Supporting Materials

Magnetic Nanocrystalline Cellulose-Poly(Methacrylic Acid-co-Acrylonitrile) Composite: A Versatile Material for Analytical and Biological Applications

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S1. Characterization of P(MAA-co-AN)-g-MNCC

The synthesized P(MAA-co-AN)-g-MNCC was characterized with various analytical techniques such as FTIR, SEM, EDX, TGA, and the E_g, PZC, and surface area. The FTIR spectral analysis was recorded using a Presige-21 (FT-IR-8400S, Shimadzu, Japan) spectrophotometer with the spectral range of 480 cm^{-1} to 4000 cm^{-1}. The SEM-EDX analyses were carried out by using an EDX spectrometer (INCA-200, Oxford Instruments, UK) coupled with a scanning electron microscope (JEOL JSM-5910 SEM, Japan). For this purpose, the sample was stuck with carbon conducting tape on a sample stub and sputtered with gold in a fine coater (SPI-module) for 30 s. The stub bearing sample was inserted in the sample chamber of the instrument, where the machine was evacuated, and the morphology of the sample was determined at 10 kV with a 10 mm gap between the sample and the electron gun tip. For EDX analysis, the sample was prepared in the same way but without sputtering with gold and analyzed at 10 keV. The TGA was carried out by using PerkinElmer Diamond TG/DTA (USA). For this purpose, in the alumina ceramic pan, the sample was placed for one min at room temperature. Increase the temperature up to 600 ^oC at a rate of heating of 10 ^oC/min under the N_2 gas environment. The study of UV-visible spectrophotometric analysis was recorded using a UV-visible spectrophotometer (PerkinElmer, UV Win Lab Lambda 900 UV/VIS/NIR, USA). For such a purpose, a small amount of the sample was mixed with isopropanol (10 mL) and dispersed completely using a sonicator for 30 min at room temperature. The absorbance of the resultant mixture was measured in the range from 200-800 nm. From the absorbance, E_g was determined using the Tauc equation.

$$(\alpha\text{-}h\nu)^{1/n} = C(h\nu - E_g)$$

where α is the absorption coefficient of P(MAA-co-AN)-g-MNCC composite, h is the Planck's constant (6.62×10^{-34} Js), ν is the photon's frequency, n factor depends on the nature of the electron transition and is equal to 1/2 or 2 for the direct and indirect transition band gaps, respectively, C is a constant (3×10^{8} m/s) and E_g is the band gap energy. For the determination of E_g, $\alpha h\nu^{1/2}$ was plotted vs E_g.

The PZC was also determined as per the reported method. For this purpose, the synthesized P(MAA-co-AN)-g-MNCC (0.05 g) was mixed with 0.1 M $NaNO_3$ solution (50 mL) with different $pH_{initial}$ values, i.e., from pH 1 to pH 12, using 0.1 M NaOH and 0.1 M HCl solution. The mixtures were shaken for 4 h at room temperature at 200 rpm. Afterward, the pH of the solutions was recorded again as pH_{final} using a digital pH-meter (3505, Jenway, UK). For the PZC measurement, ΔpH was obtained by subtracting pH_{final} from $pH_{initial}$ and plotting $pH_{initial}$. Similarly, the surface area analysis of the synthesized P(MAA-co-AN)-g-MNCC was performed via N_2 gas adsorption-desorption isotherms at 77.350 K using a surface area analyzer (TriStar-II-3020, TriStar-II Series, Micromeritics, USA). The Brunauer Emmett-Teller (BET) method was adopted for the determination of surface area, and the De-Boer protocol was used to calculate the pore radius and pore volume.

Table S1. The kinetic model equations for the adsorption of GA in the aqueous environment using P(MAA-co-AN)-g-MNCC.

Kinetic Model	**Equation**
Pseudo-first-order kinetic	$\log(qe - qt) = \log qe - \frac{K_1 t}{2.303}$
Pseudo-second-order kinetic	$\frac{t}{qt} = \frac{t}{qe} - \frac{1}{K_2 q_e^2}$
Intraparticle diffusion	$qt = K_{int} t^{1/2} + C$
Elovich	$qt = \frac{1}{\beta}\ln(\alpha\beta) + \frac{1}{\beta}\ln(t)$

Table S2. The equilibrium models applied for the adsorption of GA in the aqueous environment using P(MAA-co-AN)-g-MNCC.

Adsorption Isotherm	**Equation**
Freundlich	$logqe = logK_F + \frac{1}{n} logCe$
Langmuir	$\frac{Ce}{qe} = \frac{1}{K_L} + \frac{a_L C_e}{K_L}$
Temkin	$qe = B_T lnA_T + B_T lnC_e$
Dubinin-Radushkevich (D-R)	$lnqe = lnQ_m - K_{\epsilon}{}^2$
Separation factor (R_L, g/L)	$R_L = \frac{1}{1 + K_L C_i}$
Mean Free Kinetic Energy	$E = \frac{1}{\sqrt{2K}}$

Table S3. Thermodynamic models applied for the adsorption of GA in the aqueous environment using P(MAA-co-AN)-g-MNCC.

