

Supporting Information

Boric Acid in Magnetized Water: Clean and Powerful Media for Synthesis of 3,4-dihydropyrimidin-2(1H)-ones

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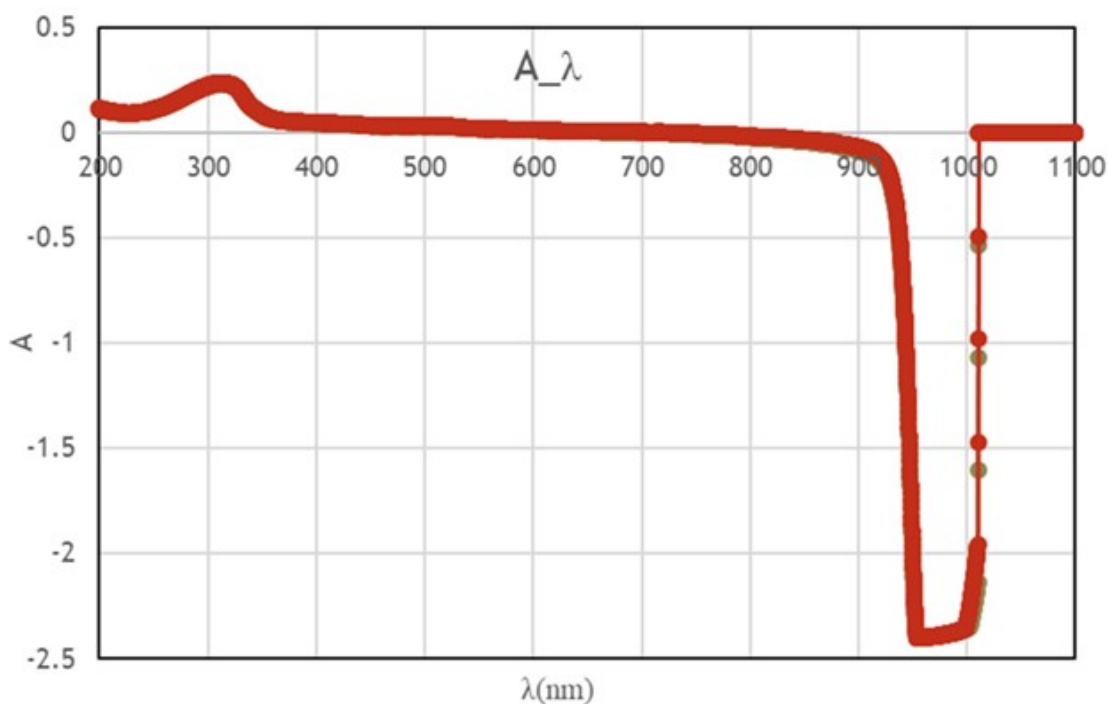
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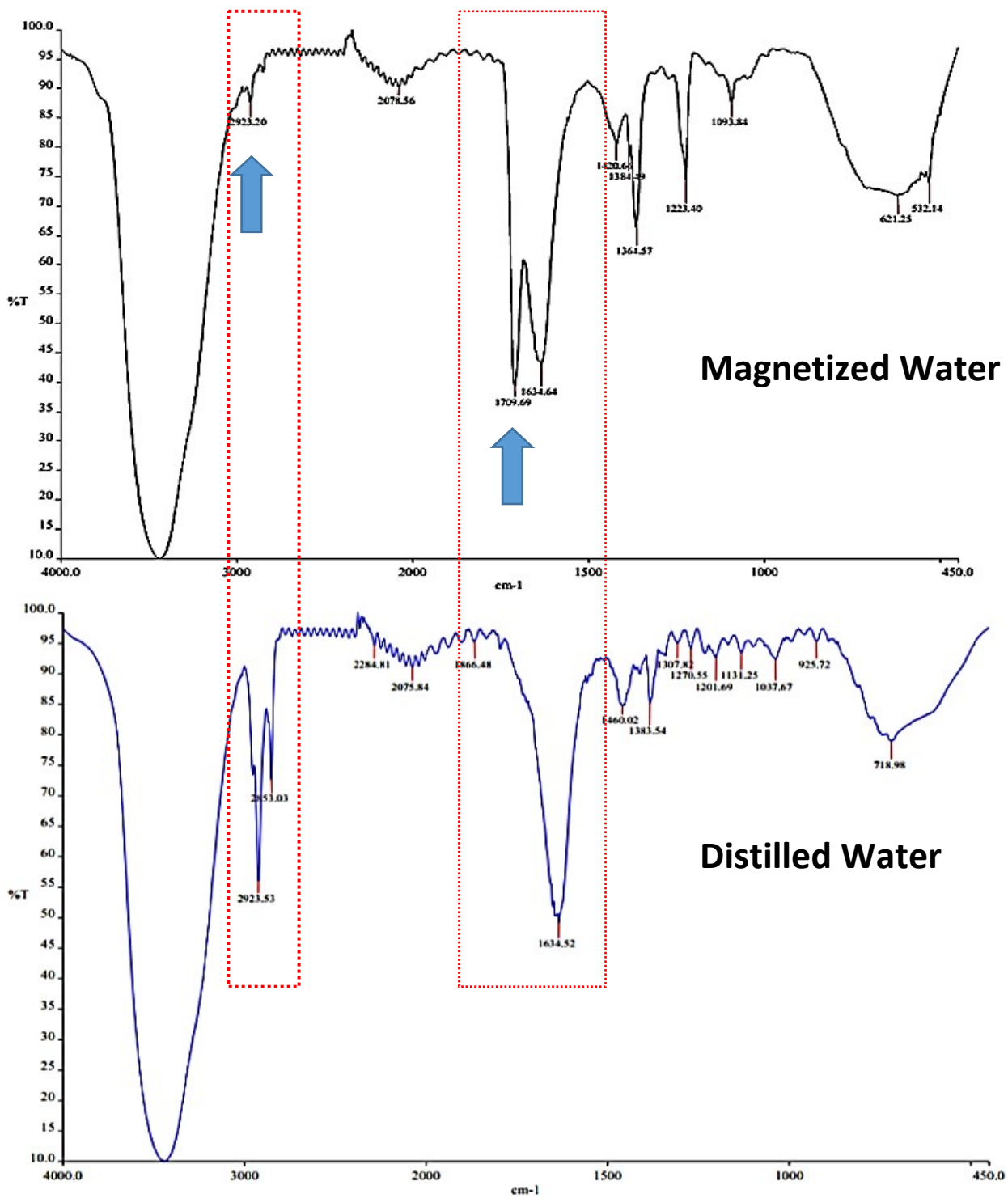
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General Methods. All chemicals were purchased from Merck or Fluka Chemical Companies. The known products were identified by comparison of their melting points and spectral data with those in the authentic samples. The ^1H NMR (250 MHz) and ^{13}C NMR (62.5 MHz) were run on a Bruker Avance DPX-250 FT-NMR spectrometer (δ in ppm). Melting points were recorded on a Büchi B-545 apparatus in open capillary tubes. Tetra-test-kit (Tetra®) was used to measure the amount of dissolved oxygen in magnetic water and ordinary water. The pH changes of the water were measured by Canaway's pH meter at different temperatures.



S1. The UV spectrum of magnetized and distilled water.



S2. FT-IR spectroscopy of magnetized and distilled water.

