Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Modelling scenarios of environmental recovery after implementation of controls on emissions of persistent organic pollutants

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Table S1 Substances – an approximate initial prioritisation for searching for source data

Substance	Notes as guidance in prioritising data searches
a) Data likely to be available in a suitable form and of appropriate quality	*The main focus for data gathering. No requirement to devote too much effort on concentrations from effluents. Surface water values might be useful as check on calculation outputs*
TBT	Much data likely to be available – possible issue with focus on contaminated sites
methyl-mercury	Data for mercury are available –estimation of likely proportion of me-Hg required
PCBs (126,118)	Data for all commonly determined or total PCBs useful – not these congeners only
HBCDD	Sewage the major source – half-life moderate
Cypermethrin	Sewage the major source – half-life short
PFOS	Likely requirement to consider sources generally
PFOA	Likely requirement to consider sources generally
Benzo(a)pyrene	Need estimates of non-sewage sources for load inputs
Fluoranthene	Need estimates of non-sewage sources for load inputs
DEHP	Fate with respect to sediment crucial – need Kp values as priority – might put in category c)
b) Data not likely to be so readily available	*Need to look carefully, but not to the detriment of progress on category a) substances – will take forward if suitable data are there*
HCB	Historic contaminant – less likely to have up to date information – possible issue with historic data quality – focus on contaminated sites
HCBD	Historic contaminant – less likely to have up to date information – possible issue with historic data quality – focus on contaminated sites
HCH	Historic contaminant – less likely to have up to date information – possible issue with historic data quality – focus on contaminated sites
Pentachloro-benzene (PeCB)	Never routinely monitored in UK?
Dioxins & dioxin-like compounds	Do not expect much of the essential information necessarily to be available – possibly more of an overview needed – could be category c)
Heptachlor/H-epoxide	Do not expect much of the essential information necessarily to be available – possibly more of an overview needed
Quinoxyfen	Data?
c) Not suited to this approach? / likely no worthwhile data?	
Lead	Infinitely persistent hence no mechanism for reduction in concentration other than by dilution or translocation (which are not part of the project)
Cadmium	Infinitely persistent hence no mechanism for reduction in concentration other than by dilution or translocation
Chloroalkanes (SCCPs)	Definition of the determinand is based on methodology that might be better defined – hence likely high uncertainty in data quality and what data might mean
Anthracene	Is there a compliance issue?
Dicofol	Not a persistent pollutant

Table S2 Key inputs and notes

Input	Units	Notes
initial sediment concentration	µg/kg	Can be set at the likely equilibrium value based on previous inputs – or at any other starting value.
initial rate of addition	µg/kg/year	Requires derivation based on concentrations-in/loads-from input sources and the size of the "sediment target" (see Table S2 below)
reduced rate of addition	percentage of initial input per year	Reduction in input as a percentage of initial input per year - based on the "measures" taken to reduce inputs
Biota-Sediment Concentration Factor (BSCF) to biota	n/a	Biota-Sediment Concentration Factor – the ratio of concentration in biota to that in sediment[1]. From literature – though care needed in assessment of relevance and credibility
half-life (t ½) in sediment	years	From literature – though care needed in assessment of relevance and credibility
Water/sediment partition coefficient, kp	l/kg	Used to estimate the proportion of inputs that are associated-with/accumulated-in sediment – should be relevant to the type of suspended particulate material envisaged Likely to require derivation from a number of different inputs – k(ow) k(oc) various k(spm) values

[1] BSCF - also known as a BSAF Biota Sediment Accumulation Factor

Table S3 Data for input and to support the input values – for derivation purposes

Input	Units	Notes
Input concentration – point source	µg/l	We stipulate that the point source is a sewage effluent discharges Note influence of local sources – how relevant and representative is the reported value? Is monitoring related to “unusual” pollution?
Input load to sediment – non- point source	µg/yr	An estimate of generic non-point sources to input rate – to be added to the point source-derived input rate
Half-life (t ½) of substance in sediment	years	A range of reported values in likely – why is this?
BSCF to biota	n/a	Biota-sediment concentration factor – the ratio of concentration in biota to that in sediment From literature – though care needed in assessment of relevance and credibility
Various measures of partitioning kp values	l/kg	Expressed on various ways and (possibly) translatable to a generic kp. The key challenge here is to understand what is being quoted
Sediment concentration value	µg/kg	As check on plausibility of initial value in above table Note influence of local sources – how relevant and representative is the reported value? Is monitoring related to “unusual” pollution?
Mass of sediment target	kg	Plausible value derived from notional point source (sewage works) inputs and in-river dilution **So NOT required from literature**

S1 Review of available data

Table S3 provides some preliminary guidance on the approach to a search for literature data. The search prioritised key substances for which the publication of sufficient data of a suitable quality would make it possible to progress to the stage of estimating the likely decline in contaminant concentrations. The first stage was to divide the substances of interest into three categories:

a) Those that are of primary interest in that they are regulated under the Water Framework Directive and have been identified as likely to be associated with EQS non-compliance;

b) Those of secondary interest by reason of likely lack of suitable data;

c) Those of questionable suitability for the chosen approach and therefore least likely to be taken forward.

The next stage prior to the estimation of changes in contaminant concentrations is to assess the suitability of the data obtained. Reasons for discounting the use of data include:

- Clear focus of the monitoring on polluted sites that are irrelevant to the generic risk assessment aims of the project;
- Lack of relevance to UK conditions;
- Likely data quality issues, often linked to historically high limits of analytical detection;
- Poor comparability amongst different estimated values.

In particular, the relative uncertainty between different categories of inputs can be very different as well as difficult to comprehend. For instance, reported values for BSCF can be highly variable according to the type of biota concerned and the exposure concentration and time. It is virtually impossible to infer the BSCF for other conditions from one reported value other than possibly the relative differences between substances.

Similarly, partition coefficients, expressed on a logarithmic scale (always difficult to envisage), can be given as k-octanol-water or k-organic carbon or true partition coefficient in a particular sediment concerned. Generally, the first in the list is the highest value and the last the lowest. Assumptions about the sorptive power of octanol and organic carbon and the carbon content of sediment can provide a “translation” between these values – but it has to be borne in mind that these involve generalising assumptions. Half-life values too can be influenced greatly by the conditions under which and the concentrations at which they are determined. This tends to lead to the observed wide range of reported values and calls into question their ready transferability to different situations.

In summary, the above discussion emphasises the caveat that this approach to estimating the possible decline in contaminant concentrations is not an attempt to model environmental conditions at a particular site. Rather, it is a way of comparing the likely effects of different controls on contamination on the likely rate of environmental recovery in response to measures to reduce the inputs of trace substances.

