

Supporting Information for

Understanding and Modeling Removal of Anionic Organic Contaminants (AOCs) by Anion Exchange Resins

Huichun Zhang*, Anthony J. Shields, Nastaran Jadbabaei, Maurice Nelson, Bingjun Pan and
Rominder P.S. Suri

Department of Civil and Environmental Engineering, Temple University
1947 North 12th Street, Philadelphia, PA 19122

*Corresponding Author, contact e-mail: hjzhang@temple.edu, phone: (215)204-4807, fax:
(215)204-4696

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Text S1. Polanyi Dubinin-Astakhov Model

The Polanyi theory was originally developed to account for sorption of gas molecules to porous materials.¹ It has been widely accepted as a powerful theory for the sorption of both gas and aqueous solutes toward heterogeneous surfaces and pores such as activated carbon and carbon nanomaterials.²⁻⁴ Briefly, the sorption potential (ε) in the theory was defined as the energy that is required to move a molecule from the attractive force field of the solid surface to bulk solution. The sorption potential varies with solute concentration and can be calculated by the following equation:

$$\varepsilon = -RT \ln(C_w / C_w^{sat}) \quad (S1)$$

where C_w^{sat} ($\mu\text{mol/L}$) is the aqueous solubility of the solute. In the Polanyi-Dubinin or Dubinin-Astakhov model (D-A model):⁵⁻⁷

$$\log q_e = \log Q^0 - \left(\frac{\varepsilon}{E_o}\right)^b \quad (S2)$$

Q^0 ($\mu\text{mol/g}$) is the maximum sorption capacity of the solute, and E_o and b are the fitting parameters. E_o (KJ/mol) is the correction factor and was supposed to account for all the interaction forces involved in sorption,^{3,4,8} b likely describes the heterogeneity of the interaction energy.⁹ The model fitting results are in Table S1.

Text S2. Calculation of $\Delta G_{S-W,i}$ for neutral compounds.

Similar to our recent work¹⁰:

$$\Delta G_{S-W,i} = -RT \ln K_{S-W,i} + \text{Const} \quad (S3)$$

$$\ln K_{S-W,i} = \ln \frac{1000 \times Q_e}{C_e} \quad (S4)$$

Based on Zhu and Pignatello 2005¹¹,

$$\text{Const} / RT = \ln \gamma_{w,i} + \ln \frac{V_w}{V_i} - \left[\left(1 - \frac{V_i}{V_s}\right) + X_{S-i} \right] \quad (S5)$$

where $\gamma_{w,i}$ is the solute activity coefficient in water; V_i , V_w , and V_s are the molar volumes of solute, water, and sorbent, respectively; and X_{S-i} is the Flory-Huggins solute-sorbent interaction parameter that corrects for the entropy loss upon mixing when the polymer suffers certain restriction on its orientation.¹² Given the non-ideal behavior of neutral OCs in water, we calculated $\gamma_{w,i}$ based on solute solubility and melting point¹³. Because there is entropy loss upon sorption, we assume $X_{S-i} = -1$. Given that $V_i \ll V_s$, Const/RT is calculated based on the eq below:

$$\text{Const} / RT = \ln \gamma_{w,i} + \ln \frac{\bar{V}_w}{\bar{V}_i} \quad (S6)$$

Text S3. Analytical methods.

Agilent Technologies 1200 Infinity Series HPLC was used to analyze aromatic solutes except BS. Each of the carboxylic acids has a pKa value between 2.3 and 4.5. Because of this, the mobile phase needed to be acidified to make sure speciation of the compounds resulted in predominately neutral species. This was performed using diluted phosphoric acid at a pH of 3.00. For the acidified mobile phases a Zorbax RX-C18 column was used. The neutral compounds used a mobile phase of nanopure water and methanol while using a Zorbax XDB-C18 column. The DAD detector was set at 230 – 382 nm.

UV/visible spectroscopy was used to measure the concentrations of benzenesulfonate at 215 nm. TOC analysis using a Shimadzu TOC-V_{CSH} was necessary to determine the concentrations of the aliphatic carboxylates which do not have sufficient ability for UV/Visible detection. Potassium hydrogen phthalate was used to calibrate the total carbon measurements from a range of 0.25 – 10 mg of carbon per liter. Injections of 100 µL were used to measure sample concentrations and were repeated three times for accuracy. Inorganic carbon tests were found to be negligible when measuring these samples. Concentrations from the TOC machine were converted from mg/L of carbon to molar concentrations based on the number of carbons within the compound. The detection limit of TOC analysis (~700 µM) was higher than the other two methods and thus was used only on compounds that are incapable of detection via the other analytical methods.

Text S4. Experiments on pH Effects.