S3. Selected Data of Compounds:

Ethyl 4-(4-(benzyloxy)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate:

Mp 200-202 °C; ¹H NMR: (250 MHz, DMSO-*d*₆) δ = 1.04-1.09 (t, *J* = 6.75 Hz, 3H, CH₃), 2.21 (s, 3H, CH₃), 3.93-3.99 (m, 2H, CH₂), 5.04 (s, 3H), 6.91-6.94 (d, *J*=8.0 Hz, 2H), 7.10-7.13 (d, *J*=8.0 Hz, 2H), 7.32-7.38 (m, 5H), 7.65 (s, 1H), 9.13 (s, 1H); ¹³C NMR (62.5 MHz, DMSO-*d*₆) δ 14.5, 18.1, 53.7, 59.5, 69.6, 100.0, 115.0, 127.8, 128.0, 128.8, 137.7, 148.4, 152.6.

Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Mp 204-207 °C; ¹H NMR (250 MHz, DMSO-*d*₆) δ 9.13 (d, *J* = 2.1 Hz, 1H), 7.67 (dd, *J* = 3.5, 2.1 Hz, 1H), 7.24 (dd, *J* = 8.1, 6.9 Hz, 2H), 7.18 – 7.11 (m, 3H), 5.07 (d, *J* = 3.3 Hz, 1H), 3.90 (q, *J* = 7.1 Hz, 2H), 2.17 (s, 3H), 1.01 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (62.5 MHz, DMSO-*d*₆) δ 165.94, 152.77, 148.97, 145.47, 129.00, 127.87, 126.86, 99.86, 59.81, 54.58, 18.41, 14.69.

Ethyl 6-methyl-2-oxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Mp 203-204 °C; ¹H NMR (250 MHz, DMSO-*d*₆) δ 9.17 (d, *J* = 2.0 Hz, 1H), 7.70 (dd, *J* = 3.5, 2.1 Hz, 1H), 7.13 (s, 4H), 5.22 – 5.00 (m, 1H), 4.06 – 3.79 (m, 2H), 2.35 – 2.16 (m, 6H), 1.12 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (62.5 MHz, DMSO-*d*₆) δ 165.85, 152.68, 148.62, 142.44, 136.85, 129.37, 126.63, 99.91, 59.69, 54.11, 21.12, 18.24, 14.57.

Ethyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

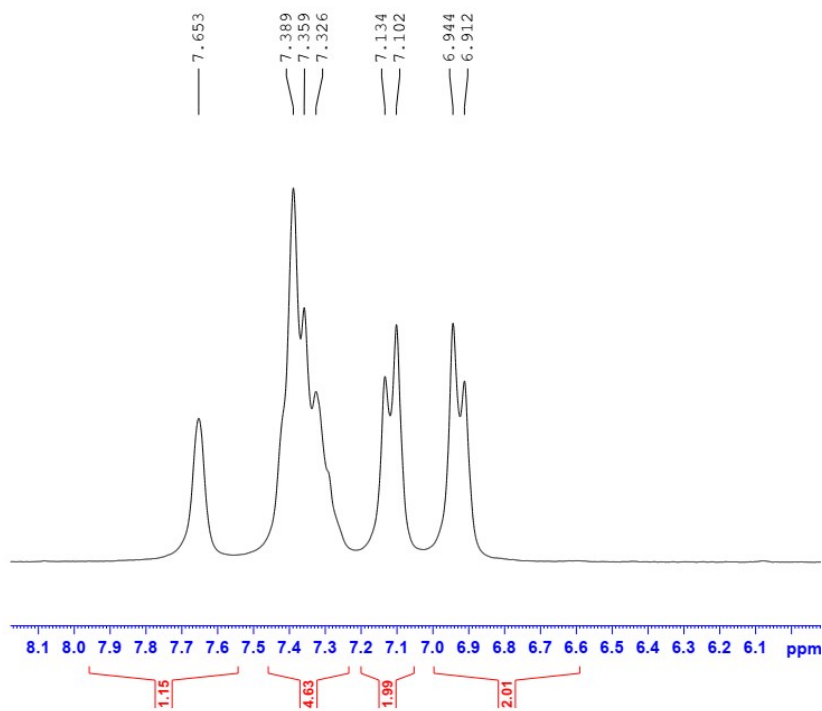
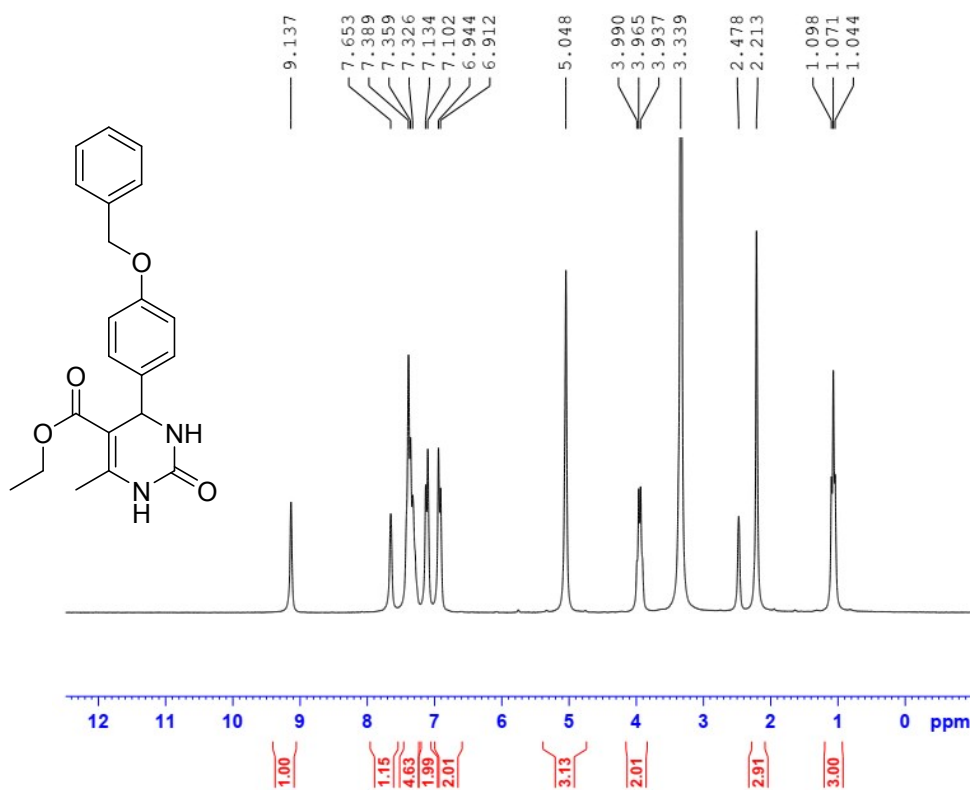
Mp 210-213 °C; ¹H NMR (250 MHz, DMSO-*d*₆) δ 9.33 (s, 1H), 9.11 (d, *J* = 2.1 Hz, 1H), 7.62 (dd, *J* = 3.4, 2.0 Hz, 1H), 7.11 – 6.90 (m, 2H), 6.76 – 6.59 (m, 2H), 5.04 (d, *J* = 3.2 Hz, 1H), 3.97 (q, *J* = 7.1 Hz, 2H), 2.23 (s, 3H), 1.09 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (62.5 MHz, DMSO-*d*₆) δ 165.86, 156.98, 152.64, 148.18, 135.88, 127.85, 115.43, 100.20, 59.56, 53.89, 40.43, 40.26, 40.09, 39.93, 39.76, 39.59, 39.42, 18.19, 14.55.

