

Supplementary Information

Solketal Removal from Aqueous Solutions Using Activated Carbon and a Metal–Organic Framework as Adsorbents

Leticia Santamaría, Sophia A. Korili and Antonio Gil *

INAMAT², Departamento de Ciencias, Universidad Pública de Navarra, Campus de Arrosadía, 31006 Pamplona, Spain; leticia.santamaria@unavarra.es (L.S.); sofia.korili@unavarra.es (S.A.K.)

* Correspondence: andoni@unavarra.es; Tel.: +34-948-169-602

Table S1. Pseudo-first and pseudo-second-order parameters for the adsorption of organic molecules by the activated carbon.

Sample		Pseudo-First Order					Pseudo-Second Order					
		10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³	10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³	
		20 mg	20 mg	20 mg	10 mg	30 mg	20 mg	20 mg	20 mg	10 mg	30 mg	
Diclofenac	k_1 (1/min)	0.041	0.036	0.051	0.034	0.042	k_2 (1/min)	8.73×10^{-4}	6.48×10^{-4}	8.45×10^{-4}	5.43×10^{-4}	8.29×10^{-4}
	χ^2	1836	2044	3388	1372	2436	χ^2	439	823	815	1128	520
	R	0.95	0.96	0.93	0.93	0.93	R	0.99	0.99	0.98	0.98	0.99
Caffeine	k_1 (1/min)	0.098	0.108	0.117	0.072	0.079	k_2 (1/min)	2.68×10^{-3}	2.10×10^{-3}	2.12×10^{-3}	9.61E-4	1.69×10^{-3}
	χ^2	319	943	1646	1096	1470	χ^2	216	101	199	533	240
	R	0.98	0.97	0.95	0.99	0.94	R	0.99	0.997	0.995	0.994	0.991
		50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³						
		1.5 g	1.5 g	1.5 g	1 g	2 g	1.5 g	1.5 g	1.5 g	1 g	2 g	
Solketal	k_1 (1/min)	0.072	0.089	0.092	0.060	0.12	k_2 (1/min)	0.027	0.027	0.024	0.014	0.054
	χ^2	4	3.7	5.8	6	1.75	χ^2	0.52	0.40	0.87	0.97	0.18
	R	0.95	0.97	0.97	0.97	0.96	R	0.993	0.997	0.995	0.996	0.996

Table S2. Pseudo-first and pseudo-second-order parameters for the adsorption of organic molecules by the metal organic framework.

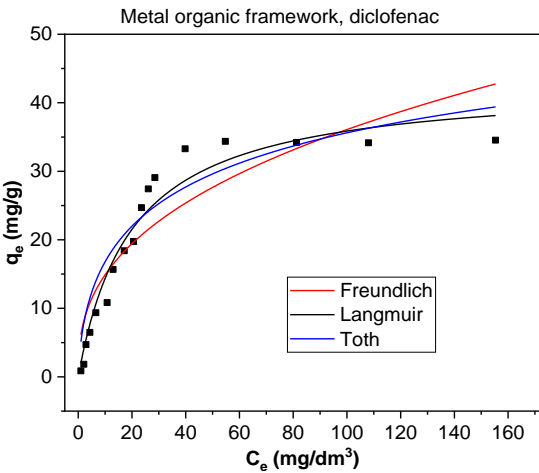
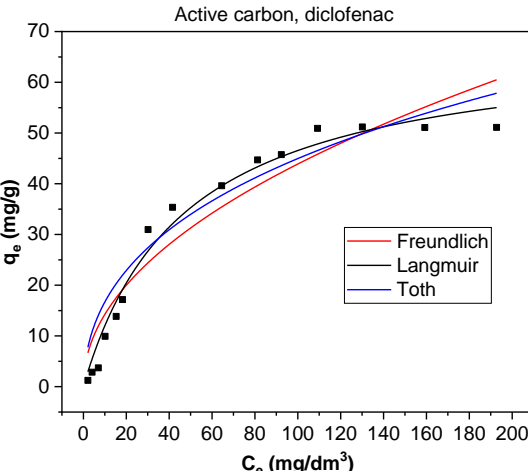
Sample		Pseudo-First Order					Pseudo-Second Order						
		10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³	10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³		
		75 mg	75 mg	75 mg	50 mg	100 mg	75 mg	75 mg	75 mg	50 mg	100 mg		
Diclofenac	k_1 (1/min)	0.044	0.245	0.178	0.011	0.041	k_2 (1/min)	0.040	0.014	6.94×10^{-3}	3.80×10^{-3}	0.032	
	χ^2	14	130	263	593	40.4	χ^2	10.2	9.3	25	125	3.82	
	R	0.991	0.97	0.97	0.94	0.98	R	0.993	0.996	0.997	0.99	0.998	
Caffeine	k_1 (1/min)	0.14	0.100	0.081	0.082	0.14	k_2 (1/min)	0.016	6.92×10^{-3}	4.31×10^{-3}	4.96×10^{-3}	0.011	
	χ^2	46	254	177	220	140	χ^2	7.7	76	27.9	54	34	
	R	0.95	0.87	0.96	0.93	0.90	R	0.991	0.96	0.994	0.98	0.98	
		50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³			50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³
		1.5 g	1.5 g	1.5 g	1 g	2 g			1.5 g	1.5 g	1.5 g	1 g	2 g
Solketal	k_1 (1/min)	0.56	0.51	0.41	0.29	0.48	k_2 (1/min)	0.56	0.36	0.234	0.18	0.39	
	χ^2	0.07	0.20	0.44	0.43	0.42	χ^2	0.032	0.27	0.30	0.29	0.09	
	R	0.991	0.991	0.99	0.99	0.98	R	0.996	0.99	0.992	0.99	0.994	

