

Supporting Information

Glucose-assisted synthesis of magnetic monohydroxy aluminium oxide @carbon (γ -AlOOH/Fe₃O₄@C) nanocomposite as an innovative sorbent for extraction and pre-concentration of deferasirox from plasma and urine samples

Payam Arabkhani ^a , Negar Sadegh, ^b, Mahmoud Shahamat ^a, Arash Asfaram ^{*a}

^a *Medicinal Plants Research Center, Yasuj University of Medical Sciences, Yasuj, Iran*

^b *Department of Chemistry, Faculty of Sciences, Shahrekord University, P.O. Box 115, Shahrekord, Iran.*

* Corresponding authors: E-mail address:
arash.asfaram@yums.ac.ir (A. Asfaram)

Table S1. Design matrix for the CCD.

Independent variables	Unit	Levels ($\alpha = 2$)				
		$-\alpha$	Low (-1)	Center (0)	High (+1)	$+\alpha$
(X ₁) pH	-	3.0	4.5	6.0	7.0	9.0
(X ₂) Sorbent mass	mg	4.0	6.0	8.0	10	12
(X ₃) Ultrasound time	min	3.0	6.0	9.0	12	15
(X ₄) Eluent volume	mL	0.050	0.125	0.200	0.275	0.350
Run	Independent variables				ER% DEX	
	X ₁	X ₂	X ₃	X ₄		
1	6.0	8.0	9.0	0.050	46.63	
2	6.0	4.0	9.0	0.200	63.39	
3	7.5	6.0	12	0.125	72.33	
4	7.5	10	12	0.275	90.54	
5	7.5	6.0	6.0	0.275	75.52	
6	7.5	10	12	0.125	86.52	
7	7.5	6.0	6.0	0.125	50.24	
8	4.5	10	6.0	0.275	77.13	
9	4.5	6.0	6.0	0.275	62.38	
10	6.0	8.0	9.0	0.200	86.12	
11	6.0	12	9.0	0.200	99.56	
12	4.5	10	12	0.275	84.41	
13	6.0	8.0	9.0	0.200	85.30	
14	6.0	8.0	3.0	0.200	64.99	
15	4.5	10	6.0	0.125	57.57	
16	7.5	10	6.0	0.275	85.47	
17	6.0	8.0	9.0	0.350	76.13	
18	7.5	10	6.0	0.125	74.25	
19	6.0	8.0	9.0	0.200	84.24	
20	6.0	8.0	9.0	0.200	82.69	
21	6.0	8.0	9.0	0.200	87.08	
22	6.0	8.0	9.0	0.200	86.61	
23	9.0	8.0	9.0	0.200	55.50	
24	3.0	8.0	9.0	0.200	33.72	
25	4.5	6.0	12	0.125	51.41	
26	4.5	10	12	0.125	79.52	
27	4.5	6.0	12	0.275	71.18	
28	4.5	6.0	6.0	0.125	32.52	
29	7.5	6.0	12	0.275	78.11	
30	6.0	8.0	15	0.200	94.14	

Table S2. Analysis of variance (ANOVA) for UA-DSPME of DFX.

Source	SS	DF	MS	F-value	P-value	
Model	8498	14	607	69.03	< 0.0001	
X ₁	821.6	1	822	93.43	< 0.0001	
X ₂	1909	1	1909	217.1	< 0.0001	
X ₃	1030	1	1030	117.2	< 0.0001	
X ₄	1341	1	1341	152.5	< 0.0001	
X ₁ X ₂	26.42	1	26.42	3.005	0.1035	
X ₁ X ₃	13.88	1	13.88	1.578	0.2283	
X ₁ X ₄	48.23	1	48.23	5.485	0.0334	
X ₂ X ₃	2.102	1	2.102	0.239	0.6319	
X ₂ X ₄	105.1	1	105.1	11.95	0.0035	
X ₃ X ₄	165.5	1	165.5	18.82	0.0006	
X ₁ ²	2500	1	2500	284.3	< 0.0001	
X ₂ ²	3.006	1	3.006	0.342	0.5675	
X ₃ ²	17.93	1	17.93	2.039	0.1738	
X ₄ ²	786.5	1	786.5	89.44	< 0.0001	
Residual	131.9	15	8.793			
Lack of Fit	118.4	10	11.84	4.391	0.0581	
Pure Error	13.48	5	2.697			
Corr. Total	8630	29				
Model Summary Statistics						
Response	Std. Dev.	CV %	R²	Adjusted-R²	Predicted-R²	Adeq Precision
ER%	2.965	4.090	0.9847	0.9705	0.9187	34.07

SS: Sum of squares

DF: Degree of freedom

MS: Mean square

Table S3. Analytical parameters of established UA-DSPME/HPLC–UV method for DFX in real samples.