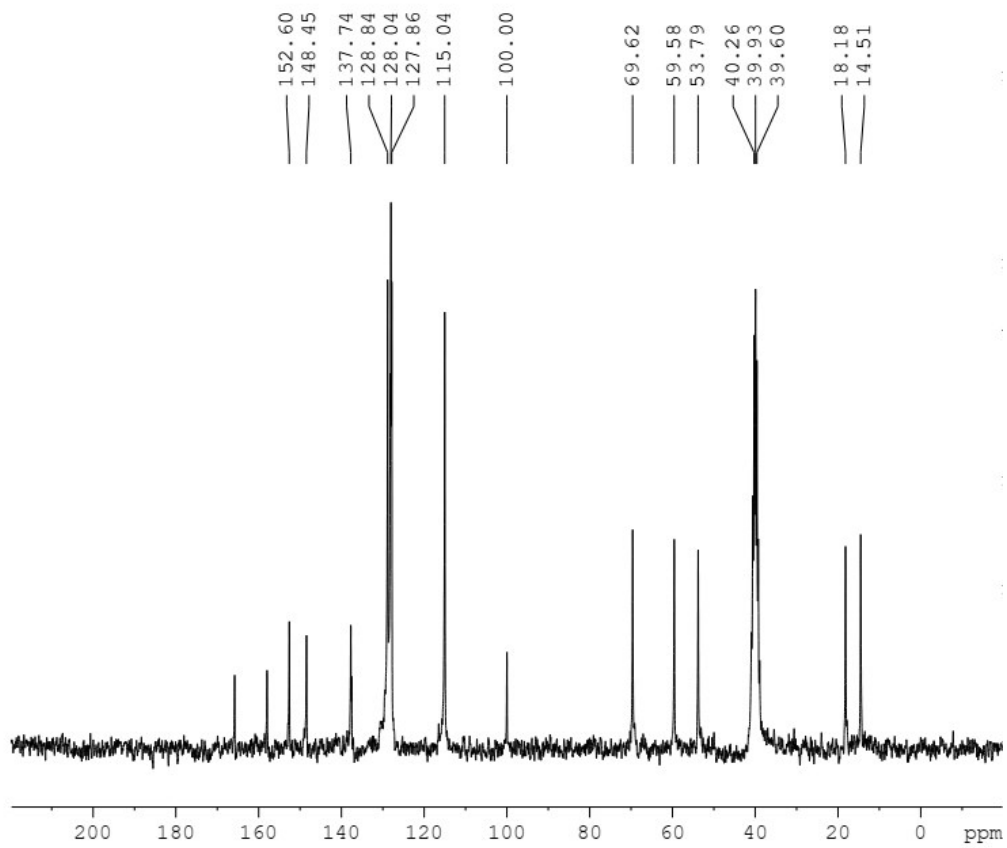
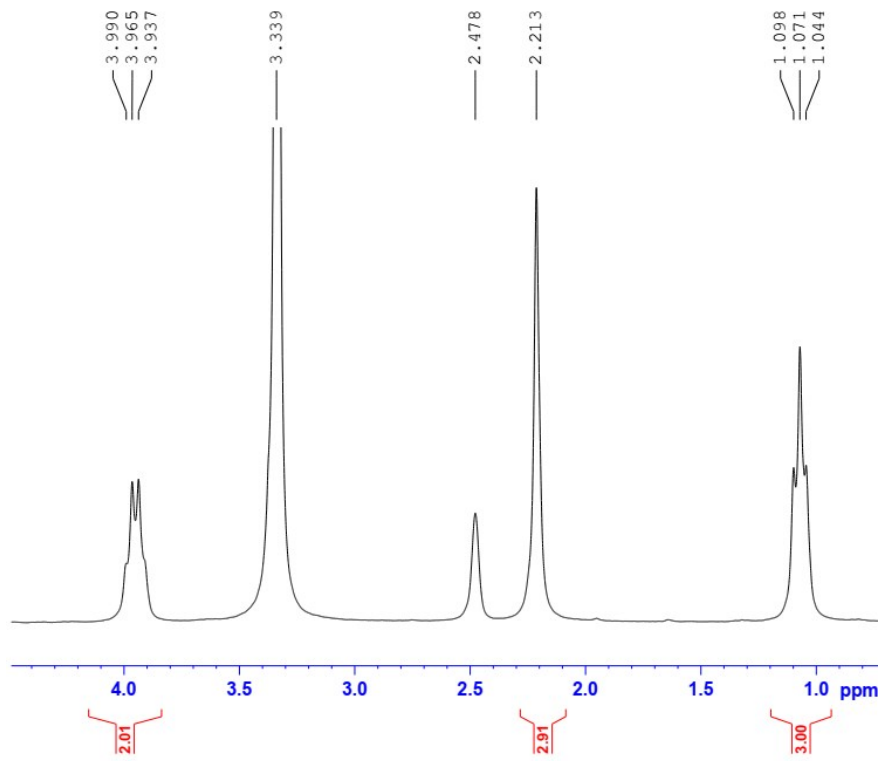
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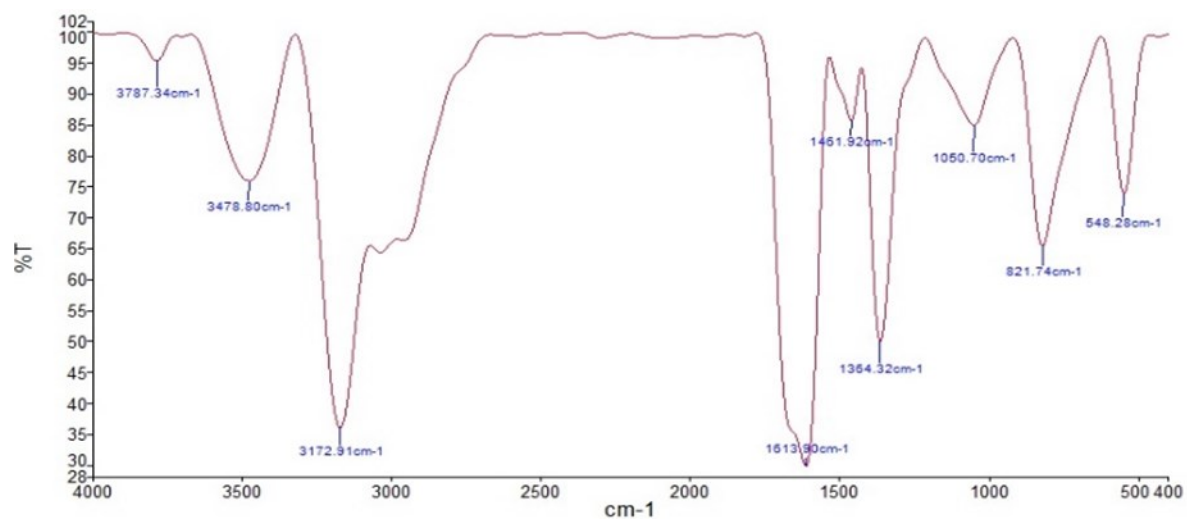
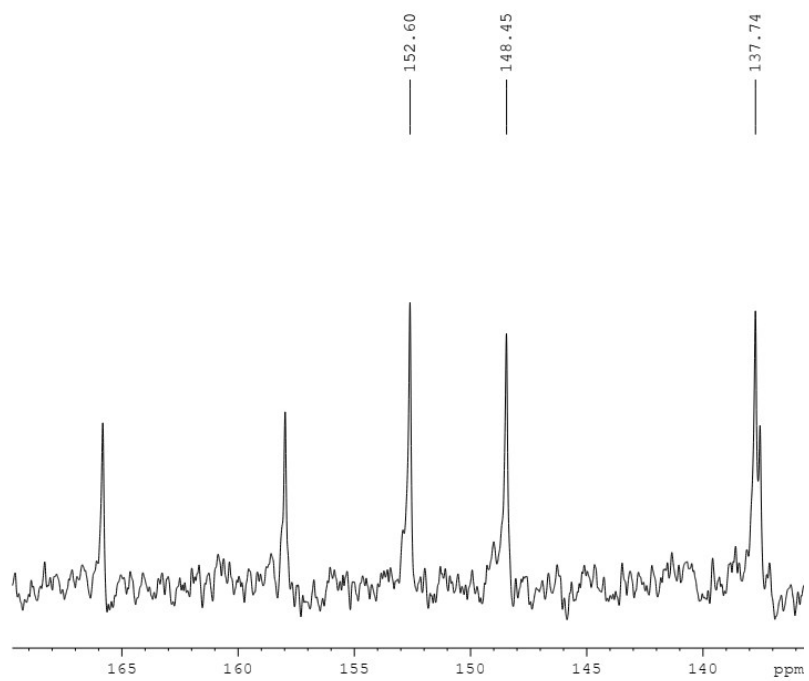
Mp 259-260 °C; ¹H NMR (250 MHz, DMSO-*d*₆) δ 9.10 (d, *J* = 2.0 Hz, 1H), 7.60 (dd, *J* = 3.5, 2.1 Hz, 1H), 7.20 – 6.90 (m, 2H), 6.78 – 6.46 (m, 2H), 5.05 (d, *J* = 3.3 Hz, 1H), 3.99 (qd, *J* = 7.1, 1.9 Hz, 2H), 2.86 (s, 6H), 2.24 (s, 3H), 1.13 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (62.5 MHz, DMSO-*d*₆) δ 165.97, 152.78, 150.24, 148.02, 133.13, 127.36, 112.70, 100.38, 59.57, 53.78, 18.21, 14.62.

