Supporting Information

Elimination of persistent anthropogenic pollutants by micro-mesoporous carbon xerogels. Natural organic matter on surface water and textural properties influences.

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Table SI 1. Physico-chemical properties of ICM and pharmaceutical compounds

	MW ($g\ mol^{-1}$)	pKa	log Kow	Solubility ($mg\ L^{-1}$)	Molar volume ($cm^3\ mol^{-1}$)	Dimensions (Å)	λ (nm)
Phenol	94.11	9.99	1.46	82000	87,8 ± 3	4.383*0.00031*5.767	269.9
Salicylic acid	138.12	2.97	2.26	2240	100,3 ± 3	5.391*2.426*6.077	295.0
Paracetamol	151.16	9.38	0.46	14000	120,9 ± 3	4.767*1.582*8.762	242.0
Caffeine	194.19	10.4	-0.07	21600	133,3 ± 7	6.453*1.595*7.309	273.1
Levodopa	197.19	2.32	-2.39	5000	134,2 ± 3	4.887*2.807*9.551	280.0
Diclofenac sodium	318.13	4.4 ± 0.4	3.91	2430	206,8 ± 3	7.424*1.809*10.251	276.2
DTZ	613.91	1.4±0.8*	1.37	50000	234,3 ± 3	7.002*1.587*11.423	238.1
IPM	777.08	10.7	-2.42	120000	340,6 ± 3	11.974*3.520*13.521	242.8
IMPRL	777.09	10.7	-2.42	120000	342,2 ± 3	8.228*0.929*15.908	244.0
IPRD	791.10	10.6 ± 1.1	-2.05	23.80	364,0 ± 3	8.545*3.110*17.025	242.4
IOX	821.13	11.8 ± 0.7	-3.05	107	373,1 ± 3	11.924*2.967*15.186	245.5
IDXL	1550.18	7.2-7.6	-3.37	0.00184*	675,3 ± 3	10.162*2.912*26.995	246.0

*pKa Basic PhysiChem Properties (Advanced Chemistry Development, Inc. (ACD/Labs)

SI Analytical method

The specifications of the analysis of pharmaceutical and ICM compounds are: injection volume 10 μL, column Waters ACQUITY BEH C18 (100 x 2.1 mm, 1.7mm particle size) equipped with a guard column (5 x 2.1 mm). Simple binary gradient consisting of a) 0.1% HCOOH or 20 mM of NH4OAc for acid and neutral conditions, respectively, and b) acetonitrile was employed for chromatographic separation. Exact mass measurements of the compounds were carried out in full-scan and product ion scan mode by HR mass spectrometer using heated electrospray ionization. Eight compounds were analyzed in positive ion (PI) mode and three in negative ion (NI) mode, diclofenac sodium was analyzed with both modes. Quantification of the compounds in the samples extracts was performed by internal standard method based on the peak areas obtained for each analyte and its deuterated analogue, using Thermo Xcalibur 2.2 software.

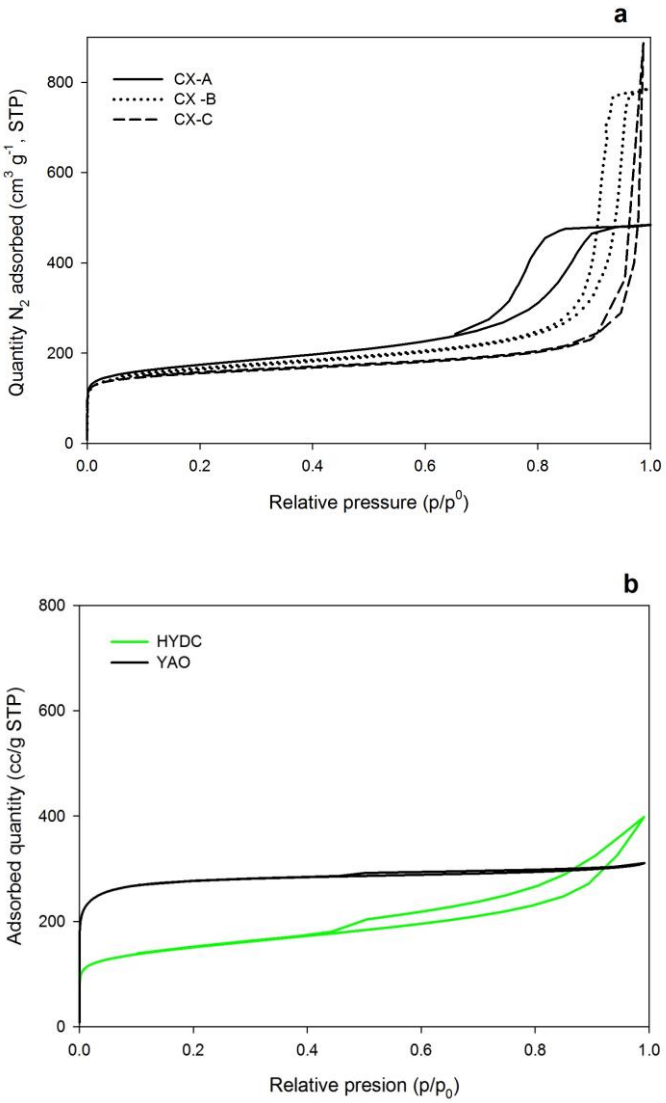

Figure SI 1. Nitrogen adsorption isotherms a) Carbon Xerogels, b) Commercial activated carbons

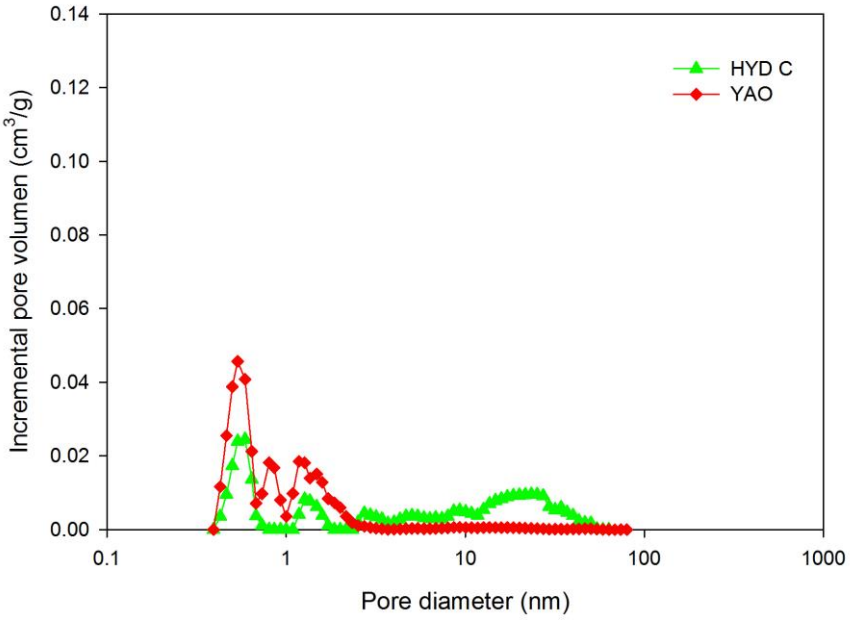

Figure SI 2 Pore size distribution obtained by application of the DFT model to the N_2 adsorption data of activated carbons

