

Supporting Information for Publication

Multicomponent Adsorption of Pharmaceutical Compounds by Batch and Fixed-Bed Column Processes: Application of Monte Carlo Bayesian Modeling

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Table S1. ANOVA Table for the Variables: i) Removal and ii) Adsorption Capacity.

i)

Factor	SS	df	MS	F	p
x ₁	8.82	1	8.82	0.87	0.449
x ₂	10.51	1	10.51	1.04	0.415
x ₃	675.28	1	675.28	66.79	0.015
x ₁ ²	43.63	1	43.63	4.32	0.173
x ₂ ²	1287.78	1	1287.78	127.38	0.008
x ₃ ²	125.13	1	125.13	12.38	0.072
Lack of Fit	32.01	6	5.33	0.53	0.770
Pure Error	20.22	2	10.11		
Total SS	2120.42	14			

R²= 0.9754; R²_{Adj}: 0.9569

ii)

Factor	SS	df	MS	F	p
x ₁	0.13	1	0.13	5.36	0.147
x ₂	0.25	1	0.25	10.56	0.083
x ₃	0.45	1	0.45	19.34	0.048
x ₁ ²	1.05	1	1.05	45.01	0.022
x ₂ ²	9.03	1	9.03	387.05	0.003
x ₃ ²	0.37	1	0.37	15.99	0.057
Lack of Fit	1.41	6	0.24	10.05	0.093
Pure Error	0.05	2	0.02		
Total SS	13.14	14			

R²= 0.8893; R²_{Adj}: 0.8063

ii) Factor	SS	df	MS	F	p
x ₁	0.13	1	0.13	5.36	0.147
x ₂	0.25	1	0.25	10.56	0.083
x ₃	0.45	1	0.45	19.34	0.048
x ₁ ²	1.05	1	1.05	45.01	0.022
x ₂ ²	9.03	1	9.03	387.05	0.003
x ₃ ²	0.37	1	0.37	15.99	0.057
Lack of Fit	1.41	6	0.24	10.05	0.093
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R²= 0.8893; R²_{Adj}: 0.8063

Figure S1. Pareto diagrams for simultaneous pharmaceuticals batch adsorption (A, removal is the response variable; B; Q_e is the response variable).