NMR Spectra of Compounds (S4)

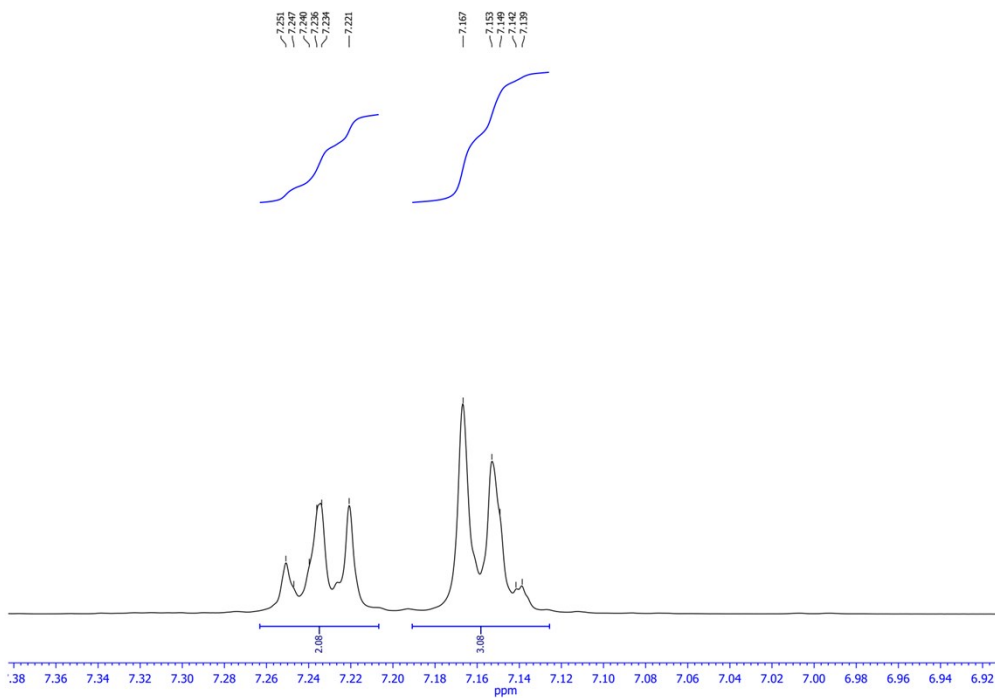
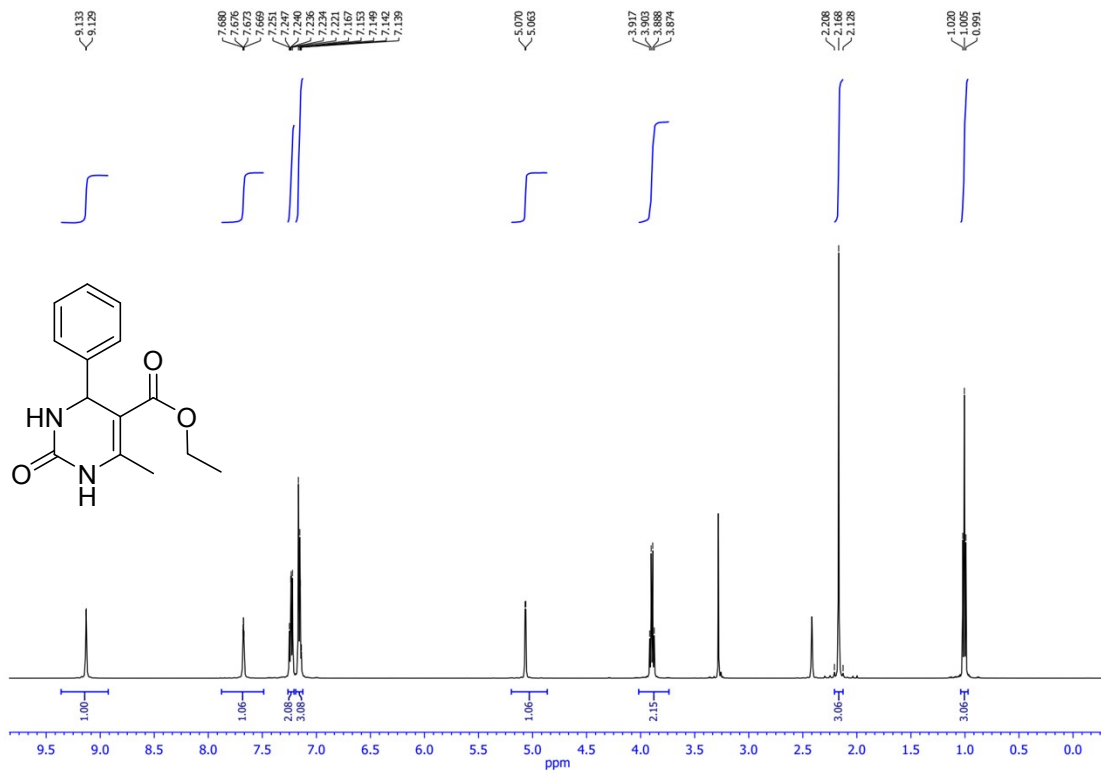
