Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Covalent triazine framework-decorated phenyl-functionalized SBA-15: Synthesis and application as a novel nanoporous adsorbent

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Table S1. The list of adsorption equilibrium, kinetics, and thermodynamic equations.

Adsorption equilibrium equations	$\%\text{Removal} = 100 \cdot (C_0 - C_e)/C_0$ (1)		$Q_e = (C_0 - C_e) \cdot V/W$ (2)	
	$K_d = Q_e/C_e$ (3)		$R_L = 1/(1 + (K_L \cdot C_e))$ (4)	
	Thermodynamic			
	$\Delta G° = -R \cdot T(\ln K_d)$ (5)		$\ln K_d = (-\Delta H°/R \cdot T) + (-\Delta S°/R)$ (6)	
	Isotherms			
	Non-linear		Linear	
Langmuir	$Q_e = (Q_m \cdot K_L \cdot C_e)/(1 + K_L \cdot C_e)$	(7)	$C_e/Q_e = (1/K_L \cdot Q_m) + (C_e/Q_m)$	(8)
Freundlich	$Q_e = K_F \cdot C_e^{1/n_F}$	(9)	$\log Q_e = \log K_F + (1/n_F) \log C_e$	(10)
Temkin	$Q_e = (R \cdot T/b_T) \ln(K_T \cdot C_e)$	(11)	$Q_e = (R \cdot T/b_T) \ln K_T + (R \cdot T/b_T) \ln C_e$	(12)
Dubinin-Radushkevich (D-R)	$Q_e = Q_m^{DR} \cdot \exp(-K_{DR} \cdot \varepsilon^2)$	(13)	$\ln Q_e = \ln Q_m^{DR} - K_{DR} \cdot \varepsilon^2$	(14)
Redlich-Peterson (R-P)	$Q_e = (K_{RP} \cdot C_e)/(1 + \alpha_{RP} \cdot C_e^g)$ where $g \leq 1$	(15)	-	
Sips	$Q_e = (Q_{max}^S \cdot K_S \cdot C_e^{1/nS})/(1 + K_S \cdot C_e^{1/nS})$	(16)	-	
Koble-Corrigan (K-C)	$Q_e = (A \cdot C_e^\beta)/(1 + B \cdot C_e^\beta)$	(17)	-	
	Kinetics			
	Non-linear		Linear	
Pseudo-First order (PFO)	$Q_t = Q_e \cdot (1 - \exp(-k_1 \cdot t))$	(18)	$\log(Q_e - Q_t) = \log Q_e - (k_1 \cdot t/2.303)$	(19)
Pseudo-Second order (PSO)	$Q_t = (k_2 \cdot Q_{e,calc}^2 \cdot t)/(1 + k_2 \cdot Q_{e,calc} \cdot t)$	(20)	$(t/Q_t) = (1/k_2 \cdot Q_e^2) + (t/Q_e)$	(21)
Elovich	$Q_t = (1/\beta) \ln h \cdot \beta + (1/\beta) \ln t$	(22)	$Q_t = (1/\beta) \ln h \cdot \beta + (1/\beta) \ln t$	(23)
Intra-particle diffusion (IPD)	$Q_t = k_{IPD} \cdot t^{0.5} + C$	(24)	$Q_t = k_{IPD} \cdot t^{0.5} + C$	(25)

Nomenclature:

C₀ (mg·L^{-1}): Adsorbate initial concentration; ***Cₑ*** (mg·L^{-1}): Equilibrium concentration; ***Qₑ*** (mg·g^{-1}): Amount of adsorbate in the adsorbent at equilibrium (adsorption capacity); ***Qₜ*** (mg·g^{-1}): Amount of adsorbate in the adsorbent at any time *t*; ***Qₑ,calc*** (mg·g^{-1}): calculated amount of adsorbate in equilibrium; ***Qₘ*** (mg·g^{-1}): Maximum monolayer coverage capacities; ***Qₘ^{DR}*** (mg·g^{-1}): D-R maximum adsorption capacity; ***R_L***: Separation factor; Calculated adsorption capacity; ***K_d*** (L·g^{-1}): distribution coefficient; ***K_L*** (L·mg^{-1}): Langmuir isotherm constant; ***K_DR*** (mol^2·kJ^{-2}): Dubinin–Radushkevich isotherm constant; ***K_F*** (mg·g^{-1}): Freundlich constant related to the rate of adsorption; ***K_RP*** (L·g^{-1}); Redlich–Peterson isotherm constant; ***K_max^S*** (L·mg^{-1}): Sips isotherm model constant; ***K_T*** (L·g^{-1}): Temkin isotherm equilibrium binding constant; ***k₁*** (min^{-1}): Rate constant of the pseudo-first-order kinetic model; ***k₂*** (g·mg^{-1}·min^{-1}): Rate constant of the pseudo-first-order kinetic model; ***K_ipd*** (mg·g^{-1}·min^{-1}): ; ***α_RP*** (mg^{-1}): Redlich–Peterson isotherm constant; ***b_T*** (kJ·mol^{-1}): Temkin isotherm constant related to the heat of sorption; ***n_F***: adsorption intensity; ***n_s***: Sips isotherm model exponent; ▯▯: Adsorption intensity; ▯ : Dubinin–Radushkevich isotherm constant (▯ (Polanyi potential) is equal to $RT \ln (1 + 1/C_e)$); ***A*** (L^n·mg^{1-n}·g^{-1}): Koble–Corrigan isotherm constant; ***B*** ((L·mg^{-1})^n): Koble–Corrigan isotherm constant (L·mg^{-1})^n; ***R*** (8.314 j·K^{-1}·mol^{-1}): Universal gas constant ; ***V*** (L): Volume of the aqueous phase; ***W*** (g): Dry weight of the adsorbent; **T** (K): Temperature; **Δ*G*°** (kJ·mol^{-1}): Standard Gibbs free energy change; **Δ*H*°** (kJ·mol^{-1}): Standard enthalpy change; **Δ*S*°** (J·K^{-1}·mol^{-1}): Standard entropy change.

Table S2. Comparison of the adsorption isotherms, kinetics, and thermodynamic constants.

Thermodynamic					
$\Delta G°/(\mathrm{kJ}\cdot\mathrm{mol}^{-1})$			$\Delta H°/(\mathrm{kJ}\cdot\mathrm{mol}^{-1})$	$\Delta S°/(\mathrm{J}\cdot\mathrm{K}\cdot\mathrm{mol}^{-1})$	
293 K	313 K	333 K	-75.8570	-223.4637	
-10.670	-5.2550	-1.8150			

Isotherm					
Langmuir		R^2	$Q_\mathrm{m}/\mathrm{mg}\cdot\mathrm{g}^{-1}$	$K_\mathrm{L}/\mathrm{L}\cdot\mathrm{mg}^{-1}$	
	Nonlinear	0.9688	569.049	0.0307	
	Linear	0.9910	555.555	0.0508	
Freundlich		R^2	$K_\mathrm{F}/\mathrm{mg}\cdot\mathrm{g}^{-1}$	n_F	
	Nonlinear	0.8851	38.897	1.000	
	Linear	0.9012	56.754	2.236	
Temkin		R^2	$K_\mathrm{T}/\mathrm{L}\cdot\mathrm{g}^{-1}$	$b_\mathrm{T}/\mathrm{kJ}\cdot\mathrm{mol}^{-1}$	
	Nonlinear	0.9373	1.9172	32.5338	
	Linear	0.9321		31.7312	
D-R		R^2	$Q_\mathrm{m}^\mathrm{DR}/\mathrm{mg}\cdot\mathrm{g}^{-1}$	ε	
	Nonlinear	0.8179	449.0837	1	
	Linear	0.7779			
R-P		R^2	$K_\mathrm{RP}/\mathrm{L}\cdot\mathrm{g}^{-1}$	$\alpha_\mathrm{RP}/\mathrm{mg}^{-1}$	g
	Nonlinear	0.9798	94.884	0.8006	0.7237
Sips		R^2	$Q_\mathrm{m}^S/\mathrm{mg}\cdot\mathrm{g}^{-1}$	$K_\mathrm{S}/\mathrm{L}\cdot\mathrm{mg}^{-1}$	n_S
	Nonlinear	0.9625	569.473	7.407	2.415
K-C		R^2	A	B	β
	Nonlinear	0.9623	17.830	0.0312	1