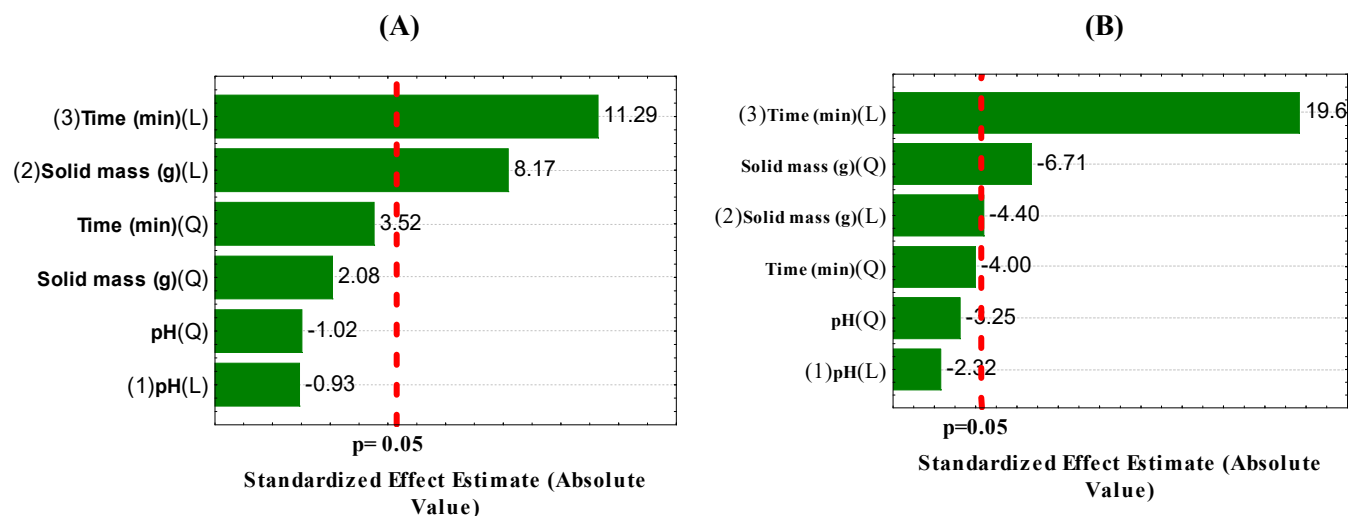
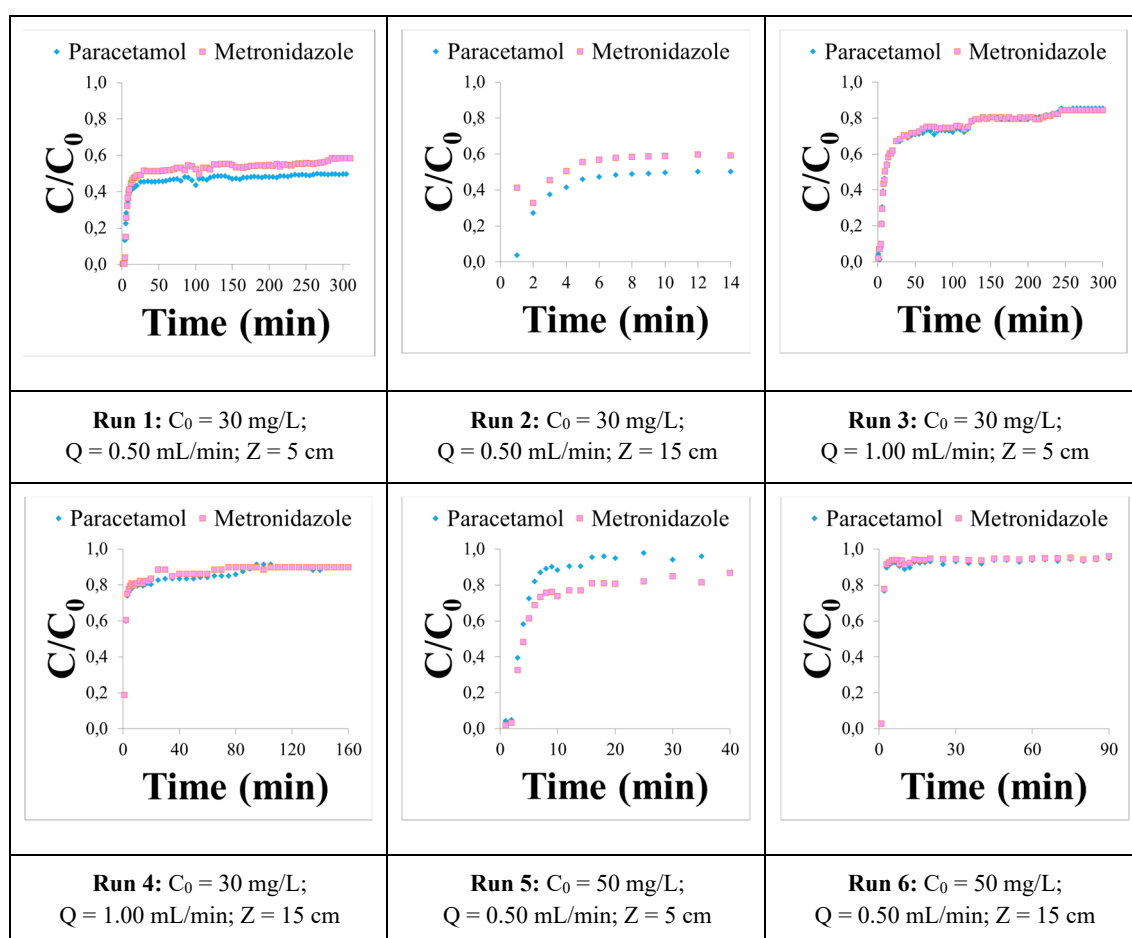


Figure S2. Breakthrough Curves Obtained by Simultaneous Adsorption of Pharmaceuticals in a Fixed-Bed Column.