Thermodynamic Parameters	**Equation**
Adsorption distribution coefficient	$K_D = \frac{q_e}{C_e}$
Van't Hoff Equation	$lnK_D =- \frac{\Delta H^o}{RT} + \frac{\Delta S^o}{R}$
Gibbs free energy (ΔG^o)	$\Delta G^o = \Delta H^o - T\Delta S^o$
Arrhenius Equation	$\ln(1-\theta) = \frac{E_a}{RT} + lnS^*$

where q_t (mg/L) is the amount of GA adsorbed at given time (t) (1/min), q_e (mg/L) is the amount of GA adsorbed at equilibrium, where K_1 (1/min) and K_2 (g/mg.min) is the sorption rate constant of PS order and PS order kinetics equations at any given time (t) (min), respectively, at t → 0 the K_2 is used to analyze the initial adsorption rate (h) (mg/g.min) as h = K_2qe_2, K_{int} (mg/gg.min) is the diffusion rate constant, C is intercept, while α and β are Elovich coefficient, respectively, α (mg/g.min) showing the initial rate of adsorption and β (mg/g.min) to explain the extent of surface coverage and the activation energy for the adsorption, respectively, q_e is the amount of GA adsorbed (g/L), KF (mg/g) or $[(mg/g)(g/L)^n]$ and n (L/g) are the Freundlich adsorption constants, C_e is the equilibrium concentration of GA in the solution (g/L), K_L and aL are the Langmuir adsorption constants, the constant B_T (mg/g) is related to the adsorption capacity of an adsorbent which is equal to; BT = (RT)/bT, T is the absolute temperature in Kelvin (K), R is the universal gas constant (8.314 J/mol.K), b_T is the Temkin constant related to the heat of adsorption (J/mol), A_T (L/g) is the equilibrium binding constant corresponding to the maximum binding energy, Q_m (mg/g) is the theoretical capacity of saturation, K (mol^2/kJ^2) is a constant for the adsorption energy, ε is for Polanyi potential and can be calculated from the equation given below.

$$\varepsilon = RTln\left(1 + \frac{1}{C_e}\right)$$

ΔG° is Gibbs' free energy, ΔH° is the enthalpy, and ΔS° is the entropy, θ is the surface coverage, E_a (kJ/mol) is the activation energy or heat of adsorption, T (K) is the absolute temperature, and S* is the sticking probability.

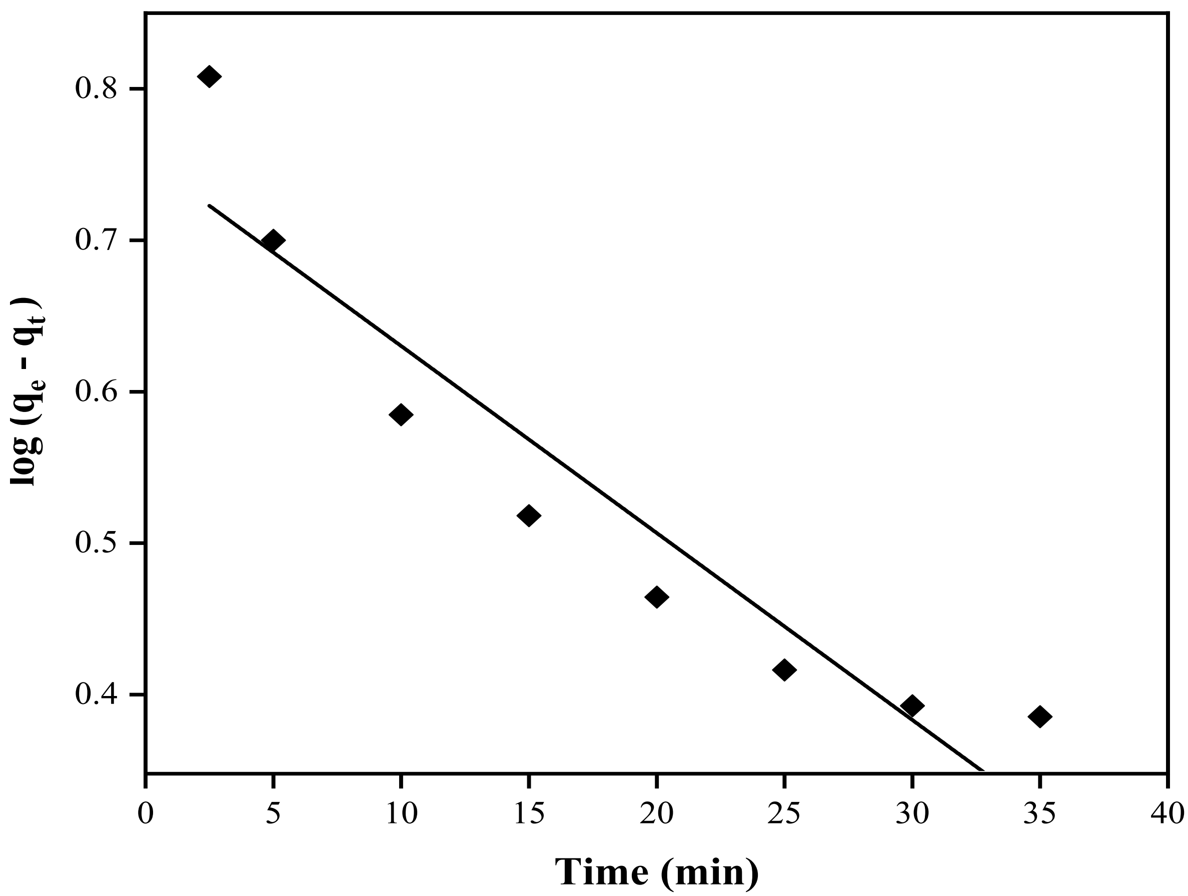

Fig. S1. Pseudo first-order kinetic model for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

