

Supporting Information

Assessment of metal toxicity in marine ecosystems - Comparative Toxicity Potentials for nine cationic metals in coastal seawater

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44 pages in total, including 9 tables and 13 figures

Table S1: Environmental and water chemistry parameters of 64 Large Marine Ecosystems (LMEs)

LME	SRT ^{1,a}	Surface Area ^{2,a}	Estuary discharge ^{2,a}	Temp ¹	pH ^b	Salinity ^b	DOC ^c	POC ^d	SPM ^e
	years	km ²	m ³ /second	°C	unit	‰	mg/l	µg/l	mg/l
1. East Bering Sea	2.00	1.2E+06	1.0E+04	5.08	7.97	33.01	0.69 ³	209.6	0.58
2. Gulf of Alaska	0.25	1.5E+06	1.4E+04	9.56	7.84	32.43	0.67 ³	148.7	0.47
3. California Current	0.25	2.2E+06	1.6E+04	17.38	7.96	33.62	0.79 ³	52.8	0.31
4. Gulf of California	1.50	2.2E+05	6.5E+02	24.50	7.96	34.63	0.90 ³	154.7	0.41
5. Gulf of Mexico	90.00	1.5E+06	3.6E+04	26.13	8.12	36.04	1.28 ⁴	57.3	0.28
6. Southeast U.S. Continental Shelf	0.25	3.0E+05	3.3E+03	24.78	8.15	36.17	1.99 ⁵	53.4	0.32
7. Northeast U.S. Continental Shelf	0.25	3.1E+05	6.7E+03	12.62	7.80	32.06	1.71 ^{6,7}	265.2	0.62
8. Scotian Shelf	0.88	4.1E+05	1.0E+04	8.43	7.80	31.33	0.74 ³	227.6	0.56
9. Newfoundland-Labrador Shelf	0.25	6.7E+05	2.4E+04	5.58	7.83	32.29	0.80 ³	182.9	0.49
10. Insular Pacific-Hawaiian	0.25	9.8E+05	1.7E+01	24.95	7.98	34.83	0.86 ³	31.0	0.16
11. Pacific Central-American Coastal	0.25	2.0E+06	1.9E+04	27.46	7.92	34.62	0.87 ³	71.0	0.40
12. Caribbean Sea	0.21	3.3E+06	1.7E+04	27.80	8.10	36.05	0.84 ³	44.3	0.21
13. Humboldt Current	0.03	2.6E+06	8.7E+03	16.55	7.75	34.80	0.73 ³	106.6	0.45
14. Patagonian Shelf	0.25	1.2E+06	2.7E+04	10.85	8.05	33.84	0.60 ³	208.5	0.60
15. South Brazil Shelf	0.25	5.7E+05	5.0E+03	22.85	8.10	35.27	0.79 ³	68.9	0.29
16. East Brazil Shelf	0.25	1.1E+06	5.6E+03	27.19	8.10	35.09	0.84 ³	32.5	0.19
17. North Brazil Shelf	0.25	1.0E+06	5.4E+04	27.90	8.05	35.35	0.92 ³	115.8	0.25
18. West Greenland Shelf	0.25	3.6E+05	1.1E+01	1.03	8.05	33.72	0.73 ³	111.7	0.60
19. Greenland Sea	0.25	1.2E+06	1.8E+02	1.87	8.14	34.90	0.97 ⁸	113.0	0.56
20. Barents Sea	2.00	2.0E+06	9.0E+03	3.29	8.14	34.93	0.74 ³	128.4	0.83
21. Norwegian Sea	2.00	1.1E+06	0.0E+00	8.55	8.13	35.03	1.07 ⁹	135.1	0.58
22. North Sea	2.00	6.9E+05	7.8E+03	10.55	8.06	34.00	1.76 ¹⁰⁻¹²	242.0	0.79
23. Baltic Sea	25.00	4.0E+05	1.0E+04	8.33	7.85	6.17	6.48 ^{6,13}	801.6	1.03
24. Celtic-Biscay Shelf	2.00	7.7E+05	1.9E+03	13.11	8.14	35.18	0.74 ³	154.5	0.59
25. Iberian Coastal	0.25	3.0E+05	1.5E+03	16.98	7.93	35.80	0.76 ³	91.4	0.40
26. Mediterranean Sea	90.00	2.5E+06	1.3E+05	19.97	8.18	38.43	1.69 ¹⁴⁻¹⁷	47.1	0.28
27. Canary Current	0.25	1.1E+06	1.0E+03	22.01	8.16	35.96	0.84 ³	78.8	0.30
28. Guinea Current	3.10	2.0E+06	7.2E+04	27.56	7.96	35.39	0.89 ³	80.3	0.28
29. Benguela Current	0.25	1.5E+06	4.7E+04	20.69	7.93	35.14	0.77 ³	143.8	0.39
30. Agulhas Current	2.00	2.6E+06	7.0E+03	25.49	8.06	35.13	0.77 ³	49.2	0.25
31. Somali Coastal Current	0.25	8.4E+05	1.4E+03	27.34	8.06	35.04	0.80 ³	66.9	0.25
32. Arabian Sea	6.50	4.0E+06	7.8E+03	27.66	7.90	35.80	0.77 ¹⁸	91.9	0.28
33. Red Sea	40.00	4.8E+05	0.0E+00	28.13	8.09	40.28	1.64 ¹⁹	63.9	0.23
34. Bay of Bengal	12.00	3.7E+06	6.3E+04	28.68	8.03	34.74	1.41 ²⁰	57.3	0.22
35. Gulf of Thailand	0.04	3.9E+05	4.1E+03	28.89	8.20	32.12	0.93 ³	73.0	0.32
36. South China Sea	25.00	5.7E+06	6.7E+04	28.04	8.17	34.01	0.93 ²¹	48.8	0.26
37. Sulu-Celebes Sea	25.00	1.0E+06	4.9E+03	28.97	8.00	34.46	0.78 ³	42.1	0.27
38. Indonesian Sea	0.75	2.3E+06	1.0E+04	28.74	7.91	34.20	0.76 ³	57.3	0.27
39. North Australian Shelf	0.25	7.7E+05	9.0E+02	28.19	8.21	34.59	0.77 ³	107.2	0.41
40. Northeast Australian Shelf	0.25	1.3E+06	1.1E+03	26.71	8.32	35.23	0.78 ³	36.3	0.18
41. East-Central Australian Shelf	0.25	6.6E+05	7.0E+02	23.01	8.19	35.46	0.76 ³	50.7	0.23
42. Southeast Australian Shelf	0.25	1.2E+06	1.5E+03	14.86	8.19	35.33	0.68 ³	86.0	0.38
43. Southwest Australian Shelf	0.25	1.0E+06	8.5E+01	17.22	8.23	35.62	0.76 ³	60.1	0.31
44. West-Central Australian Shelf	0.25	5.4E+05	4.6E+01	22.45	8.09	35.44	0.83 ³	46.1	0.20
45. Northwest Australian Shelf	0.25	9.1E+05	2.5E+02	27.75	8.00	34.77	0.81 ³	43.0	0.20
46. New Zealand Shelf	0.25	9.8E+05	2.9E+03	15.42	8.19	34.85	0.68 ³	84.9	0.36
47. East China Sea	1.90	1.0E+06	3.6E+04	22.19	8.19	34.39	1.03 ^{22,23}	126.9	0.50
48. Yellow Sea	2.00	4.4E+05	4.3E+03	15.43	8.09	32.30	2.02 ²⁴	340.6	2.88
49. Kuroshio Current	2.30	1.3E+06	2.4E+03	22.97	8.19	34.42	0.74 ³	45.4	0.30
50. Sea of Japan/East Sea	25.00	1.1E+06	1.4E+04	13.42	8.10	34.02	0.85 ²⁵	130.5	0.43
51. Oyashio Current	0.25	6.6E+05	0.0E+00	7.01	7.99	33.37	0.68 ³	186.1	0.52
52. Sea of Okhotsk	2.00	1.6E+06	1.1E+03	4.58	8.10	32.88	3.14 ²⁶	183.4	0.57
53. West Bering Sea	0.25	2.2E+06	1.1E+03	5.16	8.00	33.12	0.69 ³	202.9	0.57
54. Chukchi Sea	3.50	7.8E+05	1.2E+03	-0.08	8.13	32.23	0.76 ²⁷	158.6	0.87
55. Beaufort Sea	3.50	6.6E+05	8.1E+03	-1.24	7.86	31.58	1.52 ⁶	108.5	0.63
56. East Siberian Sea	3.50	1.0E+06	8.0E+03	-1.13	7.88	29.47	1.00 ³	365.2	1.62
57. Laptev Sea	3.50	5.4E+05	2.2E+04	-0.75	7.88	28.44	0.92 ³	319.4	1.64
58. Kara Sea	3.50	9.7E+05	3.7E+04	-0.55	8.10	31.13	0.95 ³	156.9	0.93
59. Iceland Shelf	0.25	5.2E+05	0.0E+00	5.95	8.15	34.90	0.70 ³	138.2	0.59
60. Faroe Plateau	0.25	1.5E+05	0.0E+00	9.58	8.16	35.24	0.65 ³	136.4	0.53
61. Antarctic	6.00	3.5E+06	0.0E+00	-1.19	7.95	34.43	0.61 ¹⁸	145.0	0.58
62. Black Sea	90.00	4.6E+05	1.1E+04	14.90	8.35	18.24	2.19 ²⁸	168.8	0.58
63. Hudson Bay	6.60	1.2E+06	2.0E+04	0.99	7.86	31.59	1.31 ²⁹	186.0	1.52
64. Arctic Ocean	11.00	3.5E+06	1.1E+03	-1.20	7.91	32.47	0.82 ¹⁸	123.1	0.71

a. In USEtox, the waterflow in coastal seawater compartment is calculated as Eq. S1

$$Inflow \text{ (from open ocean)} = \frac{Surface \text{ area} \times depth}{SRT \text{ (coastal seawater)}} - Estuary \text{ discharge} \quad \text{Eq.S1}$$

When calculating metal FFs in each LME, surface area, SRT and estuary discharge were replaced by LME-specific data presented above. Water depth was kept at the default value as shown in Table S3.

Water flow in the freshwater compartment was calculated as Eq. S2

$$Freshwater \text{ residence time} = \frac{Freshwater \text{ volume}}{Estuary \text{ discharge}} \quad \text{Eq. S2}$$

The introduced change of estuary discharge has an impact on freshwater residence time. To ensure consistency with freshwater metal CTP³⁰, the freshwater residence time should not be changed. Therefore, for each LME we modified the freshwater volume by changing land surface area proportionally to estuary discharge, to achieve a constant freshwater residence time in the freshwater compartment.

- b. 2.5×10^5 individual and localized pH values and 3.3×10^6 values for salinity were collected from NODC's World Ocean Database³¹. The median value of pH and salinity in each Large Marine Ecosystem (LME) regardless of season and location is shown here. In the absence of pH data for LME 4, 57 and 63, the pH value of their adjunct LME 3, 56 and 55 were taken here respectively.
- c. If *in situ* DOC concentration data is reported for an LME the geometric mean of minimum and maximum reported DOC values is taken as representative for that LME. For LMEs where no *in situ* DOC is reported, we adopted DOC concentration from a global ocean DOC model³.
- d. POC data were taken from Sea Viewing Wide-Field of view Sensor (SeaWiFS)³² project. The median value of the POC concentration in 2010 across seasons and locations within the LME was taken here.
- e. SPM data were taken from GlobColour project³³. Median values of the SPM concentration were calculated for each month in 2011 across locations within the LME. Then the annual average of the 12 month-median SPMs was taken as the representative SPM concentration for the LME.

Table S2: Salinity and ion concentrations in standard seawater³⁴

Water chemistry	concentration
Salinity [%]	35
Na⁺ [mol/kg]	0.468
Mg²⁺ [mol/kg]	0.0532
K⁺ [mol/kg]	0.0102
Ca²⁺ [mol/kg]	0.0102
Cl⁻ [mol/kg]	0.545
SO₄²⁻ [mol/kg]	0.0282

Table S3: Landscape and fate parameters used in default USEtox

Parameter	Value	Unit
Continental scale		
Land area	LME specific	
Sea area	LME specific	
Fraction of freshwater	3.00×10^{-2}	-
Fraction of natural soil	4.85×10^{-1}	-
Fraction of agricultural soil	4.85×10^{-1}	-
Temperature	1.20×10^1	°C
Wind speed	3.00×10^0	m.s ⁻¹
Rain rate	7.00×10^2	mm.yr ⁻¹
Freshwater depth	2.50×10^0	m
Run off fraction	2.50×10^{-1}	-
Infiltration fraction	2.50×10^{-1}	-
Soil erosion	3.00×10^{-2}	mm.yr ⁻¹
Suspended matter concentration in seawater	LME specific	
Seawater residence time	LME specific	
Suspended matter concentration in seawater	LME specific	
Suspended solids/water partition coefficient	LME and metal specific	
Dissolved (colloidal) organic carbon/water partition coefficient	LME and metal specific	
Sediment/water partition coefficient sea water	Metal specific	
DOC concentration in seawater	LME specific	
Suspended particle settling velocity	2.89×10^{-5}	m.s ⁻¹
Marine sediment compartment depth	3.00×10^0	cm
Seawater compartment depth	1.00×10^2	m
Bulk density of sediment	1.23×10^3	kg.m ⁻³
Suspended matter in freshwater	1.50×10^1	mg.L ⁻¹
Autochthonous production of suspended matter in seawater	1.00×10^1	g.m ⁻² .yr ⁻¹
Volume fraction of solids in sediment	2.00×10^{-1}	-
Volume fraction of water in sediment	8.00×10^{-1}	-
Fate content of seawater fish	5.00×10^{-2}	-
Biota concentration in seawater	1×10^0	mg.L ⁻¹
Partial mass transfer coefficient water side of water/sed interface	2.78×10^{-6}	m.s ⁻¹
Partial mass transfer coefficient sediment side of water/sed interface	2.78×10^{-8}	m.s ⁻¹

Parameter	Value	Unit
Global scale		
Land area	1.41×10^8	km^2
Sea area	3.29×10^8	km^2
Fraction of freshwater	3.00×10^{-2}	-
Fraction of natural soil	4.85×10^{-1}	-
Fraction of agricultural soil	4.85×10^{-1}	-
Temperature	1.20×10^1	$^\circ\text{C}$
Wind speed	3.00×10^0	m.s^{-1}
Rain rate	7.00×10^2	mm.yr^{-1}
Freshwater depth	2.50×10^0	m
Run off fraction	2.50×10^{-1}	-
Infiltration fraction	2.50×10^{-1}	-
Soil erosion	3.00×10^{-2}	mm.yr^{-1}
Suspended matter concentration in seawater	5.00×10^0	mg.L^{-1}
General		
Water flow of global freshwater to continental scale	0.00×10^0	$\text{m}^3.\text{s}^{-1}$
Mineral density in sediment and soil	2.50×10^3	kg.m^3

Table S4: Background concentration of metals in coastal seawater and metal-specific input parameters for FF calculation in USEtox, including metal molecular weight (MW), metal partitioning coefficient between sediment particles and water (K_{psd}), metal partitioning coefficient between soil particles and water (K_{psi}) and metal bioaccumulation factor in fish/biota (BAF_{fish})

Metal	Background concentration ³⁵ [nmol/l]	MW [g/mol]	K_{psd} [L/kg]	K_{psi} [L/kg]	BAF_{fish} [L/kg fish]
Cd	0.5	112.41 ³⁶	2.00×10^3 ³⁶	1.50×10^2 ³⁶	2.70×10^2 ³⁶
Co	0.02	58.93 ³⁶	1.26×10^3 ³⁶	4.80×10^2 ³⁶	4.00×10^2 ³⁶
Cr	4	52.00 ³⁶	7.94×10^4 ³⁶	4.00×10^1 ³⁶	2.10×10^2 ³⁶
Cu	4	63.55 ³⁶	3.16×10^3 ³⁶	5.30×10^2 ³⁶	2.70×10^2 ³⁶
Fe	0.5	55.85 ^{37,38}	1.60×10^5 ³⁹	8.80×10^2 ⁴⁰	1.40×10^2 ⁴⁰
Mn	0.3	54.94 ^{37,38}	2.80×10^4 ³⁹	1.20×10^3 ⁴⁰	4.50×10^2 ⁴⁰
Ni	8	58.69 ³⁶	7.94×10^3 ³⁶	2.80×10^2 ³⁶	7.10×10^1 ³⁶
Pb	0.1	207.20 ³⁶	3.98×10^4 ³⁶	2.00×10^3 ³⁶	3.70×10^2 ³⁶
Zn	5	65.38 ³⁶	1.26×10^4 ³⁶	9.50×10^2 ³⁶	4.70×10^3 ³⁶

Table S5: EC₅₀ data obtained from literature, reported with water chemistry

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Cd							
Algae	15	8.08 ^e	35	0	Chronic	8.38E-07 ⁴¹	8.56E-09
Algae	25	8	6	2.29	Chronic	2.56E-06 ⁴²	1.79E-07
Algae	25	8	25	2.29	Chronic	2.89E-06 ⁴²	4.35E-08
Algae	25	8	6	2.29	Chronic	3.11E-06 ⁴²	2.18E-07
Algae	25	8	25	2.29	Chronic	3.44E-06 ⁴²	5.18E-08
Algae	25	8	6	2.29	Chronic	4.36E-06 ⁴²	3.06E-07
Algae	18	8.2	35	2.29	Chronic	1.22E-04 ⁴³	1.23E-06
Algae	18	8.2	35	2.29	Chronic	1.22E-04 ⁴⁴	1.23E-06
Algae	18	7.8	35	2.29	Chronic	2.67E-04 ⁴⁵	2.71E-06
Algae	15	8.08	34.58 ^f	0	Chronic	3.40E-07 ⁴⁶	3.53E-09
Algae	15	7.95 ^d	30 ^d	0	Chronic	1.78E-06 ⁴⁷	2.21E-08
Algae	12	8.08 ^e	34.58 ^f	2.29	Chronic	1.17E-05 ⁴⁸	1.22E-07
Algae	24	8.08 ^e	7.6	2.29	Chronic	4.09E-07 ⁴⁹	2.26E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	1.04E-06 ⁴⁹	5.76E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	4.42E-07 ⁴⁹	2.44E-08
Algae	21	8.08 ^e	24	2.29	Chronic	2.65E-03 ⁵⁰	4.29E-05
Crustaceans	18.7	8	32.1	2.29	Chronic	1.25E-05 ⁵¹	1.41E-07
Crustaceans	20	8.08 ^e	10	2.29	Chronic	1.16E-04 ⁵²	4.96E-06
Crustaceans	20	8.08 ^e	20	2.29	Chronic	1.25E-04 ⁵²	2.49E-06
Crustaceans	20	8.08 ^e	30	2.29	Chronic	1.61E-04 ⁵²	1.97E-06
Crustaceans	10	8.08 ^e	10	2.29	Chronic	2.78E-04 ⁵²	1.22E-05
Crustaceans	30	8.08 ^e	20	2.29	Chronic	2.84E-05 ⁵²	5.51E-07
Crustaceans	30	8.08 ^e	30	2.29	Chronic	4.15E-05 ⁵²	4.94E-07
Crustaceans	17.1	8.08 ^e	34.58 ^f	2.29	Chronic	9.11E-05 ⁵¹	9.40E-07
Crustaceans	20	7.8	20	2.29	Chronic	3.82E-06 ⁵³	7.60E-08
Crustaceans	18.7	8	32.1	2.29	Chronic	1.01E-05 ⁵¹	1.14E-07
Crustaceans	17.8	8.1	32.6	2.29	Chronic	7.64E-05 ⁵¹	8.46E-07
Crustaceans	19.5	8.08 ^e	35	2.29	Chronic	1.09E-06 ⁵⁴	1.10E-08
Crustaceans	19.5	8.08 ^e	35	2.29	Chronic	2.78E-06 ⁵⁴	2.80E-08
Crustaceans	19.5	8.08 ^e	35	2.29	Chronic	1.09E-06 ⁵⁴	1.10E-08
Crustaceans	19.5	8.08 ^e	35	2.29	Chronic	6.00E-07 ⁵⁴	6.04E-09
Crustaceans	19.5	8.08 ^e	35	2.29	Chronic	1.17E-05 ⁵⁴	1.18E-07
Crustaceans	19 ^d	8.05 ^d	35.8 ^d	2.29	Chronic	5.29E-06 ⁵⁵	5.19E-08
Crustaceans	22.5 ^d	8.08 ^e	25	0	Chronic	5.45E-06 ⁵⁶	8.27E-08
Crustaceans	20	8.08 ^e	20	2.29	Chronic	9.00E-05 ⁵²	1.79E-06
Crustaceans	20	8.08 ^e	10	2.29	Chronic	9.82E-05 ⁵²	4.20E-06
Crustaceans	20	8.08 ^e	30	2.29	Chronic	1.15E-04 ⁵²	1.40E-06
Crustaceans	10	8.08 ^e	10	2.29	Chronic	1.55E-04 ⁵²	6.80E-06
Crustaceans	30	8.08 ^e	10	2.29	Chronic	1.64E-05 ⁵²	6.83E-07
Crustaceans	30	8.08 ^e	20	2.29	Chronic	2.02E-05 ⁵²	3.92E-07
Crustaceans	30	8.08 ^e	10	2.29	Chronic	2.18E-05 ⁵²	9.08E-07
Crustaceans	10	8.08 ^e	20	2.29	Chronic	2.84E-04 ⁵²	5.82E-06
Crustaceans	30	8.08 ^e	30	2.29	Chronic	3.55E-05 ⁵²	4.22E-07
Crustaceans	20	8.08 ^e	10	2.29	Chronic	6.44E-05 ⁵²	2.75E-06
Crustaceans	10	8.08 ^e	10	2.29	Chronic	8.56E-05 ⁵²	3.75E-06

