Supporting information

Applicability of passive sampling to bioanalytical screening of bioaccumulative chemicals in marine wildlife

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Section SI-1: Additional information on linear regression of K_{lipw} and K_{PDMSw} against K_{ow}.

Literature data of K_{lipw} (reviewed by Endo et al.[1]) and K_{PDMSw} (reviewed by DiFilippo et al.[2] plus some recent entries[3, 4]) were sought for linear regression analyses against K_{ow}. For both regression analyses, chemicals with $logK_{ow}$ lower than 2 were excluded due to a leveling off effect. If a chemical has multiple values for the partition coefficients, a geometric mean was taken. The slope of the regression line was fixed at 1 (close to 1 when it was not fixed with similar residual error) (Figure SI-1A). As demonstrated by the regression equations, K_{lipw} is in general 1:1 and K_{PDMSw} 1:10 in relation to hydrophobicity as indicated by octanol-water partition coefficients (K_{ow}) (Figure SI-1B). The difference in intercept between the two parallel lines represents the theoretical value of $logK_{lip\text{-}PDMS}$ (1.01, thus $K_{lip\text{-}PDMS}$ ~10) (Figure SI-1B).

$logK_{lipw}=logK_{ow}+0.14$, n=156, $R^2=0.92$
$logK_{PDMSw}=logKow-0.87$, n=68, $R^2=0.93$

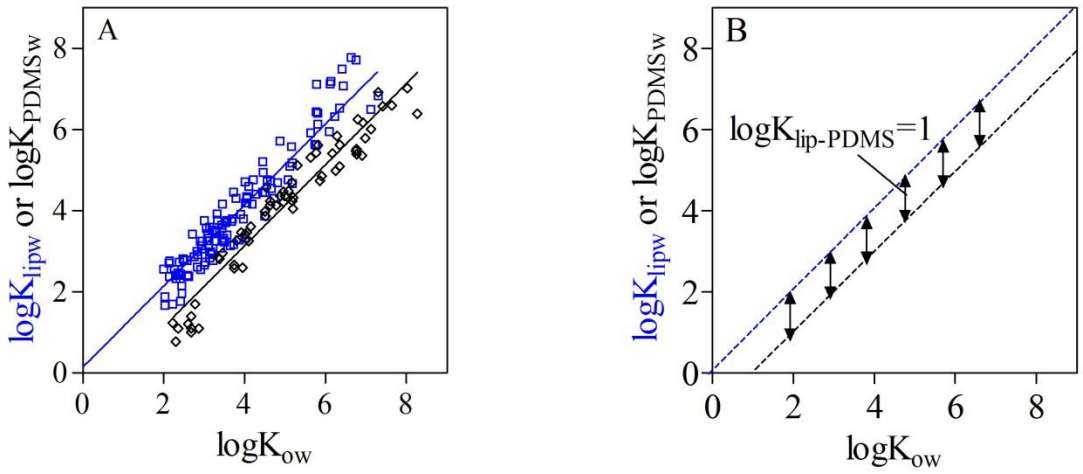


Figure SI-1: A) $logK_{lipw}$ (blue empty square) and $logK_{PDMSw}$ (black empty diamond) in relation to $logK_{ow}$ indicative of hydrophobicity; B) Conceptual figure showing the theoretical relationship between $logK_{lipw}$ and $logK_{ow}$ (1:1 blue dashed line) and between $logK_{PDMSw}$ and $logK_{ow}$ (1:10 black dashed line).

Section SI-2: Additional information on the mathematics of BEQ.

The steps to derive the BEQs from experimental data are summarized in Figure SI-2.

If analytical data are available, BEQ_{chem} is defined as the summation of the instrumentally determined concentration of a chemical (i) multiplied by its REP to a reference compound towards the biological endpoint (equation 2).

$$BEQ_{chem,lip}(ng\ g^{-1}{}_{lip}) = \sum(C_{i,lip} \times REP_i) \quad \text{(SI-1)}$$

$BEQ_{chem,\ lip}$ is the lipid-normalized BEQ_{chem} concentrations of the chemical mixture present in the tissue, $C_{i,lip}$ is the lipid normalized concentration of a chemical and REP_i is the relative effect potency of the chemical in relation to the reference compound if it is assessed in the same assay as the environmental samples are tested.

$$REP_i = \frac{EC_{50}\ (\text{reference compound})\ (ng\ L^{-1})}{EC_{50}\ (i)\ (ng\ L^{-1})} \quad \text{(SI-2)}$$

By substituting equation 2 (main text) into equation SI-2, $BEQ_{chem,\ lip}$ can be back estimated from the BEQ of the chemical mixture fraction transferred into PDMS ($BEQ_{chem,PDMS}$) (equation SI-3) and as $K_{lip\text{-}PDMS}$ is largely independent of hydrophobicity, the geometric mean K (equation SI-4) of all measured $K_{lip\text{-}PDMS,i}$ values can be used to convert $BEQ_{chem,PDMS}$ into $BEQ_{chem,lip}$.

