

SUPPORTING INFORMATION

Regularities of encapsulation of tolfenamic acid and some other non-steroidal anti-inflammatory drugs in metal organic frameworks based on γ -cyclodextrin

Ekaterina Delyagina ^{a,*}, Anna Garibyan ^b, Mikhail Agafonov ^b, Irina Terekhova ^b

^a*Institute of Mathematics, Information Technology and Natural Sciences, Ivanovo State University*

^b*G.A. Krestov Institute of Solution Chemistry of RAS*

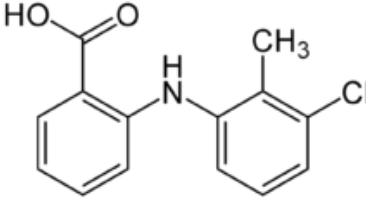
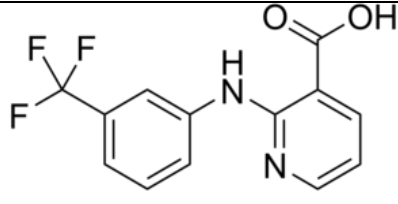
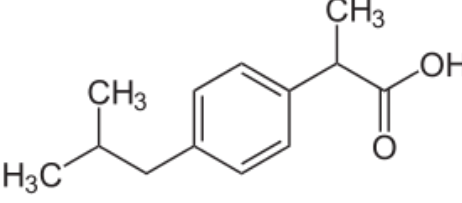
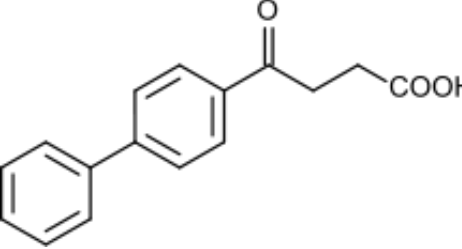
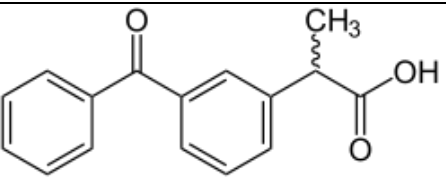
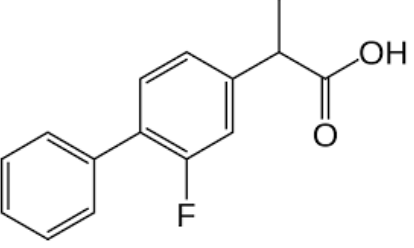
Table S1. Models for adsorption isotherms

Model	Equation	R ²
Langmuir	$\frac{1}{Q_e} = \frac{1}{Q_m \cdot b} + \frac{1}{C_e}$ <p>where Q_e (mg·g⁻¹) - is the amount of TA that can be absorbed by a unit mass of the adsorbent at equilibrium; C_e (mg·L⁻¹) – is the concentration of TA in solution at equilibrium; Q_m – is the maximum adsorption capacity (mg·L⁻¹); b (L·mg⁻¹) – is the Langmuir constant, which is related to the affinity between the adsorbent and adsorbate.</p>	0.020
Freindlich	$\log Q_e = \log k_F + \frac{1}{n} \log C_e$ <p>where k_F ((mg/g)/(mg/L)^{1/n}) – is the constant related to the sorption capacity of the adsorbent, indicative of the affinity between the species; n is the constant related to the sorption intensity.</p>	0.454
Temkin	$Q_e = \frac{RT}{b_T} \ln K_T + \frac{RT}{b_T} \ln C_e$ <p>where b_T – is the Temkin constant related to the heat of adsorption (J·mol⁻¹); K_T – is the Temkin isotherm equilibrium binding constant (L·g⁻¹); R – is the gas constant (8.314 J·mol⁻¹·K⁻¹); T – is the temperature (K).</p>	0.961

