Tuning Crystal Structures of Iron-Based Metal-Organic Frameworks for Drug Delivery Applications

Hao Pham,[1] Kimberly Ramos,[2] Andy Sua,[3] Jessica Acuna,[3] Katarzyna Slowinska,[3] Travis Nguyen,[3] Angela Bui,[3] Mark D. R. Weber[3] and Fangyuan Tian[3]*

1. Department of Physical Sciences, Long Beach City College, Long Beach, CA 90808

2. Chemistry Department, Cerritos College, Norwalk, CA 90650

3. Department of Chemistry and Biochemistry, California State University Long Beach, Long Beach, CA 90840

Supporting Information

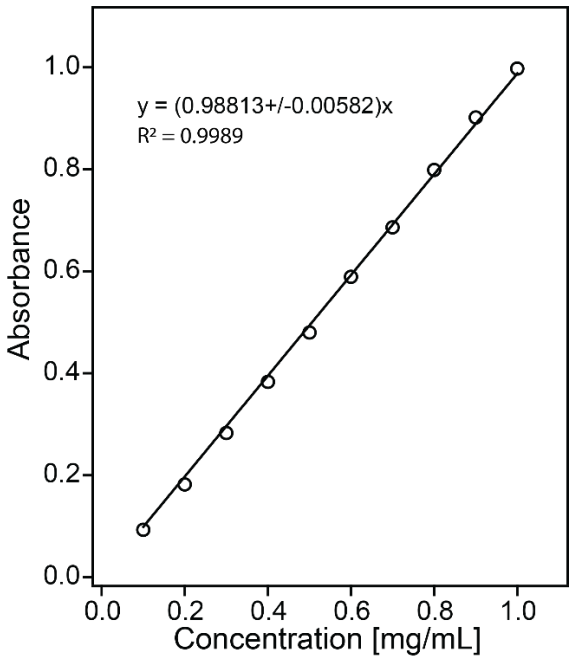


Figure S1. Absorbance of ibuprofen at 264 nm corresponding to increasing concentrations in hexane. Data were collected using a Shimadzu UV-Vis photospectrometer. The standard curve was used to evaluate ibuprofen concentration changes after being adsorbed by MIL materials.