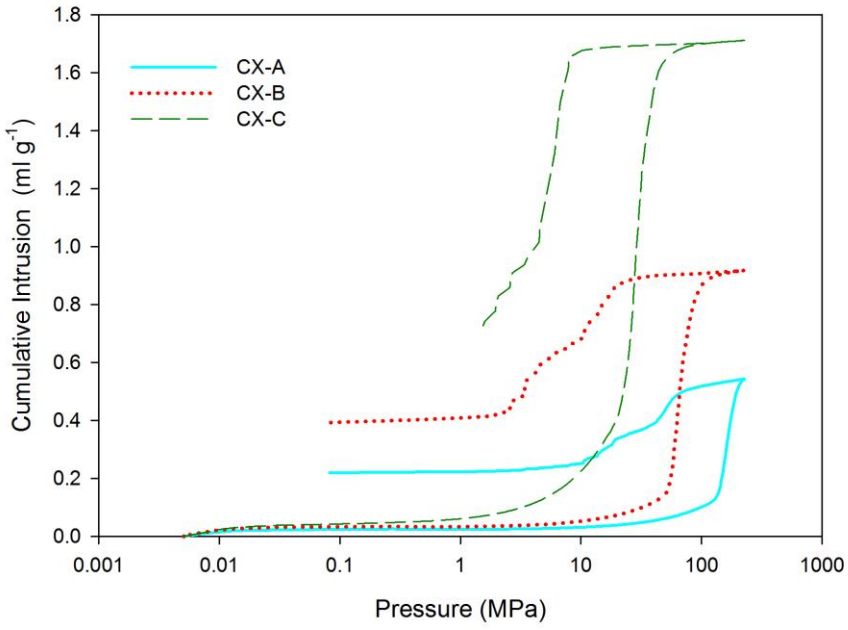

Figure SI 3. Cumulative mercury intrusion volume vs. Pressure on carbon xerogels.

Table SI 2. Mercury porosimetry parameters for the carbon xerogels.

				Mesopore Volume 5.5-50 nm	Macropore Volume 50-250000 nm	Total pore Volume 5.5-250000 nm		
	Density (at 0.005 Mpa) (g/cm^3)	Density (at 0.1013 Mpa) (g/cm^3)	Skeletal Density (at 228 Mpa) (g/cm^3)	Vol intrus Hg ($cm^3\ g^{-1}$)	Vol intrus Hg ($cm^3\ g^{-1}$)	Vol intrus Hg ($cm^3\ g^{-1}$)	Porosity (%)	Average pore diameter (4V/A) (nm)
CX-A	0.76	0.78	1.30	0.50	0.04	0.54	41.5	8.8
CX-B	0.58	0.59	1.25	0.83	0.08	0.92	53.4	19.3
CX-C	0.40	0.41	1.28	1.09	0.63	1.71	68.6	45.6

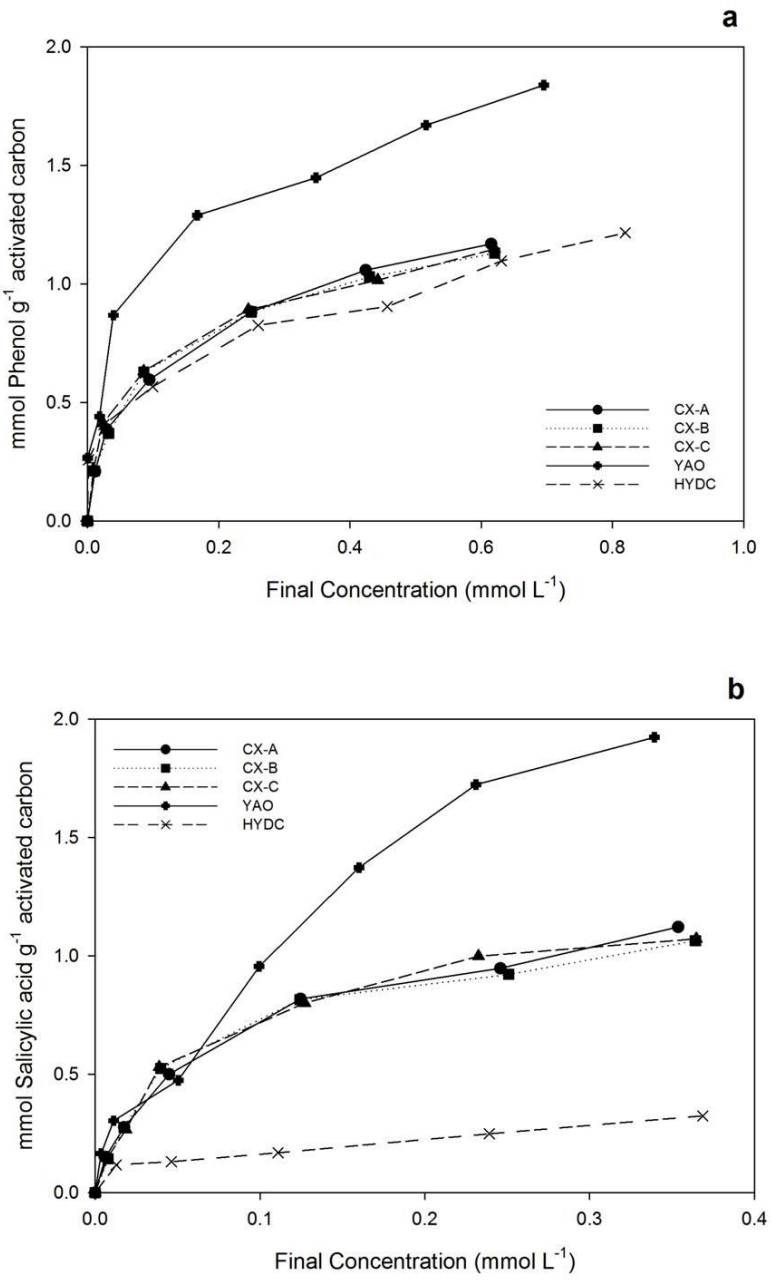

Figure SI 4. Pharmaceutical adsorption isotherms a) Phenol, b) Salicylic acid, onto the different adsorbents

