Novel Aminothiazole- supported chlorocellulose for efficient removal of cationic dyes from wastewater

Abdelrahman S El-Zeny[1], El-Sayed RH El-Gharkawy[1], Tarek A. Gad-Allah[2] and Magda A Akl[1*]

[1]Department of Chemistry, Faculty of Science, Mansoura University, Mansoura 35516, Egypt

[2]Water Pollution Research Department, National Research Centre, 33 El Buhouth St., Dokki, 12622 Giza, Egypt

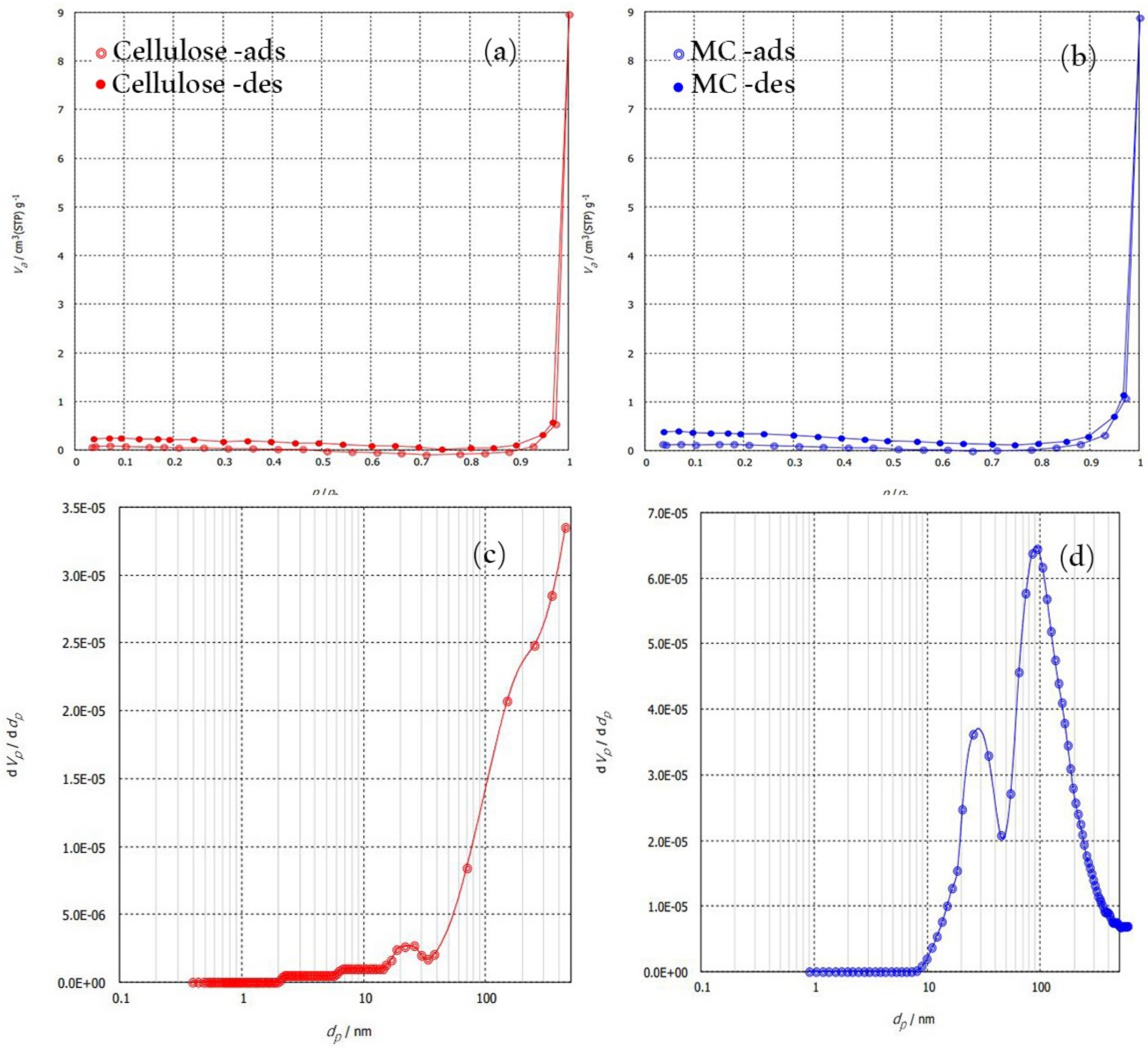

Fig. 1S: (a,b) Nitrogen adsorption- desorption isotherms, (c,d) average pore diameter
Note:(a,c for cellulose) &(b,d for MC)