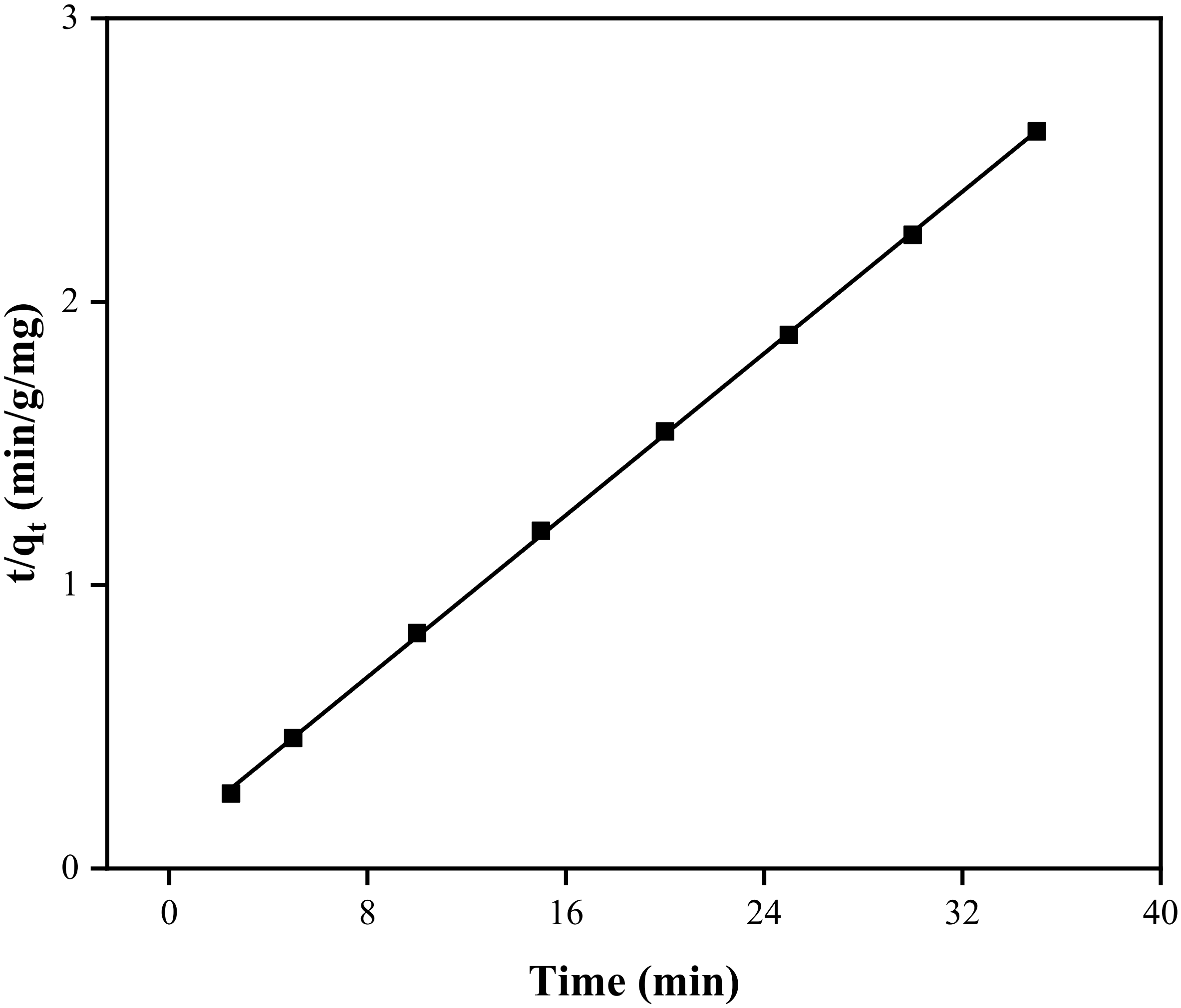

Fig. S2. Pseudo-second order kinetic model for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

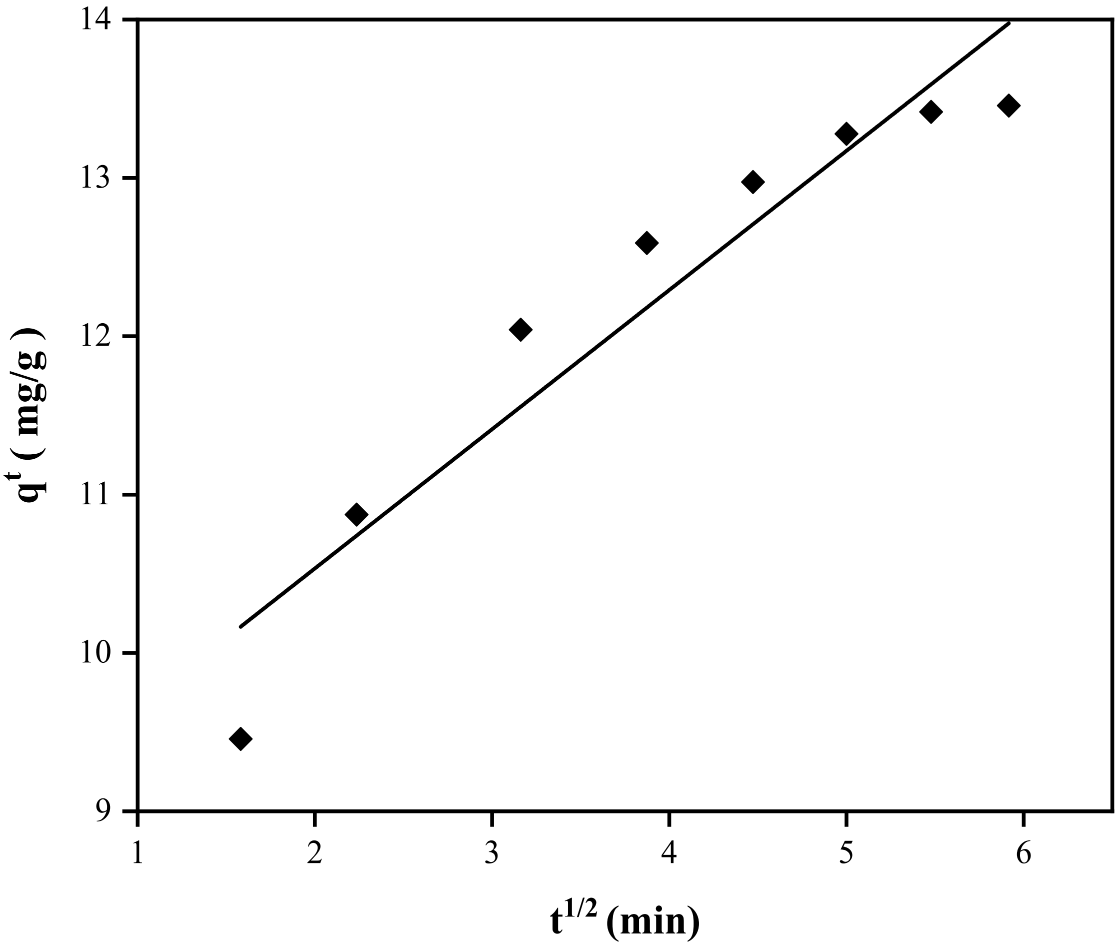

Fig. S3. Intra-particle diffusion model for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

