Electronic Supporting Information

L-Asparagine-EDTA-amide silica-coated MNPs: a highly efficient and nano-ordered multifunctional core-shell organocatalyst for green synthesis of 3,4-dihydropyrimidin-2(1*H*)-one compounds

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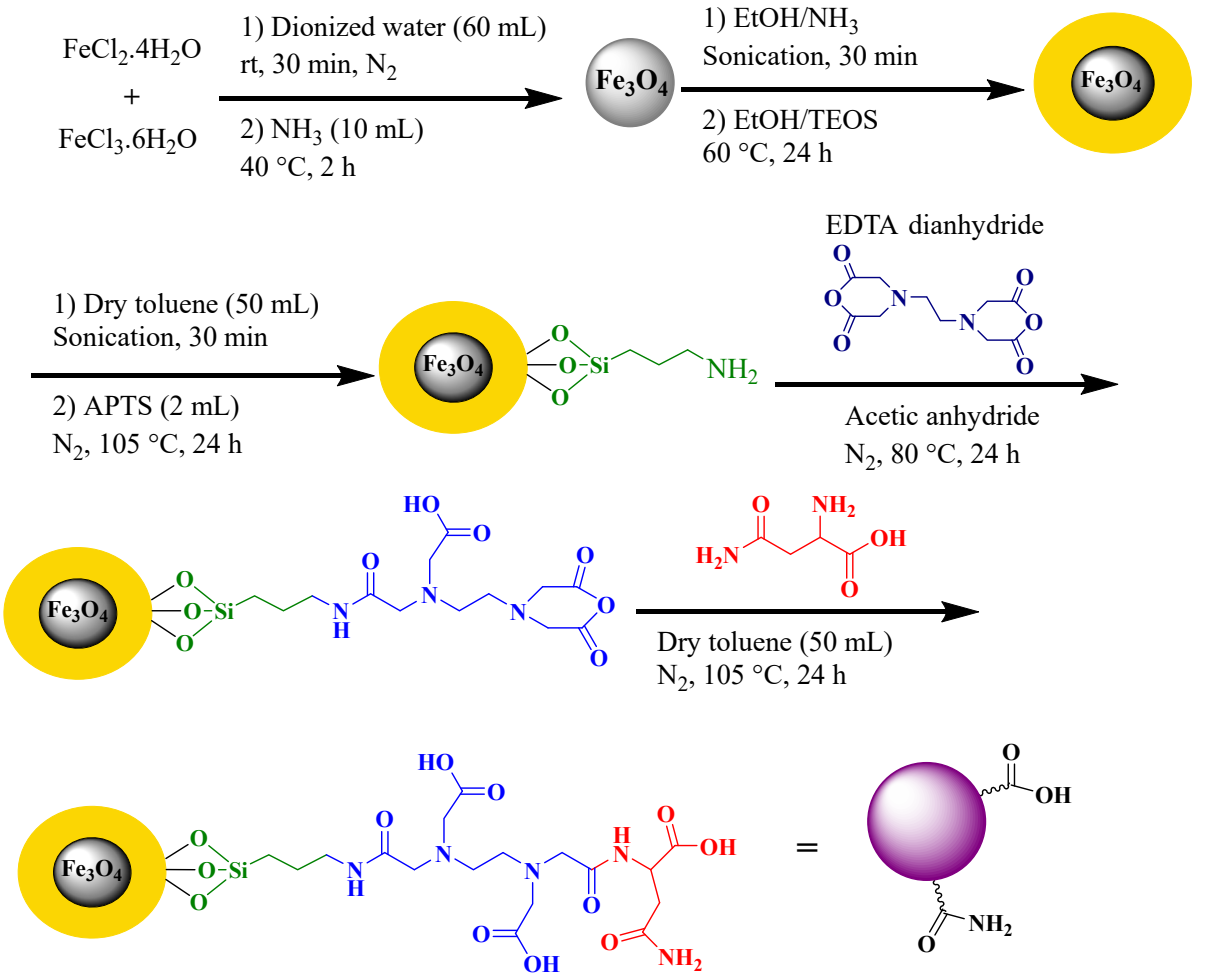
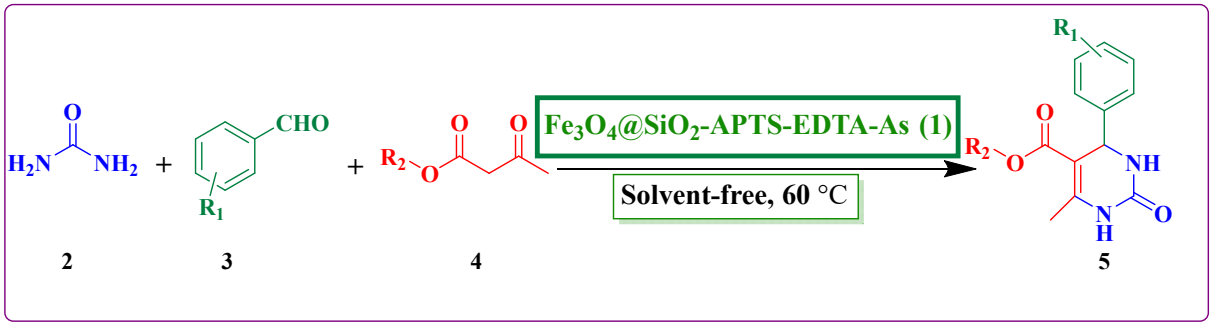


Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**)



Scheme S1. Schematic preparation of Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**), as a heterogeneous nanocatalyst, for the synthesis of 3,4-dihydropyrimidin-2(1*H*)-one **5** derivatives

Characterization of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (1)