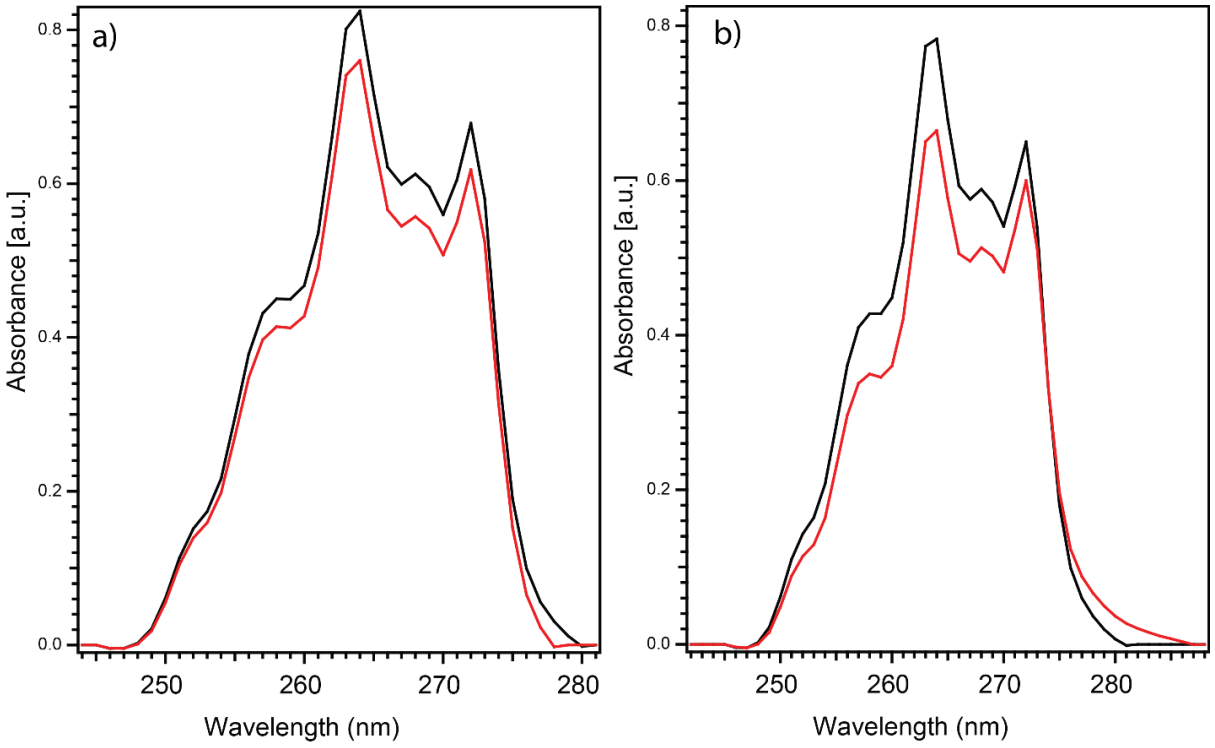


Figure S2. Absorbance of ibuprofen in hexane before (black) and after (red) being adsorbed by MIL-88B (a) and MIL-53 (b) materials. The ibuprofen solution was diluted before measurements.