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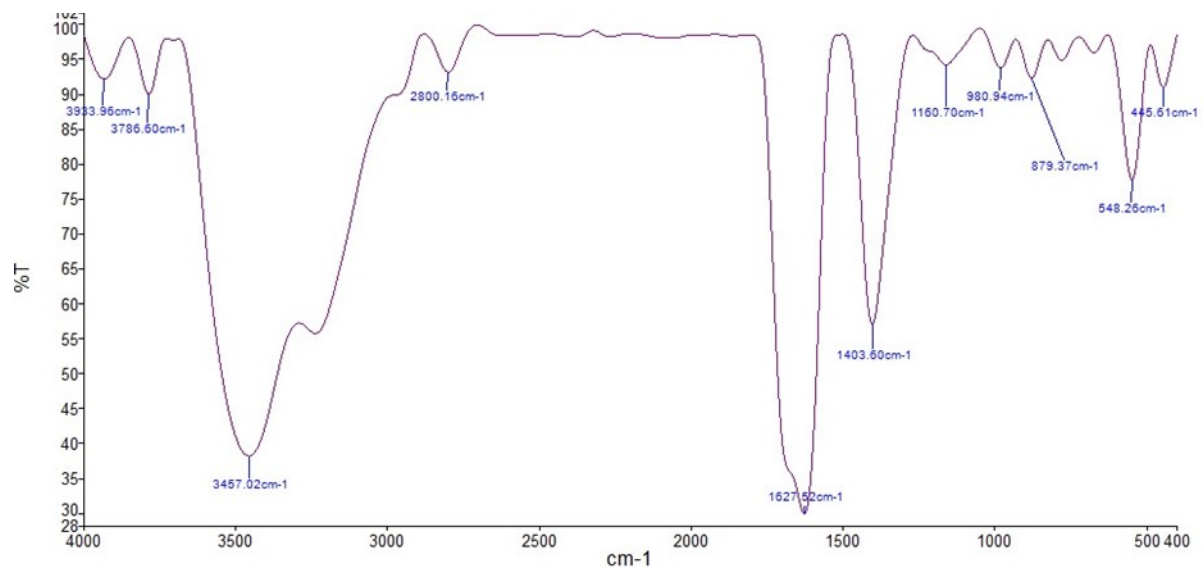
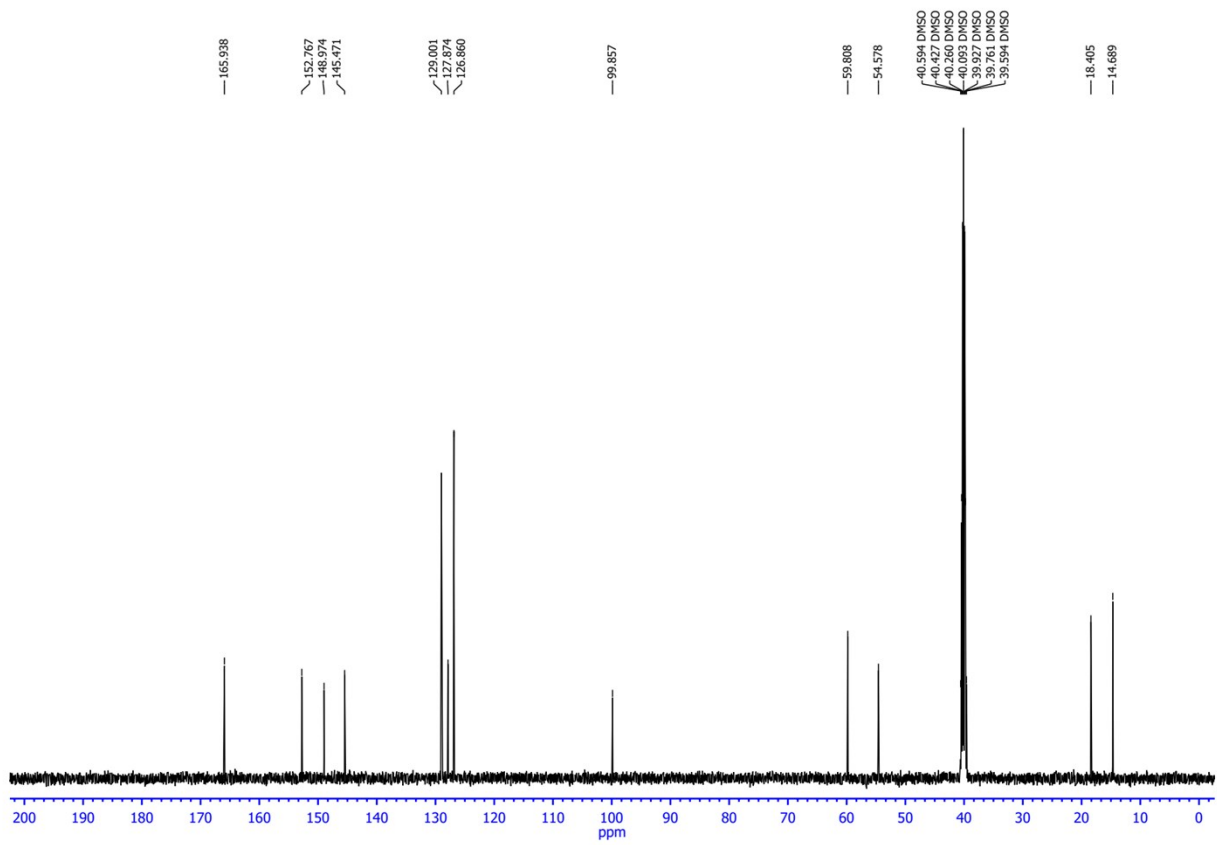