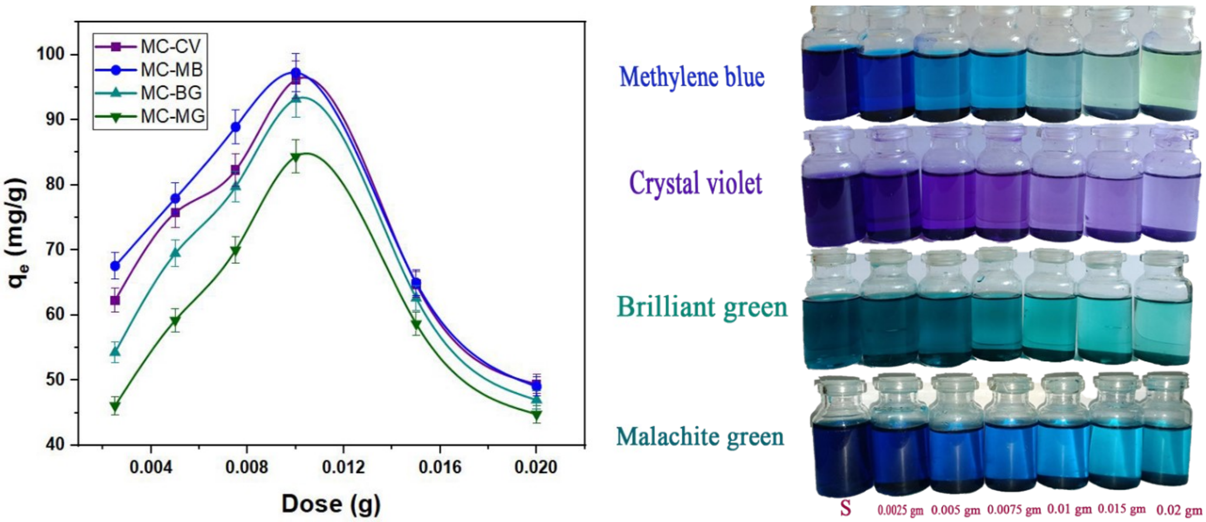

Fig. 2S: Effect of adsorbent dosage on of the dyes adsorption on MC studied dyes (100 mg L^{-1}), sorbent (1g/L), pH =6 for BG, MG and pH= 10 for CV, MB, at 308 K