Table S4 Data from the literature

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
TBT	Concentration (Point Source)	0.47	ng/L	Mean	Estuarine	3 WWTWs, Amour estuary, (SW) France	*n* = 9	1
	In-River Concentration	<50 – 960 288 – 1150 96 – 479	ng/L (as Sn)	Range	Riverine	Arosa Rias, Spain Muros Rias, Spain Corcubion Rias, Spain	*n = ?* *n = ?* *n = ?*	2
		0.5 – 425		Range	Riverine	Qiangtang, Huangpu and Yellow River, China	*n = 32*	3
		1.13 – 21.13		Range	Riverine	Tagus estuary, Portugal	*n = 15*	
		<3.1 – 29		Range	Riverine	Various rivers, Portugal	*n = 46*	
		<3.0 – 44.8 <3.0 – 71.2		Range Range	Riverine	River Deben, England Rover Orwell, England	*n = 6* *n = 11*	
		0.2 mean d.s **0.12median d/s**					***n=172***	4
	Half – Life in Sediment	578	Days		Canal	Forth and Cylde Canal (Glasgow, UK)	Sediment extracted and spiked with TBT.	5
	BSCF to Biota Clam (*Ruditapes philippinarum*)	67.3 85.6 196.4 81.6 100.5 8.1 346.7 67.8		Mean	Estuarine Coastal	Site 1, Guaidianna estuary, (SW) Spain Site 2 Site 3 Site 8, Huelva, (SW) Spain Site 9, Bay of Cadiz, (SW) Spain Site 10 Site 11 Site 13, Bay of Algeciras, (SW) Spain	28 days exposure to contaminated sediments.	6
	Partitioning Values	3.9 – 4.9 3.64	log K_{ow} log K_d	Mean	Canal	Forth and Cylde Canal (Glasgow, UK)		7

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	Sediment Concentration 1ng/g =1 ppb = 2.43 ug/kg TBT Tool predicits 0.15 ug/kg as TBT This is	1.5 (0.1 – 8.6) 153 (10) 573 (22) 340 (11) 171 (8) 81 (5) 57 (7) 48 (7) 390 (12) 17 (2) 258 (11)	ppb ng Sn/g dw	Mean (Range) Mean (SD)	Estuarine	Tolka estuary (Dublin, Ireland) Site 1, Guaidianna estuary, (SW) Spain Site 2 Site 3 Site 4, Huelva, (SW) Spain Site 5 Site 8 Site 9, Bay of Cadiz, (SW) Spain Site 11, Port of Babarte Site 13, Bay of Algeciras, (SW) Spain Site 14	 *n* = 14. Surface sediment.	8 6
Methyl-Mercury	Concentration (Point Source) *WWTP Primary effluent* *WWTP Secondary effluent* *WWTP Final effluent*	 1.92 ± 0.90 2.76 ± 1.96 1.53 ± 0.93	ng/L	Mean ± SD	Effluent	Syracuse, New York, USA	 *n = 12* *n = 12* *n = 12*	9
	In-River Concentration	0.191 0.102 ~0.33 ~0.15 ~0.18	ng/L	Median	Riverine	Colusa Basin Drain, CA, USA Mid-Sacramento River, CA, USA Sacramento Slough, CA, USA Sacramento River at Verona, CA, USA Sacramento River at Freeport, CA, USA		11
	Half – Life in Sediment	1.4 (0.2)	Hours	Mean (SD)	Estuarine	Saltmarsh, Portugal		11
	BSCF to Biota *Phytoplankton* pH < 4.0 pH 4.0 – 7.0 pH ~ 7.0 *Zooplankton* pH < 4.0 pH 4.0 – 7.0 pH ~ 7.0 *Benthic macroinvertebrates* pH < 4.0 pH 4.0 – 7.0	 107.92 ± 148.4 82.99 ± 85.9 53.00 ± 51.4 125.68 ± 165.9 105.86 ± 126.9 68.51 ± 89.8 255.61 ± 345.8 305.48 ± 705.6 181.95 ± 263.7		 Mean ± SD	 Riverine	 Rio Madeira, Brazilian Amazon	 *n = 54* *n = 144* *n = 162* *n = 54* *n = 144* *n = 162* *n = 54* *n = 144* *n = 162*	12

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	pH ~ 7.0 *Invertebrate – detritivore* Headwater stream Mid-order stream *Invertebrate – predator* Headwater stream Mid-order stream *Fish – forage* Headwater stream Mid-order stream *Fish – predator* Headwater stream Mid-order stream	 200 36.9 770 95 1140 342 2125 513		Mean	Riverine	New York, USA	 *n = 5* *n = 11* *n = 5* *n = 2* *n = 5* *n = 25* *n = 15* *n = 15*	
	Partitioning Values	<2.53 – 4.15 6.46	log K_d	Median	Riverine	OR, WI, FL, USA E Anglia	8 streams across 3 USA states.	13 14
	Sediment Concentration	19.1 (8.9 – 28.6) 5.7 (2.9 - 10.6) 19.7 (16.9 – 23.5) 12.1 (6.2 – 20.5) 18.4 (15.7 – 21.9) 0.27 0.36 0.52 2.84	µg/kg ng/g	Mean (Range) Mean	Lacustrine Riverine Lacustrine Riverine Lacustrine Riverine	Surlingham Broad (Norfolk, UK) Adjacent River Site (Norfolk, UK) Rockland Broad (Norfolk, UK) Adjacent River Site (Norfolk, UK) Wheatfen Broad (Norfolk, UK) Putah Creek, CA Cottonwood Creek, CA Colusa Basin Drain Sacramento Slough, CA	*n* = 8. Surficial sediment (0-2 cm) concentrations. Sediment collected by selecting a 100-m reach of river and collecting material from sediment	15 10