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Cd							
Crustaceans	20	8.08 ^e	30	2.29	Chronic	9.76E-05 ⁵²	1.19E-06
Crustaceans	30	8.08 ^e	10	2.29	Chronic	1.58E-05 ⁵²	6.58E-07
Crustaceans	30	8.08 ^e	20	2.29	Chronic	1.91E-05 ⁵²	3.70E-07
Crustaceans	10	8.08 ^e	20	2.29	Chronic	2.29E-04 ⁵²	4.69E-06
Crustaceans	10	8.08 ^e	30	2.29	Chronic	2.56E-04 ⁵²	3.22E-06
Crustaceans	30	8.08 ^e	30	2.29	Chronic	3.11E-05 ⁵²	3.70E-07
Crustaceans	20	8.08 ^e	20	2.29	Chronic	5.18E-05 ⁵²	1.03E-06
Crustaceans	19 ^d	8.05 ^d	35.8 ^d	2.29	Chronic	3.33E-06 ⁵⁵	3.27E-08
Crustaceans	21	8.1 ^d	30	2.29	Chronic	2.56E-06 ⁵⁷	3.11E-08
Crustaceans	21 ^d	8.08 ^e	7	2.29	Chronic	5.45E-07 ⁵⁸	3.30E-08
Crustaceans	21 ^d	8.08 ^e	15	2.29	Chronic	8.18E-08 ⁵⁸	2.23E-09
Crustaceans	21 ^d	8.08 ^e	15	2.29	Chronic	2.18E-07 ⁵⁸	5.97E-09
Crustaceans	21 ^d	8.08 ^e	15	2.29	Chronic	3.27E-08 ⁵⁸	8.89E-10
Crustaceans	19 ^d	8.05 ^d	35.8 ^d	2.29	Chronic	2.67E-06 ⁵⁸	2.62E-08
Crustaceans	22.5 ^d	8.08 ^e	25	0	Chronic	1.01E-06 ⁵⁶	1.53E-08
Crustaceans	21	8.08 ^e	30	2.29	Chronic	8.07E-08 ⁵⁹	9.78E-10
Crustaceans	19.5	8.08 ^e	35	2.29	Chronic	2.73E-06 ⁵⁴	2.75E-08
Crustaceans	20	8.08 ^e	30	2.29	Chronic	3.17E-07 ⁶⁰	3.86E-09
Crustaceans	21	8.08 ^e	30	2.29	Chronic	1.06E-07 ⁵⁹	1.29E-09
Fish	19.5	7.9	34	2.29	Chronic	7.80E-05 ⁶¹	8.17E-07
Fish	20	7.8	20	2.29	Chronic	1.20E-04 ⁵³	2.39E-06
Fish	19.5	7.9	34	2.29	Chronic	8.73E-05 ⁶¹	9.14E-07
Fish	19.5	7.9	34	2.29	Chronic	6.93E-05 ⁶¹	7.26E-07
Fish	19.5	7.9	34	2.29	Chronic	9.06E-05 ⁶¹	9.49E-07
Fish	19.5	7.9	34	2.29	Chronic	1.15E-04 ⁶¹	1.20E-06
Fish	26.25 ^d	8.07 ^d	20	2.29	Chronic	3.86E-05 ⁶²	7.56E-07
Fish	26.25 ^d	8.07 ^d	30	2.29	Chronic	7.75E-05 ⁶²	9.31E-07
Fish	26.25 ^d	8.07 ^d	20	2.29	Chronic	2.00E-05 ⁶²	3.91E-07
Fish	26.25 ^d	8.07 ^d	5	2.29	Chronic	4.09E-06 ⁶²	3.38E-07
Fish	26.25 ^d	8.07 ^d	15	2.29	Chronic	4.89E-05 ⁶²	1.33E-06
Fish	26.25 ^d	8.07 ^d	15	2.29	Chronic	1.38E-05 ⁶²	3.76E-07
Fish	26.25 ^d	8.07 ^d	30	2.29	Chronic	4.36E-05 ⁶²	5.24E-07
Fish	20	8.15 ^d	30	0	Chronic	1.97E-05 ⁶³	2.41E-07
Fish	20	8.15 ^d	30	0	Chronic	1.92E-05 ⁶³	2.34E-07
Fish	20	8.15 ^d	30	0	Chronic	1.87E-05 ⁶³	2.28E-07
Fish	20 ^g	8.08 ^e	10.4	2.29	Chronic	8.18E-07 ⁶⁴	3.33E-08
Fish	20 ^g	8.08 ^e	30.4	2.29	Chronic	6.11E-06 ⁶⁴	7.34E-08
Fish	20 ^g	8.08 ^e	20 ^d	2.29	Chronic	3.11E-06 ⁶⁴	6.18E-08
Fish	20 ^g	8.08 ^e	20.3	2.29	Chronic	3.98E-06 ⁶⁴	7.76E-08
Fish	20 ^g	8.08 ^e	12.7	2.29	Chronic	8.73E-07 ⁶⁴	2.88E-08
Fish	20 ^g	8.08 ^e	29.9	2.29	Chronic	5.29E-06 ⁶⁴	6.49E-08
Fish	20 ^g	8.08 ^e	20.3	2.29	Chronic	2.95E-06 ⁶⁴	5.75E-08
Fish	20 ^g	8.08 ^e	20 ^d	2.29	Chronic	3.55E-06 ⁶⁴	7.05E-08
Standard deviation						2.85E-04	4.83E-06
Co							
Algae	20 ^g	8.05 ^d	34.58 ^f	0	Chronic	6.58E-05 ⁶⁵	8.39E-06
Algae	24	8.08 ^e	7.6	2.29	Chronic	3.13E-05 ⁴⁹	6.12E-06

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Co							
Algae	24	8.08 ^e	7.6	2.29	Chronic	1.82E-05 ⁴⁹	3.56E-06
Algae	24	8.08 ^e	7.6	2.29	Chronic	5.52E-05 ⁴⁹	1.08E-05
Algae	24	8.08 ^e	7.6	2.29	Chronic	7.09E-06 ⁴⁹	1.38E-06
Crustaceans	20	8	7	2.29	Acute	3.47E-05 ⁶⁶	1.92E-06
Fish	20	8.08 ^e	7.9	2.29	Acute	8.41E-03 ⁶⁷	5.05E-04
Fish	20	8.08 ^e	7.9	2.29	Acute	8.41E-03 ⁶⁷	5.05E-04
Fish	20	8.08 ^e	7.9	2.29	Acute	8.41E-03 ⁶⁷	5.05E-04
Fish	20	8.08 ^e	7.9	2.29	Acute	8.41E-03 ⁶⁷	5.05E-04
Fish	20	8.08 ^e	18.8	2.29	Acute	8.41E-03 ⁶⁷	3.93E-04
Fish	20	8.08 ^e	18.8	2.29	Acute	8.41E-03 ⁶⁷	3.93E-04
Fish	20	8.08 ^e	18.8	2.29	Acute	8.41E-03 ⁶⁷	3.93E-04
Fish	20	8.08 ^e	18.8	2.29	Acute	8.41E-03 ⁶⁷	3.93E-04
Fish	20	8.08 ^e	5	2.29	Acute	2.43E-03 ⁶⁷	1.63E-04
Fish	20	8.08 ^e	25.3	2.29	Acute	4.24E-03 ⁶⁷	1.79E-04
Fish	20	8.08 ^e	5	2.29	Acute	2.12E-03 ⁶⁷	1.43E-04
Fish	20	8.08 ^e	5	2.29	Acute	2.43E-03 ⁶⁷	1.63E-04
Fish	20	8.08 ^e	25.3	2.29	Acute	2.12E-03 ⁶⁷	8.98E-05
Fish	20	8.08 ^e	5	2.29	Acute	2.43E-03 ⁶⁷	1.63E-04
Fish	20	8.08 ^e	25.3	2.29	Acute	2.12E-03 ⁶⁷	8.98E-05
Fish	20	8.08 ^e	25.3	2.29	Acute	2.12E-03 ⁶⁷	8.98E-05
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	3.39E-04 ⁶⁸	1.27E-05
Standard deviation						3.59E-03	1.94E-04
Cr							
Algae	25	8.1	34.58 ^f	2.29	Chronic	4.23E-06 ⁶⁹	3.13E-13
Algae	25	8.1	34.58 ^f	2.29	Chronic	3.85E-06 ⁶⁹	2.73E-13
Crustaceans	22.5 ^d	8 ^d	30	2.29	Acute	3.90E-05 ⁷⁰	2.44E-12
Crustaceans	14	8.08 ^e	34.58 ^f	2.29	Acute	8.10E-05 ⁷¹	1.66E-11
Fish	19.5	7.9	34	2.29	Acute	2.23E-04 ⁶¹	5.94E-11
Fish	24 ^d	8 ^d	34.9	2.29	Acute	2.50E-03 ⁷²	2.00E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	1.92E-03 ⁷²	1.54E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	1.63E-03 ⁷²	1.31E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	1.54E-03 ⁷²	1.23E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	7.69E-03 ⁷²	6.19E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	6.54E-03 ⁷²	5.27E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	2.98E-03 ⁷²	2.39E-10
Fish	24 ^d	8 ^d	34.9	2.29	Acute	5.58E-03 ⁷²	4.48E-10
Standard deviation						2.65E-03	2.10E-10
Cu							
Algae	21	8.08 ^e	34.58 ^f	2.29	Chronic	9.06E-06 ⁷³	1.64E-07
Algae	18	8.05 ^d	20	2.29	Chronic	2.83E-07 ⁷⁴	2.16E-09
Algae	18	8.05 ^d	15	2.29	Chronic	3.30E-07 ⁷⁴	2.69E-09
Algae	15	8.08 ^e	35	0	Chronic	6.29E-07 ⁴¹	1.46E-08
Algae	20	8	34.58 ^f	2.29	Chronic	1.38E-06 ⁷⁵	2.41E-08
Algae	20	8	34.58 ^f	2.29	Chronic	9.13E-07 ⁷⁵	1.41E-08
Algae	20	8	34.58 ^f	2.29	Chronic	2.16E-06 ⁷⁵	4.16E-08
Algae	20	8	34.58 ^f	2.29	Chronic	7.55E-07 ⁷⁵	1.09E-08
Algae	20	8	34.58 ^f	2.29	Chronic	5.19E-06 ⁷⁵	1.13E-07

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Cu							
Algae	15	8.08 ^e	34.58 ^f	0	Chronic	5.63E-08 ⁴⁶	1.31E-09
Algae	20	8.2	33	2.29	Chronic	8.93E-08 ⁷⁶	2.01E-10
Algae	20	8.2	33	2.29	Chronic	2.57E-08 ⁷⁶	9.81E-12
Algae	20	8.2	33	2.29	Chronic	4.17E-08 ⁷⁶	3.08E-11
Algae	20	8.2	33	2.29	Chronic	5.21E-08 ⁷⁶	5.62E-11
Algae	20	8.2	33	2.29	Chronic	5.58E-08 ⁷⁶	6.75E-11
Algae	19	8.08 ^e	34.58 ^f	0	Chronic	2.18E-06 ⁷⁷	4.73E-08
Algae	20	8.08 ^e	34.58 ^f	0	Chronic	2.89E-04 ⁷⁸	6.18E-06
Algae	20	8.08 ^e	34.58 ^f	0	Chronic	1.18E-05 ⁷⁸	2.52E-07
Algae	25	8	17	0	Chronic	7.44E-07 ⁴²	2.04E-08
Algae	18	7.6	35	2.29	Chronic	1.72E-06 ⁷⁹	7.52E-08
Algae	20	8.08 ^e	30.5	2.29	Chronic	8.85E-06 ⁸⁰	1.65E-07
Algae	20	8.05 ^d	34.58 ^f	0	Chronic	1.48E-06 ⁶⁵	3.45E-08
Algae	20	8.05 ^d	34.58 ^f	0	Chronic	2.06E-07 ⁶⁵	4.80E-09
Algae	20	8.08 ^e	5.5	2.29	Chronic	1.94E-05 ⁶⁷	4.40E-07
Algae	24	8	34.58 ^f	0	Chronic	1.88E-07 ⁸¹	4.74E-09
Algae	24	8	36	0	Chronic	1.21E-07 ⁸²	3.03E-09
Algae	24	8	36	0	Chronic	2.40E-07 ⁸²	6.02E-09
Algae	24	8	36	0	Chronic	6.01E-08 ⁸²	1.51E-09
Algae	24	8	36	0	Chronic	2.51E-09 ⁸²	6.30E-11
Algae	24	8	36	0	Chronic	2.26E-08 ⁸²	5.67E-10
Algae	24	8	36	0	Chronic	2.76E-08 ⁸²	6.92E-10
Algae	24	8	36	0	Chronic	1.05E-07 ⁸²	2.63E-09
Algae	24	8	36	0	Chronic	1.71E-07 ⁸²	4.29E-09
Algae	24	8	36	0	Chronic	2.89E-07 ⁸²	7.25E-09
Algae	24	8	36	0	Chronic	2.16E-07 ⁸²	5.42E-09
Algae	24	8	36	0	Chronic	2.19E-07 ⁸²	5.49E-09
Algae	24	8	36	0	Chronic	6.14E-08 ⁸²	1.54E-09
Algae	20	8.2	26	2.29	Chronic	2.76E-07 ⁸³	1.36E-09
Algae	21	8.08 ^e	34.58 ^f	2.29	Chronic	6.14E-06 ⁸⁴	1.07E-07
Algae	15	8.15 ^d	30	2.29	Chronic	5.64E-07 ⁸⁵	5.50E-09
Algae	15	8.15 ^d	30	2.29	Chronic	1.38E-06 ⁸⁵	1.80E-08
Algae	20	8	10	0	Chronic	3.19E-06 ⁸⁶	1.00E-07
Algae	25	8.25	33	0	Chronic	6.08E-06 ⁸⁷	7.13E-08
Algae	-1	8.2	34.58 ^f	2.29	Chronic	6.58E-07 ⁸⁸	9.56E-09
Algae	25	8.25	33	0	Chronic	7.96E-06 ⁸⁹	9.34E-08
Algae	25	8.25	33	0	Chronic	4.82E-06 ⁸⁹	5.66E-08
Algae	25	8.25	33	0	Chronic	1.82E-06 ⁸⁹	2.14E-08
Algae	15	7.95 ^d	30 ^d	0	Chronic	4.54E-07 ⁴⁷	1.54E-08
Algae	21	8.25 ^d	30	2.29	Chronic	5.33E-07 ⁹⁰	3.18E-09
Algae	-1	8.2	34.58 ^f	2.29	Chronic	5.64E-07 ⁸⁸	7.79E-09
Algae	-1	8.2	34.58 ^f	2.29	Chronic	5.14E-07 ⁸⁸	6.88E-09
Algae	15	8.08 ^e	30	0	Chronic	6.00E-05 ⁹¹	1.42E-06
Algae	25	8.08 ^e	25	2.29	Chronic	9.36E-07 ⁹²	1.04E-08
Algae	25	8.08 ^e	40	2.29	Chronic	1.18E-05 ⁹²	2.01E-07
Algae	25	8.08 ^e	35	2.29	Chronic	1.48E-05 ⁹²	2.60E-07
Algae	25	8.08 ^e	30	2.29	Chronic	2.96E-06 ⁹²	4.41E-08

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Cu							
Algae	25	8.08 ^e	20	2.29	Chronic	3.82E-06 ⁹²	6.06E-08
Algae	-1	8.2	34.58 ^f	2.29	Chronic	3.82E-07 ⁸⁸	4.57E-09
Algae	-1	8.2	34.58 ^f	2.29	Chronic	6.64E-06 ⁸⁸	1.41E-07
Algae	25	8.25 ^d	33	0	Chronic	2.00E-05 ⁸⁹	2.35E-07
Algae	21.85 ^d	8.09 ^d	31.15 ^d	0	Chronic	3.12E-07 ⁹³	6.48E-09
Algae	21.85 ^d	8.09 ^d	31.15 ^d	0.1	Chronic	2.83E-07 ⁹³	5.60E-09
Algae	21.85 ^d	8.09 ^d	31.15 ^d	0.5	Chronic	3.72E-07 ⁹³	6.28E-09
Algae	21.85 ^d	8.09 ^d	31.15 ^d	1.6	Chronic	5.21E-07 ⁹³	6.20E-09
Algae	21.85 ^d	8.09 ^d	31.15 ^d	2.0	Chronic	8.55E-07 ⁹³	1.06E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	4.39E-06 ⁴⁹	7.49E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	2.16E-06 ⁴⁹	3.07E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	5.95E-06 ⁴⁹	1.01E-07
Algae	24	8.08 ^e	7.6	2.29	Chronic	5.95E-06 ⁴⁹	9.76E-08
Crustaceans	19 ^d	8.05 ^d	35.8 ^d	2.29	Chronic	2.13E-06 ⁵⁵	3.65E-08
Crustaceans	15	7.9	30	2.29	Chronic	8.93E-06 ⁹⁴	2.94E-07
Crustaceans	21	8.1 ^d	30	2.29	Chronic	7.07E-06 ⁹⁵	1.20E-07
Crustaceans	21	8.1 ^d	30	2.29	Chronic	1.41E-06 ⁹⁵	1.86E-08
Crustaceans	21	8.1 ^d	30	2.29	Chronic	1.12E-06 ⁹⁵	1.38E-08
Crustaceans	21	8.1 ^d	30	2.29	Chronic	1.64E-06 ⁹⁵	2.24E-08
Crustaceans	21	8.1 ^d	30	2.29	Chronic	1.34E-06 ⁹⁵	1.74E-08
Crustaceans	19 ^d	8.05 ^d	35.8 ^d	2.29	Chronic	1.38E-06 ⁵⁵	2.16E-08
Crustaceans	16	7.8	30	0	Chronic	6.93E-07 ⁹⁶	3.29E-08
Crustaceans	16	7.8	30	0	Chronic	1.55E-03 ⁹⁶	7.36E-05
Crustaceans	21	8.1 ^d	30	2.29	Chronic	1.13E-06 ⁵⁷	1.40E-08
Crustaceans	21	8.1 ^d	30	2.29	Chronic	2.26E-07 ⁹⁷	1.26E-09
Crustaceans	21	8.1 ^d	30	2.29	Chronic	4.76E-07 ⁹⁷	4.14E-09
Crustaceans	27	7.85 ^d	20	0	Chronic	2.00E-06 ⁹⁸	7.75E-08
Crustaceans	27	7.85 ^d	20	0	Chronic	5.00E-06 ⁹⁸	1.94E-07
Crustaceans	27	7.85 ^d	20	0	Chronic	8.00E-06 ⁹⁸	3.10E-07
Crustaceans	19 ^d	8.05 ^d	35.8 ^d	2.29	Chronic	1.19E-06 ⁵⁵	1.79E-08
Crustaceans	10	8.08 ^e	33	0	Chronic	2.40E-06 ⁹⁹	6.21E-08
Crustaceans	10	8.08 ^e	33	0	Chronic	5.10E-06 ⁹⁹	1.32E-07
Crustaceans	10	8.08 ^e	33	0	Chronic	9.20E-06 ⁹⁹	2.38E-07
Crustaceans	20	8.1	33	0	Chronic	2.31E-07 ¹⁰⁰	4.68E-09
Crustaceans	20	8.1	33	0	Chronic	1.54E-07 ¹⁰⁰	3.12E-09
Crustaceans	20	8.1	33	0	Chronic	1.24E-07 ¹⁰⁰	2.51E-09
Crustaceans	20	8.1	33	0	Chronic	1.09E-07 ¹⁰⁰	2.21E-09
Crustaceans	20	8.1	33	0	Chronic	1.74E-07 ¹⁰⁰	3.53E-09
Crustaceans	20	8.1	33	0	Chronic	1.91E-07 ¹⁰⁰	3.87E-09
Crustaceans	20	8.08 ^e	30	2.29	Chronic	3.23E-07 ⁶⁰	2.45E-09
Crustaceans	21	8.1 ^d	30	2.29	Chronic	1.86E-06 ⁹⁵	2.61E-08
Fish	21	8	25	2.29	Chronic	9.98E-07 ¹⁰¹	1.56E-08
Fish	21	8	34	2.29	Chronic	1.53E-06 ¹⁰¹	2.68E-08
Fish	21	8	10	2.29	Chronic	3.25E-07 ¹⁰¹	2.52E-09
Fish	21	8	17	2.29	Chronic	5.36E-07 ¹⁰¹	6.25E-09
Standard deviation						1.57E-04	7.34E-06

