

Supporting Information (SI)

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Metal bioaccumulation in aquatic species: quantification of uptake and elimination rate constants using physico-chemical properties of metals and physiological characteristics of species

This Supporting Information contains 5 Tables and 1 Figure.

Metal ion characteristics

Covalent indices ($\chi^2_m r$) were calculated using Pauling's electronegativity values (χ_m) provided by Allred (1) and effective ionic radii (r) (in Ångstrom units) corresponding to octahedral coordination from Shannon and Prewitt (2,3). Electronegativity values for the correct oxidation state of the metal-ion were used, except for Cr (III) and Cu (II) as χ_m is provided for Cr (II) and Cu (I) only. For lead an ionic radius of 0.94 Å, corresponding to tetrahedral coordination, was used as the resulting covalent index is more in line with the known solution coordination chemistry of Pb²⁺ (4). Electronegativity data, ionic radii and covalent indices compiled per metal included in this study are presented in Table SI-S1.

Table SI-S1: Metal ion characteristics: electronegativity values, ionic radii and covalent indices

Metal	Ionic radius	Electronegativity	Covalent index
	r (in Å)	χ_m	$\chi^2_m r$
Ag ⁺	1.15	1.93	4.28
Cd ²⁺	0.95	1.69	2.71
Co ²⁺	0.75*	1.88	2.65
Cr ³⁺	0.62	1.66**	1.69
Cs ⁺	1.7	0.79	1.06
Cu ²⁺	0.73	1.9***	3.29
Hg ²⁺	1.02	2	4.08
Ni ²⁺	0.69	1.91	2.52
Pb ²⁺	0.94****	1.87	3.29
Zn ²⁺	0.74	1.65	2.01

* Ionic radius for high spin state of Co²⁺, radius for low spin state is 0.65 Å

** Electronegativity value for Cr²⁺ instead of Cr³⁺

*** Electronegativity value for Cu⁺ instead of Cu²⁺

**** Ionic radius of Pb²⁺ for tetrahedral coordination instead of octahedral coordination (19)

Filtration rates

Absorption efficiencies for mollusks were preferentially calculated using filtration rates determined in the same study as the absorption rate constants. These filtration rates were available for the following studies: Shi and Wang (5,6) (*Ruditapes philippinarum*, *Perna viridis*), Ng and Wang (7) (*Perna viridis*), Baines et al., (8) (*Mytilus edulis*), Wang and Fisher (9) (*Macoma balthica*, *Mytilus edulis*) and Wang et al. (10) (*Mytilus edulis*).

For other data, filtration rates from table SI-S2 were used. The filtration rate used for *Daphnia magna* is also provided in this table.

Table SI-S2. Species – specific filtration rates used

Species	Filtration rate $L \cdot kg^{-1} \text{ wet weight} \cdot d^{-1}$	References
<i>Perna viridis</i>	$2.9 \cdot 10^4$	Geometric mean (n = 39), this study 5,7
<i>Mytilus edulis</i>	$1.8 \cdot 10^4$	11
<i>Ruditapes philippinarum</i>	$6.9 \cdot 10^3$	Geometric mean (n = 2), this study 6
<i>Dreissena polymorpha</i>	$2.5 \cdot 10^4$	12
<i>Macoma balthica</i>	$9.0 \cdot 10^3$	9
<i>Daphnia magna</i>	$3.3 \cdot 10^4$	Geometric mean (n = 4), this study 13,14,15,16

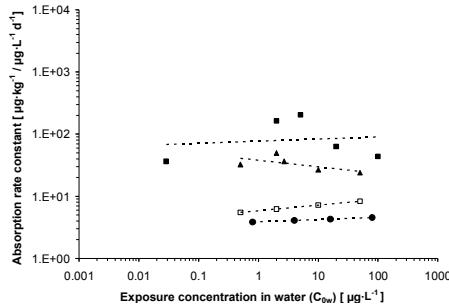
Absorption rate constants and exposure concentration in water

In our approach absorption rate constants determined at different exposure concentrations were combined to calculate mean species – specific absorption rate constants. This is only allowed if absorption rate constants are independent of the exposure concentration in water. We found that metal influx from the dissolved phase is generally linearly related to the dissolved metal concentration in water under laboratory conditions (Figure SI-S1, Table SI-S3). Absorption rate constants determined at different exposure concentrations can therefore be combined.