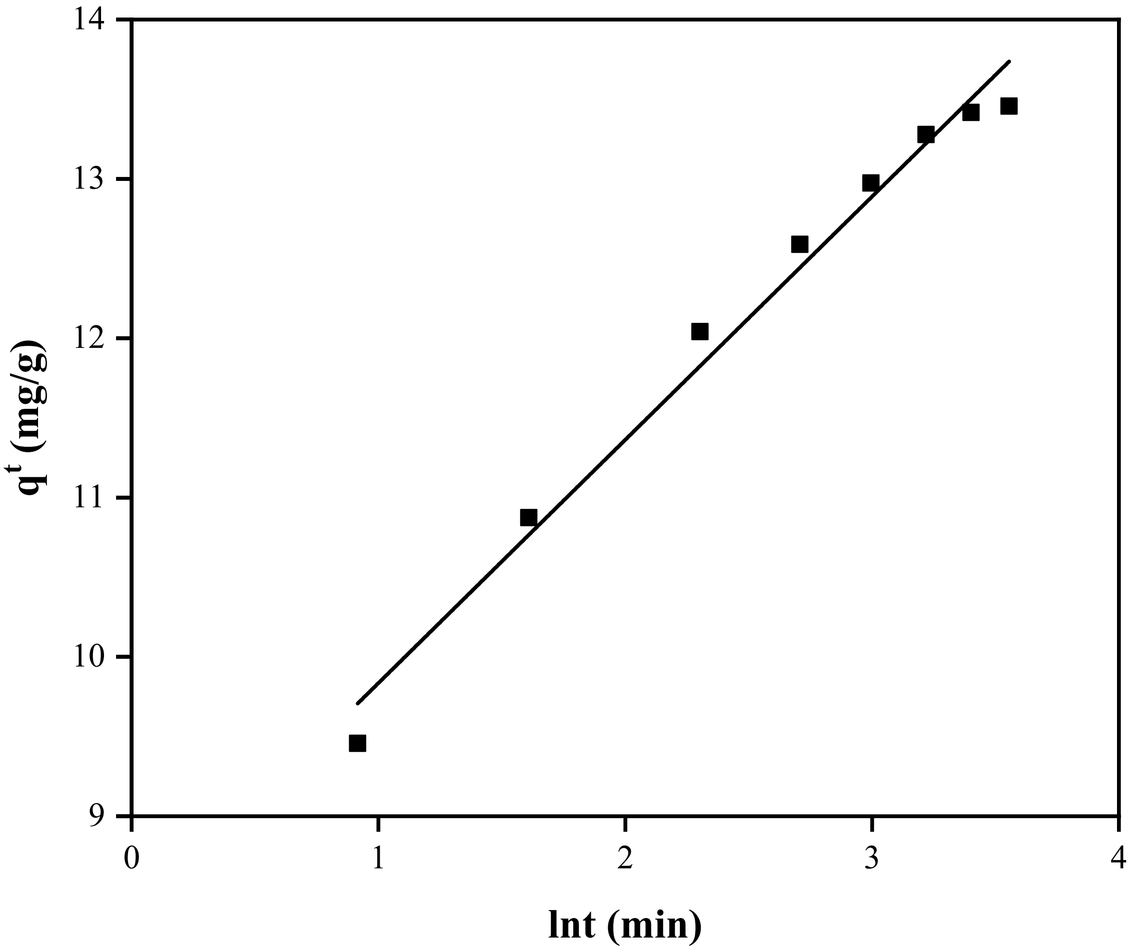

Fig. S4. Elovich model for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

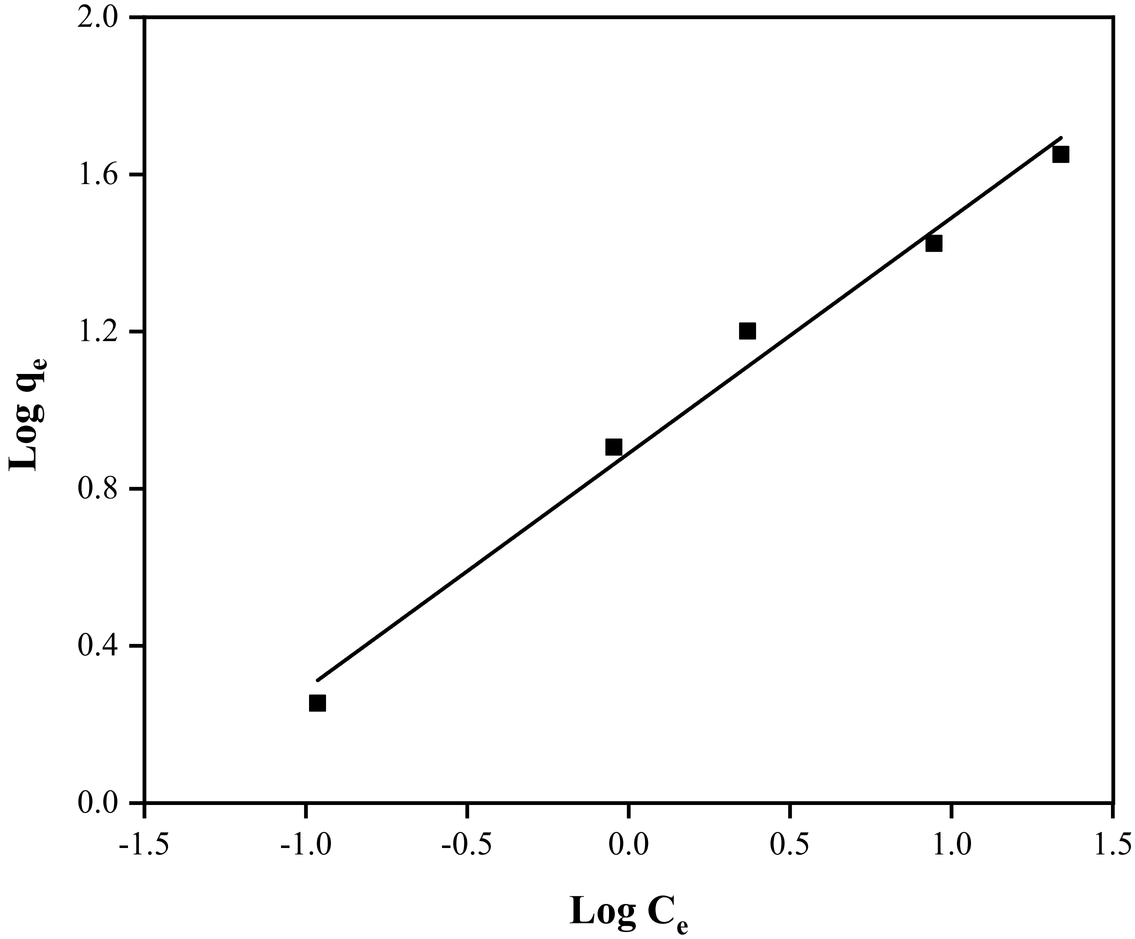

