Electronic Supplementary Material (ESI) for RSC Advances.

Fabrication of hydrochar functionalized Fe-Mn binary oxide nanocomposites: characterization and 17β-estradiol removal

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Thermodynamic studies

The thermodynamic parameters, such as standard free-energy change ($\Delta G°$), standard enthalpy change ($\Delta H°$) and standard entropy change ($\Delta S°$), were provided from a change in temperature according to following equations:

$$\Delta G^{o} = -\mathrm{R}T \ln K^{o} \quad (1)$$

$$\ln K^{o} = \frac{\Delta S^{o}}{\mathrm{R}} - \frac{\Delta H^{o}}{\mathrm{R}T} \quad (2)$$

where R (8.314 J/mol K) is universal gas constant and T (K) is the solution temperature. K^{o} is the adsorption equilibrium constant, calculated by plotting $\ln K_d$ ($K_d = q_e/C_e$) versus C_e and extrapolating C_e to zero.

The thermodynamic parameters calculated at the data of Fig. S2 on the basis of above equations are exhibited in Table S2. As seen, $\Delta G°$ values were negative at all temperatures and decreased with decreasing temperature. It revealed that the adsorption process was spontaneous; besides, the lower temperature was favorable to the E2 adsorption onto hydrochar-FMBO. $\Delta H°$ value was also negative, suggesting that the adsorption process was exothermic. It was the explanation for the decrease in adsorption at higher temperature. In addition, the negative values of $\Delta S°$ indicated the decrease in the degree of freedom at the solid–liquid interface was due to the immobilization of E2 on the surface of hydrochar-FMBO. Generally, the negative values of $\Delta G°$, $\Delta H°$ and $\Delta S°$ demonstrated that the removal process was an enthalpy-driven.

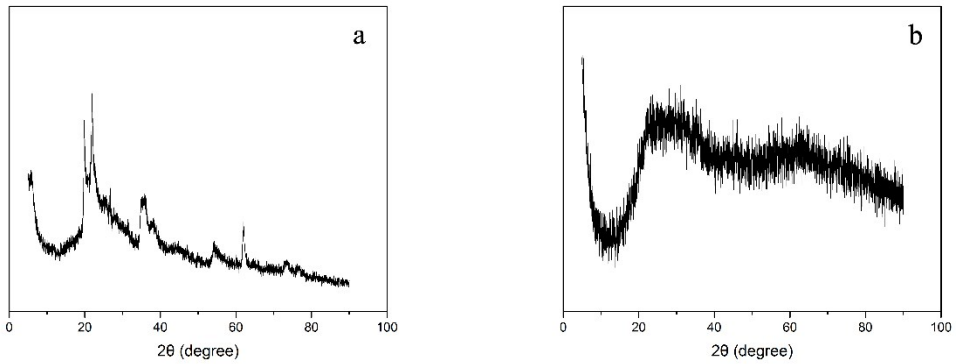

Fig. S1 XRD patterns for hydrochar (a) and hydrochar-FMBO (b).

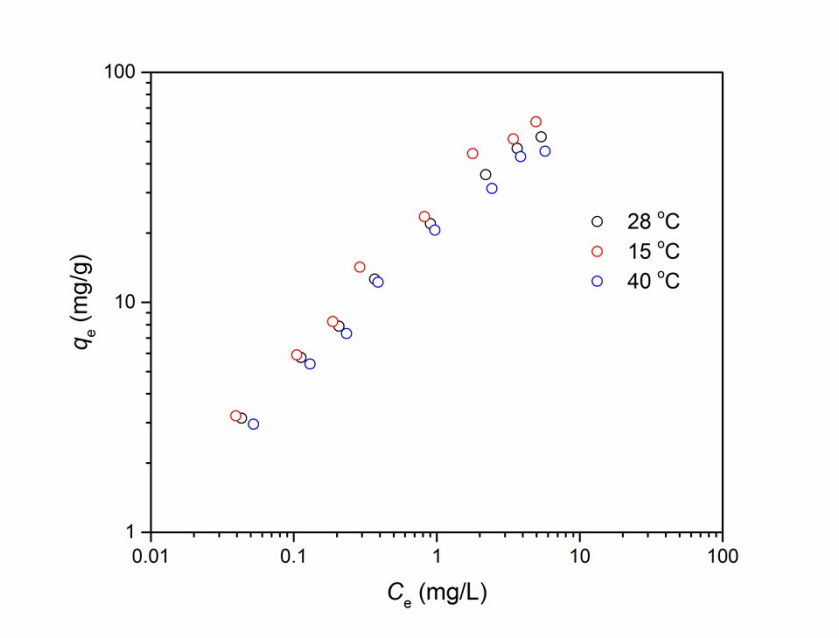

Fig. S2 Adsorption isotherms of E2 onto hydrochar-FMBO at three different temperatures.

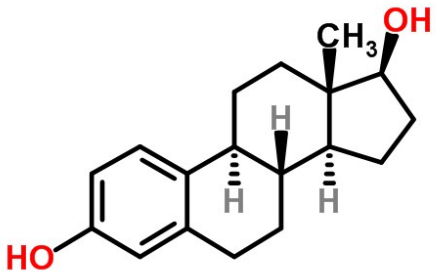

Fig. S3. Molecular structure of E2 (obtained from ChemSpider: http://www.chemspider.com).

Table S1 Parameters calculated from intra-particle diffusion model for E2 adsorption onto hydrochar-FMBO.

C_o (mg/L)	k_{d1} (mg/g min$^{0.5}$)	L_1	R^2	k_{d2} (mg/g min$^{0.5}$)	L_2	R^2
6	2.11	7.18	0.971	0.22	38.74	0.964
0.8	0.43	0.97	0.894	0.06	7.10	0.970

Table S2 Thermodynamic parameters of E2 adsorption onto hydrochar-FMBO.

T (K)	ΔG^0 (kJ/mol)	ΔS^0 (J/K mol)	ΔH^0 (kJ/mol)
288.15	-0.95		
301.15	-0.96	-3.58	-1.06
313.15	-0.94		