Quantitative analysis	Values
Sample volume (mL)	15
Elution solvent (mL)	0.2
Linear range (ng mL ⁻¹)	10-3500
Coefficients of determination (R ²)	0.9938
Limit of detections (LOD) (ng mL ⁻¹)	0.163
limit of quantification (LOQ) (ng mL ⁻¹)	5.421
Preconcentration factor	75
Enrichment factor	128.85
Precision (RSD, %)	2.09-5.22

Table S4. Sorption isotherm parameters of DFX by γ -AlOOH/Fe₃O₄@C in various isotherm models.

Isotherm	Plot	Parameters	Value
Langmuir $\frac{C_e}{q_e} = \frac{1}{Q_m k_L} + \frac{C_e}{Q_m}$	C_e/q_e vs. C_e	Q_m (mg g ⁻¹)	40.28
		K_L (L mg ⁻¹)	1.519
		R^2	0.996
		$R_L=1/(1+(K_L \times C_0))$	0.013-0.568
Freundlich $\ln q_e = \ln K_F + \frac{1}{n} \ln C_e$	$\ln q_e$ vs. $\ln C_e$	1/n	0.467
		K_F (L mg ⁻¹)	3.257
		R^2	0.975

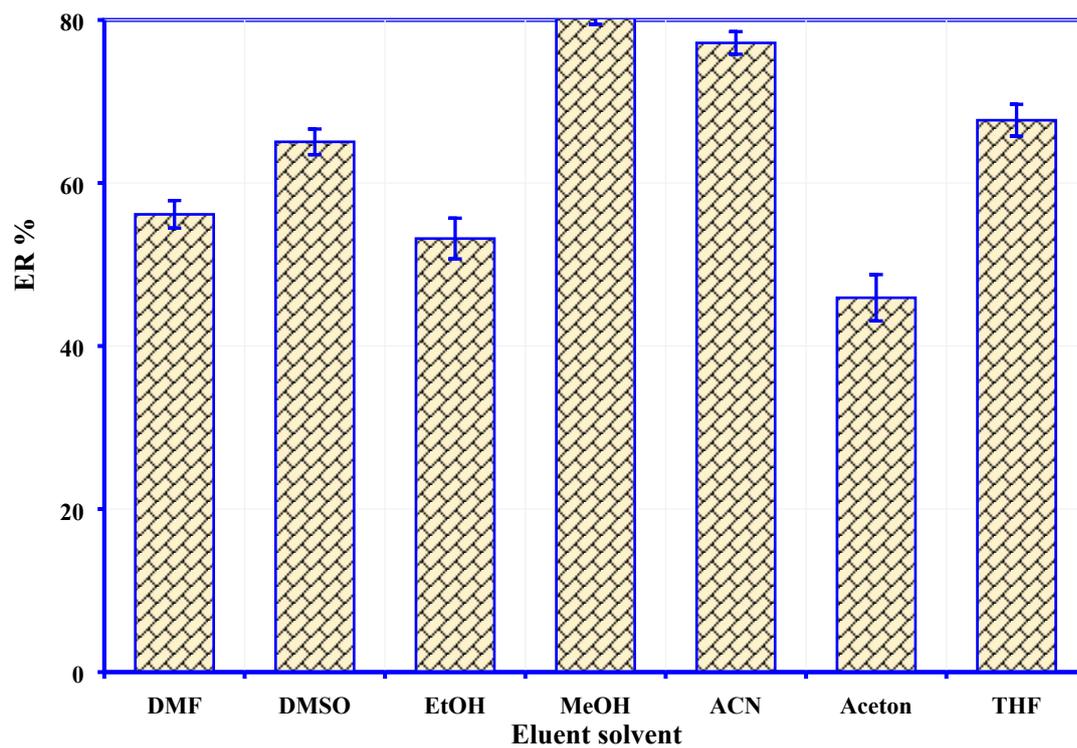


Fig. S1. Eluents types effect to extraction recovery (ER%) of DFX by γ -AlOOH/Fe₃O₄@C.