$$BEQ_{chem,lip} = \sum_{i=1}^{n}(C_{i,\ PDMS} \times K_{lip\text{-}PDMS,\ i} \times REP_i) = K\sum_{i=1}^{n}(C_{i,\ PDMS} \times REP_i) = K \times BEQ_{chem,PDMS} \quad \text{(SI-3)}$$

$$K = \sqrt[n]{\prod_{i=1}^{n} K_{lip\text{-}PDMS,\ i}} \quad \text{(SI-4)}$$

The BEQ_{bio} is defined as the concentration of a reference compound that causes the same effect as the sample and can be calculated as the ratio of the EC_{50} of the reference compound to the EC_{50} (in units of concentration factor) of the sample in the bioassay (equation SI-5).

$$BEQ_{bio,PDMS}\,(ng\,g^{-1}{}_{PDMS}) = \frac{EC_{50}\ of\ reference\ compound\,(ng\,L^{-1}{}_{w})}{EC_{50}\ of\ sample\,(g_{PDMS}\,L^{-1}{}_{w})} \qquad (SI\text{-}5)$$

In the present study, the dose metric of a sample (PDMS extract) was the concentration factor (CF), which was defined by equation SI-6.

$$CF\,(g_{PDMS}\,L^{-1}{}_{w}) = \frac{PDMS\ mass\ equivalent\ transferred\ to\ bioassay\,(g)}{volume\ of\ bioassay\,(L)} \qquad (SI\text{-}6)$$

With the constant K, $BEQ_{bio,lip}$ can be deduced from $BEQ_{bio,PDMS}$ analogously to BEQ_{chem} (equation SI-7).

$$BEQ_{bio,lip} = K \times BEQ_{bio,PDMS} \qquad (SI\text{-}7)$$

For validation purposes in the spiked experiments, BEQ_{chem} equals BEQ_{bio} provided that all effect is caused by the spiked chemicals. For samples with unknown composition of pollutants, we can quantitatively estimate the overall mixture effect burden of chemical mixtures present in the biological tissue from screening the fraction extracted by PDMS in *in vitro* bioassays. The difference between BEQ_{chem} and BEQ_{bio} is then a measure of how much unknown AhR inducers are in the sample in addition to the ones quantified with chemical analysis.

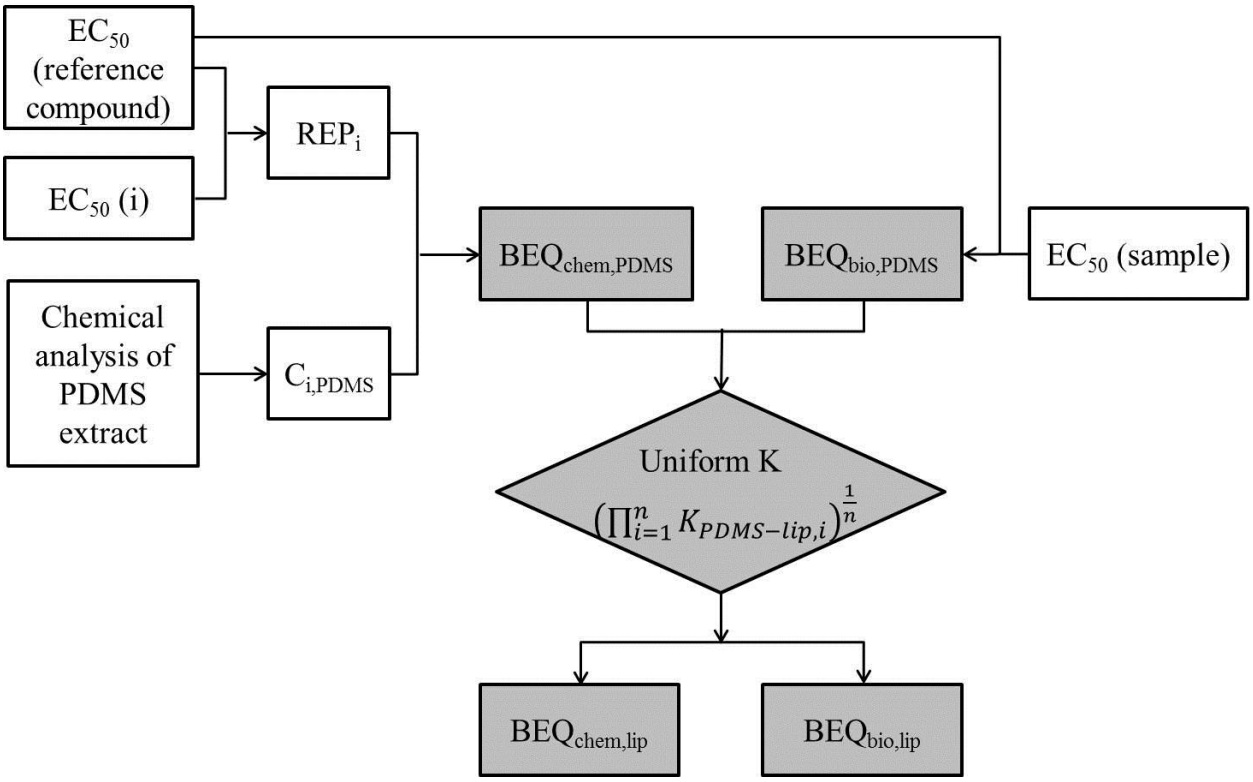


Figure SI-2: Steps of mathematical induction of BEQ.

