

Affinity adsorption for the removal of organic micropollutants in drinking water sources; proof of principle

LANGMUIR DATA FOR ADSORPTION ON MODIFIED SILICA PARTICLES

Table SI-1 | Langmuir best-fit values for adsorption of carbamazepine on silica with phenyl groups at the surface. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water	Nieuwegein tap water
Bmax	11699	~ 1.812e+007
Kd	0.1213	~ 2.336e-005
Std. Error Bmax	2333	
Std. Error Kd	0.04658	
95% Confidence Intervals Bmax	6182 to 17216	~ 2.261e+010
95% Confidence Intervals Kd	0.01112 to 0.2314	~ 0.02916
Degrees of Freedom	7	5
R ²	0.9620	0.9445
Absolute Sum of Squares	1.906e+006	1.273e+006
Sy.x	521.9	504.6
Number of points analyzed	9	7

Table SI-2 | Langmuir best-fit values for adsorption of diclofenac on silica with TBA-chloride groups at the surface. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water	Nieuwegein tap water
Bmax	11778	6010
Kd	2.281	0.1266
Std. Error Bmax	1293	3170
Std. Error Kd	1.045	0.1227
95% Confidence Intervals Bmax	8898 to 14658	-2141 to 14160
95% Confidence Intervals Kd	-0.04788 to 4.611	-0.1888 to 0.4420
Degrees of Freedom	10	5
R ²	0.8805	0.8652
Absolute Sum of Squares	2.567e+007	1.716e+006
Sy.x	1602	585.9
Number of points analyzed	12	7

Table SI-3 | Langmuir best-fit values for adsorption of benzoic acid on silica with TBA-chloride groups at the surface. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water
Bmax	24441
Kd	0.09318
Std. Error Bmax	2987
Std. Error Kd	0.02833
95% Confidence Intervals Bmax	17933 to 30948
95% Confidence Intervals Kd	0.03145 to 0.1549
Degrees of Freedom	12
R ²	0.9126
Absolute Sum of Squares	6.551e+007
Sy.x	2337
Number of points analyzed	14

Table SI-4 | Langmuir best-fit values for adsorption of ibuprofen on silica with TBA-chloride groups at the surface. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water
Bmax	29758
Kd	0.1195
Std. Error Bmax	13028
Std. Error Kd	0.09294
95% Confidence Intervals Bmax	1995 to 57522
95% Confidence Intervals Kd	-0.07859 to 0.3175
Degrees of Freedom	15
R ²	0.8636
Absolute Sum of Squares	9.939e+007
Sy.x	2574
Number of points analyzed	17

Table SI-6 | Langmuir best-fit values for adsorption of carbamazepine on Oasis MAX. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water	Nieuwegein tap water
Bmax	27098	29334
Kd	0.8491	0.6726
Std. Error Bmax	962.8	2119
Std. Error Kd	0.1189	0.1324
95% Confidence Intervals Bmax	25057 to 29140	24149 to 24519
95% Confidence Intervals Kd	0.5969 to 1.101	0.3488 to 0.9965
Degrees of Freedom	16	6
R ²	0.9896	0.9730
Absolute Sum of Squares	1.689e+007	1.122e+006
Sy.x	1027	1368
Number of points analyzed	18	8

LANGMUIR DATA FOR ADSORPTION ON OASIS[®] POLYMER ADSORBENTS

Table SI-5 | Langmuir best-fit values for adsorption of carbamazepine on Oasis[®] HLB. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water	Nieuwegein tap water
Bmax	61691	68686
Kd	1.808	3.006
Std. Error Bmax	3004	9529
Std. Error Kd	0.3061	1.205
95% Confidence Intervals Bmax	55290 to 68092	44188 to 93184
95% Confidence Intervals Kd	1.156 to 2.460	-0.09264 to 6.105
Degrees of Freedom	15	5
R ²	0.9791	0.9095
Absolute Sum of Squares	1.410e+008	2.483e+008
Sy.x	3066	7047
Number of points analyzed	17	7

Table SI-7 | Langmuir best-fit values for adsorption of ibuprofen on Oasis[®] MAX. The reliability of the fit is characterized by the number of degrees of freedom, R², the absolute sum of squares and Sy.x

Best-fit values	Milli-Q water	Nieuwegein tap water
Bmax	53714	39249
Kd	14.98	15.76
Std. Error Bmax	2326	711.7
Std. Error Kd	2.587	2.644
95% Confidence Intervals Bmax	48454 to 58975	37273 to 41225
95% Confidence Intervals Kd	9.130 to 20.83	8.422 to 23.10
Degrees of Freedom	9	4
R ²	0.9160	0.9592