

Supplementary Information

Ultrasound-assisted synthesis of 3,4-dihydropyrimidine-2(1H)-ones catalyzed by nanocomposites: An efficient and green approach

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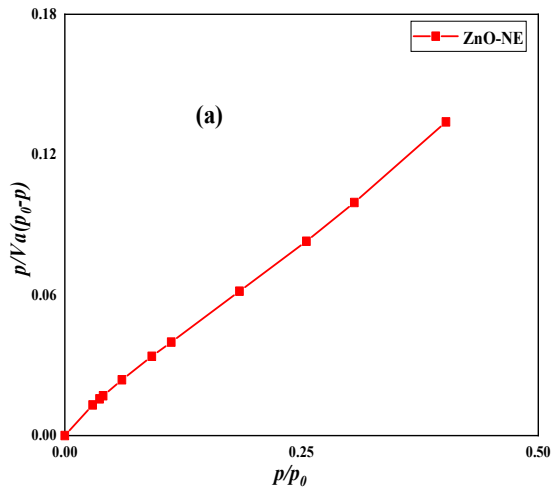
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1. BET Analysis:

1.1. BET Plot.



1.2. BJH Plot

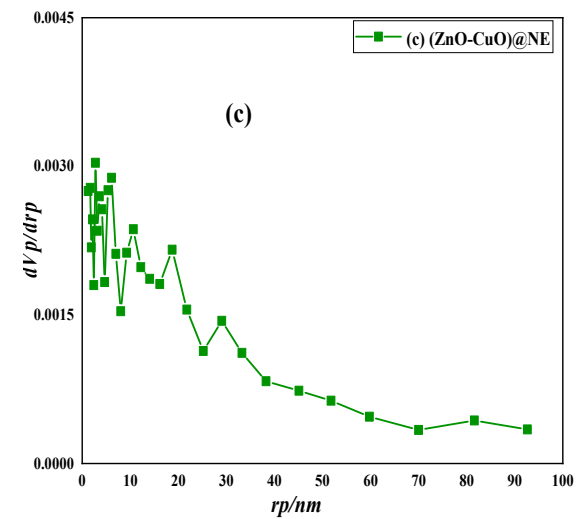
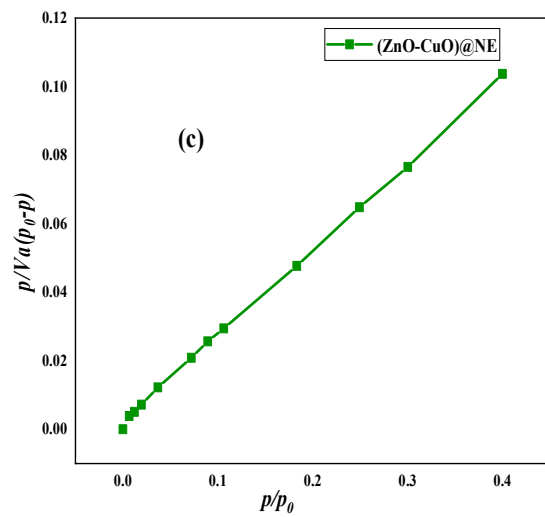
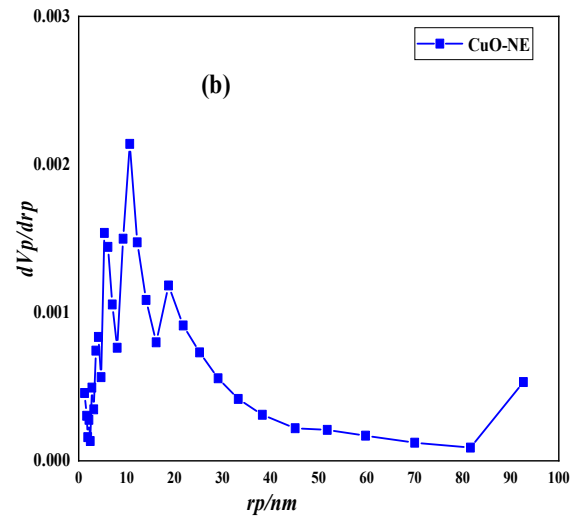
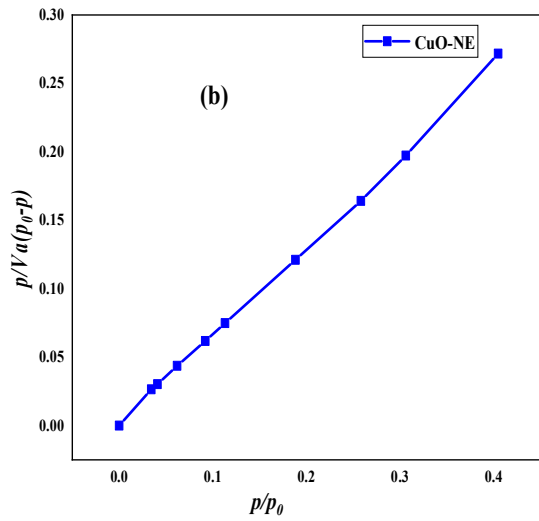
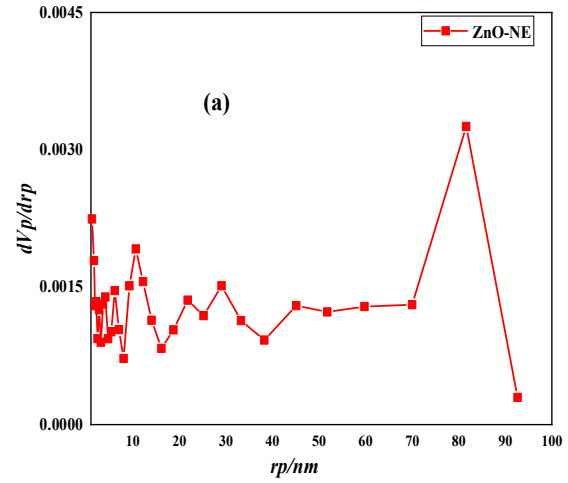
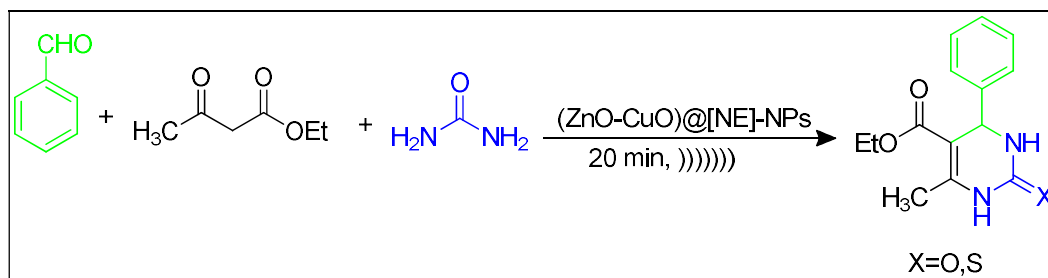