For these experiments, solutions of 10-20 mL were prepared in amber bottles with Teflon sealed caps each with the same concentration of 2.0-5.0 mM benzoic acid (BA), nitrobenzene (NB) or benzenesulfonate (BS) and 0.020 M NaCl. These solutions were added to 10-70 mg of resin in order to achieve a removal percentage between 20-80% and placed on a shaker at 175 rpm. pHs were adjusted using either NaOH or HCl solutions and repeatedly adjusted over a 48 hour period to maintain a constant pH over the course of the experiment. Aliquots of the reactors were taken for initial and equilibrium concentrations. Samples were analyzed using HPLC (for BA and NB) or UV-spectrometry (for BS).

Text S5. Titration Experiments.

The resins were prepared by crushing with a mortar and pestle to shorten the time required to reach a pH equilibrium with the solution. 20 mL reactors were prepared of DI water and equal amounts of crushed resin. The solution of DI water and resin was allowed to reach an equilibrium pH where titration was then started by adding increasing increments of NaOH and HCl. The samples were then allowed to shake for 24-48 hours until a new pH equilibrium was achieved. pH's were then read from the pH meter and analyzed.

Table S1. Isotherm modeling results: a) D-A model fitting parameters:

Solute	C_w^{Sat} ($\mu\text{mol/L}$)*	IRA-910				IRA-96				A860			
		Q_0	E_0	b	R^2	Q_0	E_0	b	R^2	Q_0	E_0	b	R^2
BA	23700	3755	8.99	1.11	0.978	2912.3	9.74	1.34	0.995	1753	7.89	1.27	0.992
CBA	511	642	6.70	1.02	0.999	871	8.30	1.06	0.988	162	3.90	0.68	0.997
2-NBA	1480	1084	7.62	1.10	0.998	1182	8.81	1.16	0.998	220	5.49	0.95	0.999
4-NBA	1020	1232	7.18	1.02	0.999	1108	10.43	1.36	0.999	138	4.90	0.88	1.000
MBA	1970	942	6.87	1.05	0.999	706	8.65	1.36	0.998	209	5.67	1.05	1.000
Naph	635	774	7.51	1.12	1.000	553	10.20	1.54	0.989	205	4.70	0.82	0.999
BS	soluble ^a	2162290	6.12	1.01	0.972	5718	20.98	2.47	0.993	4608	18.73	2.35	0.997
IBU	soluble ^b	5029	13.54	1.60	0.998	—	—	—	—	—	—	—	—
Acetate	soluble ^c	441677	8.01	1.17	0.985	—	—	—	—	—	—	—	—
IB	soluble ^c	1982500	6.49	1.10	0.879	—	—	—	—	13711	16.11	1.66	0.984
DCA	soluble ^c	532887	12.57	1.50	0.965	—	—	—	—	249	31.51	11.45	0.887
NPN	115025	10544	15.78	1.54	0.989	—	—	—	—	—	—	—	—
2,6-DCP	46000	11220	13.73	1.68	1.000	—	—	—	—	—	—	—	—
PHTH	36114	1396	19.12	2.30	0.988	—	—	—	—	—	—	—	—
TERE	102	716	9.03	1.53	0.982	—	—	—	—	—	—	—	—
FLU	1000	424	5.53	1.00	0.975	—	—	—	—	—	—	—	—
CIP	90541	1523	15.78	1.63	0.994	—	—	—	—	—	—	—	—
4-CA	21596	693	7.37	1.18	0.994	2694	6.11	0.89	0.984	—	—	—	—
4-NA	5792	472	7.79	1.12	0.970	717	9.43	1.29	0.999	—	—	—	—
Phenol	852088	16299	6.10	1.00	0.999	9996	9.02	1.15	1.000	—	—	—	—
4-MP	175714	2983	7.67	1.11	1.000	1784	12.53	1.55	1.000	—	—	—	—
NB	16982	124	8.37	1.20	0.996	813	6.47	0.96	0.996	—	—	—	—

* For solutes with high solubility, the following hypothetical solubility was used in the D-A model fitting: ^a 5,162,000 $\mu\text{mol/L}$, ^b 100,000 $\mu\text{mol/L}$, and ^c 10^8 $\mu\text{mol/L}$. Although the obtained D-A model fitting parameters may be different from the real numbers, we mainly used them to estimate C_e at any given Q_e . Therefore, the selection of these solubility values should not affect later calculations.

b) Freundlich model ($q_i = K_F C_i^n$) fitting parameters ^a:

Solute	IRA-96			A860		
	K_f	n	R^2	K_f	n	R^2
Acetate	3.56	0.3763	0.919	0.5084	0.6	0.945
IB	0.891	0.590	0.817	—	—	—
DCA	0.44	0.994	0.879	—	—	—

^a For these isotherms, equilibrium concentrations were within a narrow range due to the analytical limitation in TOC analysis. Although the D-A model fittings were very good for these isotherms, larger errors in the predicted Q_e were observed particularly at lower equilibrium concentrations because the D-A model has three fitting parameters (data not shown). The Freundlich model with only two fitting parameters was thus applied to fit the isotherms.