Table S2. Kinetic models of drug release

Model	Equation	R ²	
		γ CD-MOF/TA-1	γ CD-MOF/TA-2
Zero order	$C = K_0t$ K ₀ is zero order rate constant, t is the time	0.462	0.429
First order	$\log C_t = \log C_0 - k_1t/2.303$ C _t is amount of drug released in t time; C ₀ is the initial amount of drug	0.412	0.355
Hixson-Crowell	$Q_0^{1/3} - Q_t^{1/3} = K_{HC}t$ Q ₀ is the initial amount of drug; Q _t is the amount of drug remained after t time; K _{HC} is Hixson-Crowell dissolution rate constant	0.462	0.380
Korsemeyer -Peppas	$\log(M_t/M_\infty) = \log k + n \log t$ k is dissolution rate constant; n is release exponent; M _t /M _∞ is the drug release fraction in the media	0.979 (n=0.46)	0.925 (n=0.43)

Table S3. Summary of NSAIDs loaded in γ CD-MOF by impregnation in ethanol and lipophilicity coefficients of NSAIDs

Name	Structural formula	Loaded amount (wt.%)	logP*
Tolfenamic acid (TA)		7	5.17
Niflumic acid (NA)		1.4 [30]	4.43
Ibuprofen (IBU)		12 [24]	3.97
Fenbufen (FEN)		16.4 [26]	3.2
Ketoprofen (KET)		14 [27]	3.12
Flurbiprofen (FLU)		12 [28]	4.16

* - pubchem.ncbi.nlm.nih.gov.

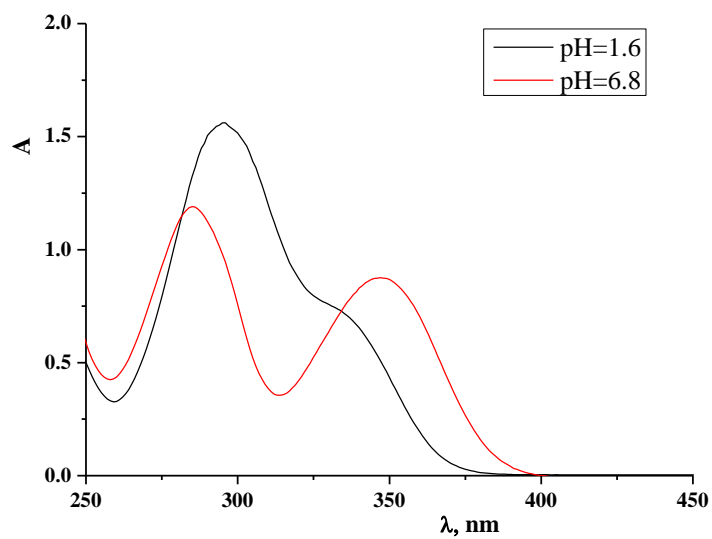


Figure S1. UV/vis spectra of TA in different buffers

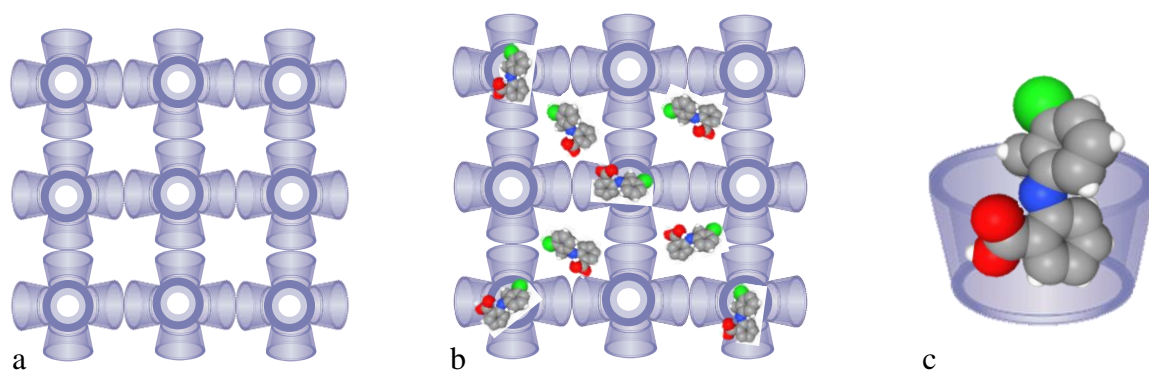


Figure S2. Schematic representation of γ CD-MOF (a), γ CD-MOF/TA (b) and inclusion complex γ -CD/TA (c).

