

Supporting information

Toxicokinetics of crude oil components in Arctic copepods

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Figure S 2. Microscopy images of lipid-rich (CV, left) and lipid-poor (CIII, right) *Calanus hyperboreus*. Regions of interest (ROI) are indicated; the prosome outline in yellow, the lipid sack in red. Note different scale on the images.

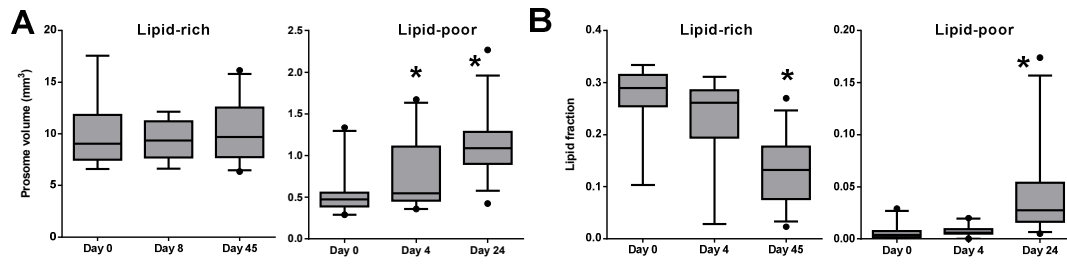


Figure S 3. Prosome volume (mm^3 , A) and the lipid sac volume fraction (B) of lipid-rich and lipid-poor *Calanus hyperboreus* from the control groups before (day 0) and at the end of the exposure period (day 4 or 8), and at the end of the recovery period (day 45 or 24). Median, 25/75% box, 95% CI, range. * indicate significant difference from day zero (ANOVA, TukeyHSD, $p < 0.05$). Note different scales on the y-axis.

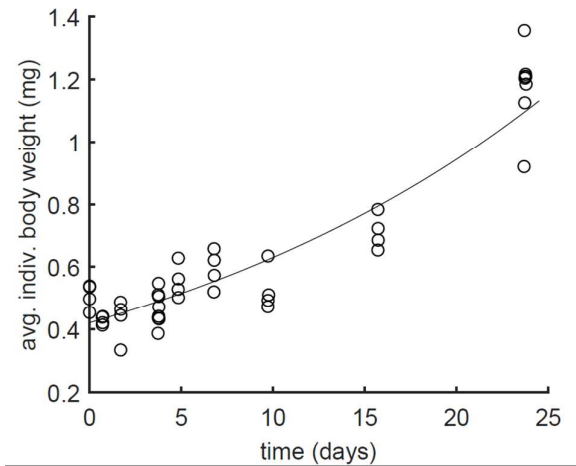


Figure S 4. Average body weight of *Calanus hyperboreus* stage CIII/CIV sampled for body residue analysis of oil components at intervals over 25 days. The log-linear regression for $t \geq 0$ d gives a growth rate of $0.040/\text{d}$ ($R^2 = 0.857$).

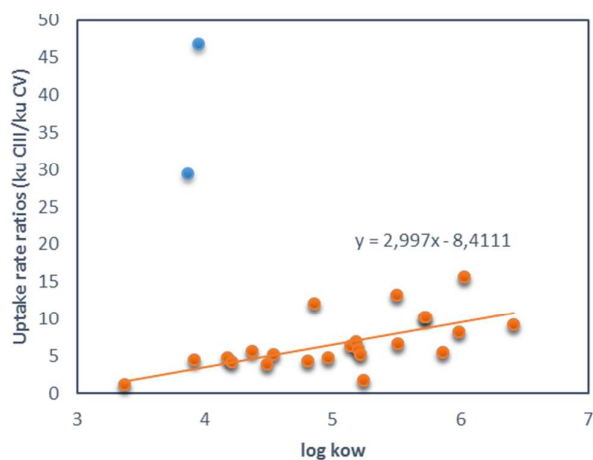


Figure S 5. Oil component uptake rate (k_u) ratios between lipid-rich (CV) and lipid-poor (CIII) *Calanus hyperboreus* as function of $\log K_{OW}$. The outliers (N1 and B) are not included in the regression.

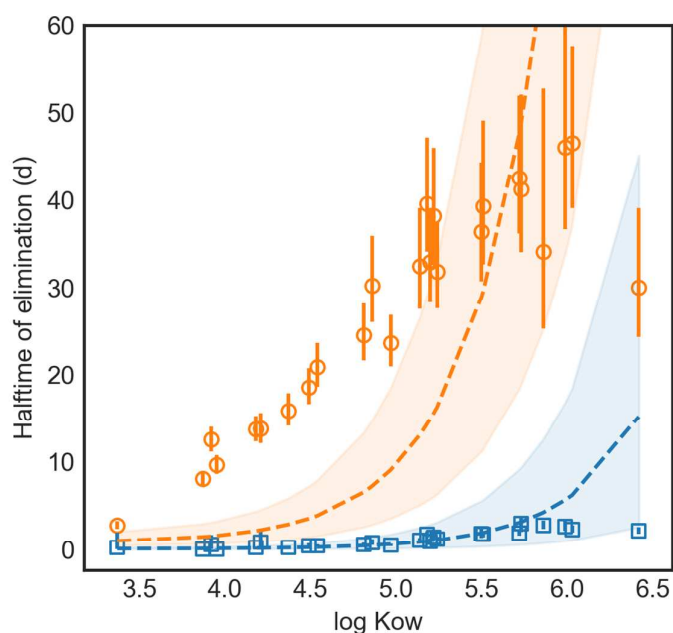


Figure S6. Half-time of elimination ($T_{1/2}$, days) as function of octanol-water partitioning coefficients ($\log K_{OW}$) for 26 oil components in lipid-rich CV (orange circles) and lipid-poor CIII (blue squares) *C. hyperboreus* exposed to the water-soluble fraction (WFS) of crude oil. $T_{1/2}$ is calculated from the model parameter k_e : $T_{1/2} = \ln 2/k_e$. Error bars: 95% CI from the MCMC posterior, see section 2.4. The lines are predictions from the OMEGA model for the mean weight (0.5 and 12.5 mg) and estimated lipid content (5% and 28%) of the two stages. Shaded area indicates the realistic range for each stage in the present study (CIII: weight 0.1 – 1, lipid: 1 – 10%; CV: weight 1-20 mg, lipid: 20 – 50%).

