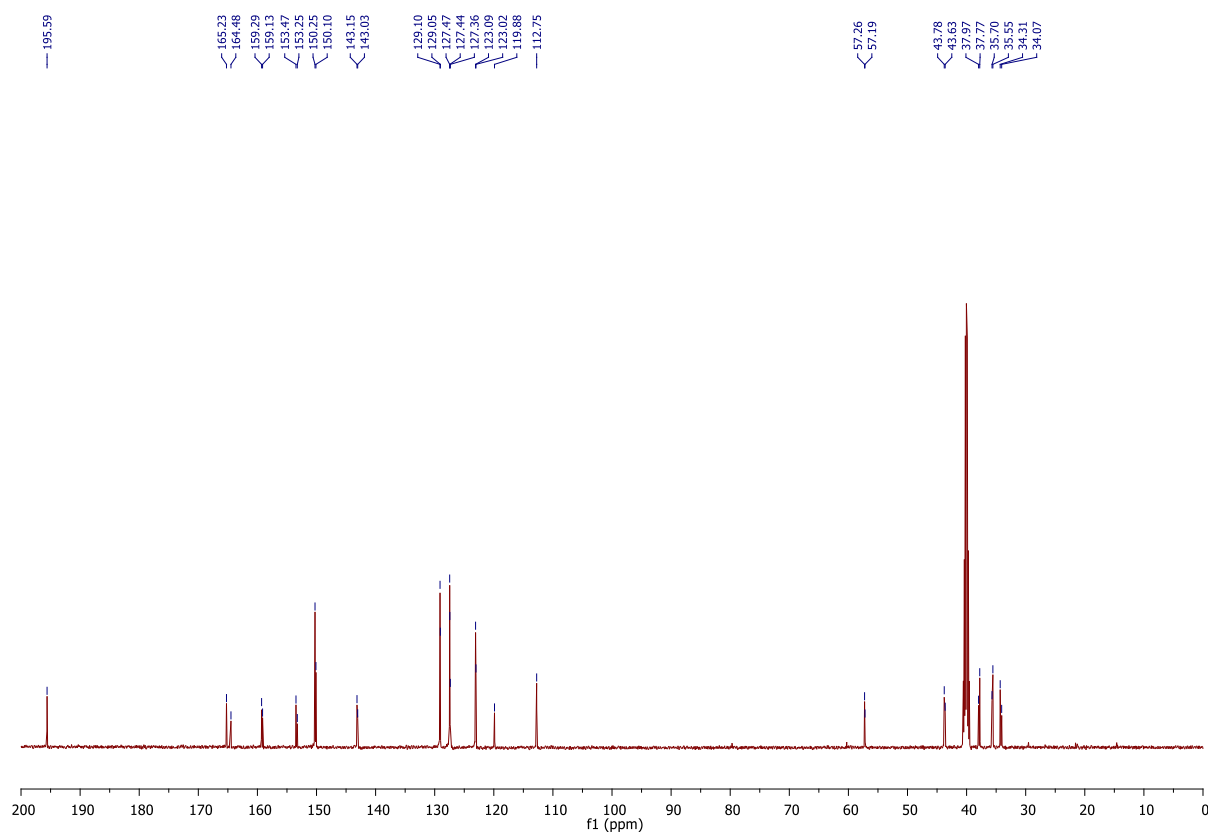


2-amino-5-oxo-7-phenyl-4-(pyridin-4-yl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (10o)



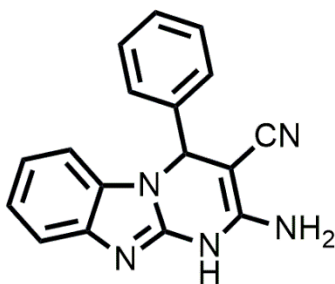
M.F. C₂₁H₁₇N₃O₂ (343.38). Yield: (0.282 g, 82%). Light yellow powder. ¹H NMR (500 MHz, DMSO d₆, ppm) δ 8.51, 8.45 (d, d, J = 4.5, 5.0 Hz, 2H), 7.31-7.38 (m, 4H), 7.23-7.26 (m, 2H), 7.20 (d, J = 16.0 Hz, 2H), 7.12 (d, J = 4.5 Hz, 1H), 4.27 (d, J = 5.0 Hz, 1H) 3.41-3.46 (m, 1H), 2.96-3.11 (m, 1H), 2.67-2.79 (m, 2H), 2.41-2.50 (m, 2H), ¹³C NMR (125 MHz, DMSO d₆, ppm) δ 195.6, 165.2, 164.8, 159.3, 153.4, 153.2, 150.2, 143.1, 129.1, 127.4, 123.0, 119.8, 112.7, 57.2, 43.7, 37.9, 35.9, 34.3.



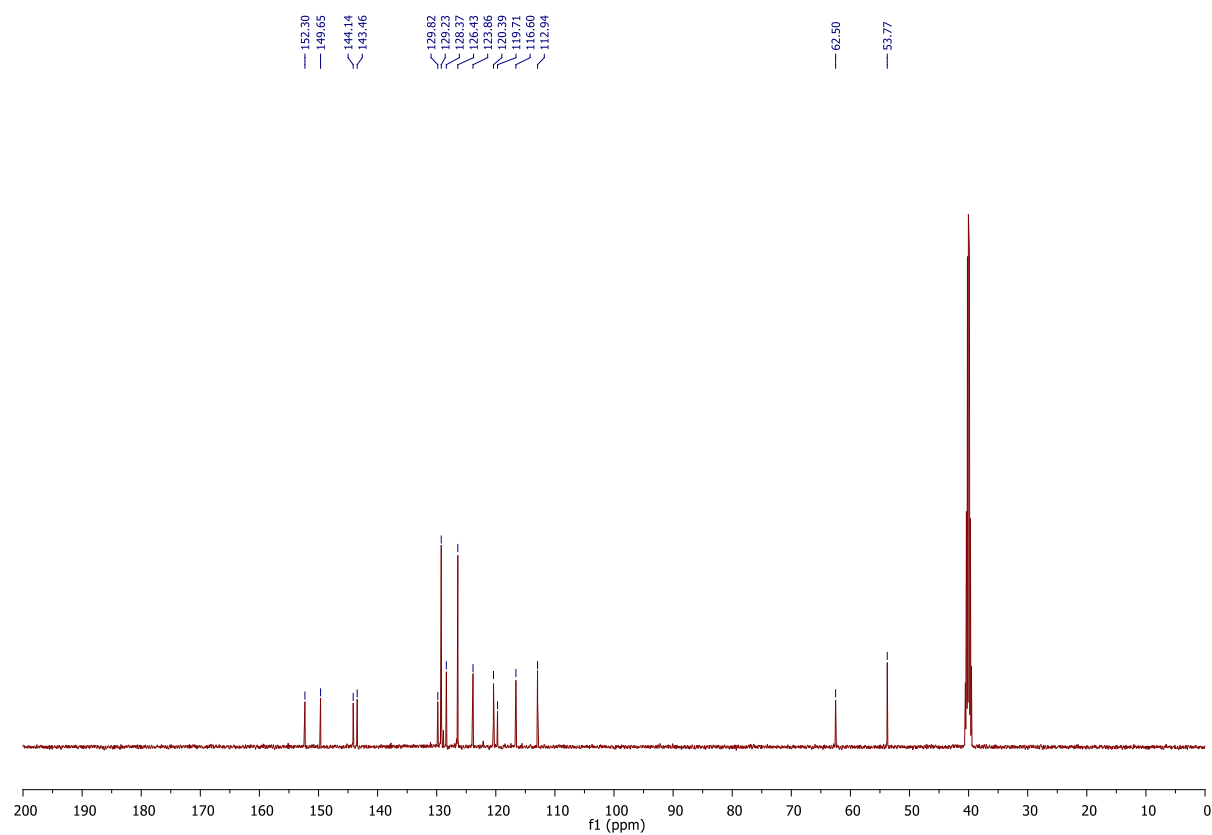
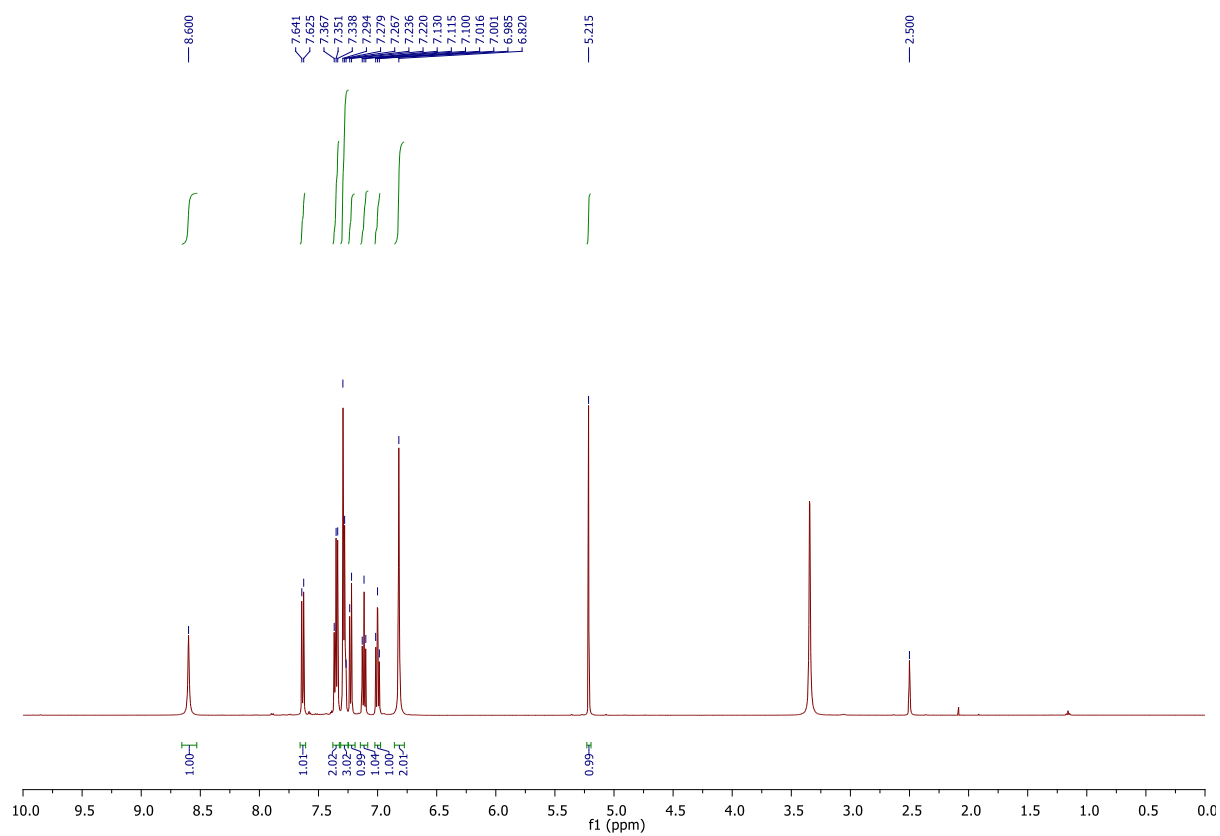


Characterization Data and spectra (^1H , ^{13}C) of the Multicomponent reaction Products Imidazopyrimidine derivatives (11a-11L)

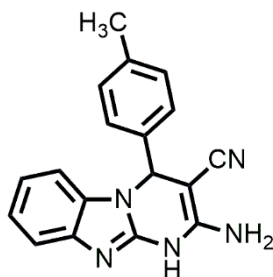
2-amino-4-phenyl-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11a)