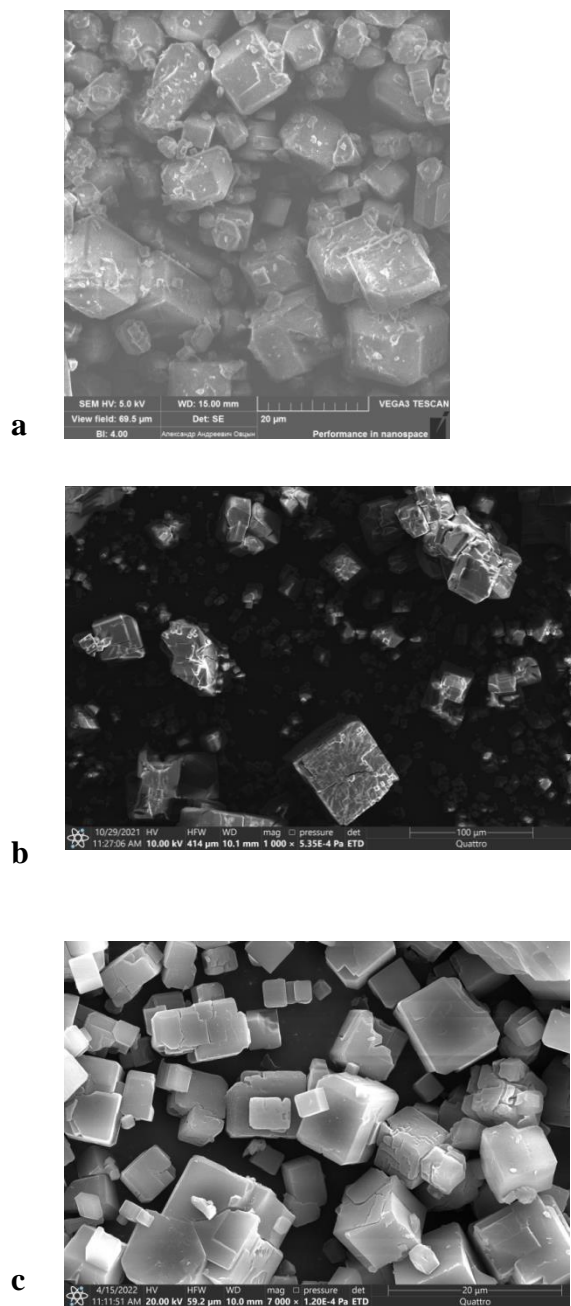


Figure S3. SEM images of γ CD-MOF (a), γ CD-MOF/TA-1 (b) and γ CD-MOF/TA-2 (c).

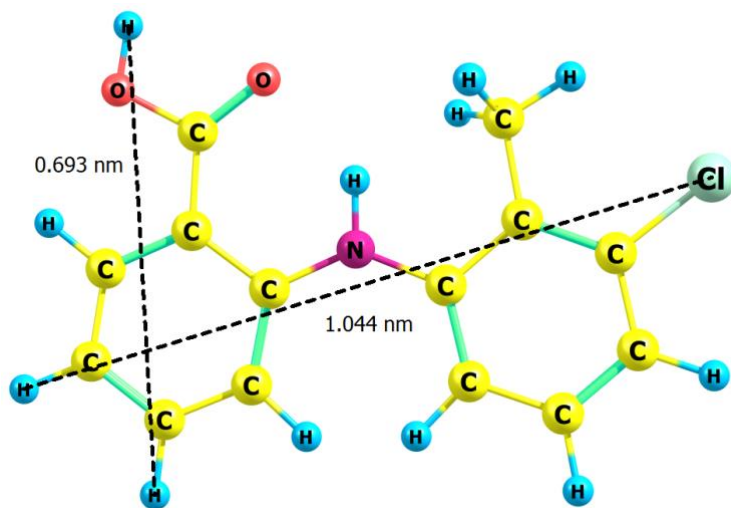


Figure S4. Geometric dimensions of TA.