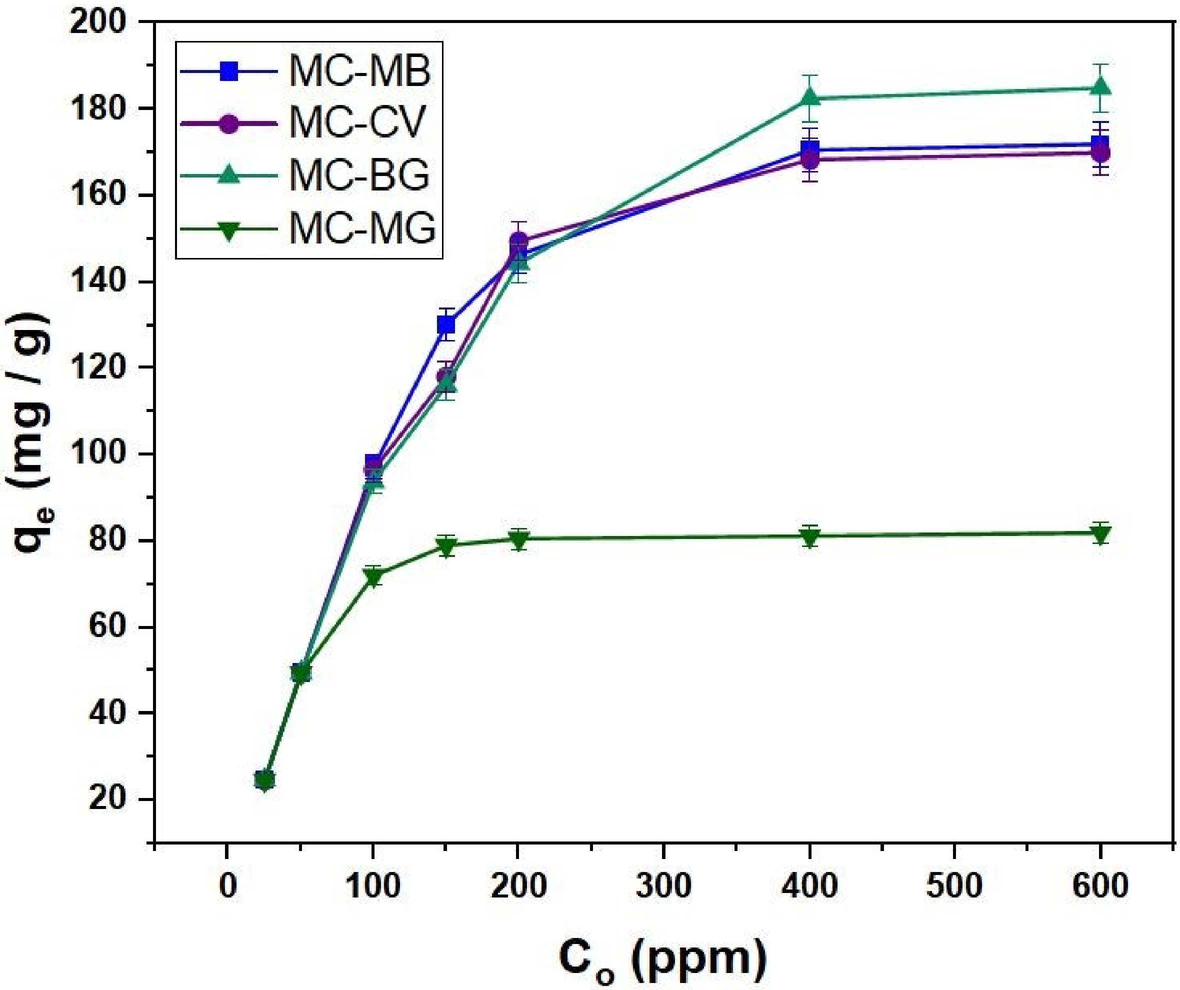

Fig. 3S: Adsorption isotherms at different MC dosages ((25-600) mg/L) initial concentrations, studied dyes (100 mg L^{-1}), sorbent (1g/L), pH =6 for BG, MG and pH= 10 for CV, MB, at 308 K