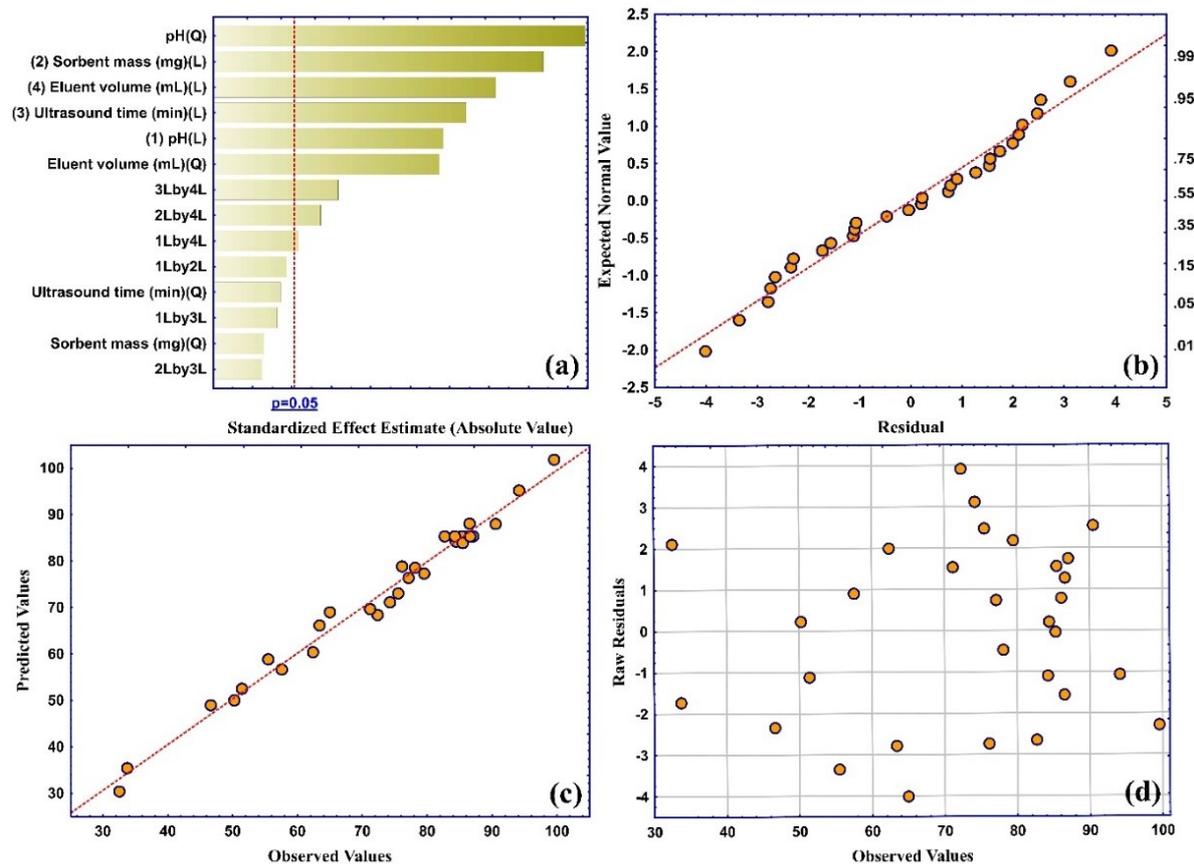


Fig. S2. (a) Pareto chart of standardized effects for variables ($p:0.05$), (b) normal plot of residuals, (c) observed versus predicted plot, and (d) observed values versus raw residuals for the ER% of DFX in predicted model.