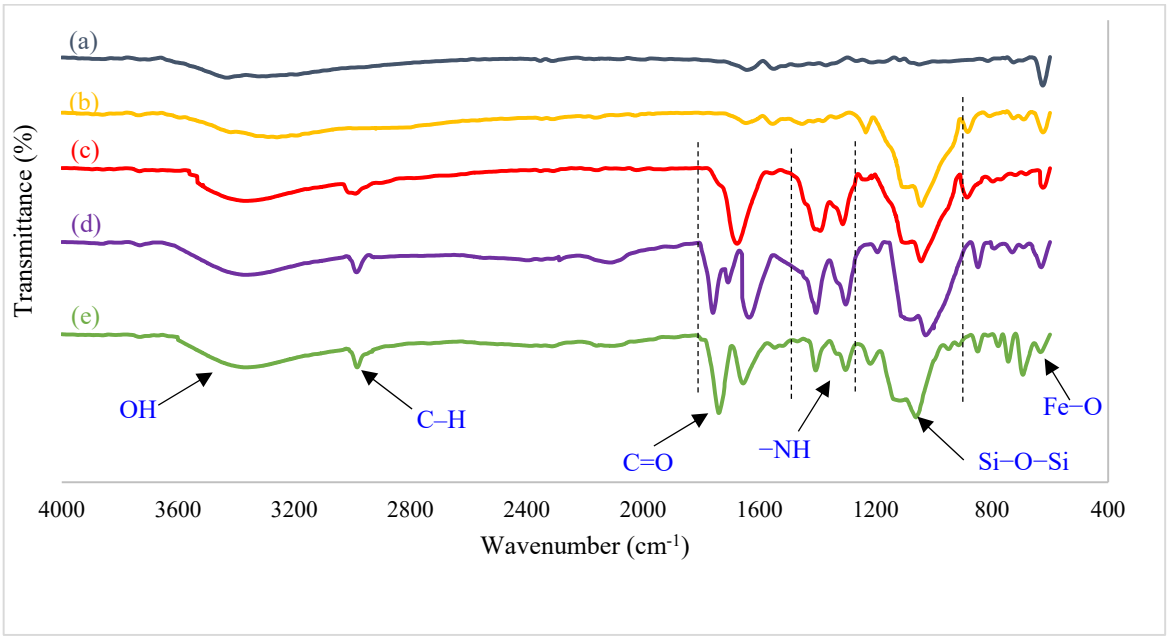
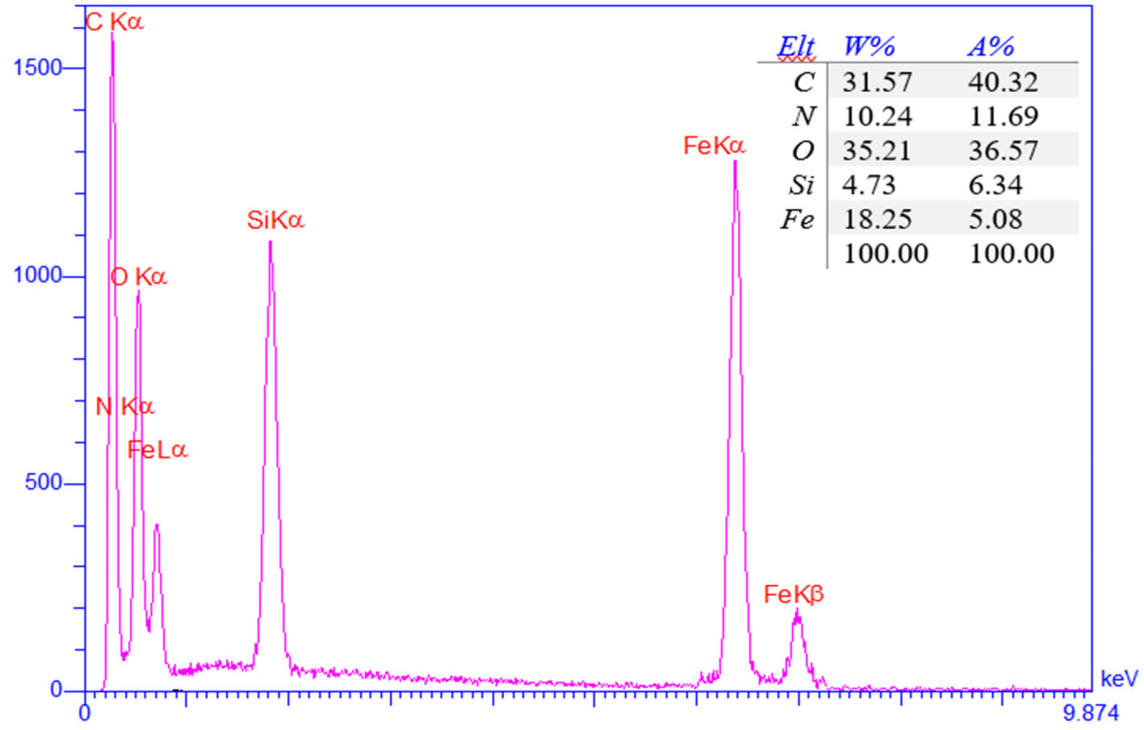


Fig S1. FT-IR spectra of the Fe_3O_4 (**a**), Fe_3O_4@SiO_2 (**b**), Fe_3O_4@SiO_2-APTS (**c**), Fe_3O@SiO_2-APTS-EDTA (**d**) and Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**, **e**).



Elt	W%	A%
C	31.57	40.32
N	10.24	11.69
O	35.21	36.57
Si	4.73	6.34
Fe	18.25	5.08
	100.00	100.00

Fig S2. The EDX spectra of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**).