Section SI-3: Additional information on the lipid content of the tested blubber samples.

The lipid content of the dugong samples used in this study was determined gravimetrically. Briefly, approximately 8 grams of soft blubber and 4 grams of hypodermis were accurately weighed into glass beakers and 40 mL of 4 M HCl was added. The samples were then heated at 70-80˚C for 3-4 hours. The acid digest was liquid-liquid extracted with 100 mL hexane and 150 mL warm water, followed by double extractions with a mix of 50 mL of hexane and 100 mL water. The water fractions were then discarded. The hexane fractions were filtered through sodium sulphate and concentrated on a rotary evaporator to approximately 1 mL. Subsequently, the fraction was transferred to preweighed pear-shaped flasks and further concentrated under a gentle high purity nitrogen stream until the weight was stable, and the percent lipid was calculated.

Table SI-1: Lipid content of the tested blubber samples.

Sample ID	Lipid content (%)
1	11
2	86
3	72
4	68
5	77
6	9.9
7	32
8	72
9	76
10	81
11	91
12*	85

*This blubber sample was used for method validation; all the others for method application.

Section SI-4: Additional information on the procedure and algorithms of the partitioning experiment.

For PDMS→Blubber partitioning experiments, PDMS disks were uploaded with dioxins using a method modified from Endo et al.[4]: PDMS disks (1 mm in thickness, 16 mm in diameter and ~235 mg in weight) were cut from medical grade PDMS sheet (Specialty Silicone Products, Inc. Ballston, Spa, NY, USA), soxhlet cleaned (300 ml hexane followed by 300 mL methanol, for 2 hours each) and air-dried. 87 μL of PCDD stock solution in toluene (5 μg mL^{-1}) (a total mass of 435 ng for each congener) was added to each of six 20 mL glass vials and gently blown down under nitrogen at 40°C. 500 μL methanol was then added to each vial. A single clean PDMS disk was placed in each vial and left overnight on an orbital shaker at 100 rpm at 25°C to allow dissolution and uptake of chemicals into PDMS. The following day Milli-Q water was added in hourly increasing volume (50, 50, 100, 100, 200 and 1000 μL every hour amounting to a total water volume of 1.5 mL) to each vial to force the diffusion of dioxins into PDMS disks, and the vials left overnight on the shaker.

For Blubber→PDMS partitioning experiments, 620 μL of PCDD stock solution (5 μg mL^{-1}) was gently blown down to near dryness under nitrogen at 40°C in an amber glass vial, and taken up in 71 μL in toluene, resulting in a concentration of 43.5 μg mL^{-1}. 16 thin blubber slices (approximately 0.25 g each) were cut, weighed and each of 8 pairs placed in individual wells of a 24-well plate. Three of these pairs were spiked with 10 μL of the concentrated PCDD standard and left overnight for diffusion of the spiked chemicals into the tissue, and evaporation of the solvent. The remaining pairs served as untreated control. The following day, a PDMS disk was

sandwiched between each blubber pair and left for 24 hours. A full mass balance equation (SI-8) was applied to calculate the $K_{lip\text{-}PDMS}$.

$$K_{lip\text{-}PDMS} = \frac{C_{lip}}{C_{PDMS}} = \frac{\frac{m_{PCDD,lipid}}{m_{lipid}}}{\frac{m_{PCDD,PDMS}}{m_{PDMS}}} = \frac{\frac{m_{PCDD,total} - m_{PCDD,PDMS}}{m_{lipid}}}{\frac{m_{PCDD,PDMS}}{m_{PDMS}}} = \frac{\frac{C_{t_0,extract} \cdot V - C_{t_{24},extract} \cdot V}{m_{blubber} \cdot \%lipid}}{\frac{C_{t_{24},extract} \cdot V}{m_{PDMS}}} \quad \text{(SI-8)}$$

Where C_{PDMS} and C_{lip} are the concentration of a dioxin congener in PDMS and lipid, respectively, after 24 hour partitioning, which are calculated by dividing the mass of the dioxin congener in PDMS ($m_{PCDD,PDMS}$) or lipid ($m_{PCDD,lipid}$) by the mass of the corresponding phase m_{PDMS} or m_{lipid}. m_{lipid} is calculated using the blubber slice weight ($m_{blubber}$) and its representative percentage lipid content. Assuming negligible loss of dioxins into other phases (which is justified as the results showed that both directions yielded the same partition coefficient), $m_{PCDD,lipid}$ is the difference between the mass uploaded into PDMS ($m_{PCDD,total}$) and $m_{PCDD,total}$ and $m_{PCDD,PDMS}$ are the product of the concentration of the PDMS extract at the intial time t_0 ($C_{to,extract}$) or after 24 h ($C_{t24,extract}$) and its volume (V).