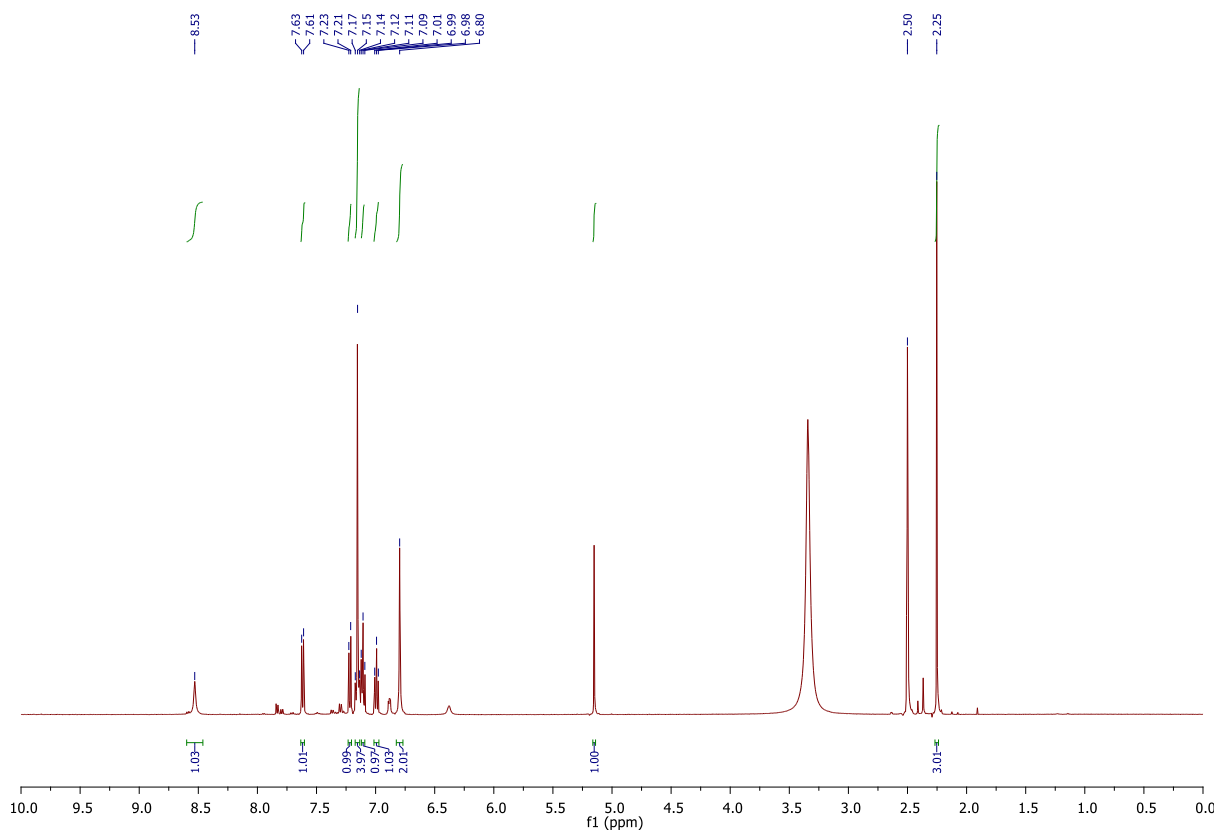
M.F. $\text{C}_{17}\text{H}_{13}\text{N}_5$ (287.32). Yield: (0.241 g, 82%). Off white powder. ^1H NMR (500 MHz, DMSO-d_6 , ppm) δ 8.60 (s, 1H, NH), 7.63 (d, $J = 8.0$ Hz, 1H), 7.37 – 7.33 (m, 2H), 7.27 (t, $J = 6.0$ Hz, 3H), 7.23 (d, $J = 8.0$ Hz, 1H), 7.12 (t, $J = 7.5$ Hz, 1H), 7.00 (t, $J = 8.0$ Hz, 1H) 6.82 (s, 2H), 5.21 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6 , ppm) δ 152.3, 149.6, 144.1, 143.5, 129.8, 129.2, 128.4, 126.4, 123.8, 120.4, 119.7, 116.6, 112.9, 62.5, 53.7.

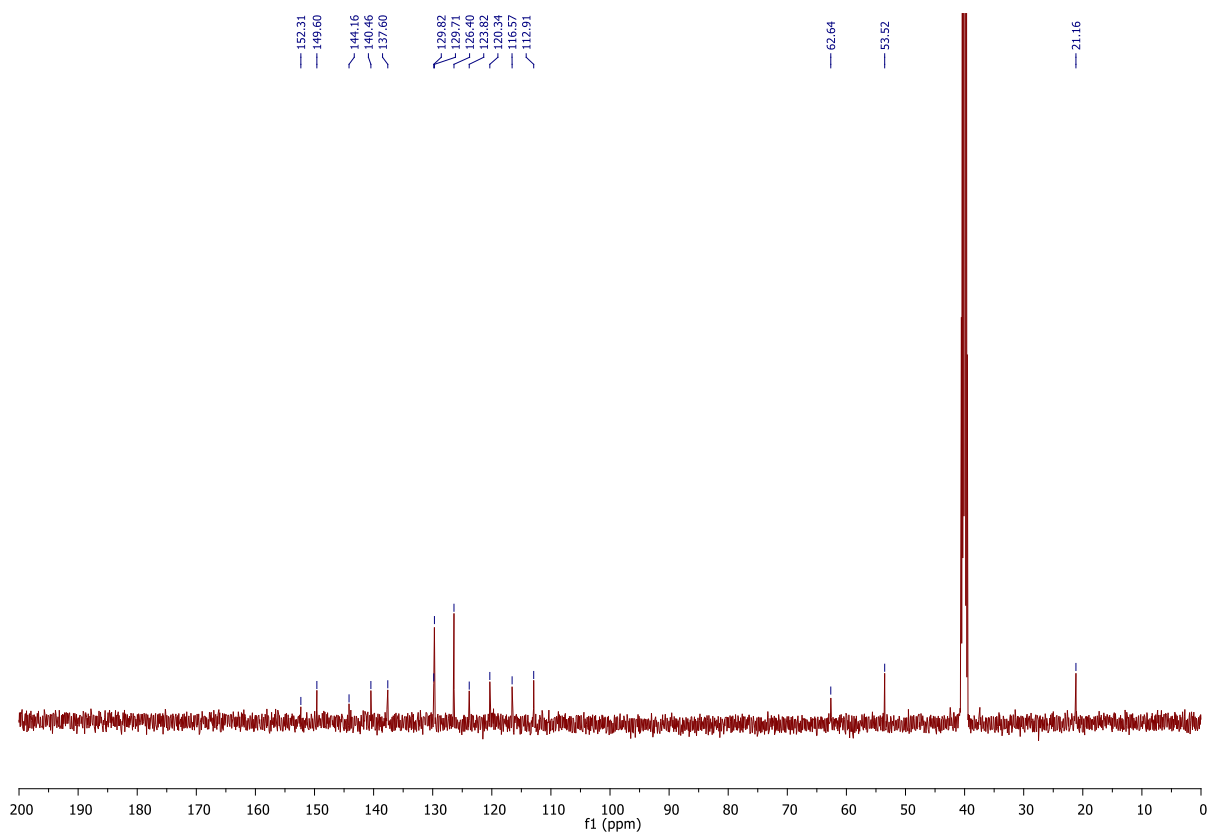


2-amino-4-(p-tolyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11b)

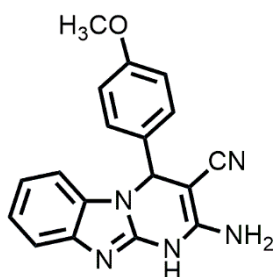


M.F. C₁₈H₁₅N₅ (301.35). Yield: (0.255 g, 85%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.57 (s, 1H, NH), 7.63 (d, J = 8.0 Hz, 1H), 7.31 – 7.34 (m, 2H), 7.17-7.23 (m, 3H), 7.11 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.85 (s, 2H), 5.24 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 152.3, 149.6, 144.1, 140.4, 137.6, 129.8, 129.7, 126.4, 123.8, 120.4, 116.6, 112.9, 62.6, 53.5, 21.2.

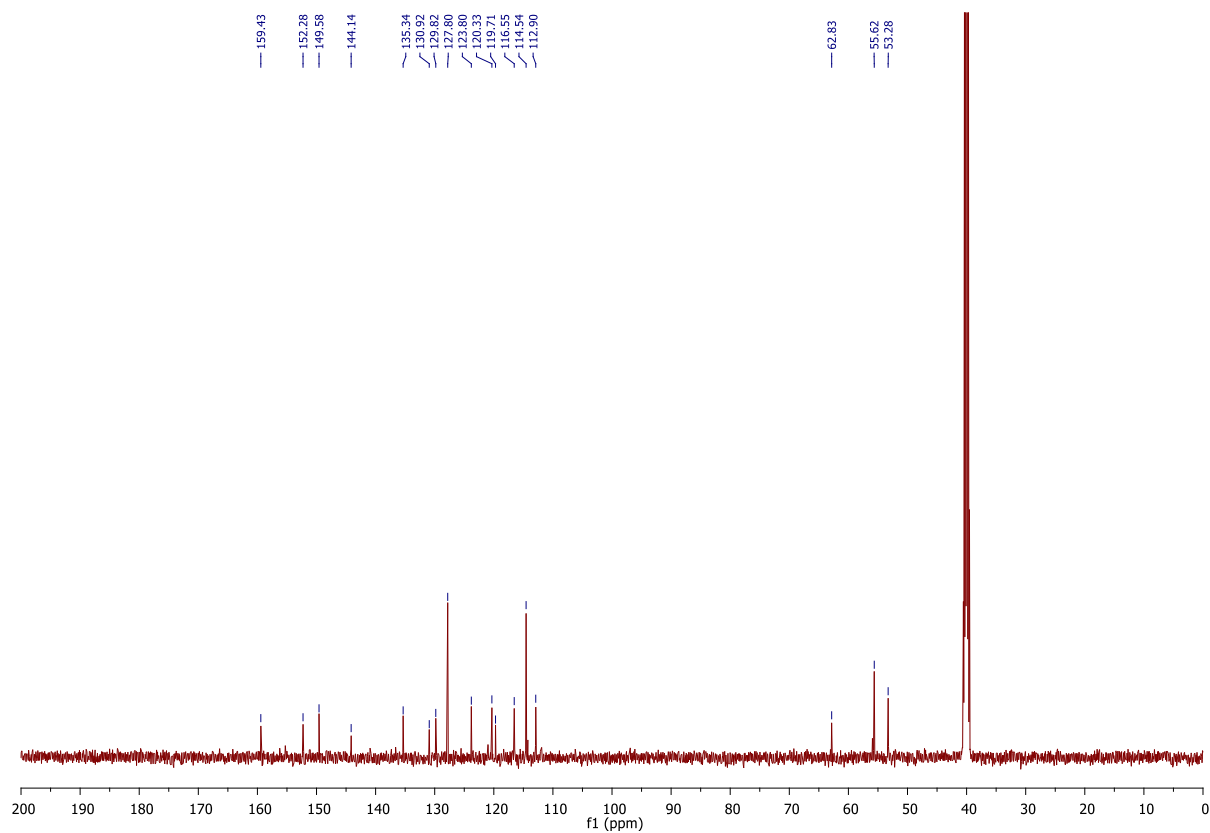
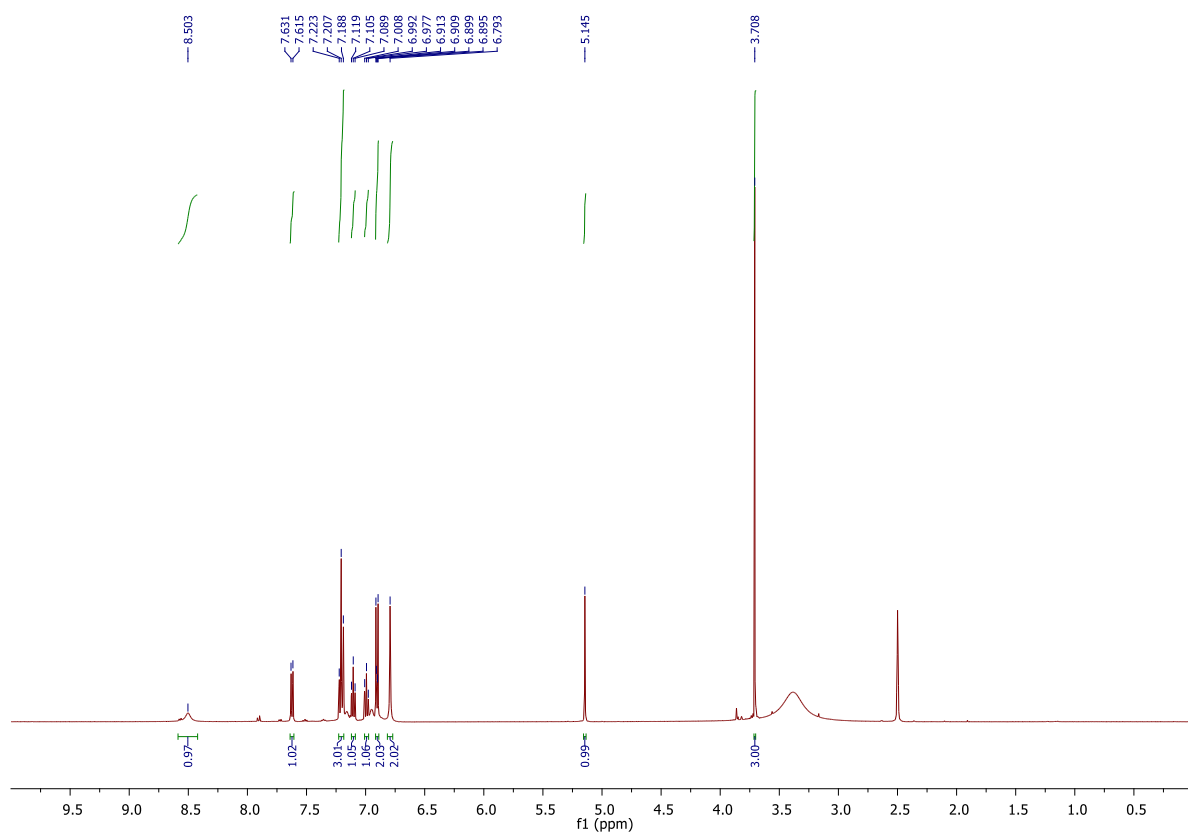




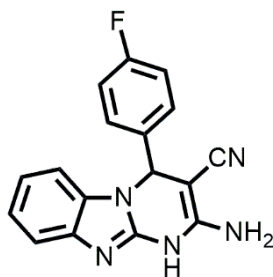
2-amino-4-(4-methoxyphenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11c)