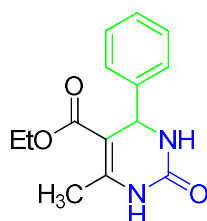
Fig.1 BET plot and BJH plot for (a) ZnO-NE, (b) CuO-NE and (c) (ZnO-CuO)@NE.

2. Spectral Analysis of some selected compounds.

Scheme-1 Synthesis of DHPMs (Biginelli reaction)-



(a) 5-(Ethoxycarbonyl)-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one.



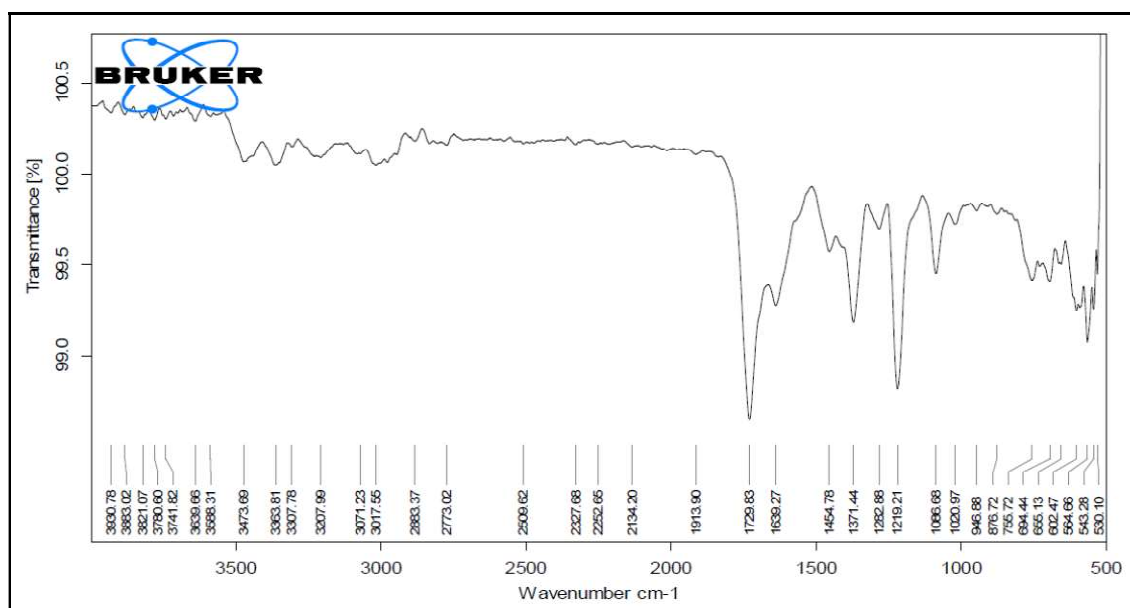
Melting point- 200⁰C (Lit: 201⁰C).

FT-IR: 3307, 3207, 3071.23, 3017.55, 2883.37, 1729.83, 1639.27, 1454.78, 1371.44, 1219.21, 1086.68, 946.88, 876.72, 755.72, 694.44 cm^{-1} .

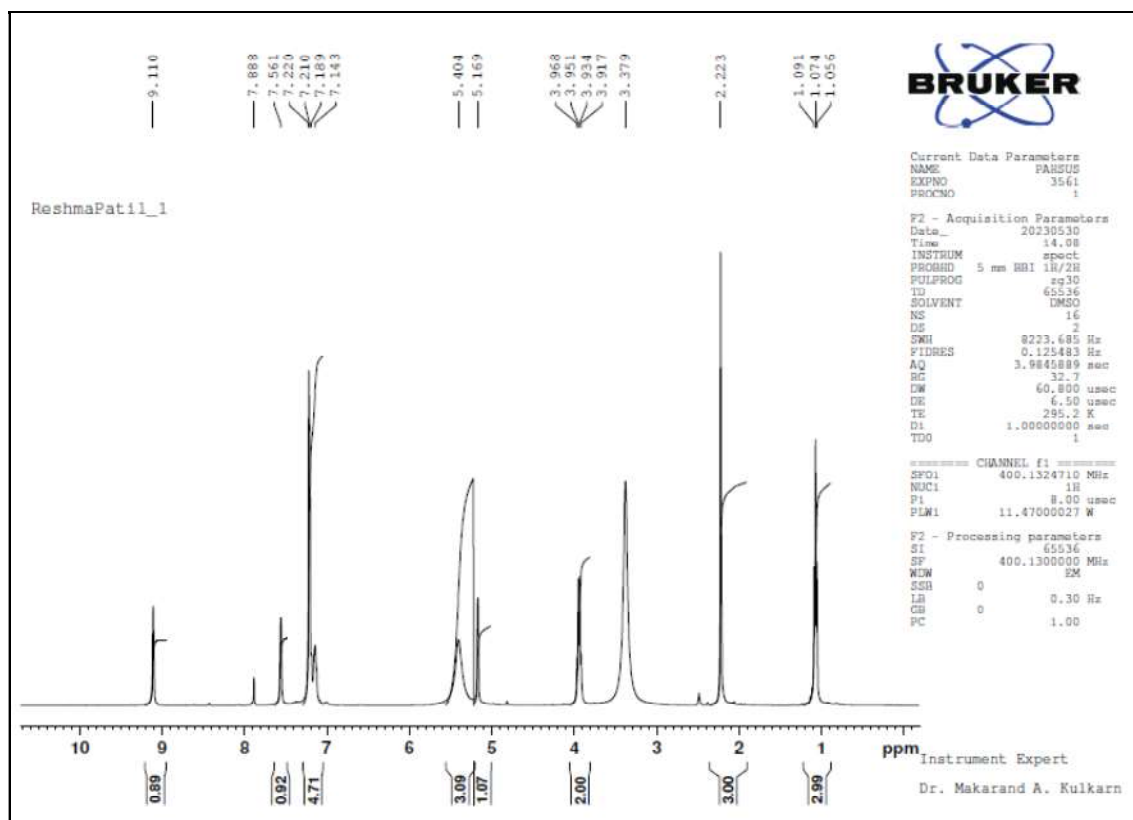
¹H-NMR (DMSO, 400 MHz) δ : 1.07 (t, 3H), 2.22 (s, 3H), 3.968 (q, 2H), 5.404 (s, 1H), 5.169 (d, 1H), 7.22 (d, 4H), 7.561 (s, 1H), 9.110 (s, 1H).