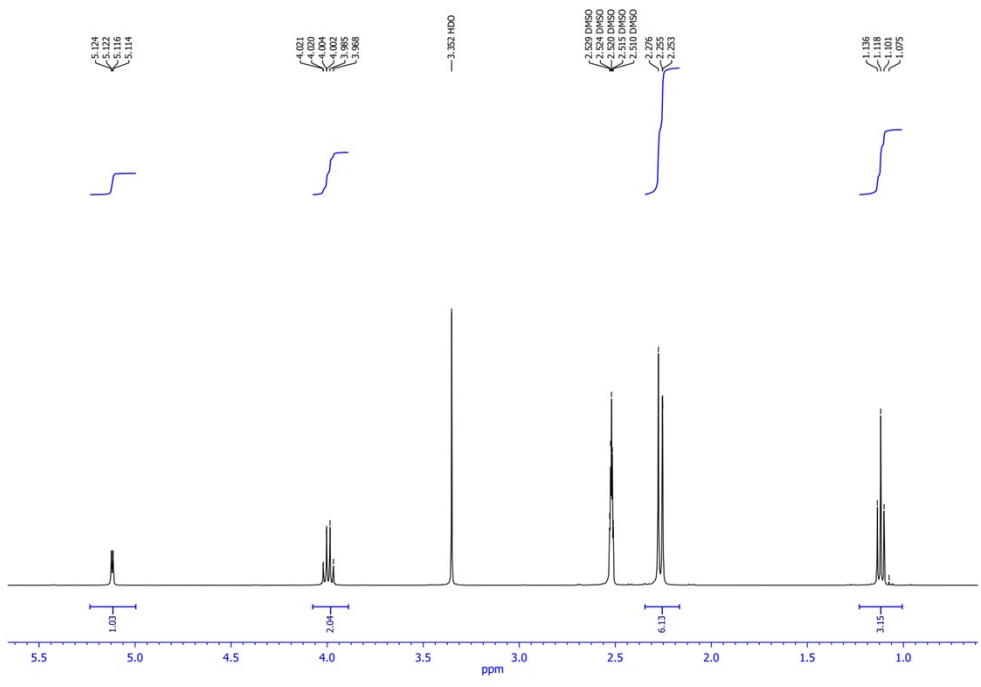
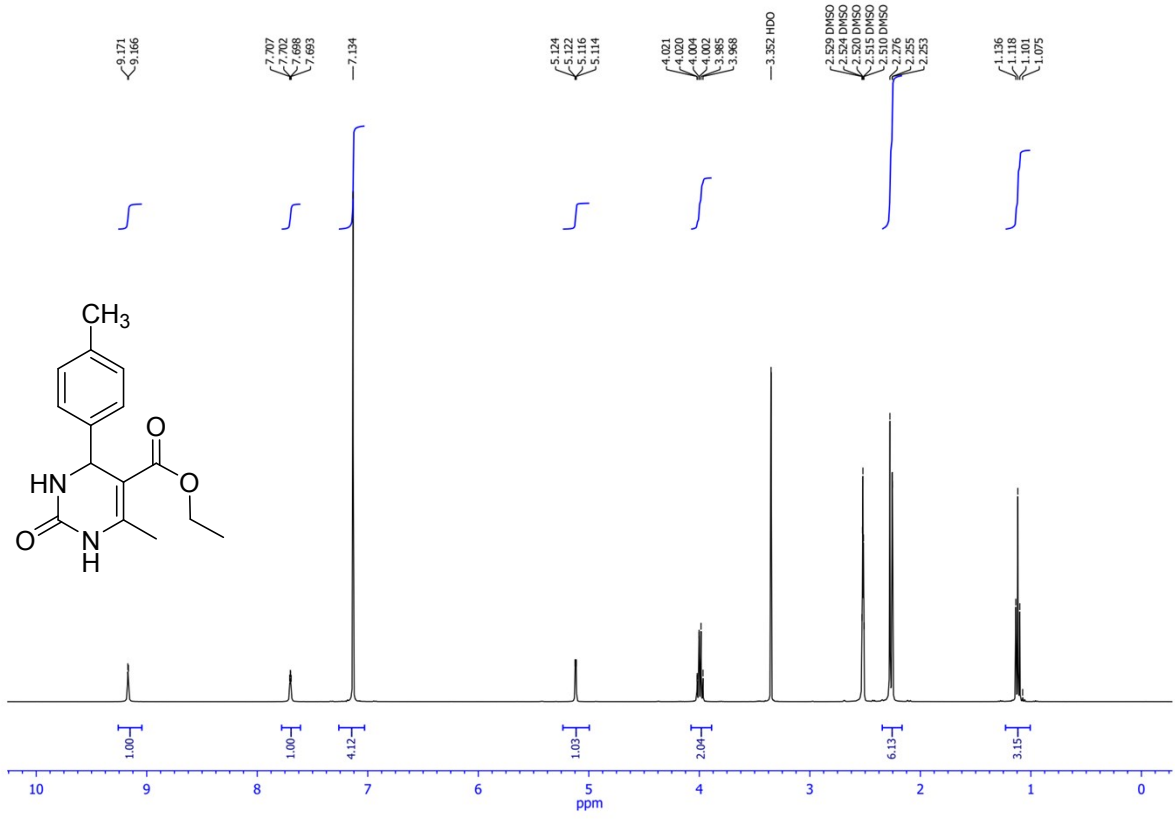


