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11 Supporting Information

12 Table S1. Values of seven ion characteristics for all metals or metalloids

Metals	σp	$\log\beta_n$	$X_m^2 r$	AN/ ΔIP	Z/r	$ \log K_{OH} $	ΔE_0
Ag	0.074	20.6	4.284	6.209	0.87	12.4	0.80
Al	0.136	14.11	1.4	1.351	5.556	4.3	1.66
As(III)	0.106	19.3	2.756	3.395	5.172	2.2	0.68
Ba	0.183	7.78	1.069	11.69	1.481	13.4	2.9
Be	0.172	9.3	1.109	0.45	4.444	3.7	1.85
Ca	0.181	11	1	3.47	2.02	12.7	2.76
Cd	0.081	18.78	2.713	6.068	2.105	10.1	0.4
Co	0.13	10.2	2.65	2.94	2.685	9.7	0.28
Cr(III)	0.107	11.2	1.708	1.66	4.839	4.0	0.41
Cr(VI)	0.107	11.2	1.212	1.134	13.64	4.0	0.13
Cu	0.104	18.5	2.635	2.309	2.74	8.0	0.16
Fe(III)	0.103	15.77	1.842	1.798	5.455	2.2	0.77
Hg	0.065	21.7	4.08	9.62	1.96	3.4	0.91
K	0.232	1.6	0.93	4.38	0.725	14.5	2.92
La	0.171	15.5	1.27	7.36	2.828	8.5	2.37
Li	0.247	2.79	0.71	0.56	1.316	13.6	3.05
Mg	0.167	8.64	1.24	1.62	2.778	11.6	2.38
Mn	0.125	14.2	1.61	3.045	2.985	10.6	1.185
Na	0.211	1.66	0.88	2.14	0.98	14.2	2.71
Ni	0.126	11.33	2.517	2.662	2.899	9.9	0.23
Pb	0.131	18.3	6.46	10.78	1.681	7.7	0.126
Sb	0.119	10.9	3.194	6.439	3.947	0	0.66
Sr	0.174	8.8	1.02	7.12	1.786	13.2	2.89
Tl	0.097	18.47	3.557	5.133	2.67	2.6	0.502
Zn	0.115	16.4	2.015	3.501	2.703	8.2	0.76

14 Table S2. Acute toxicities of 25 metals or metalloids to representative species from eight taxonomic
15 families (log-EC₅₀)

Metals	<i>C. tentans</i>	<i>C. pseudogracilis</i>	<i>D. magna</i>	<i>L. acuminata</i>	<i>C. carpio</i>	<i>B. calyciflorus</i>	<i>B. melanostictus</i>	<i>L. minor</i>
Ag	-0.194	-0.615	-0.832	-2.225	-0.326	-1.12	-1.193	0.998
Al	2.524	3.495	1.487	2.853	3.678	1.707	3.763	3.832
As(III)	0.901	0.986	-0.37	0.409	2.517	0.399	1.427	1.618
Ba	4.796	6.97	3.753	6.019	3.571	2.577	4.61	6.859
Be	4.258	6.147	3.209	3.268	4.424	3.202	4.47	5.015
Ca	4.257	6.073	2.595	4.219	4.888	1.698	4.704	6.6
Cd	0.276	0.125	-0.18	1.135	0.417	-0.32	1.321	0.575
Co	2.942	4.25	2.897	0.53	2.295	2.269	1.76	1.62
Cr(III)	2.145	3.083	2.543	2.261	2.413	2.605	3.078	1.24
Cr(VI)	0.653	0.978	2.557	3.208	4.267	2.605	3.488	-0.503
Cu	2.66	3.804	2.491	0.751	2.249	1.911	1.941	1.446
Fe(III)	1.347	1.763	0.899	2.004	2.533	1.447	2.84	1.678
Hg	-0.612	-1.252	-1.226	-0.976	-0.178	-0.447	-0.935	0.938
K	7.102	10.49	5.965	4.586	4.898	4.29	5.168	8.113
La	3.3	4.532	0.978	4.558	3.725	0.828	4.211	5.767
Li	7.345	10.78	5.532	4.156	5.643	4.037	5.618	8.682
Mg	4.217	6.116	3.448	3.263	3.57	2.521	4.23	5.682
Mn	2.201	3.036	1.458	2.801	2.251	0.981	3.357	2.855
Na	6.502	9.636	5.949	4.163	4.301	4.306	5.101	7.274
Ni	0.965	1.11	-0.08	0.413	1.448	-0.01	1.603	0.791
Pb	1.755	2.233	-0.02	1.396	5.663	0.085	1.791	1.421
Sb	2.527	3.636	2.648	0.184	2.447	3.138	0.83	1.913
Sr	4.39	6.353	3.389	5.041	3.396	2.296	4.624	6.619
Tl	0.773	0.839	-0.07	-0.91	1.185	0.601	0.108	1.127
Zn	1.59	2.08	0.669	2.034	1.8	0.594	2.652	1.963

16 Table S3. SSD fitting parameters and CMCs derivation for 25 metals or metalloids ($\mu\text{g/L}$), with coefficients, standard error, RSS, F and P values.