¹³C-NMR (DMSO, 100MHz) δ : 14.34, 18.22, 54.65, 59.53, 99.99, 126.70, 127.46, 128.47, 145.09, 148.26, 153.09, and 165.81 ppm.

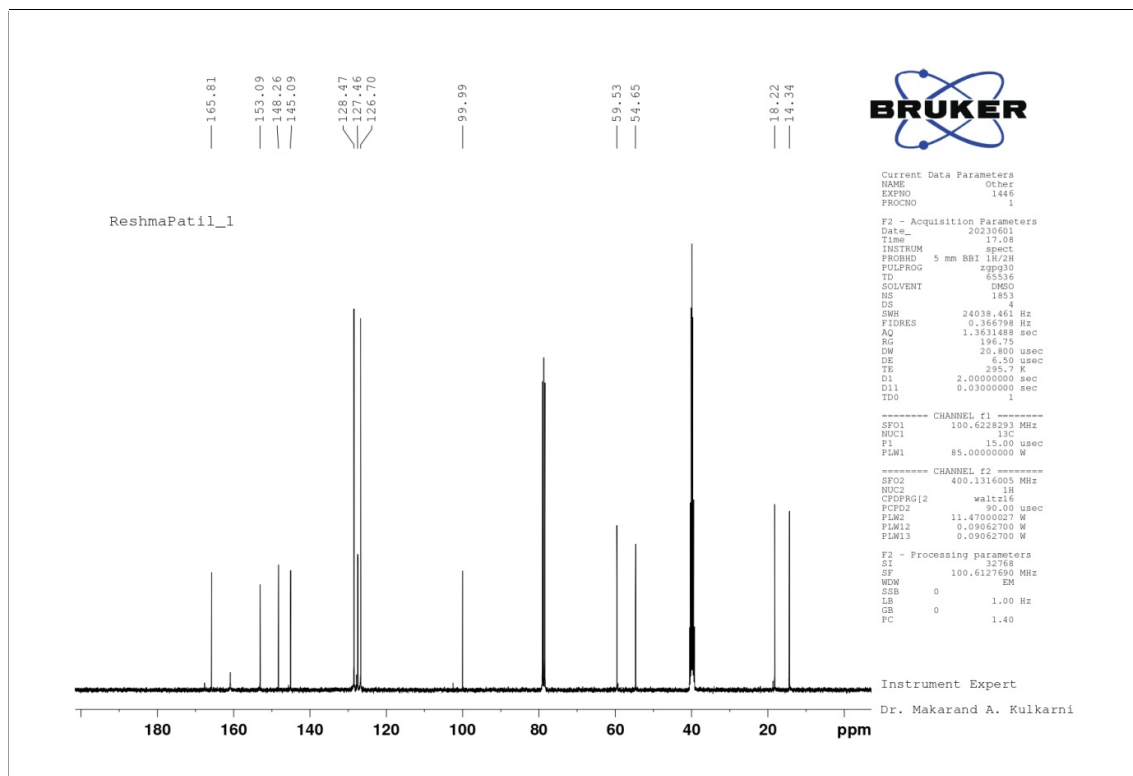
DEPT (DMSO, 100 MHz) δ : 59.53.



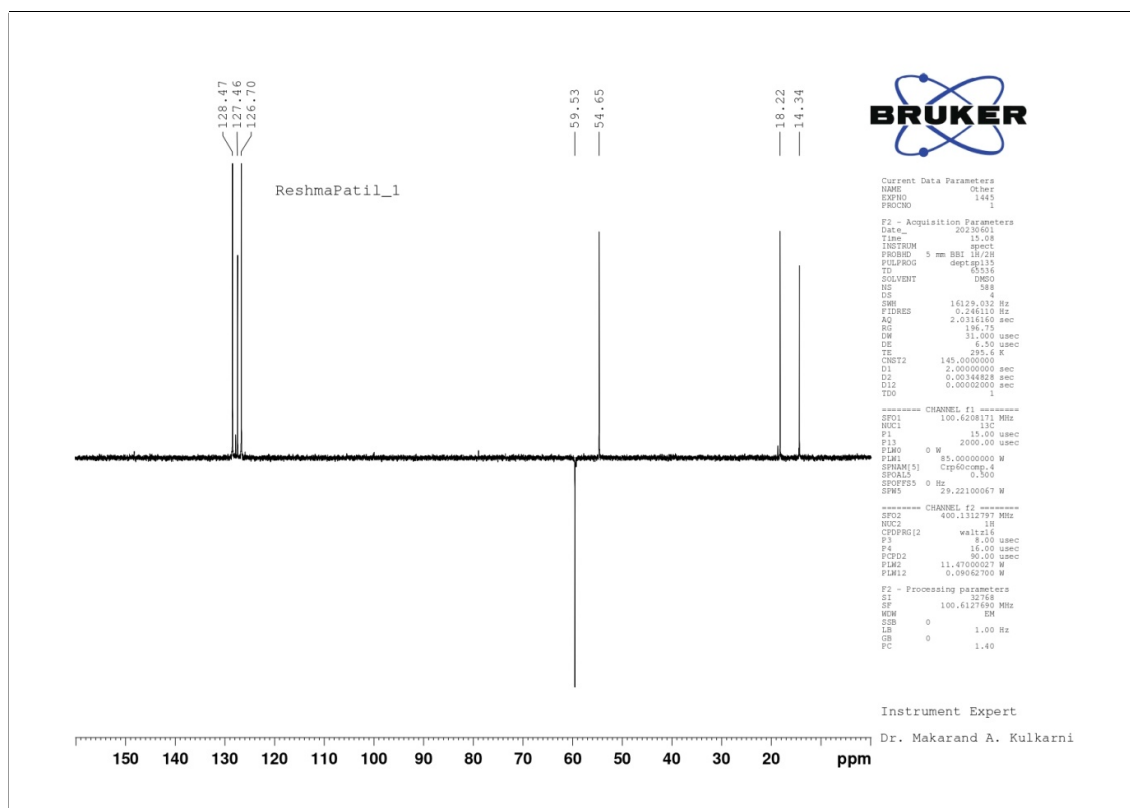
IR spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one (a).