Table S3. Intraparticle rate parameters for the adsorption of organic molecules by the AC and MOF.

Sample		Active Carbon					MOF				
		10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³	10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³
		20 mg	20 mg	20 mg	10 mg	30 mg	75 mg	75 mg	75 mg	50 mg	100 mg
Diclofenac	K_3' (mg/g·min ^{0.5})	8.54	9.18	10.31	10.27	8.71	5.03	7.00	9.14	8.32	5.64
	R	0.99	0.99	0.97	0.99	0.99	0.80	0.94	0.96	0.97	0.89
	K_3'' (mg/g·min ^{0.5})	1.99	1.64	2.00	2.94	2.02	0.01	0.12	0.27	0.71	0.03
	R	0.92	0.97	0.95	0.98	0.98	0.55	0.77	0.77	0.91	0.74
Caffeine	K_3' (mg/g·min ^{0.5})	9.40	11.76	11.64	17.14	8.92	2.64	3.35	4.93	3.95	3.30
	R	0.99	0.96	0.94	0.98	0.95	0.97	0.93	0.99	0.97	0.91
	K_3'' (mg/g·min ^{0.5})	0.12	0.51	0.77	0.77	1.13	0.19	0.51	0.52	0.52	0.35
	R	0.63	0.93	0.91	0.76	0.95	0.86	0.95	0.90	0.90	0.93
		50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³	50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³
		1.5 g	1.5 g	1.5 g	1 g	2 g	1.5 g	1.5 g	1.5 g	1 g	2 g
Solketal	K_3' (mg/g·min ^{0.5})	0.41	0.71	0.80	0.84	0.50	0.49	0.72	0.86	0.83	0.64
	R	0.97	0.97	0.96	0.98	0.97	0.90	0.92	0.92	0.97	0.92
	K_3'' (mg/g·min ^{0.5})	0.093	0.064	0.067	0.10	0.055	5E-4	0.002	0.001	0.002	0.002
	R	0.97	0.97	0.91	0.94	0.95	0.10	0.61	0.19	0.72	0.68

Table S4. Effective diffusion coefficients for the adsorption of organic molecules by the AC and MOF.

Sample		Active Carbon					MOF				
		10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³	10 mg/dm ³	15 mg/dm ³	20 mg/dm ³	15 mg/dm ³	15 mg/dm ³
		20 mg	20 mg	20 mg	10 mg	30 mg	75 mg	75 mg	75 mg	50 mg	100 mg
Diclofenac	D/r^2 (1/s)	2.66×10^{-5}	2.41×10^{-5}	3.26×10^{-5}	2.21×10^{-5}	2.56×10^{-5}	4.03×10^{-4}	2.08×10^{-4}	1.45×10^{-4}	7.85×10^{-5}	3.78×10^{-4}
	χ^2	0.031	0.020	0.050	0.038	0.064	0.0069	0.017	0.017	0.055	0.0096
	R	0.994	0.997	0.99	0.993	0.99	0.998	0.994	0.995	0.99	0.996
Caffeine	D/r^2 (1/s)	7.61×10^{-5}	8.05×10^{-5}	8.55×10^{-5}	5.19×10^{-5}	5.21×10^{-5}	1.02×10^{-4}	5.97×10^{-5}	5.66×10^{-5}	5.38×10^{-5}	9.66×10^{-5}
	χ^2	0.008	0.015	0.042	0.014	0.066	0.052	0.17	0.024	0.058	0.15
	R	0.998	0.996	0.99	0.997	0.98	0.985	0.95	0.994	0.99	0.95
		50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³	50 g/dm ³	75 g/dm ³	100 g/dm ³	75 g/dm ³	75 g/dm ³
		1.5 g	1.5 g	1.5 g	1 g	2 g	1.5 g	1.5 g	1.5 g	1 g	2 g
Solketal	D/r^2 (1/s)	4.73×10^{-5}	6.35×10^{-5}	6.45×10^{-5}	4.15×10^{-5}	8.9×10^{-5}	4.95×10^{-4}	4.61×10^{-4}	3.72×10^{-4}	2.56×10^{-4}	3.88×10^{-4}
	χ^2	0.049	0.015	0.028	0.013	0.045	0.0057	0.014	0.012	0.0092	0.012
	R	0.99	0.996	0.993	0.998	0.99	0.997	0.993	0.995	0.996	0.996