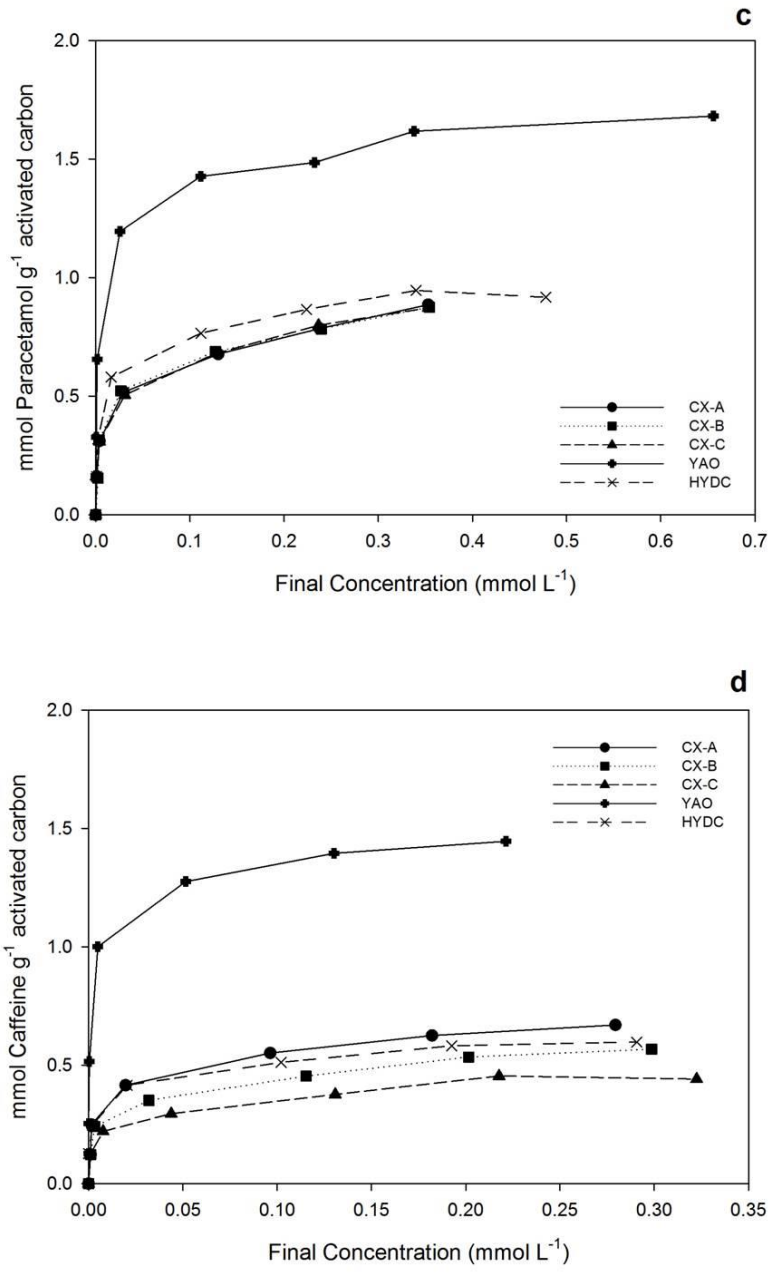

Figure SI 4. Pharmaceutical adsorption isotherms c) Paracetamol, d) Caffeine, onto the different adsorbents

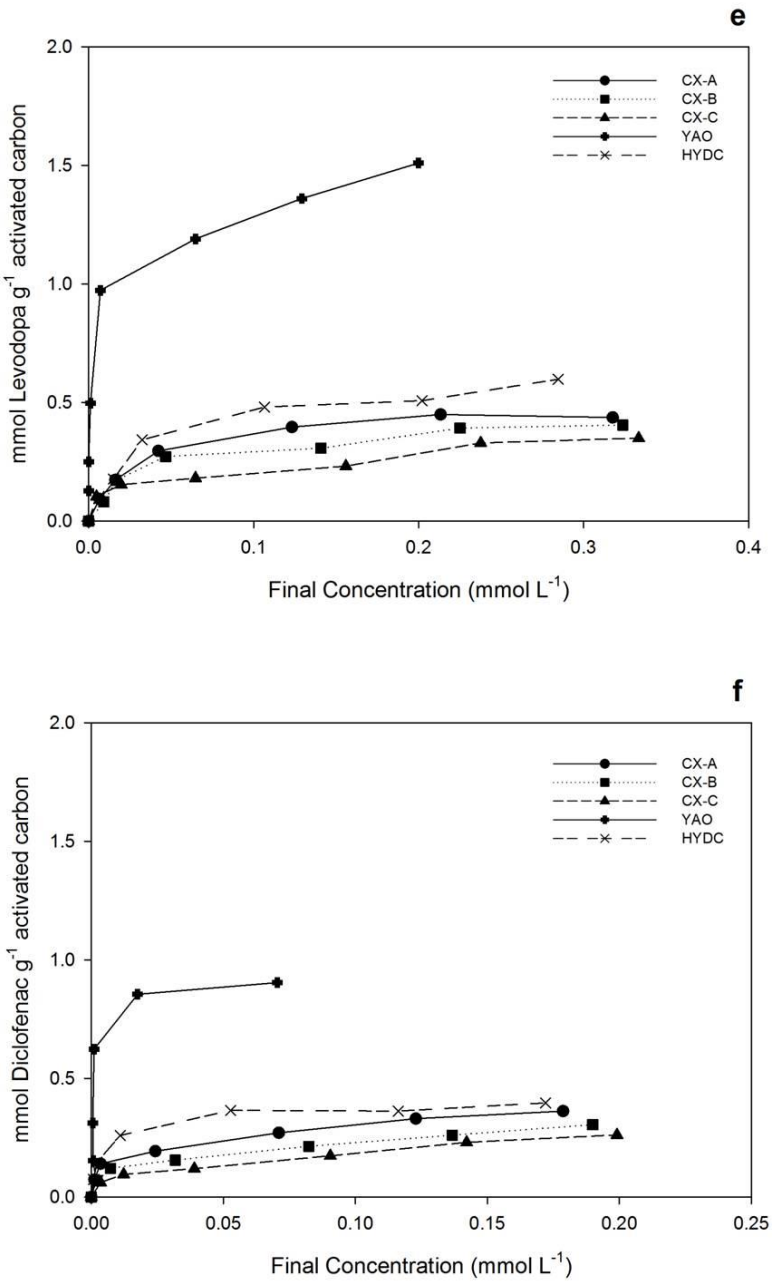

Figure SI 4. Pharmaceutical adsorption isotherms e) Levodopa, f) Diclofenac onto the different adsorbents