¹H NMR Spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one (a).

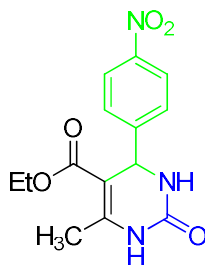


¹³C NMR Spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one (a).



DEPT of 5-(Ethoxy carbonyl)-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one (a).

(b) 5-(Ethoxy carbonyl)-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one.



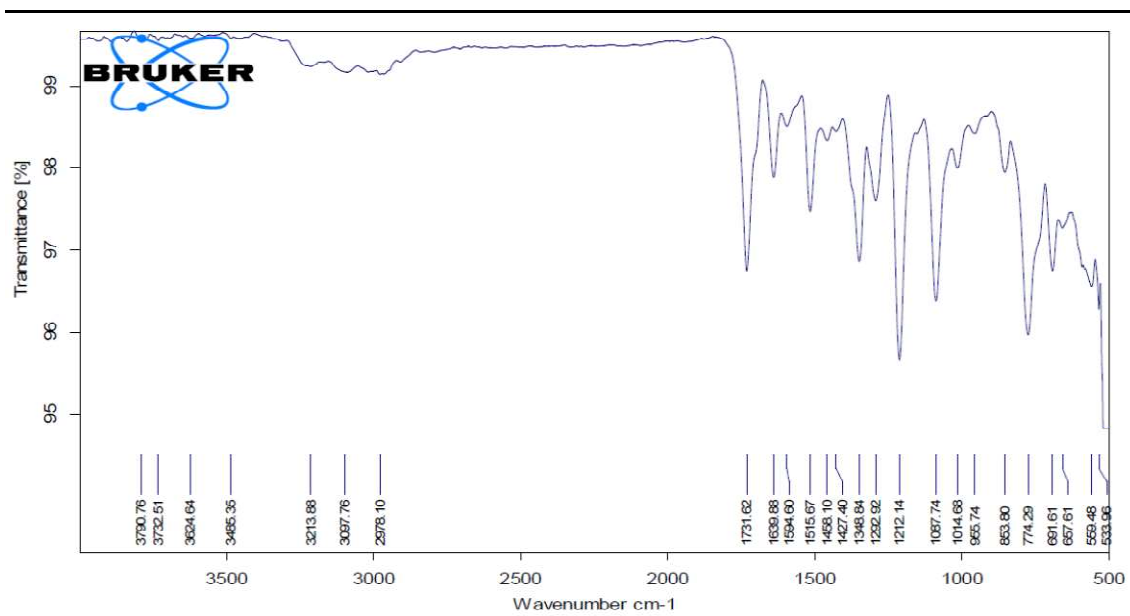
Melting point- 204⁰C (Lit: 206⁰C).

FT-IR- 3213.88, 3097.76, 2978.10, 1731.62, 1639.88, 1515.67, 1348.84, 1292.92, 1212.14, 1087.74, 774.29, 691.61 cm⁻¹.

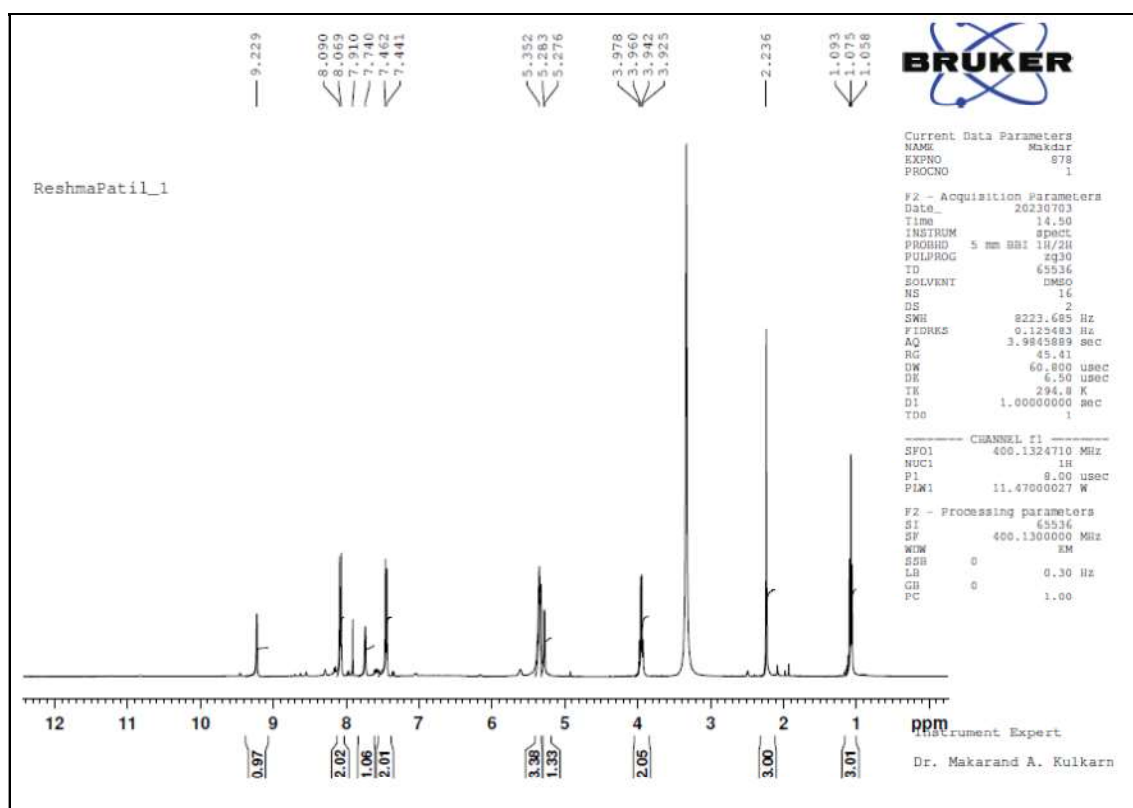
¹H-NMR (DMSO, 400 MHz) δ: 1.093 (t, 3H), 2.236 (s, 3H), 3.978 (q, 2H), 5.283 (d, 1H), 7.462 (d, 2H), 7.910 (s, 1H), 8.090 (d, 2H), 9.229 (s, 1H).