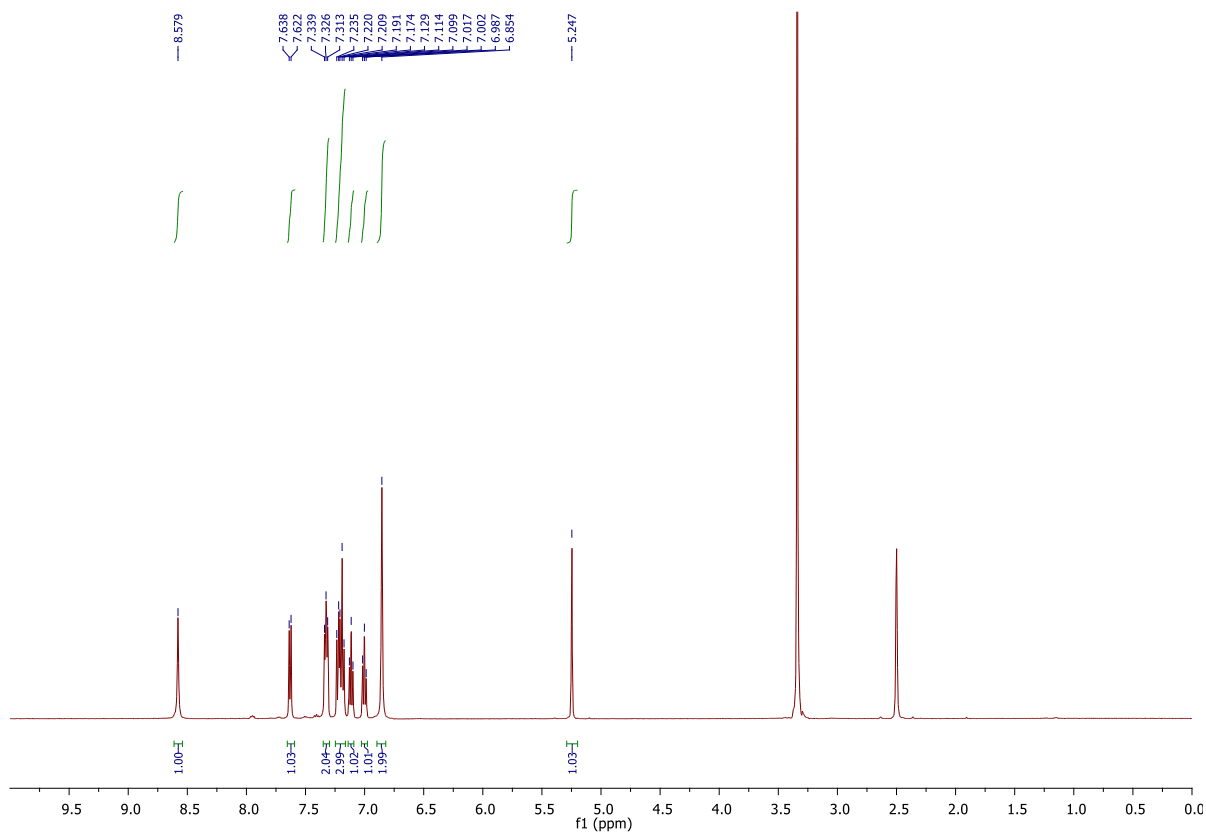
M.F. $C_{18}H_{15}N_5O$ (317.34). Yield: (0.272 g, 86%). White powder. 1H NMR (500 MHz, DMSO- d_6 , ppm) δ 8.50 (s, 1H, NH), 7.62 (d, J = 8.0 Hz, 1H), 7.20 (t, J = 9.5 Hz 1H), 7.10 (t, J = 7.5 Hz 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.89-6.91 (m, 2H), 6.79 (s, 2H), 5.14 (s, 1H), 3.71(s, 3H) ; ^{13}C NMR (125 MHz, DMSO- d_6 , ppm) δ 159.4, 152.3, 149.6, 144.1, 135.3, 130.9, 129.8, 127.8, 123.8, 120.3, 119.7, 116.6, 114.5, 112.9, 62.8, 55.3, 53.3.

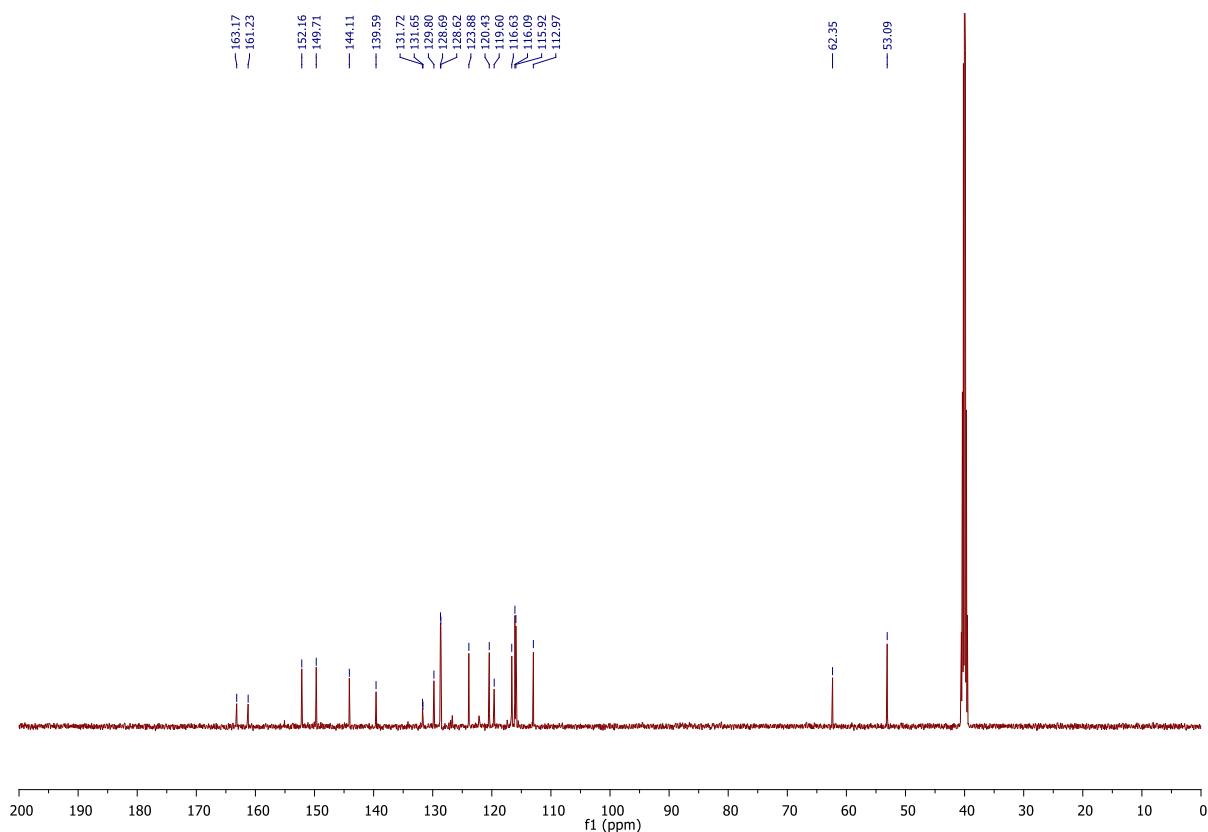


2-amino-4-(4-fluorophenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11d)

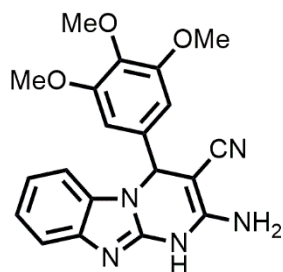


M.F. C₁₇H₁₂FN₅ (305.31). Yield: (0.253 g, 83%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.57 (s, 1H, NH), 7.63 (d, J = 8.0 Hz, 1H), 7.32 (t, J = 6.5 Hz, 2H), 7.17-7.23 (m, 3H), 7.11 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.85 (s, 2H), 5.24 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 163.2, 161.2, 152.1, 149.7, 144.1, 139.6, 131.7, 129.8, 128.6, 123.8, 120.4, 119.6, 116.6, 116.0, 115.9, 112.9, 62.3, 53.1.

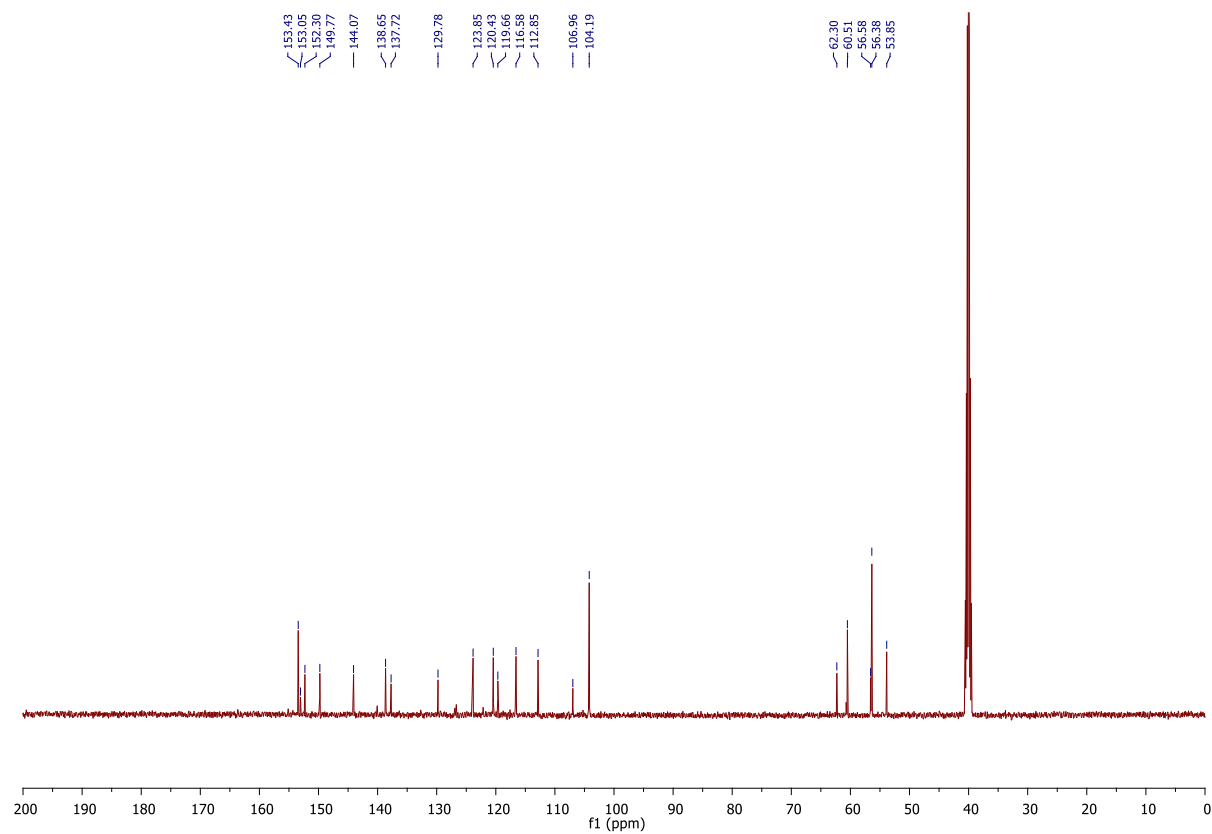
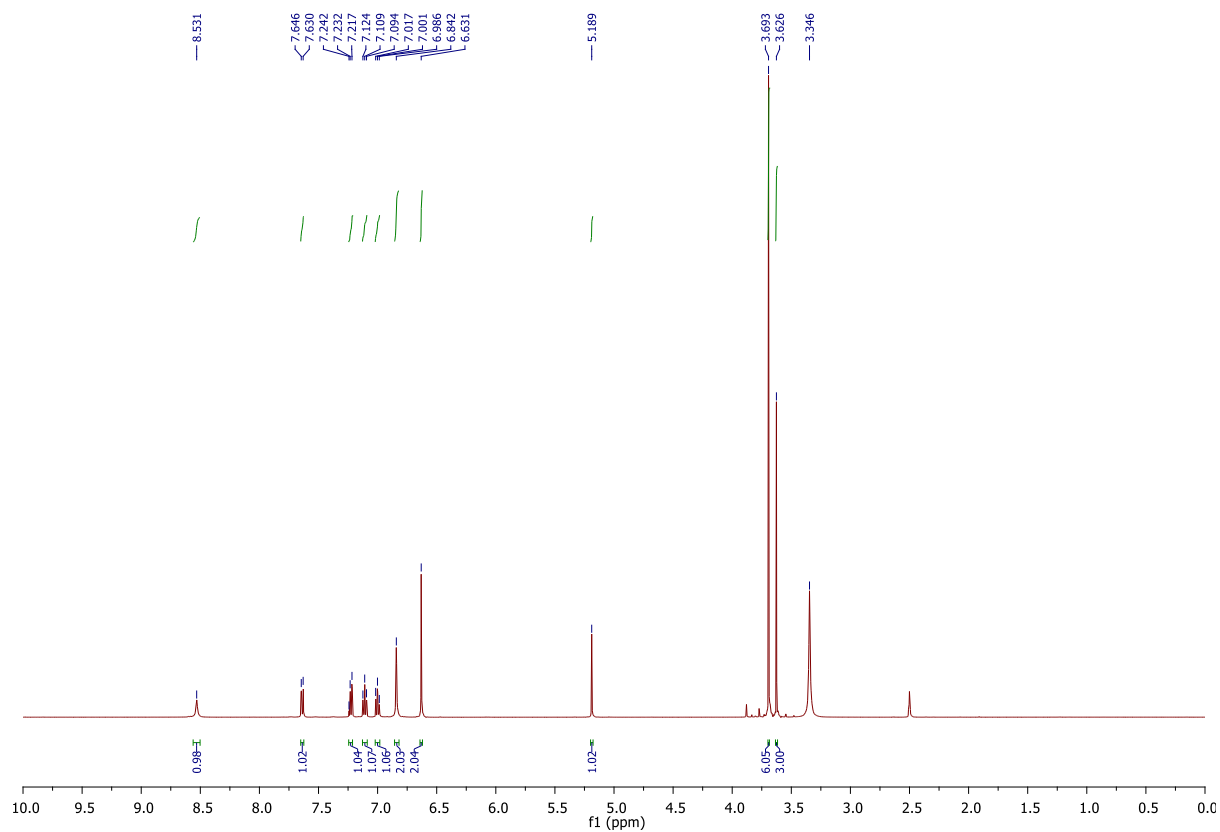