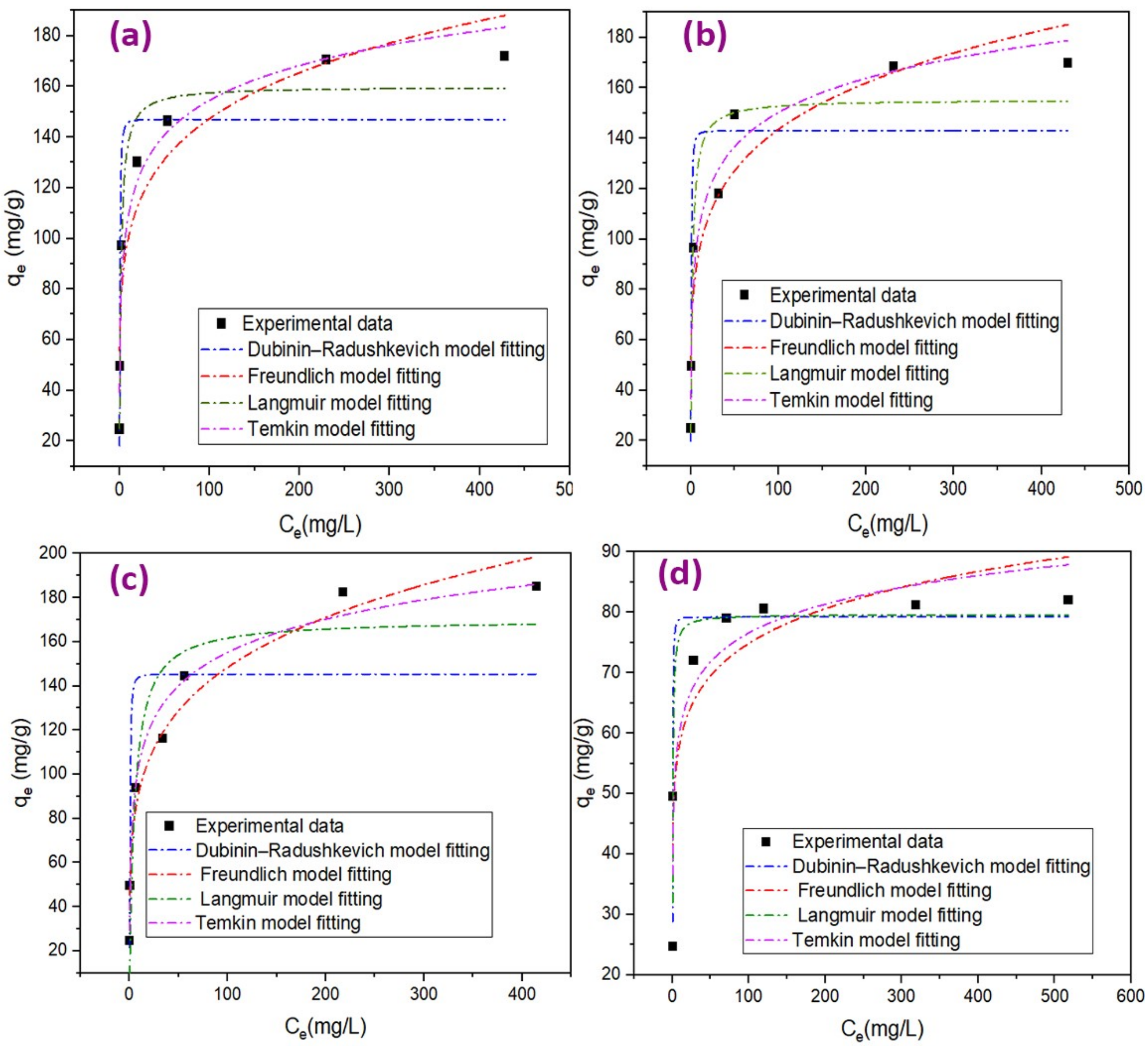

Fig.4S: adsorption isotherms models by MC the nonlinear curve fittings

a) MC-MB b) MC-CV c) MC-BG d) MC-MG

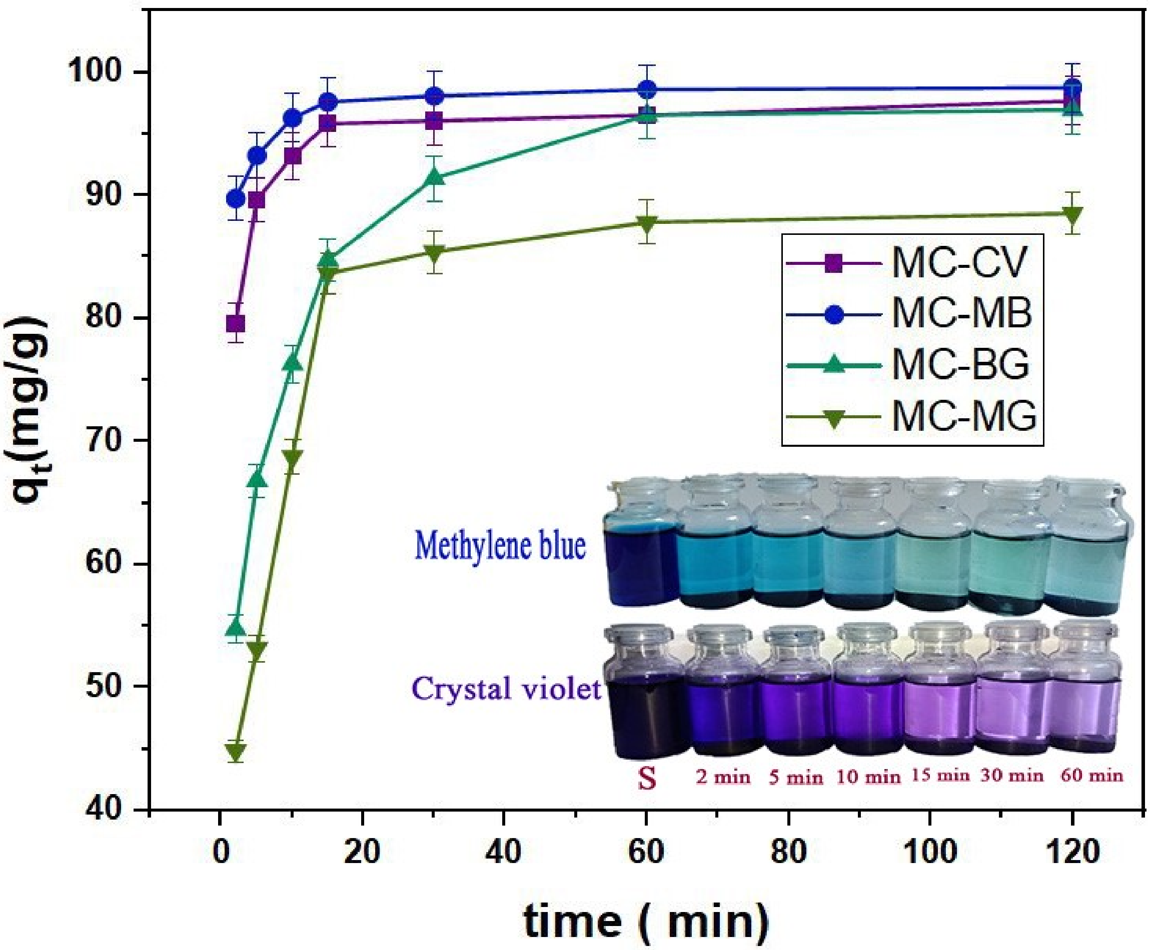

Fig. 5S: Effect of contact time on the removal efficiency of the studied dyes by MC: studied dyes (100 mg L^{-1}), sorbent (1g/L), pH =6 for BG, MG and pH= 10 for CV, MB, at 308 K.