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Mn							
Algae	15	8.05 ^d	34.58 ^f	2.29	Chronic	1.70E-04 ⁶⁵	2.34E-05
Algae	24	8.08 ^e	7.6	2.29	Chronic	7.95E-05 ⁴⁹	2.08E-05
Algae	24	8.08 ^e	7.6	2.29	Chronic	7.95E-05 ⁴⁹	2.08E-05
Algae	24	8.08 ^e	7.6	2.29	Chronic	2.73E-05 ⁴⁹	7.02E-06
Crustaceans	28	7.95 ^d	33.24 ^d	2.29	Acute	5.96E-04 ¹⁰²	2.04E-05
Crustaceans	28	7.95 ^d	33.24 ^d	2.29	Acute	4.12E-04 ¹⁰²	1.41E-05
Crustaceans	27.2 ^d	8.05 ^d	34	0	Acute	9.54E-04 ¹⁰³	3.25E-05
Crustaceans	27.2 ^d	8.05 ^d	34	0	Acute	1.41E-03 ¹⁰³	4.82E-05
Crustaceans	27.2 ^d	8.05 ^d	34	0	Acute	5.56E-04 ¹⁰³	1.89E-05
Crustaceans	27.2 ^d	8.05 ^d	34	0	Acute	1.03E-03 ¹⁰³	3.52E-05
Crustaceans	20	8	7	2.29	Acute	5.56E-04 ⁶⁶	3.86E-05
Fish	28	8.5	26	2.29	Acute	1.75E-03 ¹⁰⁴	7.35E-05
Fish	28	8.5	26	2.29	Acute	1.99E-03 ¹⁰⁴	8.35E-05
Standard deviation						6.49E-04	2.28E-05
Ni							
Algae	25	8	33	2.29	Chronic	1.31E-04 ⁴²	1.51E-05
Algae	24	8.08 ^e	7.6	2.29	Chronic	7.03E-05 ⁴⁹	1.11E-05
Algae	24	8.08 ^e	7.6	2.29	Chronic	9.26E-06 ⁴⁹	1.46E-06
Algae	24	8.08 ^e	7.6	2.29	Chronic	2.90E-05 ⁴⁹	4.59E-06
Algae	24	8.08 ^e	7.6	2.29	Chronic	7.02E-07 ⁴⁹	1.09E-07
Crustaceans	26	8.08 ^e	33	2.29	Chronic	1.00E-05 ¹⁰⁵	1.05E-06
Crustaceans	20	7.8	20	2.29	Chronic	2.31E-04 ⁵³	3.79E-05
Crustaceans	10	8.08 ^e	15	2.29	Chronic	8.49E-05 ¹⁰⁶	1.24E-05
Crustaceans	5	8.08 ^e	25	2.29	Chronic	1.16E-04 ¹⁰⁶	1.52E-05
Crustaceans	5	8.08 ^e	35	2.29	Chronic	1.23E-04 ¹⁰⁶	1.44E-05
Crustaceans	10	8.08 ^e	35	2.29	Chronic	1.23E-04 ¹⁰⁶	1.38E-05
Crustaceans	10	8.08 ^e	5	2.29	Chronic	2.47E-05 ¹⁰⁶	4.67E-06
Crustaceans	15	8.08 ^e	15	2.29	Chronic	3.86E-05 ¹⁰⁶	5.40E-06
Crustaceans	5	8.08 ^e	10	2.29	Chronic	5.40E-05 ¹⁰⁶	9.23E-06
Crustaceans	10	8.08 ^e	10	2.29	Chronic	5.40E-05 ¹⁰⁶	8.75E-06
Crustaceans	15	8.08 ^e	25	2.29	Chronic	5.56E-05 ¹⁰⁶	6.71E-06
Crustaceans	15	8.08 ^e	35	2.29	Chronic	5.79E-05 ¹⁰⁶	6.27E-06
Crustaceans	10	8.08 ^e	25	2.29	Chronic	6.56E-05 ¹⁰⁶	8.21E-06
Crustaceans	5	8.08 ^e	15	2.29	Chronic	7.33E-05 ¹⁰⁶	1.12E-05
Crustaceans	21	8.1	30	2.29	Chronic	2.00E-05 ⁵⁷	2.15E-06
Crustaceans	20	8.08 ^e	30	2.29	Chronic	4.09E-05 ⁶⁰	4.54E-06
Fish	20	7.8	20	2.29	Acute	3.09E-03 ⁵³	6.01E-04
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	2.34E-04 ⁶⁸	2.90E-05
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	1.58E-04 ⁶⁸	1.95E-05
Fish	12	7.7	34.6	2.29	Acute	9.32E-04 ¹⁰⁷	1.58E-04
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	1.37E-04 ⁶⁸	1.69E-05
Fish	12	7.7	34.6	2.29	Acute	5.14E-04 ¹⁰⁷	8.66E-05
Fish	20	7.8	20	2.29	Acute	2.70E-03 ⁵³	5.26E-04
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	1.25E-04 ⁶⁸	1.56E-05
Fish	12	7.7	34.6	2.29	Acute	4.07E-04 ¹⁰⁷	6.87E-05
Fish	20	7.8	20	2.29	Chronic	1.16E-03 ⁵³	1.90E-04
Standard deviation						7.28E-04	1.41E-04

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Pb							
Algae	20	8	34.58 ^f	2.29	Chronic	5.07E-07 ⁷⁵	6.24E-09
Algae	15	8.08 ^e	35	0	Chronic	2.36E-06 ⁴¹	2.95E-08
Algae	25	8	33	2.29	Chronic	1.44E-05 ⁴²	1.87E-07
Algae	15	7.95 ^d	30 ^d	0	Chronic	2.65E-06 ⁴⁷	4.97E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	1.97E-05 ⁴⁹	2.85E-07
Algae	24	8.08 ^e	7.6	2.29	Chronic	4.35E-06 ⁴⁹	5.74E-08
Algae	24	8.08 ^e	7.6	2.29	Chronic	9.03E-06 ⁴⁹	1.25E-07
Algae	24	8.08 ^e	7.6	2.29	Chronic	3.42E-06 ⁴⁹	4.43E-08
Crustaceans	15	8.1	33.79	2.29	Acute	1.74E-06 ¹⁰⁸	7.54E-09
Crustaceans	28	7.95 ^d	33.24 ^d	2.29	Acute	5.13E-06 ¹⁰²	2.73E-08
Crustaceans	22	8	35	2.29	Acute	1.71E-05 ¹⁰⁹	9.06E-08
Crustaceans	28	7.95 ^d	33.24 ^d	2.29	Acute	4.23E-06 ¹⁰²	2.23E-08
Crustaceans	22	8	35	2.29	Acute	9.50E-06 ¹⁰⁹	4.95E-08
Crustaceans	22	8	35	2.29	Acute	7.29E-06 ¹⁰⁹	3.77E-08
Crustaceans	8.5	8.1	30	2.29	Acute	2.16E-06 ¹¹⁰	1.11E-08
Crustaceans	15	8.1	17	2.29	Acute	1.87E-06 ¹¹¹	9.30E-09
Crustaceans	22	8	35	2.29	Acute	3.30E-06 ¹⁰⁹	1.66E-08
Crustaceans	20	8.08 ^e	5	2.29	Acute	3.44E-06 ¹¹²	1.82E-08
Crustaceans	21	8.1 ^d	30	2.29	Acute	5.50E-06 ⁵⁷	2.31E-08
Crustaceans	8.5	8.1	30	2.29	Acute	7.55E-06 ¹¹⁰	4.01E-08
Crustaceans	21	8.1 ^d	30	2.29	Acute	1.08E-05 ⁵⁷	4.62E-08
Crustaceans	20	8.08 ^e	25	2.29	Acute	1.29E-05 ¹¹²	6.30E-08
Crustaceans	15	8.1	17	2.29	Acute	1.39E-05 ¹¹¹	7.47E-08
Crustaceans	29	11	20	2.29	Acute	1.42E-05 ¹¹³	4.29E-18
Crustaceans	45	7.2	20	2.29	Acute	1.46E-05 ¹¹³	1.76E-07
Crustaceans	19	8.08 ^e	34.58 ^f	2.29	Acute	1.80E-05 ¹¹⁴	8.16E-08
Crustaceans	29	2.8	20	2.29	Acute	1.58E-05 ¹¹³	3.05E-07
Crustaceans	29	7.2	29	2.29	Acute	1.67E-05 ¹¹³	1.97E-07
Crustaceans	15	8.1	17	2.29	Acute	1.78E-05 ¹¹¹	9.62E-08
Crustaceans	10	7.2	20	2.29	Acute	2.09E-05 ¹¹³	4.52E-07
Crustaceans	29	7.2	20	2.29	Acute	2.21E-05 ¹¹³	3.59E-07
Crustaceans	29	8.08 ^e	20	2.29	Acute	2.21E-05 ¹¹³	1.04E-07
Crustaceans	19	8.08 ^e	34.58 ^f	2.29	Acute	3.60E-05 ¹¹⁴	1.66E-07
Crustaceans	22.5 ^d	8 ^d	30	2.29	Acute	1.51E-05 ⁷⁰	8.45E-08
Crustaceans	21	8.1 ^d	30	2.29	Chronic	4.57E-06 ⁵⁷	4.76E-08
Crustaceans	20	8.08 ^e	30	2.29	Chronic	1.46E-05 ⁶⁰	1.69E-07
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	9.29E-06 ⁶⁸	2.96E-08
Fish	12	7.7	34.6	2.29	Acute	1.36E-05 ¹⁰⁷	1.02E-07
Fish	28	7.19	9.8	2.29	Acute	3.22E-04 ¹¹⁵	7.52E-06
Fish	28	7.19	9.8	2.29	Acute	5.15E-04 ¹¹⁵	1.22E-05
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	6.72E-06 ⁶⁸	2.12E-08
Fish	12	7.7	34.6	2.29	Acute	1.36E-05 ¹⁰⁷	1.02E-07
Fish	28	7.19	9.8	2.29	Acute	2.29E-04 ¹¹⁵	5.30E-06
Fish	28	7.19	9.8	2.29	Acute	3.67E-04 ¹¹⁵	8.57E-06
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	4.89E-06 ⁶⁸	1.52E-08
Fish	12	7.7	34.6	2.29	Acute	1.36E-05 ¹⁰⁷	1.02E-07
Fish	28	7.19	9.8	2.29	Acute	2.12E-04 ¹¹⁵	4.90E-06

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Pb							
Fish	28	7.19	9.8	2.29	Acute	3.39E-04 ¹¹⁵	7.95E-06
Fish	19.75 ^d	8.08 ^e	32.5	2.29	Acute	1.53E-08 ¹¹⁶	4.03E-11
Fish	20 ^g	8.08 ^e	36.1 ^d	2.29	Acute	3.76E-06 ⁶⁸	1.17E-08
Fish	8.3	7.9	27	2.29	Acute	5.39E-06 ¹¹⁰	3.59E-08
Fish	12	7.7	34.6	2.29	Acute	1.36E-05 ¹⁰⁷	1.02E-07
Fish	28	7.19	9.8	2.29	Acute	1.95E-04 ¹¹⁵	4.49E-06
Fish	28	7.19	9.8	2.29	Acute	3.12E-04 ¹¹⁵	7.28E-06
Standard deviation						1.15E-04	2.73E-06
Zn							
Algae	18	8.08	34.58	2.29	Chronic	1.18E-04 ⁸⁵	1.58E-05
Algae	18	8.08	34.58	2.29	Chronic	1.30E-04 ⁸⁵	1.74E-05
Algae	15	8.08	35	0	Chronic	8.74E-06 ⁴¹	1.20E-06
Algae	20	8.05	34.58	2.29	Chronic	1.68E-06 ⁶⁵	2.21E-07
Algae	15	7.95	30	0	Chronic	3.90E-06 ⁴⁷	5.92E-07
Crustaceans	17.5	7.9	34.7	2.29	Chronic	7.70E-05 ⁵¹	1.09E-05
Crustaceans	20	7.8	20	2.29	Chronic	1.47E-06 ⁵³	2.56E-07
Crustaceans	19	8.05	35.8	2.29	Chronic	1.45E-05 ⁵⁵	1.91E-06
Crustaceans	15	8	35	2.29	Chronic	4.39E-07 ¹¹⁷	5.94E-08
Crustaceans	20	8	34	2.29	Chronic	1.42E-06 ¹¹⁷	1.91E-07
Crustaceans	20	8	34	2.29	Chronic	1.42E-06 ¹¹⁷	1.91E-07
Crustaceans	12	8.08	33	2.29	Chronic	1.98E-07 ¹¹⁸	2.71E-08
Crustaceans	12	8.08	33	2.29	Chronic	2.91E-07 ¹¹⁸	3.99E-08
Crustaceans	12	8.08	33	2.29	Chronic	3.66E-07 ¹¹⁸	5.03E-08
Crustaceans	12	8.08	33	2.29	Chronic	3.84E-07 ¹¹⁸	5.28E-08
Crustaceans	12	8.08	33	2.29	Chronic	4.03E-07 ¹¹⁸	5.55E-08
Crustaceans	12	8.08	33	2.29	Chronic	4.27E-07 ¹¹⁸	5.88E-08
Crustaceans	26.5	8	30	2.29	Chronic	1.19E-06 ¹¹⁷	1.60E-07
Crustaceans	5	8.08	10	2.29	Chronic	6.20E-06 ¹⁰⁶	1.40E-06
Crustaceans	15	8.08	25	2.29	Chronic	6.81E-06 ¹⁰⁶	1.05E-06
Crustaceans	5	8.08	15	2.29	Chronic	1.05E-05 ¹⁰⁶	2.08E-06
Crustaceans	10	8.08	35	2.29	Chronic	1.05E-05 ¹⁰⁶	1.46E-06
Crustaceans	10	8.08	15	2.29	Chronic	1.18E-05 ¹⁰⁶	2.27E-06
Crustaceans	10	8.08	25	2.29	Chronic	1.67E-05 ¹⁰⁶	2.66E-06
Crustaceans	5	8.08	25	2.29	Chronic	1.86E-05 ¹⁰⁶	3.06E-06
Crustaceans	5	8.08	35	2.29	Chronic	2.73E-05 ¹⁰⁶	3.92E-06
Crustaceans	19	8.05	35.8	2.29	Chronic	1.13E-05 ⁵⁵	1.49E-06
Crustaceans	21	8.1	30	2.29	Chronic	1.42E-05 ⁹⁵	1.94E-06
Crustaceans	21	8.1	30	2.29	Chronic	5.21E-06 ⁹⁵	7.10E-07
Crustaceans	21	8.1	30	2.29	Chronic	5.36E-06 ⁹⁵	7.30E-07
Crustaceans	21	8.1	30	2.29	Chronic	6.60E-06 ⁹⁵	9.00E-07
Crustaceans	21	8.1	30	2.29	Chronic	5.58E-06 ⁹⁵	7.60E-07
Crustaceans	20	8.08	30	2.29	Chronic	5.24E-06 ⁶⁰	7.25E-07
Crustaceans	20	8.08	20	2.29	Chronic	1.70E-05 ¹¹⁹	2.77E-06
Crustaceans	20	8.08	20	2.29	Chronic	3.30E-05 ¹¹⁹	5.39E-06
Crustaceans	21	8.08	7	2.29	Chronic	1.25E-06 ⁵⁸	2.72E-07
Crustaceans	21	8.08	15	2.29	Chronic	1.24E-06 ⁵⁸	2.16E-07
Crustaceans	21	8.08	25	2.29	Chronic	1.24E-06 ⁵⁸	1.81E-07

Species group	Temp. [°C]	pH	Salinity [%o]	DOC [mg/l] ^a	Acute/Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Zn							
Crustaceans	19	8.05	35.8	2.29	Chronic	7.78E-06 ⁵⁵	1.02E-06
Crustaceans	19	8.05	35.8	2.29	Chronic	8.44E-06 ⁵⁵	1.11E-06
Crustaceans	10	8.08	33	0	Chronic	1.35E-05 ⁹⁹	1.95E-06
Crustaceans	10	8.08	33	0	Chronic	3.80E-05 ⁹⁹	5.50E-06
Crustaceans	10	8.08	33	0	Chronic	6.00E-06 ⁹⁹	8.68E-07
Fish	20	7.8	20	2.29	Acute	9.17E-04 ⁵³	9.77E-05
Fish	20	8.08	6.1	2.29	Acute	3.48E-04 ⁶⁷	5.08E-05
Fish	20	8.08	22.9	2.29	Acute	1.08E-03 ⁶⁷	1.00E-04
Fish	20	8.08	6	2.29	Acute	1.70E-03 ⁶⁷	2.53E-04
Fish	20	8.08	6.1	2.29	Acute	2.02E-04 ⁶⁷	2.92E-05
Fish	20	8.08	24	2.29	Acute	2.31E-04 ⁶⁷	2.08E-05
Fish	20	8.08	6	2.29	Acute	8.36E-04 ⁶⁷	1.23E-04
Fish	20	8.08	22.9	2.29	Acute	2.94E-04 ⁶⁷	2.72E-05
Fish	20	8.08	6.1	2.29	Acute	1.69E-04 ⁶⁷	2.44E-05
Fish	20	8.08	24	2.29	Acute	2.31E-04 ⁶⁷	2.08E-05
Fish	20	8.08	22.9	2.29	Acute	1.70E-04 ⁶⁷	1.57E-05
Fish	20	8.08	6	2.29	Acute	1.98E-04 ⁶⁷	2.89E-05
Fish	20	8.08	6.1	2.29	Acute	1.28E-04 ⁶⁷	1.85E-05
Fish	20	8.08	24	2.29	Acute	2.31E-04 ⁶⁷	2.08E-05
Fish	20	8.08	22.9	2.29	Acute	1.70E-04 ⁶⁷	1.57E-05
Fish	20	8.08	6	2.29	Acute	1.98E-04 ⁶⁷	2.89E-05
Fish	14.5	7.7	36.5	2.29	Acute	1.12E-03 ¹²⁰	9.55E-05
Fish	20	8.08	36.1	2.29	Acute	1.21E-04 ⁶⁸	9.31E-06
Fish	28	7.19	9.8	2.29	Acute	7.91E-04 ¹¹⁵	1.17E-04
Fish	28	7.19	9.8	2.29	Acute	1.80E-04 ¹¹⁵	2.65E-05
Fish	14.5	7.7	36.5	2.29	Acute	4.96E-04 ¹²⁰	4.23E-05
Fish	20	8.08	36.1	2.29	Acute	9.29E-05 ⁶⁸	7.11E-06
Fish	13	7.65	29.5	2.29	Acute	5.90E-05 ¹²¹	5.57E-06
Fish	28	7.19	9.8	2.29	Acute	1.39E-04 ¹¹⁵	2.04E-05
Fish	28	7.19	9.8	2.29	Acute	6.10E-04 ¹¹⁵	9.05E-05
Fish	12	7.7	34.6	2.29	Acute	1.95E-04 ¹⁰⁷	1.72E-05
Fish	20	8.08	36.1	2.29	Acute	8.05E-05 ⁶⁸	6.16E-06
Fish	28	7.19	9.8	2.29	Acute	1.06E-04 ¹¹⁵	1.56E-05
Fish	28	7.19	9.8	2.29	Acute	4.66E-04 ¹¹⁵	6.90E-05
Fish	12	7.7	34.6	2.29	Acute	1.19E-04 ¹⁰⁷	1.05E-05
Fish	22	8.2	38	2.29	Acute	1.87E-07 ¹²²	1.25E-08
Fish	20	7.8	20	2.29	Acute	4.40E-04 ⁵³	4.68E-05
Fish	13	8	29	2.29	Acute	1.40E-06 ¹¹⁰	1.23E-07
Fish	19.5	7.9	34	2.29	Acute	8.44E-05 ⁶¹	7.01E-06
Fish	19.5	7.9	34	2.29	Acute	1.03E-04 ⁶¹	8.54E-06
Fish	19.5	7.9	34	2.29	Acute	2.46E-04 ⁶¹	2.05E-05
Fish	19.5	7.9	34	2.29	Acute	2.97E-04 ⁶¹	2.47E-05
Fish	19.75	8	32.5	2.29	Acute	1.09E-06 ¹¹⁶	8.78E-08
Fish	19.75	8	32.5	2.29	Acute	1.98E-07 ¹¹⁶	1.57E-08
Fish	26	8.08	14	0.916	Acute	8.02E-04 ¹²³	8.48E-05
Fish	26	8.08	14	0.916	Acute	7.39E-04 ¹²³	7.82E-05
Fish	26	8.08	14	0.916	Acute	1.09E-03 ¹²³	1.16E-04

Species group	Temp. [°C]	pH	Salinity [%]	DOC [mg/l] ^a	Acute/ Chronic ^b	Reported EC ₅₀ in literature [mol/l]	WHAM calculated free ion EC ₅₀ [mol/l] ^c
Zn							
Fish	20	8.08	36.1	2.29	Acute	6.81E-05 ⁶⁸	5.21E-06
Fish	28	7.19	9.8	2.29	Acute	8.49E-05 ¹¹⁵	1.24E-05
Fish	28	7.19	9.8	2.29	Acute	3.74E-04 ¹¹⁵	5.52E-05
Fish	12	7.7	34.6	2.29	Acute	1.14E-04 ¹⁰⁷	1.00E-05
Fish	10	7.8	7	2.29	Acute	2.35E-04 ¹²⁴	3.87E-05
Fish	25	8.08	18	2.29	Acute	8.29E-05 ¹²⁵	7.98E-06
Fish	10	7.8	7	2.29	Acute	2.60E-04 ¹²⁴	4.26E-05
Fish	12	8	32	2.29	Acute	8.98E-05 ¹²⁶	7.77E-06
Fish	20	7.8	20	2.29	Chronic	3.81E-04 ⁵³	6.87E-05
Standard deviation						3.08E-04	3.87E-05

- a. DOC is based on estimation. If the test medium is diluted with artificial seawater, a DOC value of 0 mg/l was used, assuming distilled water is used to prepared the test medium. If the test medium is diluted with filtered natural seawater, the arithmetic mean of global near shore DOC concentrations⁶ (2.29mg/l) was used.
- b. For crustacean and fish, EC₅₀ estimated in toxicity tests with a duration of up to 96h is considered acute. EC₅₀ from toxicity tests with a duration longer than 96h is considered chronic¹²⁷. For Algae, EC₅₀ estimated in toxicity tests with a duration up to 72h is considered acute. EC₅₀ from toxicity tests with a duration equal to or longer than 72h is considered chronic¹²⁸.
- c. When there were less than 3 chronic EC₅₀ data available from literature, acute EC₅₀ were used to estimate chronic free ion EC₅₀ applying an Acute to Chronic Ratio (ACR, Table S5) on the reported acute EC₅₀ to derive the corresponding chronic EC₅₀ and then the chronic free ion EC₅₀.
- d. Parameter is given as a range of values. The arithmetic mean of maximum and minimum value was taken.
- e. pH is not given. Median value of global coastal seawater pH³¹ (8.08) was taken.
- f. Salinity is not given. Median value of global coastal seawater salinity³¹ (34.58‰) was taken.
- g. Temperature is not given. Room temperature (20 °C) was assumed.