Kinetic				
PFO		R^2	k_1/min^{-1}	
	Nonlinear	0.8855	1.9321	
	Linear	0.9932	0.0836	
PSO		R^2	$Q_\mathrm{e,calc}/mg\cdot\mathrm{g}^{-1}$	$k_2/g\cdot\mathrm{mg}^{-1}\cdot min^{-1}$
	Non-linear	0.8122	296.794	0.0511
	Linear	0.9999	294.118	0.0385
Elovich		R^2	β	h
	Nonlinear	0.7401	0.3448	2.6×10^{43}
	Linear	0.9790	0.5415	2.6×10^{68}
IPD		R^2	K_IPD/ L·g^{-1}	C
	Non-linear	0.9505	0.9563	290.45
	Linear 1 (y_1)	0.9956	1.3082	289.49
	Linear 2(y_2)	0.9486	0.2121	295.37

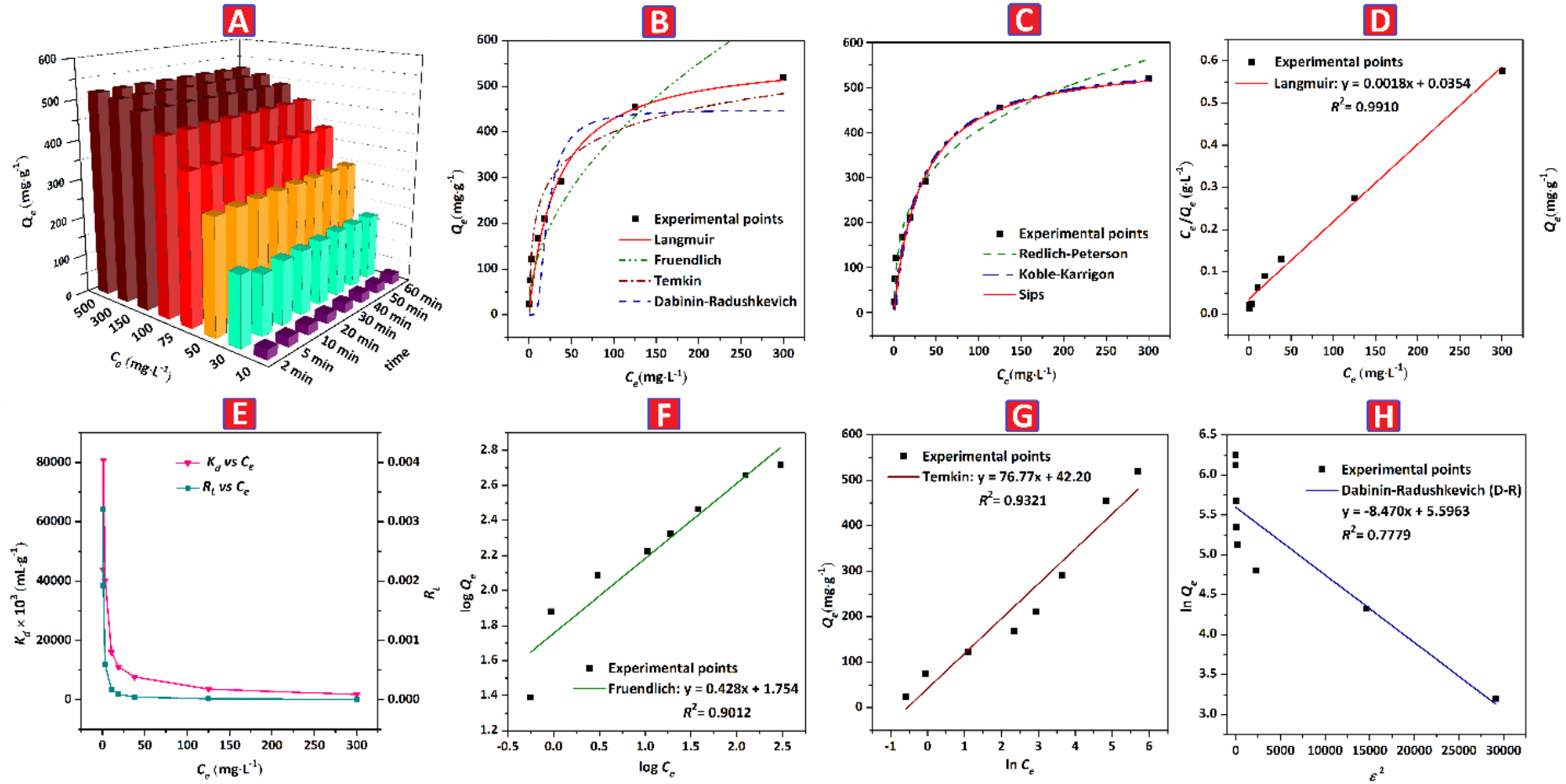