Text section 2: Chemical analyses – detailed description

Exposure characterization, water samples

Samples of exposure media were analysed for volatile organic compound (VOC, 40 mL, n=48; Table S 2), semi volatile organic compound (SVOC, 800 mL, n=48; Table S3), and total extractable material (TEM). VOC in the C₅ to C₁₀ range (n=35) were determined by Purge and Trap (P&T) GC/MS using a modification of EPA method 8260C (US EPA,²¹ SI: Table S 2). The samples were spiked with SIS (toluene-*d*₈ and ethylbenzene-*d*₈) and RIS (chlorobenzene-*d*₅). The quantification of individual compounds was performed by using the RFs of the individual compounds relative to the internal standards. All standards and samples were analysed in a full scan mode. SVOC in the exposure media (800 mL, n=24 in each experiment) were determined by GC/FID (gas chromatography/flame ionization detection) and GC/MS (gas chromatography/mass spectrometry) following a modified EPA Method 8270D (US EPA,²² SI: Table S3). Surrogate internal standards (SIS; o-terphenyl, naphthalene-*d*₈, phenanthrene-*d*₁₀, chrysene-*d*₁₂, phenol-*d*₆, 4-methylphenol-*d*₈) were added to each sample prior to serial extraction with dichloromethane (45-30-30 mL). The combined extracts were dried with sodium sulphate and concentrated to approximately 1 mL, before addition of recovery internal standard (RIS; 5 α -androstane, fluorene-*d*₁₀, and acenaphthene-*d*₁₀). The mass spectrometer was operated in the selective ion monitoring mode to achieve optimum sensitivity and specificity. The quantification of target compounds was performed by the method of internal standards, using average response factors (RF) for the parent compounds. The PAH and phenol alkyl homologues were quantified using the straight baseline integration of each level of alkylation and the RF for the respective parent PAH compound. The response factors were generated for all targets and surrogates versus fluorene-*d*₁₀.

TEM in dichloromethane extracts of water samples (the same as for SVOC analyses) were measured using GC/FID according to a modification of US EPA Method 8100²³. Resolved and unresolved (Figure S 7) total petroleum hydrocarbon (TPH; C₁₀–C₃₆) were quantified by the method of internal standards using the baseline-corrected total area of the chromatogram and the average response factor (RF) for the individual C₁₀ to C₃₆ n-alkanes.

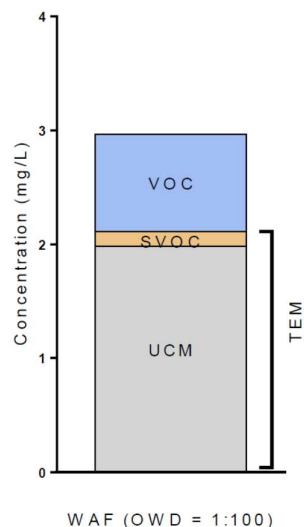


Figure S 7. Composition of fresh 100% WAF of Troll 200°C+ residue. TEM; total extractable material (C9 - C36), UCM; unresolved complex material, SVOC; resolved semi-volatile organic components > C9, VOC; resolved volatile organic components.

Body residue analyses

Extraction of organic compound from homogenate of *Calanus hyperboreus* was performed as described in Sørensen *et al.*²⁴ After transfer to glass vials and addition of surrogate standards (naphthalene-*d*8, phenanthrene-*d*10, chrysene-*d*12 and perylene-*d*12, 100 ng/g sample), the samples were homogenized in *n*-hexane-dichloromethane (1:1 v/v, 2 mL) using a microprocessor, followed by addition of sodium sulphate (150 mg), vortex extraction (30 s) and centrifugation (2000 rpm, 2 min). The supernatant was collected and the extraction step was repeated two additional times. The combined organic extract was concentrated to ~1 mL prior to clean-up by solid phase extraction (SPE) using silica (Agilent Bond Elut SI, 500 mg, Agilent Technologies, USA). The extract was eluted with dichloromethane in *n*-hexane (1:9, v/v, 6 mL). Immediately prior to the analysis, the volume of the cleaned extract was reduced to 100 µL under a gentle stream of N₂ and spiked with recovery standard (fluorene-*d*10, 100 ng/g sample). Laboratory blank samples (empty vials) were included in the extraction daily. Background levels of PAHs identified in laboratory blanks were subtracted from the samples.

Text section 3: Toxicokinetic model and body residue calculations

Uptake of dissolved organic compounds from the water phase into tissue of an aquatic organism (body residue) is traditionally modelled using a one-compartment model by a rate equation containing an uptake and a depuration term:

$$\frac{dC_i}{dt} = k_u C_w - k_e C_i(t) \quad (\text{Eq. S1})$$

where t is time (days), C_w is the ambient concentration (mg/L), $C_i(t)$ is the concentration in tissue (body residue, mg/kg wet weight), k_u is the uptake rate (L/kg/day), k_e is the elimination rate (1/day). This formulation uses two rates, while the alternative formulation uses one rate (k_e) and the partition coefficient between internal and water (P_{iw} , equal to the bioconcentration factor), and they are related via

$$P_{iw} = \frac{k_u}{k_e} \quad (\text{Eq. S2})$$

To account explicitly for measurable properties of the individual, such size and fat, we use a formulation of the uptake rate as proposed by Hendriks *et al*¹,

$$k_u = \frac{w^{-\kappa}}{\rho_0 + \frac{\rho_1}{K_{OW}}} \quad (\text{Eq. S3})$$

where w = wet weight of organism (kg), $\kappa=0.25$ is a shape factor, and K_{OW} is the octanol-water partition coefficient. In addition, the lipid layer permeation resistance $\rho_1 = 68$ (day·kg^{-κ}), and water layer diffusion resistance $\rho_0 = 0.0023$ (day·kg^{-κ}) are defined, with values taken from De Hoop *et al.*¹. The depuration rate is given by^{1, 2}:

$$k_e = \frac{k_u}{f_L(K_{OW}-1)+1} \quad (\text{Eq. S4})$$

where f_L is the lipid content of the organism (volume fraction). For high K_{OW} , the denominator of this equation, which is P_{iw} , reduces to $f_L \times K_{OW}$. If the water concentrations remain constant over time, Eq. S1 can be integrated analytically to give an explicit expression for $C_i(t)$,

$$C_i(t) = C_w P_{iw} (1 - e^{-k_e t}) + C_i(0) e^{-k_e t} \quad (\text{Eq. S5})$$

For sufficiently long exposure time, that is $t \rightarrow \infty$, Eq. S5 reduces to

$$\lim_{t \rightarrow \infty} C_i(t) = P_{iw} \times C_w \quad (\text{Eq. S6})$$

1. Hendriks, J.; van der Linde, A.; Cornelissen, G.; Sijm, D., The power of size. 1. Rate constants and equilibrium ratios for accumulation of organic substances related to octanol-water partition ratio and species weight. *Environmental Toxicology and Chemistry* **2001**, *20*, (7), 1399-420.

2. de Hoop, L.; Schipper, A. M.; Leuven, R.; Huijbregts, M. A. J.; Olsen, G. H.; Smit, M. G. D.; Hendriks, A. J., Sensitivity of Polar and Temperate Marine Organisms to Oil Components. *Environmental Science & Technology* **2011**, *45*, (20), 9017-9023.

Table S 2. Volatile organic compounds (VOC) with limit of quantification (LOQ) in µg/L for detection in seawater samples.