Table S6: Acute to Chronic Ratio (ACR) used to derive chronic EC₅₀s from reported acute EC₅₀.

All reported seawater EC₅₀ for algae, crustacean and fish in USEPA ECOTOX database¹²⁹, regardless of water chemistry, were labeled as acute or chronic respectively, according to the criteria mentioned in Table S5. For each metal and each trophic level, the ratio between the geometric mean of reported acute EC₅₀ and the geometric mean of reported chronic EC₅₀ was calculated as the ACR. Where an ACR cannot be calculated for a combination of metal and trophic level due to lack of EC₅₀ data, an X was put in the table. Here the average ACR for the concerned trophic level was applied. The arithmetic mean of ACR across all available metals for one trophic level was recorded as the average ACR for that trophic level.

ACR used in paper	Algae	Crustacean	Fish
Cd	1.23	0.93	6.51
Co	X	X ^a	X ^a
Cr	11.11	X ^a	X ^a
Cu	1.49	1.80	4.04
Mn	X	X ^a	X ^a
Ni	6.70	2.23	0.84 ^a
Pb	0.65	2.43 ^a	X ^a
Zn	2.45	12.55	1.69 ^a
Average	3.94	3.99	3.27

- a. ACR were applied in the study to derive chronic EC₅₀s from reported acute EC₅₀.

Table S7: Calculated Fate Factors (FFs [day]), Bioavailability Factors (BF [dimensionless]), Effect Factors (EF, [(PAF)·m³/kg]) and Comparative Toxicity Potentials (CTP, [(PAF)·day·m³/kg]) for nine metals in 64 LME seawaters

	Cd				Co				Cr				Cu				Fe			
	FF	BF	EF	CTP																
LME 1	7.8E+02	1.0E+00	2.7E+02	2.1E+05	8.2E+02	1.0E+00	1.0E+02	8.2E+04	8.4E+01	5.3E-04	1.0E+04	4.6E+02	1.9E+02	3.9E-02	2.2E+04	1.7E+05	8.2E+01	8.3E-04	0.0E+00	0.0E+00
LME 2	1.9E+02	1.0E+00	2.7E+02	5.0E+04	2.3E+02	1.0E+00	1.0E+02	2.4E+04	8.6E+00	6.7E-04	8.8E+03	5.1E+01	1.3E+01	3.6E-02	2.7E+04	1.3E+04	8.6E+00	9.0E-04	0.0E+00	0.0E+00
LME 3	3.7E+02	1.0E+00	2.5E+02	9.3E+04	5.0E+02	1.0E+00	9.5E+01	4.7E+04	6.0E+00	1.5E-03	1.3E+03	1.2E+01	1.3E+01	3.2E-02	1.7E+04	7.2E+03	6.0E+00	1.7E-03	0.0E+00	0.0E+00
LME 4	5.5E+02	1.0E+00	2.4E+02	1.3E+05	5.6E+02	1.0E+00	9.2E+01	5.1E+04	4.6E+01	2.0E-03	3.9E+02	3.5E+01	9.5E+01	1.8E-02	1.6E+04	2.7E+04	4.5E+01	1.8E-03	0.0E+00	0.0E+00
LME 5	2.0E+04	1.0E+00	2.3E+02	4.4E+06	2.0E+04	1.0E+00	8.0E+01	1.6E+06	5.8E+02	2.2E-03	1.3E+02	1.6E+02	3.0E+03	1.3E-02	9.7E+03	3.9E+05	5.6E+02	2.2E-03	0.0E+00	0.0E+00
LME 6	1.3E+02	1.0E+00	2.3E+02	3.0E+04	1.6E+02	1.0E+00	7.8E+01	1.2E+04	6.8E+00	9.4E-04	1.4E+02	8.8E-01	1.3E+01	7.0E-03	9.0E+03	8.1E+02	7.2E+00	1.2E-03	0.0E+00	0.0E+00
LME 7	1.0E+02	1.0E+00	2.7E+02	2.8E+04	1.1E+02	1.0E+00	1.1E+02	1.2E+04	1.1E+01	1.5E-04	6.3E+03	1.1E+01	1.5E+01	7.9E-03	2.8E+04	3.4E+03	1.1E+01	1.1E-04	0.0E+00	0.0E+00
LME 8	3.3E+02	1.0E+00	2.8E+02	9.4E+04	3.4E+02	1.0E+00	1.1E+02	3.7E+04	3.5E+01	4.2E-04	1.3E+04	1.9E+02	6.0E+01	2.7E-02	3.0E+04	4.8E+04	3.5E+01	4.4E-04	0.0E+00	0.0E+00
LME 9	1.3E+02	1.0E+00	2.7E+02	3.5E+04	1.4E+02	1.0E+00	1.1E+02	1.5E+04	9.0E+00	3.3E-04	1.8E+04	5.3E+01	1.3E+01	2.7E-02	3.0E+04	1.1E+04	9.0E+00	3.2E-04	0.0E+00	0.0E+00
LME 10	2.0E+02	1.0E+00	2.4E+02	4.7E+04	2.5E+02	1.0E+00	9.0E+01	2.2E+04	3.4E+00	2.7E-03	3.2E+02	3.0E+00	7.7E+00	2.3E-02	1.5E+04	2.6E+03	3.4E+00	2.8E-03	0.0E+00	0.0E+00
LME 11	3.4E+02	1.0E+00	2.4E+02	8.1E+04	4.4E+02	1.0E+00	9.3E+01	4.1E+04	8.0E+00	2.7E-03	2.9E+02	6.2E+00	1.2E+01	1.8E-02	1.7E+04	3.8E+03	7.8E+00	2.4E-03	0.0E+00	0.0E+00
LME 12	4.3E+02	1.0E+00	2.2E+02	9.8E+04	6.1E+02	1.0E+00	8.1E+01	5.0E+04	3.9E+00	5.2E-03	1.0E+02	2.1E+00	6.7E+00	2.3E-02	9.9E+03	1.5E+03	4.0E+00	6.1E-03	0.0E+00	0.0E+00
LME 13	2.5E+02	1.0E+00	2.4E+02	6.1E+04	3.3E+02	1.0E+00	1.0E+02	3.4E+04	1.0E+00	9.6E-04	4.1E+03	4.0E+00	1.4E+00	3.0E-02	2.8E+04	1.2E+03	1.0E+00	9.3E-04	0.0E+00	0.0E+00
LME 14	1.6E+02	1.0E+00	2.5E+02	4.2E+04	2.0E+02	1.0E+00	9.2E+01	1.9E+04	1.1E+01	1.3E-03	2.6E+03	3.8E+01	1.6E+01	4.7E-02	1.5E+04	1.2E+04	1.1E+01	3.0E-03	0.0E+00	0.0E+00
LME 15	1.5E+02	1.0E+00	2.3E+02	3.4E+04	1.7E+02	1.0E+00	8.3E+01	1.4E+04	5.9E+00	3.3E-03	2.5E+02	4.9E+00	1.0E+01	2.9E-02	1.1E+04	3.3E+03	6.0E+00	4.5E-03	0.0E+00	0.0E+00
LME 16	2.3E+02	1.0E+00	2.3E+02	5.3E+04	3.0E+02	1.0E+00	8.2E+01	2.5E+04	4.5E+00	4.8E-03	1.2E+02	2.5E+00	8.9E+00	2.3E-02	1.0E+04	2.1E+03	4.6E+00	5.7E-03	0.0E+00	0.0E+00
LME 17	1.4E+02	1.0E+00	2.3E+02	3.2E+04	1.7E+02	1.0E+00	8.5E+01	1.4E+04	4.8E+00	3.4E-03	1.4E+02	2.2E+00	6.8E+00	1.7E-02	1.2E+04	1.3E+03	4.8E+00	3.5E-03	0.0E+00	0.0E+00
LME 18	1.3E+02	1.0E+00	2.6E+02	3.5E+04	1.5E+02	1.0E+00	9.8E+01	1.5E+04	1.1E+01	4.5E-04	1.5E+04	7.4E+01	2.0E+01	4.8E-02	2.0E+04	1.9E+04	1.1E+01	7.3E-04	0.0E+00	0.0E+00
LME 19	2.2E+02	1.0E+00	2.5E+02	5.6E+04	2.9E+02	1.0E+00	9.1E+01	2.6E+04	1.0E+01	3.7E-04	8.4E+03	3.2E+01	2.0E+01	3.9E-02	1.5E+04	1.2E+04	1.0E+01	5.1E-04	0.0E+00	0.0E+00
LME 20	1.0E+03	1.0E+00	2.5E+02	2.5E+05	1.2E+03	1.0E+00	9.0E+01	1.0E+05	1.2E+02	6.5E-04	6.5E+03	5.1E+02	3.0E+02	5.3E-02	1.4E+04	2.3E+05	1.2E+02	1.2E-03	0.0E+00	0.0E+00
LME 21	8.2E+02	1.0E+00	2.5E+02	2.0E+05	8.8E+02	1.0E+00	8.7E+01	7.7E+04	8.6E+01	5.4E-04	2.7E+03	1.2E+02	2.4E+02	3.0E-02	1.3E+04	9.1E+04	8.4E+01	7.0E-04	0.0E+00	0.0E+00
LME 22	7.6E+02	1.0E+00	2.5E+02	1.9E+05	7.9E+02	1.0E+00	9.2E+01	7.2E+04	1.1E+02	2.2E-04	2.6E+03	6.5E+01	2.4E+02	1.1E-02	1.5E+04	4.1E+04	1.1E+02	2.5E-04	0.0E+00	0.0E+00
LME 23	6.9E+03	7.7E-01	1.7E+03	9.0E+06	7.6E+03	9.4E-01	1.9E+02	1.3E+06	1.0E+03	7.9E-07	1.3E+04	1.0E+01	1.6E+03	3.9E-05	3.5E+04	2.2E+03	1.0E+03	5.7E-06	0.0E+00	0.0E+00
LME 24	7.8E+02	1.0E+00	2.4E+02	1.9E+05	8.2E+02	1.0E+00	8.4E+01	6.9E+04	8.8E+01	1.5E-03	1.1E+03	1.5E+02	2.2E+02	4.3E-02	1.1E+04	1.1E+05	8.7E+01	2.6E-03	0.0E+00	0.0E+00
LME 25	1.2E+02	1.0E+00	2.3E+02	2.9E+04	1.3E+02	1.0E+00	9.4E+01	1.3E+04	7.6E+00	1.4E-03	1.6E+03	1.7E+01	1.3E+01	3.3E-02	1.9E+04	8.1E+03	7.6E+00	1.6E-03	0.0E+00	0.0E+00
LME 26	1.9E+04	1.0E+00	2.1E+02	4.1E+06	2.0E+04	1.0E+00	7.5E+01	1.5E+06	4.0E+02	9.2E-04	2.7E+02	1.0E+02	3.0E+03	1.2E-02	8.7E+03	3.3E+05	4.0E+02	1.2E-03	0.0E+00	0.0E+00
LME 27	1.9E+02	1.0E+00	2.3E+02	4.3E+04	2.5E+02	1.0E+00	7.8E+01	1.9E+04	6.0E+00	3.3E-03	2.1E+02	4.2E+00	1.1E+01	3.0E-02	9.1E+03	2.9E+03	6.2E+00	4.6E-03	0.0E+00	0.0E+00
LME 28	1.3E+03	1.0E+00	2.3E+02	2.9E+05	1.3E+03	1.0E+00	9.1E+01	1.2E+05	6.4E+01	2.9E-03	2.3E+02	4.3E+01	1.9E+02	1.8E-02	1.5E+04	5.1E+04	6.2E+01	2.6E-03	0.0E+00	0.0E+00
LME 29	1.8E+02	1.0E+00	2.4E+02	4.4E+04	2.2E+02	1.0E+00	9.4E+01	2.1E+04	7.3E+00	1.7E-03	8.5E+02	1.1E+01	1.1E+01	2.6E-02	1.8E+04	4.9E+03	7.3E+00	1.9E-03	0.0E+00	0.0E+00
LME 30	1.0E+03	1.0E+00	2.3E+02	2.4E+05	1.2E+03	1.0E+00	8.5E+01	9.8E+04	4.2E+01	4.2E-03	1.9E+02	3.4E+01	1.3E+02	2.7E-02	1.2E+04	4.0E+04	4.3E+01	5.4E-03	0.0E+00	0.0E+00
LME 31	1.6E+02	1.0E+00	2.3E+02	3.7E+04	2.0E+02	1.0E+00	8.5E+01	1.7E+04	5.2E+00	4.5E-03	1.4E+02	3.3E+00	8.3E+00	2.3E-02	1.1E+04	2.2E+03	5.2E+00	5.3E-03	0.0E+00	0.0E+00
LME 32	2.5E+03	1.0E+00	2.3E+02	5.7E+05	2.6E+03	1.0E+00	9.3E+01	2.4E+05	1.4E+02	3.2E-03	3.1E+02	1.4E+02	5.5E+02	2.1E-02	1.7E+04	2.0E+05	1.3E+02	3.2E-03	0.0E+00	0.0E+00
LME 33	1.1E+04	1.0E+00	1.9E+02	2.2E+06	1.1E+04	1.0E+00	7.9E+01	9.0E+05	5.0E+02	1.7E-03	1.0E+02	8.8E+01	2.5E+03	8.3E-03	1.0E+04	2.1E+05	4.7E+02	1.7E-03	0.0E+00	0.0E+00
LME 34	4.3E+03	1.0E+00	2.3E+02	1.0E+06	4.4E+03	1.0E+00	8.7E+01	3.8E+05	1.9E+02	1.8E-03	1.3E+02	4.4E+01	9.5E+02	9.2E-03	1.2E+04	1.1E+05	1.7E+02	1.5E-03	0.0E+00	0.0E+00
LME 35	4.5E+01	1.0E+00	2.6E+02	1.2E+04	7.0E+01	1.0E+00	7.6E+01	5.4E+03	1.1E+00	5.7E-03	5.0E+01	3.0E-01	1.4E+00	1.8E-02	7.4E+03	1.9E+02	1.1E+00	7.1E-03	0.0E+00	0.0E+00
LME 36	8.2E+03	1.0E+00	2.4E+02	2.0E+06	8.6E+03	1.0E+00	7.8E+01	6.6E+05	4.1E+02	5.2E-03	6.9E+01	1.4E+02	1.9E+03	2.0E-02	8.2E+03	3.1E+05	4.0E+02	6.2E-03	0.0E+00	0.0E+00

