**Polymer Grafting of Graphene Oxide through Esterification of Terephthalic Acid and Allyl Alcohol for Metronidazole Drug Delivery:** **Central Composite Design Optimization Study**

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The following is included as additional **Supporting Information** for this paper:

**Figure Captions:**

**Fig. S1.** TGA thermogram of GO/TPAA cl-poly (AA)/TPA.

**Fig. S2.** XRD pattern of GO/TPAA cl-poly (AA)/TPA.

**Fig. S3.** FT-IR spectra of GO/TPAA (a) and GO/TPAA cl-poly (AA)/TPA (b).

**Fig. S4.** N2 adsorption–desorption isotherm of GO/TPAA cl-poly (AA)/TPA.

**Fig. S5.** plot of ln (KL) versus 1/T.

**Fig. S6.** Influence of reusability on MNZ adsorption.

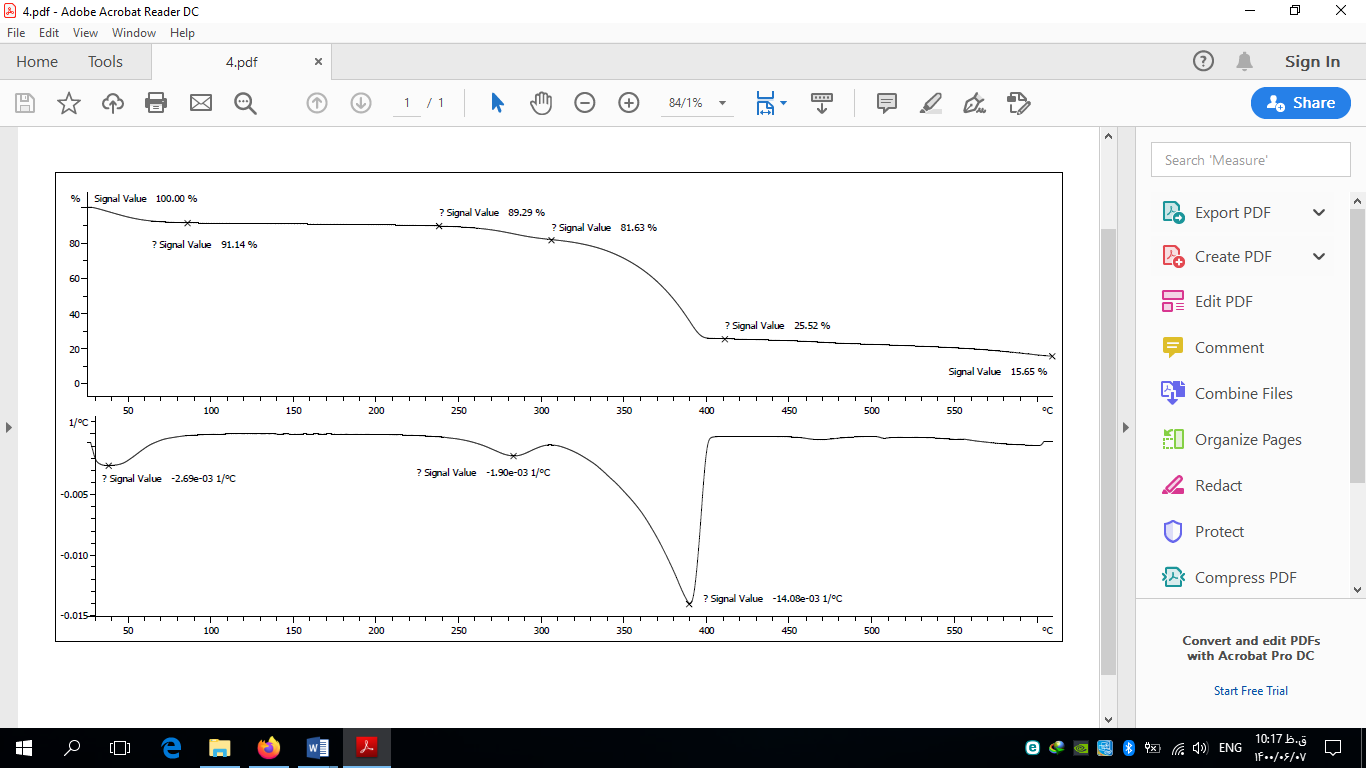