Figure S1. (A) Time-concentration profile for the MB adsorption onto the RS-3. (B) The Langmuir, Freundlich, Temkin, D-R and (C) R-P, K-C and Sips isotherms plots in the non-linear regression analysis. (D) The Langmuir, (F) Freundlich, (G) Temkin, and (H) D-R isotherms plots in the linear regression analysis. (E) the values of R_L and K_d.

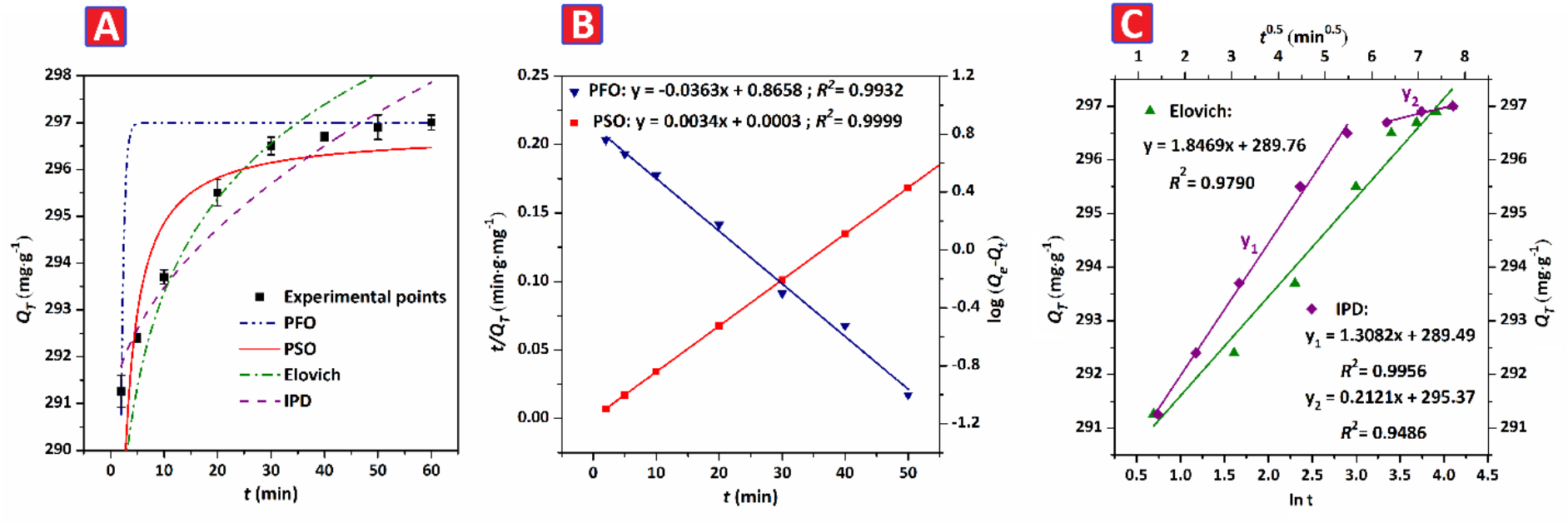

Figure S2. (A) The PFO, PSO, Elovich, and IPD kinetics plots in the non-linear regression analysis. (B) The PFO, PSO, (C) Elovich, and IPD kinetics plots in the linear regression analysis.