	Cd				Co				Cr				Cu				Fe			
	FF	BF	EF	CTP																
LME 37	7.8E+03	1.0E+00	2.4E+02	1.8E+06	7.9E+03	1.0E+00	8.9E+01	7.0E+05	4.2E+02	4.8E-03	1.5E+02	3.0E+02	2.0E+03	2.2E-02	1.3E+04	5.6E+05	4.0E+02	5.2E-03	0.0E+00	0.0E+00
LME 38	5.1E+02	1.0E+00	2.4E+02	1.2E+05	6.0E+02	1.0E+00	9.4E+01	5.7E+04	1.7E+01	3.8E-03	2.5E+02	1.6E+01	3.3E+01	2.2E-02	1.7E+04	1.2E+04	1.7E+01	3.9E-03	0.0E+00	0.0E+00
LME 39	1.5E+02	1.0E+00	2.4E+02	3.6E+04	2.0E+02	1.0E+00	7.4E+01	1.5E+04	8.5E+00	7.5E-03	5.3E+01	3.4E+00	1.2E+01	2.4E-02	7.2E+03	2.1E+03	8.9E+00	1.1E-02	0.0E+00	0.0E+00
LME 40	2.2E+02	1.0E+00	2.3E+02	5.2E+04	3.5E+02	1.0E+00	6.3E+01	2.2E+04	4.9E+00	9.9E-03	3.7E+01	1.8E+00	8.9E+00	3.3E-02	5.0E+03	1.5E+03	5.9E+00	1.7E-02	0.0E+00	0.0E+00
LME 41	1.6E+02	1.0E+00	2.3E+02	3.7E+04	2.0E+02	1.0E+00	7.6E+01	1.5E+04	4.9E+00	4.8E-03	1.5E+02	3.6E+00	9.9E+00	3.5E-02	8.2E+03	2.8E+03	5.3E+00	7.9E-03	0.0E+00	0.0E+00
LME 42	2.1E+02	1.0E+00	2.4E+02	5.0E+04	2.9E+02	1.0E+00	7.9E+01	2.3E+04	7.3E+00	2.5E-03	6.5E+02	1.2E+01	1.5E+01	5.3E-02	9.3E+03	7.2E+03	7.6E+00	5.3E-03	0.0E+00	0.0E+00
LME 43	2.1E+02	1.0E+00	2.3E+02	5.0E+04	3.0E+02	1.0E+00	7.4E+01	2.2E+04	6.2E+00	3.0E-03	3.5E+02	6.4E+00	1.4E+01	4.6E-02	7.8E+03	5.1E+03	6.6E+00	5.5E-03	0.0E+00	0.0E+00
LME 44	1.5E+02	1.0E+00	2.3E+02	3.4E+04	1.7E+02	1.0E+00	8.4E+01	1.5E+04	4.2E+00	3.0E-03	2.8E+02	3.6E+00	9.0E+00	2.9E-02	1.1E+04	2.9E+03	4.3E+00	3.8E-03	0.0E+00	0.0E+00
LME 45	1.8E+02	1.0E+00	2.4E+02	4.3E+04	2.3E+02	1.0E+00	8.9E+01	2.0E+04	4.4E+00	4.0E-03	1.8E+02	3.2E+00	7.8E+00	2.2E-02	1.3E+04	2.3E+03	4.4E+00	4.3E-03	0.0E+00	0.0E+00
LME 46	1.8E+02	1.0E+00	2.4E+02	4.4E+04	2.5E+02	1.0E+00	7.9E+01	1.9E+04	7.0E+00	2.6E-03	5.9E+02	1.1E+01	1.4E+01	5.2E-02	9.2E+03	6.7E+03	7.3E+00	5.7E-03	0.0E+00	0.0E+00
LME 47	7.6E+02	1.0E+00	2.4E+02	1.8E+05	8.2E+02	1.0E+00	7.7E+01	6.3E+04	7.1E+01	2.3E-03	1.8E+02	2.9E+01	1.7E+02	2.1E-02	8.3E+03	3.0E+04	7.1E+01	3.0E-03	0.0E+00	0.0E+00
LME 48	7.9E+02	9.9E-01	2.7E+02	2.1E+05	8.4E+02	1.0E+00	8.9E+01	7.4E+04	4.0E+02	2.5E-04	9.7E+02	9.9E+01	4.8E+02	7.3E-03	1.3E+04	4.4E+04	4.0E+02	3.3E-04	0.0E+00	0.0E+00
LME 49	1.0E+03	1.0E+00	2.4E+02	2.4E+05	1.1E+03	1.0E+00	7.6E+01	8.6E+04	5.9E+01	4.9E-03	1.5E+02	4.5E+01	2.0E+02	3.6E-02	8.2E+03	6.0E+04	6.3E+01	8.4E-03	0.0E+00	0.0E+00
LME 50	7.7E+03	1.0E+00	2.5E+02	1.9E+06	7.8E+03	1.0E+00	8.7E+01	6.8E+05	5.0E+02	1.1E-03	1.3E+03	7.4E+02	1.8E+03	3.4E-02	1.3E+04	7.8E+05	4.9E+02	1.5E-03	0.0E+00	0.0E+00
LME 51	1.3E+02	1.0E+00	2.6E+02	3.4E+04	1.5E+02	1.0E+00	9.8E+01	1.5E+04	9.6E+00	6.8E-04	6.8E+03	4.4E+01	1.5E+01	4.1E-02	2.0E+04	1.2E+04	9.6E+00	1.1E-03	0.0E+00	0.0E+00
LME 52	8.2E+02	9.9E-01	2.7E+02	2.2E+05	8.8E+02	1.0E+00	9.4E+01	8.2E+04	8.4E+01	3.9E-05	6.2E+03	2.0E+01	2.0E+02	3.7E-03	1.6E+04	1.1E+04	8.3E+01	8.7E-05	0.0E+00	0.0E+00
LME 53	2.2E+02	1.0E+00	2.7E+02	5.8E+04	2.8E+02	1.0E+00	9.9E+01	2.8E+04	1.0E+01	5.7E-04	8.9E+03	5.4E+01	1.6E+01	4.1E-02	2.0E+04	1.3E+04	1.0E+01	9.3E-04	0.0E+00	0.0E+00
LME 54	1.3E+03	1.0E+00	2.8E+02	3.7E+05	1.4E+03	1.0E+00	9.6E+01	1.3E+05	2.2E+02	4.1E-04	1.3E+04	1.1E+03	4.9E+02	4.7E-02	1.6E+04	3.8E+05	2.1E+02	7.0E-04	0.0E+00	0.0E+00
LME 55	1.3E+03	1.0E+00	2.9E+02	3.8E+05	1.3E+03	1.0E+00	1.1E+02	1.5E+05	1.5E+02	7.2E-05	5.3E+04	5.9E+02	4.2E+02	1.2E-02	3.4E+04	1.7E+05	1.5E+02	5.9E-05	0.0E+00	0.0E+00
LME 56	1.3E+03	1.0E+00	3.1E+02	4.1E+05	1.4E+03	1.0E+00	1.1E+02	1.5E+05	3.9E+02	1.2E-04	4.7E+04	2.1E+03	5.5E+02	1.7E-02	3.2E+04	3.0E+05	3.8E+02	1.0E-04	0.0E+00	0.0E+00
LME 57	1.3E+03	1.0E+00	3.3E+02	4.2E+05	1.3E+03	1.0E+00	1.1E+02	1.5E+05	3.7E+02	1.4E-04	4.4E+04	2.2E+03	5.3E+02	1.9E-02	3.2E+04	3.2E+05	3.6E+02	1.3E-04	0.0E+00	0.0E+00
LME 58	1.3E+03	1.0E+00	2.9E+02	3.9E+05	1.4E+03	1.0E+00	9.9E+01	1.4E+05	2.1E+02	2.5E-04	1.6E+04	8.5E+02	4.7E+02	3.3E-02	1.8E+04	2.9E+05	2.1E+02	3.4E-04	0.0E+00	0.0E+00
LME 59	1.4E+02	1.0E+00	2.5E+02	3.5E+04	1.7E+02	1.0E+00	8.7E+01	1.5E+04	1.1E+01	9.0E-04	3.8E+03	3.8E+01	1.9E+01	5.5E-02	1.3E+04	1.4E+04	1.1E+01	1.8E-03	0.0E+00	0.0E+00
LME 60	1.0E+02	1.0E+00	2.4E+02	2.5E+04	1.1E+02	1.0E+00	8.4E+01	9.4E+03	9.9E+00	1.5E-03	1.9E+03	2.8E+01	1.7E+01	5.8E-02	1.1E+04	1.1E+04	1.0E+01	3.3E-03	0.0E+00	0.0E+00
LME 61	2.4E+03	1.0E+00	2.6E+02	6.2E+05	2.5E+03	1.0E+00	1.0E+02	2.6E+05	2.4E+02	4.3E-04	3.4E+04	3.5E+03	6.6E+02	5.0E-02	2.7E+04	8.9E+05	2.3E+02	8.8E-04	0.0E+00	0.0E+00
LME 62	2.0E+04	9.8E-01	5.3E+02	1.0E+07	2.0E+04	1.0E+00	7.4E+01	1.5E+06	9.7E+02	2.8E-04	3.1E+02	8.4E+01	3.0E+03	7.8E-03	5.7E+03	1.3E+05	9.7E+02	6.6E-04	0.0E+00	0.0E+00
LME 63	2.5E+03	1.0E+00	2.9E+02	7.1E+05	2.6E+03	1.0E+00	1.1E+02	2.8E+05	6.2E+02	1.1E-04	3.6E+04	2.3E+03	1.0E+03	1.4E-02	3.2E+04	4.6E+05	6.2E+02	8.4E-05	0.0E+00	0.0E+00
LME 64	4.1E+03	1.0E+00	2.8E+02	1.1E+06	4.3E+03	1.0E+00	1.1E+02	4.6E+05	4.9E+02	2.3E-04	4.1E+04	4.6E+03	1.2E+03	3.2E-02	3.0E+04	1.2E+06	4.8E+02	2.5E-04	0.0E+00	0.0E+00
Mn					Ni				Pb				Zn							
				FF	BF	EF	CTP													
LME 1	7.1E+02	9.9E-01	4.1E+01	2.9E+04	7.0E+02	9.8E-01	9.7E+01	6.7E+04	5.4E+02	8.6E-01	6.6E+02	3.1E+05	6.6E+02	9.6E-01	4.2E+02	2.7E+05				
LME 2	1.1E+02	9.9E-01	4.1E+01	4.6E+03	9.8E+01	9.8E-01	1.0E+02	9.9E+03	6.8E+01	8.5E-01	7.9E+02	4.5E+04	8.8E+01	9.6E-01	4.3E+02	3.6E+04				
LME 3	1.6E+02	9.9E-01	3.9E+01	6.1E+03	1.2E+02	9.9E-01	9.0E+01	1.1E+04	7.8E+01	8.5E-01	5.4E+02	3.6E+04	1.0E+02	9.6E-01	4.0E+02	3.8E+04				
LME 4	5.3E+02	9.9E-01	3.8E+01	2.0E+04	5.2E+02	9.8E-01	8.7E+01	4.5E+04	3.7E+02	7.8E-01	4.8E+02	1.4E+05	4.9E+02	9.5E-01	3.7E+02	1.8E+05				
LME 5	1.8E+04	9.9E-01	3.7E+01	6.6E+05	1.9E+04	9.8E-01	7.2E+01	1.3E+06	1.2E+04	7.7E-01	3.1E+02	2.9E+06	1.7E+04	9.4E-01	3.4E+02	5.6E+06				
LME 6	1.0E+02	9.8E-01	3.7E+01	3.6E+03	9.5E+01	9.7E-01	7.0E+01	6.4E+03	7.8E+01	7.1E-01	2.8E+02	1.6E+04	8.9E+01	9.2E-01	3.4E+02	2.8E+04				
LME 7	9.2E+01	9.8E-01	4.1E+01	3.7E+03	8.8E+01	9.6E-01	1.0E+02	8.8E+03	6.5E+01	6.8E-01	8.1E+02	3.6E+04	8.2E+01	9.1E-01	4.3E+02	3.2E+04				
LME 8	3.1E+02	9.9E-01	4.2E+01	1.3E+04	3.0E+02	9.8E-01	1.1E+02	3.2E+04	2.2E+02	8.1E-01	8.8E+02	1.5E+05	2.8E+02	9.5E-01	4.4E+02	1.2E+05				
LME 9	9.8E+01	9.9E-01	4.2E+01	4.0E+03	9.1E+01	9.8E-01	1.1E+02	9.4E+03	6.5E+01	8.2E-01	8.7E+02	4.6E+04	8.4E+01	9.5E-01	4.4E+02	3.5E+04				
LME 10	1.1E+02	9.9E-01	3.8E+01	4.3E+03	1.0E+02	9.9E-01	8.5E+01	8.5E+03	6.9E+01	8.2E-01	4.6E+02	2.6E+04	9.0E+01	9.6E-01	3.7E+02	3.2E+04				
LME 11	1.5E+02	9.9E-01	3.8E+01	5.6E+03	1.2E+02	9.8E-01	9.0E+01	1.0E+04	7.3E+01	7.9E-01	5.1E+02	2.9E+04	9.8E+01	9.6E-01	3.7E+02	3.5E+04				

	Mn				Ni				Pb				Zn			
	FF	BF	EF	CTP												
LME 12	1.5E+02	9.9E-01	3.7E+01	5.6E+03	1.2E+02	9.9E-01	7.4E+01	8.6E+03	5.8E+01	8.2E-01	3.2E+02	1.5E+04	8.6E+01	9.6E-01	3.4E+02	2.8E+04
LME 13	6.7E+01	9.9E-01	3.9E+01	2.6E+03	3.5E+01	9.8E-01	1.0E+02	3.5E+03	1.1E+01	8.4E-01	7.7E+02	6.9E+03	2.1E+01	9.6E-01	4.1E+02	8.2E+03
LME 14	1.1E+02	9.9E-01	4.0E+01	4.2E+03	9.7E+01	9.9E-01	8.6E+01	8.2E+03	7.1E+01	8.8E-01	4.8E+02	3.0E+04	8.6E+01	9.6E-01	4.0E+02	3.3E+04
LME 15	1.0E+02	9.9E-01	3.8E+01	3.8E+03	9.6E+01	9.9E-01	7.5E+01	7.1E+03	7.1E+01	8.5E-01	3.4E+02	2.1E+04	8.7E+01	9.6E-01	3.6E+02	3.0E+04
LME 16	1.2E+02	9.9E-01	3.7E+01	4.5E+03	1.1E+02	9.9E-01	7.5E+01	7.9E+03	7.1E+01	8.2E-01	3.3E+02	1.9E+04	9.2E+01	9.6E-01	3.4E+02	3.1E+04
LME 17	1.0E+02	9.9E-01	3.7E+01	3.7E+03	9.2E+01	9.8E-01	7.9E+01	7.2E+03	5.4E+01	7.8E-01	3.7E+02	1.6E+04	8.2E+01	9.5E-01	3.5E+02	2.7E+04
LME 18	1.0E+02	9.9E-01	4.1E+01	4.0E+03	9.4E+01	9.9E-01	9.4E+01	8.7E+03	8.0E+01	8.9E-01	5.9E+02	4.2E+04	8.8E+01	9.6E-01	4.2E+02	3.6E+04
LME 19	1.2E+02	9.9E-01	4.0E+01	4.7E+03	1.1E+02	9.8E-01	8.4E+01	8.7E+03	8.3E+01	8.8E-01	4.4E+02	3.2E+04	9.2E+01	9.5E-01	4.1E+02	3.6E+04
LME 20	7.7E+02	9.9E-01	4.0E+01	3.0E+04	7.4E+02	9.9E-01	8.3E+01	6.0E+04	6.6E+02	9.0E-01	4.3E+02	2.5E+05	7.0E+02	9.6E-01	4.0E+02	2.7E+05
LME 21	7.2E+02	9.9E-01	3.9E+01	2.8E+04	7.1E+02	9.8E-01	7.9E+01	5.6E+04	6.2E+02	8.6E-01	3.9E+02	2.1E+05	6.8E+02	9.5E-01	3.9E+02	2.5E+05
LME 22	7.1E+02	9.8E-01	4.0E+01	2.8E+04	7.0E+02	9.7E-01	8.5E+01	5.8E+04	5.9E+02	7.6E-01	4.7E+02	2.1E+05	6.7E+02	9.1E-01	4.0E+02	2.4E+05
LME 23	5.9E+03	7.0E-01	8.7E+01	3.6E+05	5.8E+03	6.3E-01	1.8E+02	6.7E+05	4.2E+03	1.1E-01	1.5E+03	7.2E+05	4.9E+03	3.8E-01	8.1E+02	1.5E+06
LME 24	7.1E+02	9.9E-01	3.8E+01	2.7E+04	7.1E+02	9.9E-01	7.5E+01	5.3E+04	6.0E+02	8.9E-01	3.5E+02	1.8E+05	6.8E+02	9.6E-01	3.8E+02	2.4E+05
LME 25	9.7E+01	9.9E-01	3.8E+01	3.7E+03	9.2E+01	9.9E-01	9.1E+01	8.2E+03	7.3E+01	8.5E-01	5.6E+02	3.5E+04	8.7E+01	9.6E-01	3.9E+02	3.3E+04
LME 26	1.7E+04	9.9E-01	3.6E+01	6.2E+05	1.8E+04	9.8E-01	6.6E+01	1.2E+06	1.3E+04	7.9E-01	2.7E+02	2.7E+06	1.7E+04	9.3E-01	3.4E+02	5.4E+06
LME 27	1.1E+02	9.9E-01	3.7E+01	4.1E+03	1.0E+02	9.9E-01	6.9E+01	7.0E+03	7.2E+01	8.6E-01	2.8E+02	1.8E+04	8.9E+01	9.6E-01	3.5E+02	3.0E+04
LME 28	1.1E+03	9.9E-01	3.7E+01	4.1E+04	1.1E+03	9.8E-01	8.6E+01	9.2E+04	7.6E+02	7.8E-01	4.6E+02	2.8E+05	1.0E+03	9.6E-01	3.6E+02	3.6E+05
LME 29	1.1E+02	9.9E-01	3.8E+01	4.2E+03	9.7E+01	9.8E-01	9.0E+01	8.6E+03	6.4E+01	8.2E-01	5.3E+02	2.8E+04	8.6E+01	9.6E-01	3.8E+02	3.2E+04
LME 30	7.7E+02	9.9E-01	3.8E+01	2.9E+04	7.4E+02	9.9E-01	7.8E+01	5.7E+04	5.6E+02	8.3E-01	3.7E+02	1.7E+05	6.9E+02	9.6E-01	3.6E+02	2.4E+05
LME 31	1.1E+02	9.9E-01	3.7E+01	3.9E+03	9.7E+01	9.9E-01	7.9E+01	7.5E+03	6.5E+01	8.1E-01	3.7E+02	1.9E+04	8.7E+01	9.6E-01	3.5E+02	2.9E+04
LME 32	2.2E+03	9.9E-01	3.7E+01	8.2E+04	2.2E+03	9.9E-01	9.0E+01	2.0E+05	1.5E+03	8.0E-01	5.1E+02	6.4E+05	2.1E+03	9.6E-01	3.7E+02	7.4E+05
LME 33	1.1E+04	9.9E-01	3.5E+01	3.6E+05	1.1E+04	9.8E-01	7.2E+01	7.7E+05	8.0E+03	7.1E-01	3.2E+02	1.8E+06	1.0E+04	9.4E-01	3.2E+02	3.2E+06
LME 34	3.8E+03	9.9E-01	3.8E+01	1.4E+05	3.9E+03	9.8E-01	8.1E+01	3.1E+05	2.8E+03	7.0E-01	3.9E+02	7.8E+05	3.7E+03	9.4E-01	3.5E+02	1.2E+06
LME 35	2.1E+01	9.9E-01	3.8E+01	8.1E+02	1.9E+01	9.9E-01	6.6E+01	1.2E+03	1.1E+01	7.9E-01	2.4E+02	2.0E+03	1.5E+01	9.5E-01	3.3E+02	4.5E+03
LME 36	7.4E+03	9.9E-01	3.7E+01	2.7E+05	7.5E+03	9.9E-01	6.8E+01	5.1E+05	5.7E+03	8.0E-01	2.7E+02	1.2E+06	7.2E+03	9.6E-01	3.3E+02	2.3E+06
LME 37	7.4E+03	9.9E-01	3.8E+01	2.8E+05	7.5E+03	9.9E-01	8.4E+01	6.2E+05	5.7E+03	8.0E-01	4.2E+02	1.9E+06	7.2E+03	9.6E-01	3.6E+02	2.5E+06
LME 38	3.2E+02	9.9E-01	3.8E+01	1.2E+04	2.9E+02	9.9E-01	9.1E+01	2.6E+04	2.0E+02	8.0E-01	5.1E+02	8.2E+04	2.7E+02	9.6E-01	3.7E+02	9.5E+04
LME 39	1.0E+02	9.9E-01	3.7E+01	3.8E+03	9.8E+01	9.9E-01	6.4E+01	6.2E+03	6.8E+01	8.2E-01	2.3E+02	1.3E+04	8.7E+01	9.6E-01	3.2E+02	2.7E+04
LME 40	1.2E+02	9.9E-01	3.6E+01	4.3E+03	1.1E+02	9.9E-01	5.1E+01	5.8E+03	7.3E+01	8.7E-01	1.5E+02	9.8E+03	9.2E+01	9.7E-01	2.9E+02	2.6E+04
LME 41	1.0E+02	9.9E-01	3.7E+01	3.9E+03	9.9E+01	9.9E-01	6.6E+01	6.4E+03	7.3E+01	8.7E-01	2.6E+02	1.6E+04	8.8E+01	9.7E-01	3.4E+02	2.9E+04
LME 42	1.2E+02	9.9E-01	3.8E+01	4.4E+03	1.1E+02	9.9E-01	6.9E+01	7.2E+03	7.9E+01	9.1E-01	2.8E+02	2.0E+04	9.1E+01	9.7E-01	3.6E+02	3.2E+04
LME 43	1.2E+02	9.9E-01	3.7E+01	4.3E+03	1.1E+02	9.9E-01	6.3E+01	6.8E+03	8.0E+01	9.0E-01	2.4E+02	1.7E+04	9.2E+01	9.7E-01	3.5E+02	3.1E+04
LME 44	1.0E+02	9.9E-01	3.7E+01	3.8E+03	9.6E+01	9.9E-01	7.6E+01	7.2E+03	7.1E+01	8.5E-01	3.5E+02	2.1E+04	8.8E+01	9.6E-01	3.6E+02	3.0E+04
LME 45	1.1E+02	9.9E-01	3.8E+01	4.2E+03	1.0E+02	9.9E-01	8.4E+01	8.2E+03	6.7E+01	8.1E-01	4.2E+02	2.3E+04	8.9E+01	9.6E-01	3.6E+02	3.1E+04
LME 46	1.1E+02	9.9E-01	3.8E+01	4.2E+03	1.0E+02	9.9E-01	6.9E+01	7.0E+03	7.8E+01	9.0E-01	2.8E+02	2.0E+04	9.0E+01	9.7E-01	3.6E+02	3.1E+04
LME 47	6.8E+02	9.9E-01	3.8E+01	2.5E+04	6.8E+02	9.8E-01	6.7E+01	4.5E+04	5.5E+02	8.2E-01	2.6E+02	1.2E+05	6.4E+02	9.5E-01	3.5E+02	2.1E+05
LME 48	7.3E+02	9.8E-01	4.0E+01	2.9E+04	7.2E+02	9.6E-01	8.1E+01	5.7E+04	6.9E+02	7.0E-01	4.0E+02	1.9E+05	7.1E+02	8.9E-01	3.9E+02	2.5E+05
LME 49	8.5E+02	9.9E-01	3.8E+01	3.2E+04	8.3E+02	9.9E-01	6.7E+01	5.5E+04	6.9E+02	8.7E-01	2.6E+02	1.6E+05	7.9E+02	9.7E-01	3.4E+02	2.6E+05
LME 50	7.4E+03	9.9E-01	3.9E+01	2.9E+05	7.4E+03	9.8E-01	8.0E+01	5.8E+05	5.7E+03	8.6E-01	3.9E+02	1.9E+06	6.9E+03	9.6E-01	3.9E+02	2.6E+06
LME 51	9.8E+01	9.9E-01	4.1E+01	3.9E+03	9.2E+01	9.8E-01	9.4E+01	8.5E+03	6.9E+01	8.6E-01	6.0E+02	3.6E+04	8.4E+01	9.6E-01	4.2E+02	3.4E+04
LME 52	7.2E+02	9.7E-01	4.1E+01	2.9E+04	7.1E+02	9.5E-01	8.7E+01	5.8E+04	6.1E+02	6.8E-01	4.8E+02	2.0E+05	6.7E+02	8.6E-01	4.1E+02	2.4E+05