**Table captions:**

**Table S1.** Isotherm model parameters for the adsorption of MNZ onto GO/TPAA cl-poly (AA)/TPA.

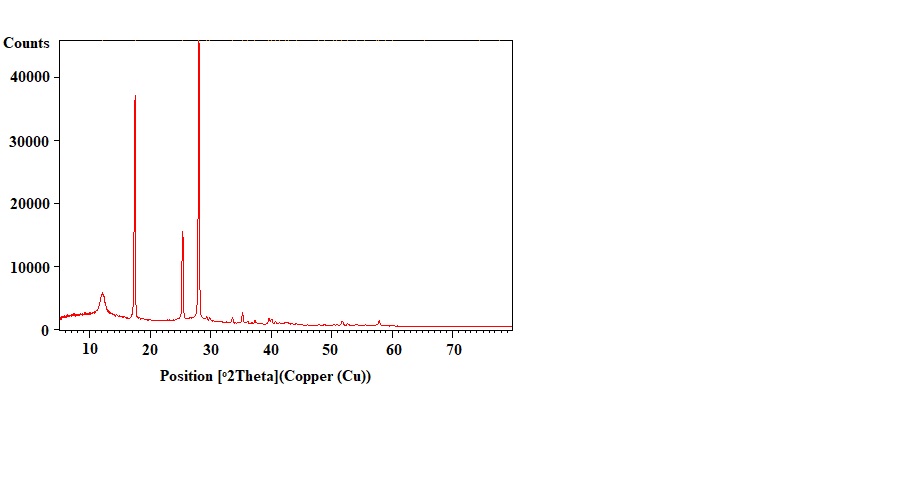
**Table S2.** Kinetic model parameters for the adsorption of MNZ onto GO/TPAA cl-poly (AA)/TPA.

**Table S3.** Thermodynamics parameters for the adsorption of MNZ onto GO/TPAA cl-poly (AA)/TPA.

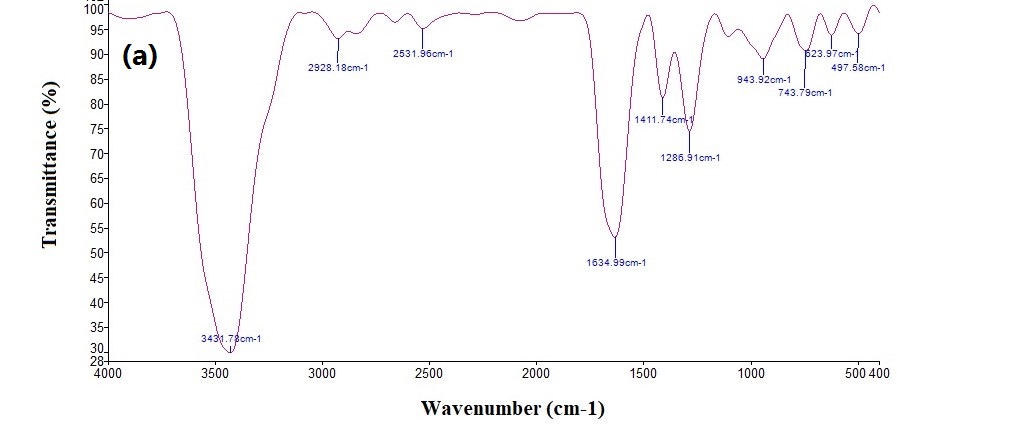
**Table S4.** Results of the correlation coefficients and rate constants of different models for release curve of MNZ from GO/TPAA cl-poly (AA)/TPA (pH=1.2 and 7.4).