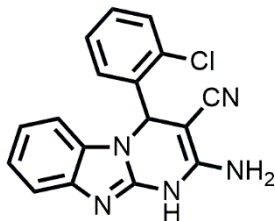
2-amino-4-(3,4,5-trimethoxyphenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11e)



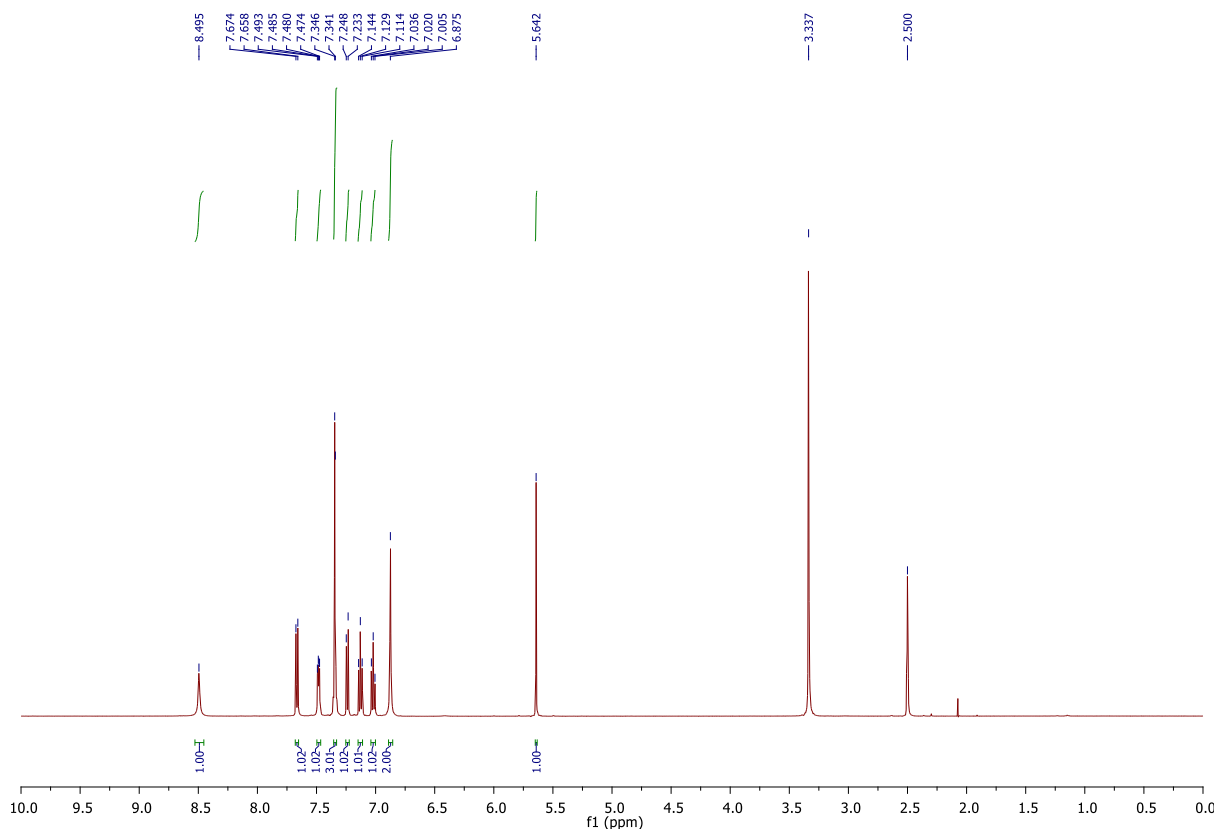
M.F. C₂₀H₁₉N₅O₃ (377.40). Yield: (0.339 g, 90%). Light yellow powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.53 (s, 1H, NH), 7.64 (d, J = 8.0 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.84 (s, 2H), 6.63 (s, 2H), 5.19 (s, 1H), 3.69 (s, 6H), 3.63 (s, 3H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 153.4, 153.0, 152.2, 149.7, 144.1, 138.7, 137.7, 129.8, 123.8, 120.4, 119.6, 116.6, 112.9, 106.9, 104.2, 62.3, 60.5, 56.5, 53.1.

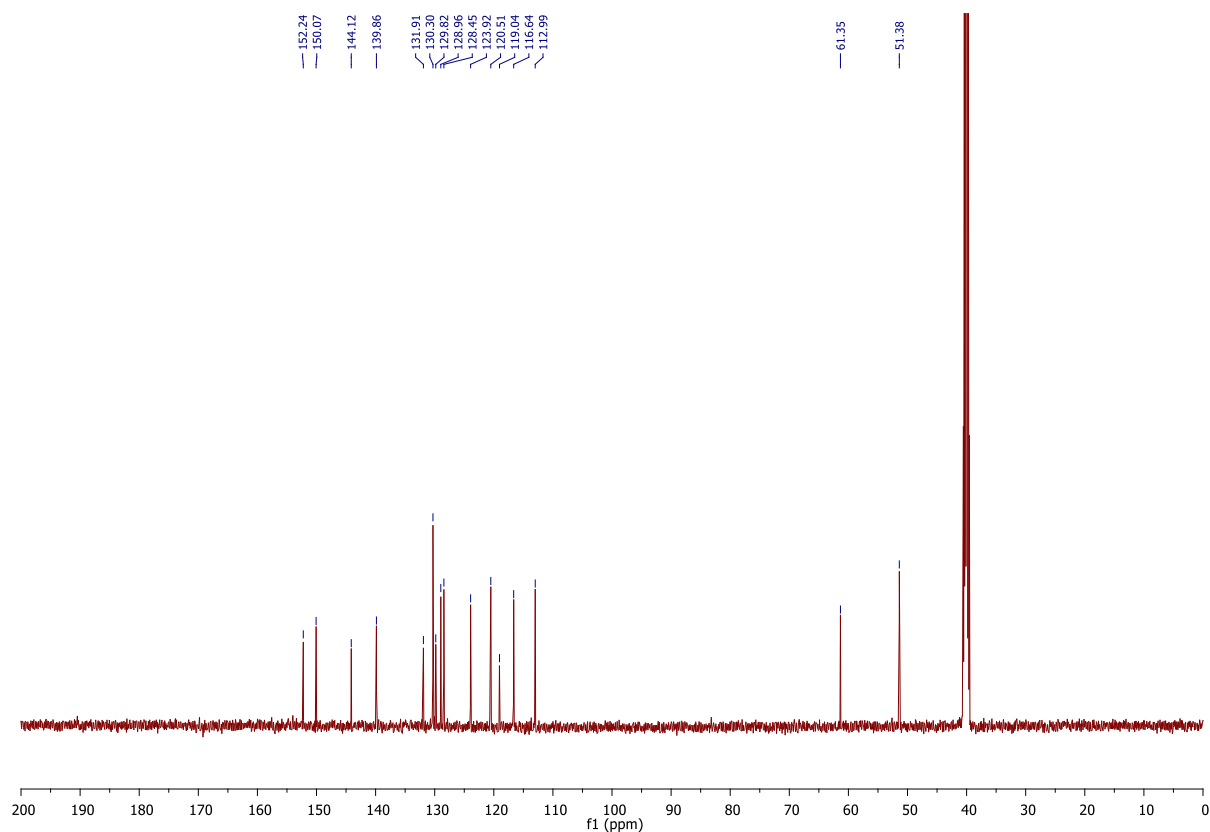


2-amino-4-(2-chlorophenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11f)

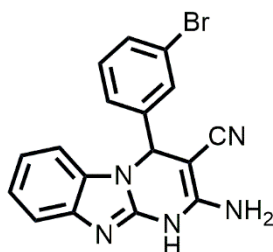


M.F. C₁₇H₁₂N₅Cl (321.76). Yield: (0.244 g, 76%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.50 (s, 1H, NH), 7.66 (d, J = 8.0 Hz, 1H), 7.47-7.49 (m, 1H), 7.34 (d, J = 2.5 Hz, 3H), 7.24 (d, J = 7.5 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.5 Hz, 1H), 6.87 (s, 2H), 5.64 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 152.2, 150.1, 144.1, 139.8, 131.9, 130.3, 129.8, 123.8, 128.9, 128.4, 123.9, 120.5, 119.0, 116.6, 112.9, 61.3, 51.4.

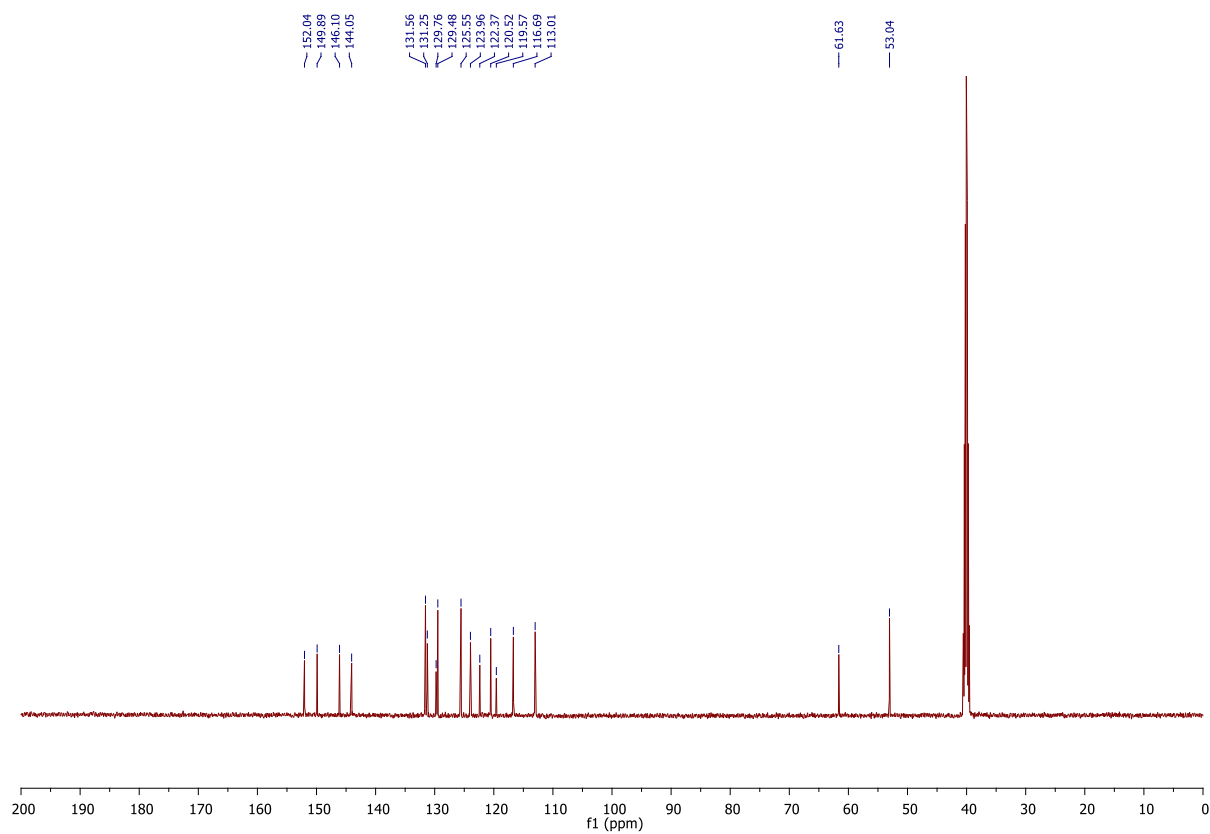
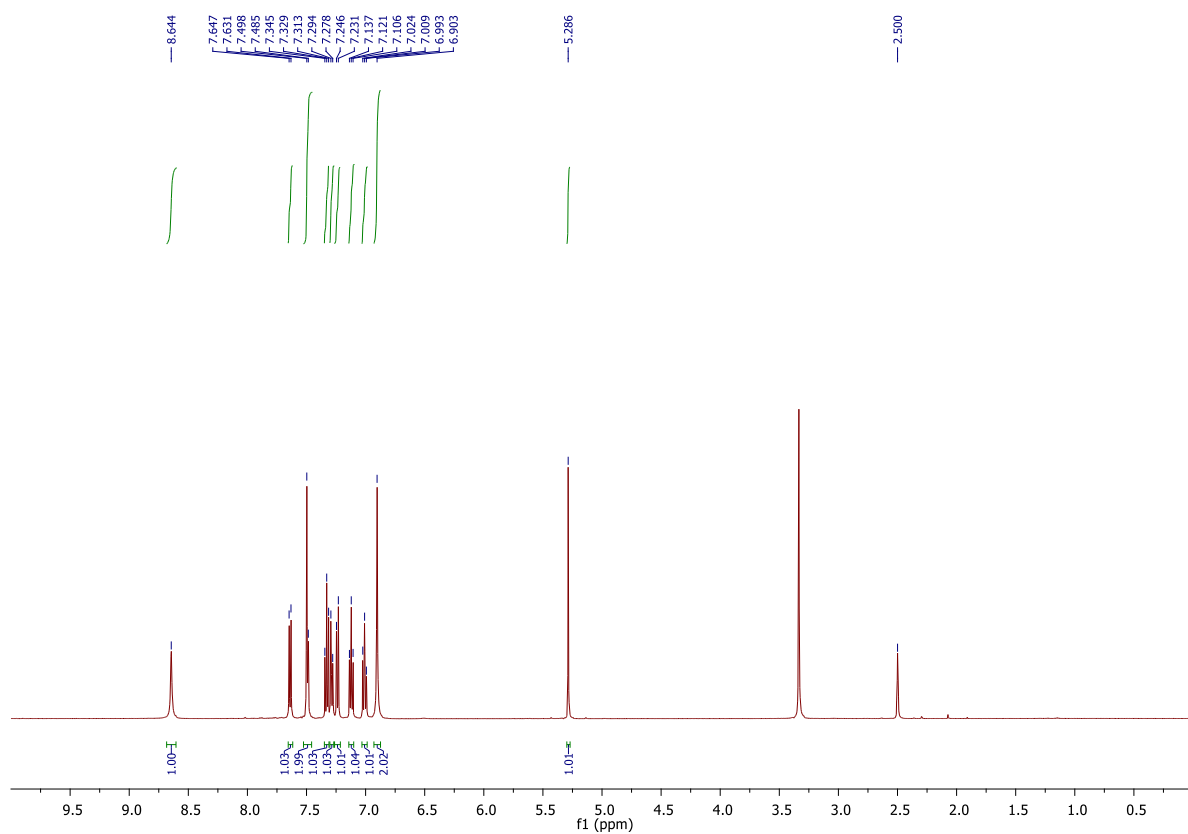