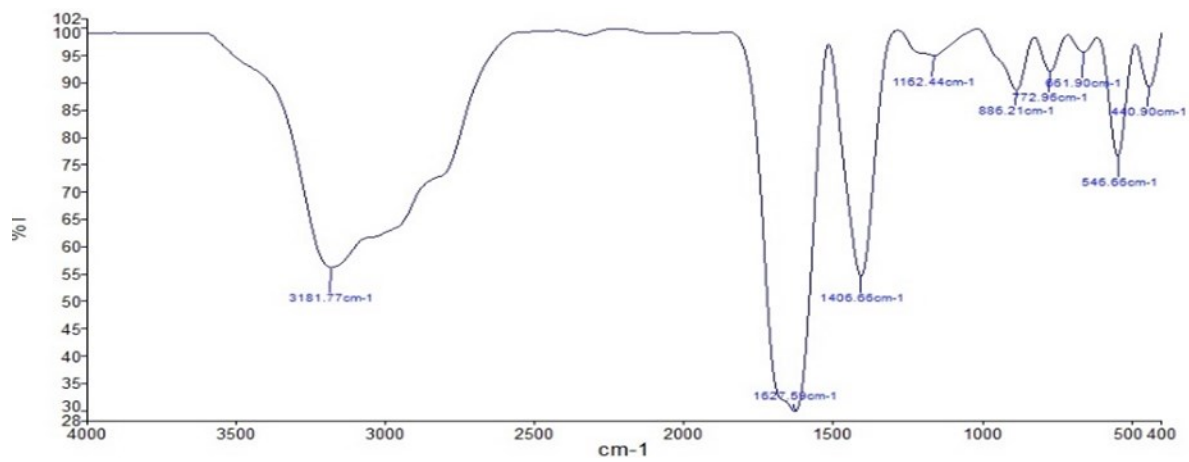
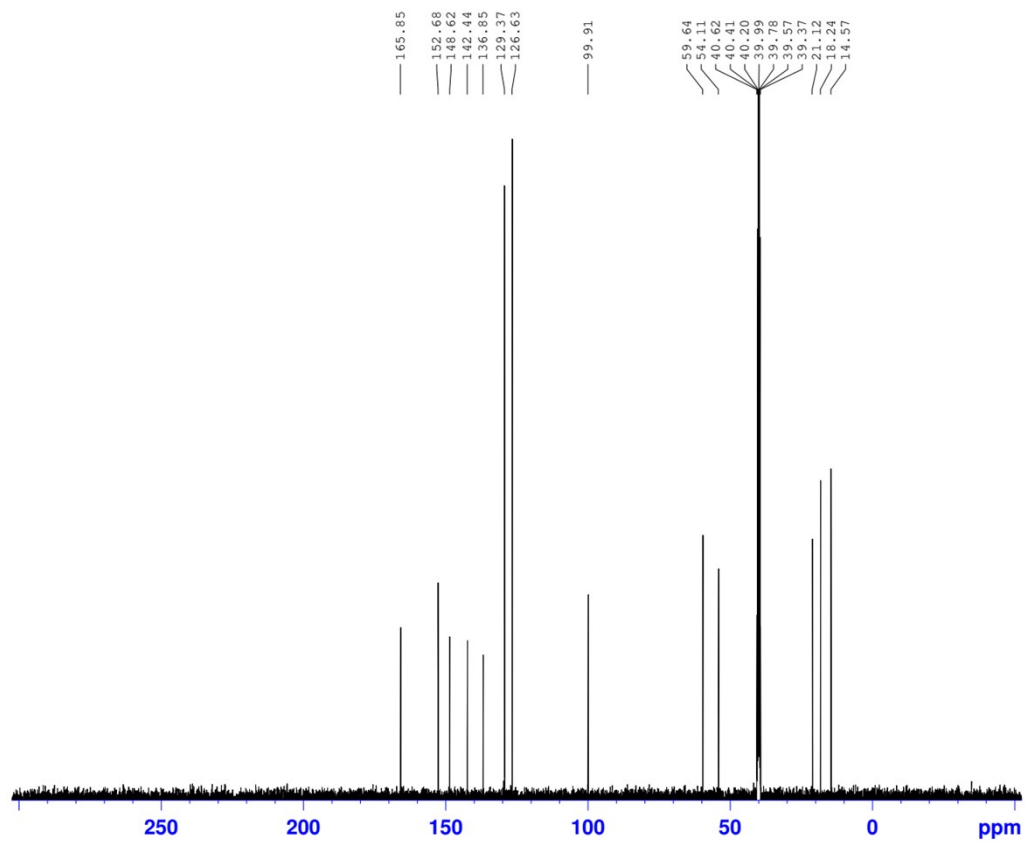
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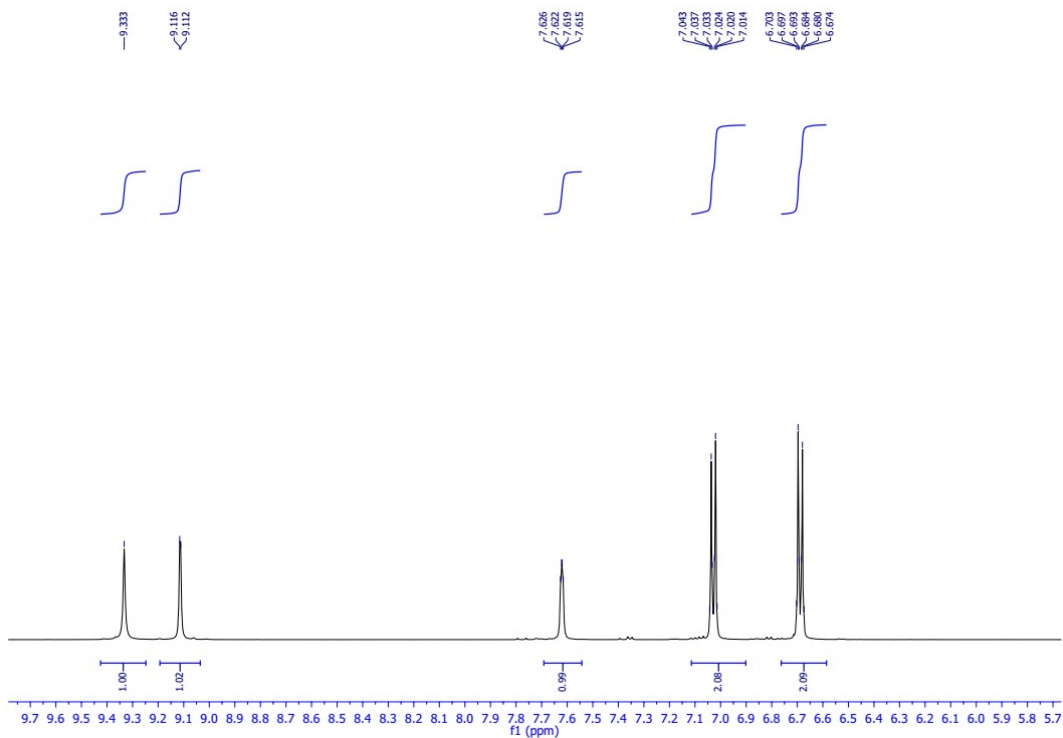
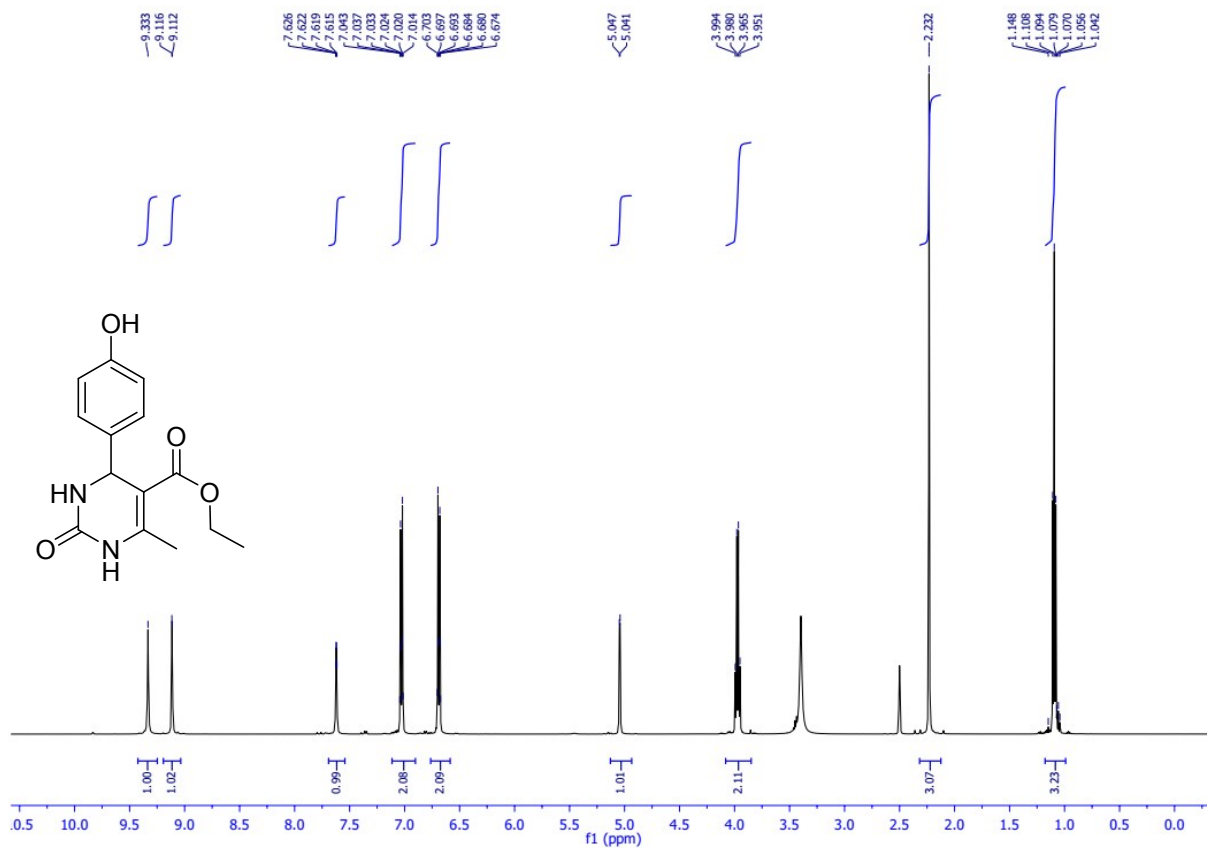