¹³C-NMR (DMSO, 100MHz) δ: 14.35, 18.33, 54.21, 59.69, 98.75, 123.73, 127.86, 147.01, 149.49, 152.56, 160.53, 165.47.

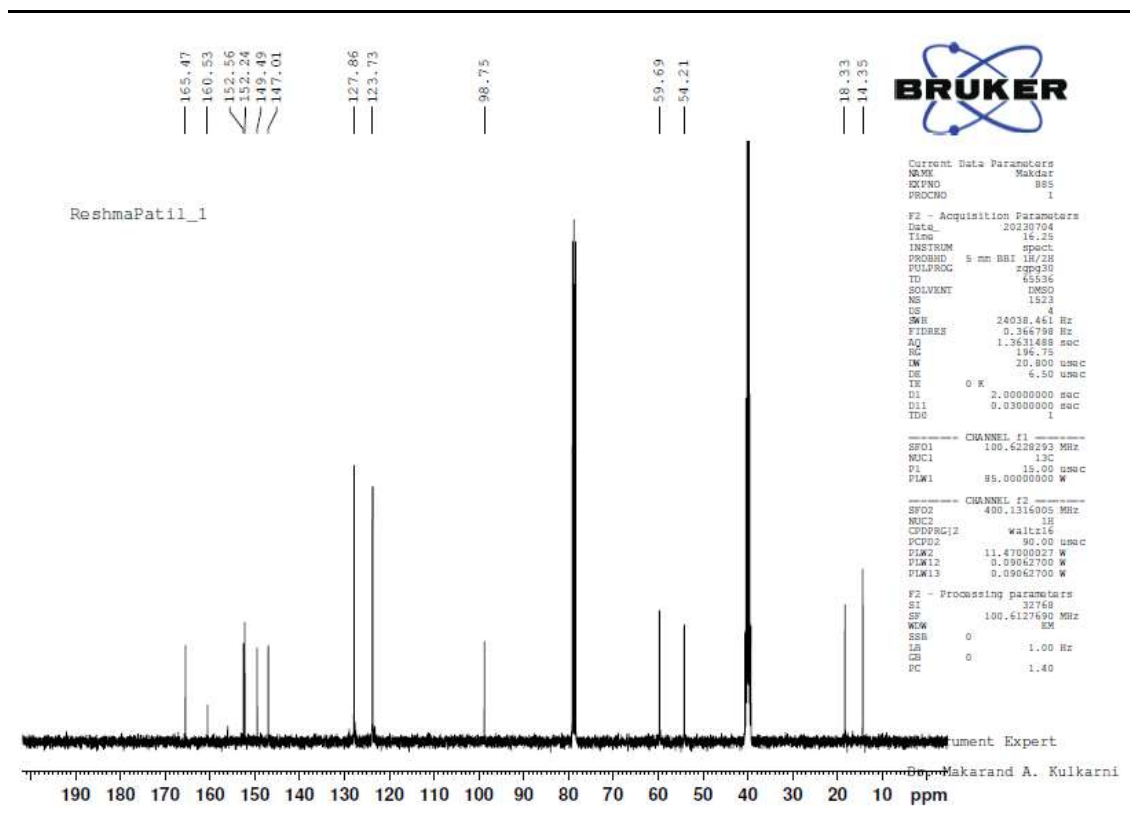
DEPT (DMSO, 100 MHz) δ: 59.69.