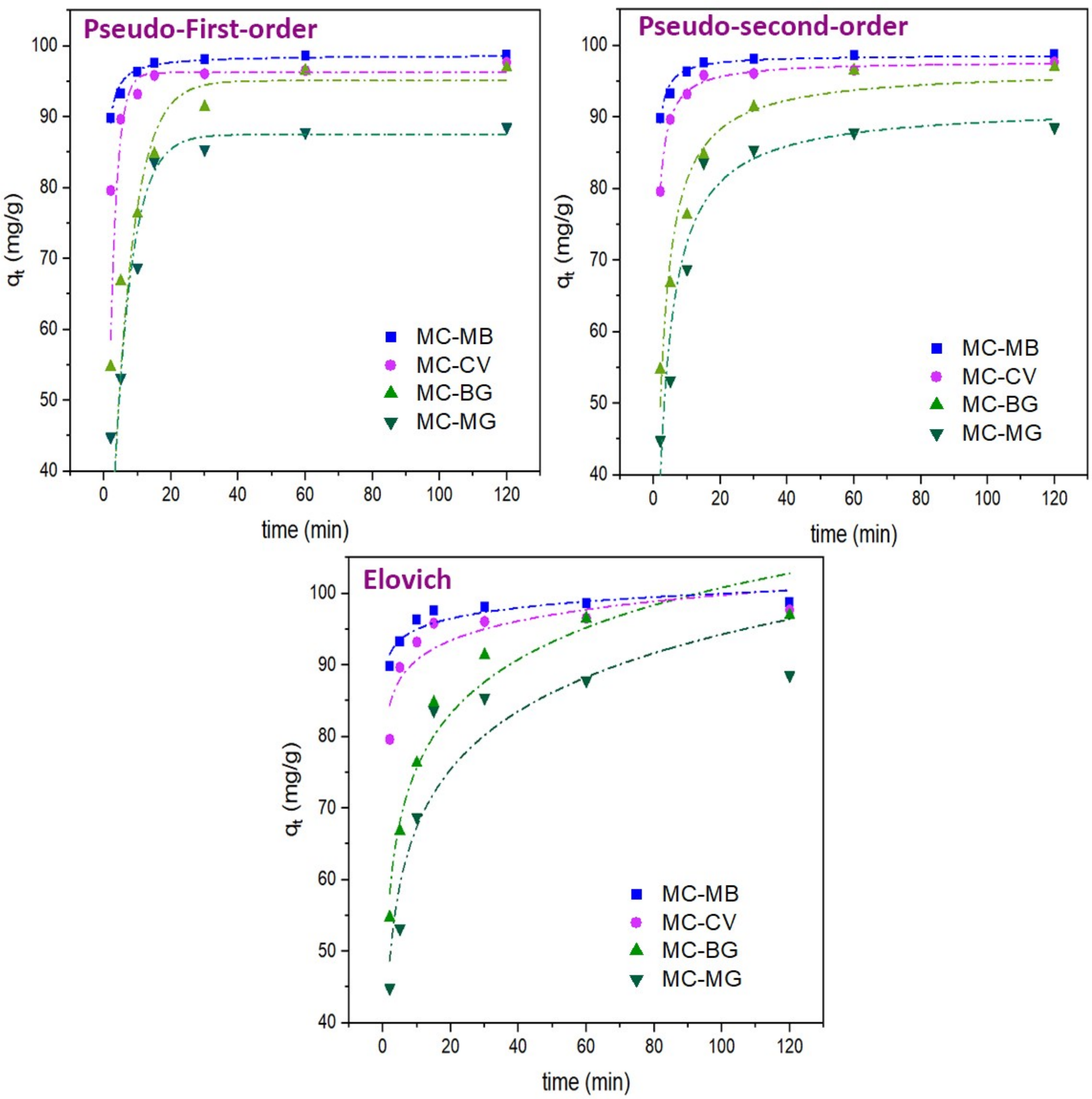

Fig. 6S: Kinetic models fittings for the studied dyes adsorption on MC.

