

Supplemental material to

Demographic toxicokinetic-toxicodynamic modeling of lethal effects

André Gergs, Faten Gabsi, Armin Zenker, Thomas G. Preuss

33 Pages, 17 Figures, 21 Tables

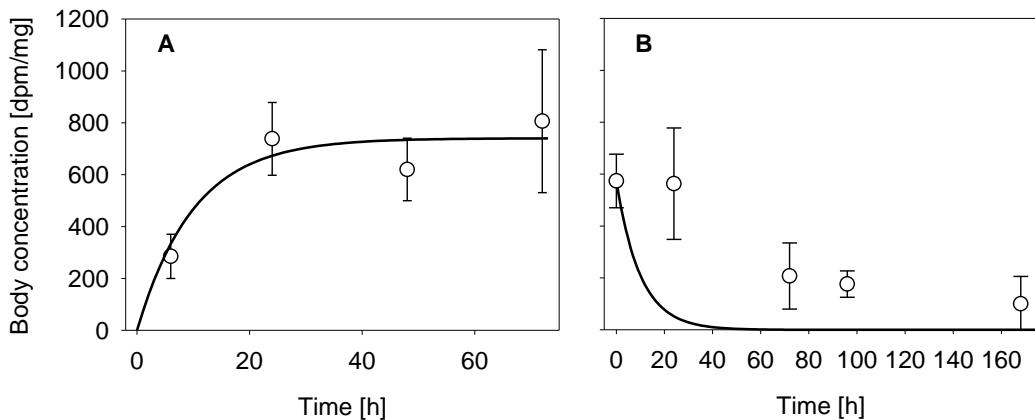


Figure S1: Bioconcentration of TPT in intermediate sized *Daphnia magna*. Uptake (A) and Elimination (B) is described by a one-compartment toxicokinetic model for computing the internal concentration [1] (lines). Estimated parameters are $k_i=14.06 \text{ h}^{-1}$ and $k_e = 0.095 \text{ h}^{-1}$. Dots represent measured data.

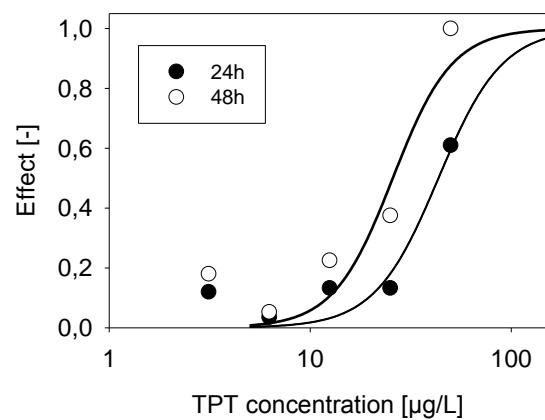


Figure S2: Concentration responses of *D. magna* for TPT as determined in a 48h acute toxicity test. $\text{EC}_{50}(24\text{h})=43.49$, slope(24h)=2.74; $\text{EC}_{50}(48\text{h})= 25.76$, slope(48h)=2.95; data (dots) from [2].

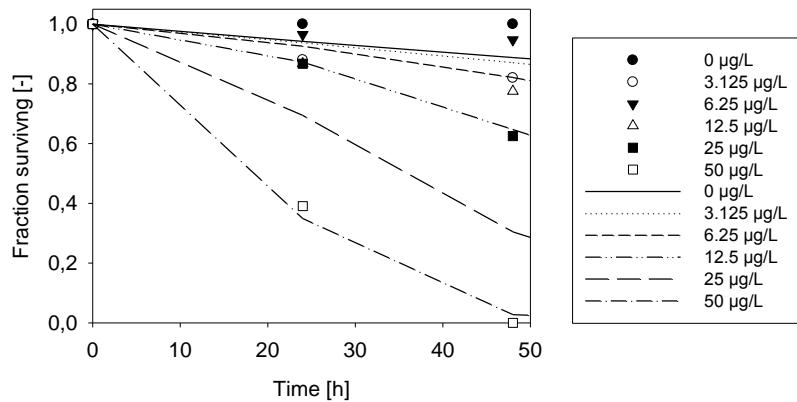


Figure S3: GUTS fits to TPT survival data derived from a *D. magna* 48h acute toxicity test using neonate daphnids ($<24\text{h}$, $1.01 \pm 0.12 \text{ mm}$), under the tk-td assumptions of **scaled internal concentration** and **individual tolerance** (for explanations see main text). Data (dots) from [2], lines represent model fit. Estimated background hazard rate is $h_b=0.0025 \text{ h}^{-1}$.