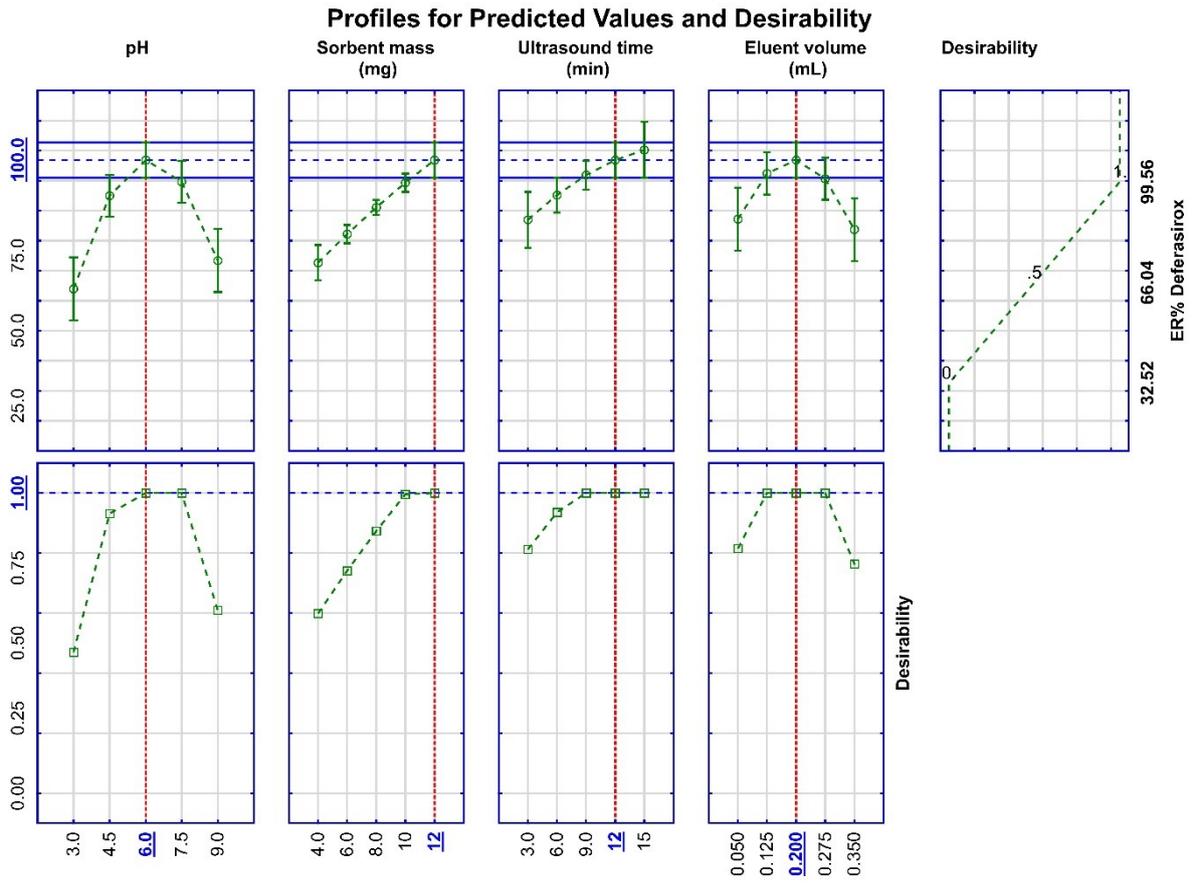


Fig. S3. Profile of predicted values of independent variables along with desirability. The dotted red line indicates the optimal value of each variable.