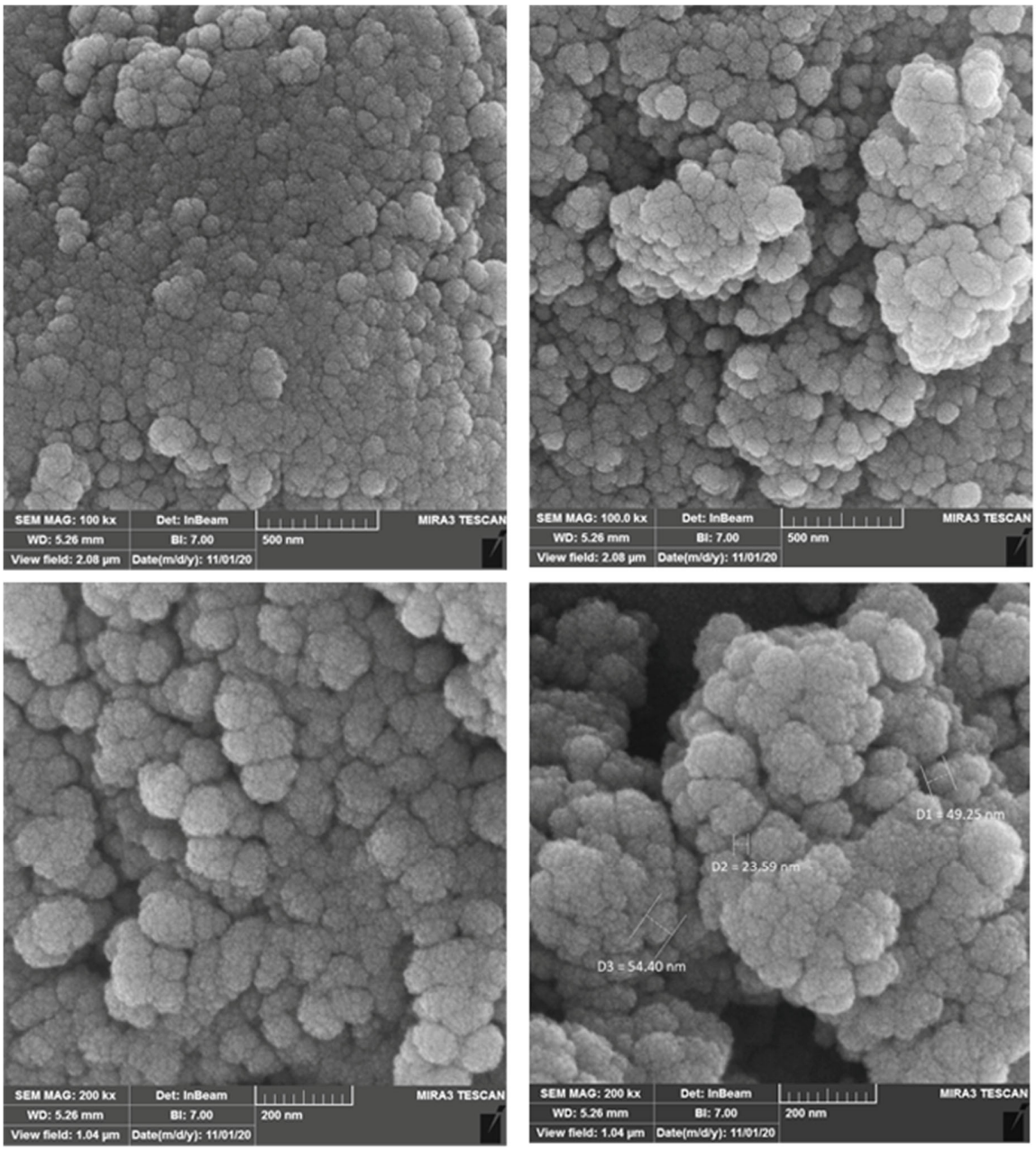


Fig S3. FESEM images of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**).

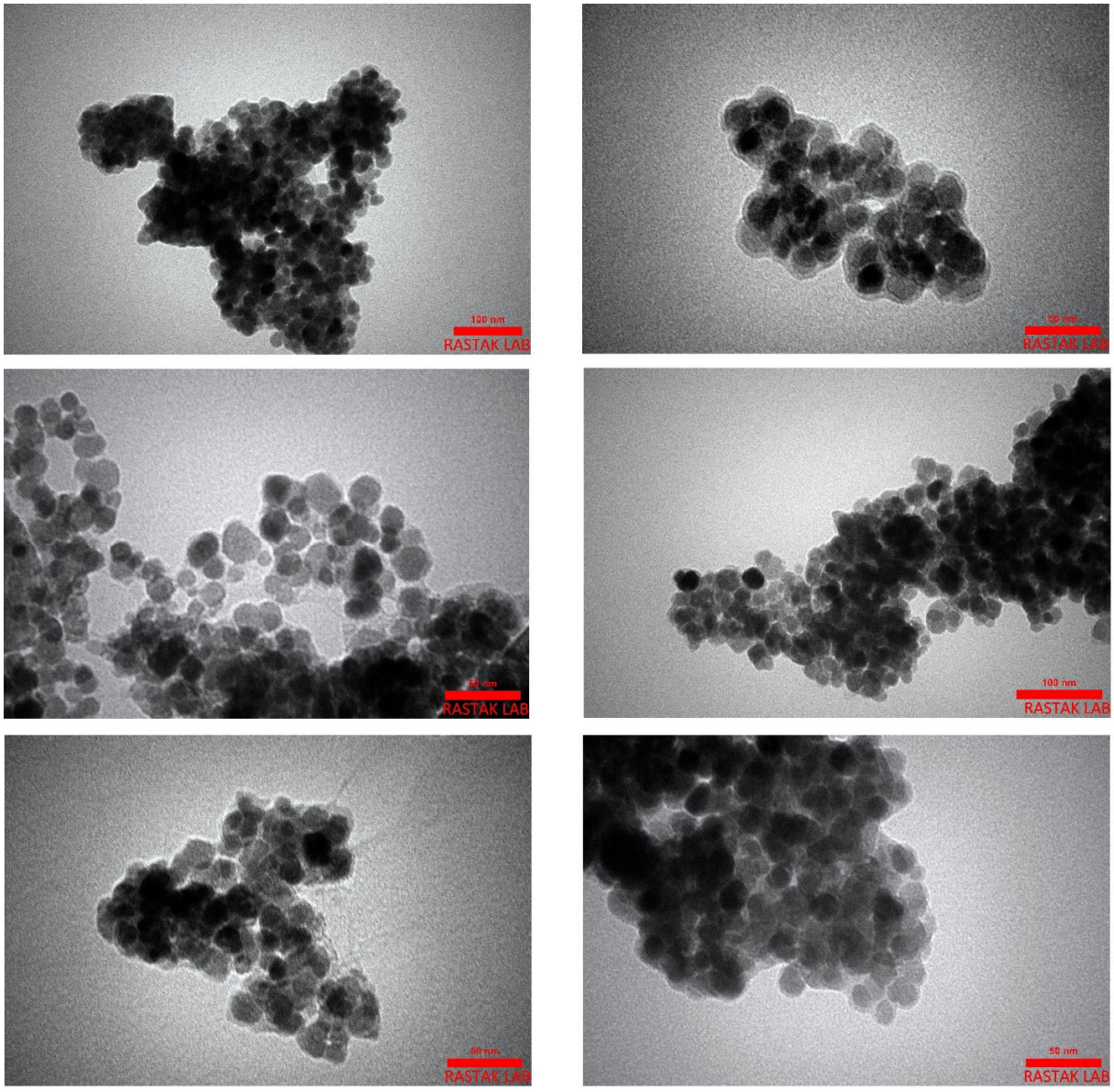


Fig S4. TEM images of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**).