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
							deposition zones.	
PCBs [number]	Concentration (Point Source)	**[101]** 397 (326) **[105]** 63 (60) **[118]** 229 (252) **[128]** 25 (50) **[138]** 357 (205) **[153]** 164 (39) **[170]** 37 (45) **[180]** 155 (87) **[183]** 21 (33)	pg/L	Mean (SD)	Effluent	MUC WWTP, Quebec, Canada	*n* = 6. The MUC wastewater treatment plant typically treats an average effluent flow of 19.8 m^3/s.	16
	In-River Concentration	**[total]** 123 (51) [U/S] **[total]** 221 (60) [Outfall] **[total]** 189 (94) [0.3km D/S] **[total]** 171 (107) [4km D/S] **[total]** 161 (70) [8.5km D/S]	pg/L	Mean (SD) [Location or distance from WWTWs discharge]	Riverine	St Lawrence River, Quebec, Canada		16
	Half – Life Water; Sediment	**[28]** 1,450; 26,000 **[52]** 30,000; 87,600 **[77]** 30,000; 87,600 **[101]** 60,000; 87,600 **[105]** 60,000; 87,600 **[118]** 60,000; 60,000 **[126]** 60,000; 87,600 **[138]** 120,000; 165,000 **[153]** 120,000; 165,000 **[169]** 120,000; 165,000 **[180]** 240,000; 333,000	Hours		Maritime	Baltic Sea		17
	BSCF to Biota Eel; Pike	**[28/31]** 0.16; 1.98 **[52]** 3.92; 2.54 **[99/113]** 1.44; 3.77 **[101/90]** 1.49; 2.92 **[105]** 2.55; 7.16 **[118]** 2.16; 4.77 **[138/164]** 4.61; 7.38		Mean	Riverine	River Severn at Stourport-on-Severn, Worcestershire, UK	*n* = 5.	18

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	   White Sucker Sculpins Bivalve (*Corbicula manilensis*)	**[153]** 10.1; 9.84 **[180]** 1.93; 12.2 **[total]** 11 **[total]** 5.7 **[total]** 5.7 **[total]** 4.4 **[total]** 3.3 **[total]** 2.4 **[total]** 2.0 **[total]** 1.8 **[total]** 1.8 **[total]** 1.1 **[total]** 21 **[total]** 2.1 - 3.3		 Mean Range	 Riverine	 Conestoga River, PA, USA Quinebaug River, MA, USA Codorus Creek, PA, USA Lind Coulee Nr. Moses Lake, WA, USA East Branch Housatonic, MA, USA Quinnipac River, CT, USA Winchester Wasteway, WA, USA Mattabasset River, CT, USA Qunittapahilla Creek, PA, USA Salt Creek, IN, USA White River, IN, USA		 19
	Partitioning Values	**[28]** 5.31 **[31]** 5.31 **[52]** 5.91 **[77]** 5.75 **[83]** 6.04 **[87]** 6.07 **[95]** 6.16 **[101]** 6.14 **[136]** 6.42 **[138]** 6.49 **[153]** 6.57	log K_{oc}	Mean	Riverine	Hudson River, USA	Theoretical values of log K_{oc}.	20
	Sediment Concentration	**[28/31]** 620 **[52]** 200 **[99/113]** 140 **[101/90]** 320 **[105]** 110 **[118]** 220 **[138/164]** 170 **[153]** 83 **[180]** 160	ng/kg dw	Mean	Riverine	River Severn at Stourport-on-Severn (Worcestershire, UK)	Samples taken to a depth of 5 cm along a 200 m stretch of river.	18
		[28] 2.51 (0-10cm) 2.65 (10-20cm) 5.65 (20-30cm)	µg/kg	Mean (Depth)	Estuarine	Site M34, Mersey (Inner) Estuary, UK		21

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		8.31 (30-40cm) 12.2 (40-50cm) 11.7 (50-60cm) 1.63 (60-70cm) <0.1 (70-80cm) <0.1 (80-90cm)					Two sites chosen to report here as full sediment profile was analysed. Reference also contains further sites with various depths measured. Sampling was carried out from May 2000 to November 2002.	
		3.35 (0-10cm) 3.21 (10-20cm) 2.95 (20-30cm) 2.96 (30-40cm) 3.15 (40-50cm) 1.59 (50-60cm) 3.61 (60-70cm)				Site M165, Mersey (Inner) Estuary, UK		
		[52] 2.07 (0-10cm) 1.46 (10-20cm) 2.91 (20-30cm) 4.86 (30-40cm) 4.98 (40-50cm) 6.04 (50-60cm) 1.29 (60-70cm) <0.1 (70-80cm) <0.1 (80-90cm)				Site M34, Mersey (Inner) Estuary, UK		
		1.3 (0-10cm) 1.26 (10-20cm) 1.29 (20-30cm) 1.57 (30-40cm) 1.7 (40-50cm) 1.03 (50-60cm) 1.55 (60-70cm)				Site M165, Mersey (Inner) Estuary, UK		
		[101] 2.39 (0-10cm) 2.17 (10-20cm) 4.29 (20-30cm) 5.38 (30-40cm) 5.90 (40-50cm) 7.67 (50-60cm) 0.45 (60-70cm) <0.1 (70-80cm)				Site M34, Mersey (Inner) Estuary, UK		

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		<0.1 (80-90cm)						
		2.16 (0-10cm) 2.04 (10-20cm) 2.13 (20-30cm) 2.65 (30-40cm) 2.33 (40-50cm) 1.24 (50-60cm) 2.67 (60-70cm)				Site M165, Mersey (Inner) Estuary, UK		
		[118] 1.83 (0-10cm) 0.30 (10-20cm) <0.15 (20-30cm) 3.71 (30-40cm) 4.84 (40-50cm) 7.27 (50-60cm) <0.15 (60-70cm) <0.15 (70-80cm) <0.15 (80-90cm)				Site M34, Mersey (Inner) Estuary, UK		
		2.15 (0-10cm) 1.84 (10-20cm) 1.71 (20-30cm) 2.19 (30-40cm) 2.01 (40-50cm) 1.21 (50-60cm) 2.03 (60-70cm)				Site M165, Mersey (Inner) Estuary, UK		
		[153] 1.30 (0-10cm) 1.56 (10-20cm) 2.89 (20-30cm) 2.52 (30-40cm) 3.62 (40-50cm) 1.80 (50-60cm) 0.38 (60-70cm) <0.15 (70-80cm) <0.15 (80-90cm)				Site M34, Mersey (Inner) Estuary, UK		
		1.83 (0-10cm) 1.70 (10-20cm) 1.86 (20-30cm)						

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		1.96 (30-40cm) 1.81 (40-50cm) 1.06 (50-60cm) 1.90 (60-70cm)						
		[138] 2.23 (0-10cm) 2.36 (10-20cm) 4.24 (20-30cm) 3.19 (30-40cm) 5.25 (40-50cm) 6.85 (50-60cm) 0.54 (60-70cm) <0.15 (70-80cm) <0.15 (80-90cm)				Site M165, Mersey (Inner) Estuary, UK		
		2.46 (0-10cm) 2.53 (10-20cm) 2.35 (20-30cm) 2.74 (30-40cm) 2.69 (40-50cm) 1.73 (50-60cm) 2.28 (60-70cm)				Site M34, Mersey (Inner) Estuary, UK		
		[180] 0.84 (0-10cm) 1.20 (10-20cm) 2.22 (20-30cm) <0.20 (30-40cm) 3.07 (40-50cm) 3.68 (50-60cm) <0.2 (60-70cm) <0.2 (70-80cm) <0.2 (80-90cm)				Site M165, Mersey (Inner) Estuary, UK		
		1.19 (0-10cm) 1.33 (10-20cm) 0.99 (20-30cm) 1.40 (30-40cm) 1.38 (40-50cm) 0.79 (50-60cm) 1.45 (60-70cm)				Site M34, Mersey (Inner) Estuary, UK		