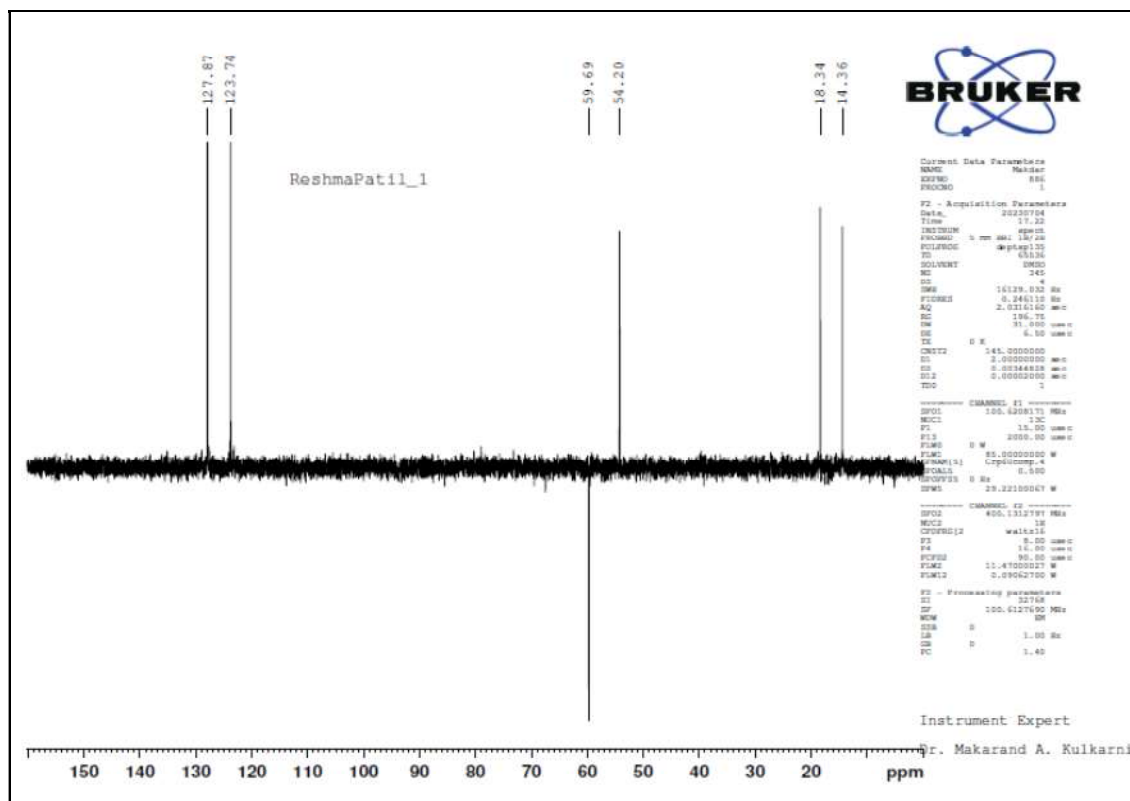
IR spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one (b).



¹H NMR Spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one (b).

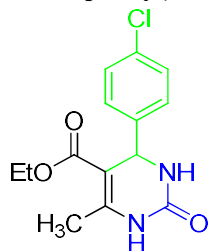


¹³C NMR Spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one (b).



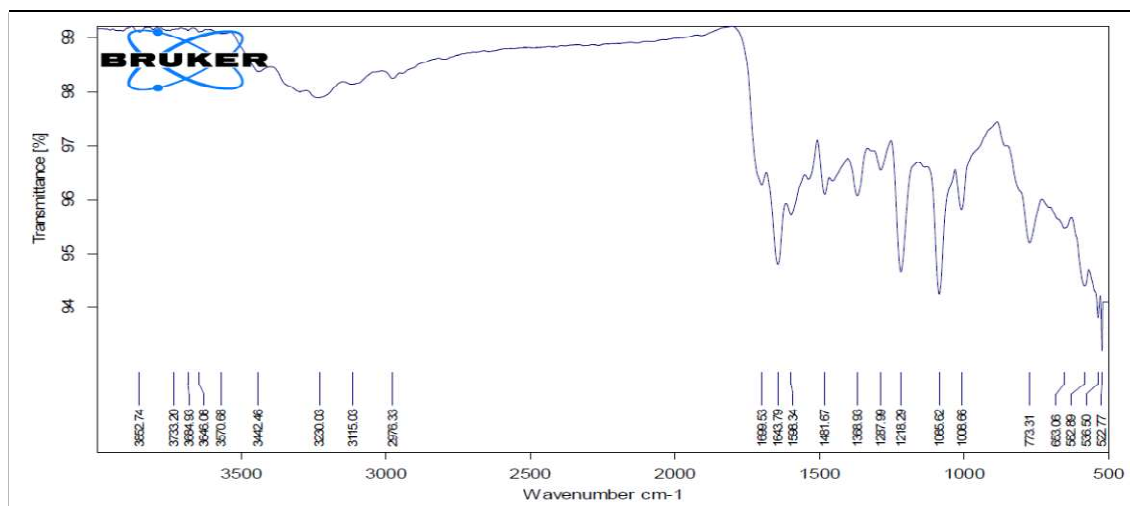
DEPT of 5-(Ethoxy carbonyl)-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one (b).

(c) 5-(Ethoxy carbonyl)-6-methyl-4-(4-chlorophenyl)-3,4-dihdropyrimidin-2(1H)-one.

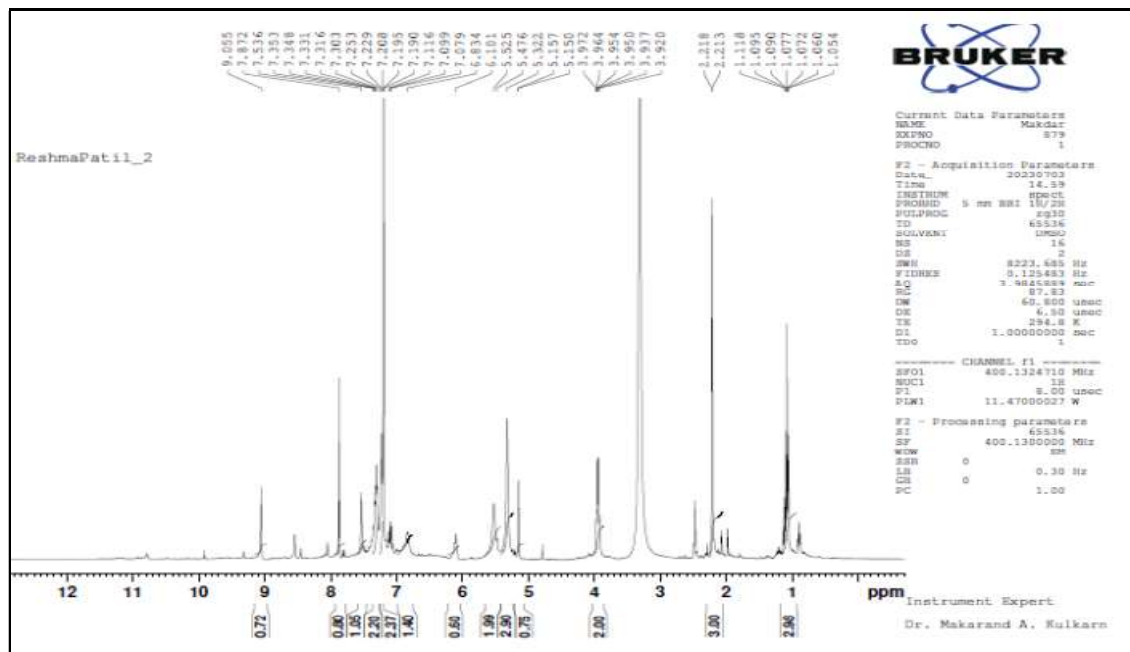


Melting point- 212⁰C (Lit: 215⁰C).