Figure SI-S1. Metal absorption rate constants ($k_{X,w,in}$ in $\text{L}\cdot\text{kg}^{-1}\cdot\text{d}^{-1}$) vs. exposure concentrations in water (C_{0w} in $\mu\text{g}\cdot\text{L}^{-1}$). Absorption rate constants are plotted against exposure concentration, if rate constants are determined at three or more exposure concentrations.

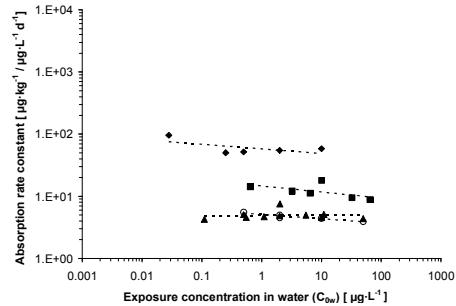
a. *Perna viridis*

(Cd, Zn, Cs, Cr (III))



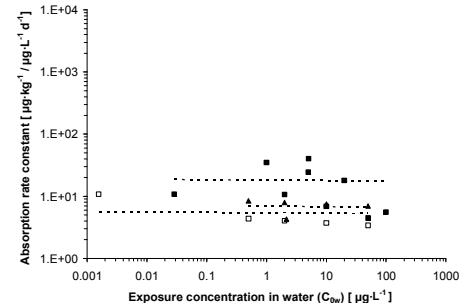
b. *Macoma balthica*

(Ag, Zn, Cd, Co)



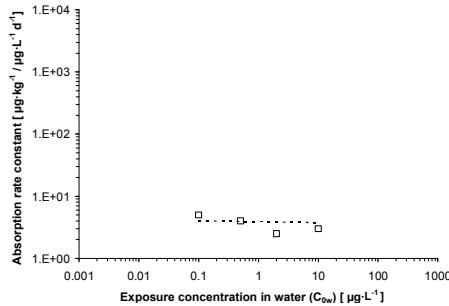
c. *Ruditapes philippinarum*

(Cd, Zn, Cr (III))



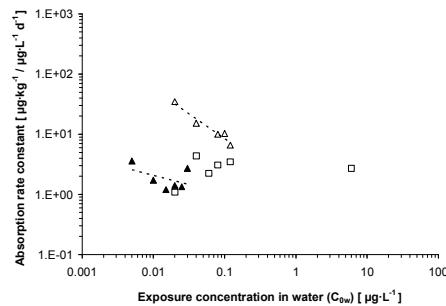
d. *Mytilus edulis*

(Cr (III))



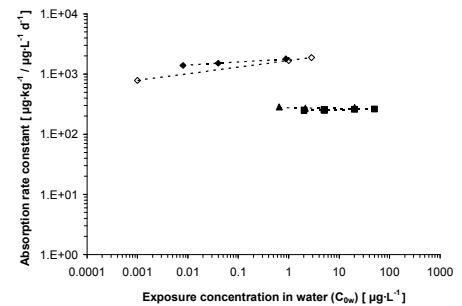
e. *Gammarus oceanicus*

(Pb, Cd, Cr (III))



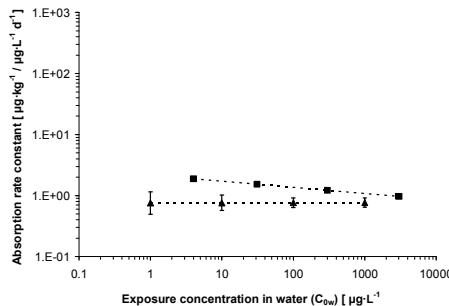
f. *Daphnia magna*

(Cd, Zn, Ag, Hg)



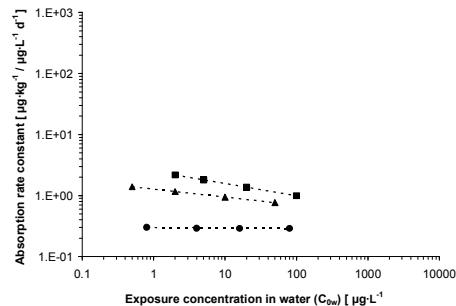
g. *Acanthopagrus schlegeli*

(Cd, Zn)



h. *Lutjanus argentimaculatus*

(Cd, Zn, Cs)