For the direction from blubber to PDMS, $K_{lip\text{-}PDMS}$ was calculated using equation SI-9:

$$K_{lip\text{-}PDMS} = \frac{C_{lip}}{C_{PDMS}} = \frac{\frac{m_{PCDD,lip}}{m_{lip}}}{\frac{m_{PCDD,PDMS}}{m_{PDMS}}} = \frac{\frac{m_{PCDD,spike} - m_{PCDD,PDMS}}{m_{blubber} \cdot \%lipid}}{\frac{C_{t_{24},extract} \cdot V}{m_{PDMS}}} = \frac{\frac{C_{spike} \cdot V_{spike} - C_{t_{24},extract} \cdot V}{m_{blubber} \cdot \%lipid}}{\frac{C_{t_{24},extract} \cdot V}{m_{PDMS}}} \quad \text{(SI-9)}$$

Where $m_{PCDD,spike}$ represents the mass of a dioxin congener spiked into the blubber, which is calculated by multiplying the spiked concentration (C_{spike}) by the spiked volume (V_{spike}), and the other parameters bear the same meaning of those in eq (SI-1).

Table SI-2: Determination of $K_{lip\text{-}PDMS}$ in the bi-directional partitioning experiment.

PDMS → Blubber		TCDD	PeCDD	HxCDD	HpCDD	OCDD
Concentration in the GC vial (ng μl^{-1})	t0 1	9.1	8.8	9.3	9.2	9.1
	t0 2	8.4	7.5	8.5	8.5	8.3
	t0 3	8.2	7.6	8.1	8.3	8.3
	t24 1	0.15	0.11	0.098	0.089	0.077
	t24 2	0.15	0.092	0.089	0.081	0.089
	t24 3	0.18	0.12	0.11	0.098	0.094
Calculation for concentration in PDMS at t=24 h (m_{PDMS} = 0.236 g)	t24 1 mass in PDMS (ng)	11	7.8	7.4	6.7	5.8
	t24 2 mass in PDMS (ng)	11	6.9	6.6	6.1	6.7
	t24 3 mass in PDMS (ng)	14	8.9	8.6	7.3	7.0
	C_{PDMS} 1 (ng g^{-1})	48	33	31	28	24
	C_{PDMS} 2 (ng g^{-1})	47	29	28	26	28
	C_{PDMS} 3 (ng g^{-1})	57	37	36	31	30
Calculation for concentration in lipid at t=24 h (m_{lipid} = 0.43 g)	t0 1 mass in PDMS (ng)	454	437	462	459	454
	t0 2 mass in PDMS (ng)	419	375	423	424	415
	t0 3 mass in PDMS (ng)	410	378	407	414	413
	Mass depleted into blubber 1 (ng)	416	389	423	426	422
	Mass depleted into blubber 2 (ng)	416	390	424	426	421
	Mass depleted into blubber 3 (ng)	414	388	422	425	421
	C_{lip} 1 (ng g^{-1})	971	907	989	993	984
	C_{lip} 2 (ng g^{-1})	975	913	993	998	986
	C_{lip} 3 (ng g^{-1})	972	911	992	998	987
Calculation for $K_{lip\text{-}PDMS}$ (g_{PDMS} $g^{-1}{}_{lip}$)	$K_{lip\text{-}PDMS}$ 1	20	27	31	35	40
	$K_{lip\text{-}PDMS}$ 2	20	31	35	38	35
	$K_{lip\text{-}PDMS}$ 3	17	24	27	32	33

Table SI-2 (continued)

Blubber → PDMS		TCDD	PeCDD	HxCDD	HpCDD	OCDD
Concentration in the GC vial (ng μl^{-1})	t=24 h 1	0.19	0.14	0.13	0.11	0.10
	t=24 h 2	0.15	0.11	0.092	0.086	0.085
	t=24 h 3	0.15	0.10	0.095	0.082	0.080
Calculation for concentration in PDMS at t=24 h	Mass in PDMS 1 at t=24 h (ng)	14	10	9.7	8.0	7.6
	Mass in PDMS 2 at t=24 h (ng)	12	8.0	6.9	6.5	6.4
	Mass in PDMS 3 at t=24 h (ng)	11	7.5	7.1	6.2	6.0
	C_{PDMS} 1 (ng g^{-1})*	61	34	29	27	27
	C_{PDMS} 2 (ng g^{-1})*	47	43	41	34	32
	C_{PDMS} 3 (ng g^{-1})*	48	32	30	26	26
Calculation for concentration in lipid at t=24 h	Spiked concentration (ng μl^{-1})	48	43	46	45	46
	Mass spiked into blubber (ng)	481	434	457	454	457
	Mass remaining in blubber 1 (ng)	466	471	471	473	473
	Mass remaining in blubber 2 (ng)	469	473	474	474	474
	Mass remaining in blubber 3 (ng)	469	473	474	475	475
	C_{lip} 1 (ng g^{-1})	1,089	1,099	1,100	1,104	1,105
	C_{lip} 2 (ng g^{-1})	1,105	1,113	1,115	1,116	1,117
	C_{lip} 3 (ng g^{-1})	1,101	1,111	1,111	1,113	1,113
Calculation for $K_{lip\text{-}PDMS}$ (g_{PDMS} g^{-1}_{lip})	$K_{lip\text{-}PDMS}$ 1	18	32	37	40	40
	$K_{lip\text{-}PDMS}$ 2	23	25	27	32	34
	$K_{lip\text{-}PDMS}$ 3	22	34	36	42	43

*These three extracts correspond to those in Table SI-5 and 6 and the concentrations of PCDD congeners are used to calculate BEQ_{chem} values

Section SI-5: Additional information on lipid uptake into PDMS.