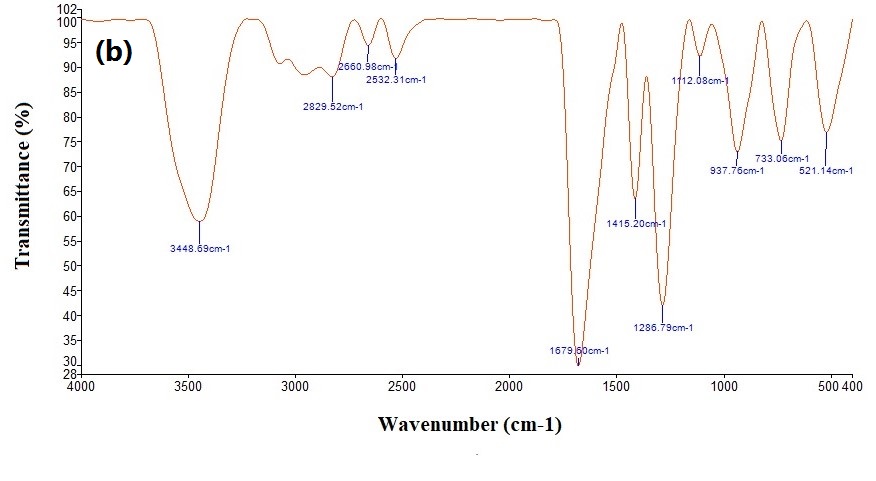


**Fig. S1**

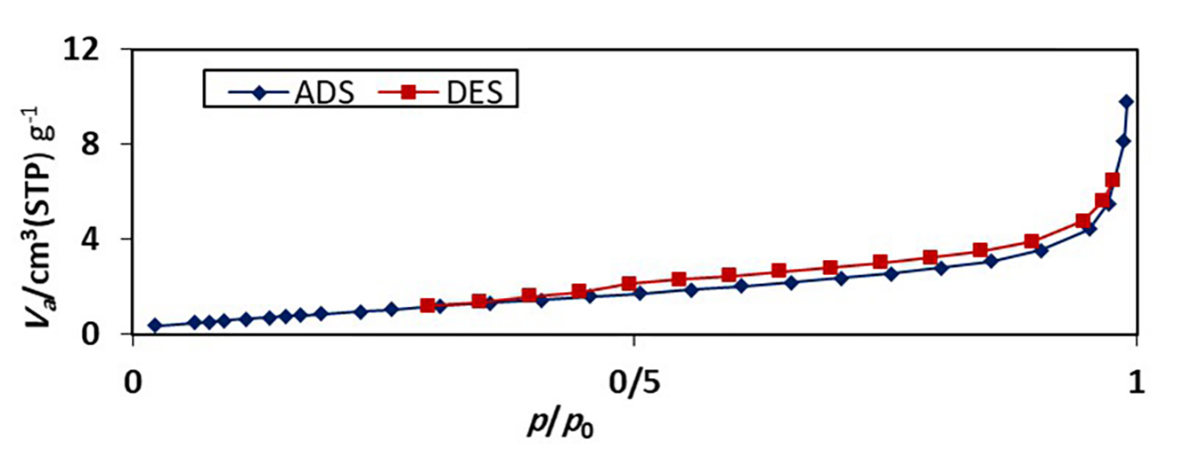
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**Fig. S2**