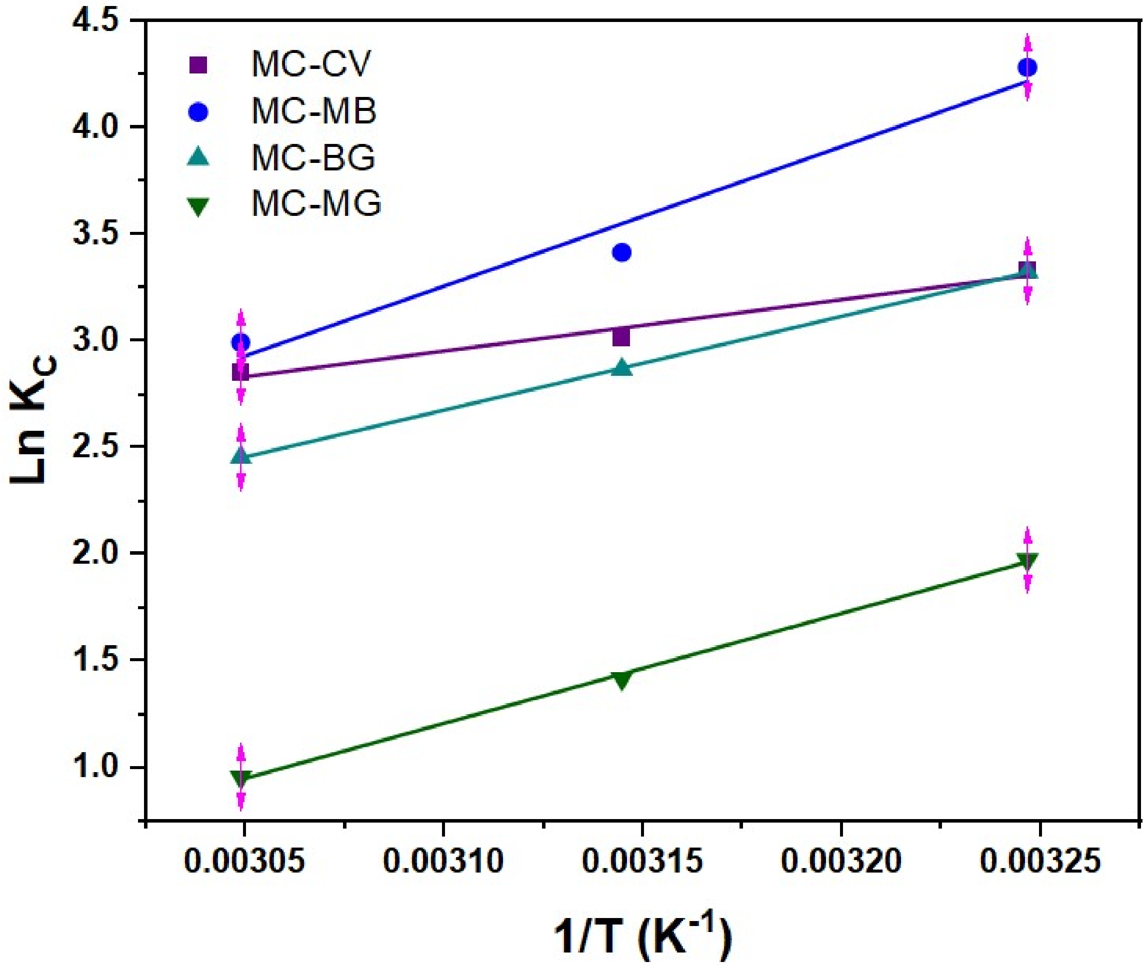

Fig. 7S: Plot of ln K_C vs 1/T absolute temperature.

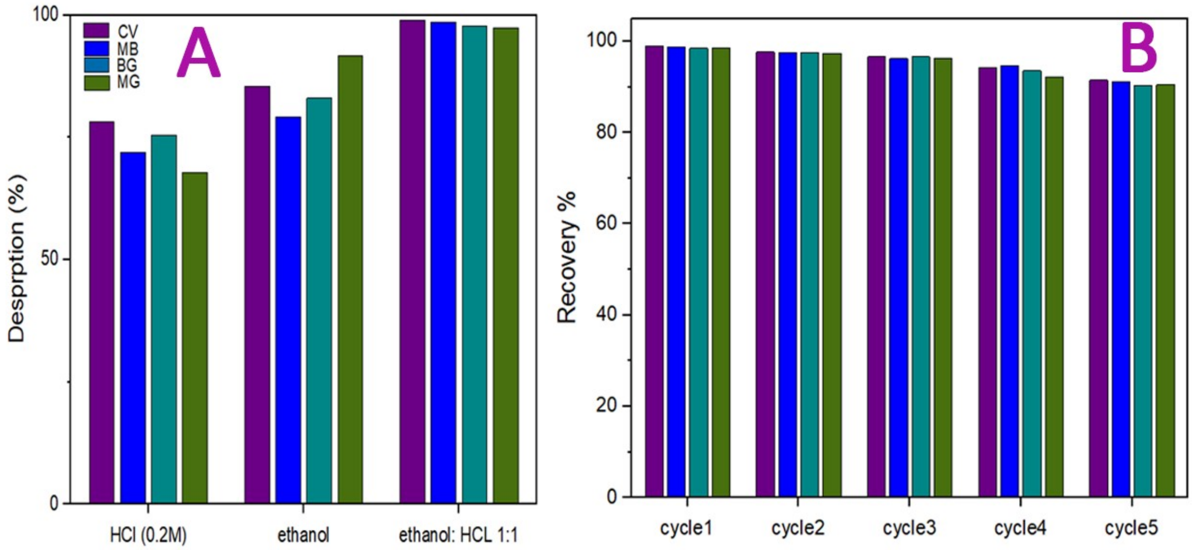

Fig 8S: A) Various eluents were used to desorb CV, MB, BG, and MG from the MC adsorbent. B) Ethanol and HCl in a 1:1 ratio served as an eluent for five cycles of adsorption and desorption of CV, MB, BG, and MG..