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
						Site M165, Mersey (Inner) Estuary, UK		
HBCDD	Concentration (Point Source)	<3.9 4.9 (7.6)	µg/kg	Mean (SD)		SE England Netherlands	*n* = 5.	22
	In-River Concentration	2.64E-04 **(query these)** 9.55E-04 5.61E-04 2.29E-04 1.40E-03 **0.0027 (0.0030) d/s** **0.0016**	µg/L	Mean Mean Mean Mean Mean **Mean (SD)**	Riverine	River Arun, England River Erewash, England River Ouzel, England River Team, England River Alt, England **Rivers England**	N = 1 N = 12 N = 15 N = 9 N = 17 **N=172**	4
	Half – Life in Sediment Aerobic Anaerobic	101 66	Days					23
	BSCF to Biota *Bleak* *Barbel*	0.10 – 0.68 0.10 – 1.44 0.23 – 1.23 0.14 – 0.47		Range	Riverine	Cinca River, Spain		24
	Partitioning Values	7.74 6.72		log K_{ow} log K_{oc}			Values modelled with EPI suite (US EPA)	25
	Sediment Concentration	60 (223) 10 (25) 3.3 (5.2) 199 (364)	µg/kg	Mean (SD)	Riverine Estuarine Estuarine + Riverine	Scheldt Basin, Netherlands Western Scheldt, Netherlands Dublin Bay, Ireland 6 England Rivers	*n* = 19.	22

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		Nd - 514	ng/g	Range	Riverine	Cinca River, Spain	Samples collected up and downstream of industrialized town draining to the river.	26
Cyper--methrin	Concentration (Point Source)	269.1 568.7 79.16 **0.3 (0.9)** **0.14 (0.31) mean (sd)** **0.064 median**	ng/L	Mean	Effluent Effluent River d/s	El Gallo WWTWs, Mexico El Naranjo WWTWs, Mexico El Sauzal WWTWs, Mexico	24hr composite samples.	27 4
	In-River Concentration	5.8 - 30.4 [2008] 0.73 – 57.2 [2009]	ng/L	Range [Year]	Riverine	Ebro Delta River, (NE) Spain	*n* = 12.	28
	Half – Life in Sediment Hydrolysis Aerobic	6-20 1.9 – 619 6 - 20	days days	Range Range	Estuarine + Coastal Riverine	Punta Banda Estuary and Todos Santos Bay, Mexico Ebro Delta River, (NE) Spain		27 28
	BSCF to Biota *Daphina magna* *Chironomus tentans*	 0.31 (0.28-0.34) [1] 0.14 (0.12-0.16) [3] 0.08 (0.06-0.10) [13] 0.63 (0.5-0.76) [1] 0.19 (0.17-0.21) [3] 0.08 (0.06-0.10) [13]		 Mean (95% CL) [OC content %]	 Natural Sediments	 Mississippi, Florissant, Duluth, USA		 29

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	Partitioning Values	2,360 [1] 15,700 [3] 23,600 [13] 238,000 (16) [1] 502,000 (5) [3] 177,000 (13) [13] 5 – 6.3	Mean Range	K_ds [OC content %] K_{oc} (CoV) [OC content %] log K_{oc}	Natural Sediments Riverine	Mississippi, Florissant, Duluth, USA Ebro Delta River, (NE) Spain		29 28)
	Sediment Concentration	0.24 (0.30) 0.46 (1.47) 8.3 – 71.9 (Jun 2009) 0.13 – 2.92 (Oct 2009)	ng g/dw ng/g	Mean (SD) Range [Date]	Estuarine Coastal Riverine	Punta Banda Estuary, Mexico Todos Santos Bay, Mexico Ebro Delta River, (NE) Spain	*n* = 19. Top 2cm sediment. *n* = 13. *n* = 8.	27 28
PFOS	Concentration (Point Source)	5.5 (0.6) 4.7 (0.8) 2.5 (0.7) 5.8 (0.5) 82.2 (6.5) 2.1 (0.4) < 0.06 < 0.06 0.5 (0.1) 45 [Apr 2005] 140 [Jul 2005] 31 [Mar 2006] 30 [13 Jul 2005] 12 [27 Jul 2005] 12	ng/L	Mean (SD) Mean [Date]	Effluent	WWTW a, River Elbe, Germany WWTW b, River Elbe, Germany WWTW c, River Elbe, Germany WWTW d, River Elbe, Germany WWTW e, River Elbe, Germany WWTW f, River Elbe, Germany WWTW g, River Elbe, Germany WWTW h, River Elbe, Germany WWTW i, River Elbe, Germany WWTW a, Bayreuth, Germany WWTW b, Bayreuth, Germany WWTW c, Bayreuth, Germany		30 31

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	In-River Concentration	1.2 (0.2) 2.1 (0.03) 1.9 (0.04) 2.2 (0.1) 2 (0.1) 2.9 (0.3) 1.5 (0.7) 0.6 (0.1) 0.5 (0.3) 1.6 (1.1) 2.1 (0.2) 2 (0.1) 1.6 (0.0003) 1.2 (0.03) 1 (0.2)	ng/L	Mean (SD)	Riverine Estuarine	Site 1, River Elbe, Germany Site 2, River Elbe, Germany Site 3, River Elbe, Germany Site 4, River Elbe, Germany Site 5, River Elbe, Germany Site 6, River Elbe, Germany Site 7, River Elbe, Germany Site 8, River Elbe, Germany Site 9, River Elbe, Germany Site 10, River Elbe, Germany Site 11, River Elbe, Germany Site 12, River Elbe, Germany Site 13, River Elbe, Germany Site 14, River Elbe, Germany Site 15, River Elbe, Germany		30
		1.7 (0.3) [1km U/S] 16 (0.3) [0.1km D/S] 14 (0.5) [0.5km D/S] 11 (0.2) [1km D/S]		Mean (SD) [Distance from WWTWs discharge)	Riverine	Rotor Main river, Bayreuth, Germany	*n* = 3.	32
		17.4 (2.2)		Mean (SD)	Riverine	Orge River, Paris, France	*n* = 3	33
		6.6 (9.2) mean (Sd) **4.0 median**			**River d/s**		**n-172**	4
	Half – Life in Sediment	> 41 (in water)	Years				Could not find half-life in sediment	34
	BSCF to Biota European Chub: Plasma Liver Gills Gonads Muscle	 1.5 (0.1) 0.6 (0.2) 0.3 (0.1) 0.2 (0.1) -0.3 (0.2)		Mean (SD)	Riverine	Orge River, Paris, France	*n* = 3.	33