Component	LOQ
Isopentane	0.0058
n-C5 (Pentane)	0.0420
Cyclopentane	0.0168
2-methylpentane	0.0090
3-Methylpentane	0.0145
n-C6 (Hexane)	0.0222
Methylcyclopentane	0.0109
Benzene	0.0275
Cyclohexane	0.0185
2.3-Dimethylpentane	0.0048
3-methylhexane	0.0044
n-C7 (Heptane)	0.0224
Methylcyclohexane	0.0192
Toluene	0.0173
2.4 dimethylhexane	0.0045
2-Methylheptane	0.0116
n-C8 (Octane)	0.0226
Ethylbenzene	0.0252
m-Xylene	0.0083
p-Xylene	0.0178
o-Xylene	0.0083
n-C9 (Nonane)	0.0231
Propylbenzene	0.0160
1-Methyl-3-ethylbenzene	0.0080
1-Methyl-4-ethylbenzene	0.0072
1.3.5-Trimethylbenzene	0.0040
1-Methyl-2-ethylbenzene	0.0081
1.2.4-Trimethylbenzene	0.0090
n-C10 (Decane)	0.0230
1.2.3-Trimethylbenzene	0.0100
n-Butylbenzene	0.0077
1.2.4.5-Tetramethylbenzene	0.0008
n-Pentylbenzene	0.0156
C4-Benzenes	0.0000
C5-Benzenes	0.0000

Table S3. Semi-volatile organic compounds (SVOC) with abbreviation and limit of quantification (LOQ) in µg/L for detection in seawater samples. LOQ for parent compounds are used when not determined (ND)

Component	Abb.	LOQ	Component	Abb.	LOQ
Decalin	DE	0.0035	Fluoranthene	FL	0.0033
C1-decalins	DE1	ND	Pyrene	PY	0.0032
C2-decalins	DE2	ND	C1-fluoranthrenes/pyrenes	FL1	ND
C3-decalins	DE3	ND	C2-fluoranthrenes/pyrenes	FL2	ND
C4-decalins	DE4	ND	C3-fluoranthrenes/pyrenes	FL3	ND
Benzo(b)thiophene	BT	0.0030	Benz(a)anthracene	BA	0.0030
Naphthalene	N	0.0066	Chrysene	C	0.0035
C1-naphthalenes	N1	0.0032	C1-chrysenes	C1	ND
C2-naphthalenes	N2	0.0018	C2-chrysenes	C2	ND
C3-naphthalenes	N3	0.0022	C3-chrysenes	C3	ND
C4-naphthalenes	N4	ND	C4-chrysenes	C4	ND
Biphenyl	B	0.0032	Benzo(b)fluoranthene	BBF	0.0033
Acenaphthylene	ANY	0.0029	Benzo(k)fluoranthene	BKF	0.0031
Acenaphthene	ANA	0.0029	Benzo(e)pyrene	BEP	0.0028
Dibenzofuran	DBF	0.0027	Benzo(a)pyrene	BAP	0.0026
Fluorene	F	0.0032	Perylene	PE	0.0023
C1-fluorenes	F1	0.0026	Indeno(1.2.3-c.d)pyrene	IN	0.0038
C2-fluorenes	F2	ND	Dibenz(a.h)anthracene	DBA	0.0042
C3-fluorenes	F3	ND	Benzo(g.h.i)perylene	BPE	0.0034
Phenanthrene	P	0.0049	Phenol	PH	ND
Anthracene	A	0.0027	C1-Phenols (o- og p-cresol)	PH1	ND
C1-phenanthrenes/anthracenes	P1	0.0030	C2-Phenols	PH2	ND
C2-phenanthrenes/anthracenes	P2	0.0028	C3-Phenols	PH3	ND
C3-phenanthrenes/anthracenes	P3	ND	C4-Phenols	PH4	ND
C4-phenanthrenes/anthracenes	P4	ND	C5-Phenols	PH5	ND
Dibenzothiophene	D	0.0028	30 ab hopane	HOP	ND
C1-dibenzothiophenes	D1	ND			
C2-dibenzothiophenes	D2	0.0019			
C3-dibenzothiophenes	D3	ND			
C4-dibenzothiophenes	D4	ND			

Table S 4. Target compounds for body residue analyses with limit of detection (LOD) and limit of quantitation (LOQ) in µg/mL extract calculated based on measurements of laboratory and matrix blank samples (n=6 of each). LOD=average + 3 standard deviations of the blanks. LOQ=3*LOD.¹

Compound	LOD	LOQ	Compound	LOD	LOQ
Decalin	0.032	0.097	Dibenzothiophene	0.0013	0.0040
C1-decalins	0.062	0.19	C1-dibenzothiophenes	0.017	0.051
C2-decalins	0.084	0.25	C2-dibenzothiophenes	0.017	0.052
C3-decalins	0.041	0.12	C3-dibenzothiophenes	0.021	0.062
C4-decalins	0.15	0.45	C4-dibenzothiophenes	0.066	0.198
Benzo(b)thiophene	0.0031	0.0092	Fluoranthene	0.0067	0.020
Naphthalene	0.0079	0.024	Pyrene	0.0050	0.015
C1-naphthalenes	0.038	0.11	C1-fluoranthrenes/pyrenes	0.024	0.072
C2-naphthalenes	0.10	0.30	C2-fluoranthrenes/pyrenes	0.013	0.038
C3-naphthalenes	0.066	0.20	C3-fluoranthrenes/pyrenes	0.018	0.055
C4-naphthalenes	0.86	0.26	Benz(a)anthracene	0.00049	0.0015
Biphenyl	0.0024	0.0073	Chrysene	0.0022	0.0065
Acenaphthylene	0.0034	0.010	C1-chrysenes	0.0031	0.0092
Acenaphthene	0.0054	0.016	C2-chrysenes	0.0083	0.025
Dibenzofuran	0.0249	0.075	C3-chrysenes	0.014	0.042
Fluorene	0.0032	0.0097	C4-chrysenes	0.046	0.14
C1-fluorenes	0.0048	0.014	Benzo(b)fluoranthene	0.0018	0.0053
C2-fluorenes	0.033	0.10	Benzo(k)fluoranthene	0.00072	0.0022
C3-fluorenes	0.020	0.061	Benzo(e)pyrene	0.0011	0.0033
Phenanthrene	0.0068	0.020	Benzo(a)pyrene	0.00086	0.0026
Anthracene	0.0021	0.0062	Perylene	0.00041	0.0012
C1-phenanthrenes/anthracenes	0.0054	0.016	Indeno(1.2.3-c.d)pyrene	0.00072	0.0022
C2-phenanthrenes/anthracenes	0.013	0.040	Dibenz(a,h)anthracene	0.00013	0.00040
C3-phenanthrenes/anthracenes	0.016	0.047	Benzo(g,h,i)perylene	0.00041	0.0012
C4-phenanthrenes/anthracenes	0.078	0.23	30 ab hopane	0.11	0.33

¹ Method validation: Spiked samples in the range 0.00001-0.1 µg/sample (~0.0006-6 µg/g wet weight copepod) were extracted and analysed to evaluate the linearity of the method. For the matrix blank, 20 un-exposed animals were used (average total wet weight 17 mg). The method gave a linear relationship between spiked and extracted values in the range 0.001-0.1 µg/sample (~0.06-6 µg/g wet weight). For most parent PAHs, linearity was observed down to 0.0001 µg/sample (~0.006 µg/g wet weight). Precision at the three highest spike levels was good (<20 % RSD. n=3). Recovery of compounds were in the range 40-100 %.