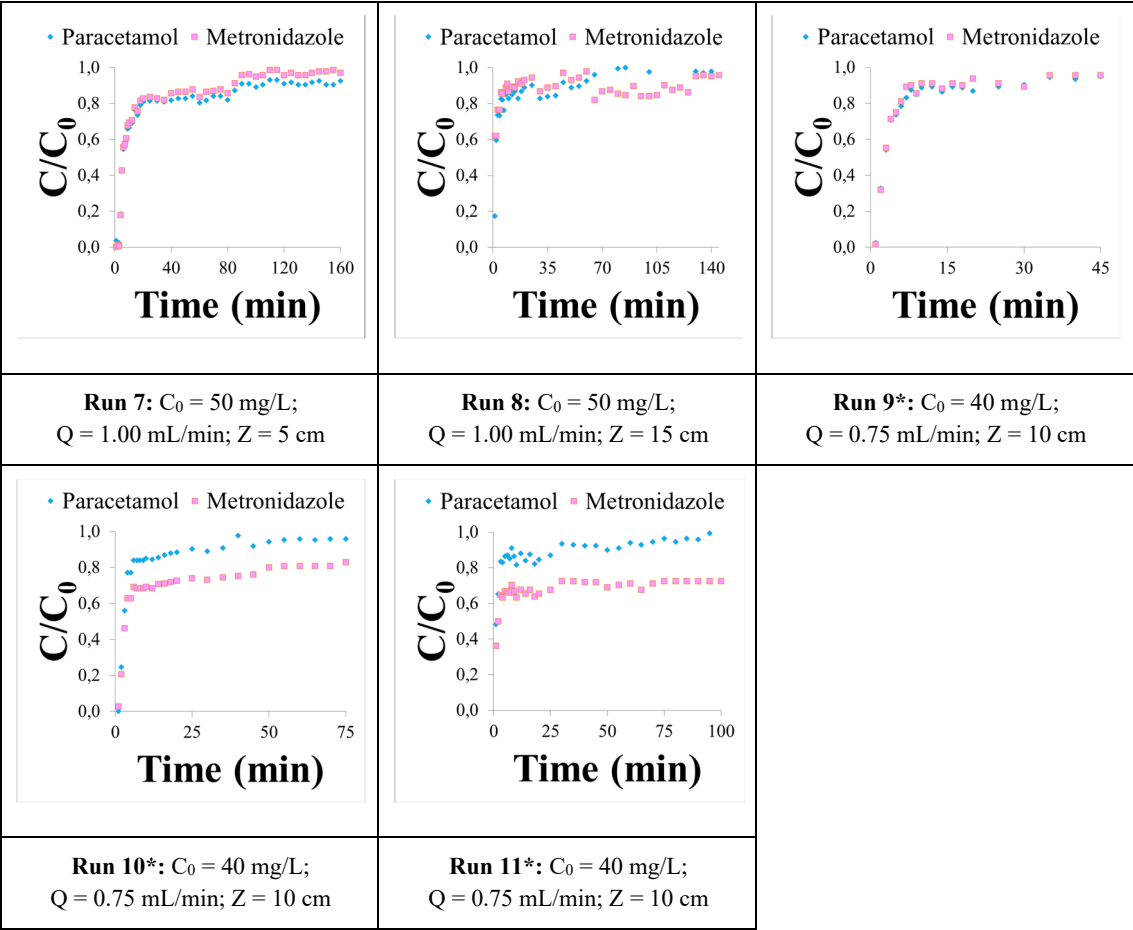
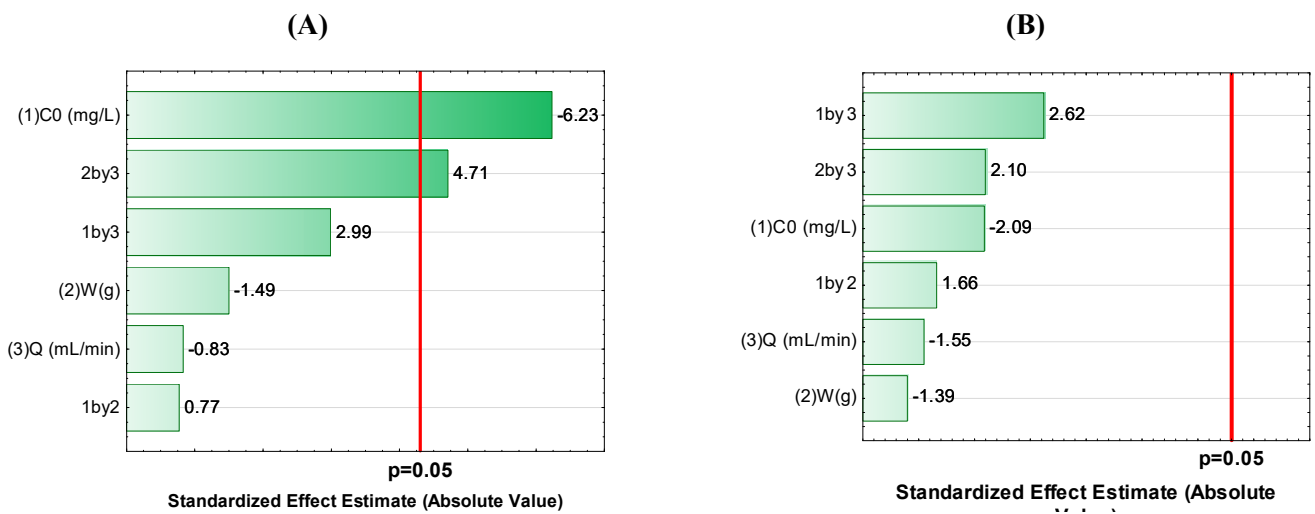