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	Partitioning Values	7.42 2.8 2.4 (0.2) 3.7 (0.2)	Mean Mean (SD)	log K_d log K_{oc} log K_d log K_{oc}	Riverine Riverine	Lake Michigan, USA Orge River, Paris, France		35 33
	Sediment Concentration	105 (85) [0.1km U/S] 280 (120) [0.05km D/S] 250 (150) [0.5km D/S] 200 (90) [1km D/S] 4.3 (0.3)	Ng/kg dw	Mean (SD) [Distance from WWTWs discharge] Mean (SD)	Riverine Riverine	Rotor Main river, Bayreuth, Germany Orge River, Paris, France	*n* = 3. *n* = 3. Surface sediment, 0-2cm.	32
PFOA	Concentration (Point Source)	239 235 663 697 165 67 12-185 0.40–926 145	ng/L ng/L ng/L ng/L	Mean Range Range Mean	Effluent Effluent Effluent	New York State, USA California, USA Germany	Measured in effluent waters of 2 activated sludge WWTW plants. Measured in reclaimed wastewater from 4 WWTW plants. Measured in landfill effluent (n = 20)	36 37 38
	In-River Concentration	30.7 10.6 10.5 7.4 5.7	ng/L	Median	Riverine	Japan England (London) Sri Lanka China Turkey	*n = 233* *n = 13* *n = 6* *n = 13* *n = 2*	40

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		5.6 4.8 3.8 2.3 1.2 0.7				Singapore Malaysia Laos Thailand Ireland Vietnam	*n = 49* *n = 63* *n = 1* *n = 125* *n= 1* *n = 15*	
		23	ng/L	Mean	Riverine	River Thames, England		41
		100	ng/L	Average	Riverine	River Wyre, England		42
		4.9 (4.6) mean (Sd) **3.6 median**			**River d/s**		***N=172***	4
	Half – Life in Sediment	No measurable half-lives available			Freshwater and Estuarine		Due to the high persistence of PFOA, no half-lives in sediment are available.	43
	BSCF to Biota Freshwater oligochaete, *Lumbriculus variegatus*	33 ± 12 95 ± 12 94 ± 12		Measured value ± SD Measured value ± SD Measured value ± SD	Riverine	California, USA	Lipid-normalised BSAF value (estimated). Lipid-normalised measured values after 56 days for 2 sediment samples taken downstream of 2 different WWTW.	44
	Partitioning Values	2.3 – 2.6 2.69		Log k_{oc} (Range) Log k_{ow}			Values determined experimentally in water containing suspended	45 46

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		0.5		pKa			solids Calculated using Advanced Chemistry Development (ACD/Labs) Software at pH 7 and 25°c Values determined experimentally in water	43
	Sediment Concentration	1.48 27 70 85 50 0.3 5	µg/kg dw ng/kg dw ng/g	Mean Mean Median Mean	Riverine Riverine Various	Danube River, Austria Roter Main River, Germany Taken at locations relative to a WWTP China, Japan, Austria, Germany, USA	Samples taken from Danube river banks 0.1 km upstream 0.05 km downstream 0.5 km downstream 1 km downstream *n = 74*	47 31 48
Benzo (a) pyrene	Concentration (Point Source)	0.0066	µg/L	95%ile of average	Effluent	UK	*n = 162* WWTW final effluent	49
	In-River Concentration	4.79E-03 0.023 0.017 0.012 0.036 **0.016 (0.015) mean (Sd)** **0.012 median**	µg/L	Average	Riverine **River d/s**	River Arun, England River Erewash, England River Ouzel, England River Team, England River Alt, England	*n = 18* *n = 11* *n = 17* *n = 11* *n = 21*	4

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	Half – Life in Sediment	17,000	Hours	Estimated	Lacustrine	Quebec, Canada		50
	BSCF to Biota Freshwater tubificid oligochaete (*Ilyodrilus templetoni)*	1.33 ± 0.06 1.34 ± 0.11		Mean ± SD	Riverine	California, USA	*n = 3* *n = 3*	51
	Partitioning Values	6.24 6.04		Log k_{oc} (Avg.) Log k_{ow}				52
	Sediment Concentration *Depth of sample (cm):* 50–60 60–70 70–80 50–60 60–70 90–100 0–10 10–20 20–30 40–50 50–60 60–70 70–80 90–100 0–10 10–20 20–30 30–40 40–50 50–60	107 86.7 138 80.8 76.3 218 315 201 144 301 289 251 227 332 368 348 440 350 363 332	μg/kg dw	Measured concentration	Estuarine	Mersey Estuary, NW England		53
Fluroanthene	Concentration (Point Source) *WWTW Effluent* *Urban Stream Stormflow* *CSO*	0.0067 0.1 0.071 0.16 0.067 – 0.082	μg/L μg/L μg/L	Median Maximum Median Maximum Range	Effluent	Lake Champlain Basin, USA	*n = 6* *n = 5* *n = 2*	54
	In-River Concentration	14 - 240	ng/L	Range	Riverine	Humber Estuary, UK	Range	55

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		0.1 ± 0.16	µg/L	Mean ± SD	Various	Europe	across 6 rivers	
		22.1 4.07 0.858 0.711 **0.032 (0.037) mean sd** **0.025 median**	ng/L	Mean	Riverine **River d/s**	USA *Elizabeth River* *York River*	Dissolved fraction Dissolved fraction Particulate Fraction Dissolved fraction Particulate Fraction	56 57 4
	Half – Life in Sediment	1.14	Years		Estuarine	Tamar Estuary, UK		58
	Depth of sample (m): 0 10 50 100 150	 95.5 100 112 125 136	Days		Marine	Gulf of Mexico	Determined experimentally at 25°C	59
	BSCF to Biota Freshwater Amphipod (*Diporeia* sp.) *Sediment concentration (nmol/g dw):* 0.1 688	 0.107 0.424		Mean	Lacustrine	Lake Michigan, USA	*n = 3*	60
	Freshwater Amphipod (*Hyalella asteca*) *Sediment concentration (nmol/g dw):* 0.1 136	 0.045 0.236					*n = 3*	
	Benthic copepod				Estuarine	Louisiana, USA		61