Table S 5: Model parameters for CIII (A) and CV (B). Estimated steady-state body concentrations (C_{inf} , $\mu\text{g/g}$), elimination rates (k_e , 1/d), partitioning coefficient internal-water (P_{iw} , L/kg) equivalent to the bioconcentration factor (BCF), $\log P_{iw}$ (\log L/kg), estimated water concentration during the recovery period (C_w Rec, $\mu\text{g/L}$) and estimated initial body concentration (C_0 , $\mu\text{g/g}$). Se text for details.

A *Calanus hyperboreus* stage CIII

Stage	Compound Name	LogKow	Piw (BCF) L/kg	log Piw	ke 1/d	ku 1/d	Cinf ug/g	T 1/2 days	C0 ug/L	cwrec ug/L	ke-2.5%	ke-50%	ke-97.5%	Piw-2.5%	Piw-50%	Piw-97.5%	
C3	N	Naphthalene	3,37	90	1,95	3,54	317,1	0,069	0,20	0,034	0,251	0,36	4,01	inf	46	87	114
C3	N1	C1-naphthalenes	3,87	186	2,27	51,40	9579,4	0,267	0,01	0,000	0,000	7,47	54,40	inf	170	186	201
C3	ANA	Acenaphthene	3,92	1384	3,14	1,30	1797,9	0,036	0,53	0,036	0,010	0,42	1,43	inf	1132	1376	1523
C3	B	Biphenyl	3,95	344	2,54	47,39	16284,2	0,083	0,01	0,029	0,066	6,72	50,02	inf	315	343	371
C3	F	Fluorene	4,18	596	2,78	3,39	2022,4	0,060	0,20	0,017	0,014	2,36	4,27	inf	550	592	635
C3	DBF	Dibenzofuran	4,21	1832	3,26	0,85	1562,6	0,055	0,81	0,079	0,010	0,28	0,89	inf	981	1823	2123
C3	N2	C2-naphthalenes	4,37	784	2,89	3,24	2539,2	1,215	0,21	0,002	0,035	2,36	4,01	inf	719	775	832
C3	D	Dibenzothiophene	4,49	1135	3,05	1,57	1781,3	0,026	0,44	0,012	0,004	1,04	1,69	inf	1023	1126	1229
C3	P	Phenanthrene	4,54	1686	3,23	1,65	2775,1	0,235	0,42	0,034	0,012	1,30	1,68	2,26	1573	1682	1789
C3	N3	C3-naphthalenes	4,81	1910	3,28	1,20	2287,0	1,934	0,58	0,025	0,071	0,94	1,19	1,52	1778	1904	2026
C3	D1	C1-dibenzothiophenes	4,86	6983	3,84	0,92	6391,6	0,262	0,76	0,007	0,007	0,58	0,90	1,35	6258	6960	7782
C3	F1	C1-fluorenes	4,97	2017	3,30	1,35	2726,0	0,351	0,51	0,037	0,023	1,06	1,38	1,84	1872	2010	2148
C3	P1	C1-phenanthrenes/anthracenes	5,14	5708	3,76	0,66	3764,9	1,099	1,05	0,029	0,008	0,53	0,66	0,82	5280	5687	6117
C3	PY	Pyrene	5,18	12557	4,10	0,40	5063,7	0,063	1,72	0,007	0,000	0,33	0,41	0,49	11590	12521	13577
C3	F2	C2-fluorenes	5,2	4292	3,63	0,78	3335,9	0,793	0,89	0,004	0,032	0,54	0,75	0,99	3944	4301	4739
C3	FL	Fluoranthene	5,22	6570	3,82	0,50	3272,3	0,042	1,39	0,005	0,001	0,40	0,50	0,62	6089	6551	7087
C3	DE	Decalin	5,24	10211	4,01	0,58	5916,0	0,733	1,20	0,017	0,002	0,48	0,58	0,70	9482	10168	10914
C3	D2	C2-dibenzothiophenes	5,5	16615	4,22	0,39	6416,8	0,418	1,79	0,019	0,002	0,29	0,39	0,53	14704	16510	18838
C3	P2	C2-phenanthrenes/anthracenes	5,51	11781	4,07	0,40	4694,8	1,577	1,74	0,040	0,012	0,32	0,40	0,49	10752	11741	12904
C3	FL1	C1-fluoranthrenes/pyrenes	5,72	22655	4,36	0,37	8443,3	0,382	1,86	0,001	0,001	0,31	0,37	0,44	20910	22659	24673
C3	D3	C3-dibenzothiophenes	5,73	34502	4,54	0,23	8047,6	0,317	2,97	0,011	0,000	0,18	0,24	0,34	28273	33778	39884
C3	C	Chrysene	5,86	21869	4,34	0,25	5496,4	0,114	2,76	0,000	0,000	0,21	0,25	0,29	19812	21724	23894
C3	P3	C3-phenanthrenes/anthracenes	5,99	28089	4,45	0,27	7467,4	0,946	2,61	0,004	0,001	0,21	0,26	0,33	24843	27908	31453
C3	FL2	C2-fluoranthrenes/pyrenes	6,03	41044	4,61	0,30	12302,5	0,401	2,31	0,000	0,000	0,25	0,30	0,36	36882	40704	44909
C3	C1	C1-chrysenes	6,42	30233	4,48	0,32	9779,1	0,092	2,14	0,000	0,000	0,27	0,32	0,39	27185	29886	32726
C3	DE1	C1-decalins		33103	4,52	0,27	8900,2	1,497	2,58	0,052	0,002	0,21	0,27	0,34	29250	32895	37390

Table S 5 cont: Model parameters for CIII (A) and CV (B). Equilibrium body concentrations (C_{inf} , $\mu\text{g/g}$), elimination rates (k_e , $1/\text{d}$), partitioning internal-water (P_{iw} , L/kg) equivalent to the bioconcentration factor (BCF), $\log P_{iw}$ ($\log \text{L/kg}$), estimated water concentration during the recovery period ($C_w \text{ Rec}$, $\mu\text{g/L}$) and estimated initial body concentration (C_0 , $\mu\text{g/g}$). Se text for details.