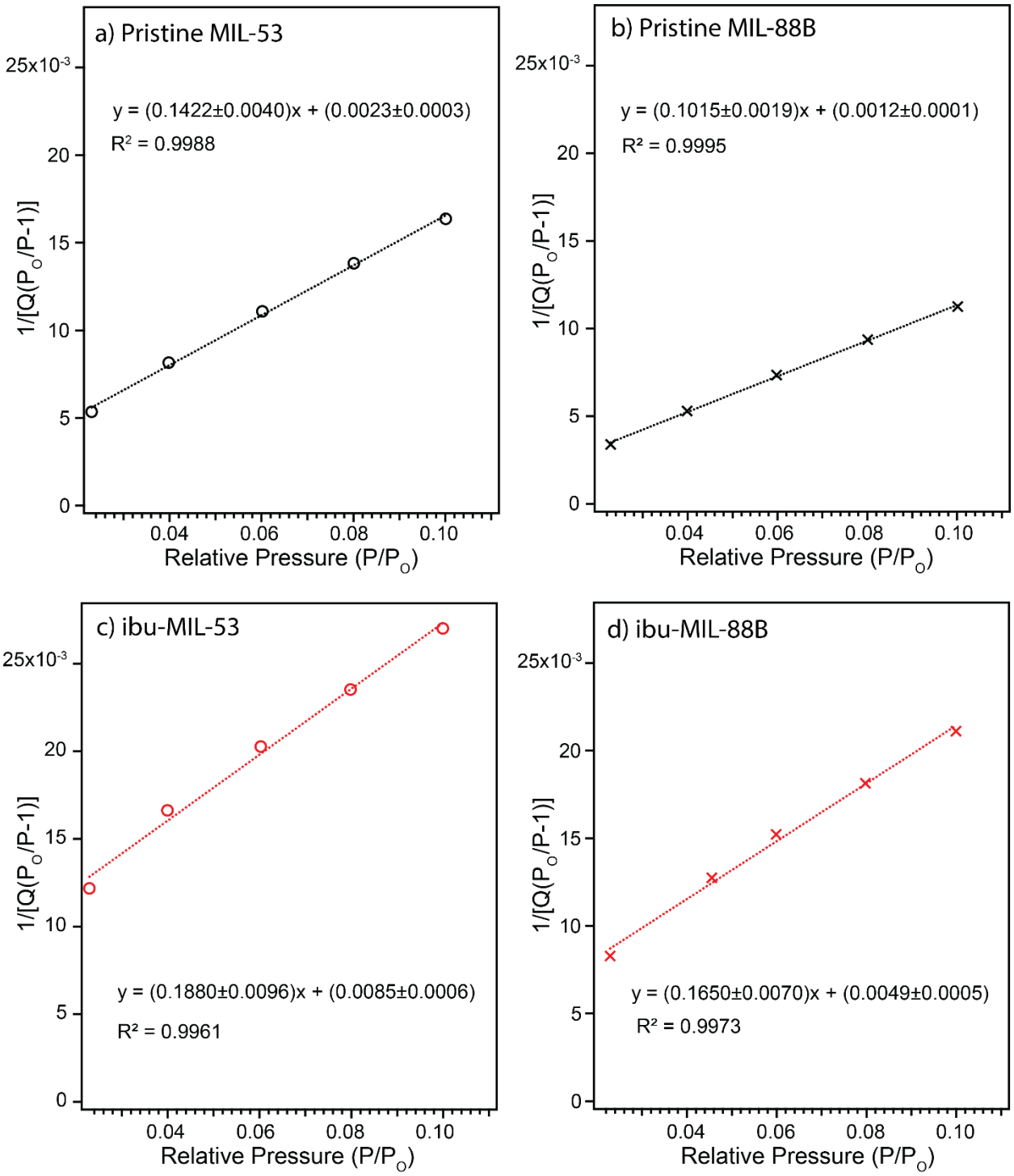


Figure S3. BET plots of a) MIL-53 (circle) and b) MIL-88B (cross) before (black) and after (red) ibuprofen loading based on nitrogen adsorption isotherms at 77 K.

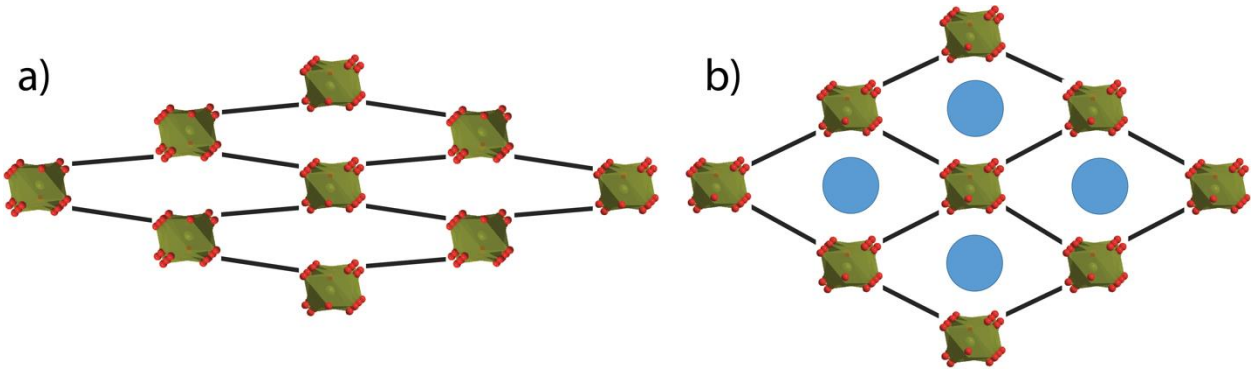
Table S1. Summary of BET parameters and SSA of MIL-53 and MIL-88B with and without ibuprofen

Sample	*C*	*V_m (cm^3/g, STP)*	*SSA (m^2/g)*
MIL-53	62.26	6.92	30.11±0.83
ibu-MIL-53	23.06	5.09	22.15±1.09
MIL-88B	86.66	9.74	42.39±0.77
ibu-MIL-88B	34.46	5.88	25.61±1.06