To understand the uptake of lipid into the PDMS disk, we used a microbalance (smallest scale of 0.001 mg) to monitor the weight change of three PDMS disks throughout the whole procedure of the partition experiment with unspiked blubber slices. To ensure there is no residue remaining on the PDMS surface, PDMS disks were quickly dipped into acetone and wiped with lint-free tissue paper, and the cleaning was repeated three times. As our tested blubber contained 85% lipid content, we assumed that the net weight gain was the amount of lipid that diffused into the PDMS not from other tissue components (proteins, water).

Table SI-3: Weight (mg) change of PDMS throughout the experimental procedure.

	PDMS 1	PDMS 2	PDMS 3
Initial weight	233.69	236.73	234.25
After 24 h contact without wiping	250.80	254.01	255.42
After thorough wiping with acetone	234.91	238.18	235.57
Weight confirmation the following day	234.90	238.17	235.59
Net weight gain	1.21	1.44	1.34
% weight gain	0.51	0.60	0.57

Section SI-6: Additional information on quantification of PCDD/Fs in dugong blubber.

Target analytes were the seventeen 2,3,7,8-substituted PCDD/Fs. Analyses were carried out using a high-resolution gas chromatograph high-resolution mass spectrometer (HRGC-HRMS) at ERGO Forschungsgesellschaft mbH in Germany, which is accredited according to ISO 17025 and regularly participates in interlaboratory studies relating to the analyses of PCDD/Fs in biological tissues, including fish.

Samples were extracted either using a cold extraction (10-40 g ww of lipid poor blubber) or acid digest (1-3 g ww lipid rich blubber) methods. For cold extraction, tissue was homogenized in a stainless steel blender, mixed with anhydrous sodium sulphate to create a free flowing mixture,, extracted ultrasonically with a mixture of n-hexane/acetone (1:1, v:v) and concentrated. Acid digestion was carried out in 150 mL of 4 molar HCl at 60 °C for 2-4 hours, followed by triplicate liquid:liquid extraction in hexane:water (1:3, v:v); extracts were then filtered through ~3 g Na_2SO_4 and concentrated. Approximately 1-3 g of yielded lipid was spiked with quantification standards (internal standards) using all PCDD/F analytes as ^{13}C-labeled compounds, except for 1,2,3,7,8,9-HexaCDD (1,2,3,6,7,8-HexaCDD was used).

The clean-up consisted of a sulfuric acid coated silica gel (~6-12 g) pre-treatment, followed by fractionation on active carbon (Supelco SupelcleanTM ENVI-Carb SPE tube). PCDD/Fs were eluted with 50 mL toluene in the reverse direction. This was followed by chromatography with a combination of columns using cesium coated silica gel, sulfuric acid coated silica gel followed by alumina (elution with 25 mL hexane:DCM (1:1, v:v)) and florisil (elution with 120 mL toluene). The fractions were evaporated and a set of four ^{13}C-PCDD/Fs were added as injection

standards. Analytical measurement was performed by HRGC/HRMS on a Waters Autospec HRMS at mass resolution R ⩾ 10,000 equipped with a DB5ms-type fused silica column (60m × 0.32mm i.d. × 0.25μm dF). Quantification was carried out by isotope dilution against daily calibration points together with a multipoint calibration.

For quality control, method blanks were run with each sample batch to monitor for possible background contamination. Reference materials (routinely run in-house pooled fish oil) were regularly monitored to test reproducibility.

Analytes were accepted for quantification if their retention times were within 2 seconds of the retention times of the relevant labelled internal standards and the ratios for the area of the two most abundant isotopes were within 20% of their calculated values. The limit of quantification (LOQ) for PCDD/F was defined as a signal–to-noise ratio greater than 3 times the average baseline variation. BEQ_{chem} of each sample was calculated using CAFLUX-derived REP values.

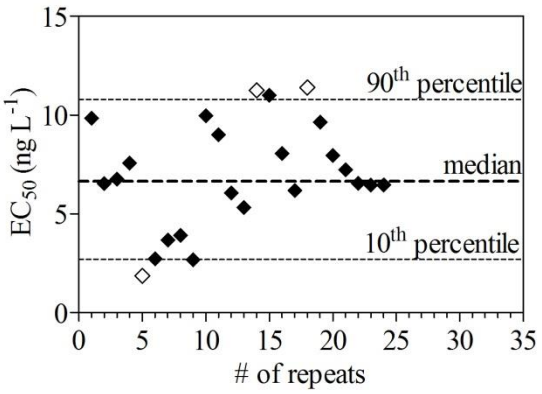


Figure SI-3: Long-term record of EC_{50} of the reference compound, TCDD. The filled diamonds are the valid repeats and the empty diamonds are the repeats that were excluded.