Table 1S: Elemental analysis of the prepared materials.

Material	C (%)	H (%)	N (%)	S (%)
Ligand	35.1	4.52	32.1	18.4
	(34.87)*	(4.68)*	(32.54)*	(18.62)*
Cellulose	41.55	6.05	--------	--------
Cellulose-Cl	39.92	5.72	--------	--------
MC	41.8	5.94	10.4	5.98

*Calculated values.

Table 2 S: Adsorption kinetics and isotherms nonlinear models

Models	**Formula**	**Descriptions**
Pseudo-first order (PFO)	$q_t = q_e\left(1 - e^{-K_1 t}\right),$	q_e (mg/g) represents the quantity that has been adsorbed when equilibrium is reached, q_t (mg/g) indicates the quantity adsorbed at a given time (min), K1 (min^{-1}) is the constant for the pseudo-first-order reactio
Pseudo-second order (PSO)	$q_t = \frac{k_2 q_e^2 t}{1 + (k_2 q_e t)}$	K_2(g/mg/min) Pseudo- second -order constant.
Elovich	$q_t = (\frac{1}{q_e}) ln(1 + a_e q_e t),$	a_e (mg/(g.min)) rate constant of adsorption
Langmuir	$q_e = q_m K_L\left(\frac{C_e}{1 + K_L C_e}\right),$ $R_L = \left(\frac{1}{1 + K_L C_O}\right)$	q_e (mg/g) represents the quantity that has been adsorbed when equilibrium is reached, q_m (mg/g) indicates the highest capacity for monolayer adsorption, K_L (L/mg) is the equilibrium constant of Langmuir, R_L (–) is the separation factor of Langmuir: $R_L = 0$ means reversible, $0 < R_L < 1$ indicates favorable conditions, $R_L = 1$ signifies a linear relationship, and $R_L > 1$ shows unfavorable conditions.
Freundlich	$q_e = K_F\left(C_e^{\frac{1}{n}}\right)$	K_F(L/g) constant for Freundlich, n exponent for Freundlich related to the affinity of adsorption.
Dubinin–Radushkevich	$q_e = q_m exp[-K_{DR}[RTl$	qe (mg/g) refers to the quantity of adsorption that occurs when equilibrium is reached, Ce (mg/L) indicates the concentration of the adsorbate at this equilibrium point, qm represents the capacity for monolayer adsorption, and KDR denotes the D-R constant that provides the energy of adsorption (E), $E = \frac{1}{\sqrt{2K_{DR}}}$. KJ/mol T (K) represents the temperature, and R denotes the universal gas constant.

Temkin	$q_e = \frac{RT}{b} ln\left(K_T C_e\right),$	q_e (mg/g) refers to the quantity of adsorbate that gets adsorbed when equilibrium is reached. C_e (mg/L) indicates the concentration of the adsorbate at equilibrium. T (K) denotes the temperature, while R represents the

Table 3S: Thermodynamic parameters of the studied adsorption processes.

System	K_c			ΔG^o_{ads} (KJ/mol)			ΔH^o_{ads} (KJ/mol)	ΔS^o_{ads} (J/mol K)
	308 K	318 K	328 K	308 K	318 K	328 K		
MC-CV	27.96667	20.4333	17.3714	-8529.77	-7976.9	-7785.09	-20057.9	-37.612
MC-MB	72.65	30.475	19.9833	-10974.3	-9033.8	-8167.06	-54384.7	-141.488
MC-BG	27.82609	17.6176	11.66	-8516.86	-7584.9	-6697.94	-36535.7	-90.993
MC-MG	7.213675	4.128492	2.6	-5059.91	-3748.7	-2605.67	-42883.1	-122.888

Table 4S: Effect ionic strength on the removal percentages of the studied dyes .

Salts	Removal (%) CV	MB	BG	MG
NaCl (0.1M)	99.0	99.3	98.3	98.4
KCl (0.1M)	98.1	98.7	98.2	98.1
$MgCl_2$ (0.1M)	97.8	98.4	98.2	97.8
$AlCl_3$ (0.1M)	97.5	96.4	95.7	96.1
CH_3COONa (0.1M)	97.8	97.4	97.2	97.1