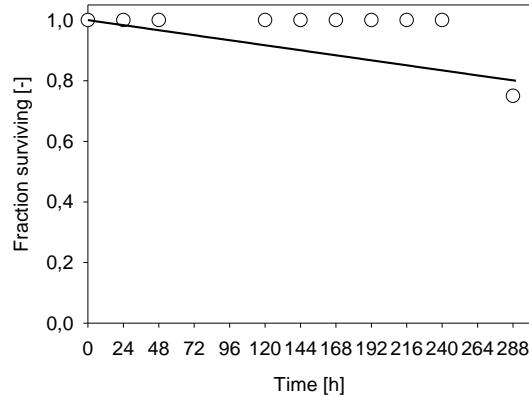


Figure S4: Survival as function of time in large bodied *D. magna*. Dots represent control data for the pulse exposure experiment used for GUTS calibration (Figure 2, main text). Lines represent model fit for the background hazard rate. Background hazard estimate rate was $h_b=0.001 \text{ h}^{-1}$.

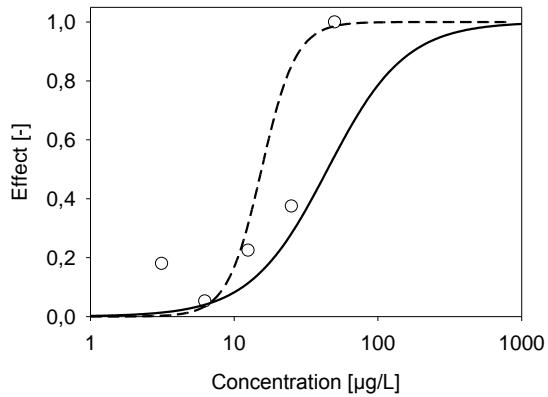


Figure S5: Predictions of the GUTS-SIDS for TPT concentration responses of neonate *D. magna* (48h, see also Figure S2) based on the adult data set parameterization with toxicokinetics being corrected for body size. Lines represent GUTS model predictions for the two toxicodynamic assumptions individual tolerance (dashed line) and stochastic death (solid line).

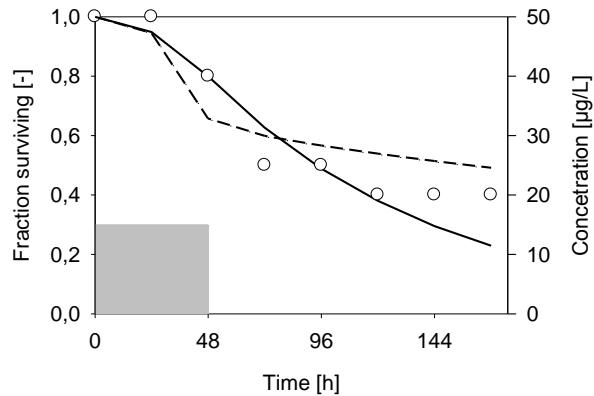


Figure S6: Predictions of the GUTS-SIDS for TPT pulse exposure of neonate *D. magna* based on the adult data set parameterization with toxicokinetics being corrected for body size. Lines represent GUTS model predictions for the two toxicodynamic assumptions individual tolerance (dashed line) and stochastic death (solid line). Assumed background hazard rate was $h_b=0.001 \text{ h}^{-1}$.