◆ Silver (Ag), ▲ Cadmium (Cd), □ Chromium (III) (Cr), ■ Zinc (Zn), ◇ Mercury (Hg), △ Lead (Pb), ● Cesium (Cs), × Copper (Cu), ○ Cobalt (Co)

Table SI-S3. Regression analysis of metal absorption rate constants ($k_{X,w,in}$ in $L \cdot kg^{-1} \cdot d^{-1}$) with exposure concentrations (C_{0w} in $\mu g \cdot L^{-1}$).

Species	Metal	Log ($k_{x,w,in}$)	r^2	SE	p	n
<i>Perna viridis</i>	Zn	$0.03 \cdot Log(C_{0w}) + 1.89$	0.02	0.39	0.83	5
<i>Perna viridis</i>	Cd	$-0.11 \cdot Log(C_{0w}) + 1.58$	0.42	0.11	0.24	5
<i>Macoma balthica</i>	Ag	$-0.07 \cdot Log(C_{0w}) + 1.76$	0.38	0.10	0.27	5
<i>Macoma balthica</i>	Cd	$0.003 \cdot Log(C_{0w}) + 0.69$	0	0.07	0.94	10
<i>Macoma balthica</i>	Zn	$-0.10 \cdot Log(C_{0w}) + 1.17$	0.36	0.10	0.21	6
<i>Macoma balthica</i>	Co	$-0.07 \cdot Log(C_{0w}) + 0.71$	0.89	0.022	0.02	5
<i>Gammarus oceanicus</i>	Pb	$-0.82 \cdot Log(C_{0w}) + 0.10$	0.95	0.07	0.005	5
<i>Gammarus oceanicus</i>	Cd	$-0.31 \cdot Log(C_{0w}) - 0.30$	0.19	0.19	0.34	6
<i>Lutjanus argentimaculatus</i>	Cs	$-0.009 \cdot Log(C_{0w}) - 0.52$	0.64	0.0051	0.13	4

Empirical absorption rate constants and elimination rate constants compiled

In Table SI-S4 species – specific geometric mean absorption rate constants per metal are given. 95% Confidence intervals represent the variability between organisms from one species. In Table SI-S5 all elimination rate constants compiled per species are provided. 95% Confidence intervals represent the variability between organisms from one species.

Table SI-S4: Species-specific and metal specific absorption rate constants and absorption efficiencies