	Mn				Ni				Pb				Zn			
	FF	BF	EF	CTP												
LME 53	1.2E+02	9.9E-01	4.1E+01	4.8E+03	1.0E+02	9.8E-01	9.5E+01	9.5E+03	7.1E+01	8.6E-01	6.2E+02	3.8E+04	8.8E+01	9.6E-01	4.2E+02	3.6E+04
LME 54	1.2E+03	9.9E-01	4.2E+01	5.1E+04	1.2E+03	9.8E-01	8.9E+01	1.1E+05	1.1E+03	8.9E-01	5.0E+02	4.9E+05	1.2E+03	9.6E-01	4.3E+02	4.8E+05
LME 55	1.2E+03	9.8E-01	4.3E+01	5.2E+04	1.2E+03	9.7E-01	1.1E+02	1.3E+05	1.1E+03	7.4E-01	9.7E+02	7.6E+05	1.2E+03	9.3E-01	4.5E+02	5.0E+05
LME 56	1.2E+03	9.8E-01	4.4E+01	5.4E+04	1.2E+03	9.7E-01	1.1E+02	1.3E+05	1.0E+03	7.5E-01	9.7E+02	7.6E+05	1.2E+03	9.3E-01	4.7E+02	5.1E+05
LME 57	1.2E+03	9.9E-01	4.5E+01	5.5E+04	1.2E+03	9.7E-01	1.1E+02	1.3E+05	1.0E+03	7.6E-01	9.8E+02	7.8E+05	1.2E+03	9.3E-01	4.7E+02	5.2E+05
LME 58	1.2E+03	9.9E-01	4.3E+01	5.2E+04	1.2E+03	9.8E-01	9.4E+01	1.1E+05	1.1E+03	8.6E-01	5.6E+02	5.2E+05	1.2E+03	9.5E-01	4.4E+02	4.9E+05
LME 59	1.0E+02	9.9E-01	3.9E+01	3.9E+03	9.5E+01	9.9E-01	7.9E+01	7.5E+03	7.9E+01	9.0E-01	3.9E+02	2.8E+04	8.8E+01	9.6E-01	3.9E+02	3.3E+04
LME 60	9.3E+01	9.9E-01	3.9E+01	3.6E+03	9.1E+01	9.9E-01	7.5E+01	6.7E+03	7.7E+01	9.1E-01	3.5E+02	2.4E+04	8.6E+01	9.6E-01	3.8E+02	3.2E+04
LME 61	2.1E+03	9.9E-01	4.1E+01	8.5E+04	2.1E+03	9.9E-01	1.0E+02	2.1E+05	1.7E+03	8.8E-01	7.8E+02	1.2E+06	2.0E+03	9.7E-01	4.3E+02	8.2E+05
LME 62	1.8E+04	9.6E-01	5.0E+01	8.5E+05	1.8E+04	9.6E-01	5.8E+01	1.0E+06	1.3E+04	7.5E-01	1.7E+02	1.7E+06	1.6E+04	8.5E-01	4.2E+02	5.5E+06
LME 63	2.3E+03	9.9E-01	4.3E+01	9.7E+04	2.3E+03	9.7E-01	1.1E+02	2.4E+05	2.1E+03	7.5E-01	9.2E+02	1.4E+06	2.2E+03	9.3E-01	4.5E+02	9.3E+05
LME 64	3.7E+03	9.9E-01	4.2E+01	1.6E+05	3.7E+03	9.8E-01	1.1E+02	3.8E+05	3.1E+03	8.4E-01	8.7E+02	2.3E+06	3.5E+03	9.6E-01	4.5E+02	1.5E+06

Table S8: Linear correlation parameters between x (Seawater residence time (SRT), pH, salinity, DOC, POC and SPM) and y ($\log K_{DOC}$, $\log K_{pss}$, Bioavailability Factor (BF), Effect Factor (EF), Fate Factor (FF) and Comparative Toxicity Potential (CTP)), assuming $y = \text{slope} * x + (\text{y-intersection})$

	log K_{DOC}	log K_{pss}	BF	EF	FF	CTP	log K_{DOC}	log K_{pss}	BF	EF	FF	CTP	log K_{DOC}	log K_{pss}	BF	EF	FF	CTP
Cd																		
R²																		
P value																		
SRT [year]	0.06	0.02	0.02	0.03	0.98	0.64	0.058	0.284	0.254	0.166	0.000	0.000	2.1E-03	1.9E-03	-2.1E-04	1.6E+00	2.2E+02	7.3E+04
Temperature [$^{\circ}\text{C}$]	0.04	0.02	0.01	0.04	0.02	0.00	0.123	0.271	0.412	0.132	0.316	0.982	-3.3E-03	-3.7E-03	2.9E-04	-3.4E+00	5.5E+01	5.0E+02
pH	0.01	0.05	0.03	0.03	0.05	0.02	0.452	0.076	0.177	0.155	0.077	0.290	-1.3E-01	-4.6E-01	3.7E-02	-2.5E+02	7.5E+03	1.8E+06
Salinity [%o]	0.93	0.69	0.67	0.81	0.04	0.49	0.000	0.000	0.000	0.000	0.105	0.000	-3.8E-02	-5.1E-02	5.4E-03	-3.8E+01	-2.1E+02	-2.9E+05
DOC [mg/L]	0.68	0.52	0.74	0.72	0.10	0.44	0.000	0.000	0.000	0.000	0.010	0.000	1.8E-01	2.4E-01	-3.0E-02	1.9E+02	1.7E+03	1.5E+06
POC [$\mu\text{g/L}$]	0.61	0.60	0.58	0.64	0.00	0.17	0.000	0.000	0.000	0.000	0.946	0.001	1.2E-03	1.8E-03	-1.9E-04	1.3E+00	3.4E-01	6.6E+03
SPM [mg/L]	0.07	0.00	0.03	0.05	0.00	0.00	0.035	0.590	0.180	0.070	0.619	0.639	1.1E-01	4.3E-02	-1.1E-02	9.7E+01	-6.6E+02	2.5E+05
Co	R²						P value						Slope					
SRT [year]	0.01	0.00	0.02	0.01	0.98	0.88	0.477	0.862	0.262	0.441	0.000	0.000	4.8E-04	2.4E-04	-5.0E-05	-8.3E-02	2.3E+02	1.8E+04
Temperature [$^{\circ}\text{C}$]	0.08	0.02	0.02	0.27	0.02	0.01	0.021	0.226	0.330	0.000	0.315	0.565	-2.9E-03	-3.2E-03	8.3E-05	-8.3E-01	5.6E+01	2.7E+03
pH	0.19	0.17	0.04	0.51	0.05	0.02	0.000	0.001	0.127	0.000	0.078	0.314	-3.4E-01	-6.6E-01	1.0E-02	-9.0E+01	7.6E-03	3.6E+05
Salinity [%o]	0.84	0.49	0.67	0.52	0.05	0.15	0.000	0.000	0.000	0.000	0.086	0.001	-2.2E-02	-3.4E-02	1.3E-03	-2.7E+00	-2.2E+02	-3.4E+04
DOC [mg/L]	0.62	0.38	0.78	0.35	0.11	0.26	0.000	0.000	0.000	0.000	0.008	0.000	1.0E-01	1.6E-01	-7.5E-03	1.2E+01	1.8E+03	2.3E+05
POC [$\mu\text{g/L}$]	0.72	0.56	0.61	0.68	0.00	0.04	0.000	0.000	0.000	0.000	0.895	0.100	7.8E-04	1.4E-03	-4.8E-05	1.2E-01	6.8E-01	6.9E+02
SPM [mg/L]	0.10	0.00	0.04	0.17	0.00	0.00	0.009	0.852	0.111	0.001	0.624	0.981	7.8E-02	1.2E-02	-3.3E-03	1.6E+01	-6.6E+02	-2.6E+03
Cr	R²						P value						Slope					
SRT [year]	0.00	0.00	0.01	0.01	0.49	0.00	0.985	0.973	0.381	0.483	0.000	0.932	6.6E-05	1.3E-04	-1.1E-05	-5.6E+01	8.1E+00	4.6E-01
Temperature [$^{\circ}\text{C}$]	0.70	0.59	0.57	0.53	0.04	0.29	0.000	0.000	0.000	0.000	0.135	0.000	-4.5E-02	-4.5E-02	1.5E-04	-8.8E+02	-4.2E+00	-4.3E+01
pH	0.23	0.25	0.19	0.24	0.00	0.08	0.000	0.000	0.000	0.000	0.907	0.022	-2.0E+00	-2.3E+00	6.7E-03	-4.6E+04	-2.6E+01	-1.8E+03
Salinity [%o]	0.45	0.49	0.09	0.09	0.40	0.02	0.000	0.000	0.015	0.017	0.000	0.323	-8.5E-02	-9.8E-02	1.4E-04	-8.5E+02	-3.3E+01	-2.4E+01
DOC [mg/L]	0.32	0.37	0.08	0.00	0.36	0.01	0.000	0.000	0.026	0.641	0.000	0.534	3.9E-01	4.6E-01	-6.9E-04	9.0E+02	1.7E+02	-8.0E+01
POC [$\mu\text{g/L}$]	0.64	0.72	0.26	0.14	0.24	0.03	0.000	0.000	0.000	0.002	0.000	0.154	3.9E-03	4.6E-03	-9.1E-06	4.2E+01	9.9E-01	1.3E+00
SPM [mg/L]	0.35	0.24	0.25	0.25	0.16	0.15	0.000	0.000	0.000	0.000	0.001	0.001	7.6E-01	7.0E-01	-2.4E-03	1.5E+04	2.1E+02	7.5E+02
Cu	R²						P value						Slope					
SRT [year]	0.06	0.03	0.12	0.04	0.85	0.10	0.061	0.156	0.004	0.138	0.000	0.009	3.5E-03	3.4E-03	-2.5E-04	-7.5E+01	3.7E+01	3.7E+03
Temperature [$^{\circ}\text{C}$]	0.06	0.03	0.11	0.42	0.00	0.11	0.049	0.163	0.007	0.000	0.676	0.006	6.9E-03	6.5E-03	-4.5E-04	-5.0E+02	4.1E+00	-7.4E+03
pH	0.06	0.09	0.05	0.76	0.02	0.02	0.059	0.019	0.076	0.000	0.245	0.311	-5.2E-01	-8.4E-01	2.4E-02	-5.2E+04	8.8E+02	-2.2E+05
Salinity [%o]	0.43	0.45	0.08	0.19	0.06	0.00	0.000	0.000	0.020	0.000	0.052	0.853	-4.3E-02	-5.8E-02	9.3E-04	-7.9E+02	-4.4E+01	-1.2E+03
DOC [mg/L]	0.77	0.70	0.34	0.05	0.13	0.00	0.000	0.000	0.000	0.082	0.004	0.585	3.1E-01	3.9E-01	-9.9E-03	2.1E+03	3.5E+02	-1.9E+04
POC [$\mu\text{g/L}$]	0.31	0.41	0.05	0.35	0.01	0.00	0.000	0.000	0.072	0.000	0.462	0.874	1.4E-03	2.1E-03	-2.8E-05	4.1E+01	6.5E-01	4.1E+01
SPM [mg/L]	0.00	0.00	0.02	0.19	0.00	0.04	0.601	0.914	0.266	0.000	0.700	0.132	4.5E-02	-1.2E-02	-4.6E-03	8.1E+03	9.0E+01	1.0E+05

	log K _{DOC}	log K _{pss}	BF	EF	FF	CTP	log K _{DOC}	log K _{pss}	BF	EF	FF	CTP	log K _{DOC}	log K _{pss}	BF	EF	FF	CTP	log K _{DOC}	log K _{pss}	BF	EF	FF	CTP		
Fe																										
R²												P value												Slope		
SRT [year]												P value												y-intersection		
Temperature [°C]												0.00 0.00 0.02 - 0.49 - 0.898 0.735 0.286 - 0.000 - -4.4E-04 -1.2E-03 -2.1E-05 - 8.0E+00 - 8.8E+00 8.3E+00 3.0E-03 - 8.1E+01 -												-		
pH												0.64 0.57 0.36 - 0.04 - 0.000 0.000 0.000 - 0.123 - -4.1E-02 -4.2E-02 1.8E-04 - -4.2E+00 - 9.5E+00 9.0E+00 -8.0E-06 - 2.1E+02 -												-		
Salinity [%o]												0.39 0.44 0.29 - 0.00 - 0.000 0.000 0.000 - 0.927 - -2.5E+00 -2.8E+00 1.2E-02 - -2.0E+01 - 2.9E+01 3.1E+01 -9.7E-02 - 3.0E+02 -												-		
DOC [mg/L]												0.30 0.36 0.07 - 0.41 - 0.000 0.000 0.033 - 0.000 - -6.7E-02 -7.8E-02 1.9E-04 - -3.3E+01 - 1.1E+01 1.1E+01 -3.4E-03 - 1.2E+03 -												-		
POC [µg/L]												0.22 0.24 0.07 - 0.36 - 0.000 0.000 0.030 - 0.000 - 3.0E-01 3.4E-01 -1.0E-03 - -1.6E+02 - 8.5E+00 7.9E+00 3.9E-03 - -3.3E+01 -												-		
SPM [mg/L]												0.36 0.25 0.19 - 0.16 - 0.000 0.000 0.000 - 0.001 - 3.3E-03 6.6E-01 -3.1E-03 - -2.1E+02 - 8.4E+00 8.0E+00 4.5E-03 - 3.3E+01 -												-		
Mn												R²												P value		
SRT [year]												0.06 0.01 0.03 0.02 0.98 0.95 0.056 0.441 0.153 0.279 0.000 0.000 1.3E-03 1.1E-03 -3.3E-04 4.5E-02 2.1E+02 8.2E+03 4.0E+00 3.5E+00 9.9E-01 4.0E+01 3.5E+02 1.4E+04												Slope		
Temperature [°C]												0.03 0.01 0.02 0.14 0.02 0.01 0.153 0.397 0.332 0.002 0.325 0.500 -1.9E-03 -2.2E-03 4.3E-04 -2.3E-01 5.0E+01 1.4E+03 4.0E+00 3.6E+00 9.8E-01 4.4E+01 1.2E+03 5.7E+04												y-intersection		
pH												0.00 0.06 0.03 0.08 0.05 0.05 0.598 0.060 0.210 0.024 0.076 0.085 -5.4E-02 -3.8E-01 4.3E-02 -1.4E+01 6.9E+03 2.7E+05 4.4E+00 6.6E+00 6.4E-01 1.5E+02 -5.4E+04 -2.1E+06												Salinity [%o]		
Salinity [%o]												0.92 0.55 0.71 0.89 0.04 0.12 0.000 0.000 0.000 0.000 0.121 0.006 -2.3E-02 -3.6E-02 6.9E-03 -1.4E+00 -1.8E+02 -1.3E+04 4.8E+00 4.7E+00 7.5E-01 8.7E+01 8.1E+03 5.1E+05												DOC [mg/L]		
DOC [mg/L]												0.68 0.43 0.81 0.66 0.10 0.15 0.000 0.000 0.000 0.000 0.013 0.001 1.1E-01 1.7E-01 -4.0E-02 6.4E+00 1.5E+03 7.9E+04 3.9E+00 3.4E+00 1.0E+00 3.3E+01 3.0E+02 -6.7E+03												POC [µg/L]		
POC [µg/L]												0.60 0.53 0.61 0.75 0.00 0.01 0.000 0.000 0.000 0.000 0.976 0.440 7.3E-04 1.4E-03 -2.5E-04 4.9E-02 1.4E-01 1.4E+02 3.9E+00 3.4E+00 1.0E+00 3.3E+01 1.9E+03 6.0E+04												SPM [mg/L]		
SPM [mg/L]												0.07 0.00 0.04 0.12 0.00 0.00 0.042 0.982 0.096 0.005 0.637 0.851 6.3E-02 -1.4E-03 -1.8E-02 5.2E+00 -5.7E+02 -9.2E+03 3.9E+00 3.5E+00 9.9E-01 3.7E+01 2.3E+03 8.3E+04												Ni		
Ni												R²												P value		
SRT [year]												0.00 0.00 0.02 0.02 0.98 0.92 0.895 0.905 0.231 0.268 0.000 0.000 8.5E-05 -1.6E-04 -3.4E-04 -1.3E-01 2.1E+02 1.4E+04 4.2E+00 3.8E+00 9.8E-01 8.6E+01 3.2E+02 4.1E+04												Slope		
Temperature [°C]												0.13 0.04 0.02 0.28 0.02 0.01 0.003 0.133 0.220 0.000 0.315 0.483 -3.5E-03 -3.9E-03 6.6E-04 -9.6E-01 5.2E+01 2.5E+03 4.3E+00 3.9E+00 9.7E-01 1.0E+02 1.2E+03 1.1E+05												y-intersection		
pH												0.35 0.24 0.05 0.63 0.05 0.02 0.000 0.000 0.085 0.000 0.071 0.257 -4.5E-01 -7.8E-01 7.2E-02 -1.1E+02 7.3E+03 3.1E+05 7.8E+00 1.0E+00 1.0E-01 9.9E+02 -5.6E+04 -2.4E+06												Salinity [%o]		
Salinity [%o]												0.73 0.45 0.70 0.42 0.04 0.06 0.000 0.000 0.000 0.000 0.137 0.051 -1.9E-02 -3.2E-02 8.4E-03 -2.8E+00 -1.8E+02 -1.6E+04 4.9E+00 4.9E+00 6.9E-01 1.8E+02 8.1E+03 6.9E+05												DOC [mg/L]		
DOC [mg/L]												0.51 0.33 0.83 0.26 0.09 0.14 0.000 0.000 0.000 0.000 0.015 0.002 8.7E-02 1.5E-01 -4.9E-02 1.2E+01 1.6E+03 1.3E+05 4.1E+00 3.6E+00 1.0E+00 7.3E+01 3.0E+02 7.6E+03												POC [µg/L]		
POC [µg/L]												0.71 0.55 0.65 0.60 0.00 0.01 0.000 0.000 0.000 0.000 0.981 0.488 7.5E-04 1.4E-03 -3.1E-04 1.3E-01 -1.1E-01 2.2E+02 4.1E+00 3.6E+00 1.0E+00 6.8E+01 2.0E+03 1.2E+05												SPM [mg/L]		
SPM [mg/L]												0.13 0.00 0.06 0.16 0.00 0.00 0.004 0.754 0.050 0.001 0.620 0.859 8.3E-02 2.0E-02 -2.5E-02 1.8E+01 -6.2E+02 -1.5E+04 5.3E+00 3.8E+00 9.9E-01 7.6E+01 2.3E+03 1.6E+05												Pb		
Pb												R²												P value		
SRT [year]												0.00 0.00 0.06 0.02 0.97 0.67 0.802 0.899 0.061 0.239 0.000 0.000 2.4E-04 1.9E-04 -1.3E-03 -1.9E+00 1.5E+02 2.9E+04 5.3E+00 4.8E+00 8.2E-01 5.1E+02 3.0E+02 2.1E+05												Slope		
Temperature [°C]												0.17 0.11 0.00 0.36 0.01 0.00 0.001 0.008 0.775 0.000 0.394 0.600 5.9E-03 7.5E-03 -3.7E-04 -1.5E+01 3.1E+01 -4.6E+03 5.2E+00 4.7E+00 8.2E-01 7.2E+02 9.7E+02 5.1E+05												y-intersection		
pH																										

Table S9: Free ion activity HC_{50} [mg/l] calculated from EC_{50} of metals in seawater (this study) and freshwater³⁰

	Cd	Co	Cr	Cu	Fe	Mn	Ni	Pb	Zn
Seawater	1.91E-07	1.24E-05	7.38E-12	1.40E-08	-	3.27E-05	1.16E-05	7.52E-08	2.77E-06
Freshwater	8.98E-08	3.90E-06	3.17E-12	1.10E-10	1.07E-16	1.86E-05	1.53E-06	1.89E-07	1.90E-06