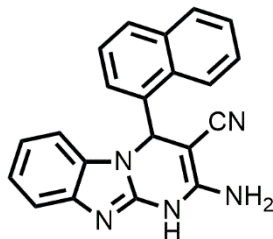
2-amino-4-(3-bromophenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11g)



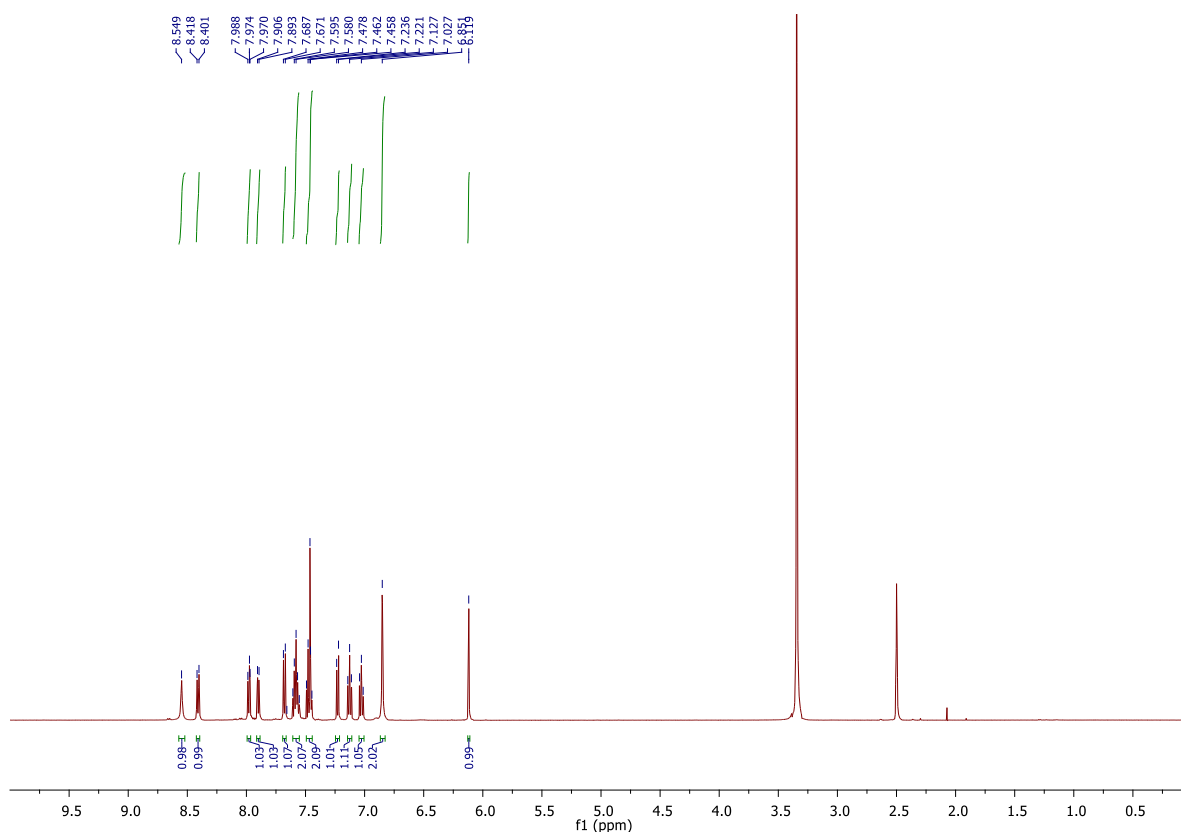
M.F. C₁₇H₁₂N₅Br (366.21). Yield: (0.303 g, 83%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.64 (s, 1H, NH), 7.64 (d, J = 8.0 Hz, 1H), 7.49 (d, J = 6.5 Hz, 2H), 7.27-7.34(m, 2H), 7.24 (d, J = 7.5 Hz 1H), 7.12 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 8.0 Hz, 1H), 6.90 (s, 2H), 5.28 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 152.0, 149.9, 146.1, 144.1, 131.5, 129.7, 125.5, 123.9, 122.4, 120.5, 119.6, 116.6, 113.0, 61.6, 53.0.

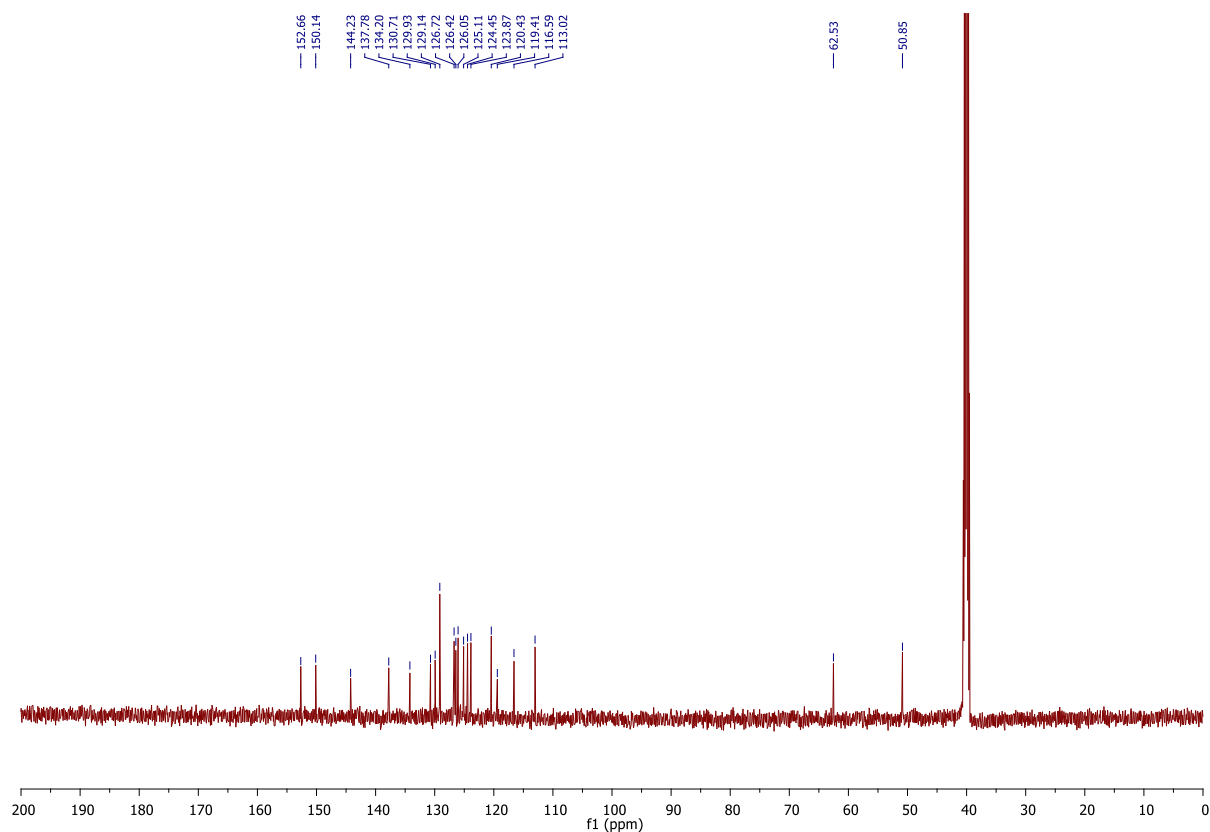


2-amino-4-(naphthalen-1-yl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11h)

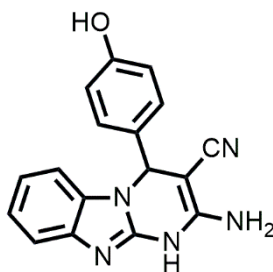


M.F. C₂₁H₁₅N₅ (337.38). Yield: (0.303 g, 83%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.58 (s, 1H, NH), 7.63 (d, J = 8.0 Hz, 1H), 7.32 (t, J = 6.5 Hz, 2H), 7.17-7.23(m, 3H), 7.11 (t, J = 7.5 Hz 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.85 (s, 2H), 5.24 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 152.7, 150.1, 144.2, 137.8, 134.2, 130.7, 129.9, 129.1, 126.7, 126.4, 126.0, 125.1, 124.4, 123.8, 120.4, 119.4, 116.6, 113.0, 62.53, 50.8.

