Supplementary Material: Removal of Salicylic and Ibuprofen by Hexadecyltrimethylammonium-Modified Montmorillonite and Zeolite

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Table S1. Physicochemical properties of raw clays.

Parameter	Montmorillonite	Zeolite
CEC (meq/100 g)	75.3	132.5
BET surface area (A_{BET}, m^2/g)	125.7	53.69
Pore size (Å)	19.07	76.25
pH_{PZC}	3.2	4.8

Calculation of Antibiotic Speciation

The neutral (α) and anionic (α^-) fractions of the antibiotics were estimated using Equations (S1)–(S2) [1]:

$$\alpha = \frac{1}{1+10^{(pK_a - pH)}} \quad \text{(S1)}$$

$$\alpha^- = 1 - \frac{1}{1+10^{(pK_a - pH)}} \quad \text{(S2)}$$

where α and α^- represent the fractions of the neutral and anionic species. The pK_a is the logarithmic dissociation constant.

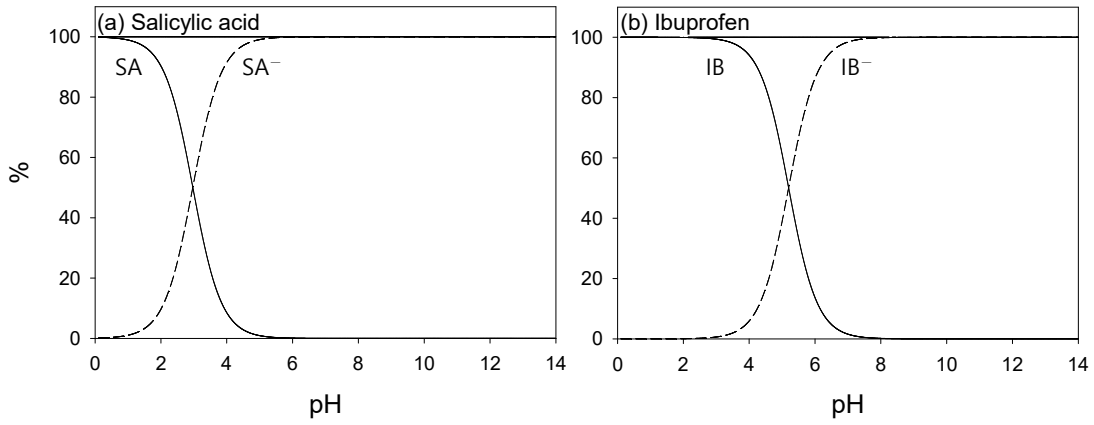

Figure S1. Distribution of speciation of (**a**) SA and (**b**) IB as a function of pH.

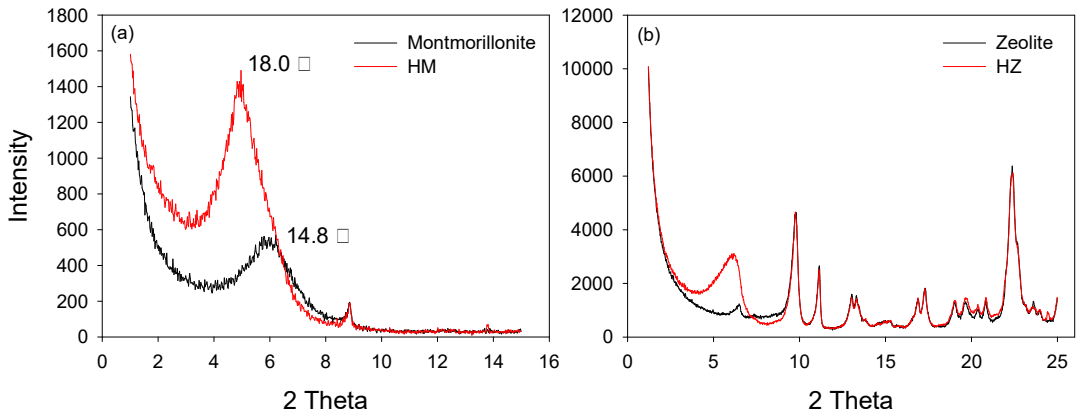

Figure S2. XRD patterns of (**a**) montmorillonite and HM; (**b**) zeolite and HZ.