Fig. S5. Freundlich isotherm for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

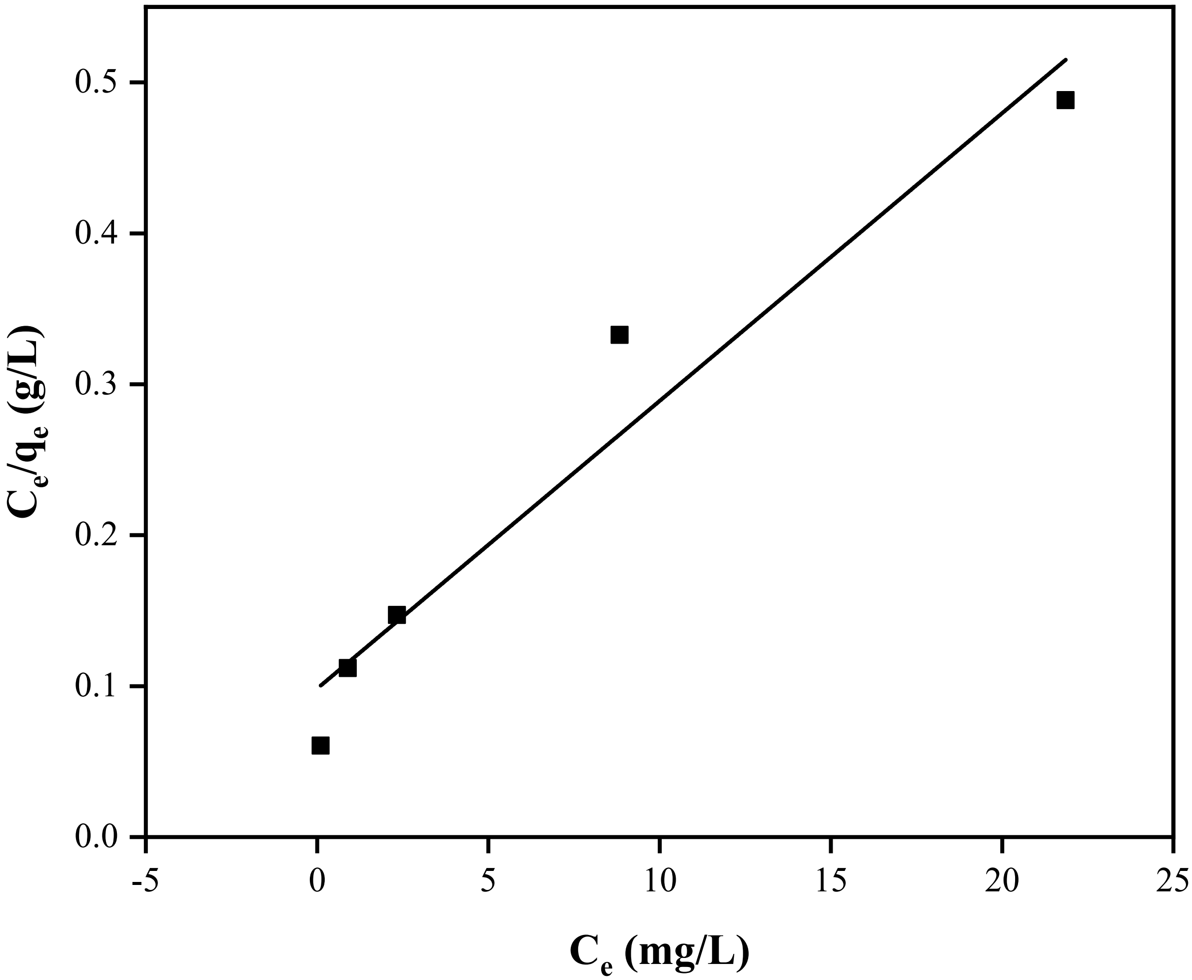

Fig. S6. Langmuir isotherm for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