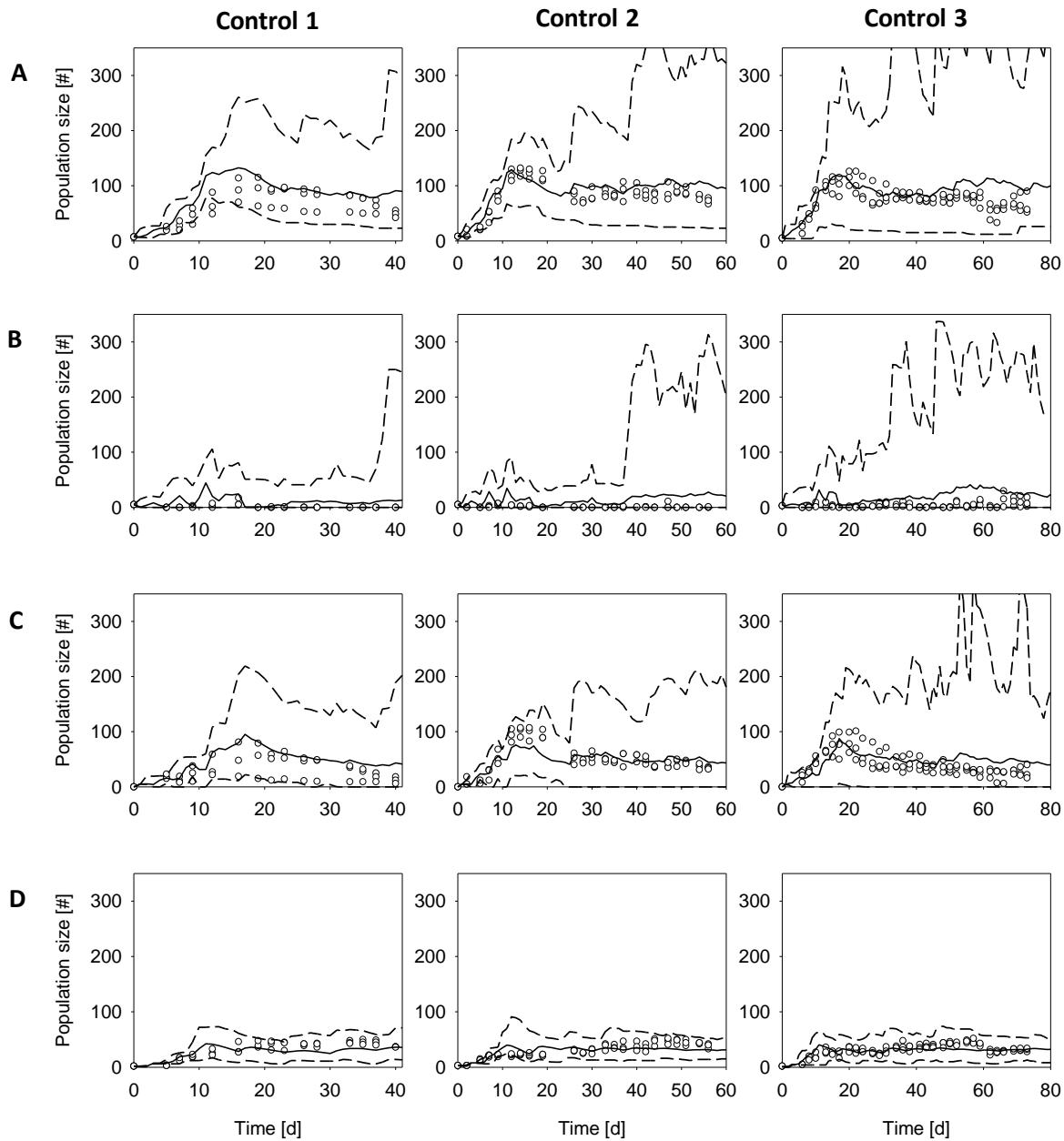


Figure S7: Control populations to single pulse experiments (Control 1), multiple pulse experiments (Control 2) and realistic exposure scenario experiments (Control 3), for exposures scenarios see Figures S5-S12. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo simulations) for A) total population size and abundances within tree size classes: B) small (<1.25 mm), C) medium ($\geq 1.25 - < 2.1$ mm) and D) large (≥ 2.1 mm).