Table S2. Linear correlation between experimentally used m/V (g/L) and Q_e ($\mu\text{mol/L}$).

Solute	IRA-910		IRA-96		A860	
	m/V=f(Q_e)	R ²	m/V=f(Q_e)	R ²	m/V=f(Q_e)	R ²
BA	$0.0036Q_e + 0.1542$	0.94	$0.0094Q_e + 0.8979$	0.90	$0.0108Q_e + 1.0521$	0.94
CBA	$0.0004Q_e + 0.1356$	0.92	$0.0008Q_e + 0.1921$	0.91	$0.1112Q_e + 3.7$	0.98
2-NBA	$0.0007Q_e + 0.1864$	0.82	$0.0008Q_e + 0.2731$	0.77	$0.0832Q_e + 2.3695$	0.77
4-NBA	$0.0004Q_e + 0.1322$	0.94	$0.0006Q_e + 0.1905$	0.93	$0.4939Q_e + 3.2088$	0.89
MBA	$0.0019Q_e + 0.3018$	0.92	$0.0011Q_e + 0.2701$	0.92	$0.0051Q_e + 3.7619$	0.42
Naph	$0.0004Q_e + 0.1303$	0.95	$0.0008Q_e + 0.2177$	0.92	$0.1033Q_e + 3.6244$	0.98
IBU	$0.0022Q_e + 0.257$	0.99	—	—	—	—
Acetate	$0.3301Q_e + 13.822$	0.87	$0.1992Q_e + 15.827$	0.84	$0.3118Q_e + 11.836$	0.78
IB	$0.26Q_e + 15.181$	0.77	$0.0919Q_e + 1.5519$	0.48	$0.1439Q_e + 6.084$	0.66
DCA	$0.0334Q_e + 8.9487$	0.91	$0.0068Q_e + 4.3451$	0.85	$0.0407Q_e + 4.8443$	0.82
NPN	$0.0001Q_e$	0.92	—	—	—	—
2,6-DCP	$0.0001Q_e + 0.0446$	0.91	—	—	—	—
PHTH	$0.0004Q_e$	0.72	—	—	—	—
TERE	$3E-05Q_e + 0.0246$	0.81	—	—	—	—
FLU	$0.0366Q_e + 0.9832$	0.79	—	—	—	—
CIP	$0.0292Q_e + 0.7091$	0.59	—	—	—	—
BS	$0.0024Q_e + 0.4362$	0.98	$0.0055Q_e + 1.0044$	0.89	$0.0196Q_e + 2.4618$	0.83

Table S3. Properties of the selected resins.

Name	Structure ^a	Functional Group ^a	Exchange Capacity (meq/g-dry) ^c	BET Surface Area ^a (m ² /g)	Moisture content % ^c
IRA-910	MP ^b , Polystyrene	Dimethyl ethanol Ammonium	5.33	NA	53.4 ± 0.2
IRA-96	MP ^b , Polystyrene	Tertiary amine	6.19	NA	58.8 ± 0.1
A860	MP ^b , polyacrylate	Quaternary Ammonium	7.13	NA	70.1 ± 0.1
MN100	MP ^b , Polystyrene	Tertiary amine	0.23	≥ 900	57.3 ± 0.1
MN200	MP ^b , Polystyrene	None	—	1021	57.6 ± 0.0

^a reported by the manufacturer, ^b macroporous, ^c this work.

Table S4. Regression coefficients of multiple linear regressions between $\ln(\alpha_{A/Cl})$ and solute descriptors for sorption of all anions except BS onto IRA-910. Q_e : $\mu\text{mol/g}$.