Figures

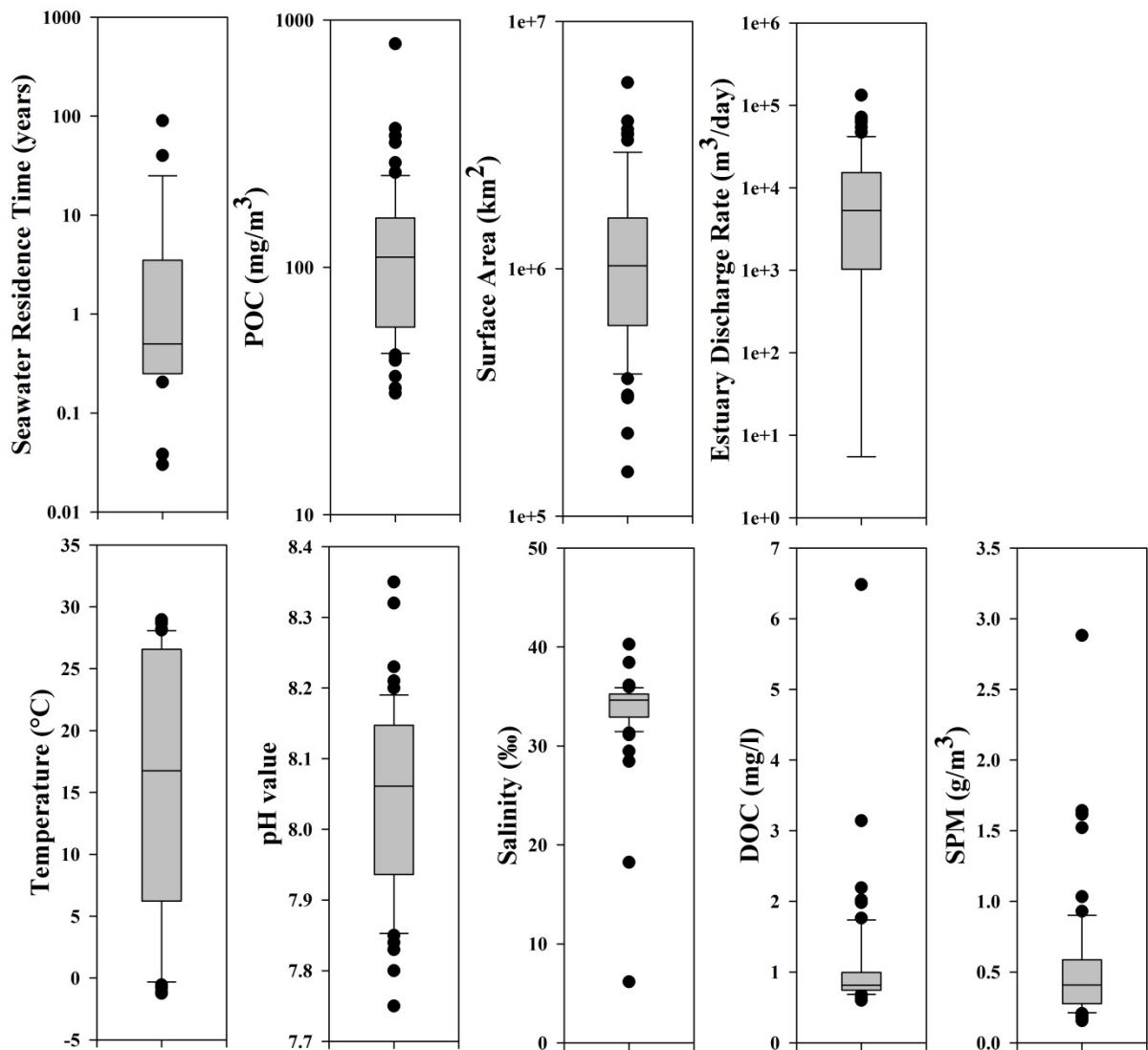


Figure S1: Seawater residence time, POC, surface area, estuary discharge rate, temperature, pH value, salinity, DOC and SPM concentration distribution across LMEs

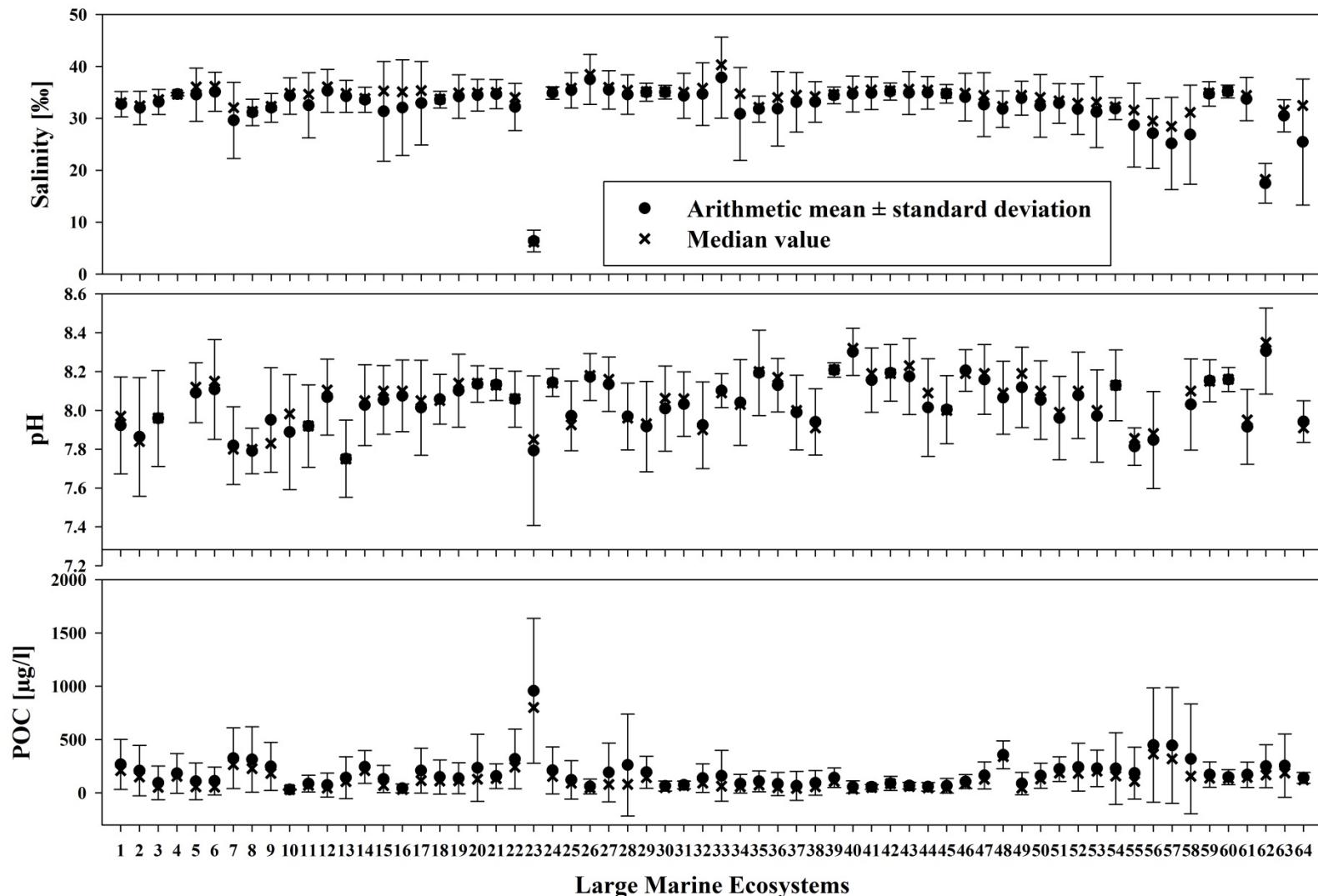


Figure S2: Variations in salinity, pH and POC within each Large Marine Ecosystem due to variations in sampling location within the LME and sampling season (pH value is not available for LME 4, 57 and 63).

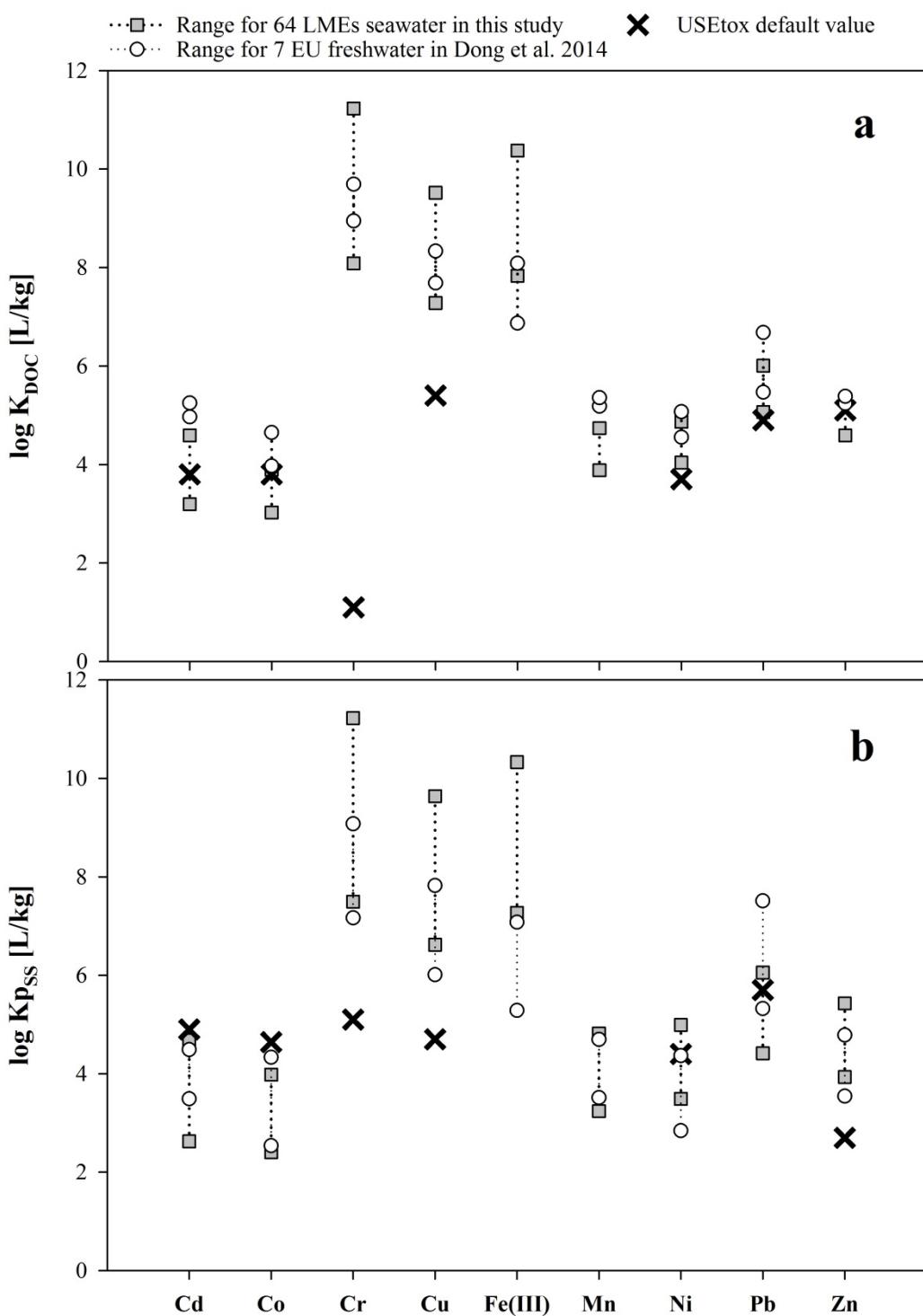


Figure S3. Range of $\log K_{DOC}$ values (ratio between concentrations of metal adsorbed to DOC and truly dissolved metal in the water) in Figure S3a and $\log K_{PSS}$ values (ratio between concentrations of metal adsorbed to SPM and truly dissolved metal in the water) in Figure S3b as determined for 64 LMEs in this study. For comparison the corresponding ranges of freshwater $\log K_{PSS}$ and $\log K_{DOC}$ in the study of Dong et al.³⁰ and their default value currently used in the USEtox database are shown for those metals that are presently covered by the models.

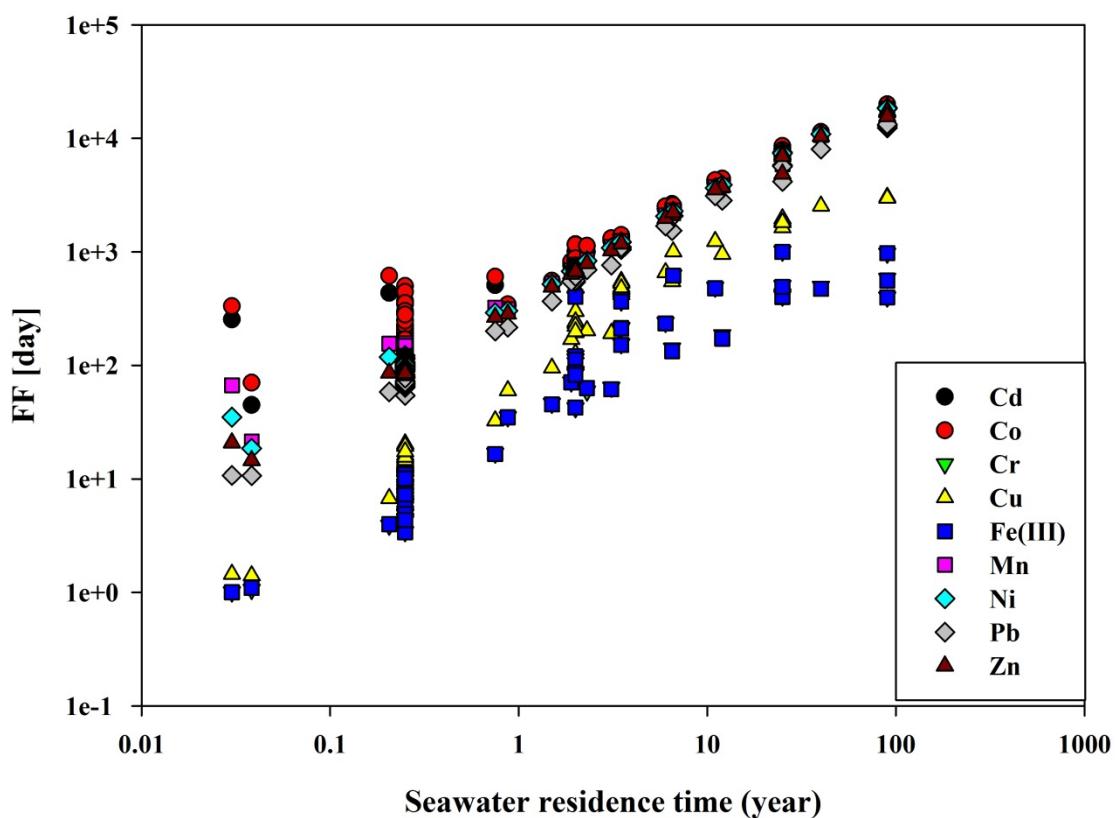


Figure S4. Relationship between Fate Factor (FF) and seawater residence time for all metals in all LMEs.

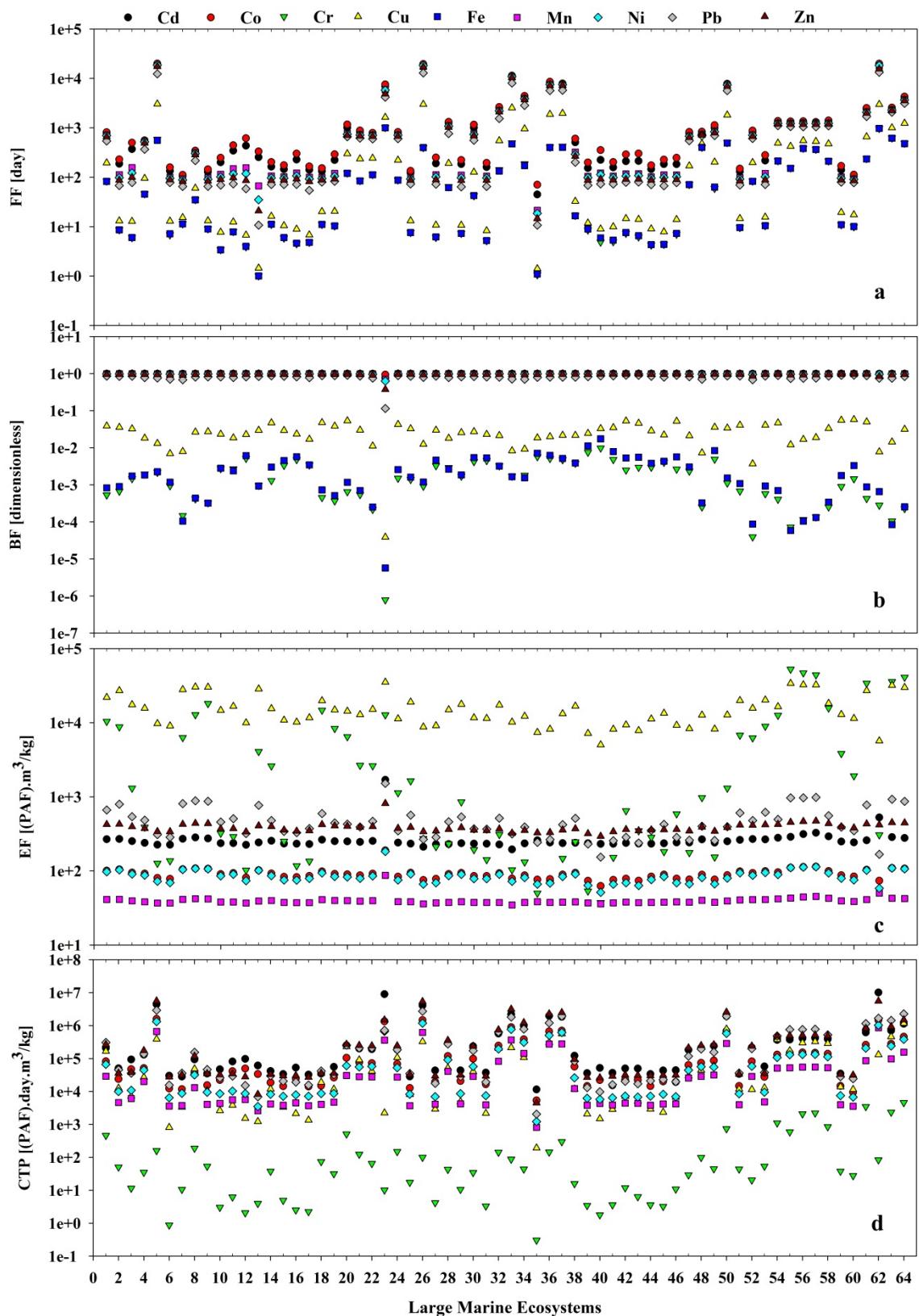


Figure S5. Fate Factor (Figure S5a), Bioavailability Factor (Figure S5b), Effect Factor (Figure S5c) and Comparative Toxicity Potential (Figure S5d) determined for nine metals in 64 LMEs.

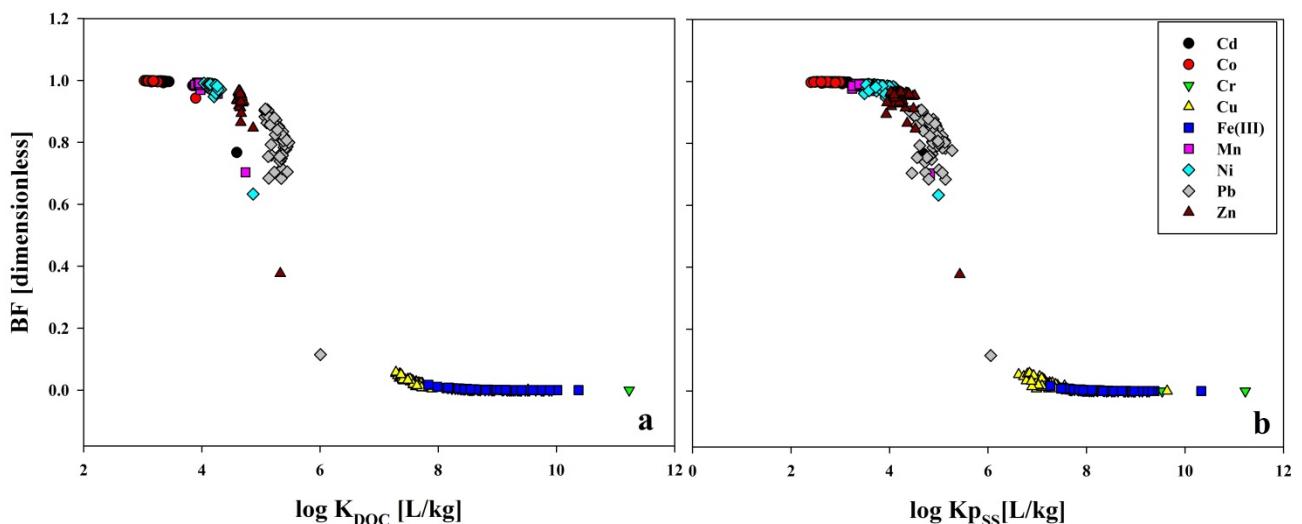


Figure S6. Relationship between Bioavailability Factor (BF) and $\log K_{DOC}$ (Figure S6a), and BF and $\log K_{pss}$ (Figure S6b) for all metals in all LMEs.