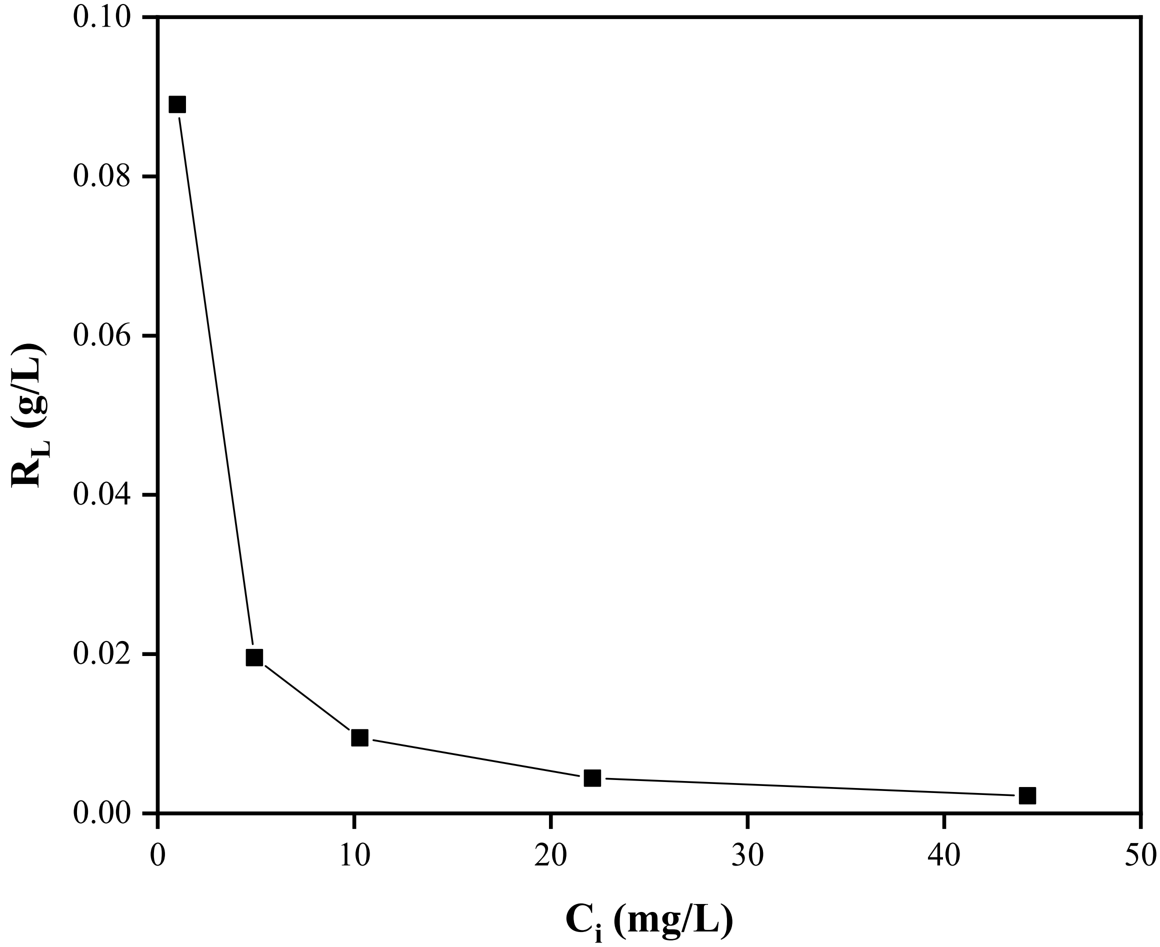

Fig. S7. The R_L values for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

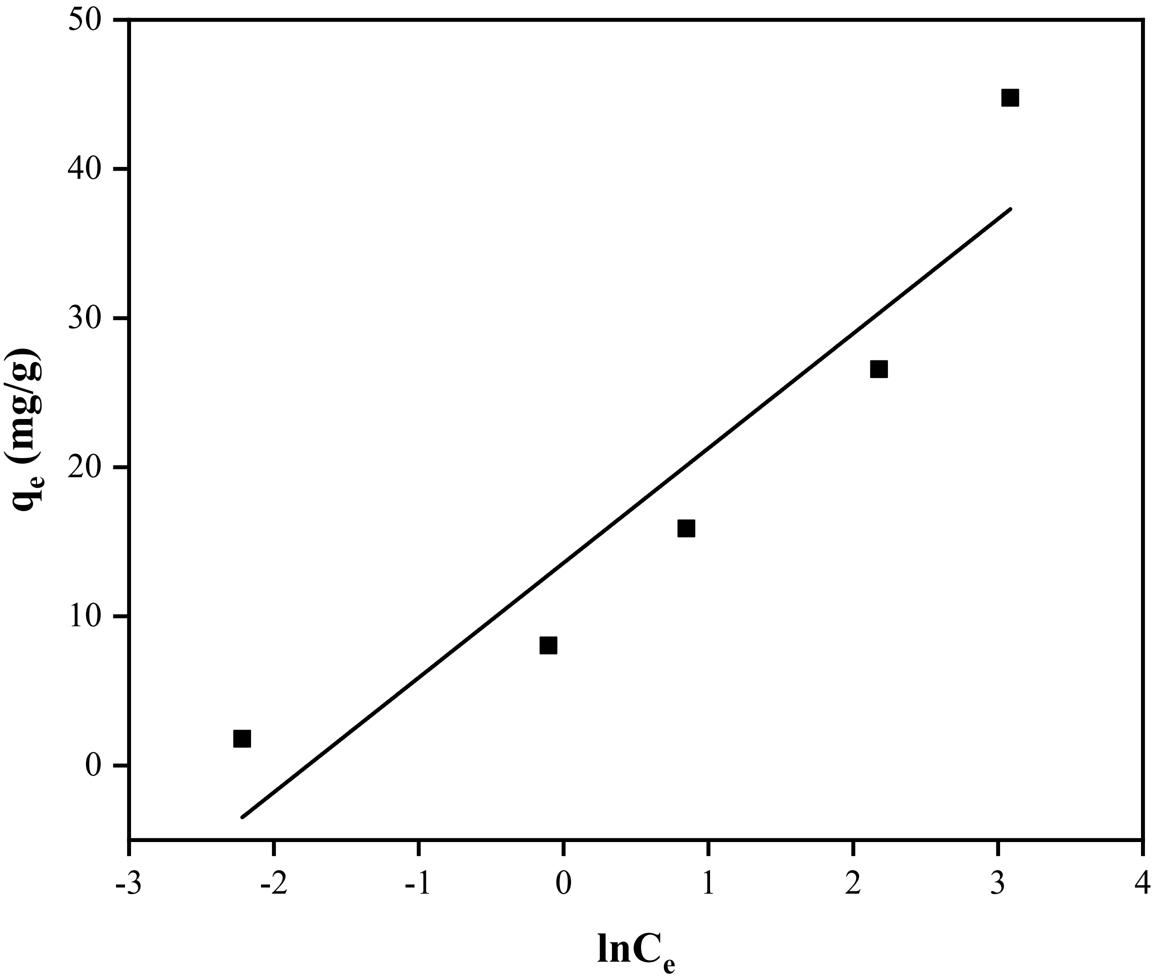

Fig. S8. Temkin isotherm for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