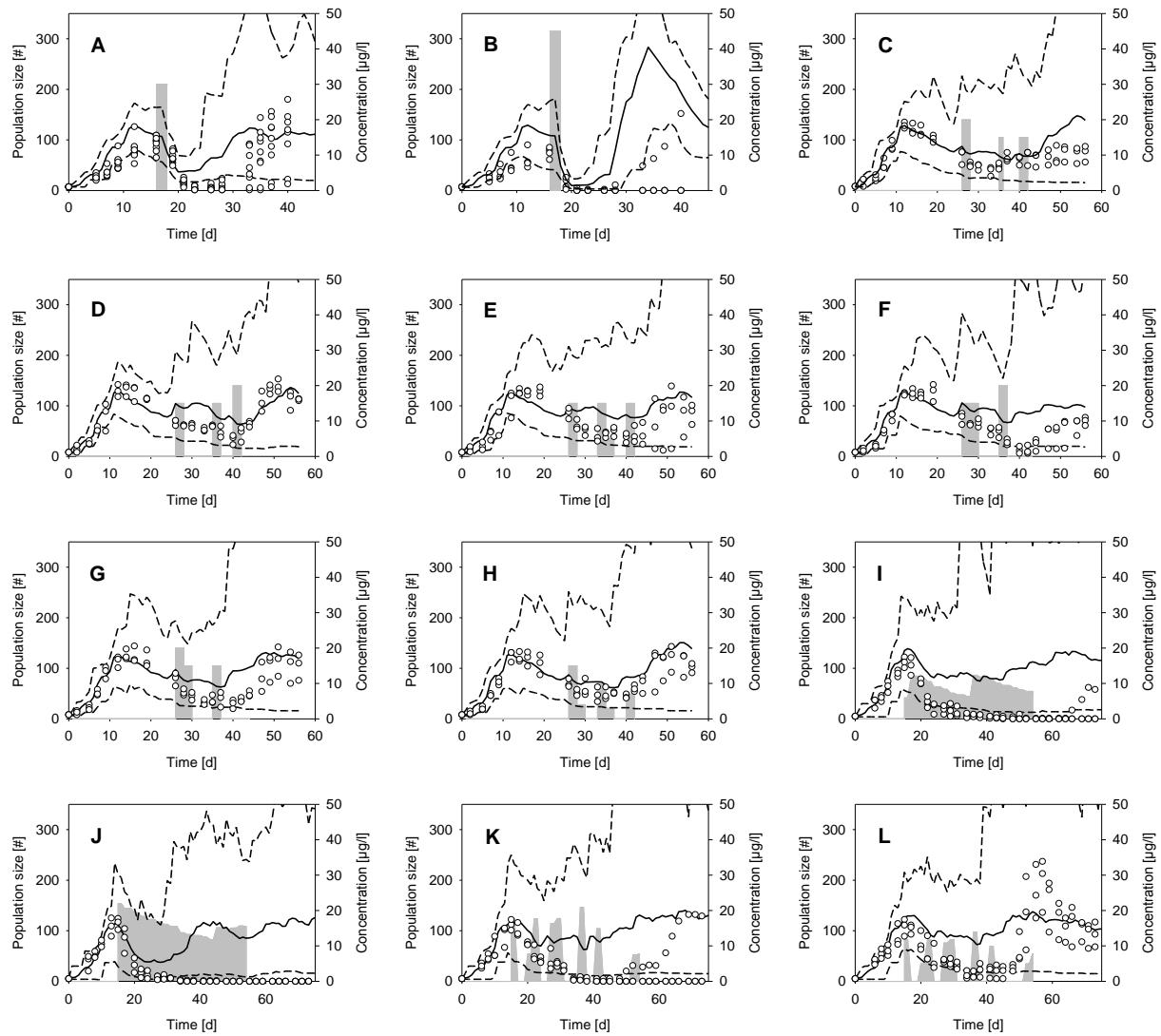


Figure S8: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the **concentration response curve** for 24h neonate acute toxicity. Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.