B *Calanus hyperboreus* stage CV

Stage	Compound Name	LogKow	Piw (BCF) L/kg	log Piw	ke 1/d	ku 1/d	Cinf ug/g	T 1/2 days	C0 ug/L	cwrec ug/L	ke-2.5%	ke-50%	ke-97.5%	Piw-2.5%	Piw-50%	Piw-97.5%	
C5	N	Naphthalene	3,37	1062	3,03	0,252	267,8	2,06	2,7	0	0	0,215	0,253	0,295	986	1060	1141
C5	N1	C1-naphthalenes	3,87	3797	3,58	0,086	325,2	15,32	8,1	0	0	0,077	0,086	0,095	3545	3790	4060
C5	ANA	Acenaphthene	3,92	7295	3,86	0,055	403,6	0,37	12,5	0	0	0,050	0,055	0,062	6750	7294	7886
C5	B	Biphenyl	3,95	4851	3,69	0,072	347,8	2,62	9,7	0	0	0,064	0,072	0,080	4506	4843	5204
C5	F	Fluorene	4,18	8371	3,92	0,051	423,5	2,00	13,7	0	0	0,046	0,051	0,056	7758	8360	9018
C5	DBF	Dibenzofuran	4,21	7486	3,87	0,050	376,6	0,56	13,8	0	0	0,044	0,050	0,057	6845	7485	8192
C5	N2	C2-naphthalenes	4,37	10392	4,02	0,044	453,4	34,85	15,9	0	0	0,039	0,044	0,049	9553	10394	11321
C5	D	Dibenzothiophene	4,49	12275	4,09	0,037	459,2	0,59	18,5	0	0	0,033	0,037	0,042	11321	12269	13338
C5	P	Phenanthrene	4,54	15929	4,20	0,033	529,1	5,42	20,9	0	0	0,029	0,033	0,037	14618	15952	17507
C5	N3	C3-naphthalenes	4,81	18930	4,28	0,028	534,4	37,65	24,6	0	0	0,025	0,028	0,032	17240	18971	20946
C5	D1	C1-dibenzothiophenes	4,86	22982	4,36	0,023	526,4	2,09	30,3	0	0	0,019	0,023	0,027	20455	23019	26189
C5	F1	C1-fluorenes	4,97	19251	4,28	0,029	565,0	7,62	23,6	0	0	0,026	0,029	0,033	17524	19246	21247
C5	P1	C1-phenanthrenes/anthracenes	5,14	27934	4,45	0,021	596,2	13,26	32,5	0	0	0,018	0,021	0,025	24616	27995	32206
C5	PY	Pyrene	5,18	41782	4,62	0,018	732,1	0,50	39,6	0	0	0,015	0,017	0,020	37146	41863	48073
C5	F2	C2-fluorenes	5,2	27030	4,43	0,021	569,2	10,47	32,9	0	0	0,018	0,021	0,024	24012	27101	30887
C5	FL	Fluoranthene	5,22	35095	4,55	0,018	637,0	0,48	38,2	0	0	0,015	0,018	0,021	30939	35167	40538
C5	DE	Decalin	5,24	152901	5,18	0,022	3330,9	15,41	31,8	0	0	0,019	0,022	0,025	136989	153025	172740
C5	D2	C2-dibenzothiophenes	5,5	25444	4,41	0,019	484,9	1,30	36,4	0	0	0,016	0,019	0,023	22340	25453	29706
C5	P2	C2-phenanthrenes/anthracenes	5,51	40188	4,60	0,018	710,0	9,45	39,2	0	0	0,014	0,018	0,021	34782	40410	48020
C5	FL1	C1-fluoranthrenes/pyrenes	5,72	50491	4,70	0,016	822,7	2,01	42,5	0	0	0,013	0,016	0,019	44391	50661	59181
C5	D3	C3-dibenzothiophenes	5,73	46786	4,67	0,017	787,0	0,74	41,2	0	0	0,013	0,017	0,020	40222	46924	56354
C5	C	Chrysene	5,86	48716	4,69	0,020	990,4	0,10	34,1	0	0	0,013	0,020	0,027	38223	49196	69414
C5	P3	C3-phenanthrenes/anthracenes	5,99	59900	4,78	0,015	901,7	3,36	46,0	0	0	0,011	0,015	0,019	49760	60608	77258
C5	FL2	C2-fluoranthrenes/pyrenes	6,03	52596	4,72	0,015	784,2	0,96	46,5	0	0	0,012	0,015	0,018	45697	52800	62505
C5	C1	C1-chrysenes	6,42	46126	4,66	0,023	1064,4	0,22	30,0	0	0	0,018	0,023	0,029	38958	46214	56495
C5	DE1	C1-decalins		238154	5,38	0,017	4157,9	12,24	39,7	0	0	0,014	0,017	0,021	208028	238573	280088

Text section 4: Exposure verification kinetics experiment. extended results

Exposure profiles based on particle characterization by Coulter Counter Multisizer (Beckman) of dispersion used for generating water soluble fractions are shown in Figure S 8. Volumetric measurements are converted to weight by multiplying with the density of the oil. The total concentrations of SVOCs in the controls were relatively low, comprising 1.6 and 2.5 % of the sum SVOC in the WSFs for lipid-rich and lipid-poor, respectively (Figure S 9). Two outliers were identified in the controls, one in each treatment group, containing primarily high concentrations of sum naphthalenes (0.52 and 1.86 $\mu\text{g/L}$), increasing the average concentrations of total SVOC and sum naphthalenes in the controls significantly. Without the outliers in the control groups, the sum SVOC of the controls comprised 0.54 and 1.15% of the sum SVOC in the WSF in the experiment with lipid-poor and lipid-rich, respectively. Accidental carryover between the exposure containers may be the cause of the high concentrations of naphthalenes in the two control samples.

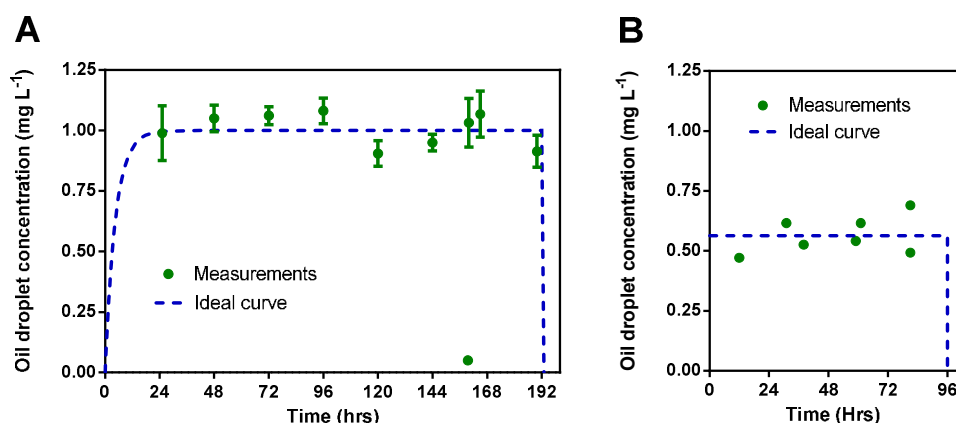


Figure S 8. Ideal exposure concentration (dashed line) and measured concentration in the setup with CVs (A; daily mean \pm SD in exposure chambers parallel to the WSF chambers. n=8) and CIIIs (B; settling chamber. n=1).