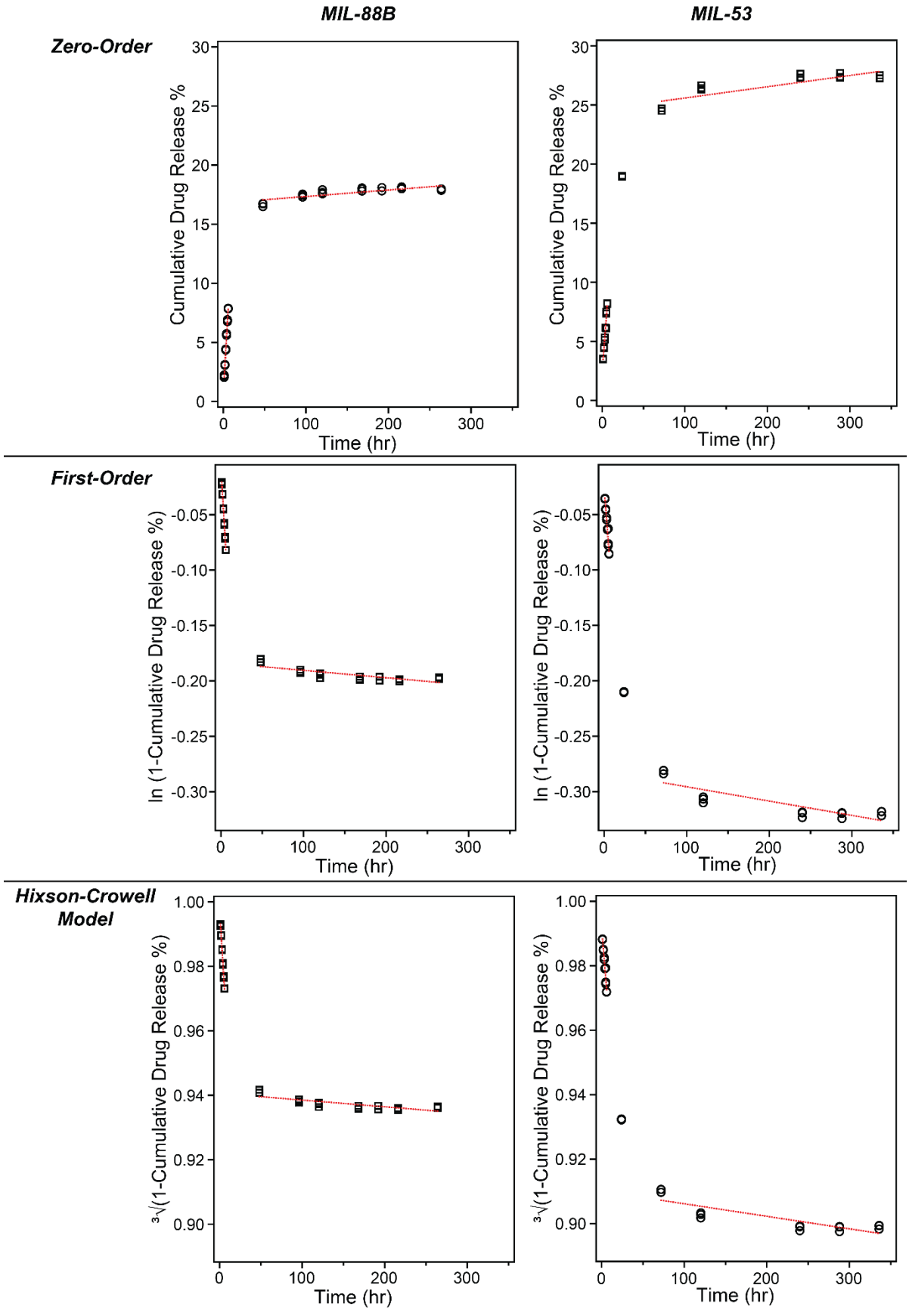
Note:

1. C is the BET constant, describing the difference in heat of adsorption between the multilayer and the first layer formation.
2. Based on the BET equation, C = 1 + slope/y-intercept; V_m = 1/(slope+y-intercept). Both slope and y-intercept were determined by BET plots shown in Fig. R1.
3. SSA was calculated based on Eq. S1.

$$SSA = \frac{V_m N_A}{V_g} A_0 \qquad \text{Eq. S1}$$



Scheme S1. Illustrative scheme of MIL-53 (Fe) with a) closed channels and b) expanded framework with guest molecules.


MIL-88B
MIL-53
Zero-Order
First-Order
Hixson-Crowell Model
Cumulative Drug Release %
ln (1-Cumulative Drug Release %)
∛(1-Cumulative Drug Release %)
Time (hr)