Section SI-7: Error propagation.

Error was propagated for EC_{50} and REP of each PCDD congener and BEQ_{chem} and BEQ_{bio} of samples using the following equations (SI-9-12). The standard error of $logEC_{50}$ for each compound and sample was initially provided in the sigmoidal curve fitting and given to propagate the error for REP and BEQ according to their mathematical relationships.

$$\sigma REP_i = \sigma 10^{logREP_i} = \sigma 10^{logEC_{50}(TCDD) - logEC_{50}(i)}$$

$$= logREP_i \times ln10 \times \sqrt{\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(TCDD)\right)^2}$$

$$= lnREP_i \times \sqrt{\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(TCDD)\right)^2} \quad \text{(SI-9)}$$

$$\sigma BEQ_{chem} = \sigma \sum (C_i \times REP_i) = \sqrt{\sum \left(\frac{\partial (C_i \times REP_i)}{\partial REP_i} \times \sigma REP_i\right)^2} = \sqrt{\sum (C_i \times \sigma REP_i)^2}$$

$$= \sqrt{\sum \left(C_i \times lnREP_i \times \sqrt{\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(i)\right)^2}\right)^2}$$

$$= \sqrt{\sum \left({C_i}^2 \times ln^2 REP_i \times \left(\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(i)\right)^2\right)\right)} \quad \text{(SI-10)}$$

$$\sigma BEQ_{bio,PDMS} = \sigma \left(\frac{EC_{50}(TCDD)}{EC_{50}(sample)}\right) = \sigma \left(10^{logEC_{50}(TCDD) - logEC_{50}(sample)}\right)$$

$$= \sqrt{\begin{array}{l} \left(\frac{\partial (10^{logEC_{50}(TCDD) - logEC_{50}(sample)})}{\partial logEC_{50}(TCDD)} \times \sigma logEC_{50}(TCDD)\right)^2 \\ + \left(\frac{\partial (10^{logEC_{50}(TCDD) - logEC_{50}(sample)})}{\partial logEC_{50}(sample)} \times \sigma logEC_{50}(sample)\right)^2 \end{array}}$$

$$= \sqrt{\left(logBEQ_{bio,PDMS} \times ln10 \times \sigma logEC_{50}(TCDD)\right)^2 + \left(-logBEQ_{bio,PDMS} \times ln10 \times \sigma logEC_{50}(sample)\right)^2}$$

$$= lnBEQ_{bio,PDMS} \times \sqrt{\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(sample)\right)^2} \quad \text{(SI-11)}$$

$$\sigma BEQ_{bio,lip} = \sigma\left(K_{lip-PDMS} \times BEQ_{bio,PDMS}\right)$$

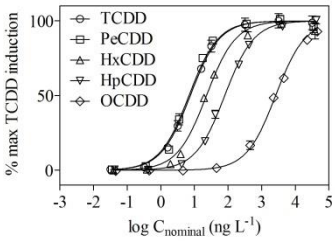
$$= \sqrt{\begin{array}{c}\left(\frac{\partial\left(K_{lip-PDMS} \times BEQ_{bio,PDMS}\right)}{\partial K_{lip-PDMS}} \times \sigma K_{lip-PDMS}\right)^2 \\ +\left(\frac{\partial\left(K_{lip-PDMS} \times BEQ_{bio,PDMS}\right)}{\partial BEQ_{bio,PDMS}} \times \sigma BEQ_{bio,PDMS}\right)^2\end{array}}$$

$$= \sqrt{\begin{array}{c}\left(BEQ_{bio,PDMS} \times \sqrt{\sum_{i=1}^{n}\left(\frac{\partial\left(\prod_{i=1}^{n} K_{lip-PDMS,i}\right)}{\partial K_{lip-PDMS,i}} \times \sigma K_{lip-PDMS,i}\right)^2}\right)^2 \\ +\left(K_{lip-PDMS} \times lnBEQ_{bio,PDMS} \times \sqrt{\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(sample)\right)^2}\right)^2\end{array}}$$

$$= \sqrt{\begin{array}{c}BEQ_{bio,PDMS}^2 \times \sum_{i=1}^{n}\left(\frac{\left(\prod_{i=1}^{n} K_{lip-PDMS,i}\right)^{\left(\frac{1}{n}-1\right)}}{n} \prod_{i=1}^{m-1} K_{lip-PDMS,i} \prod_{i=m+1}^{n} K_{lip-PDMS,i}\, \sigma K_{lip-PDMS,i}\right)^2 \\ +K_{lip-PDMS}^2 \times ln_{bio,PDMS}^2 \times \left(\left(\sigma logEC_{50}(TCDD)\right)^2 + \left(\sigma logEC_{50}(sample)\right)^2\right)\end{array}}$$

(SI-12)

Table SI-4: Combined concentration-response curves (n=21 for TCDD and n=4 for the other congeners) and EC_{50} and REP values of each PCDD congener.