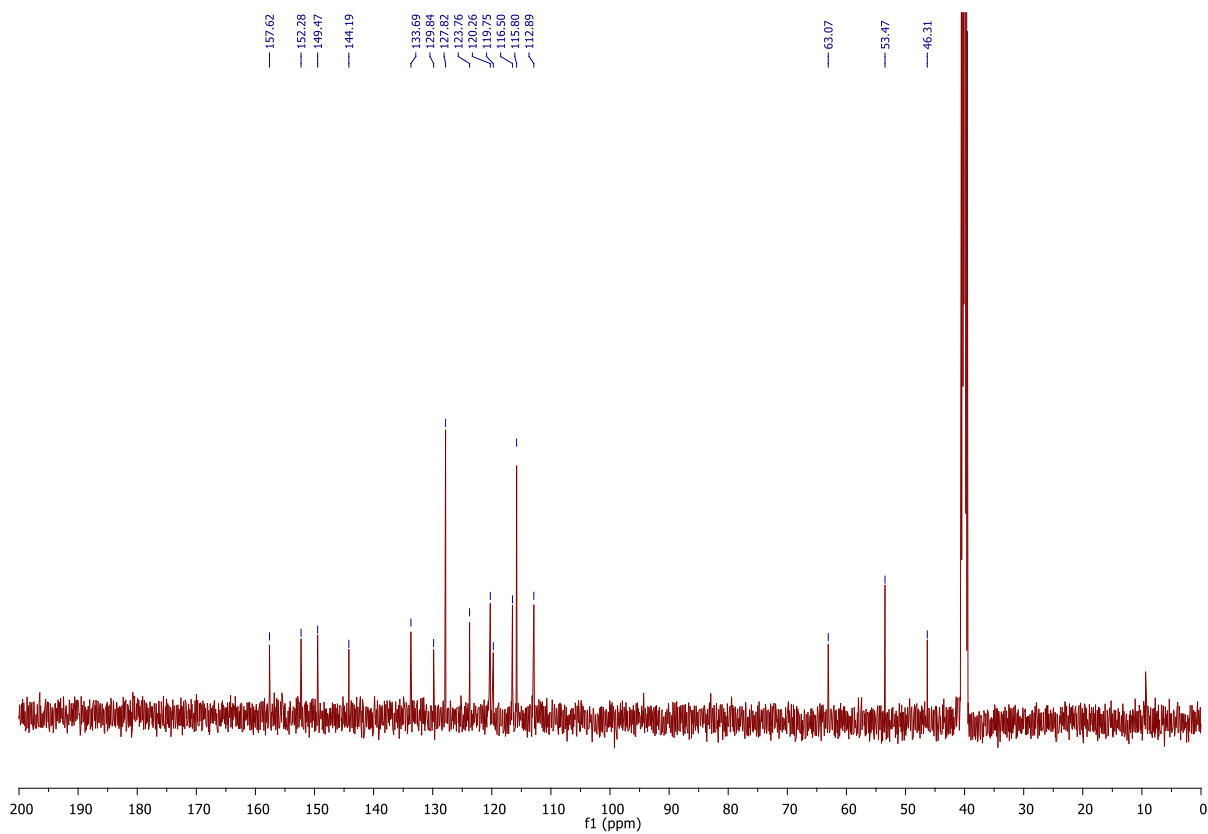
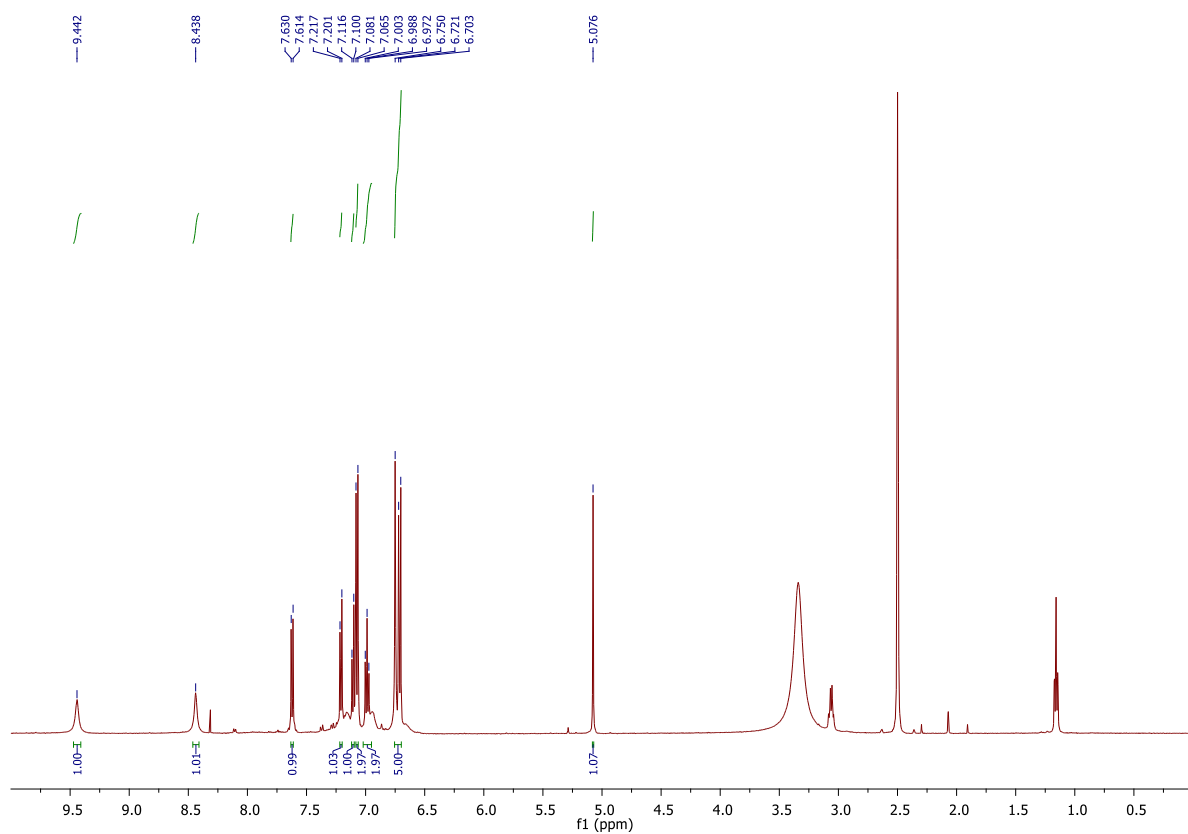




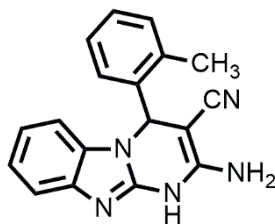
2-amino-4-(4-hydroxyphenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11i)



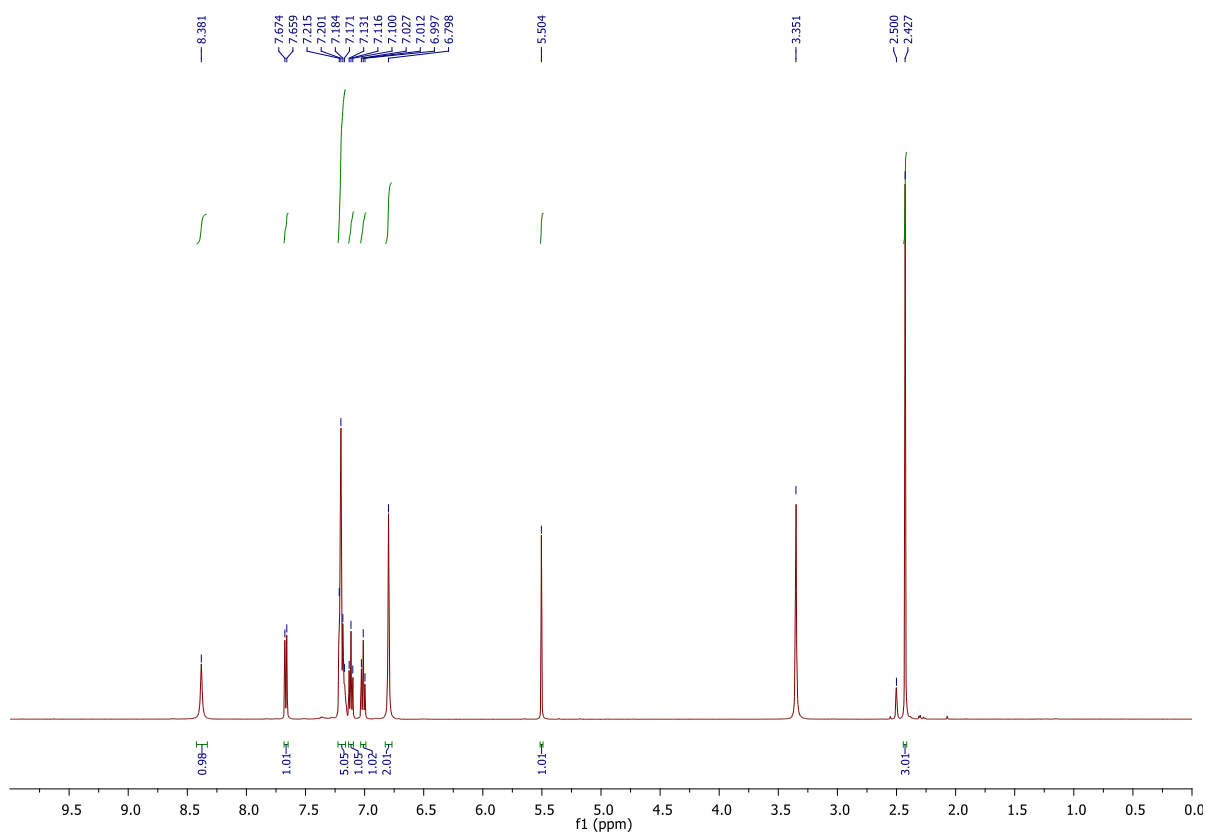
M.F. C₁₇H₁₃N₅O (303.32). Yield: (0.206 g, 68%). slaty powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 9.44 (s, 1H, OH), 8.58 (s, 1H, NH), 7.62 (d, J = 8.0 Hz, 1H), 7.21 (d, J = 8.0 Hz, 1H), 7.06-7.11(m, 3H), 6.99 (t, J = 8.0 Hz 2H), 6.73 (t, J = 9.0 Hz, 5H), 5.07 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 157.6, 152.3, 149.5, 144.1, 133.7, 129.8, 127.8, 123.8, 120.2, 119.7, 116.5, 115.8, 112.9, 63.0, 53.5, 46.3.

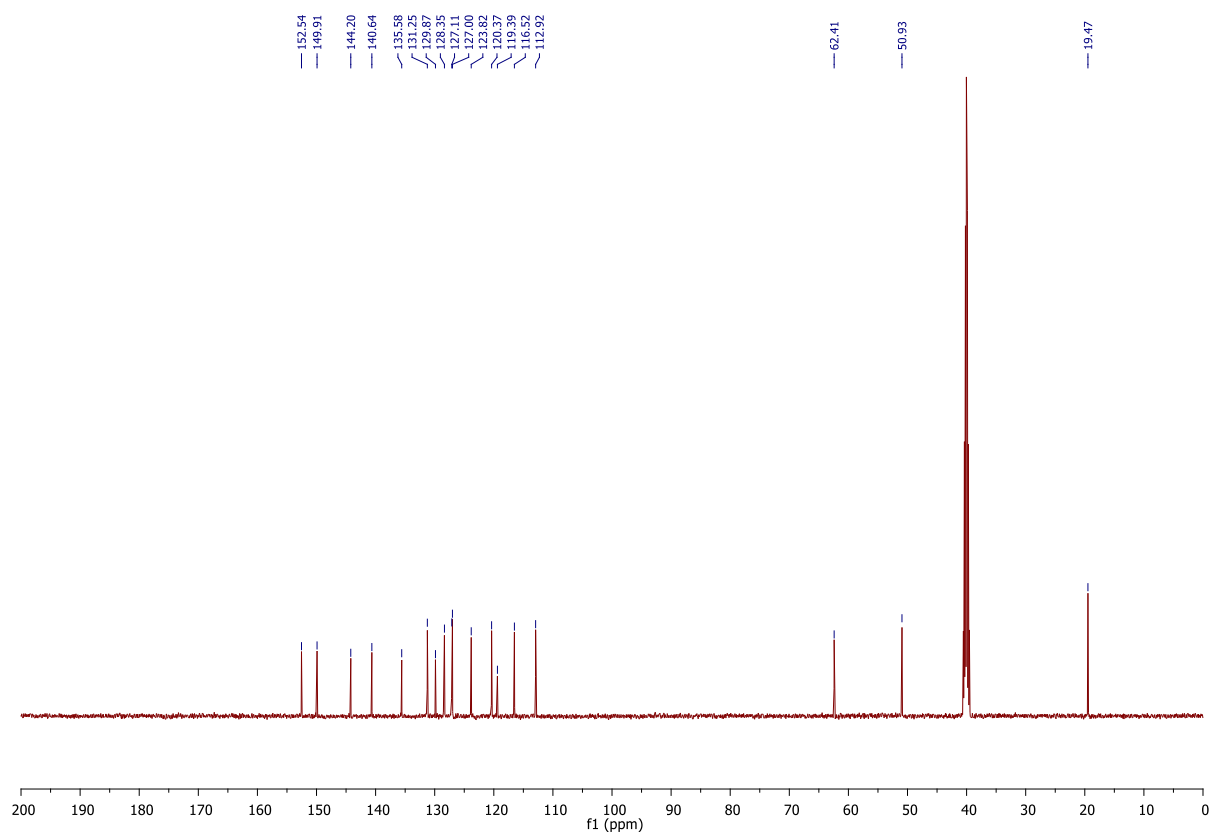


2-amino-4-(o-tolyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11j)

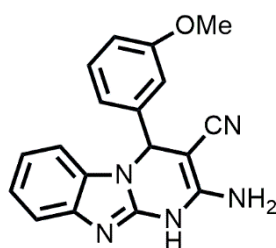


M.F. C₁₈H₁₅N₅ (301.35). Yield: (0.240 g, 80%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.38 (s, 1H, NH), 7.67 (d, J = 7.5 Hz, 1H), 7.17-7.21 (m, 5H), 7.11 (t, J = 8.0 Hz, 2H), 7.01 (t, J = 7.5 Hz, 1H), 6.79 (s, 2H), 5.50 (s, 1H), 2.43-2.50 (s, 3H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 152.5, 149.9, 144.2, 140.6, 135.6, 131.2, 129.8, 128.3, 127.1, 127.0, 123.8, 120.4, 119.4, 116.5, 112.9, 62.4, 50.9, 19.5.