FT-IR- 3230.03, 3115.03, 2976.33, 1699.53, 1643.79, 1598.34, 1481.67, 1368.93, 1287.99, 1218.29, 1085.62, 1008.66, 773.31 cm⁻¹. **¹H-NMR (DMSO, 400 MHz) δ:** 1.11 (t, 3H), 2.22 (s, 3H), 3.972 (dd, 2H), 5.32 (s, 1H), 6.10 (s, 2H), 7.20 (m, 2H), 7.52 (m, 2H).

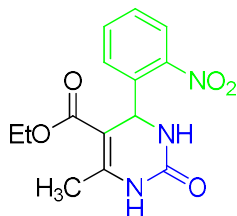


IR spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-chlorophenyl)-3,4-dihdropyrimidin-2(1H)-one (c).



¹H NMR Spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-chlorophenyl)-3,4-dihdropyrimidin-2(1H)-one (c).

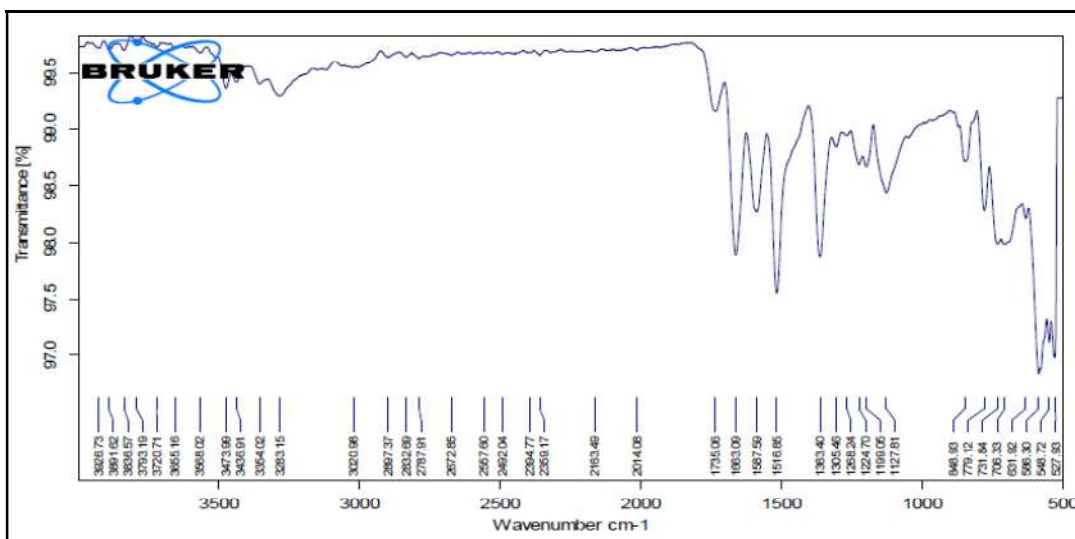
(d) 5-(Ethoxy carbonyl)-6-methyl-4-(2-nitrophenyl)-3,4-dihdropyrimidin-2(1H)-one.



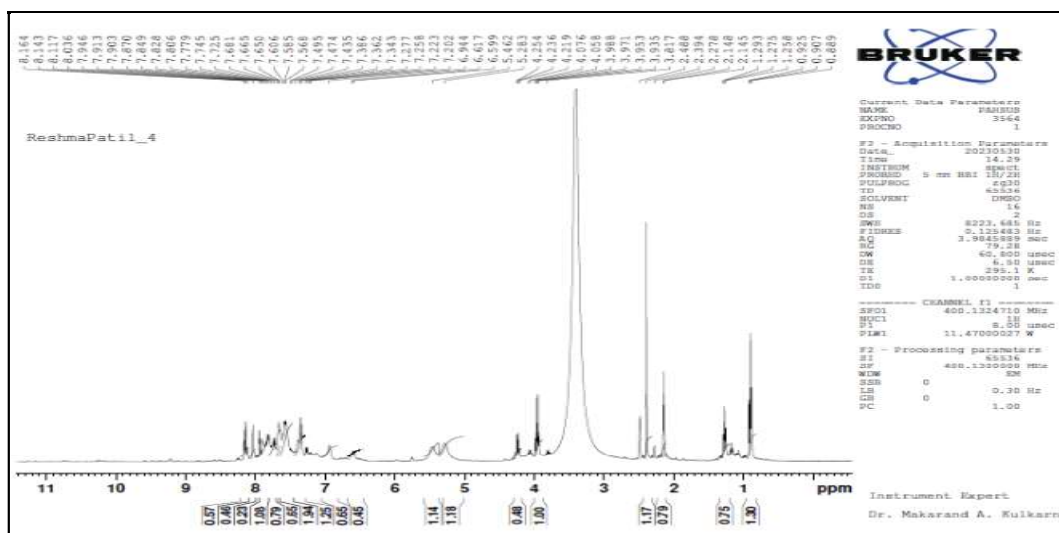
Melting point- 215⁰C (Lit: 217-220⁰C).

FT-IR- 3283.15, 3120, 1735.06, 1663.09, 1587.59, 1516.85, 1363.40, 1137.81, 779.12 cm⁻¹.

¹H-NMR (DMSO, 400 MHz) δ: 0.8 (s, 1H), 1.3 (s, 1H), 2.1 (s, 3H), 2.3-2.4 (d, 2H), 3.8-4.2 (d, 5H), 5.5 (s, 1H), 6.5 (s, 1H), 7.4-7.5 (m, 2H), 7.8-7.9 (m, 4H).