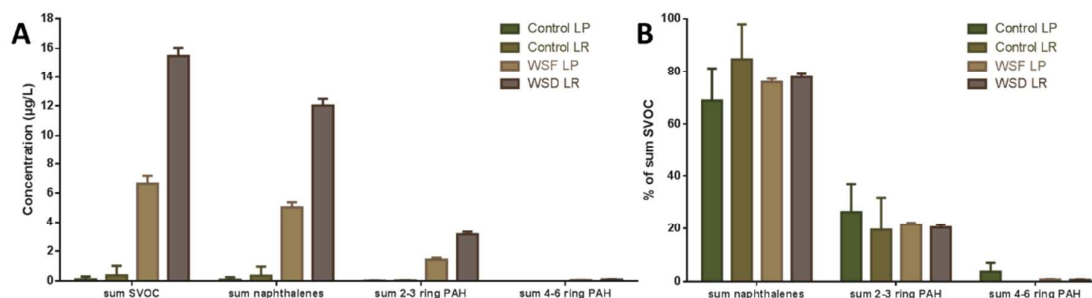


Figure S 9. A: Semi-volatile organic compounds (SVOC). naphthalenes (N-N4). 2-3 ring PAHs and 4-6 ring PAHs in $\mu\text{g/L}$ in the exposure media (water soluble fraction of crude oil and seawater controls) from the uptake and depuration experiments with lipid-rich (LR) and lipid-poor (LP) *Calanus hyperboreus*. B: Sum naphthalenes (N-N4), 2-3 ring PAHs and 4-6 ring PAHs as percentage of sum SVOC.

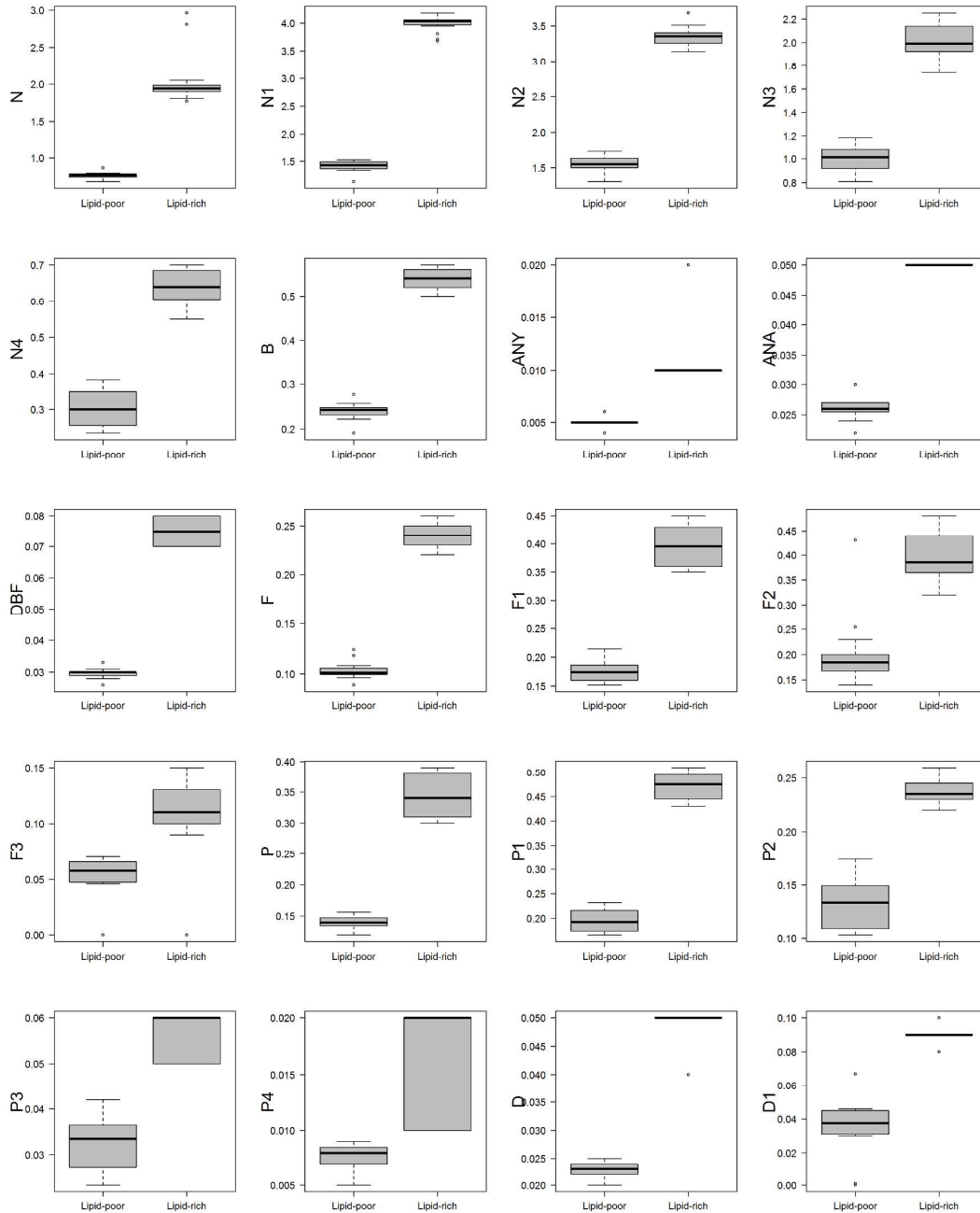


Figure S 10. Semi volatile organic compounds (SVOC) concentrations (in µg/L) in water samples containing the water-soluble fraction (WSF) of crude oil sampled during the experiments with *Calanus hyperboreus* stage CIII and CVs. Data given as mean ± SD (n=16 for each). Abbreviations are given in Table S3