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	(**S. knabeni**) *Sediment concentration (nmol/g dw):* 25 2000 Benthic copepod (**Coullana** sp.) *Sediment concentration (nmol/g dw):* 25 2000	0.57 ± 0.28 0.80 ± 0.22 0.22 ± 0.05 0.49 ± 0.06		Mean ± SD			*n = 4* *n = 3*	
	Partitioning Values	5.23 5.16 4.58		Log k_{ow} (Mean) Log k_{ow} (Mean) Log k_{oc}	Experimental	Experimental value from slow-stirring in distilled water at 25°C Reported value from literature Humber Estuary, UK	*n = 6*	62 55
	Sediment Concentration	388 ± 408	ng/g dw	Mean ± SD	Estuarine	Humber Estuary, UK	*n = 32*	55
DEHP	Concentration (Point Source) *Sewage Treatment Effluent*	1.9	µg/L	Average	Effluent	Manchester, UK	*n = ?*	63
	In-River Concentration	0.693 0.183 0.125 0.138 0.294 0.4 1.6 2.27 0.33 – 97.8 27.9 9.3	µg/L µg/L µg/L µg/L	 Average Average Median Range Median Average	Riverine Riverine Surface Water Riverine Riverine	River Mersey, England River Irwell, Manchester, UK River Etherow, Manchester, UK Germany River Rhine, Germany Taiwan	*n = 1* *n = 1* *n = 1* *n = 1* *n = 1* *n = ?* *n = ?* *n = 115* *n = ?* *n = 14*	64 63 65 66
	Half – Life in Sediment	14.8	Days	Average	Riverine			67

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	BSCF to Biota Fish (**Liza subviridis**.) **(Oreochromis miloticus niloticus)** (**Acanthopagrus schlegel)** **(Zacco platypus)**	 13.8–40.9 2.4–28.5 0.1 0.9		 Range Range Average Average	Riverine	Taiwan	 *n = 2* *n = 3* *n = 1* *n = 1*	68
	Partitioning Values	7.5	Log k_{ow}			Recommended value determined in review of several experimentally derived values.	*n = 13*	69
	Sediment Concentration	1.220 1.199 0.70 0.21 – 8.44 4.6 0.5 – 23.9	µg/g dw mg/kg dw µg/g	 Median Range Average Range	Riverine Riverine Riverine	River Speke, England River Runcorn, England Brandenburg and Berlin, Germany Taiwan	*n = 6* *n = 6* *n = 35* *n = 6*	64 65 66
HCB	Concentration (Point Source) *WWTP Effluent*	3.23 1.65 – 4.51	ng/L	Mean Range	Effluent	Gaobeidan Lake, Beijing, China	*n = 6*	70
	In-River Concentration	<0.001 – 0.002 <0.001 61.58 53.60 9.23 5.78	µg/L ng/L	Range Mean Mean	Riverine Estuarine Riverine	River Thames, Caversham, England Thames Estuary, Woolwich, England River Aire, Humber Estuary, England River Calder, Humber Estuary, England River Don, Humber Estuary, England River Trent, Humber Estuary, England	*n = 30* *n = 76* *n = 71* *n = 69* *n = 70* *n = 70*	71 72
	Half – Life in Sediment							
	BSCF to Biota							

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	Partitioning Values	6.0 4.5 – 7.3 5.5	Median Range	Log k_p Log k_{ow}				73
	Sediment Concentration	1.17 1.52 2.27 2.00 2.56 1.87 0.884 0.628 0.746 0.596 0.485 0.527 1.74 2.45 1.82 3.73 1.01 0.557	μg/kg dw		Riverine	Han River, South Korea		74
		0.18 1.3 4.2 1.6	ng/g dw	Mean Mean Mean Mean	Lacustrine	Redón Lake, Pyrenees, Spain Ladove, Tatra Mountains, Poland Starolesnianske Pleso, Tatra Mountains, Poland Dugli Staw, Tatra Mountains, Poland	Mean across sediment core. *n = 7* *n = 5*	75
HCBD	Concentration (Point Source) *Sewage Treatment Effluent*							
	In-River Concentration	<0.003 <0.003	μg/L	Mean	Riverine Estuarine	River Thames, Caversham, England Thames Estuary, Woolwich, England	*n = 30* *n = 76*	71
	Half – Life in Sediment	125- 191	Days					76
	BSCF to Biota							

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
	Partitioning Values	3.7 – 4.9 4.90 4.9 3.8 – 6.7 4.8	 Median Range	Log k_{ow} Log k_{oc} Log k_p Log k_{ow}				77 78 73
	Sediment Concentration	7.3 6.11 – 8.71	Mean Range	µg/kg dw	Riverine	Ebro River Basin, NE Spain	*Surface sediments. n = 2*	79
HCH	Concentration (Point Source) *WWTP Effluent*	18.0 13.2 – 26.7	ng/L	Mean Range	Effluent	Gaobeidan Lake, Beijing, China	*n = 6*	70
	In-River Concentration *γ-HCH*	6.93 4.41 0.81 22.94 6.4 9.45 10.26 11.33 5.28 11.69 0.017 0.06 – 0.032 0.037 0.005 – 0.136	ng/L µg/L	 Mean Range Mean Range	Riverine Riverine	Yu Rivulet, Fujian Province, China Quiulu Rivulet, Fujian Province, China Quiulu Rivulet, Fujian Province, China Hanjiang River, Fujian Province, China Hanjiang River, Fujian Province, China Yu Rivulet, Fujian Province, China Quiulu Rivulet, Fujian Province, China Quiulu Rivulet, Fujian Province, China Hanjiang River, Fujian Province, China Hanjiang River, Fujian Province, China River Lee, England Tributaries of the River Lee, England	High Tide Low Tide HCH (gamma)	80 81
	Half – Life in Sediment	90	Days				Calculated	76