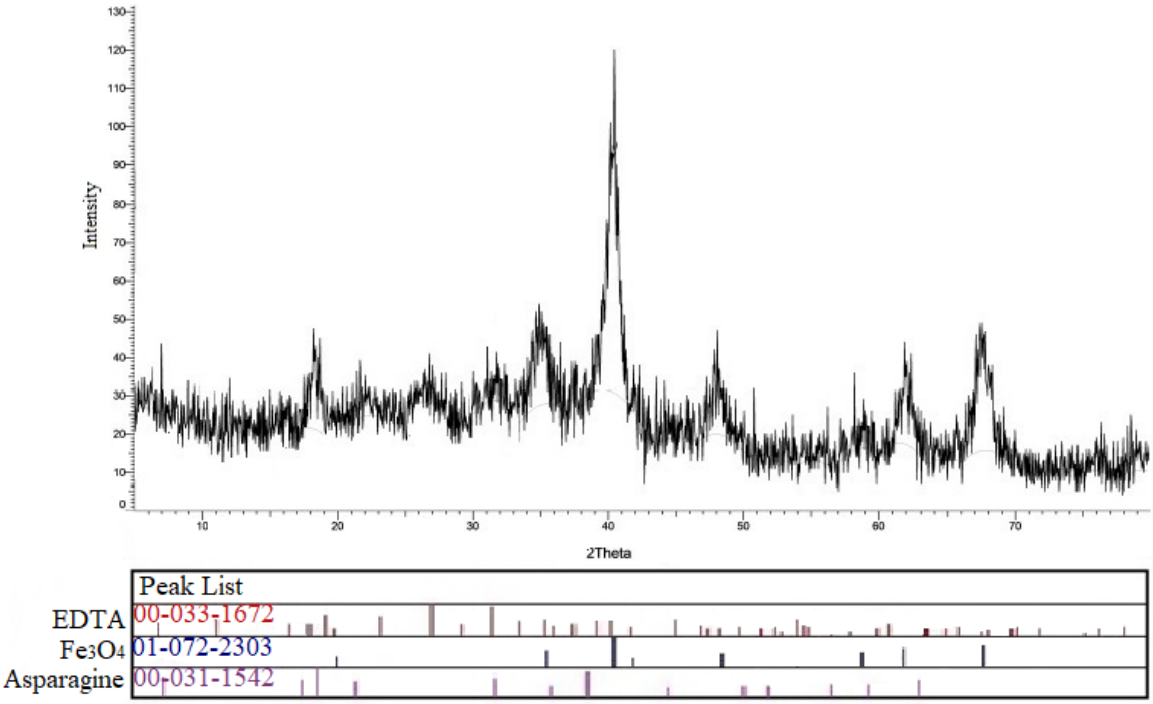


Fig S5. XRD pattern of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**).

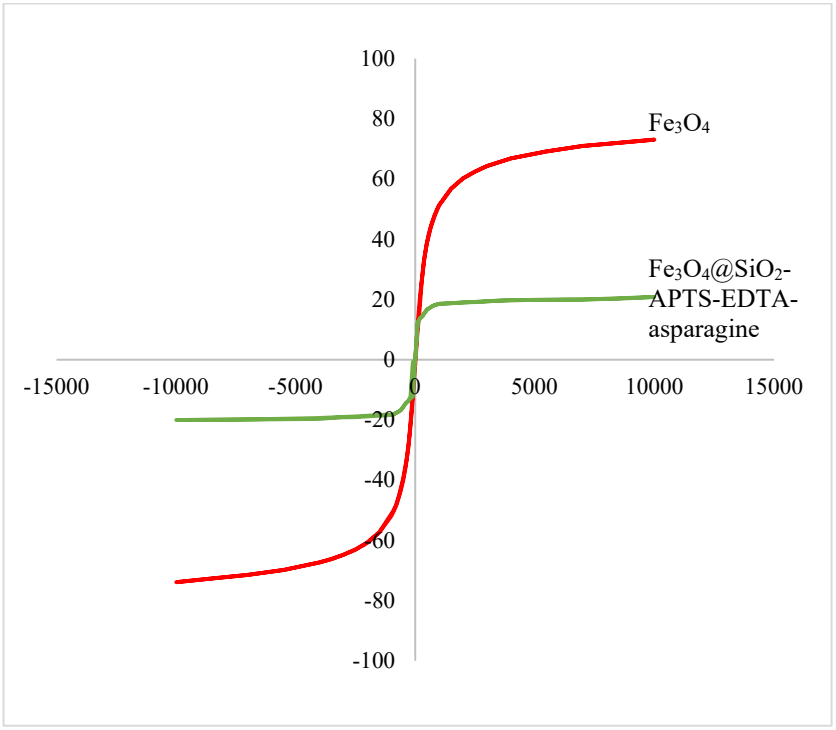


Fig S6. VSM pattern of Fe_3O_4 (red) and Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**, green).

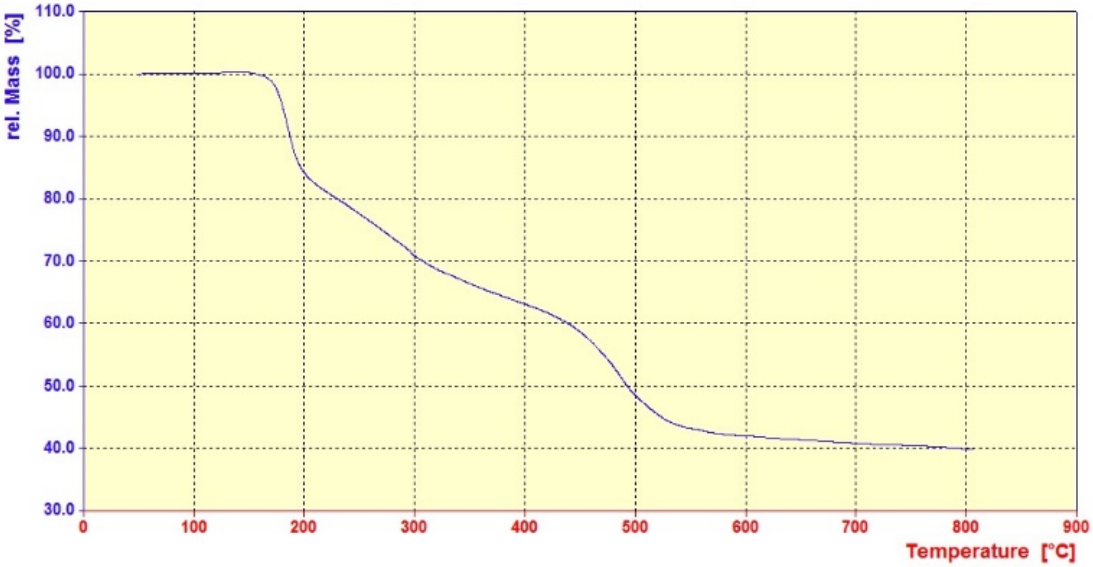


Fig S7. TGA curve of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**)