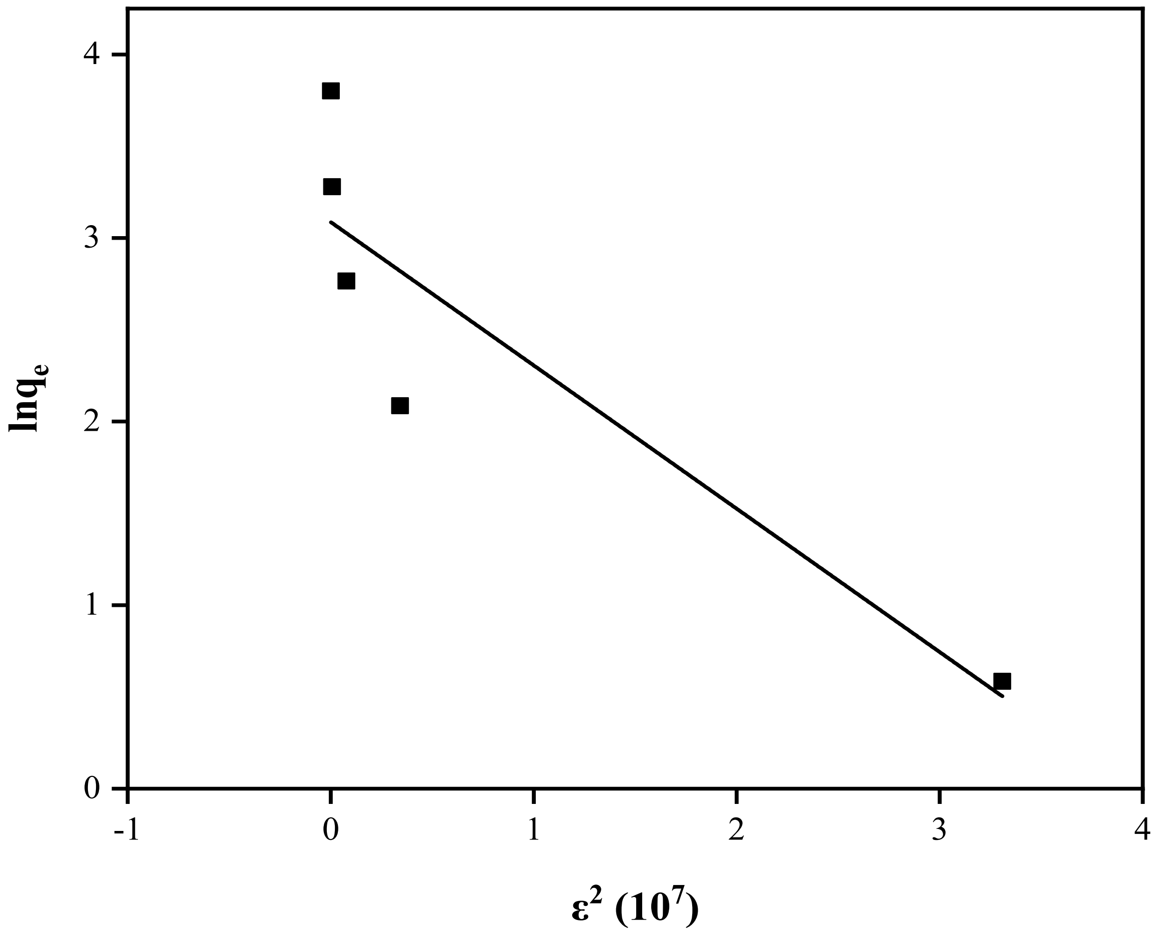

Fig. S9. Dubinin-Radushkevich for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