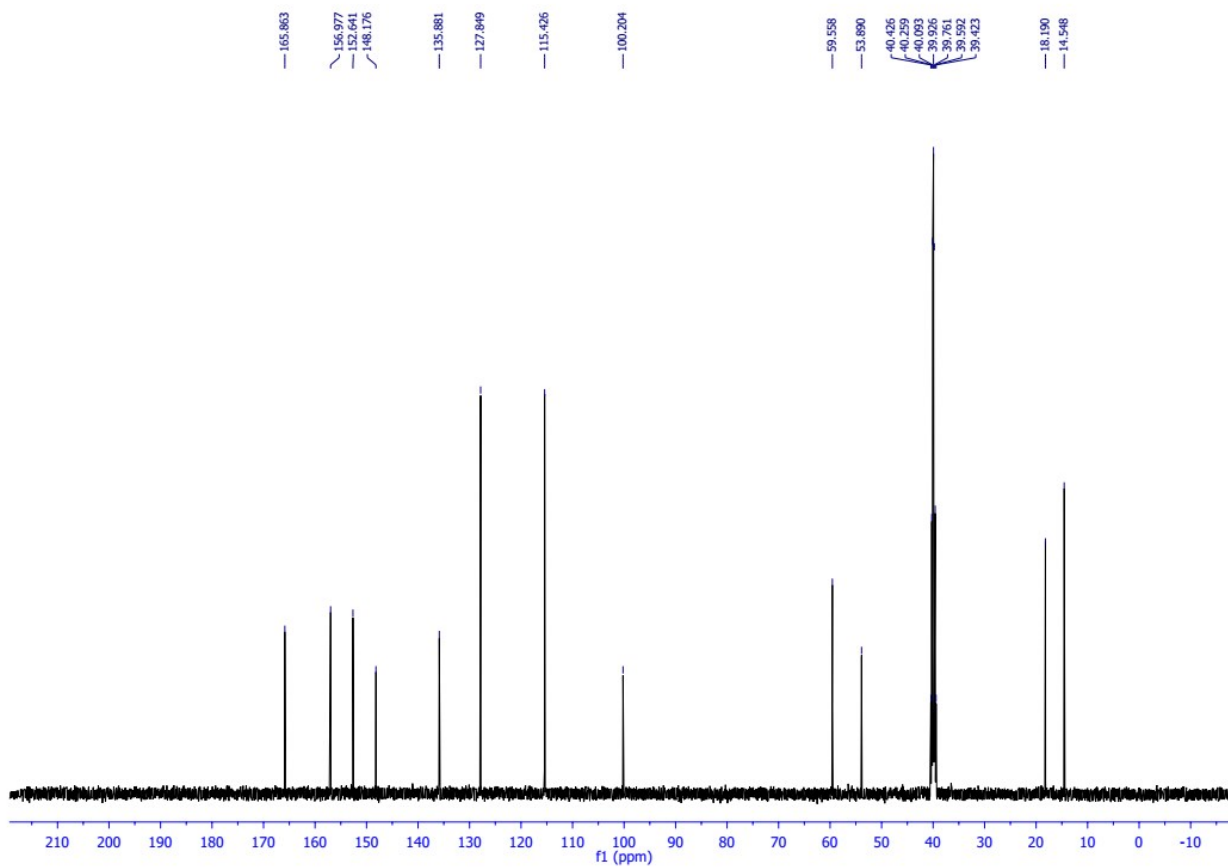
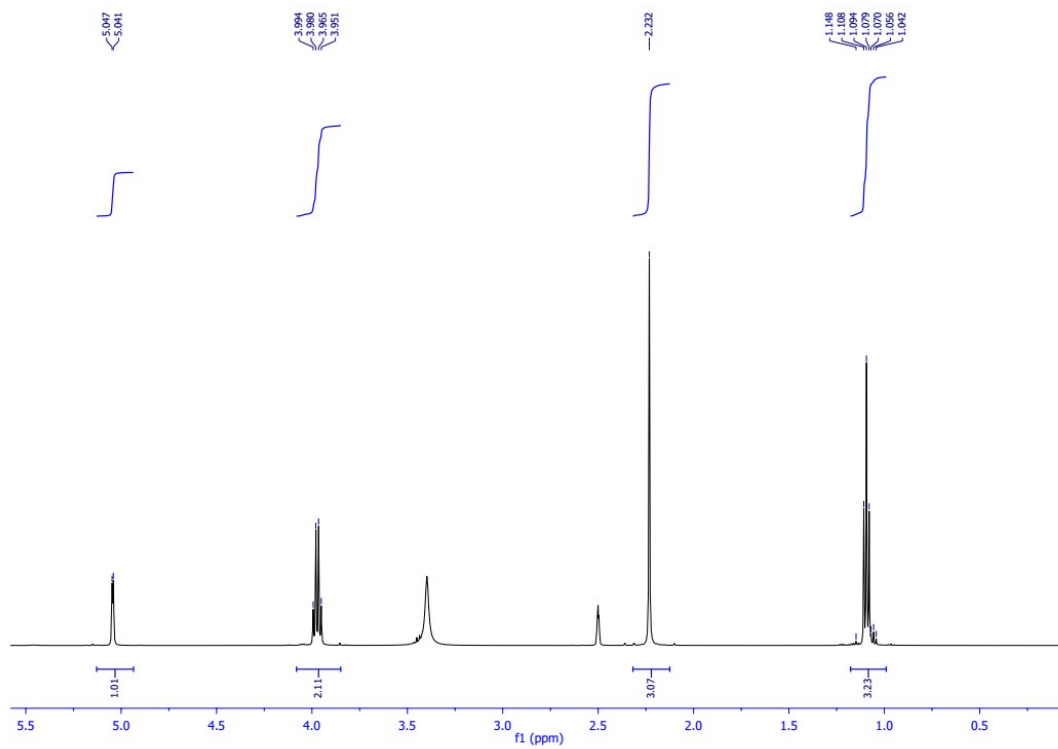
Ethyl 6-methyl-2-oxo-4-(p-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate

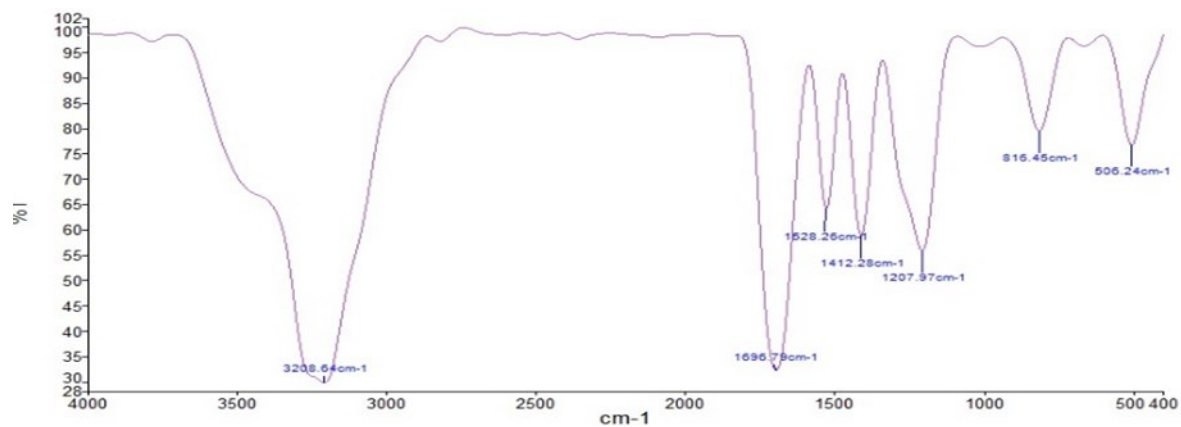




Ethyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate







Ethyl 4-(4-(dimethylamino)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