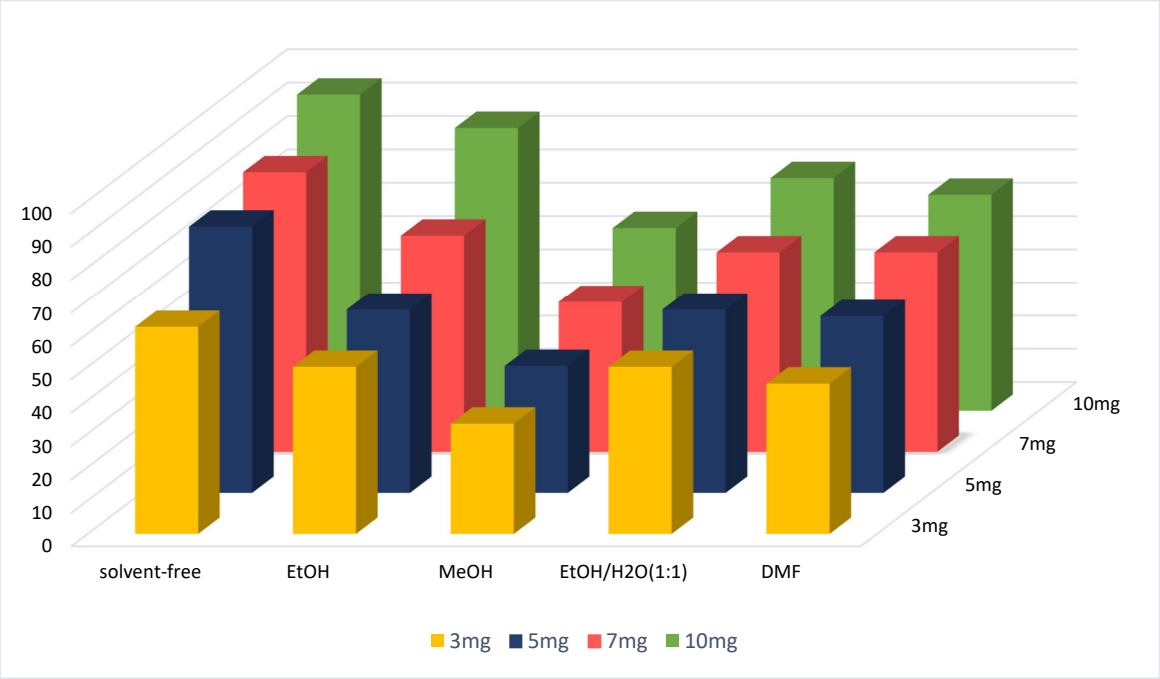


Fig S8. Effect of solvent and the amount of Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**) nanocatalyst on the model reaction.

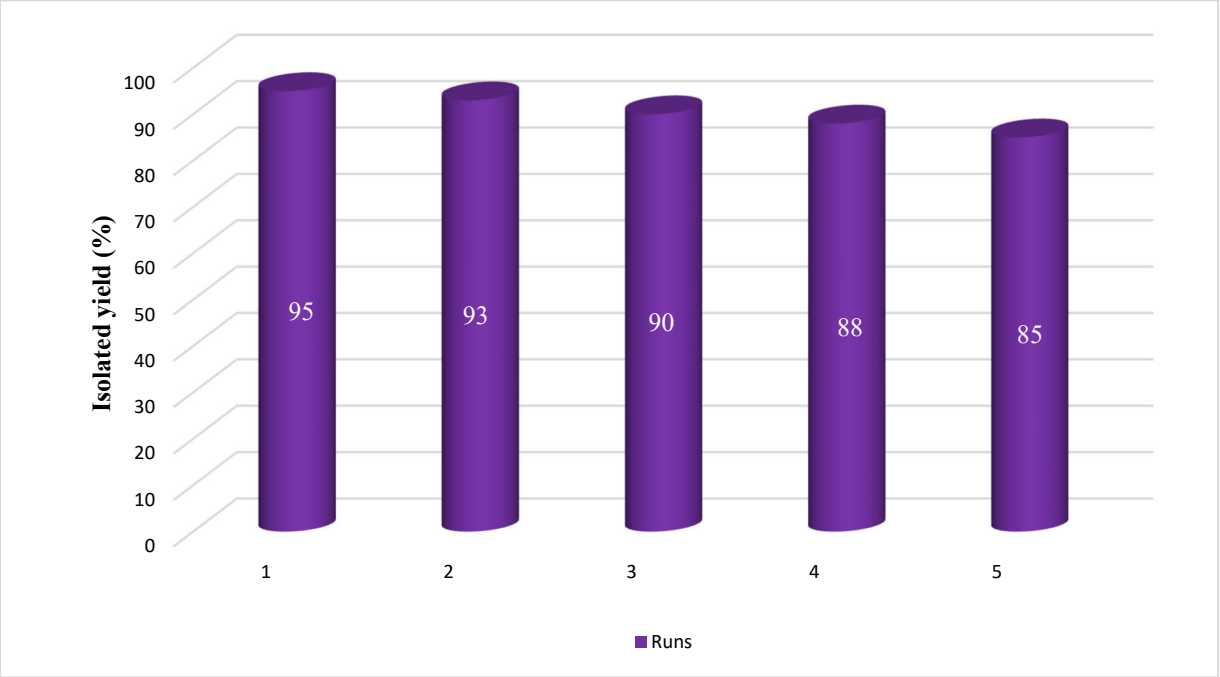
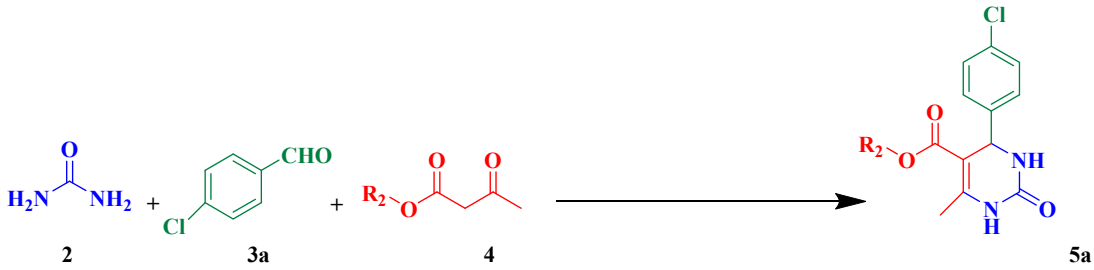


Fig S9. Reusability of the Fe_3O_4@SiO_2-APTS-EDTA-asparagine (**1**) nanocatalyst for the synthesis of **5a**.

Table S1. Calculation of green chemistry metrics for compound **5a**.