Metal	Species	Weight kg	$k_{x,w,in}$ L·kg ⁻¹ ·d ⁻¹	95%CI	5% CI	n	$p_{x,w,in}$	References
argentum	Perna viridis	1.3E-03	1.2E+03	1.6E+03	8.5E+02	33	4.11%	5,7,17
mercury	Perna viridis	1.3E-03	7.7E+02	2.4E+03	2.5E+02	4	2.69%	5,18,19
copper	Perna viridis	1.3E-03	1.7E+02			1	0.56%	20
cadmium	Perna viridis	1.3E-03	4.5E+01	6.2E+01	3.2E+01	25	0.15%	5,7,20,21,22,23,24,25
cesium	Perna viridis	1.3E-03	4.2E+00	4.7E+00	3.7E+00	4	0.01%	26,27
chromium (III)	Perna viridis	1.3E-03	6.7E+00	8.9E+00	5.1E+00	5	0.02%	24
zinc	Perna viridis	1.3E-03	1.4E+02	2.1E+02	9.0E+01	24	0.46%	5,7,21,22,23,24
lead	Perna viridis	1.3E-03	2.0E+01			1	0.06%	20
argentum	Mytilus edulis	1.9E-04	2.7E+02	1.1E+03	6.8E+01	6	0.46%	8,9,10
cadmium	Mytilus edulis	1.9E-04	5.5E+01	1.3E+02	2.4E+01	9	0.16%	8,9,10,28
chromium (III)	Mytilus edulis	1.9E-04	3.5E+00	5.7E+00	2.1E+00	4	0.02%	11
zinc	Mytilus edulis	1.9E-04	1.4E+02	2.5E+02	7.3E+01	9	0.44%	8,9,10,28
cobalt	Mytilus edulis	1.9E-04	2.0E+01	3.1E+01	1.3E+01	8	0.07%	8,9,28
cesium	Mytilus edulis	1.9E-04	3.0E+00			1	0.02%	29
argentum	Ruditapes philippinarum	1.6E-03	2.3E+02			1	0.25%	30
zinc	Ruditapes philippinarum	1.6E-03	1.0E+01	1.7E+01	6.0E+00	14	0.07%	6,22,24,30
chromium (III)	Ruditapes philippinarum	1.6E-03	4.7E+00	8.5E+00	2.6E+00	5	0.01%	22,24
mercury	Ruditapes philippinarum	1.6E-03	2.4E+02	2.4E+02	2.4E+02	1	2.12%	30
cadmium	Ruditapes philippinarum	1.6E-03	7.6E+00	8.7E+00	6.6E+00	14	0.06%	6,22,24,30
chromium	Dreissena polymorpha	5.9E-03	1.4E+02			1	0.47%	31,32
argentum	Dreissena polymorpha	5.9E-03	5.5E+02			1	1.87%	31,32
mercury	Dreissena polymorpha	5.9E-03	3.5E+02			1	1.17%	31,32
cadmium	Dreissena polymorpha	5.9E-03	3.0E+02			1	1.02%	31,32
cadmium	Macoma balthica	1.4E-03	4.9E+00	5.5E+00	4.4E+00	10	0.05%	9,33,34,35
zinc	Macoma balthica	1.4E-03	1.2E+01	1.6E+01	9.0E+00	6	0.13%	9,35
argentum	Macoma balthica	1.4E-03	6.0E+01	8.4E+01	4.3E+01	5	0.67%	9,33,34,35
cobalt	Macoma balthica	1.4E-03	4.6E+00	5.5E+00	3.9E+00	5	0.05%	9,33,34,35
copper	Chaetogammarus marinus		2.1E+02	8.4E+02	5.0E+01	3		36
lead	Chaetogammarus marinus		4.5E+01	2.8E+02	7.1E+00	3		36