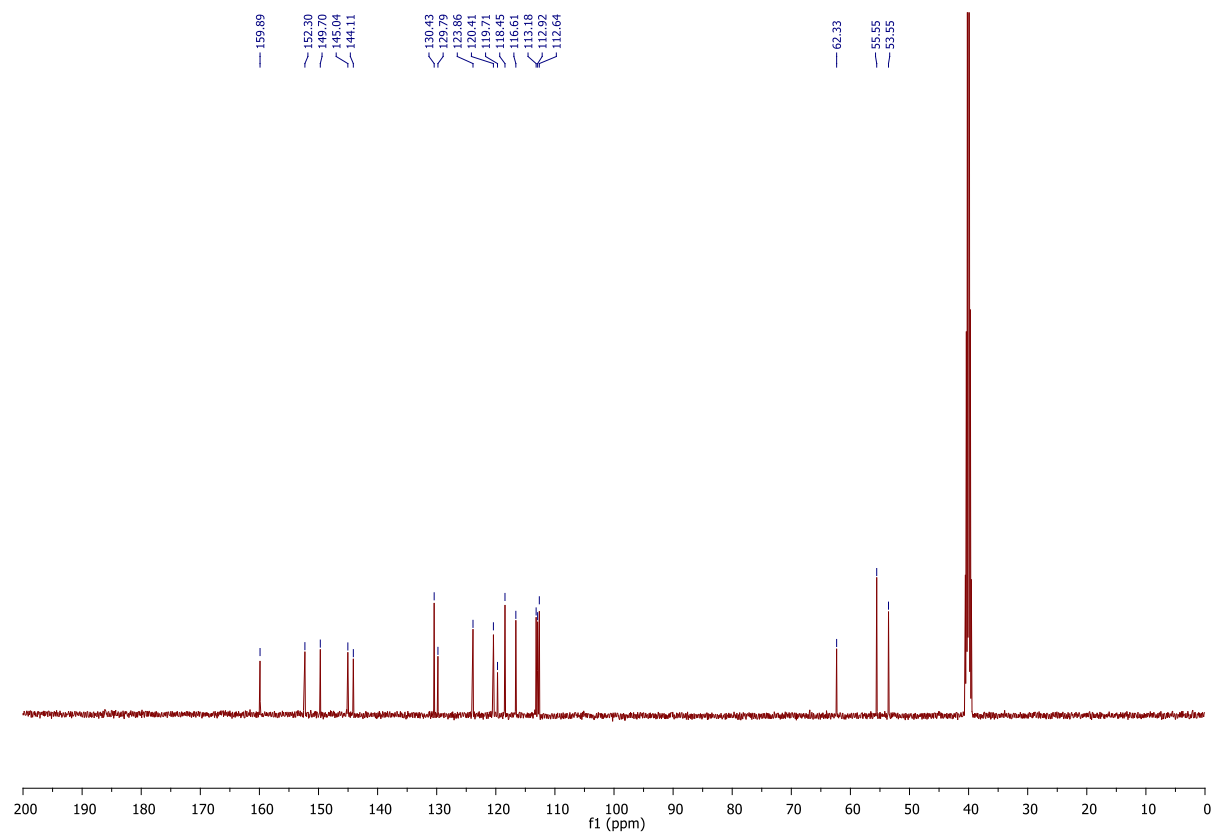
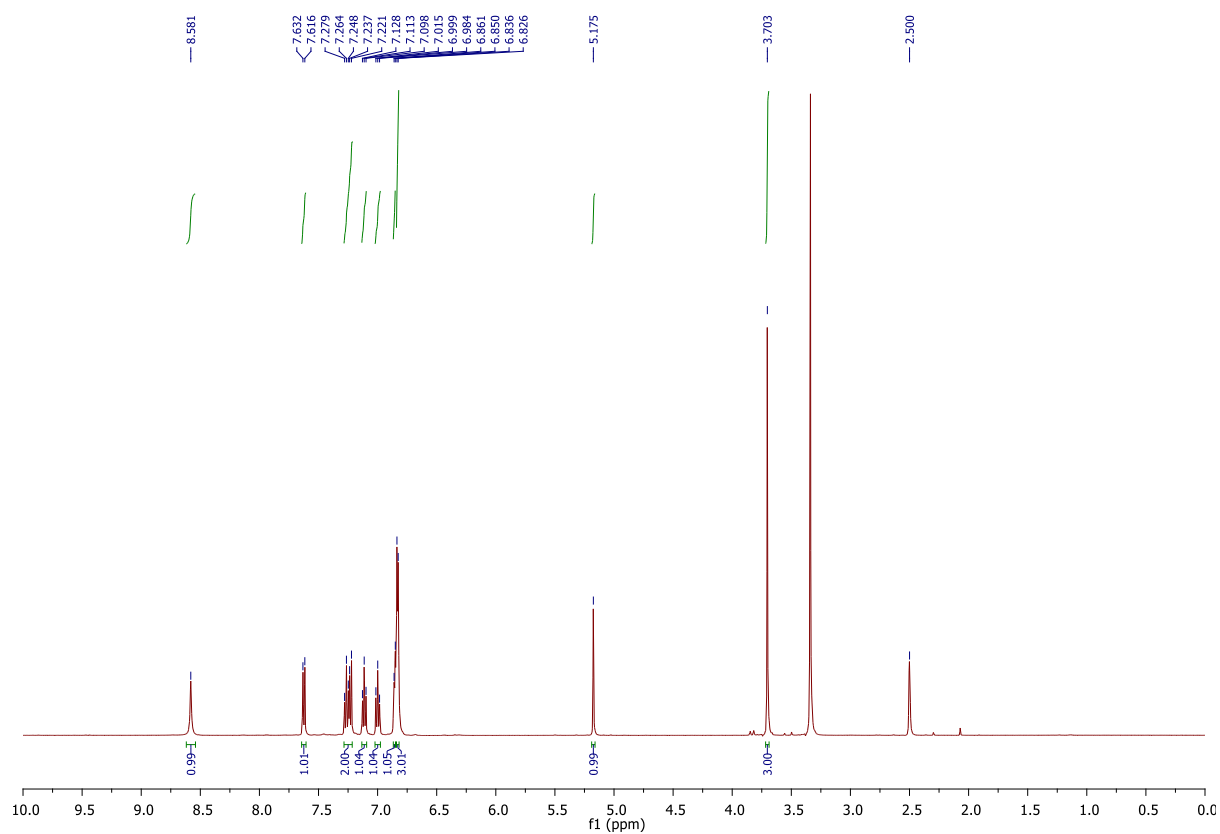




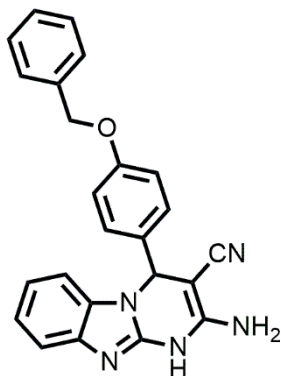
2-amino-4-(3-methoxyphenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11k)



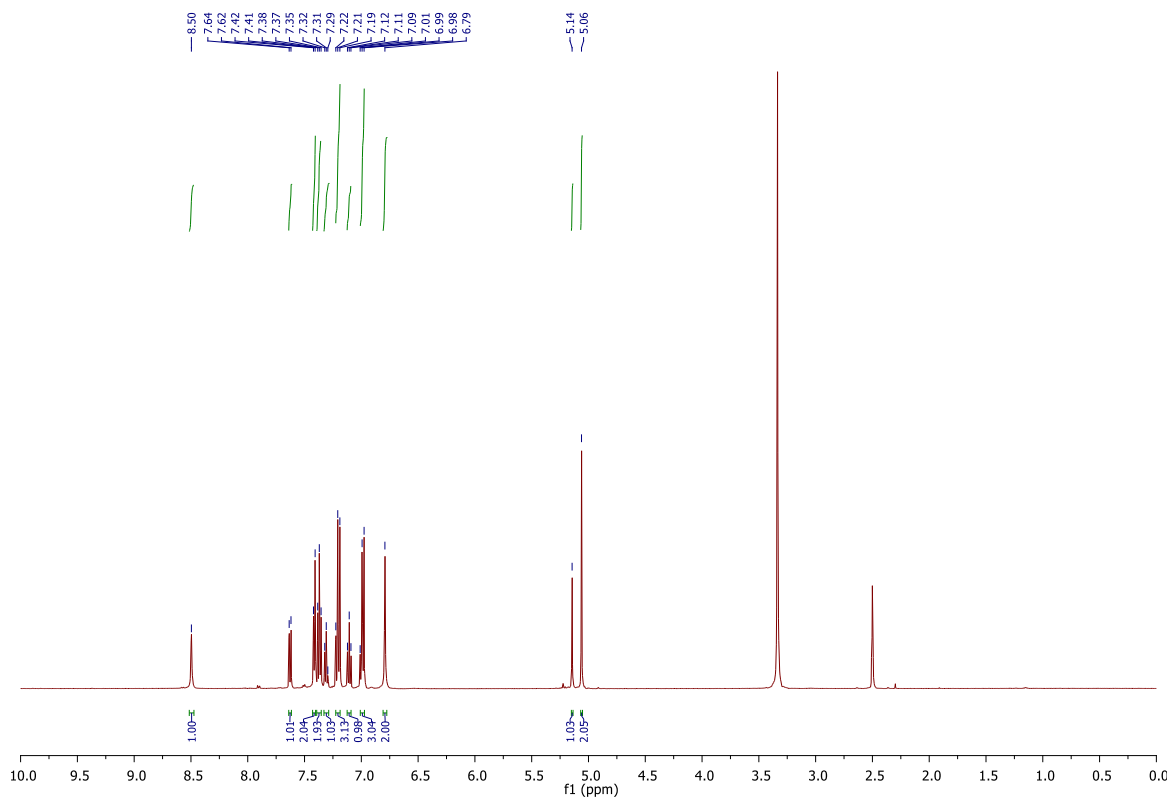
M.F. C₁₈H₁₅N₅O (317.34). Yield: (0.266 g, 84%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.58 (s, 1H, NH), 7.62 (d, J = 8.0 Hz, 1H), 7.22-7.27(m, 2H), 7.11 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.82-6.86 (m, 4H), 5.17 (s, 1H), 3.70 (s, 3H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 159.9, 152.3, 149.7, 145.0, 144.1, 130.4, 129.8, 123.8, 120.4, 119.7, 118.4, 116.6, 113.2, 112.9, 62.3, 55.5, 53.5.

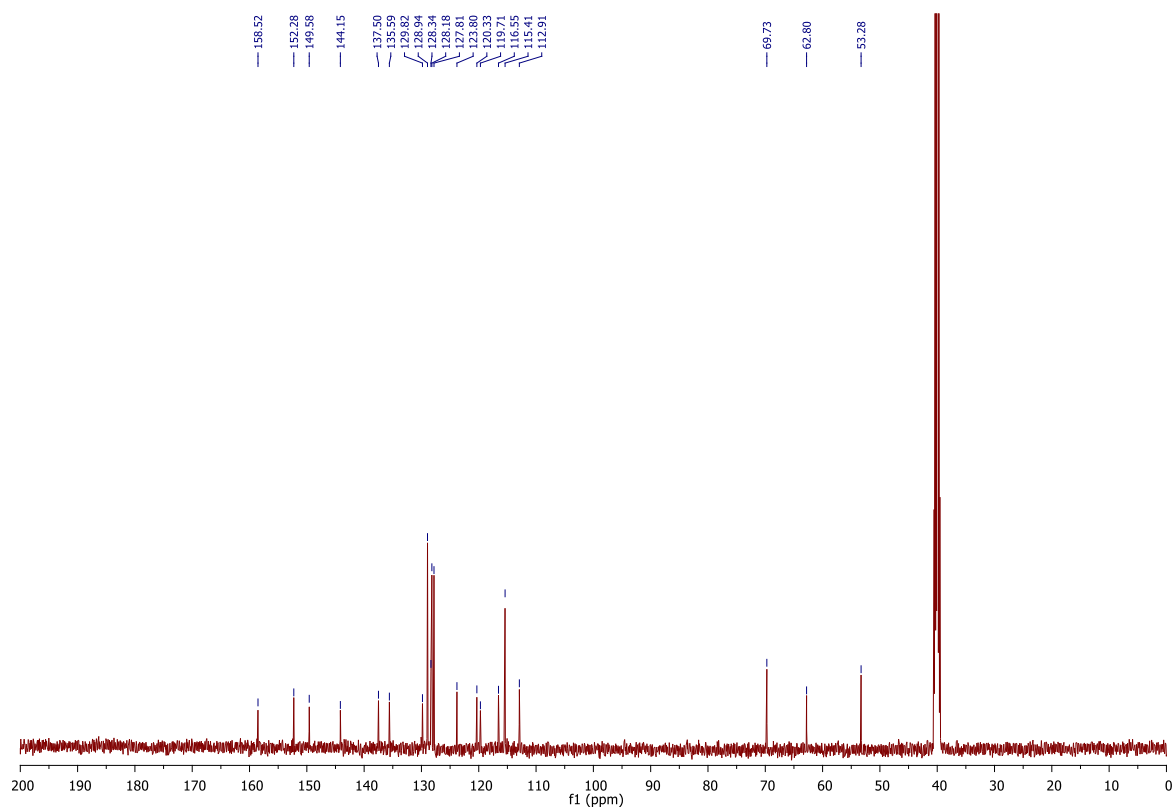


2-amino-4-(4-(benzyloxy)phenyl)-1,4-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidine-3-carbonitrile (11L)



M.F. C₂₄H₁₉N₅O (393.44). Yield: (0.341 g, 87%). White powder. ¹H NMR (500 MHz, DMSO-d₆, ppm) δ 8.49 (s, 1H, NH), 7.66 (d, J = 8.0 Hz, 1H), 7.47-7.49 (m, 1H), 7.34 (d, J = 7.5 Hz, 3H), 7.24 (d, J = 7.5 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.5 Hz, 1H), 6.87 (s, 2H), 5.64 (s, 1H); ¹³C NMR (125 MHz, DMSO-d₆, ppm) δ 158.5, 152.3, 149.6, 144.1, 137.5, 135.6, 129.8, 128.9, 128.3, 128.1, 127.8, 123.8, 120.3, 119.7, 116.5, 115.4, 112.9, 69.7, 62.8, 53.3.