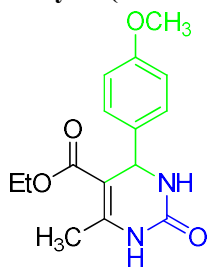


IR spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(2-nitrophenyl)-3,4-dihdropyrimidin-2(1H)-one (d).



¹H NMR Spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(2-nitrophenyl)-3,4-dihdropyrimidin-2(1H)-one (d).

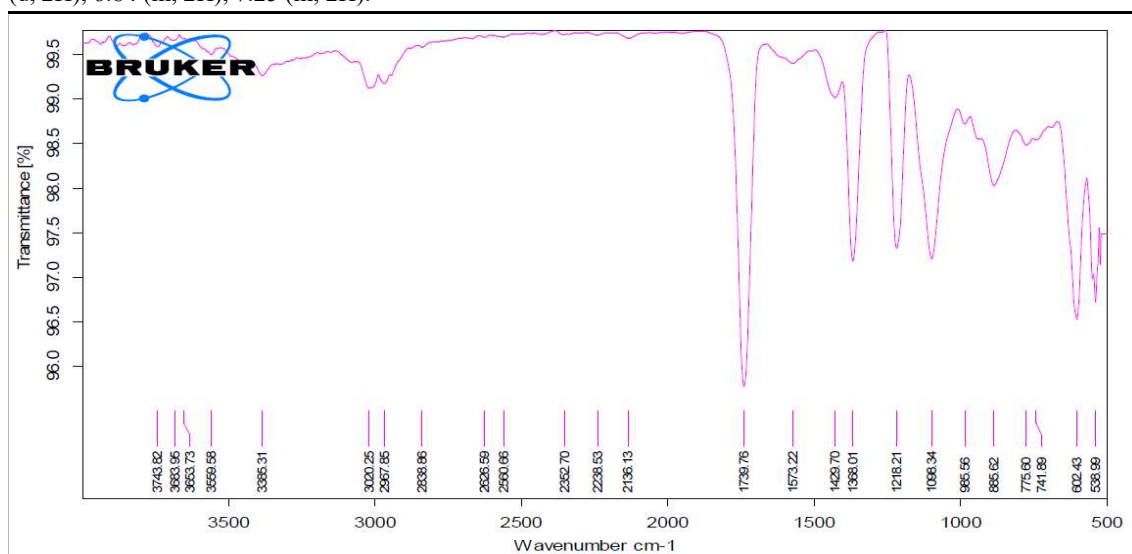
(e) 5-(Ethoxy carbonyl)-6-methyl-4-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-one.



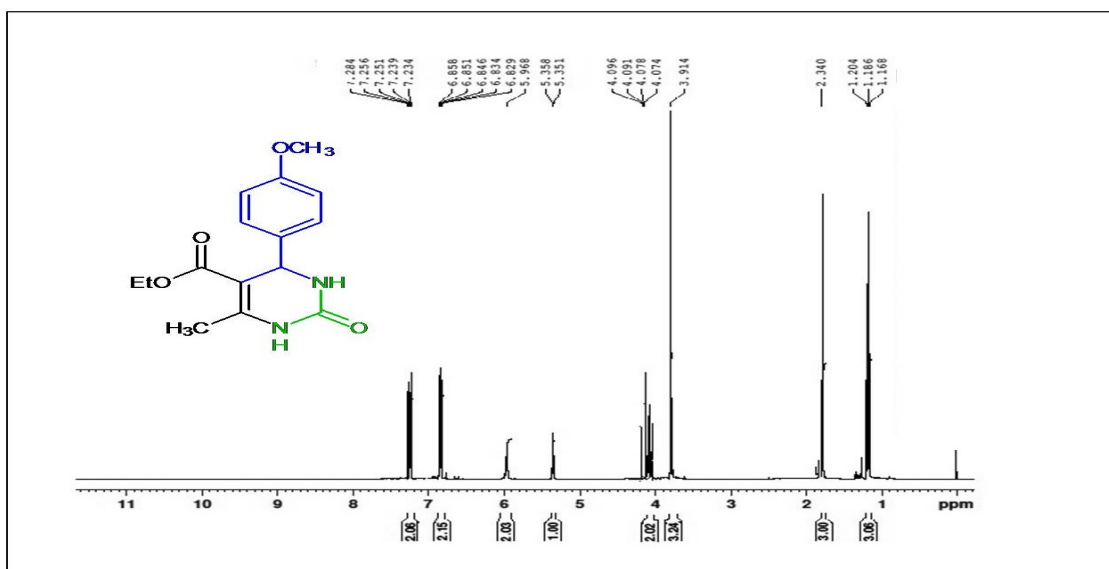
Melting point- 205⁰C (Lit: 203-207⁰C).

FT-IR- 3385.31, 3020.25, 2967.85, 1739.76, 1573.22, 1429.70, 1368.01, 1218.21, 1098.34, 985.56, 885.62, 775.60, 602.43 cm⁻¹.

¹H-NMR (DMSO, 400 MHz) δ : 1.18 (t, 3H), 2.34 (s, 3H), 3.91 (s, 3H), 4.85 (dd, 2H), 5.54 (d, 1H), 5.96 (d, 2H), 6.84 (m, 2H), 7.25 (m, 2H).



IR spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)one.



¹H NMR spectrum of 5-(Ethoxy carbonyl)-6-methyl-4-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-one (e).

3. XRD Analysis: 2θ values, hkl planes, observed 'd' values, standard 'd' values –

Sample	2θ	FWHM	θ	θ	FWHM	cosθ	βcosθ	Crystalline size
(Crystalline)	degree	degree	degree	radian	radian			nm
(a) ZnO-NE.	36.2706	0.45722	18.135275	0.3165203	0.007979	0.950324	0.007584	18.2824.
(b) CuO-NE.	33.49679	0.95732	16.748395	0.292315	0.016708	0.957579	0.015999	1.31.
(c) (Zn-CuO)@[NE]	22.71327	0.54793	11.3566	0.198210	0.009563	0.980421	0.009376	1.13.