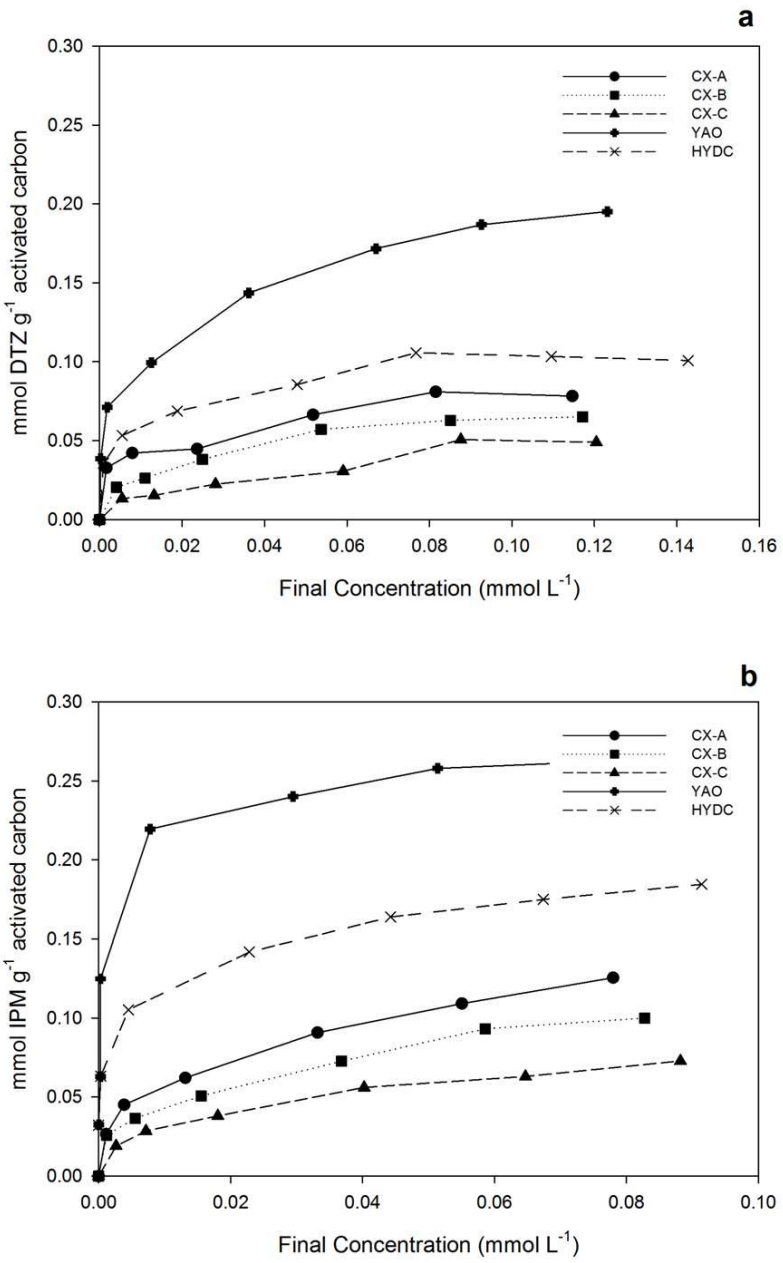

Figure SI 5. Pharmaceutical adsorption isotherms a) DTZ, b) IPM onto the different adsorbents

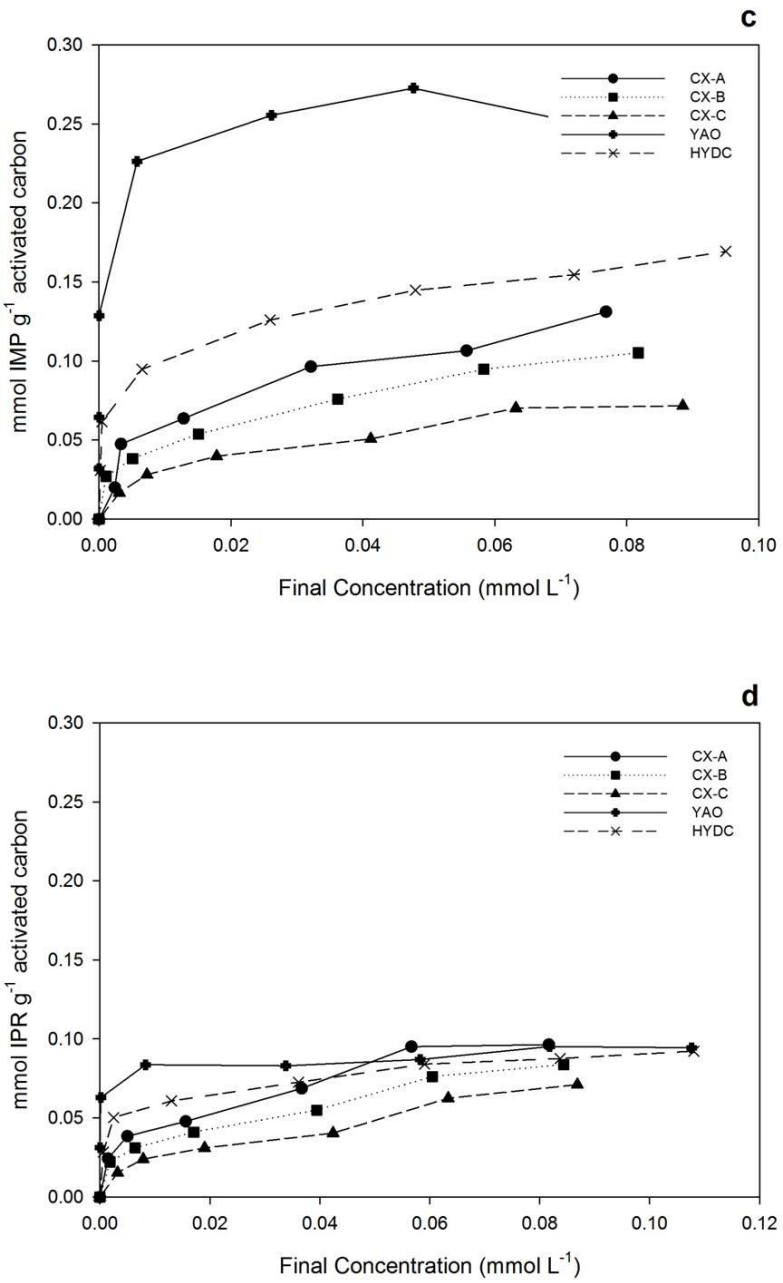

Figure SI 5. Pharmaceutical adsorption isotherms c) IMP d) IPR onto the different adsorbents