cobalt	Chaetogammarus marinus		7.0E+00	8.4E+00	5.8E+00	2		36
nickel	Chaetogammarus marinus		5.9E+00	1.8E+01	1.9E+00	3		36
cadmium	Chaetogammarus marinus		1.7E+01	2.1E+01	1.3E+01	3		36
lead	Gammarus oceanicus	1.3E+01	2.8E+01	5.9E+00		5		37
cadmium	Gammarus oceanicus	1.8E+00	2.9E+00	1.2E+00		6		37
nickel	Gammarus oceanicus	1.1E+00	1.1E+00	1.1E+00		1		37
copper	Gammarus oceanicus	3.8E+01	3.8E+01	3.8E+01		1		37
cadmium	Temora longicornis	1.0E-06	1.4E+02	1.6E+02	1.2E+02	4		38
cobalt	Temora longicornis	1.0E-06	1.2E+02	1.4E+02	1.0E+02	4		38
argentum	Temora longicornis	1.0E-06	2.1E+03	3.0E+04	1.5E+02	2		38
zinc	Temora longicornis	1.0E-06	6.5E+02	9.5E+02	4.4E+02	4		38
cadmium	Daphnia magna	1.4E-06	3.2E+02	4.4E+02	2.4E+02	9	0.83%	39
zinc	Daphnia magna	1.4E-06	2.1E+02	3.4E+02	1.3E+02	8	0.54%	39
argentum	Daphnia magna	1.4E-06	1.6E+03	2.8E+03	8.7E+02	6	3.98%	40
mercury	Daphnia magna	1.4E-06	1.4E+03	4.4E+03	4.2E+02	3	3.47%	41
cadmium	Acanthopagrus schlegelii	3.8E-04	9.3E-01	1.2E+00	7.2E-01	26	0.06%	42,43,44
zinc	Acanthopagrus schlegelii	3.8E-04	1.7E+00	2.4E+00	1.2E+00	22	0.12%	42,43
argentum	Acanthopagrus schlegelii	4.0E-04	8.3E+00	7.1E+01	9.6E-01	4	0.58%	44
cesium	Lutjanus argentimaculatus	3.7E-04	2.9E-01	3.0E-01	2.8E-01	4	0.02%	45
cadmium	Lutjanus argentimaculatus	3.7E-04	1.0E+00	1.6E+00	6.9E-01	4	0.07%	46
zinc	Lutjanus argentimaculatus	3.7E-04	1.5E+00	2.6E+00	8.9E-01	4	0.11%	46
cadmium	Terapon jarbua	1.4E-03	3.9E-01	3.0E+03	5.2E-05	2	0.04%	42
zinc	Terapon jarbua	1.4E-03	1.3E+00	2.9E+02	5.9E-03	2	0.13%	42
cadmium	Oncorhynchus mykiss	1.8E-01	3.8E-01	2.6E+00	5.5E-02	5	0.12%	47
argentum	Pleuronectes platessa	4.5E-02	7.4E+00			1	1.71%	48
mercury	Pleuronectes platessa	4.3E-02	4.3E+00			1	0.98%	49
zinc	Gambusia affinis	4.1E-04	7.4E-01	1.9E+00	2.8E-01	6	0.05%	50
mercury	Lepomis microlophus	8.5E-04	8.8E+00	5.7E+01	1.4E+00	2	0.75%	51
zinc	Oncorhynchus mykiss	5.5E-03	2.0E+00	2.0E+00	2.0E+00		0.27%	52
mercury	Gambusia affinis	4.1E-04	1.3E+01	1.7E+02	9.7E-01	2	0.91%	51
cadmium	Periophthalmus cantonensis	3.0E-03	5.0E-01	8.0E-01	3.2E-01	4	0.06%	53
zinc	Periophthalmus cantonensis	3.0E-03	1.2E+00	3.6E+00	3.9E-01	4	0.14%	53