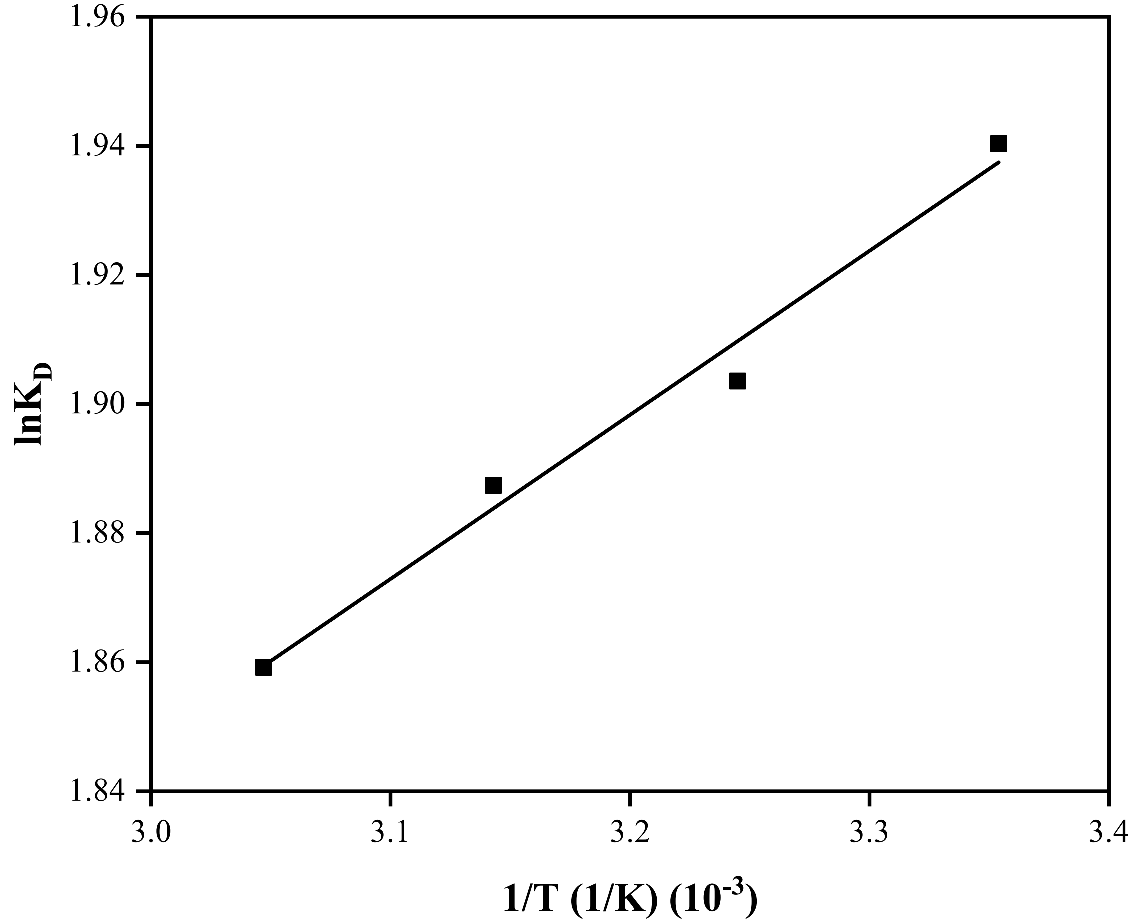

Fig. S10. Determination of thermodynamic parameters for the adsorption of GA using P(MAA-co-AN)-g-MNCC.

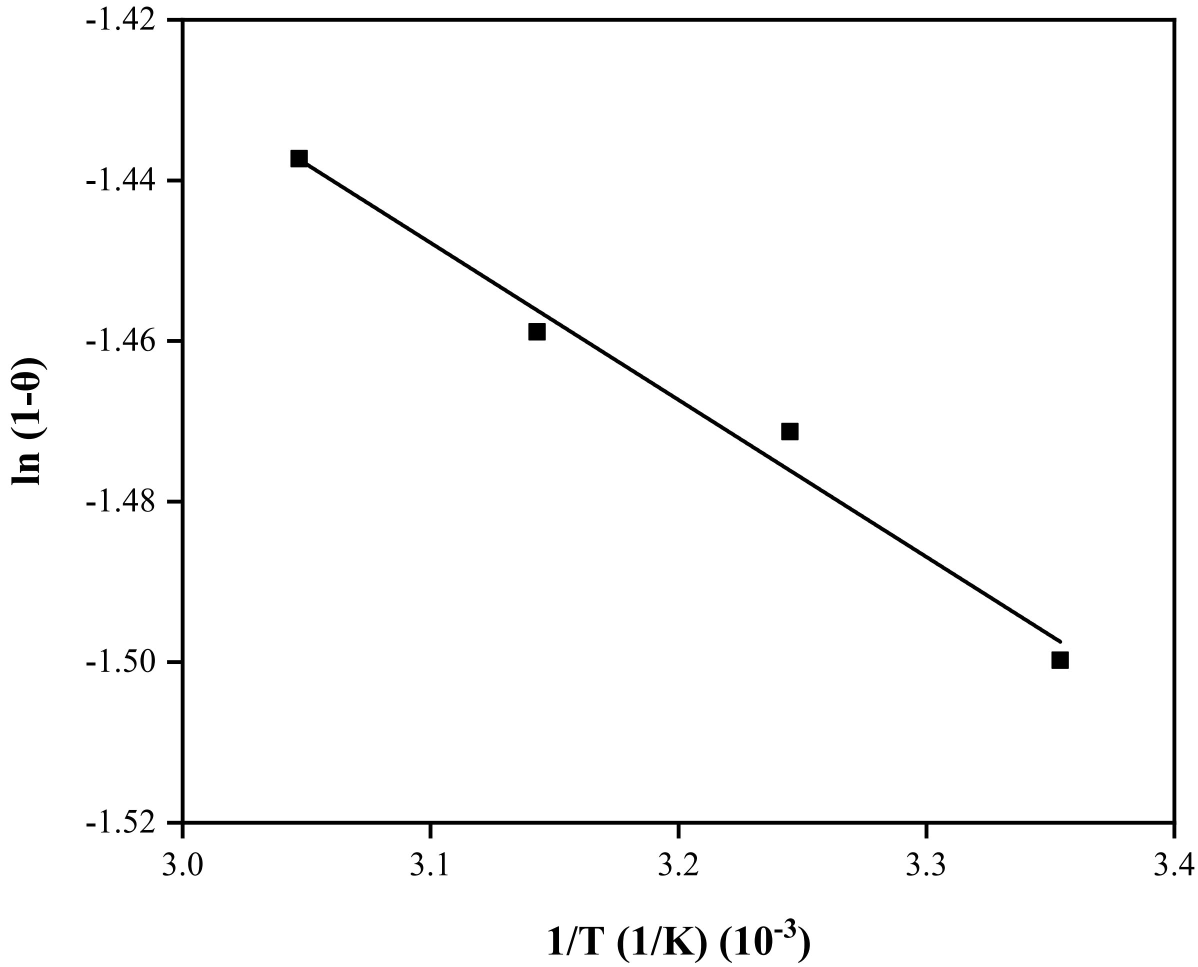

Fig. S11. Determination of heat of adsorption for the adsorption of GA using P(MAA-co-AN)-g-MNCC.