Powder X-ray analysis of catalyst 2

Powder X-rd shows a sharp and intense peak for the bulk sample that clearly indicates the crystalline nature of the bulk sample.

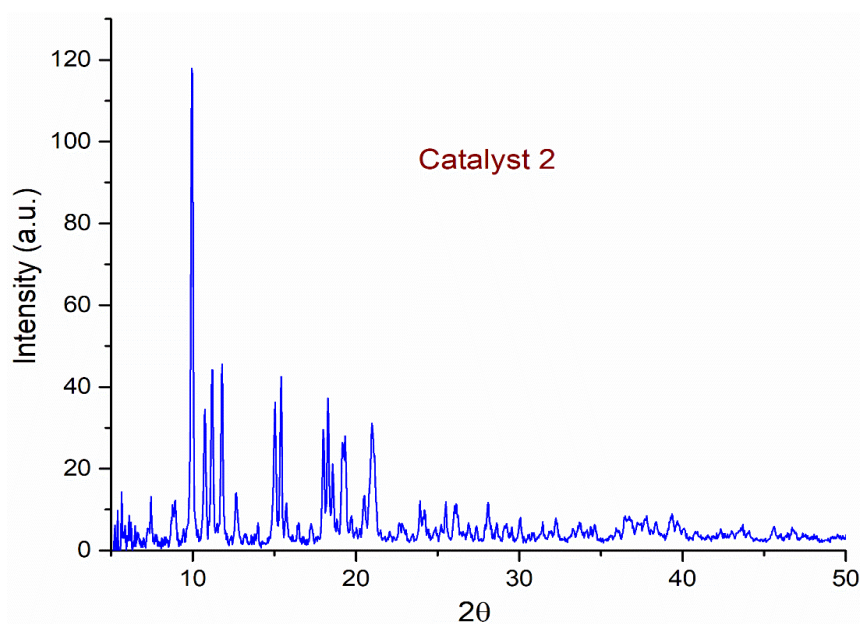


Figure S8: Powder X-ray analysis of catalyst 2

Elemental analysis:

EDAX analysis shows that the S, O, N, In and C present in the sample.

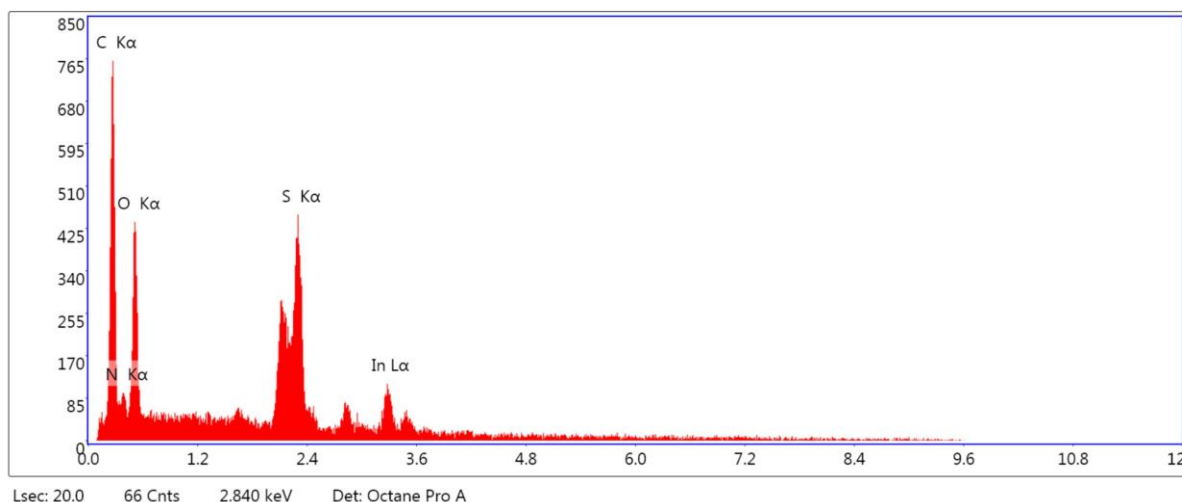


Figure S9: EDAX analysis of catalysts 2.

| Element | Weight % | Atomic % | Net Int. | Error % | Kratio | Z | A | F |
|---------|----------|----------|----------|---------|--------|--------|--------|--------|
| C K | 42.80 | 64.76 | 222.18 | 10.98 | 0.1330 | 1.1322 | 0.2745 | 1.0000 |
| N K | 1.61 | 2.09 | 6.86 | 59.15 | 0.0036 | 1.1001 | 0.2010 | 1.0000 |
| O K | 14.22 | 16.15 | 120.61 | 12.71 | 0.0449 | 1.0724 | 0.2943 | 1.0000 |
| S K | 25.57 | 14.49 | 331.75 | 4.45 | 0.2354 | 0.9314 | 0.9799 | 1.0088 |
| InL | 15.81 | 2.50 | 52.55 | 15.04 | 0.1044 | 0.6440 | 1.0268 | 0.9988 |

Materials

2,2'-bipyridine, 1,10 phenanthroline, tetramethylethylenediamine (tmeda), Indium trichloride anhydrous, copper(II)nitrate, Silver(I)nitrate, triphenylphosphine, 1,1'-bis(diphenylphosphinoferrocene) dppf, triethylamine, diisopropylamine, and 2-furoyl chloride all were purchased from Sigma-Aldrich chemicals. The solvents, chloroform, acetonitrile, and methanol were purchased from Merck Life sciences, India.

Instrumentation

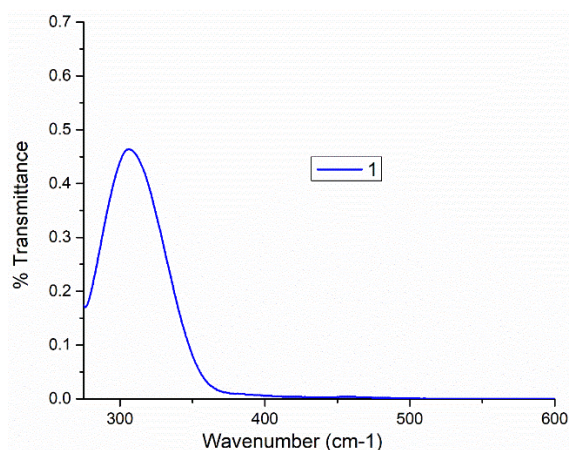
Electronic absorption spectra were recorded using a Shimadzu UV-1700 Pharma Spectrophotometer. Infrared spectra were recorded with a Varian-3100 FTIR spectrometer. NMR spectra were obtained using a JEOL ECZ500 MHz FT NMR spectrometer.

Synthesis

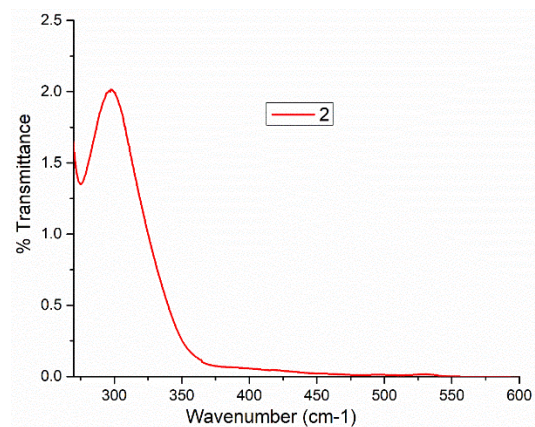
The precursor complexes $[\text{Ag}(\text{PPh}_3)_2\text{NO}_3]$, and $[\text{Cu}(\text{PPh}_3)_2\text{NO}_3]$ were prepared according to literature methods.^{1,2}

Synthesis of ligand: (furan-2-thiocarboxylic acid, fCOSH)

The ligand, fCOSH³ was synthesized using a process similar to that used to make thiobenzoic acid. 2-furoyl chloride (18.14g, 13.7 mL, 0.139 moles) was added drop-wise to a solution of KSH (15.60 g, 0.0278 moles) in ethanol (80 mL) for 1 h in an ice bath with stirring. The reaction mixture was agitated for another hour before the KCl precipitate was filtered off. The residue was dissolved in 100 mL of water and washed with 40 mL of benzene after the filtrate was dried under reduced pressure. 6 N HCl was used to acidify the aqueous solution, which was then extracted with 60 mL of diethyl ether. The ethereal layer was leftover anhydrous sodium sulfate overnight. It was dried at reduced pressure. A yellow oily liquid was obtained. Yield (13.8 g, 76%).



(a)



(b)

Figure S10. UV-Vis spectra of (a) Catalyst **1** and Catalyst and (b) **2** (DMSO solutions)

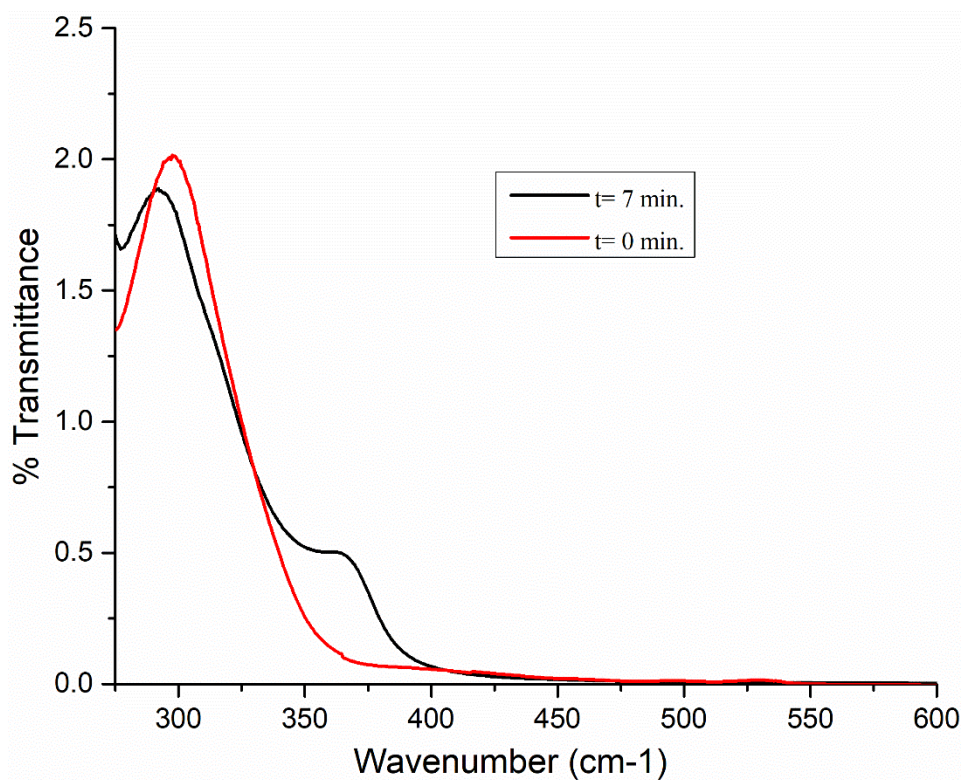


Figure S11. UV-Vis spectra of Catalyst **2** and the reaction mixture. [T= 0 min; Pure catalyst **2**; λ_{max} = 297 nm; T= 7 min (Catalyst + Substrate) λ = 292, 364 nm.]

Table S2 Important vibrational modes of Complex 1 and 2 (*via* DFT analysis)

Complex 2

| Sl. No. | Frequency (nm) | IR Intensity (a.u.) | Raman Intensity (a.u.) | Assignment |
|---------|----------------|---------------------|------------------------|--------------------------|
| 54 | 316.51 | 8.6521 | 14.7132 | In-S Stretching |
| 55 | 329.48 | 8.2773 | 14.0777 | |
| 56 | 333.63 | 20.8862 | 13.7045 | |
| 57 | 342.50 | 17.7793 | 5.0524 | |
| 58 | 398.59 | 53.7416 | 13.2512 | Scissoiring of SCO group |
| 59 | 400.17 | 55.3759 | 17.5387 | |
| 60 | 402.97 | 51.2300 | 7.3040 | |
| 61 | 410.84 | 40.3564 | 11.0262 | |
| 62 | 541.99 | 5.9239 | 3.8145 | Wagging of SCO group |
| 63 | 542.43 | 12.3207 | 9.9561 | |
| 64 | 544.42 | 11.8126 | 8.3952 | |
| 65 | 546.93 | 8.3151 | 16.0730 | |
| 66 | 558.14 | 15.9046 | 4.2607 | |
| 67 | 558.92 | 1.7567 | 40.7581 | |
| 68 | 561.50 | 3.3626 | 13.6071 | Ring Deformations |
| 69 | 563.60 | 12.3804 | 3.6988 | |
| 70 | 612.15 | 2.9517 | 30.5785 | |
| 71 | 641.62 | 1.5899 | 2.0945 | |
| 72 | 642.02 | 0.7336 | 5.0414 | |
| 73 | 645.73 | 0.6148 | 1.8849 | |
| 74 | 650.74 | 4.8313 | 88.3500 | |
| 75 | 651.87 | 5.2806 | 12.8407 | |
| 76 | 657.97 | 6.4139 | 25.8686 | |
| 77 | 675.38 | 0.8679 | 4.4551 | |
| 78 | 716.55 | 0.2910 | 14.2229 | |
| 79 | 721.97 | 0.7513 | 24.2536 | |
| 80 | 722.56 | 0.6078 | 17.7696 | |

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