Table SI-S5: Species - specific and metal - specific elimination rate constants and weight-corrected elimination rates

Metal	Species	weight kg	$k_{x,ex}$ d^{-1}	95% CI	5% CI	n	Weight-corrected $k_{x,ex}$ $kg^k d^{-1}$	95% CI	5% CI	n	References
argentum	Perna viridis	1.3E-03	1.9E-02	2.0E-02	1.0E-02	16	3.8E-03	7.0E-03	2.0E-03	16	7,17
cadmium	Perna viridis	1.3E-03	1.3E-02	1.4E-02	8.4E-03	6	2.3E-03	3.8E-03	1.4E-03	6	7,24
cesium	Perna viridis	1.3E-03	1.5E-01			1	3.0E-02			1	26,27
chromium (III)	Perna viridis	1.3E-03	2.9E-02			1	6.1E-03			1	24
zinc	Perna viridis	1.3E-03	3.1E-02	3.3E-02	1.9E-02	6	5.7E-03	8.9E-03	3.7E-03	6	7,21,24
argentum	Mytilus edulis	1.9E-04	4.5E-02	4.6E-02	3.1E-02	5	4.7E-03	7.2E-03	3.1E-03	5	8,10
cadmium	Mytilus edulis	1.9E-04	6.9E-02	6.9E-02	2.4E-02	8	6.0E-03	1.8E-02	2.0E-03	8	8,10,28
chromium (III)	Mytilus edulis	1.9E-04	1.1E-02	1.1E-02	8.7E-03	3	2.3E-03	3.0E-03	1.8E-03	3	11
zinc	Mytilus edulis	1.9E-04	5.4E-02	5.4E-02	2.3E-02	8	4.7E-03	9.7E-03	2.3E-03	8	8,10,28
cobalt	Mytilus edulis	1.9E-04	8.7E-02	8.8E-02	2.6E-02	7	7.6E-03	2.0E-02	2.9E-03	7	8,11
zinc	Ruditapes philippinarum	1.6E-03	1.7E-02	1.9E-02	5.1E-03	3	3.6E-03	1.1E-02	1.2E-03	3	6,24
chromium (III)	Ruditapes philippinarum	1.6E-03	2.3E-02			1	5.0E-03			1	24
cadmium	Ruditapes philippinarum	1.6E-03	2.0E-02	2.2E-02	4.5E-03	3	4.2E-03	1.7E-02	1.0E-03	3	6,24
argentum	Dreissena polymorpha	5.9E-03	8.8E-02			1	9.0E-03			1	31
cadmium	Dreissena polymorpha	5.9E-03	1.1E-02			1	1.1E-03			1	31
cadmium	Macoma balthica	1.4E-03	2.0E-02	2.2E-02	4.3E-03	2	4.0E-03	2.3E-02	6.8E-04	2	34,35
zinc	Macoma balthica	1.4E-03	1.2E-02			1	2.3E-03			1	35
argentum	Macoma balthica	1.4E-03	9.6E-03			1	1.9E-03			1	34
cobalt	Macoma balthica	1.4E-03	2.6E-02			1	5.2E-03			1	34
copper	Chaetogammarus marinus	3.4E-01	8.5E-01	1.4E-01		3					36
lead	Chaetogammarus marinus	1.3E-01									36
cobalt	Chaetogammarus marinus	1.8E-01				2					36
nickel	Chaetogammarus marinus	1.5E-01	3.0E-01	7.5E-02		3					36
cadmium	Chaetogammarus marinus	2.9E-01	3.5E-01	2.3E-01		3					36
lead	Gammarus oceanicus	3.6E-01	6.1E-01	2.2E-01		5					37
cadmium	Gammarus oceanicus	1.7E-01	2.6E-01	1.1E-01		6					37
nickel	Gammarus oceanicus	4.7E-01				1					37
copper	Gammarus oceanicus	1.2E+00				1					37
cadmium	Temora longicornis	1.0E-06	2.2E-01	7.1E-01	6.7E-02	3	6.9E-03	2.2E-02	2.1E-03	3	38
cobalt	Temora longicornis	1.0E-06	2.7E-01	4.6E-01	1.6E-01	3	8.7E-03	1.4E-02	5.2E-03	3	38
argentum	Temora longicornis	1.0E-06	2.2E-01	4.6E-01	1.0E-01	2	6.8E-03	1.4E-02	3.2E-03	3	38
zinc	Temora longicornis	1.0E-06	7.0E-02	1.7E-01	2.9E-02	3	2.2E-03	5.3E-03	9.2E-04	3	38
cadmium	Daphnia magna	1.4E-06	6.5E-02	1.4E-01	3.1E-02	3	2.2E-03	4.7E-03	1.0E-03	3	54
zinc	Daphnia magna	1.4E-06	2.9E-01	3.0E-01	2.7E-01	3	9.8E-03	1.0E-02	9.3E-03	3	54
argentum	Daphnia magna	1.4E-06	2.8E-01	3.2E-01	2.5E-01	4	9.6E-03	1.1E-02	8.6E-03	4	40
mercury	Daphnia magna	1.4E-06	5.1E-02	7.6E-02	3.5E-02	3	1.8E-03	2.6E-03	1.2E-03	3	41
cadmium	Acanthopagrus schlegelii	3.8E-04	8.9E-02			1	1.3E-02			1	55
zinc	Acanthopagrus schlegelii	3.8E-04	1.6E-02			1	2.2E-03			1	55
cesium	Lutjanus argentimaculatus	3.7E-04	2.1E-02			1	3.0E-03			1	45
cadmium	Lutjanus argentimaculatus	3.7E-04	2.5E-02			1	3.5E-03			1	46
zinc	Lutjanus argentimaculatus	3.7E-04	1.5E-02			1	2.1E-03			1	46
cadmium	Terapon jarbua	1.4E-03	3.0E-02	5.1E-02	1.7E-02	3	4.7E-03	8.0E-03	2.7E-03	3	56
argentum	Terapon jarbua	6.0E-04	3.4E-02	4.7E-02	2.5E-02	5	5.3E-03	7.4E-03	3.8E-03	3	56
cadmium	Oncorhynchus mykiss	1.8E-01	1.1E-02	4.0E-02	3.0E-03	5	7.0E-03	2.6E-02	1.9E-03	5	47
argentum	Pleuronectes platessa	4.5E-02	2.3E-02				1.0E-02			1	48
mercury	Pleuronectes platessa	4.3E-02	3.7E-03				1.7E-03			1	49
mercury	Gambusia affinis	5.9E-04	1.7E-02	8.9E-02	3.1E-03	5	1.7E-02	8.9E-02	3.1E-03	5	51
mercury	Lepomis microlophus	8.5E-04	1.2E-02	2.9E-01	5.1E-04	2	2.1E-03	5.0E-02	8.6E-05	2	51

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