Concentration-response curve	Congener	EC_{50} (ng L^{-1}) (95% CI)	REP (±standard error)*
	TCDD	7.7 (7.4-8.0)	1.0±0.1
	PeCDD	6.9 (6.0-7.9)	1.1±0.2
	HxCDD	22 (19-26)	0.3±0.01
	HpCDD	80 (73-87)	0.09±0.00
	OCDD	2613 (2398-2847)	0.002±0.000

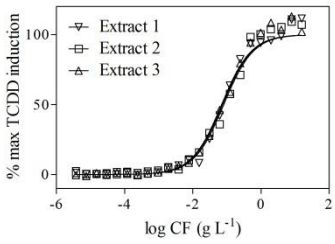
*calculated by error propagation (Section SI-7, equation SI-9).

Table SI-5: BEQ_{chem} derivation of the triplicate PDMS extracts from spiked blubber.

Extract	BEQ_{chem} of each congener (ng g^{-1}_{PDMS})*					BEQ_{chem} (ng g^{-1}_{PDMS}) (±standard error)#	Average (ng g^{-1}_{PDMS}) (±standard error)
	TCDD	PeCDD	HxCDD	HpCDD	OCDD		
1	49	41	9	2.7	0.1	101±20	109±20
2	61	52	12	3.4	0.1	128±25	
3	48	38	9	2.6	0.1	98±19	

*calculated using the concentrations in Table SI-2 and REPs in Table SI-4.
#calculated by error propagation (Section SI-7, equation SI-10).

Table SI-6: Concentration-response curves and BEQ_{bio} derivation of the triplicate PDMS extracts from spiked blubber.

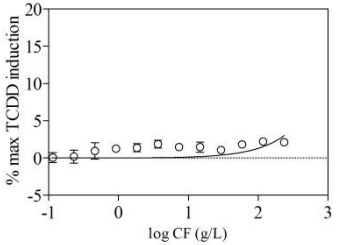
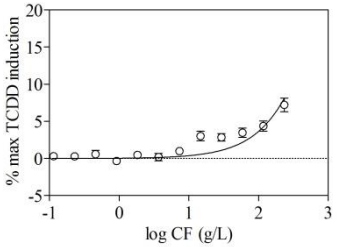
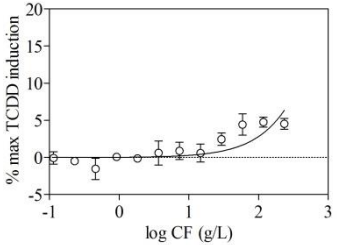
Extract	Concentration-response curve	EC_{50} (CF (g L^{-1})) (95% CI)	BEQ_{bio} (ng g^{-1}_{PDMS}) (±standard error)*	Average (ng g^{-1}_{PDMS}) (±standard error)
1		0.074 (0.061-0.091)	108±5	108±8
2		0.069 (0.056-0.085)	115±7	
3		0.080 (0.064-0.010)	100±2	

*calculated by error propagation (Section SI-7, equation SI-11).

Section SI-8: Additional information on concentration-response curves of dugong sample extracts and derivation of method detection limit, EC_{50} and BEQ.

The method detection limit (MDL) was calculated against the dose-response curve of TCDD standard. Detectable response in the bioassay (7.2%) was defined as three times of the percentage induction of controls (2.4%). Based on the sigmoidal dose-response curve averaged for all 21 replicates that were determined during the course of the study (Table SI-4 with the equation: % max TCDD induction = $100 / (1+10^{(0.8882\text{-log Cnominal})})$). The detection limit of the bioassay was calculated to be 0.6 ng L^{-1}. The detectable mass was thus 0.06 pg TCDD equivalent in a 100 µL well, which is transferred from lipid into PDMS equivalent to half a disk mass (approx. 0.235 g per PDMS), as we splitted each sample extract from one PDMS disk in half to have the optimal lipid amount that does not interfere with CAFLUX. The concentration of 0.5 pg g^{-1}_{PDMS} was then converted to the bioanalytical method detection limit of 15 pg g^{-1}_{lip} in the dugong blubber by applying the generalized $K_{lip\text{-}PDMS}$ of 30.

Table SI-7: Concentration-response curves (n=6) and BEQ derivations of dugong blubber samples.

Sample ID	Concentration-response curve	Significantly higher than PDMS blank?	R^2	EC_{50} ($g\ L^{-1}$)	$BEQ_{bio,\ PDMS}$ ($pg\ g^{-1}_{PDMS}$)	> detection limit of 0.5 $pg\ g^{-1}_{PDMS}$?	$BEQ_{bio,lip}$ ($pg\ g^{-1}_{lip}$) (±standard error)	$BEQ_{chem,lip}$ ($pg\ g^{-1}_{lip}$) (±standard error)
PDMS blank		N/A	N/A	N/A	N/A	N/A	N/A	N/A
1		Yes	0.5853	2658	2.9	Yes	81±20	18±4
2		Yes	0.2849	3466	2.2	Yes	62±15	45±9

*Section SI-7, equation SI-12; #Section SI-7, equation SI-11.