Q_e	c	e	s	b	v	j^-	R^2
1	-6.95±1.66	4.70±1.77	0.64±1.01	-1.88±0.84	0.39±0.88	3.52±1.45	0.890
2	-6.83±1.67	4.74±1.78	0.57±1.02	-1.73±0.84	0.32±0.89	3.37±1.46	0.886
5	-6.64±1.68	4.81±1.79	0.47±1.02	-1.55±0.85	0.25±0.89	3.19±1.47	0.880
10	-6.46±1.68	4.88±1.79	0.37±1.02	-1.44±0.85	0.20±0.89	3.08±1.47	0.876
20	-6.23±1.67	4.95±1.78	0.26±1.02	-1.34±0.84	0.15±0.89	2.98±1.46	0.872
50	-5.79±1.64	5.04±1.75	0.08±1.00	-1.25±0.83	0.10±0.87	2.87±1.43	0.867
100	-5.25±1.58	5.08±1.70	-0.09±0.96	-1.21±0.80	0.07±0.84	2.80±1.38	0.862
200	-4.28±1.47	5.01±1.58	-0.32±0.90	-1.16±0.78	0.02±0.78	2.69±1.29	0.854
500	-1.81±1.27	4.43±1.36	-0.70±0.77	-1.07±0.67	-0.01±0.67	2.34±1.11	0.807

Table S5. The corresponding p-values for the regression coefficients in Table S4. Q_e : $\mu\text{mol/g}$.

Q_e	c	e	s	b	v	j^-
1	0.002	0.026	0.54	0.052	0.669	0.038
2	0.003	0.026	0.586	0.071	0.723	0.046
5	0.003	0.025	0.659	0.101	0.788	0.057
10	0.004	0.024	0.725	0.125	0.831	0.065
20	0.005	0.022	0.804	0.146	0.869	0.072
50	0.006	0.018	0.936	0.164	0.909	0.076
100	0.009	0.015	0.928	0.165	0.938	0.074
200	0.018	0.011	0.732	0.153	0.978	0.067
500	0.187	0.01	0.386	0.128	0.985	0.064

Table S6. Three sets of regression coefficients for the multiple linear regressions between the net Gibbs free energy change and solute descriptors for IRA-910 with the following compounds included in the regressions: a) all solutes except BS, b) 16 solutes in the training set, and c) all anions except BS.

Set	Q_e	c	e	s	a	b	v	j^-	R^2
a) All Solute	1	-18.21±2.14	10.07±2.78	1.98±1.47	18.09±4.22	-4.64±1.72	0.50±1.55	9.40±3.05	0.917
	2	-18.07±2.15	10.12±2.78	1.85±1.47	17.93±4.23	-4.26±1.72	0.30±1.55	9.06±3.06	0.916
	5	-17.89±2.15	10.13±2.79	1.70±1.48	17.78±4.23	-3.80±1.72	0.03±1.56	8.66±3.06	0.914
	10	-17.75±2.15	10.08±2.79	1.60±1.48	17.75±4.24	-3.49±1.72	-0.20±1.56	8.40±3.06	0.912
	20	-17.59±2.15	9.97±2.79	1.51±1.48	17.80±4.23	-3.21±1.72	-0.45±1.55	8.18±3.06	0.911
	50	-17.32±2.14	9.60±2.77	1.45±1.47	18.10±4.21	-2.89±1.72	-0.84±1.55	7.96±3.05	0.909
	100	-16.10±2.13	8.94±2.77	1.51±1.47	18.72±4.21	-2.66±1.71	-1.28±1.55	7.82±3.04	0.907
	200	-13.88±2.78	8.93±2.94	0.82±1.61	13.42±6.43	-2.50±1.69	-1.25±1.62	7.22±3.01	0.862
	500	-9.05±2.75	6.13±2.91	0.93±1.60	9.51±6.37	-1.77±1.69	-1.99±1.60	5.59±3.05	0.817
b) Training Set	1	-17.42±2.85	10.63±3.52	2.07±1.78	17.71±5.38	-4.82±2.18	-0.98±2.19	9.55±3.80	0.906
	2	-17.35±2.90	10.62±3.59	1.92±1.82	17.58±5.48	-4.43±2.22	-0.98±2.23	9.2±3.872	0.902
	5	-17.29±2.96	10.51±3.67	1.74±1.86	17.52±5.60	-3.94±2.27	-0.98±2.28	8.80±3.95	0.898
	10	-17.26±3.00	10.34±3.71	1.63±1.88	17.59±5.67	-3.58±2.29	-0.99±2.30	8.48±4.00	0.895
	20	-17.26±3.02	10.07±3.74	1.56±1.89	17.79±5.71	-3.23±2.31	-0.98±2.32	8.17±4.03	0.893
	50	-17.26±3.03	9.44±3.75	1.55±1.90	18.37±5.73	-2.77±2.32	-1.00±2.33	7.74±4.04	0.892
	100	-17.24±3.01	8.50±3.73	1.70±1.89	19.37±5.70	-2.37±2.30	-1.11±2.32	7.33±4.02	0.893
	200	-14.31±4.23	8.26±4.10	1.03±2.24	14.37±9.37	-2.16±2.34	-0.89±2.40	6.75±4.04	0.828
	500	-10.72±4.11	4.76±3.98	1.62±2.20	13.06±9.22	-1.11±2.28	-1.31±2.33	4.61±3.97	0.793
c) All Anions	1	-17.21±4.10	11.64±4.39	1.59±2.50	—	-4.65±2.07	0.96±2.18	8.72±3.59	0.890
	2	-16.92±4.13	11.75±4.41	1.42±2.52	—	-4.28±2.09	0.80±2.20	8.35±3.61	0.886
	5	-16.45±4.15	11.92±4.44	1.16±2.53	—	-3.84±2.10	0.61±2.21	7.91±3.63	0.880
	10	-16.00±4.15	12.08±4.44	0.92±2.53	—	-3.56±2.10	0.48±2.21	7.63±3.63	0.876
	20	-15.43±4.13	12.26±4.42	0.65±2.52	—	-3.32±2.09	0.37±2.20	7.38±2.62	0.872
	50	-14.35±4.05	12.49±4.33	0.20±2.47	—	-3.10±2.05	0.25±2.16	7.11±3.54	0.867
	100	-13.00±3.92	12.58±4.18	-0.22±2.39	—	-2.99±1.98	0.17±2.08	6.93±3.42	0.862
	200	-10.60±3.65	12.42±3.90	-0.79±2.23	—	-2.89±1.85	0.06±1.94	6.65±3.20	0.854
	500	-4.48±3.14	10.98±3.36	-1.75±1.92	—	-2.66±1.59	-0.03±1.67	5.81±2.75	0.807