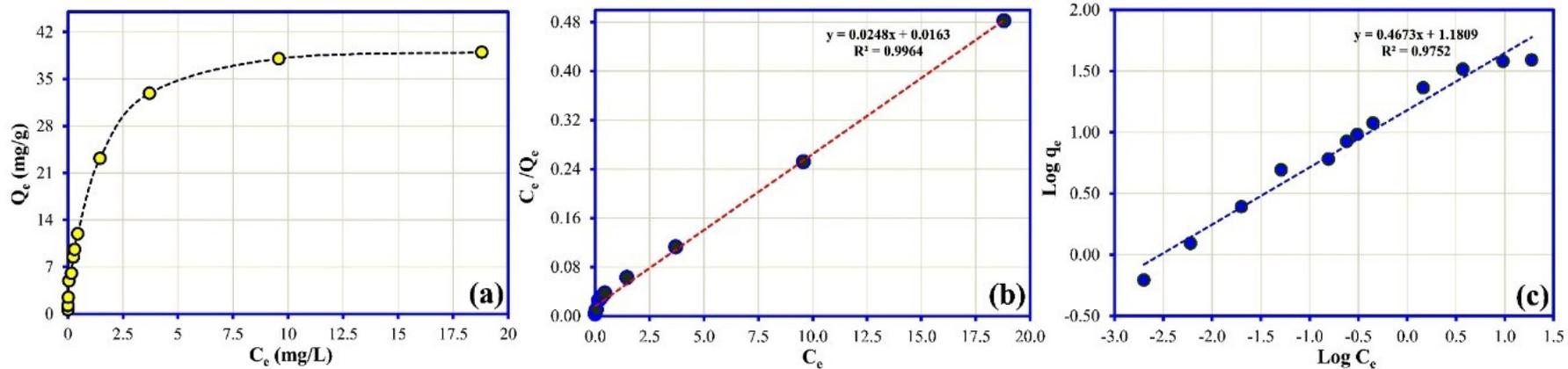


Figure S4. Linear fits of the sorption of DFX for (a) experimental, (b) Langmuir, and (c) Freundlich isotherm models.

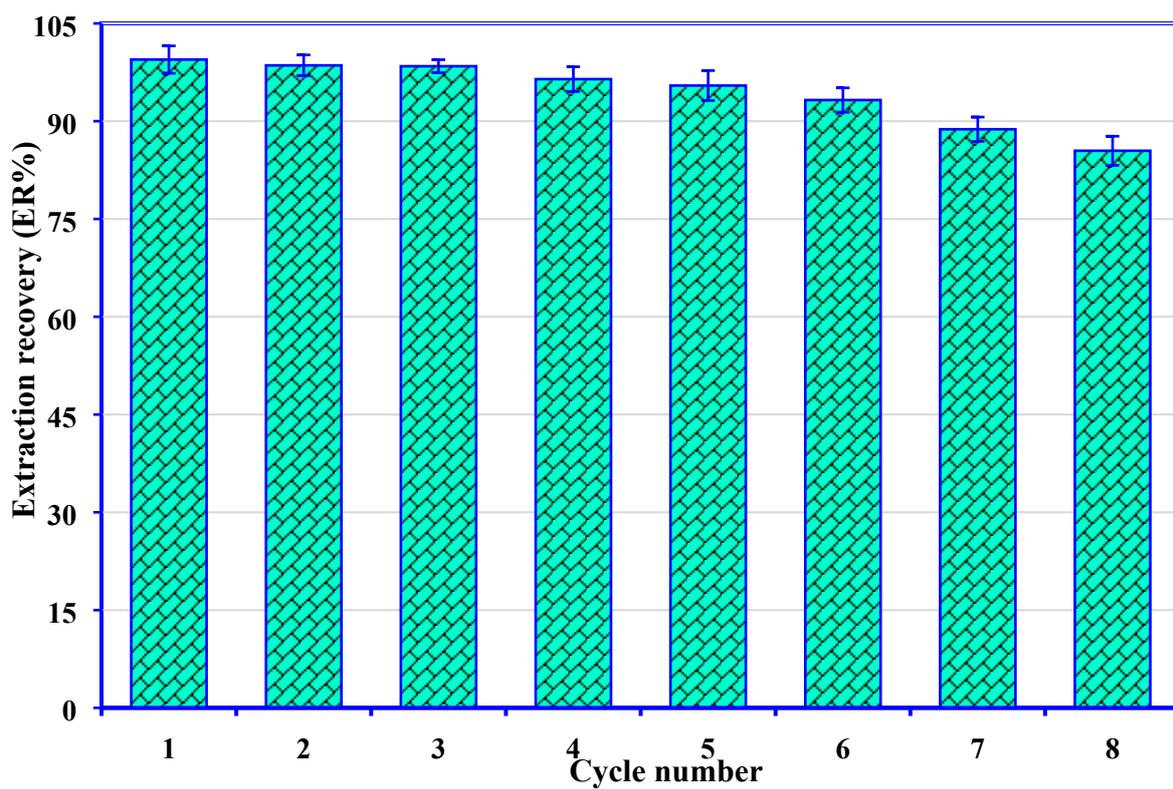


Fig. S5. Extraction recovery of DFX by γ -AlOOH/Fe₃O₄@C in reusability test.