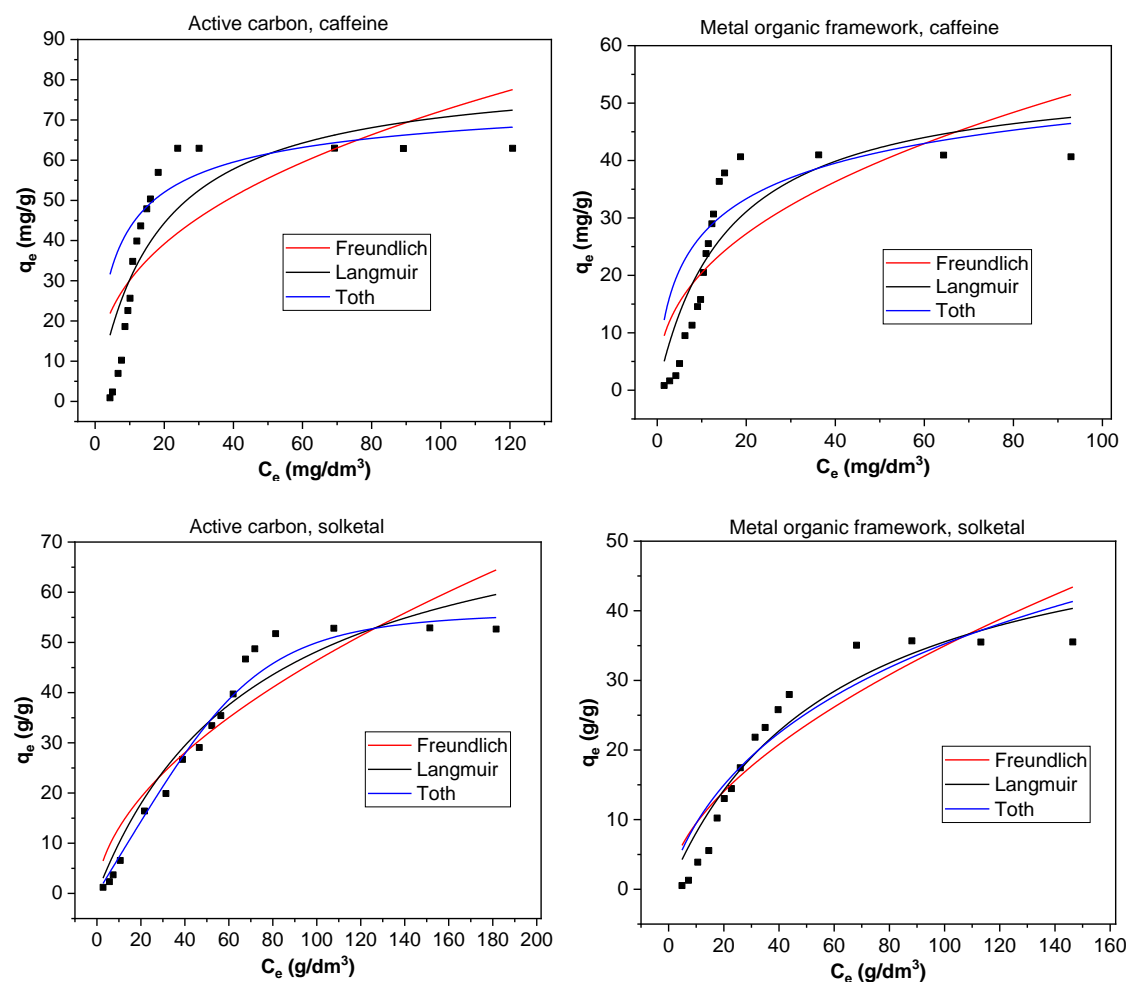


Figure S1. Experimental results (scatter) and isotherm adjustment to Langmuir, Freundlich and Toth models for diclofenac, caffeine and solketal adsorption on the AC (first column) and MOF (second column).