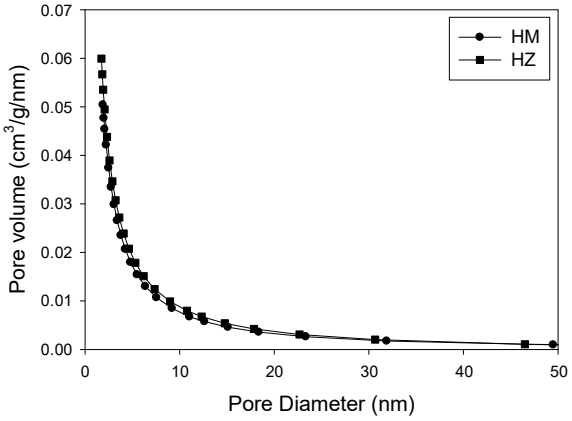

Figure S3. DFT pore size distribution of organoclays.

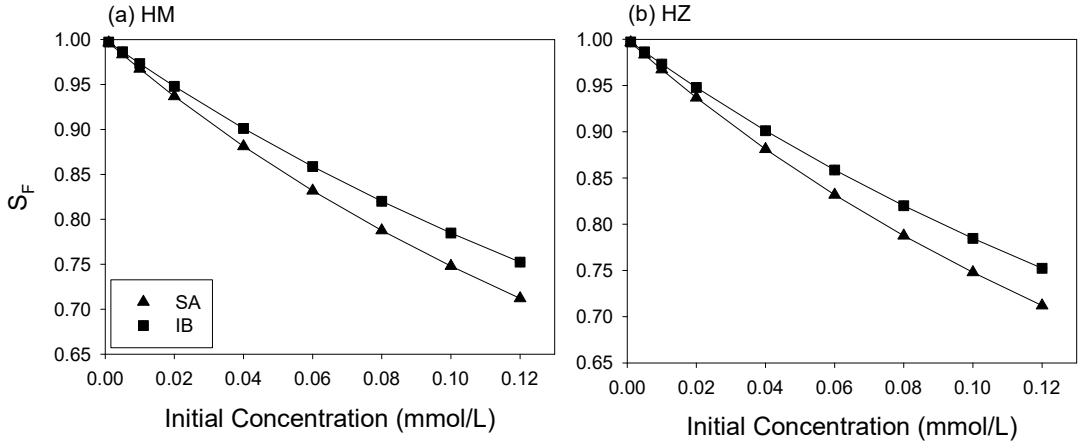

Figure S4. S_F as a function of initial concentration.

Calculation of Selectivity in Binary Sorption

The selectivity of pharmaceuticals in binary sorption system was calculated at $C_{initial}$ = 0.05 mM using Equations (S3)−(S4) as shown in Table S2.

$$\text{Selectivity of SA} = K_{d,SA}/K_{d,IB} \quad \text{(S3)}$$

$$\text{Selectivity of IB} = K_{d,IB}/K_{d,SA} \quad \text{(S4)}$$

Table S2. Selectivity of pharmaceuticals in binary sorption.

Sorbents	$\mathbf{K_{d,SA}/K_{d,IB}}$	$\mathbf{K_{d,IB}/K_{d,SA}}$
HM	0.78	1.28
HZ	0.49	2.10

References

1. Schwarzenbach, R.P.; Gschwend, P.M.; Imboden, D.M. *Environmental Organic Chemistry*, 2nd ed.; John Wiley & Sons Inc.: New York, NY, USA, 2003. pp. 246–256.