2 **3a** **4** **5a**

Molar mass: 60.06 g/mol 294.74g/mol		140.57 g/mol	130.14 g/mol		
mmol mmol	1.0 mmol	1.0 mmol	1.0 mmol		0.96
amount mg	60.06 mg	140.57 mg	130.14 mg		282.95

	Parameters	Characteristics	Formula	Ideal Value	Calculated value for compound 5a
1	Environmental (E) factor	E-factor signifies the total amount of waste generated in a chemical reaction.	[Total mass of raw materials - the total mass of product]/ mass of product	0	[(60.06 + 140.57 +130.14)- 282.95]/ 282.95 = 0.16
2	Atom economy (AE%)	Atom economy signifies the percentage of atoms wasted in chemical reaction. Higher the value of AE, greener is the reaction. Maximum value of atom economy is 100% which indicates that all the atoms present in reactants lies in the product.	[MW of product] ÷ Σ(MW of stoichiometric reactants) × 100	100%	[(294.74)/ (60.06 +140.57 + 130.14)] ×100 = 89.1%
3	Carbon efficiency (CE%)	CE signifies the percentage of carbons in the reactants that is left in the product.	[Amount of carbon in product/ Total carbon present in reactants] x 100	100%	[0.96 x 14 / (1.0 x1+ 1.0 x 7 + 1.0 x 6)]x 100 = [6.72 / (0.5 + 3.5 +3)] x 100 = 96%
4	Process mass intensity (PMI)	PMI takes into account reaction efficiency, stoichiometry, amount of solvent and all reagent used in the chemical reaction.	Σ (mass of stoichiometric reactants)/[mass of stoichiometry product]	1	(60.06 + 140.57 + 130.14) / 282.95 = 1.16
5	Reaction mass efficiency (RME %)	RME accounts into atom economy, chemical yield and stoichiometry.	[mass of product/Σ (mass of stoichiometric reactants)] × 100	100%	[282.95/ (60.06 + 140.57 +130.14)] × 100 = 85.5%

5-Ethoxycarbonyl−6-methyl-4-(3-nitrophenyl)−3,4-dihydropyrimidin-2(1*H*)-one (**nifetepimine, 5e**)

M.P. = 211-212 °C; FT-IR (KBr, cm^{-1}) ν = 3324, 3087, 2955, 1689, 1622, 1567,1453, 1218, 1082; ^{1}HNMR (500MHz, DMSO–d6) δ (ppm) = 1.10 (t, 3H, OCH_2CH_3), 2.2 8(s, 3H, CH_3), 4.0 (q, 2H, OCH_2), 5.31 (s, 1H, CH), 7.66 − 8.15 (m, 4H, Ar−H), 7.9 (brs, 1H, NH), 9.37 (brs, 1H, NH).

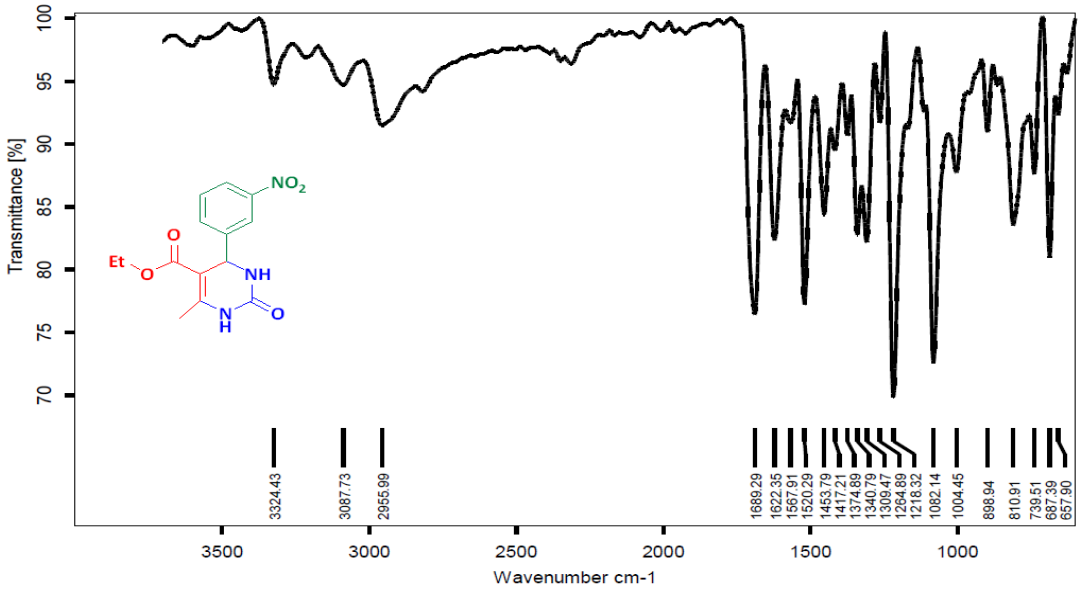


Fig S10. FT-IR spectrum of 5-Ethoxycarbonyl−6-methyl-4-(3-nitrophenyl)−3,4-dihydropyrimidin-2(1*H*)-one (**5e**).

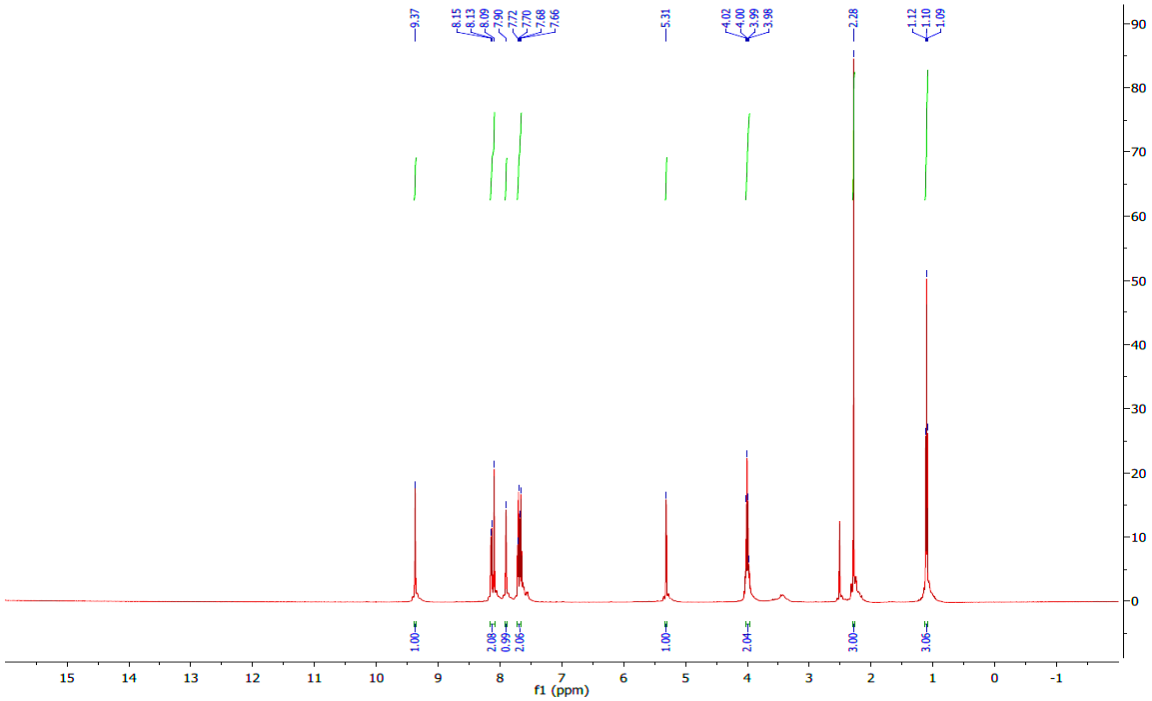


Fig S11. ^{1}H NMR spectrum of 5-Ethoxycarbonyl−6-methyl-4-(3-nitrophenyl)−3,4-dihydropyrimidin-2(1*H*)-one (**5e**).