Table S7. The corresponding p-values for the regression coefficients in Table S6.

Set	Q_e	c	e	s	a	b	v	j^-
a) All Solutes	1	0	0.003	0.203	0.001	0.018	0.754	0.009
	2	0	0.003	0.231	0.001	0.028	0.849	0.011
	5	0	0.003	0.27	0.001	0.046	0.987	0.014
	10	0	0.003	0.299	0.001	0.064	0.901	0.017
	20	0	0.003	0.324	0.001	0.085	0.779	0.019
	50	0	0.004	0.341	0.001	0.116	0.595	0.021
	100	0	0.007	0.322	0.001	0.145	0.423	0.023
	200	0	0.01	0.618	0.059	0.166	0.455	0.034
	500	0.007	0.059	0.576	0.164	0.318	0.242	0.094
b) Training Set	1	0	0.014	0.276	0.009	0.054	0.666	0.033
	2	0	0.016	0.319	0.011	0.077	0.67	0.041
	5	0	0.019	0.374	0.012	0.116	0.676	0.053
	10	0	0.021	0.409	0.013	0.153	0.681	0.063
	20	0	0.025	0.433	0.012	0.196	0.685	0.073
	50	0	0.033	0.435	0.011	0.263	0.678	0.088
	100	0	0.048	0.39	0.008	0.33	0.642	0.102
	200	0.01	0.079	0.658	0.164	0.383	0.72	0.133
	500	0.035	0.271	0.486	0.2	0.643	0.591	0.285
c) All Anions	1	0.002	0.026	0.54	—	0.052	0.669	0.038
	2	0.003	0.026	0.586	—	0.071	0.723	0.046
	5	0.003	0.025	0.659	—	0.101	0.788	0.057
	10	0.004	0.024	0.725	—	0.125	0.831	0.065
	20	0.005	0.022	0.804	—	0.146	0.869	0.072
	50	0.006	0.018	0.936	—	0.164	0.909	0.076
	100	0.009	0.015	0.928	—	0.165	0.938	0.074
	200	0.018	0.011	0.732	—	0.153	0.978	0.067
	500	0.187	0.01	0.386	—	0.128	0.985	0.064