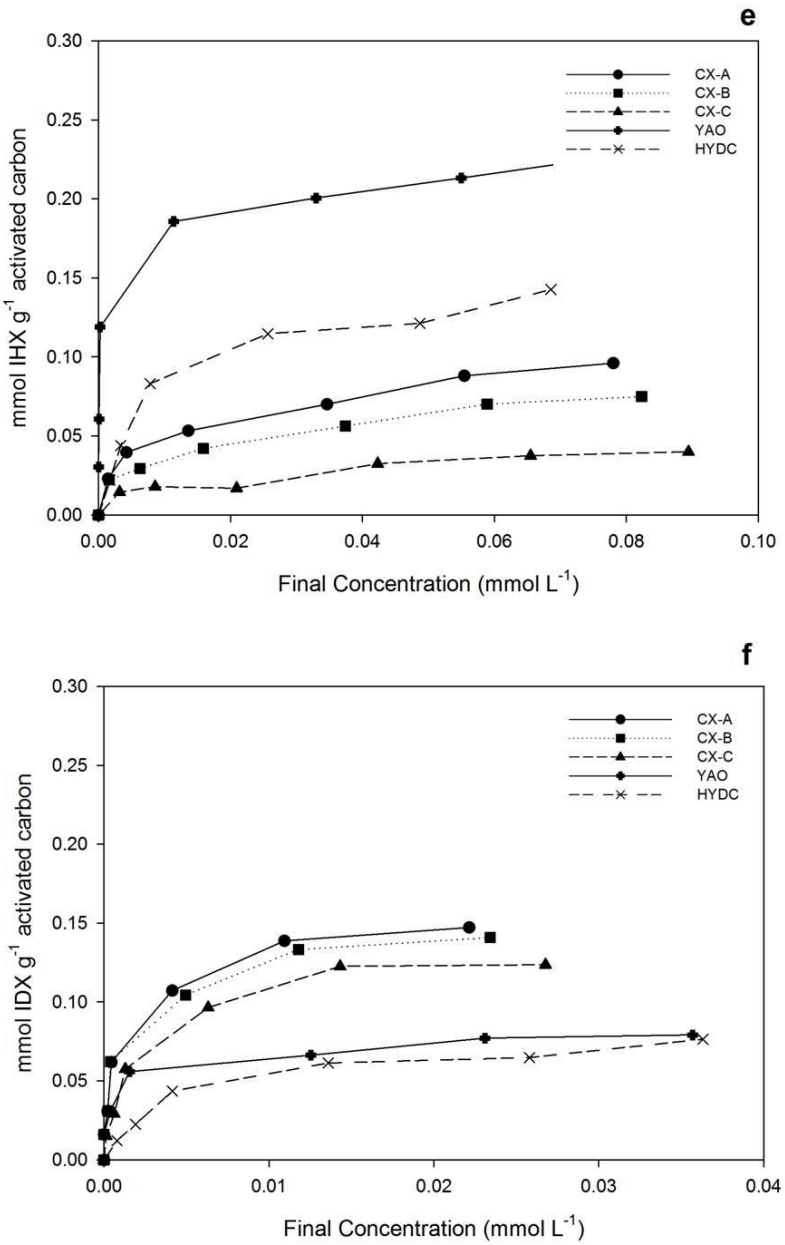

Figure SI 5. Pharmaceutical adsorption isotherms e)IHX f) IDX onto the different adsorbents

Table SI3 a. Pharmaceutical and IDM isotherm parameters on CX-A

		Langmuir			Freundlich		
		q_{max}	K_L	OF	K_F	N	OF
CX-A	Cafeine	0.6068	283.6648	0.1491	0.913	4.4869	0.0913
	Diclofenac	0.3316	135.4664	0.0936	0.59	3.5051	0.0299
	DZT	0.0763	181.3542	0.0257	0.013	4.0365	0.013
	IHX	0.0974	126.0774	0.0178	0.2268	2.9774	0.0057
	IDX	0.1445	1351.4	0.0249	0.4278	3.7929	0.0271
	IMP	0.1382	83.6012	0.0241	0.3561	2.5224	0.0187
	IPM	0.131	94.584	0.024	0.3134	2.7579	0.0047
	IPR	0.1074	76.4415	0.0237	0.2502	2.7000	0.0124
	Levodopa	0.4908	34.9972	0.0216	0.6948	3.1690	0.0917
	Paracetamol	0.7988	123.4878	0.1879	1.1393	4.0449	0.0731
	Phenol	1.2776	11.2035	0.1396	1.4467	2.6179	0.072
	Salicylic acid	1.2769	14.6968	0.087	1.7808	2.3399	0.1185

Table SI3 b. Pharmaceutical and IDM isotherm parameters on CX-B

		Langmuir			Freundlich		
		q_{max}	K_L	OF	K_F	N	OF
CX-B	Cafeine	0.5064	237.8227	0.1325	0.7523	4.4440	0.0532
	Diclofenac	0.2859	67.7961	0.0759	0.4971	3.1422	0.0259
	DZT	0.0757	52.382	0.0089	0.15	2.7539	0.0073
	IHX	0.0807	88.3012	0.0152	0.1785	2.9086	0.0047
	IDX	0.1361	1573.9	0.0274	0.3849	3.9522	0.027
	IMP	0.1134	78.9656	0.0235	0.2536	2.8172	0.0069
	IPM	0.1116	70.1287	0.0219	0.2511	2.7281	0.0079
	IPR	0.0937	58.4088	0.0198	0.219	2.5331	0.009
	Levodopa	0.4256	33.5907	0.0582	0.6089	3.0690	0.0768
	Paracetamol	0.7946	110.6908	0.1657	1.1432	3.9897	0.1234
	Phenol	1.219	13.0181	0.0972	1.3882	2.7682	0.1013
	Salicylic acid	1.1764	18.5207	0.0677	1.6456	2.5055	0.1678

Table SI3 c. Pharmaceutical and IDM isotherm parameters on CX-C

		Langmuir			Freundlich		
		q_{max}	K_L	OF	K_F	N	OF
CX-C	Cafeine	0.4207	143.9423	0.1214	0.5841	4.7731	0.039
	Diclofenac	0.2912	24.325	0.0628	0.4848	2.5187	0.0261
	DZT	0.0738	17.4211	0.0118	0.1558	1.9109	0.0096
	IHX	0.0457	58.1628	0.0115	0.0998	2.6717	0.0076
	IDX	0.1332	529.4413	0.0115	0.4342	3.1254	0.0256
	IMP	0.0834	57.5981	0.0112	0.2005	2.4419	0.0076
	IPM	0.0794	67.7967	0.0108	0.1822	2.6333	0.0032
	IPR	0.0943	27.9344	0.0158	0.2374	1.9851	0.0097
	Levodopa	0.3417	31.1048	0.1057	0.4835	3.1247	0.0531
	Paracetamol	0.7983	109.4788	0.2164	1.1191	4.2265	0.0257
	Phenol	1.2615	17.9819	0.1527	1.3591	3.0241	0.0879
	Salicylic acid	1.2387	16.7301	0.0698	1.7325	2.4292	0.168