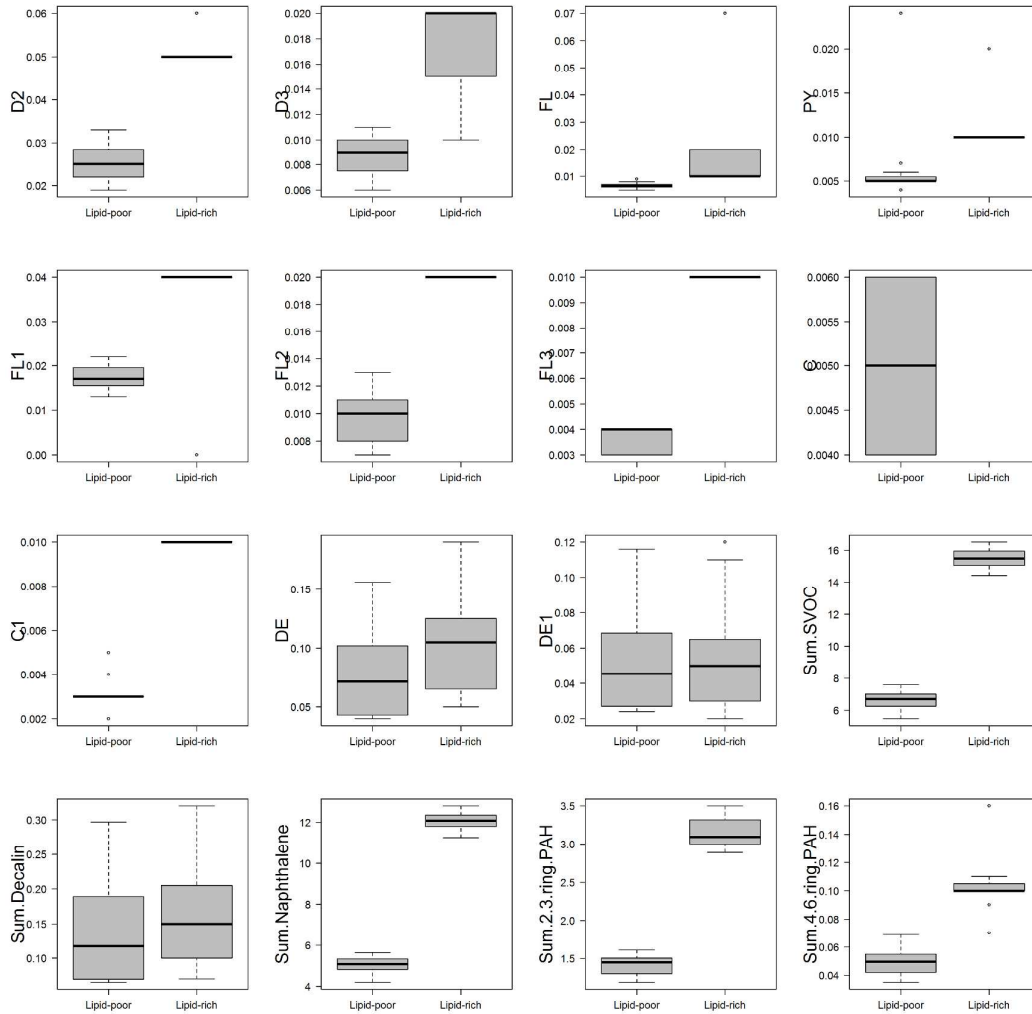


Figure S 10 cont. Semi volatile organic compounds (SVOC) concentrations (in $\mu\text{g/L}$) in water samples containing the water-soluble fraction (WSF) of crude oil sampled during the experiments with *Calanus hyperboreus* stage CIII and CVs. Data given as mean \pm SD (n=16 for each). Abbreviations are given in Table S3.

Table S 7. Volatile organic compounds (VOC) concentrations (in $\mu\text{g/L}$) in water samples containing the water-soluble fraction (WSF) of crude oil from the kinetics experiment with *Calanus hyperboreus* of stage CIII (n=7) and CVs (n=16). Data given as mean \pm SD. ND=Not detected above LOR.

Component	CIII $\mu\text{g/L}$	CV $\mu\text{g/L}$
Isopentane	ND	ND
n-C5 (Pentane)	ND	ND
Cyclopentane	ND	ND
2-methylpentane	ND	ND
3-Methylpentane	ND	ND
n-C6 (Hexane)	ND	ND
Methylcyclopentane	ND	0.04 \pm 0.08
Benzene	ND	0.004 \pm 0.01
Cyclohexane	ND	0.34 \pm 0.35
2.3-Dimethylpentane	ND	ND
3-methylhexane	ND	ND
n-C7 (Heptane)	ND	ND
Methylcyclohexane	ND	2.52 \pm 0.15
Toluene	ND	0.08 \pm 0.01
2.4 dimethylhexane	ND	ND
2-Methylheptane	ND	ND
n-C8 (Octane)	ND	ND
Ethylbenzene	0.27 \pm 0.05	0.86 \pm 0.04
m-Xylene	0.72 \pm 0.10	2.83 \pm 0.14
p-Xylene	0.23 \pm 0.05	0.85 \pm 0.07
o-Xylene	0.14 \pm 0.02	0.62 \pm 0.04
n-C9 (Nonane)	ND	0.03 \pm 0.08
Propylbenzene	ND	0.37 \pm 0.03
1-Methyl-3-ethylbenzene	0.16 \pm 0.11	1.27 \pm 0.09
1-Methyl-4-ethylbenzene	0.07 \pm 0.05	0.53 \pm 0.04
1.3.5-trimethylbenzene	0.11 \pm 0.08	0.99 \pm 0.07
1-Methyl-2-ethylbenzene	0.08 \pm 0.05	0.56 \pm 0.04
1.2.4-Trimethylbenzene	0.23 \pm 0.17	2.24 \pm 0.17
n-C10 (Decane)	ND	0.044 \pm 0.12
1.2.3-Trimethylbenzene	0.01 \pm 0.04	0.91 \pm 0.07
n-Butylbenzene	ND	0.13 \pm 0.02
1.2.4.5-Tetramethylbenzene	ND	0.11 \pm 0.05
n-Pentylbenzene	ND	0.014 \pm 0.04
C4-Benzenes	ND	5.11 \pm 0.36
C5-Benzenes	ND	4.58 \pm 0.35
sum all	2.01 \pm 0.64	25.0 \pm 1.5

Text section 5: Stage distribution of *C. hyperboreus* during the experimental periods

The duration of the experiments caused a shift in stage distribution of copepods over time, in particular during the recovery periods (Figure S 11). The majority of the lipid-rich copepods were at developmental stage copepodite five (CV) at the start of the exposure period, as this developmental stage was visually separated from copepodite four (CIV) and adult females before start. At the time of imaging at day zero, 80 % of the copepods in the controls were at stage CV, the rest had already moulted into adult females (n=16, Figure S 11A). At the end of the exposure period at day 8, 93 % of the copepods in the controls were at stage CV (n=16). The higher number of females in the controls on day 0 seems coincidental, as the total distribution over the first 8 days were 91.4 % CV, 2.3% CIV and 6.3% adult females (n=128, results not shown). The CVs gradually moulted into females during the recovery period, comprising only 37 % of the total at day 45 (Figure S 11A). The total number of copepods used in this experiment was 300.

The majority of the lipid-poor copepods were at developmental stage copepodite three (CIII) at the start of the experiment (Figure S 11B). These copepods were reared from eggs in a laboratory culture, and the experiment was started at a time when the majority of the culture had moulted into CIII. Overlapping stage durations results in some representatives of copepodite two (CII) and CIV in the samples on day zero (n=30, Figure S 11B). A visual inspection was performed when selecting the experimental individuals, however, due to the large number of copepods used in this experiment (approx. 4000), complete stage determination of each individual was not possible. At the end of the exposure period on day four, 41 % of the copepods had moulted into CIV, whereas at the end of the recovery period, only 3 % was still at stage CIII Figure S 11B).

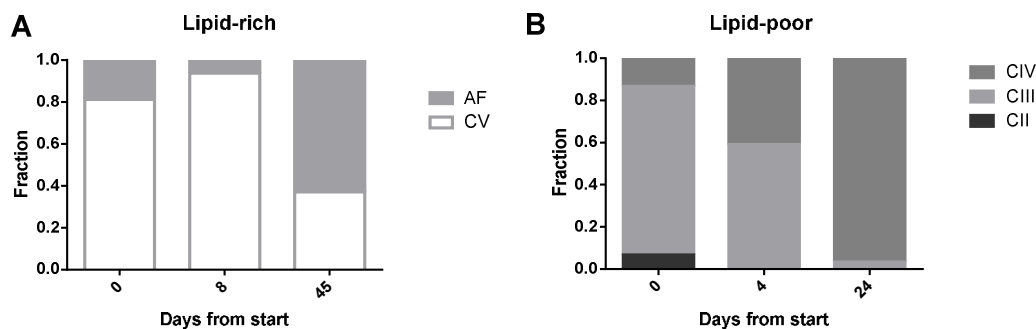


Figure S 11. Stage distribution of lipid rich (A) and lipid poor (B) *C. hyperboreus* in the control groups at the start (Day 0), after the exposure period (Day 4 or 8) and at the end of the experiment (Day 45 or 24).