5-Methoxycarbonyl-4-(2,4-dichlorophenyl)-6-methyl-3,4-dihydropyrimidine-2(1*H*)-one (**5m**)

M.P. = 252-254 °C; FT-IR (KBr, cm^{-1}) ν = 3357, 3216, 3093, 2946, 1694, 1641, 1454, 1223, 1096; ^{1}HNMR (500MHz, DMSO–d6) δ (ppm)= 2.30 (s, 3H, CH_3), 3.46 (s, 3H, OCH_3), 5.59 (s, 1H, CH), 7.31-7.42 (dd, 2H, Ar-H), 7.56 (s, 1H, Ar-H), 7.76 (brs, 1H, NH), 9.35 (brs, 1H, NH).

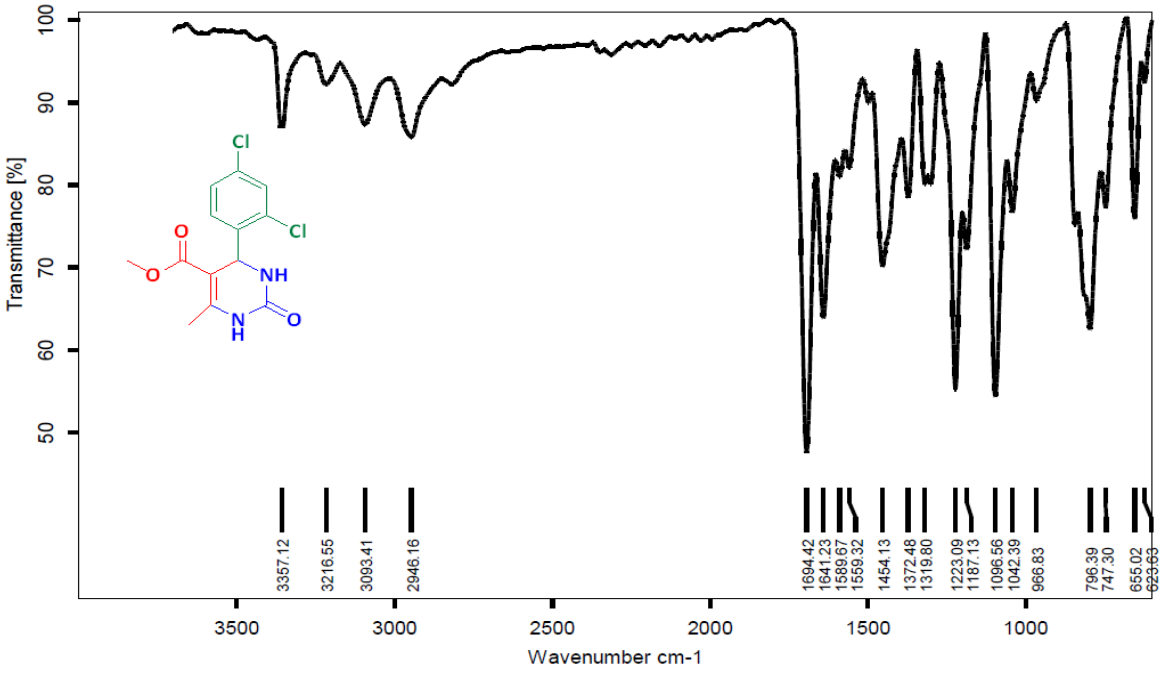


Fig S12. FT-IR spectrum of 5-Methoxycarbonyl-4-(2,4-dichlorophenyl)-6-methyl-3,4-dihydropyrimidine-2(1*H*)-one (**5m**).

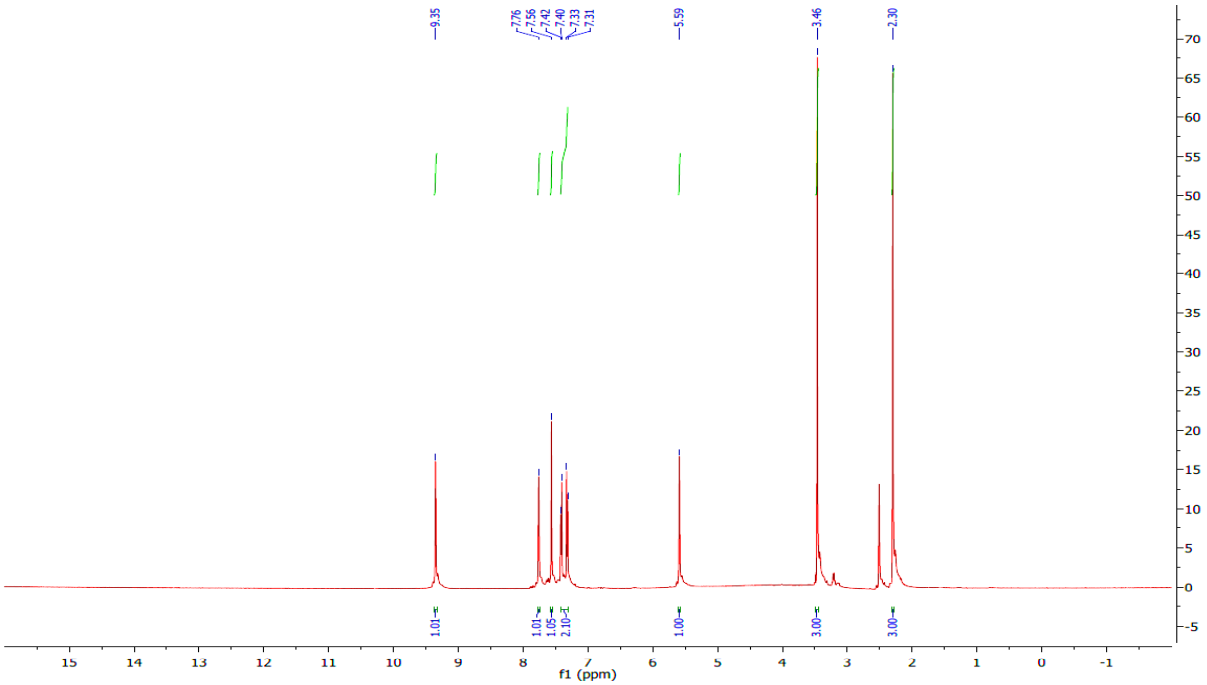


Fig S13. ^{1}H NMR spectrum of 5-Methoxycarbonyl-4-(2,4-dichlorophenyl)-6-methyl-3,4-dihydropyrimidine-2(1*H*)-one (**5m**)

5-Methoxycarbonyl-6-methyl-4-(thiophen-2-yl)-3,4-dihydropyrimidin-2(1*H*)-one (**5t**)

M.P. = 224-226°C; FT-IR (KBr, cm^{-1}) ν = 3344, 3106, 2946, 1690, 1639, 1423, 1226, 1089; ^{1}HNMR (500MHz, DMSO–d6) δ (ppm) = 2.23 (s, 3H, CH_3), 3.61 (s, 3H, OCH_3), 5.41 (s, 1H, CH), 6.90 − 6.96 (m, 2H, Ar−H), 7.37 (s, H, H−CS), 7.91 (brs, 1H, NH), 9.34 (brs, 1H, NH).