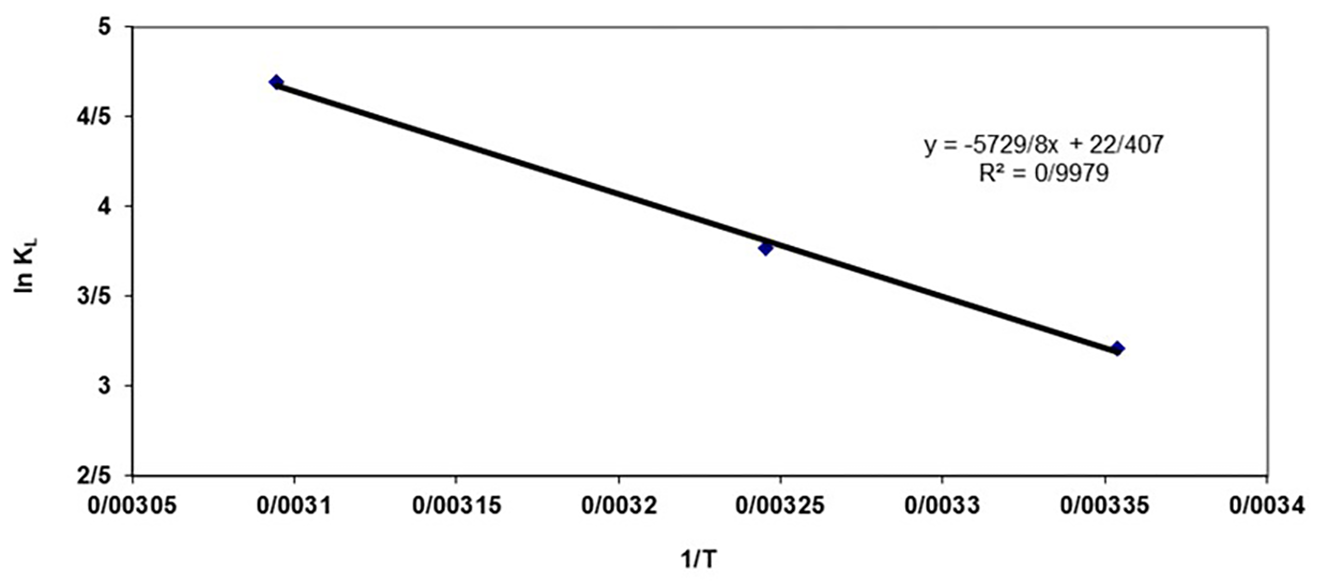




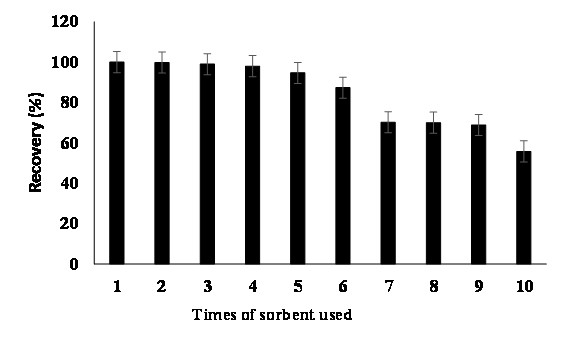
**Fig. S3**



**Fig. S4**



**Fig. S5**

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**Fig. S6**

**Table S1**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Model** | **Parameter**  **T=298.15K** | | **Value**  **T= 308.15 K T= 323**.**15K** | |
| **Langmuir** | qm (mg g-1)  kl (L mg-1)  Rl  R2 | 7.776  0.024  0.287  0.9956 | 10.582  0.043  0.186  0.9932 | 11.098  0.109  0.083  0.9913 |
| **Ferundlich** | n  Ln(kf)  kf(mg11/nL1/ng-1)  R2 | 1. 508  -1.088  0.336  0.9947 | 1.594  -0.32  0.726  0.9836 | 1.692  0.301  1.351  0.9885 |
| **Temkine** | B  AT (L mg-1)  R2 | 1.295  0.419  0.9515 | 2.227  0.469  0.9945 | 2.433  1.061  0.9828 |
| **Dubinin-Radushkevich** | Kad (mol2 kJ-2)  Ln (qs)  qs (mg g-1)  R2 | 0.00002  1.344  3.834  0.8863 | 0.000007  1.735  5.672  0.9141 | 0.000002  1.901  6.694  0.8406 |

**Table S2**

|  |  |  |
| --- | --- | --- |
| **Model** | **Parameter** | **Value** |
| **Pseudo-first-order model** | qe (mg g-1)  K1 (min-1)  R2 | 4.073  0.0039  0.9486 |
| **Pseudo-second-order model** | qe (mg g-1)  K2 (g mg-1min-1)  R2 | 1.694  1.779  0.9999 |
| **Intra-particle diffusion** | Ki (g mg-1min-1/2)  Ci (mg g-1)  R2 | 0.081  1.365  0.9419 |

**Table S3**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sample** | **Temperature (K)** | **ΔHo (J mol-1)** | **ΔSo (J mol-1 K-1)** | **ΔGo (J mol-1)** |
| **GO/TPAA cl-poly (AA)/TPA** | 298.15  308.15  323.15 | 47637.56 | 186.2918 | 7.905  9.768  12.562 |

**Table S4**

|  |  |  |  |
| --- | --- | --- | --- |
| **Zero order**  pH=1.2 pH=7.4 | **First order**  pH=1.2 pH=7.4 | **Higuchi**  pH=1.2 pH=7.4 | **Korsmeyer – Peppas**  pH=1.2 pH=7.4 |
| **K0  R2 K0  R2** | **K1  R2 K1 R2** | **KH  R2 KH  R2** | **n KKP  R2 KKP  R2** |
| 5.226 0.9919 5.362 0983 | 0.151 0.9562 0.255 0.9863 | 34.579 0.9871 34.03 0.9286 | 0.5 34.077 0.9889 34.03 0.9286  0.6 26.015 0.9937 26.132 0.9441  0.7 20.318 0.9962 20.525 0.9571  0.8 16.118 0.9966 16.37 0.9679  0.9 12.928 0.9951 13.198 0.9765  1 10.454 0.9919 10.724 0.9830 |