Table SI3 d. Pharmaceutical and IDM isotherm parameters on HYDC

		Langmuir			Freundlich		
		q_{max}	K_L	OF	K_F	N	OF
HYDC	Cafeine	0.559	312.3777	0.1605	0.7521	5.9876	0.1313
	Diclofenac	0.3866	252.9113	0.0381	0.6221	4.3984	0.083
	DZT	0.1018	223.1087	0.0266	0.1645	4.6803	0.0134
	IHX	0.1506	130.5217	0.0147	0.3796	2.7973	0.028
	IDX	0.081	236.3704	0.0075	0.2578	2.7715	0.0141
	IMP	0.1451	1161.7	0.0479	0.2817	4.5422	0.016
	IPM	0.1669	855.1358	0.059	0.2904	5.3336	0.0323
	IPR	0.084	583.6246	0.0202	0.1433	5.0966	0.0085
	Levodopa	0.633	30.3402	0.0594	0.9581	2.7779	0.1107
	Paracetamol	0.8887	173.0516	0.1544	1.1556	4.8036	0.167
	Phenol	1.2264	10.4014	0.3394	1.2377	3.297	0.132
	Salicylic acid	0.696	2.9406	0.1262	0.5973	1.9082	0.0899

Table SI3 e. Pharmaceutical and IDM iisotherm parameters on YAO

		Langmuir			Freundlich		
		q_{max}	K_L	OF	K_F	N	OF
YAO	Cafeine	1.3529	1134.7	0.3533	1.8465	7.2807	0.3349
	Diclofenac	0.9296	490.2541	0.1562	1.9427	4.0226	0.2651
	DZT	0.2491	57.7486	0.075	0.4552	3.1158	0.0436
	IHX	0.2077	6066.9	0.0418	0.3278	7.0935	0.0439
	IDX	0.0765	1784.9	0.018	0.1426	5.9147	0.0195
	IMP	0.2627	1122	0.1488	0.2932	22.3205	0.1495
	IPM	0.2511	2108.4	0.0581	0.4307	5.8477	0.0667
	IPR	0.0889	1828.1	0.0333	0.1062	17.2397	0.0324
	Levodopa	1.3773	415.2745	0.3559	1.9817	5.7032	0.3337
	Paracetamol	1.5247	464.6646	0.3439	1.9208	5.9376	0.3517
	Phenol	1.8278	18.4526	0.3574	2.0642	3.2482	0.3457
	Salicylic acid	2.6810	4.1433	0.2412	3.8733	1.6623	0.2499

Table SI 4. Linear coefficient correlation (r) between q_{max} and different physic-chemical characteristics of pharmaceuticals for the different adsorbents

	linear correlation coeficient (r) with q_{max}									
	Highest dimension		pKa		Log Kow		Log Kow (with out diclofenac)		Solubility	
CX-A	-	0.909		0.217	+	0.689	+	0.903	+	0.547
CX-B	-	0.874		0.245	+	0.690	+	0.896	+	0.558
CX-C	-	0.838		0.176	+	0.748	+	0.910	+	0.471
HYDC	-	0.636	+	0.522		0.308		0.444	+	0.835
YAO	-	0.780		0.145	+	0.585	+	0.773		0.110

Table SI 5. Lineal coefficient correlation (r) between q_{max} and different physic-chemical and molecular characteristics of ICM for the different adsorbents

	Coefficient correlation (r) with q_{max}							
	Highest dimensión		pKa		Log Kow		Solubility	
CX-A	+	0.643		0.077	-	0.740		0.326
CX-B	+	0.777		0.318	-	0.621		0.184
CX-C	+	0.819	-	0.686		0.245		0.167
HYDC	-	0.528	+	0.686		0.214	+	0.667
YAO	-	0.780		0.319		0.392	+	0.771

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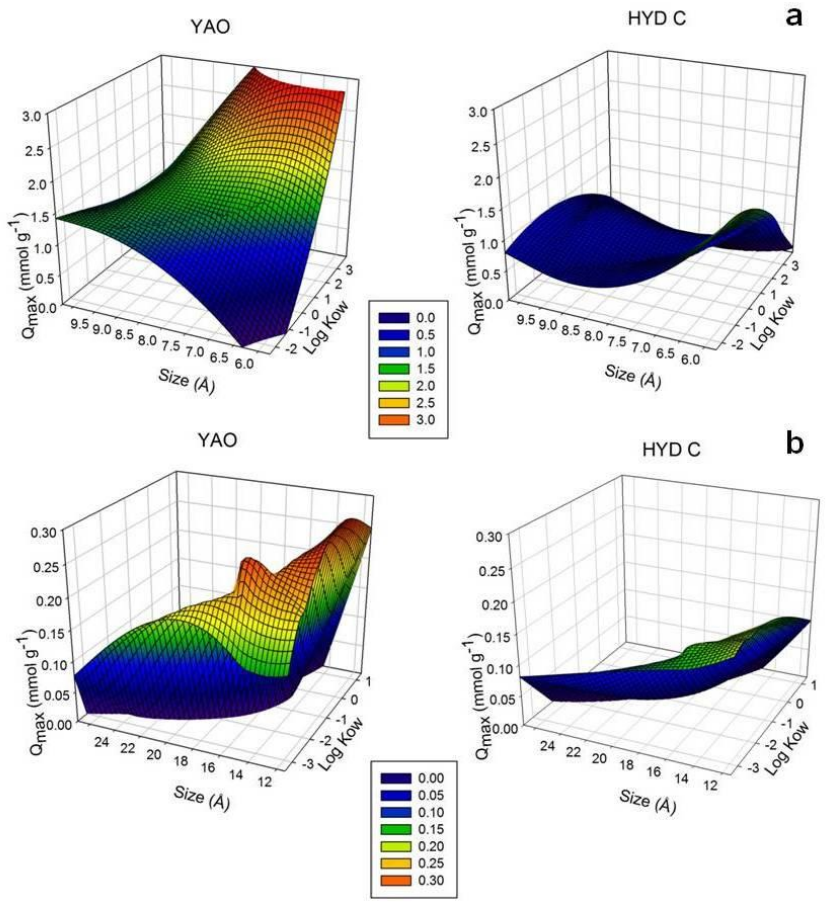

Figure SI 6. Trend of adsorption capacity (q_{max}) *vs* third compound dimension and logkow onto commercial activated carbons (YAO and HYDC) a) pharmaceuticals, b) ICM

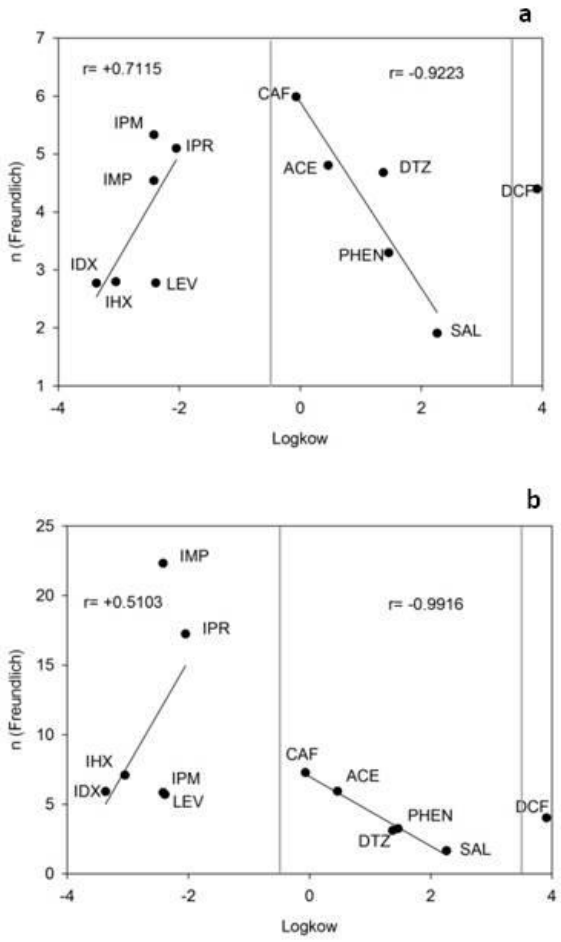

Figure SI 7 Relation between the intensity of adsorption (n) Freundlich and logkow on commercial activated carbons: a) HYDC b) YAO