Substance	Input	Value(s)	Units	Descriptive	Environment	Location	Details/Notes	Reference
		0.9 to 12.6	Years	Range		Amituk Lake, Cornwallis Island, Arctic	value	
	BSCF to Biota							
	Partitioning Values *α-HCH* *β-HCH* *γ-HCH* *α-HCH* calculated experimental *β-HCH* calculated experimental *γ-HCH* calculated experimental	 8.63×10^3 8.22×10^3 6.79×10^3 5920 9800 11160 9380 4400 8160		 K_{ow} K_{ow}			 Final adjusted values at 25°C	 82 83
	Sediment Concentration	0.1–16.7 0.2–101 0.14–1.12 0.1–2.0 0.25–6.0 3.7–13 1.2–33.7 0.02–4.55 0.086–0.33 0.85–7.87 0.008–0.02 0.11–0.40 1.26 1.02 – 1.48	ng/g dw ng/g dw	Range Mean Range	Coastal Estuarine Coastal Coastal Coastal Estuarine Coastal Coastal Coastal Coastal Coastal Coastal Lacustrine	Hong Kong, PRC Chinese river/estuaries Xiamen Harbour, PRC Manukkau Harbour, New Zealand Alexandria Harbour, Egypt Juilong river estuary, PRC Northern coast, Vietnam Ulsan Bay, Korea West coast of Sri Lanka Arabian Sea, India Eastern coast of India Northeastern coast of India Gaobeidan Lake, Beijing, China	 *n = 10* *n = 6*	84

Transport of nonpolar organic compounds from surface water to groundwater. Laboratory sorption studies.(85)

Table S5. Notes on data sources

Point source Concentration	Me-Hg	as default (me-Hg] assumed the same as [Hg-dissolved] good agreement between UK and US (Gbondo-Tugbawa et al. (2010)) data for effluents
	PCBs	data for Quebec WwTW (Phram and Proulx (1997)) for congener 118
	HCB	Meharg et al. (1998) Aire and Calder (contaminated at 0.05 ug/l, Trent and Don (not contaminated) at 0.01 ug/l
	HCBD	Jürgens et al. (2013)
	HCH	Snook et al (2004)
t1/2		
	TBT	Sakultantimetha et al. (2011) seems a little long re the 80 days I have seen elsewhere
	Me-Hg	Cesario et al. (2017) looks like a ridiculous value
	PCB(118)	Sinkkonen and Paasivirta (2000)
	HBCDD	Davis et al. (2006)
	cypermethrin	Hernandez-Guzman et al. (2017) 6-20 days
	PFOS	nd 41 yr in water
	PFOA	nd
	Benzo(a)pyrene	Mackay and Hickie (1999)
	Fluoranthene	Readman et al. (1987)
	DEHP	Chao et al. (2007)
	HCB	nd
	HCBD	Onogbosele et al. (2014) Cranfield
	HCH	Onogbosele et al. (2014) range 1-12
BSCF		*Variability on organisms can be a source of uncertainty if the species of interest is very different from that tested*
	TBT	Garg et al. (2009) variable between 8 and 50 but sediments contaminated so chose 10
	Me-Hg	Vieira et al. (2018) quite variable
	PCB (118)	Harrad and Smith (1997) Severn 2.2-4.8 chose 3 ell pike
	HBCDD	Van Beusekom et al. (2006) around 1
	cypermethrin	Labadie and Chevreuil (2011) chironomids
	PFOS	Labadie and Chevreuil (2011) chubb around 1 to plasma
	PFOA	Higgins et al. (2007) lumbriculus lipid normalised? – Need to back calculates to whole organism – assuming lumbriculus is 5% lipid the published BSCF of 33 becomes 1.65
	Benzo(a)pyrene	Lu et al. (2009) oligochaete
	Fluoranthene	Driscoll et al. (1997) amphipods
	dehp	Huang et al. (2008) very variably this value for minnow other ranges 10-30
	HCB	nd
	HCBD	nd
	HCH	nd
Kp		*Note log kp values might be log kow or log koc, in which case they require adjustment to a nominal Kp*

Point source Concentration	Me-Hg	as default (me-Hg] assumed the same as [Hg-dissolved] good agreement between UK and US (Gbondo-Tugbawa et al. (2010)) data for effluents
	TBT	Bangkedphol et al. (2009) proper logkp 3.64 Reviews of Environmental Contamination and Toxicology 166 edited by George W. Ware vol 166 p 1048 J Meador Predictign the fate and effects of tributyltin in marine ssytems logkoc 4.7
	Me-Hg	Marvin-Dipasquale et al. (2009) 2.5-4 proper - v low re mercury a value of log kp of 6.46 has been used from: Moriarty F. and French M.C. (1977) Mercury in waterways that drain into the Wash, in Eastern England. Water Research, 11, 367-372.
	PCBs	Butcher et al. (1998)
	HBCDD	Gustavsson et al. (2013) modelled koc
	Cypermethrin	EA WFD dossier Science Report: SC040038/SR7 SNIFFER log koc 5.5 Maund et al. (2002) dependent on OC this for 3%
	PFOS	Labadie and Chevreuil (2011) proper kd 2.4 koc 3.7. EA RA gives koc as 2.6
	PFOA	ECHA (2013) log kow EA RA gives koc as 2.85
	Benzo(a)pyrene	Latimer and Zhen (2003) kow
	Fluoranthene	Maagd et al. (1998) log kow
	DEHP	Staples et al. (1997) log kow
	HCB	Oliver and Kaiser (1986) range 4.5-7.3
	HCBD	Lerche et al. (2002) Taylor et al. (2003) Oliver and Kaiser (1986) range narrow
	HCH	Xiao et al. (2004) for different conformers log Kow