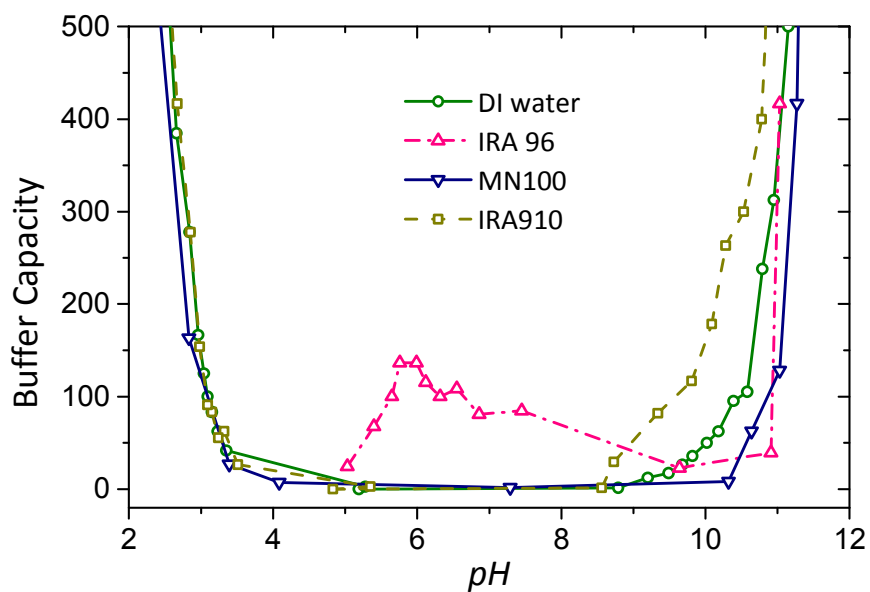


Figure S1. The buffering capacities for IRA910, IRA96, and MN100.

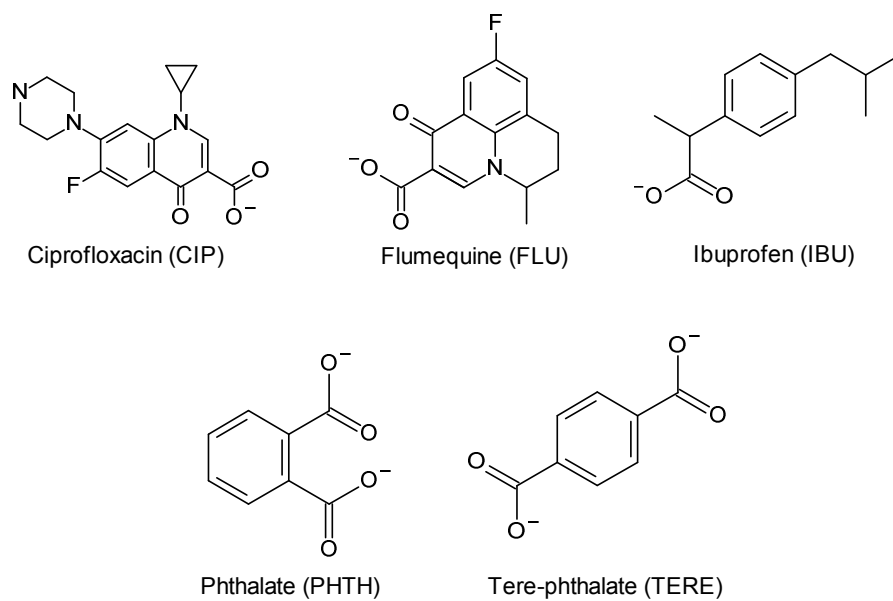


Figure S2. Structures of selected anions.