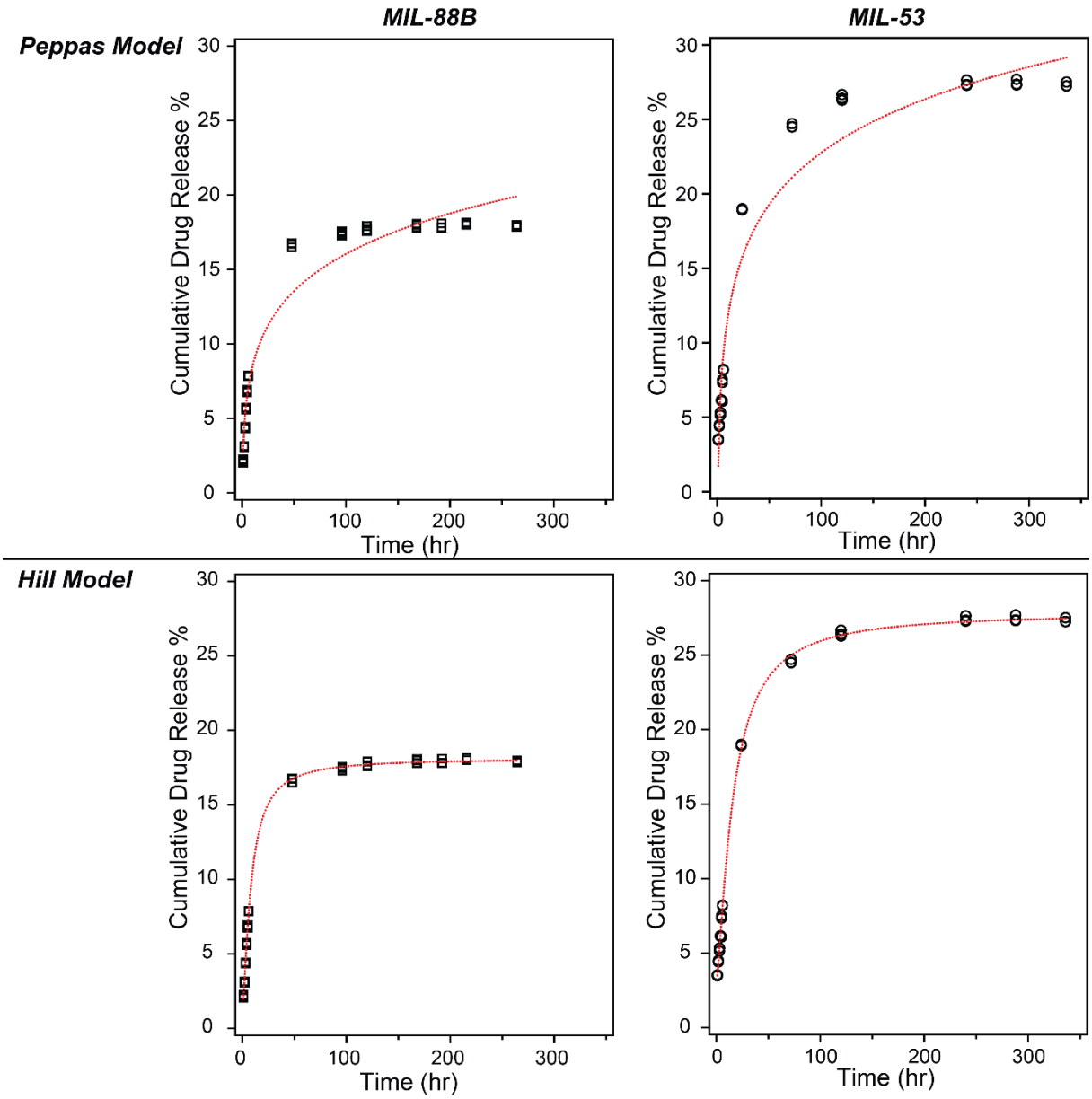


Figure S4. Drug release profiles of ibuprofen as a function of soaking time in PBS for MIL-88B and MIL-53. The data were fitted to different math models based on Eq. 2 to 6. Fitting paramethers and correlation coefficients are listed in Table S2.

Table S2. Summary of drug eluation models and their fitting correlation coefficients.

Model		MIL-88B	R^2	MIL-53	R^2
Zero-Order	Stage 1	$y = 1.1738x + 0.8909$	0.9973	$y = 0.9909x + 2.5701$	0.9684
	Stage 2	$y = 0.0055x + 16.791$	0.6651	$y = 0.0095x + 24.633$	0.7354
First-Order	Stage 1	$y = -0.0124x - 0.0083$	0.9974	$y = -0.0097x - 0.0256$	0.9672
	Stage 2	$y = -7E-05x - 0.1838$	0.6657	$y = -0.0001x - 0.2827$	0.7376
Hixson-Crowell	Stage 1	$y = -0.004x + 0.9972$	0.9974	$y = -0.0032 + 0.9915$	0.9676
	Stage 2	$y = -2E-05x + 0.9406$	0.6655	$y = -4E-05x + 0.9101$	0.7369
Peppas		$y = 3.0456x^{0.3576}$	0.9243	$y = 3.8365x^{0.3768}$	0.9498
Hill		$y = 1.1443 + 16.9707 \Big/ \left[1 + \left(\frac{8.2915}{x}\right)^{1.3811}\right]$	0.9994	$y = 2.9373 + 24.9117 \Big/ \left[1 + \left(\frac{16.022}{x}\right)^{1.3599}\right]$	0.9989