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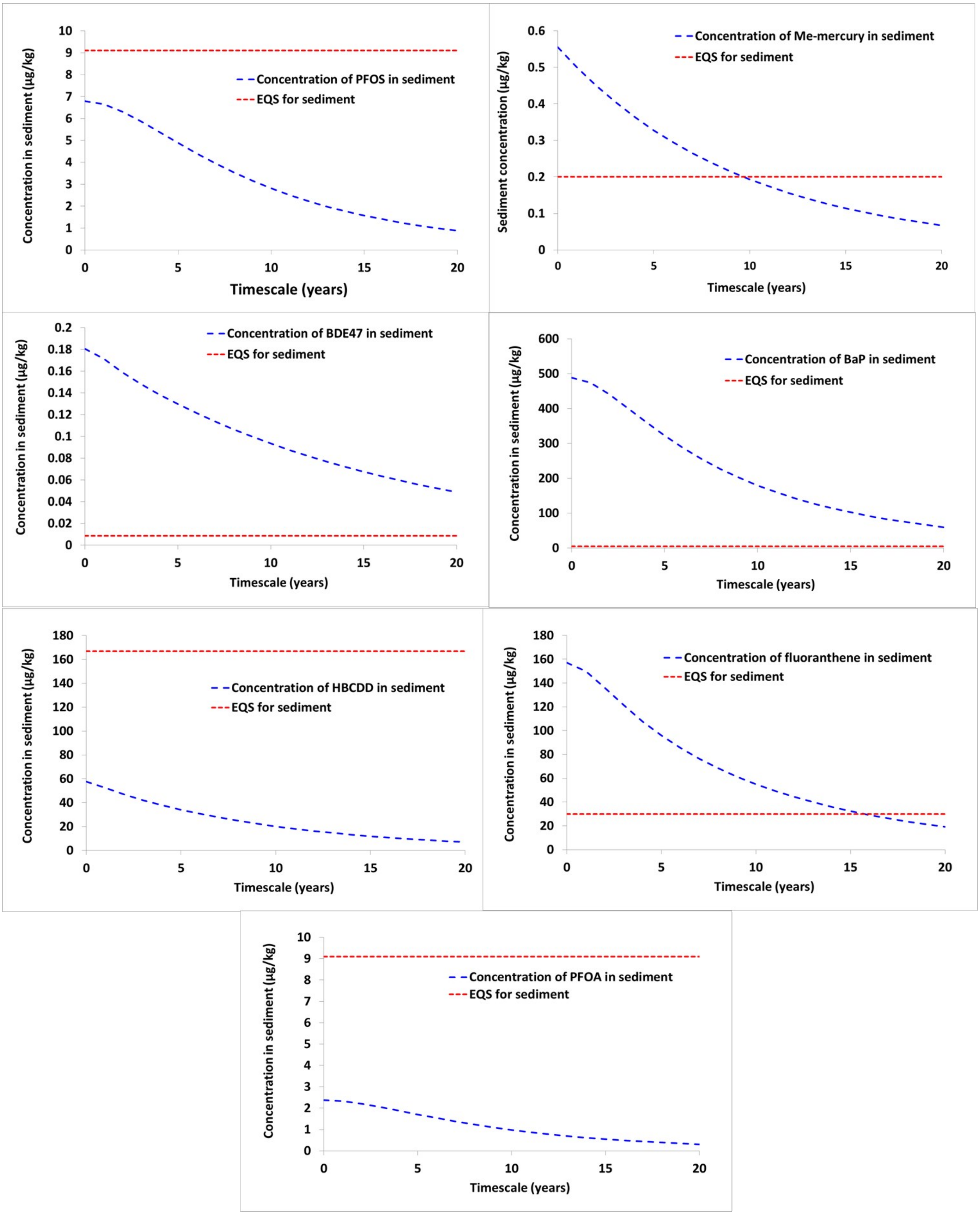

Figure S1 **Illustrations of decline in sediment contaminant concentrations for APR reductions of 10% in both types of inputs (scenario 2)**

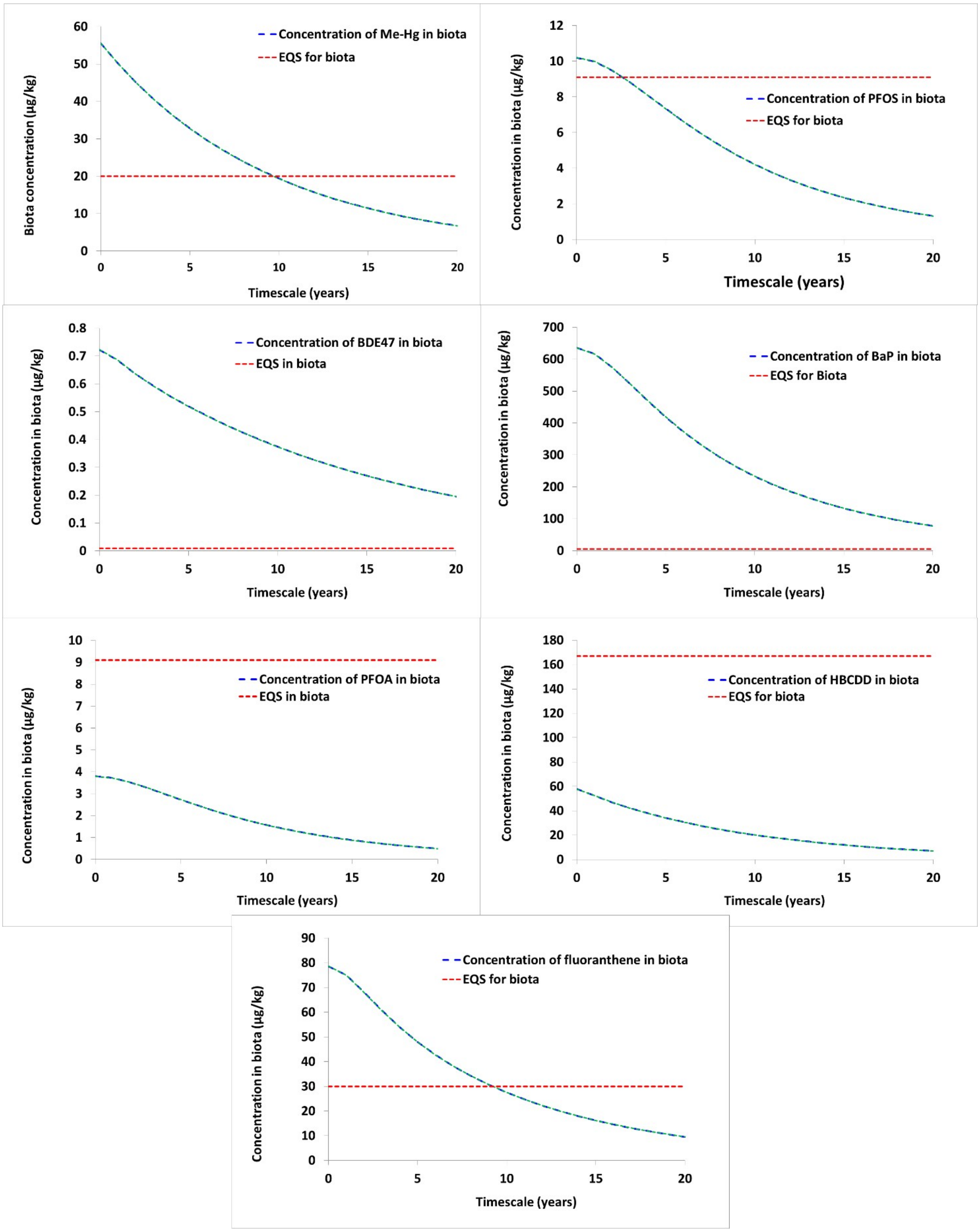

Figure S2 **Illustrations of decline in biota contaminant concentrations for APR reductions of 10% in both types of inputs (scenario 2)**