Text section 6: Acute toxicity data

Exposure verification results

The total extractable material (TEM) was determined to be 2.45 and 2.11 mg/L in the 100 % WAF of the CV and CIII experiment, respectively. In order to verify the stability of the exposure solutions with regard to SVOC, analyses were performed on the fresh WAF before exposure (n=2) and the highest (100%WAF, n=4) and lowest (nominal 12% WAF, n=4) exposure concentration after exposure. There were no significant differences in component composition in the 100% WAF before and after exposure. For SVOC with a concentration above 0.1 µg/L, the mean concentrations were 99.1% [in the 100% WAF after exposure relative to the](#) relative to the fresh WAF in the CV experiment, and 100.4 ± 12.2 in the CIII experiment. The dilution series was verified by comparing the concentration of PAHs between the fresh WAF (100%) and the nominal 12% WAF after exposure. The concentrations of the >0.1 µg/L PAHs in the nominal 12% WAF were on average 11.9 ± 1.1 % (n=10 components) and 13.6 ± 2.5 % (n=14 components) relative to the concentrations in the 100% WAF in the CV and CIII experiment, respectively (excluding phenols).

Acute toxicity results

Concentration dependent survival of lipid-poor and lipid-rich *C. hyperboreus* after WAF exposure is shown in Figure S 12. The LC₅₀ for 192 hours of exposure of stage CI - CIII of the copepod *C. hyperboreus* for WAF prepared from Troll B crude oil artificially weathered to 200 °C + residue at an oil:sea water ratio of 1:100 was calculated to be 61.6 % WAF (Table S 8). This corresponds to a concentration of total extractable material of 1.302 mg/L. The estimated LC₁₀ after 8 days of exposure was 1.2 mg/L based on total extractable material (TEM). This is considerably below the corresponding LC₁₀ of estimated for the lipid rich stages of *C. hyperboreus* of 2.1 mg/L (Table S 9). The LC₅₀ of lipid poor *C. hyperboreus* estimated after 192 hours exposure is in the same range as found for *Calanus finmarchicus* where the average LC₅₀ (96 h test) for 12 different 200° C+ crude oil residues were 1.7 (±0.9) mg/L (SINTEF; various sources). The LC50 could not be determined for the lipid-rich CV stage of *C. hyperboreus*.

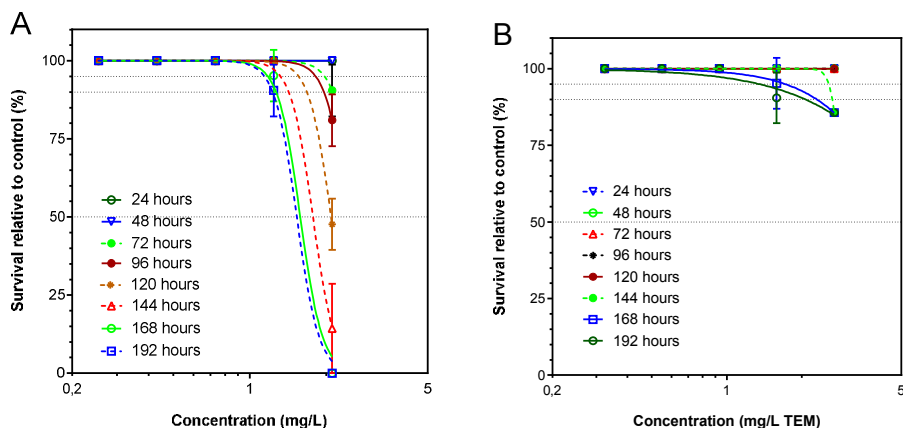


Figure S 12. Survival in percent for *Calanus hyperboreus* exposed for 24. 48. 72. 96. 120. 144. 168 and 192 hours to different concentrations of WAF from Troll B crude oil artificially weathered to 200 °C + residue and prepared at a oil:sea water ratio of 1:100. A) Lipid poor copepodites (CI-III) B) Lipid rich copepodites (CV) from previous experiment. Dots represent mean (\pm SD) of observed data and lines the data fitted to the non-linear sigmoidal mode. A fixed slope was used in Fig. A. Horizontal dotted lines indicate the LC₅, LC₁₀ and LC₅₀ effect concentrations.

Table S 8. LC_x-values for copepodite stage CI-CIII of *Calanus hyperboreus* following 192 hours of exposure to dilutions of the WAF from the artificially weathered Troll B crude oil. The values are listed as the volume-percent WAF in seawater causing the effect and the corresponding calculated nominal concentration of TEM in mg/L based on analytical data from the semi-volatile organic compounds (SVOC) in a subsample of the undiluted WAF. Values are listed with 95% Confidence Intervals (CI_{95%}) if calculated.

Effect concentration	LC ₅ 192 hours	LC ₁₀ 192 hours	LC ₅₀ 192 hours
Conc. TEM (mg/L)*	2.11	2.11	2.11
% WAF	57.9	58.8	61.6
CI _{95%}	(Very wide)	(Very wide)	(Very wide)
TEM (mg/L)	1.23	1.24	1.30
CI _{95%}	(Very wide)	(Very wide)	(Very wide)

* Concentration based on analytical data in the semi-volatile organic compound fraction (SVOC) in the undiluted WAF as TEM. The CI_{95%} are listed as '(Very wide)' rather than stating numerical data due to the few data points covering a gradual response in the model.

Table S 9. LC_x-values for *Calanus hyperboreus* CV following 192 hours of exposure to dilutions of the WAF from the artificially weathered Troll B crude oil. The values are listed as the volume-percent WAF in seawater causing the effect and the corresponding calculated nominal concentration of total extractable (organic) matter (TEM) in mg/L based on analytical data of semi-volatile organic compounds (SVOC) in the undiluted WAF as analysed after exposure. Values are listed with 95% Confidence Intervals (CI_{95%}) if calculated. NC: Not Calculated.

Effect concentration	LC ₅ 192 hours	LC ₁₀ 192 hours	LC ₅₀ 192 hours
Conc. TEM (mg/L)*	2.70	2.70	2.70
% WAF	49.9	76.5	> 100
CI _{95%}	33.4 – 74.8	62.3 – 94.0	NC
TEM (mg/L)	1.35	2.06	> 2.70
CI _{95%}	0.89 – 2.02	1.68 – 2.54	NC

* Concentration based on analytical data in the SVOC fraction in the undiluted WAF analysed after exposure as TEM.

**Text section 7: Model fits for all components including MCMC
uncertainty estimates**

See attached PDF file.