Table SI-7 (continued)

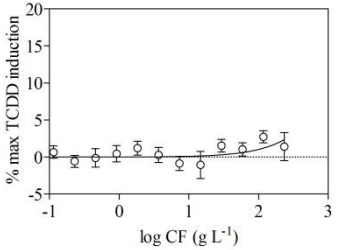
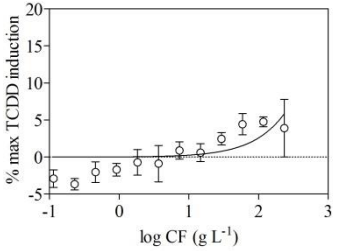
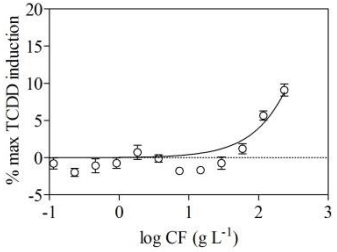
Sample ID	Concentration-response curve	Significantly higher than PDMS blank?	R^2	EC_{50} (g L^{-1})	$BEQ_{bio,PDMS}$ (pg g^{-1}_{PDMS})	> detection limit of 0.5 pg g^{-1}_{PDMS}?	$BEQ_{bio,lip}$ (pg g^{-1}_{lip}) (±standard error)*	$BEQ_{chem,lip}$ (pg g^{-1}_{lip}) (±standard error)#
3		No	N/A	N/A	N/A	N/A	N/A	5.7±1.1
4		No	N/A	N/A	N/A	N/A	N/A	13±2.7
5		Yes	0.6605	2433	3.2	Yes	89±21	53±11

Table SI-7 (continued)

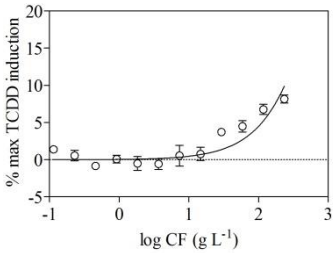
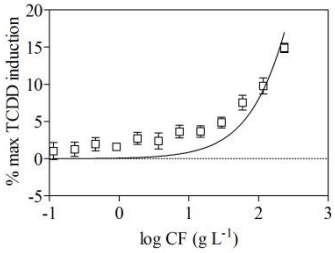
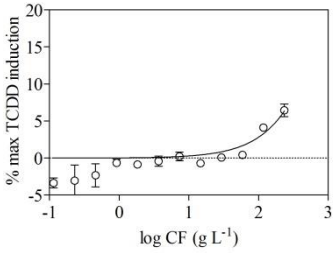
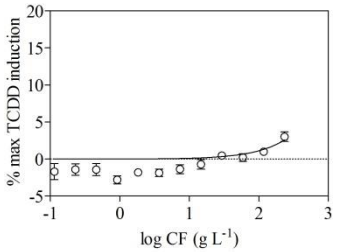
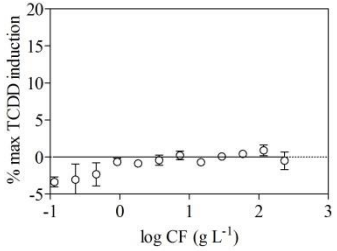
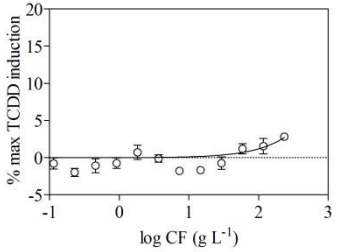
Sample ID	Concentration-response curve	Significantly higher than PDMS blank?	R^2	EC_{50} ($g\ L^{-1}$)	$BEQ_{bio,PDMS}$ ($pg\ g^{-1}_{PDMS}$)	> detection limit of 0.5 $pg\ g^{-1}_{PDMS}$?	$BEQ_{bio,lip}$ ($pg\ g^{-1}_{lip}$) (±standard error)	$BEQ_{chem,lip}$ ($pg\ g^{-1}_{lip}$) (±standard error)
6		Yes	0.6144	2140	3.6	Yes	101±25	92±18
7		Yes	0.5886	1152	6.7	Yes	188±45	259±52
8		Yes	0.4068	3475	2.2	Yes	62±14	26±5

Table SI-7 (continued)

Sample ID	Concentration-response curve	Significantly higher than PDMS blank?	R^2	EC_{50} ($g\ L^{-1}$)	$BEQ_{bio,PDMS}$ ($pg\ g^{-1}$)	> detection limit of 0.5 $pg\ g^{-1}_{PDMS}$?	$BEQ_{bio,lip}$ ($pg\ g^{-1}_{lip}$) (±standard error)	$BEQ_{chem,lip}$ ($pg\ g^{-1}_{lip}$) (±standard error)
9		No	N/A	N/A	N/A	N/A	N/A	2.4±0.5
10		No	N/A	N/A	N/A	N/A	N/A	14±2.9
11		No	N/A	N/A	N/A	N/A	N/A	10±2.1

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