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(1H)-one compounds

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| Content                                                                 | Page |
|------------------------------------------------------------------------|------|
| Title page                                                             | S1   |
| Schematic preparation of Fe\textsubscript{3}O\textsubscript{4}@SiO\textsubscript{2}-APTS-EDTA-asparagine (1), as a heterogeneous nanocatalyst, for the synthesis of 3,4-dihydropyrimidin-2(1H)-one 5 derivatives | S2   |
| Characterization of the Fe\textsubscript{3}O\textsubscript{4}@SiO\textsubscript{2}-APTS-EDTA-asparagine (1)                           | S3   |
| Reusability of the Fe\textsubscript{3}O\textsubscript{4}@SiO\textsubscript{2}-APTS-EDTA-asparagine (1) nanocatalyst for the synthesis of 5a | S9   |
| Table S1. Calculation of green chemistry metrics for compound 5a       | S10  |
| Chemical characterization of 5-ethoxycarbonyl-6-methyl-4-(3-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one (5e)                | S11  |
| Chemical characterization of 5-methoxycarbonyl-4-(2,4-dichlorophenyl)-6-methyl-3,4-dihydropyrimidine-2(1H)-one (5m)       | S12  |
| Chemical characterization of 5-methoxycarbonyl-6-methyl-4-(thiophen-2-yl)-3,4-dihydropyrimidin-2(1H)-one (5t)             | S13  |
**Scheme S1.** Schematic preparation of Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1), as a heterogeneous nanocatalyst, for the synthesis of 3,4-dihydropyrimidin-2(1H)-one 5 derivatives.
Characterization of the Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1)

Fig S1. FT-IR spectra of the Fe₃O₄ (a), Fe₃O₄@SiO₂ (b), Fe₃O₄@SiO₂-APTS (c), Fe₃O₄@SiO₂-APTS-EDTA (d) and Fe₃O₄@SiO₂-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 Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1).
Fig S3. FESEM images of the Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1).
Fig S4. TEM images of the Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1).
Fig S5. XRD pattern of the Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1).

Fig S6. VSM pattern of Fe₃O₄ (red) and Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1, green).
Fig S7. TGA curve of the Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1)
Fig S8. Effect of solvent and the amount of Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1) nanocatalyst on the model reaction.
Fig S9. Reusability of the Fe₃O₄@SiO₂-APTS-EDTA-asparagine (1) nanocatalyst for the synthesis of 5a.
Table S1. Calculation of green chemistry metrics for compound 5a.

![Chemical Structure](image)

Molar mass: 60.06 g/mol 294.74 g/mol

| 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. | \[rac{\text{Total mass of raw materials} - \text{the total mass of product}}{\text{mass of product}}\] | 0           | \[\frac{(60.06 + 140.57 + 130.14)}{282.95}\] = 0.16 |
| 2 Atom economy (AE%)                | Atom economy signifies the percentage of atoms wasted in chemical reaction.     | \[rac{\text{MW of product}}{\sum(\text{MW of stoichiometric reactants})} \times 100\] | 100%        | \[\frac{(294.74)}{\left(\frac{60.06 + 140.57 + 130.14}{282.95}\right)} \times 100\] = 89.1% |
| 3 Carbon efficiency (CE%)           | CE signifies the percentage of carbons in the reactants that is left in the product. | \[rac{\text{Amount of carbon in product}}{\sum(\text{carbon present in reactants})} \times 100\] | 100%        | \[\frac{0.96 \times 14}{(1.0 \times 1 + 1.0 \times 7 + 1.0 \times 6)} \times 100\] = 96% |
| 4 Process mass intensity (PMI)      | PMI takes into account reaction efficiency, stoichiometry, amount of solvent and all reagent used in the chemical reaction. | \[rac{\sum(\text{mass of stoichiometric reactants})}{\text{mass of stoichiometric product}}\] | 1           | \[\frac{(60.06 + 140.57 + 130.14)}{282.95}\] = 1.16 |
| 5 Reaction mass efficiency (RME %)  | RME accounts into atom economy, chemical yield and stoichiometry.              | \[rac{\text{mass of product}}{\sum(\text{mass of stoichiometric reactants})} \times 100\] | 100%        | \[\frac{282.95}{\left(\frac{60.06 + 140.57 + 130.14}{282.95}\right)} \times 100\] = 85.5% |
5-Ethoxycarbonyl–6-methyl-4-(3-nitrophenyl)–3,4-dihydropyrimidin-2(1H)-one (nifetepimine, 5e)

M.P. = 211-212 °C; FT-IR (KBr, cm⁻¹) ν = 3324, 3087, 2955, 1689, 1622, 1567, 1453, 1218, 1082; ¹H NMR (500MHz, DMSO–d6) δ (ppm) = 1.10 (t, 3H, OCH₂CH₃), 2.2 8(s, 3H, CH₃), 4.0 (q, 2H, OCH₂), 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(1H)-one (5e).

Fig S11. ¹H NMR spectrum of 5-Ethoxycarbonyl–6-methyl-4-(3-nitrophenyl)–3,4-dihydropyrimidin-2(1H)-one (5e).
5-Methoxycarbonyl-4-(2,4-dichlorophenyl)-6-methyl-3,4-dihydropyrimidine-2(1H)-one (5m)

M.P. = 252-254 °C; FT-IR (KBr, cm\(^{-1}\)) \(\nu = 3357, 3216, 3093, 2946, 1694, 1641, 1454, 1223, 1096\); \(^1\)HNMR (500MHz, DMSO–d6) \(\delta \) (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(1H)-one (5m).

Fig S13. \(^1\)H NMR spectrum of 5-Methoxycarbonyl-4-(2,4-dichlorophenyl)-6-methyl-3,4-dihydropyrimidine-2(1H)-one (5m)
5-Methoxycarbonyl-6-methyl-4-(thiophen-2-yl)-3,4-dihydropyrimidin-2(1H)-one (5t)

M.P. = 224-226°C; FT-IR (KBr, cm\(^{-1}\)) \(\nu = 3344, 3106, 2946, 1690, 1639, 1423, 1226, 1089\); \(^1\)HNMR (500MHz, DMSO-d6) \(\delta\) (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, 1H, 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(1H)-one (5t).

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