Table S2. ANOVA Table for the Response Variables: i) $q_{\max\text{PAR}}$ and ii) $q_{\max\text{MTZ}}$ of Adsorption in Fixed-Bed Column*.

i)	Factor	SS	df	MS	F	p
	X ₁	601.53	1	601.53	38.85	0.025
	X ₂	34.82	1	34.82	2.25	0.273
	X ₃	10.65	1	10.65	0.69	0.494
	X ₁ X ₂	9.22	1	9.22	0.60	0.521
	X ₁ X ₃	138.53	1	138.53	8.95	0.096
	X ₂ X ₃	343.35	1	343.35	22.18	0.042
	Lack of Fit	979.34	2	489.67	31.63	0.031
	Pure Error	30.97	2	15.48		
	Total SS	2148.41	10			
R²=0.5297; R²_{Adj}=0.0						
ii)	Factor	SS	df	MS	F	p
	X ₁	200.10	1	200.10	4.36	0.17
	X ₂	89.98	1	89.98	1.96	0.30
	X ₃	109.89	1	109.89	2.39	0.26
	X ₁ X ₂	126.64	1	126.64	2.76	0.24
	X ₁ X ₃	315.13	1	315.13	6.86	0.12
	X ₂ X ₃	201.91	1	201.91	4.40	0.17
	Lack of Fit	152.02	2	76.01	1.66	0.38
	Pure Error	91.85	2	45.92		
	Total SS	1287.52	10			
R²=0.811; R²_{Adj}=0.526						

*Effects not shown were linear combinations of other effects and could not be estimated.

Figure S3. Pareto diagrams for simultaneous pharmaceuticals removal by fixed-bed column adsorption (A, $q_{\max\text{PAR}}$ is the response variable; B; $q_{\max\text{MTZ}}$ is the response variable)*.



*Effects not shown were linear combinations of other effects and could not be estimated.