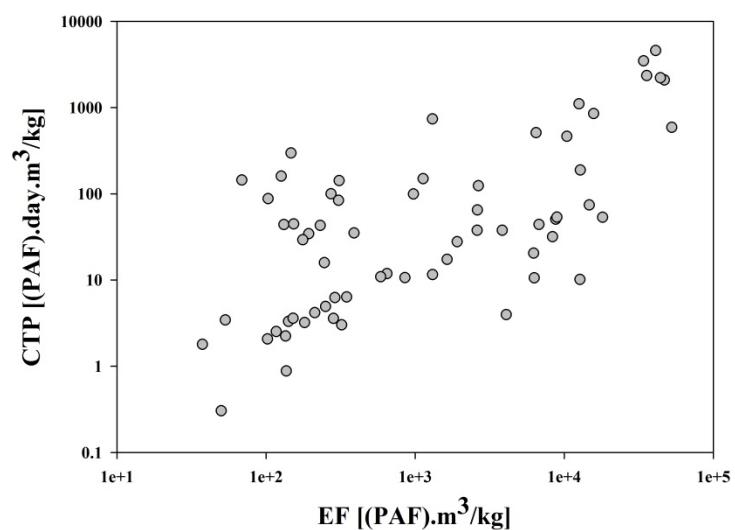


Figure S7. Relationship between Effect Factor (EF) and Comparative Toxicity Potential (CTP) for Cr in all LMEs

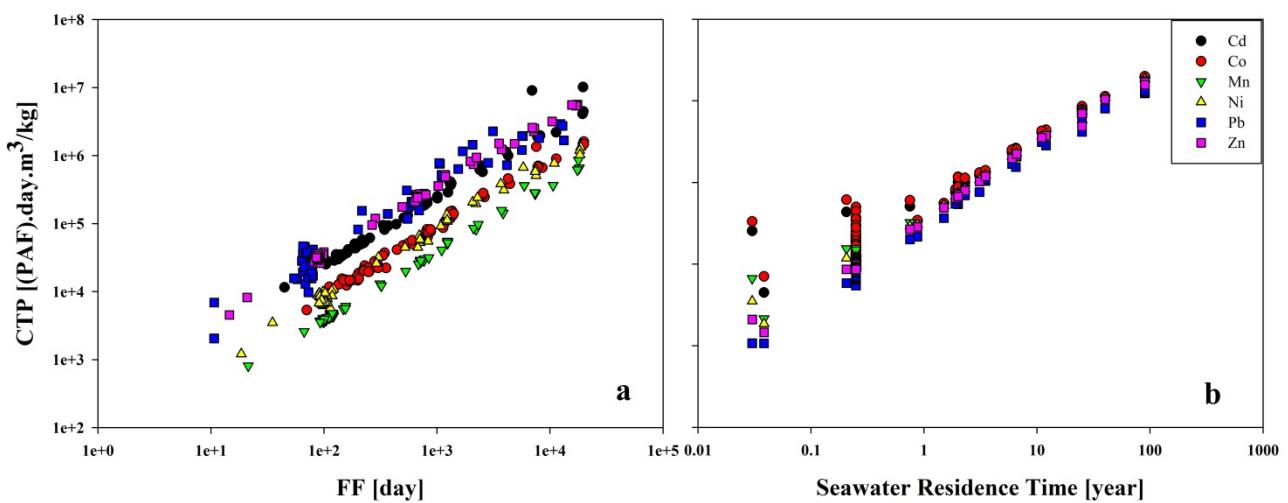


Figure S8. Relationship between Fate Factor (FF) and Comparative Toxicity Potential (CTP, Figure S8a), and Seawater residence time and CTP (Figure S8b) for Cd, Co, Mn Ni, Pb and Zn in all LMEs

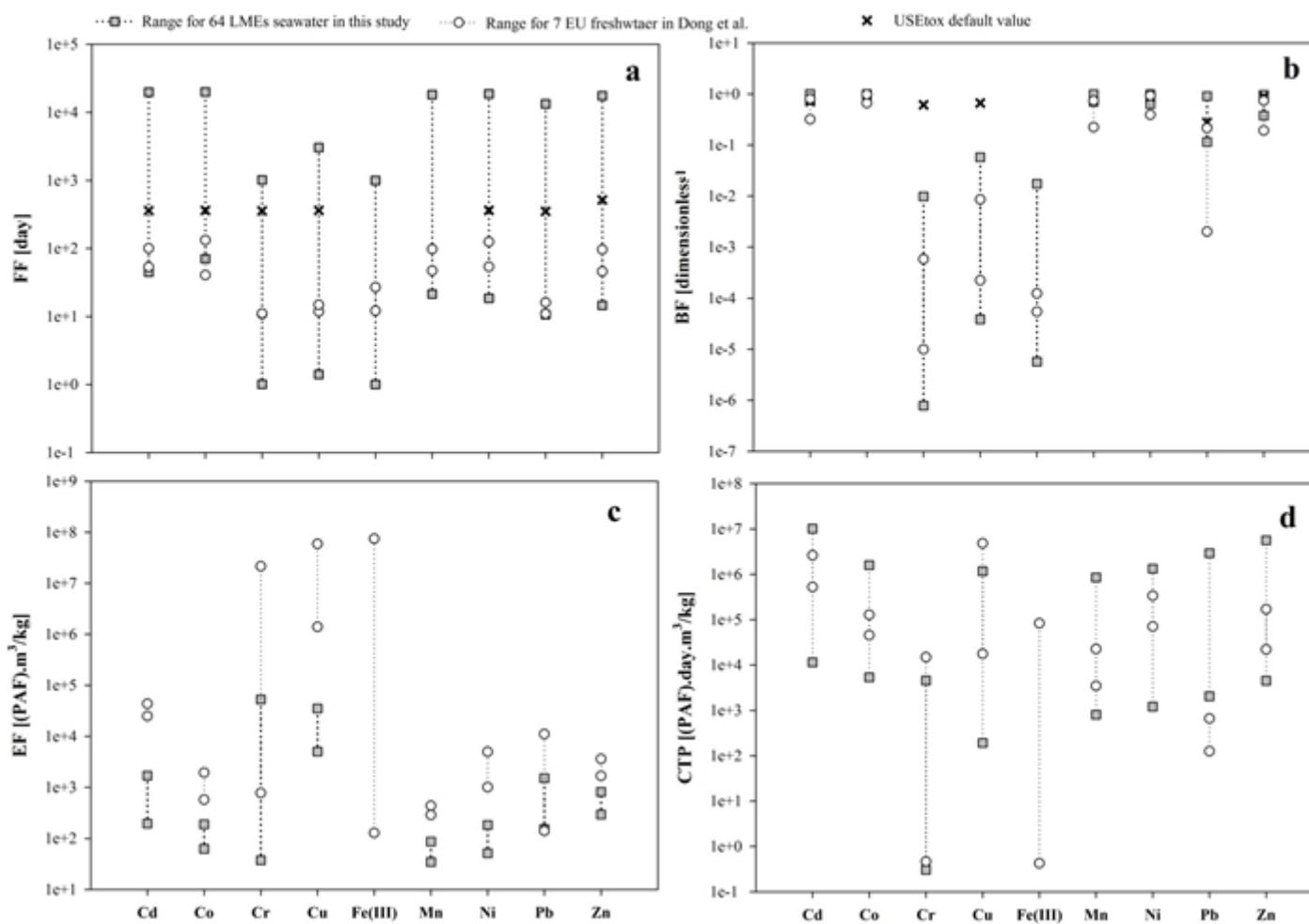


Figure S9. Ranges for Fate Factor (FF, S9a), Bioavailability Factor (BF, S9b), Effect Factor (EF, S9c) and Comparative Toxicity Potential (CTP, S9d) for nine metals determined across the 64 LMEs in this study. For comparison the corresponding ranges of freshwater FF, BF, EF and CTP in the study of Dong et al.³⁰, and the default values of FF and BF currently applied in USEtox are shown for those metals that are presently covered by the model.

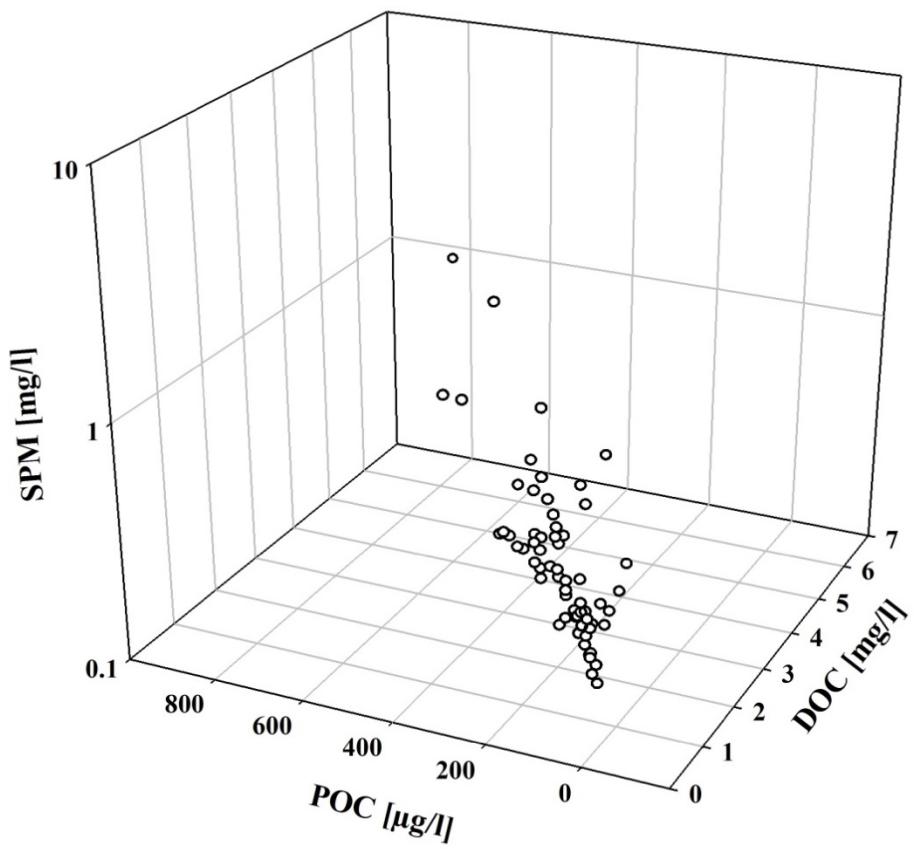


Figure S10. Relationships between POC, DOC and SPM concentrations in 64 LMEs.

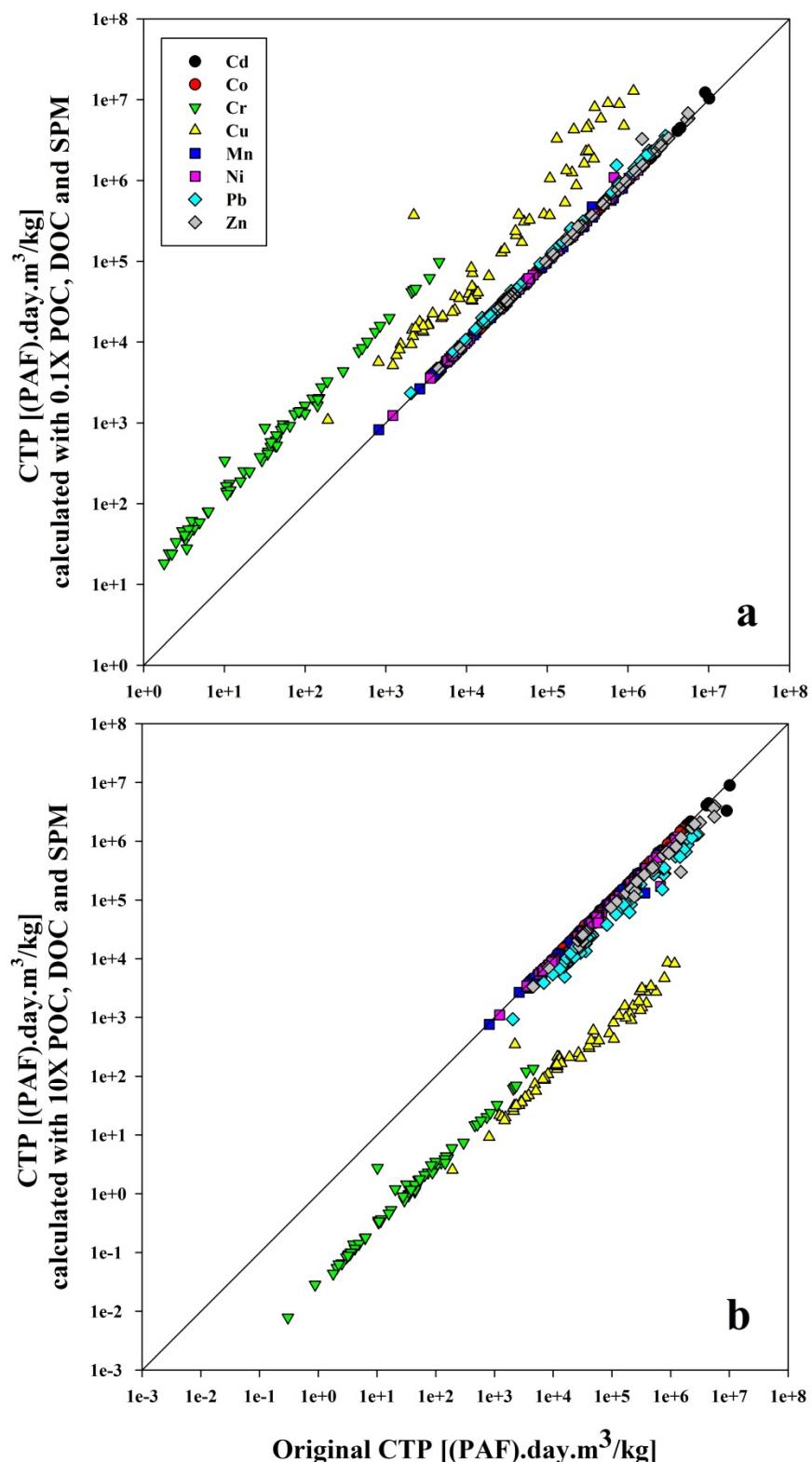


Figure S11. Comparative Toxicity Potentials (CTP) calculated with variations in POC, DOC and SPM concentrations (0.1X in Figure S11a or 10X in Figure S11b), and compared with the original CTP.

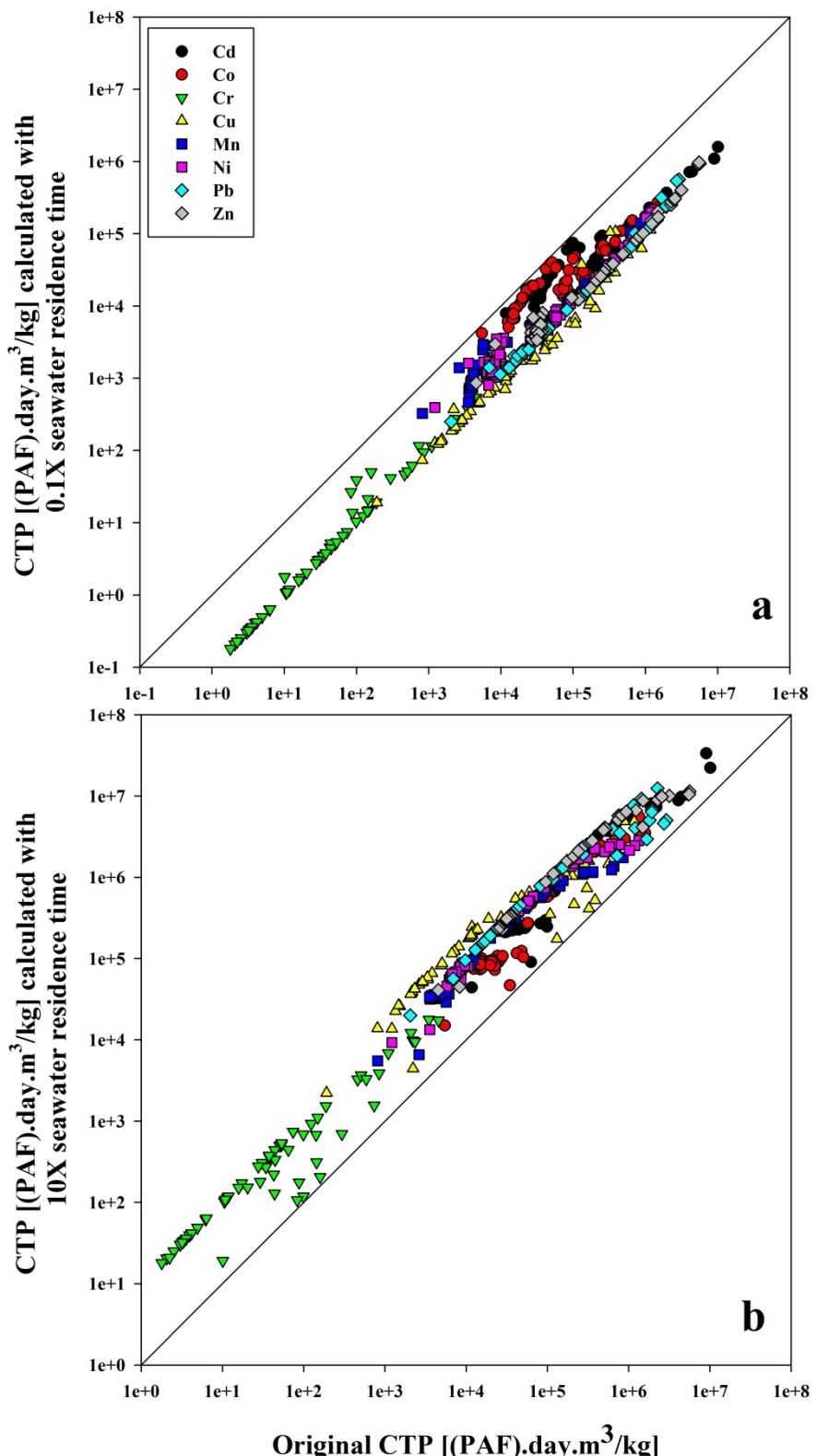


Figure S12. Comparative Toxicity Potentials (CTP) calculated with variations in seawater residence time (0.1X in Figure S12a or 10X in Figure S12b), and compared with the original CTP.

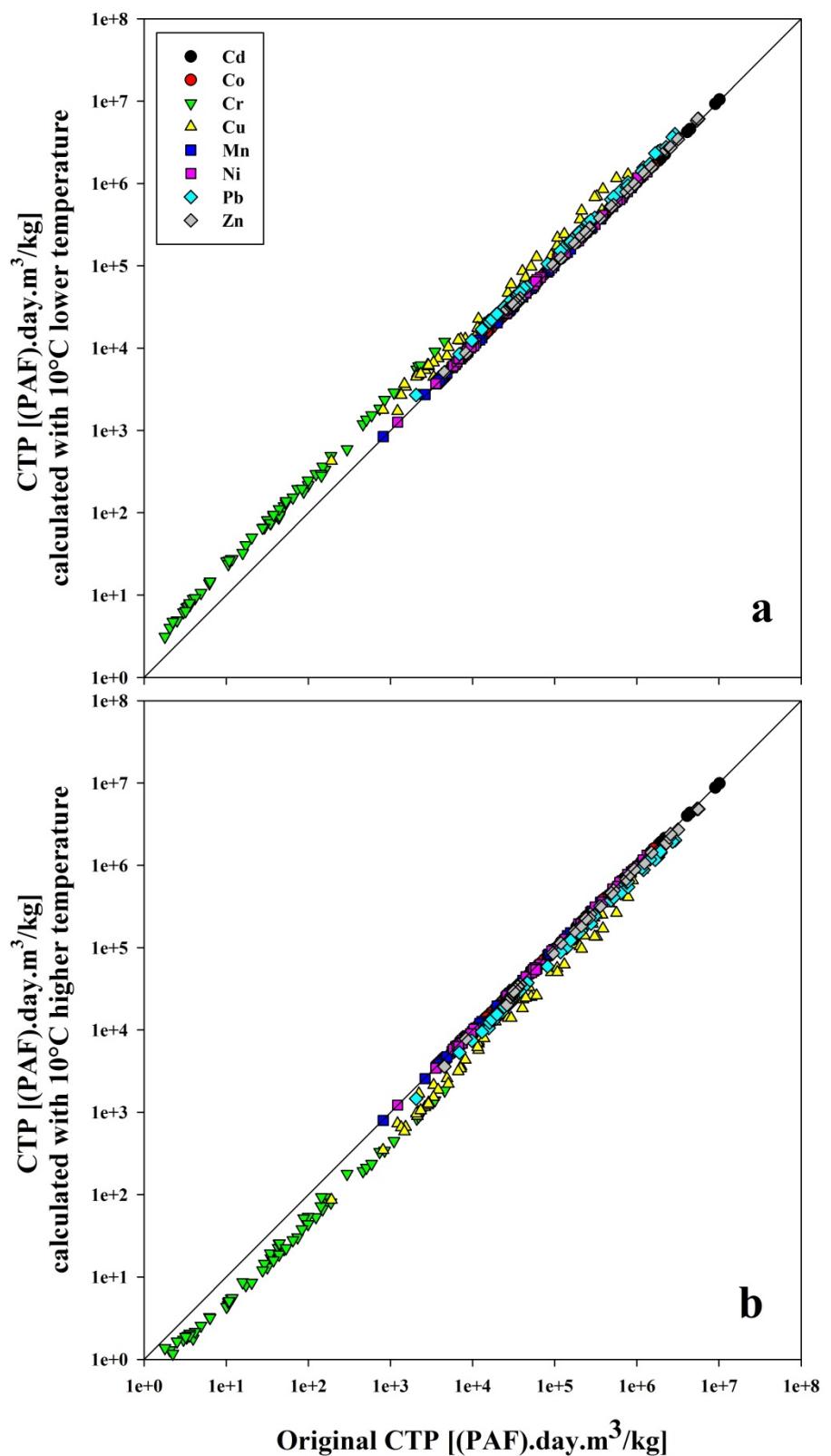


Figure S13. Comparative Toxicity Potentials (CTP) calculated with 10°C lower (Figure S13a) or 10°C higher temperature (Figure S13b), and compared with the original CTP.

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