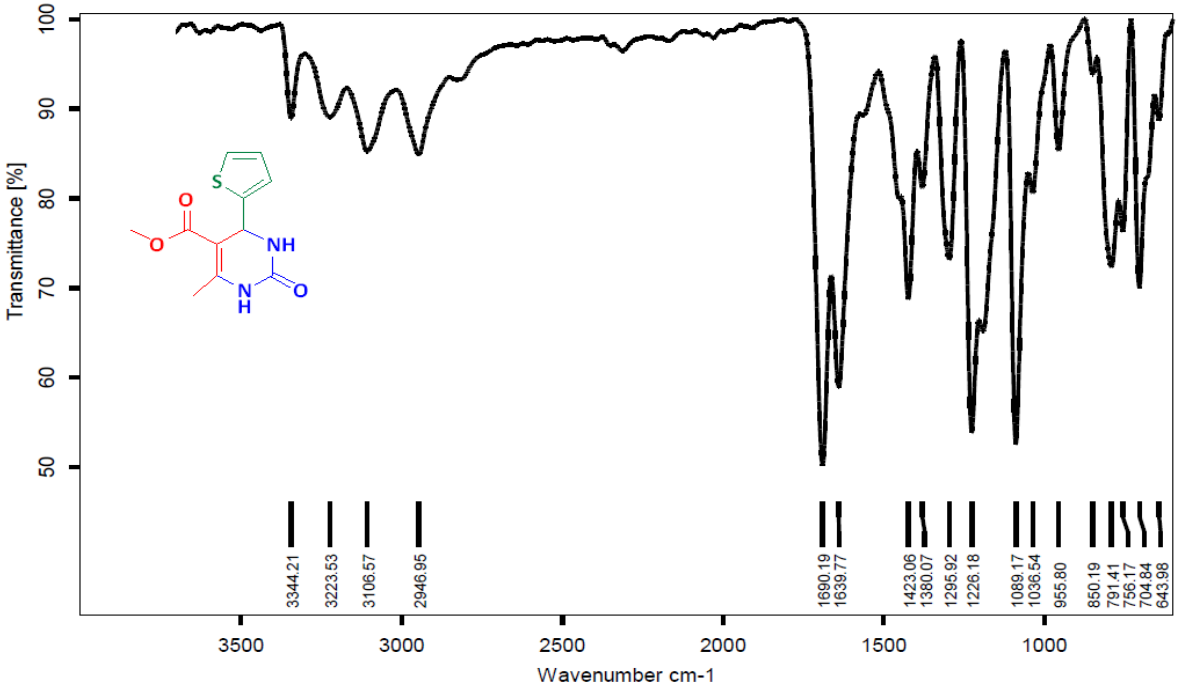


Fig S14. FT-IR spectrum of 5-Methoxycarbonyl-6-methyl-4-(thiophen-2-yl)-3,4-dihydropyrimidin-2(1*H*)-one (**5t**).

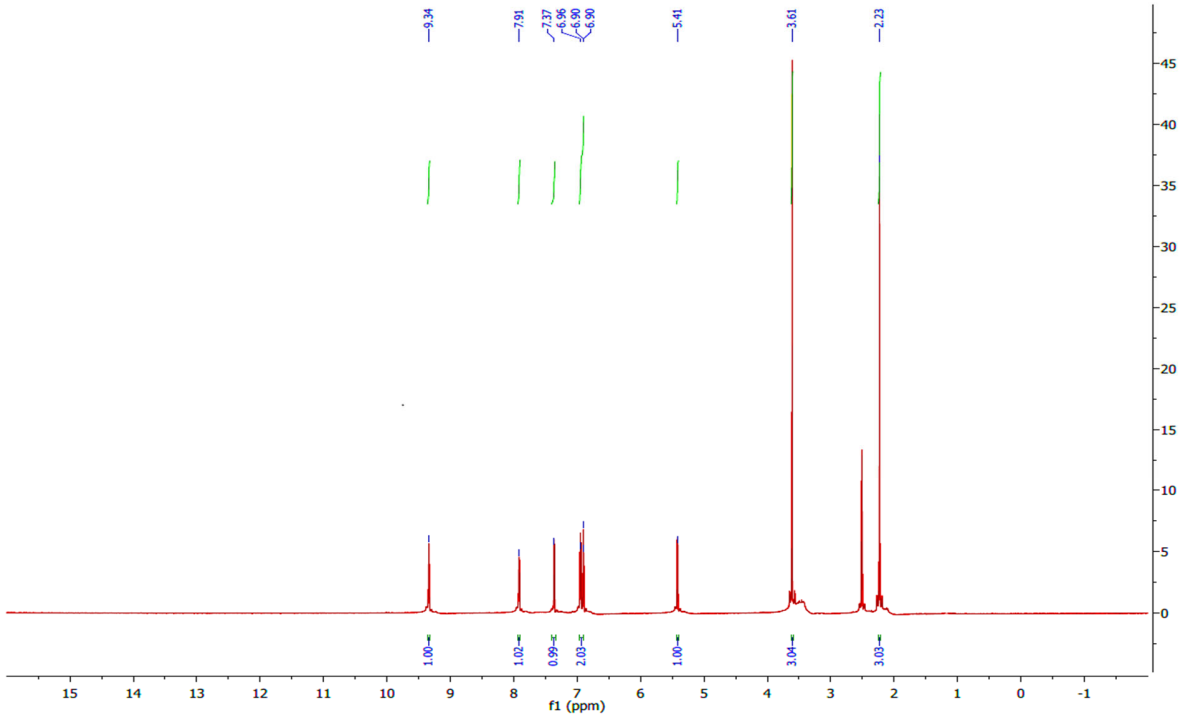


Fig S15. ^{1}H NMR spectrum of 5-Methoxycarbonyl-6-methyl-4-(thiophen-2-yl)-3,4-dihydropyrimidin-2(1*H*)-one (**5t**).