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Metals	a	Xc	k	$a-SE$	$Xc-SE$	$k-SE$	Adj. r^2	RSS	F	P	log-HC ₅	AW	CMCs	WQC
Ag	0.9545	-0.7612	2.573	0.0441	0.0552	0.3132	0.9823	0.0083	531.434	1.50×10^{-6}	-1.8865	107	0.695	3.2
Al	923.498	12.268	0.8280	0.0001	1406.4	0.5155	0.9418	0.0273	160.494	2.91×10^{-5}	0.4035	27	34.18	750
As(III)	0.9758	0.9257	2.0628	0.0659	0.0959	0.3222	0.9734	0.0125	352.93	4.15×10^{-6}	-0.4892	75	12.16	340
Ba	0.9387	4.655	1.04	0.1049	0.3305	0.2747	0.9546	0.0213	206.452	1.57×10^{-5}	1.8879	137	5292	/
Be	0.9935	4.1851	1.6012	0.1234	0.2234	0.409	0.9067	0.0437	99.542	9.40×10^{-5}	2.3505	4	448.3	/
Ca	1.0816	4.6755	0.929	0.1936	0.479	0.2874	0.9437	0.0264	166.21	2.67×10^{-5}	1.4173	40	522.8	/
Cd	0.9146	0.2901	3.5246	0.0409	0.042	0.4779	0.981	0.0089	494.711	1.79×10^{-6}	-0.5186	112	16.97	2
Co	0.9617	2.2409	1.8697	0.0682	0.1124	0.3312	0.9655	0.0162	272.42	7.89×10^{-6}	0.688	59	143.8	/
Cr(III)	0.9147	2.4172	4.7783	0.0557	0.0404	0.9387	0.9699	0.0141	312.564	5.61×10^{-6}	1.1656	52	380.7	570
Cr(VI)	1.539	3.5298	0.6637	0.6118	1.2343	0.1768	0.9596	0.019	231.794	1.18×10^{-5}	-1.5837	52	0.678	16
Cu	1.2362	1.0483	1.9225	0.2293	0.2242	0.3665	0.9776	0.0105	420.478	2.69×10^{-6}	-0.5988	64	8.06	13
Fe	0.908	1.6699	3.477	0.0386	0.0411	0.482	0.9818	0.0085	517.632	1.60×10^{-6}	0.8524	56	199.3	/
Hg	0.9273	-0.7808	3.3526	0.0593	0.0647	0.5625	0.9594	0.019	231.176	1.18×10^{-5}	-1.6352	201	2.328	1.4
K	0.8819	5.5426	1.157	0.0672	0.2544	0.2983	0.9353	0.0303	144.28	3.79×10^{-5}	3.1124	39	25263	/
La	1.2924	4.3943	0.8022	0.4173	0.8948	0.2916	0.9237	0.0358	122.172	5.69×10^{-5}	0.3894	139	170.4	/
Li	0.8987	5.7567	0.9453	0.0828	0.3412	0.2919	0.9135	0.0406	107.513	7.79×10^{-5}	2.7612	7	2019	/
Mg	0.8873	3.7525	1.9811	0.0548	0.1118	0.4185	0.9518	0.0226	194.072	1.82×10^{-5}	2.3300	24	2565	/
Mn	1.7877	3.2607	1.2941	0.9485	0.7922	0.3552	0.9669	0.0155	283.517	7.14×10^{-6}	0.5188	55	90.81	/
Na	0.9391	5.4775	1.0534	0.083	0.2785	0.2288	0.9343	0.0308	141.974	3.94×10^{-5}	2.7452	23	6396	/
Ni	0.9664	2.0934	2.4283	0.0487	0.0616	0.3178	0.9799	0.0094	468.199	2.06×10^{-6}	0.8957	59	232	470
Pb	0.9648	1.5224	1.9592	0.0869	0.14	0.5812	0.9148	0.0399	109.203	7.49×10^{-5}	0.0388	207	113.2	65
Sb	1.367	2.8647	1.1087	0.4263	0.6144	0.3247	0.9537	0.0217	202.104	1.65×10^{-5}	-0.0857	51	20.93	/
Sr	0.9595	4.3693	1.1481	0.0829	0.2228	0.2338	0.9632	0.0173	254.99	9.29×10^{-6}	1.8426	88	3063	/
Tl	3.7912	2.0502	1.334	6.469	1.9196	0.4097	0.9757	0.0114	386.453	3.31×10^{-6}	-1.1845	204	6.669	/
Zn	1.1602	1.9188	2.237	0.2848	0.2535	0.8688	0.9061	0.0465	98.865	9.55×10^{-5}	0.5330	65	110.9	120

Table S4. Correlations between metal ion characteristics and predicted log-HC₅, with intercept, slope, coefficients values, F , P and Ranks.

Metals	σp	$\log\beta_n$	ΔE_0	$X_m^2 r$	$\log K_{OH}$	Z/r	$AN/\Delta IP$
Intercept	-3.0211	3.3881	-0.7015	2.1214	-0.7487	1.2523	1.1577
Intercept-SE	0.4358	0.3735	0.3161	0.4219	0.5273	0.4457	0.4841
Slope	26.408	-0.2162	0.9998	-0.6886	0.1694	-0.1914	-0.1216
Slope-SE	2.9782	0.0269	0.1853	0.1663	0.0567	0.1089	0.0918
Adj.R^2	0.7638	0.7265	0.5394	0.4022	0.2481	0.0801	0.0306
F	78.626	64.760	29.104	17.147	8.918	3.089	1.756
P	7.02×10^9	3.88×10^8	1.76×10^5	3.96×10^4	0.0066	0.0921	0.1981
Ranks	1	2	3	4	5	6	7