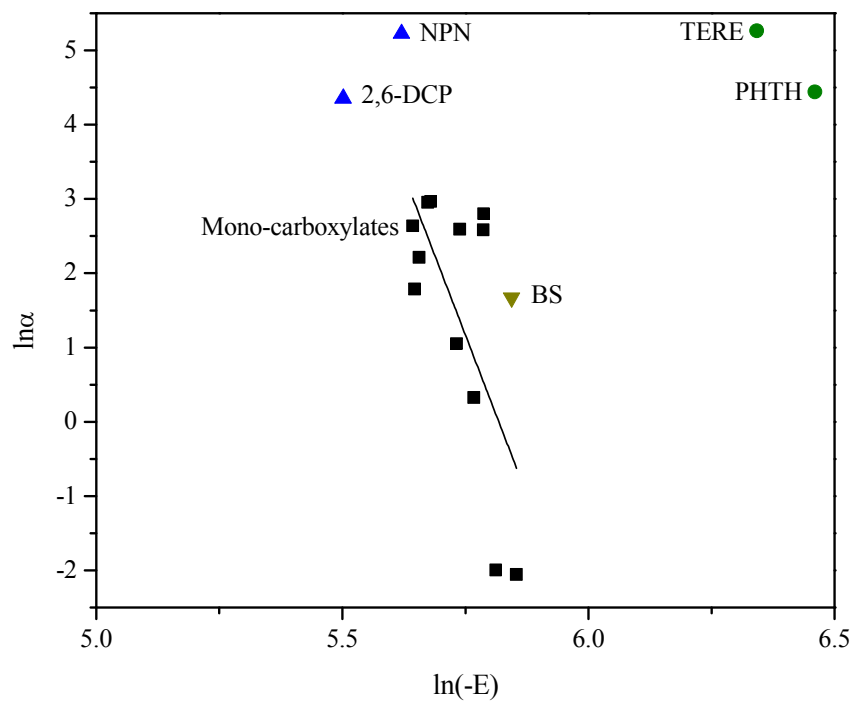
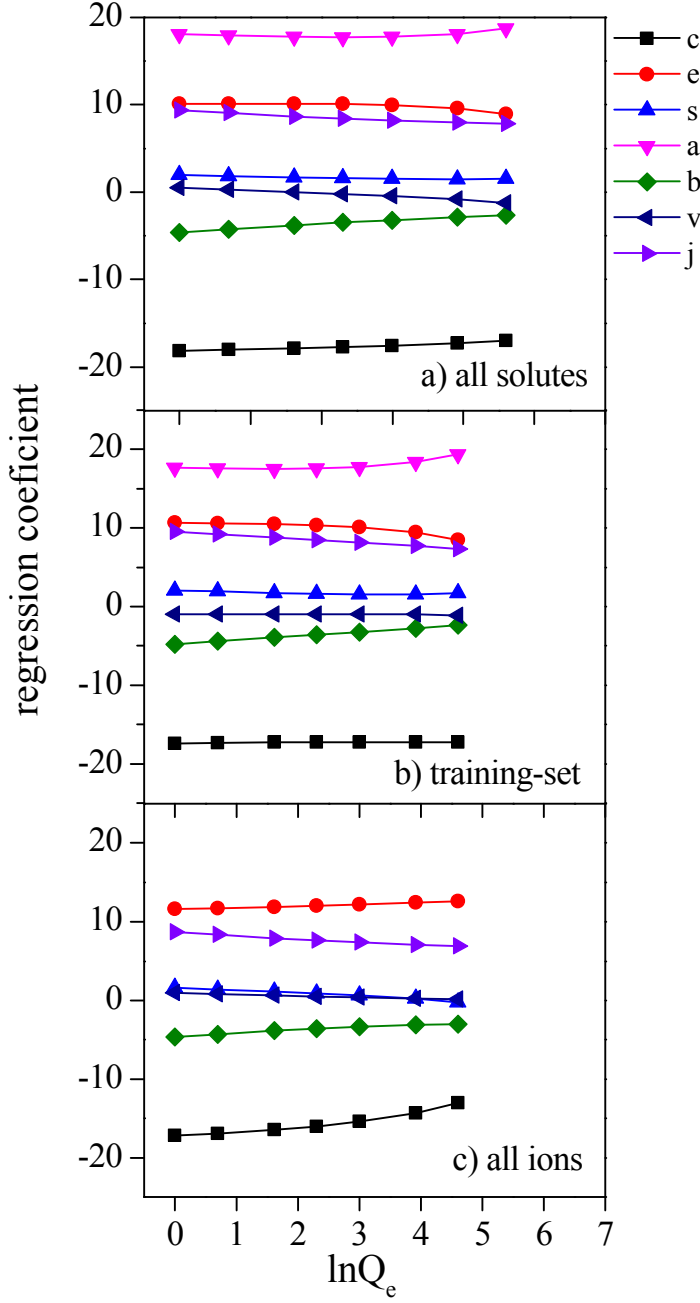


Figure S3. Relationship between selectivity (at $Q_e = 50 \mu\text{mol/g}$) and hydration energy for all anions, the regression is for mono-carboxylates only ($\ln\alpha = -17.24\ln(-E) + 100.3$, $R^2=0.45$).



a) All solutes included:

$$c = -2 \times 10^{-7} Q_e^3 + 0.0001 Q_e^2 + 0.0016 Q_e - 17.932, R^2 = 0.995$$

$$e = -1 \times 10^{-7} Q_e^3 + 0.00008 Q_e^2 - 0.0183 Q_e + 10.206, R^2 = 0.995$$

$$s = 0.008 (\ln Q_e)^3 - 0.02791 (\ln Q_e)^2 - 0.1432 (\ln Q_e) + 1.9709, R^2 = 0.999$$

$$a = 0.0141 (\ln Q_e)^3 + 0.0049 (\ln Q_e)^2 - 0.2333 (\ln Q_e) + 18.085, R^2 = 0.999$$

$$b = 0.0131 (\ln Q_e)^3 - 0.125 (\ln Q_e)^2 + 0.7308 (\ln Q_e) - 4.6707, R^2 = 0.999$$

$$v = -0.0103(\ln Q_e)^3 + 0.034(\ln Q_e)^2 - 0.3243(\ln Q_e) + 0.5024, R^2 = 0.999$$

$$j^- = -0.0005(\ln Q_e)^3 + 0.0424(\ln Q_e)^2 - 0.5298(\ln Q_e) + 9.4051, R^2 = 0.999$$

b) Training-set solutes included:

$$c = -3 \times 10^{-7} Q_e^3 + 0.0002 Q_e^2 - 0.015 Q_e - 17.218, R^2 = 0.995$$

$$e = -2 \times 10^{-7} Q_e^3 + 0.0002 Q_e^2 - 0.0341 Q_e + 10.685, R^2 = 0.999$$

$$s = 0.0118(\ln Q_e)^3 - 0.0324(\ln Q_e)^2 - 0.1808(\ln Q_e) + 2.0633, R^2 = 0.997$$

$$a = 0.0383(\ln Q_e)^3 - 0.0838(\ln Q_e)^2 - 0.0676(\ln Q_e) + 17.689, R^2 = 0.997$$

$$b = 0.0142(\ln Q_e)^3 - 0.1119(\ln Q_e)^2 + 0.7396(\ln Q_e) - 4.8562, R^2 = 0.995$$

$$v = 5E-08(\ln Q_e)^3 - 3E-05(\ln Q_e)^2 + 0.0009(\ln Q_e) - 0.9831, R^2 = 0.999$$

$$j^- = -0.0451(\ln Q_e)^3 + 0.3096(\ln Q_e)^2 - 0.9718(\ln Q_e) + 9.6444, R^2 = 0.991$$

c) All anions included:

$$c = -2 \times 10^{-7} Q_e^3 - 0.0002 Q_e^2 + 0.0559 Q_e - 16.835, R^2 = 0.996$$

$$e = -0.0198(\ln Q_e)^3 + 0.1373(\ln Q_e)^2 - 0.0242(\ln Q_e) + 11.668, R^2 = 0.99$$

$$s = -0.0102(\ln Q_e)^3 + 0.0249(\ln Q_e)^2 - 0.2977(\ln Q_e) + 1.605, R^2 = 0.9999$$

$$b = 0.0053(\ln Q_e)^3 - 0.857(\ln Q_e)^2 + 0.6493(\ln Q_e) - 4.6656, R^2 = 0.996$$

$$v = -0.0012(\ln Q_e)^3 + 0.0219(\ln Q_e)^2 - 0.2507(\ln Q_e) + 0.9639, R^2 = 0.999$$

$$j^- = -0.0199(\ln Q_e)^3 + 0.1755(\ln Q_e)^2 - 0.7877(\ln Q_e) + 8.7614, R^2 = 0.999$$

Figure S4. Correlations of the regression coefficients c , e , s , b , v , and j^- with Q_e for IRA-910 when a) all solutes; b) solutes in the training set; and c) all anions were included in the regressions. When only anions were involved in the model development, RMSE=1.44 when comparing the predicted C_e values with the experimental C_e values (data not shown).

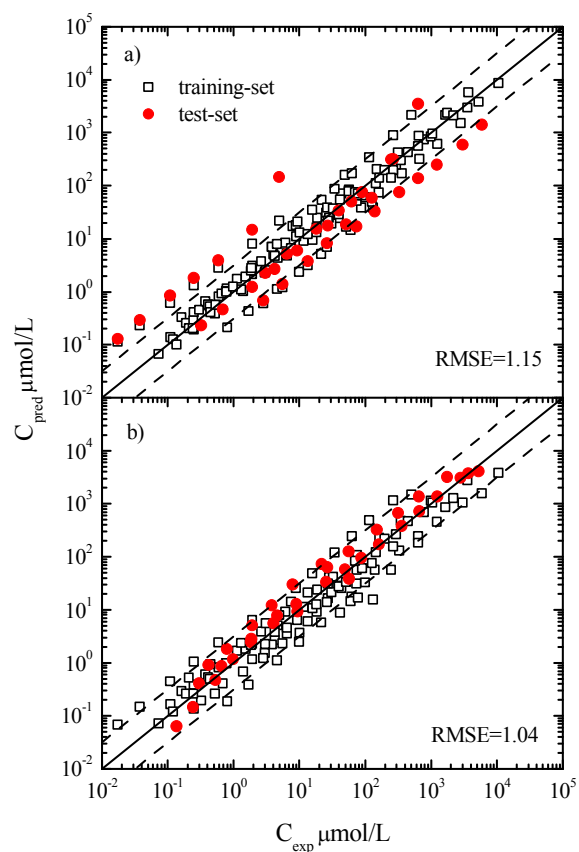


Figure S5. Model development with 16 solutes in the training set (a. 230 or b. 217 data points), a) the test set: acetate, FLU, 4-NA, 2-NBA, and NPN (73 data points), and b) the test set: CBA, 2,6-DCP, IB, IBU, and Phenol (86 data points). The test compounds in red circles were accurately predicted within the range of the training set of compounds. The solid lines show a perfect prediction, where the predicted values for C_e exactly equal the experimental values; the dashed lines are 0.5 log units above or below the solid lines.

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