Table SI 6. Lineal coefficient correlation (r) between q_{max} and different pore volume (ultramicropore, total micropore and mesopore)

	Linear coefficient correlation (r)		
	Ultramicropore	Micropore (total)	Mesopore
Phenol	(+) 0.8602	(+) 0.9746	(-) 0.7150
Salicylic acid	(+) 0.9739	(+) 0.9767	(-) 0.4363
Paracetamol	(+) 0.8509	(+) 0.9714	(-) 0.7106
Caffeine	(+) 0.8341	(+) 0.9631	(-) 0.7495
Levodopa	(+) 0.7653	(+) 0.9301	(-) 0.8154
Diclofenac sodium	(+) 0.8354	(+) 0.9643	(-) 0.7429
DTZ	(+) 0.8333	(+) 0.9633	(-) 0.7336
IDX	(-) 0.3203	(-) 0.5593	(+) 0.8019
IPM	(+) 0.5876	(+) 0.8151	(-) 0.9299
IMP	(+) 0.7087	(+) 0.8935	(-) 0.8639
IPR	(+) 0.0922	(-) 0.2445	(+) 0.3637
IHX	(+) 0.4713	(+) 0.7282	(-) 0.9627
IDX	(-) 0.3203	(-) 0.5593	(+) 0.8019

Table SI 7. Pore volume in different pore diameter sections

	Pore volume ($cm^3\ g^{-1}$)			
	1.3-5	Meso 2-5	meso 5-10	meso 2-10
CX-A	0.053	0.029	0.210	0.239
CX-B	0.038	0.017	0.061	0.078
CX-C	0.013	0.000	0.006	0.006
HYDC	0.046	0.030	0.034	0.064
YAO	0.068	0.009	0.004	0.013

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Table SI 8. Linear coefficient correlation between IDX, IHX, IMP, IPM and IPR with different pore volume diameter sections

	lineal coeficient correlation (r)			
	1.3-5 (nm)	Meso 2-5 (nm)	meso 5-10 (nm)	meso 2-10 (nm)
IDX	(-) 0.5326	0.0529	(+) 0.5828	(+) 0.5211
IHX	(+) 0.8691	0.2098	0.2337	0.5788
IMP	(+) 0.8765	0.0071	0.1876	0.1691
IPM	(+) 0.8784	0.1127	0.2291	0.1921
IPR	0.0424	0.1476	(+) 0.8525	(+) 0.7931

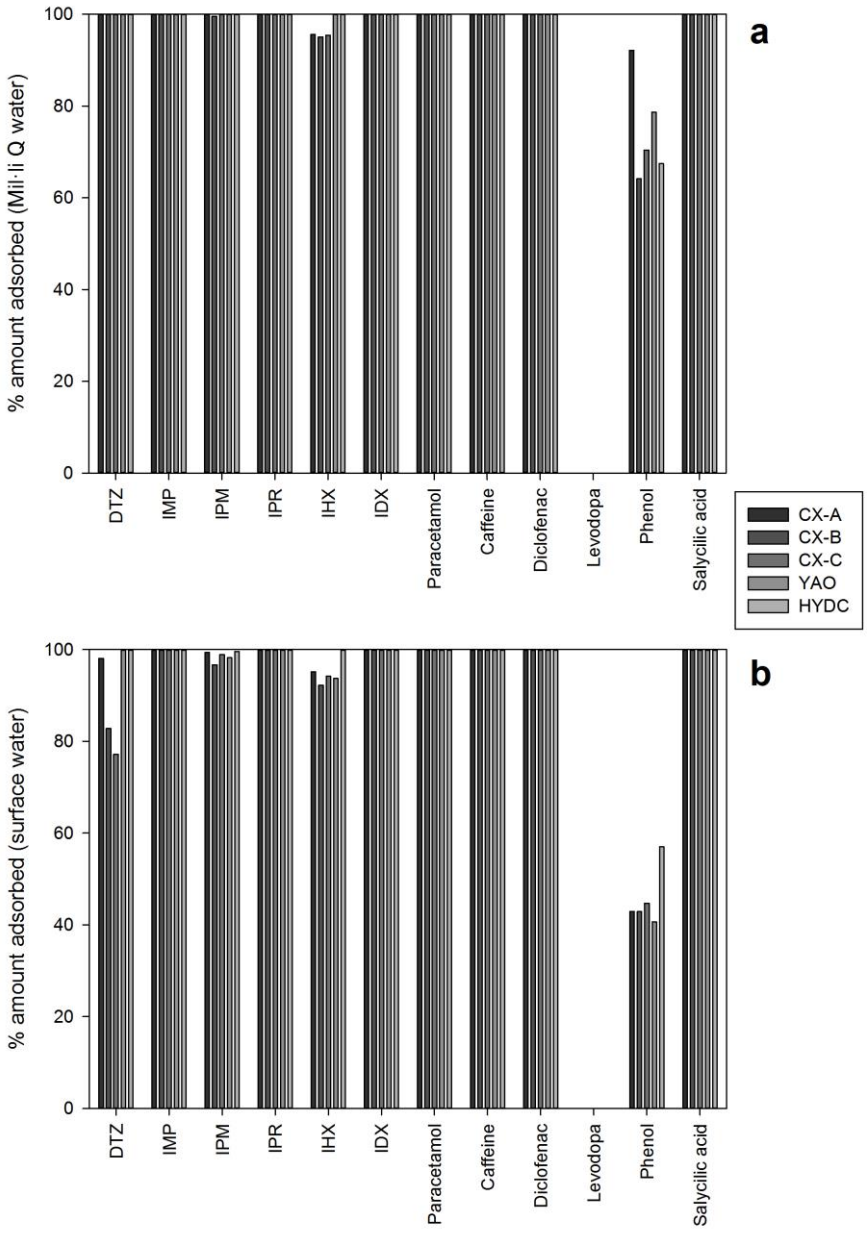

Figure SI 8. Multiadsorption of pharmaceuticals and ICM at 100 nmols a) mil·li Q water b) Surface water

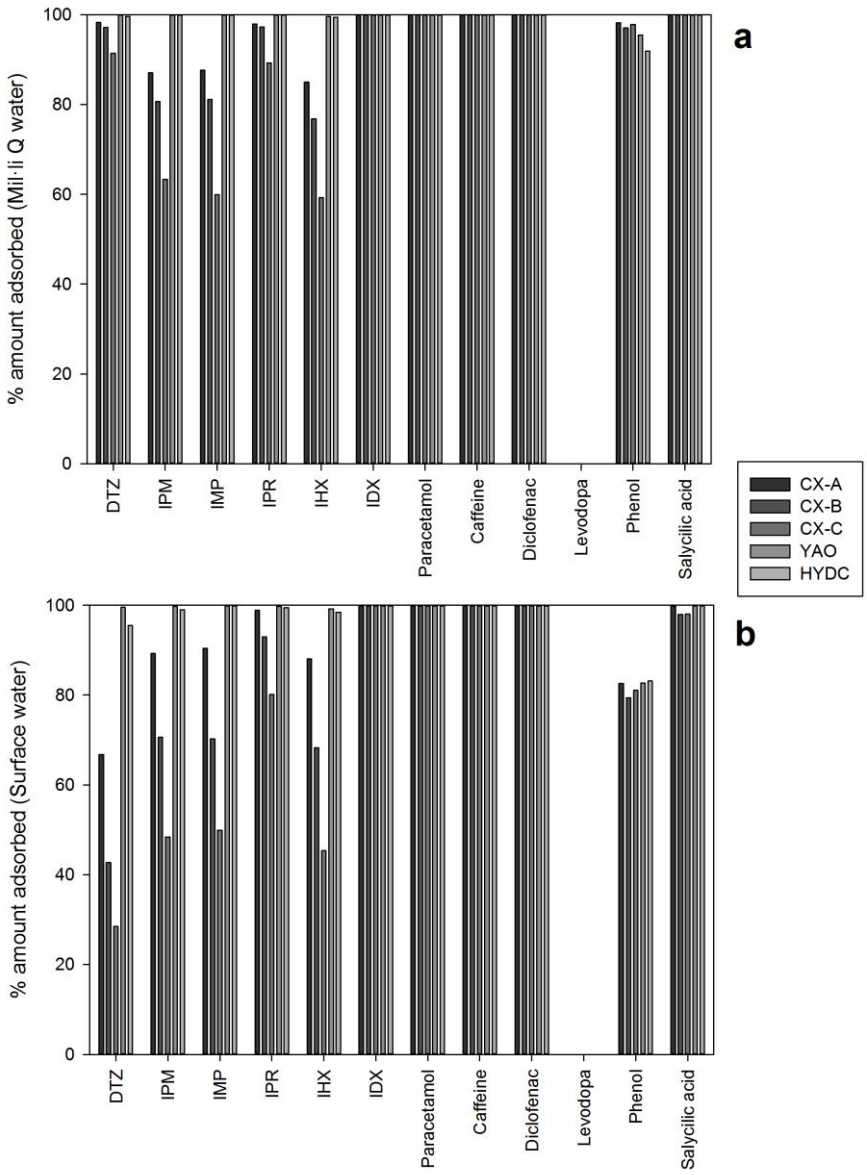

Figure SI 9. Multiadsorption of pharmaceuticals and ICM at 1 μmols a) mil·li Q water b) Surface water

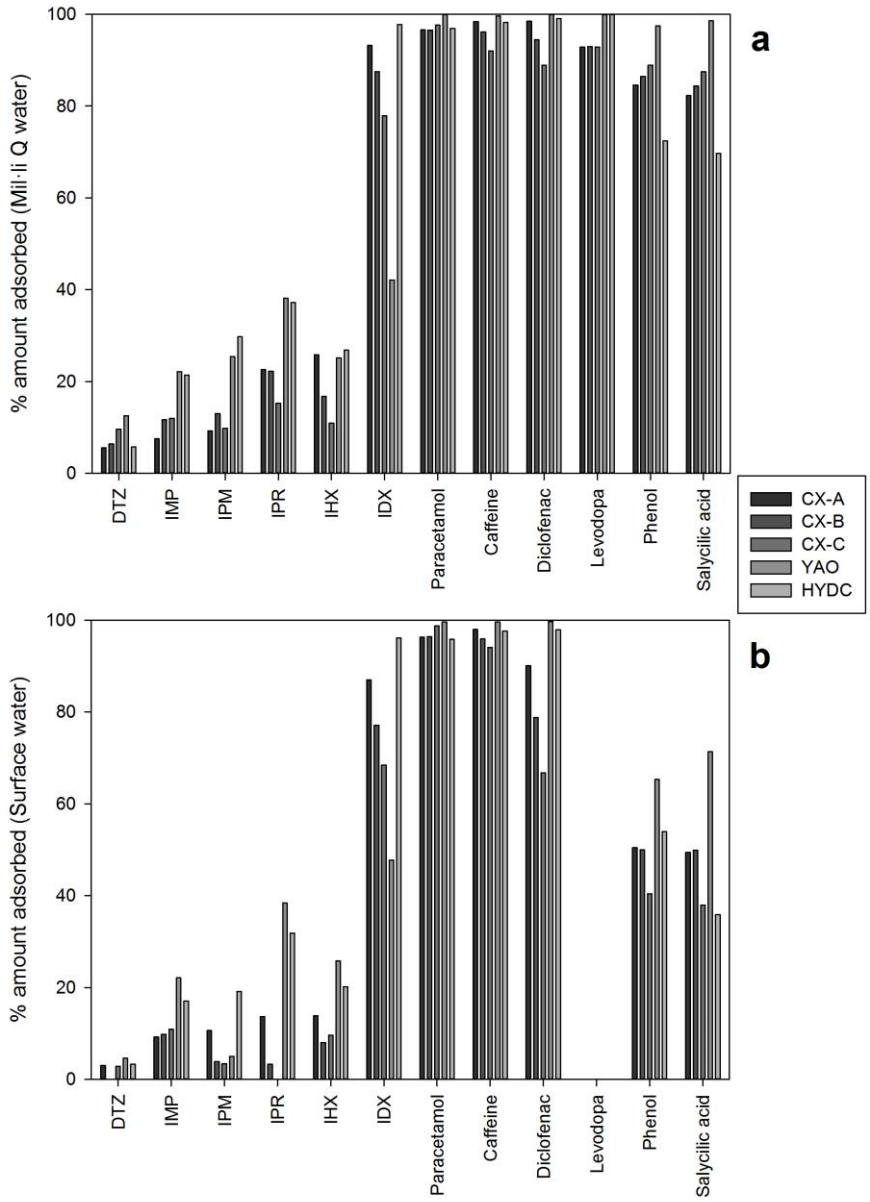

Figure SI 10 Multiadosrption of pharmaceuticals and ICM at 10 µmols a) mil·li Q water b) Surface water