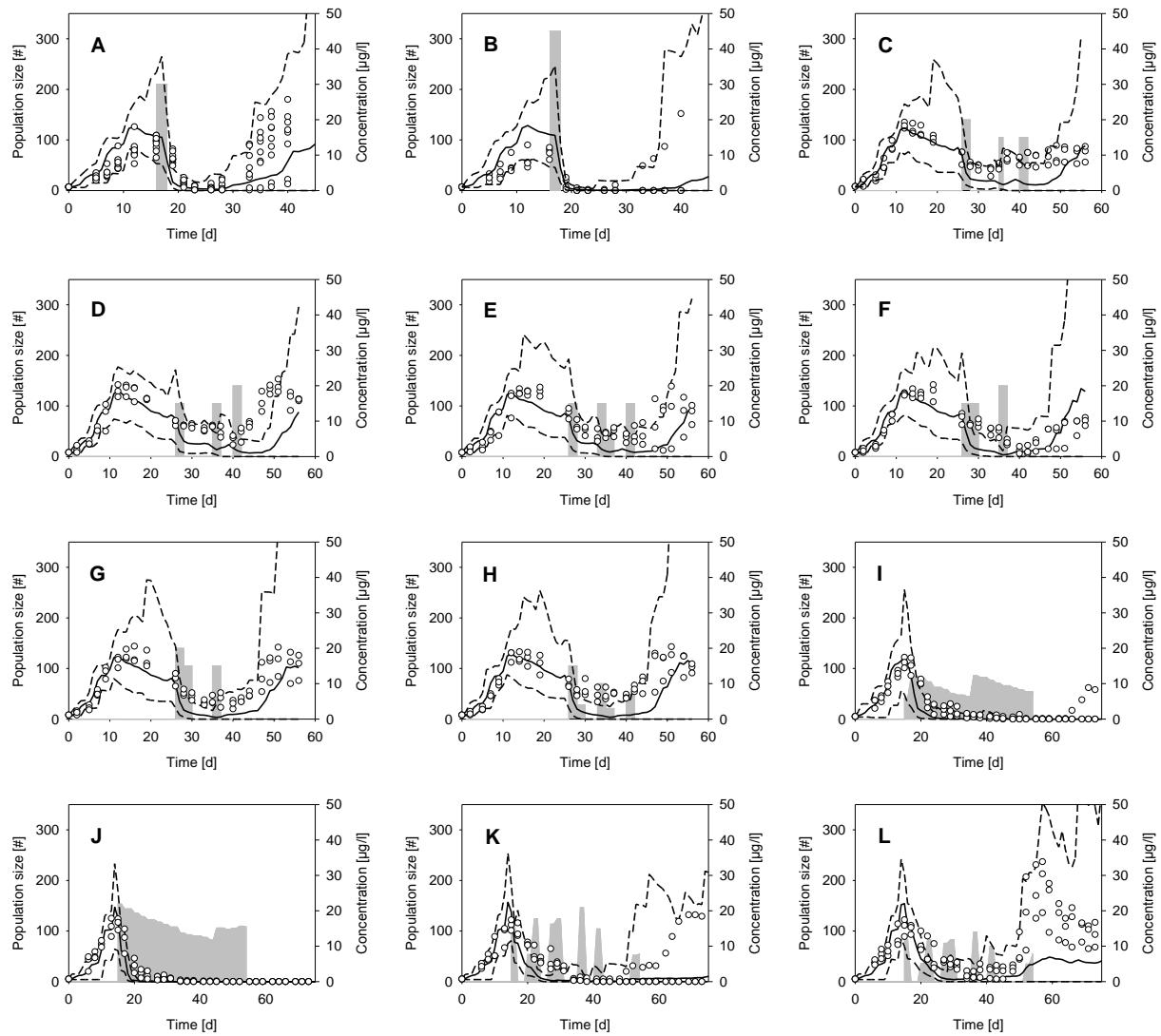


Figure S9: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the tk-td assumptions of **scaled internal concentration** and **stochastic death** (for explanations see main text). Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.

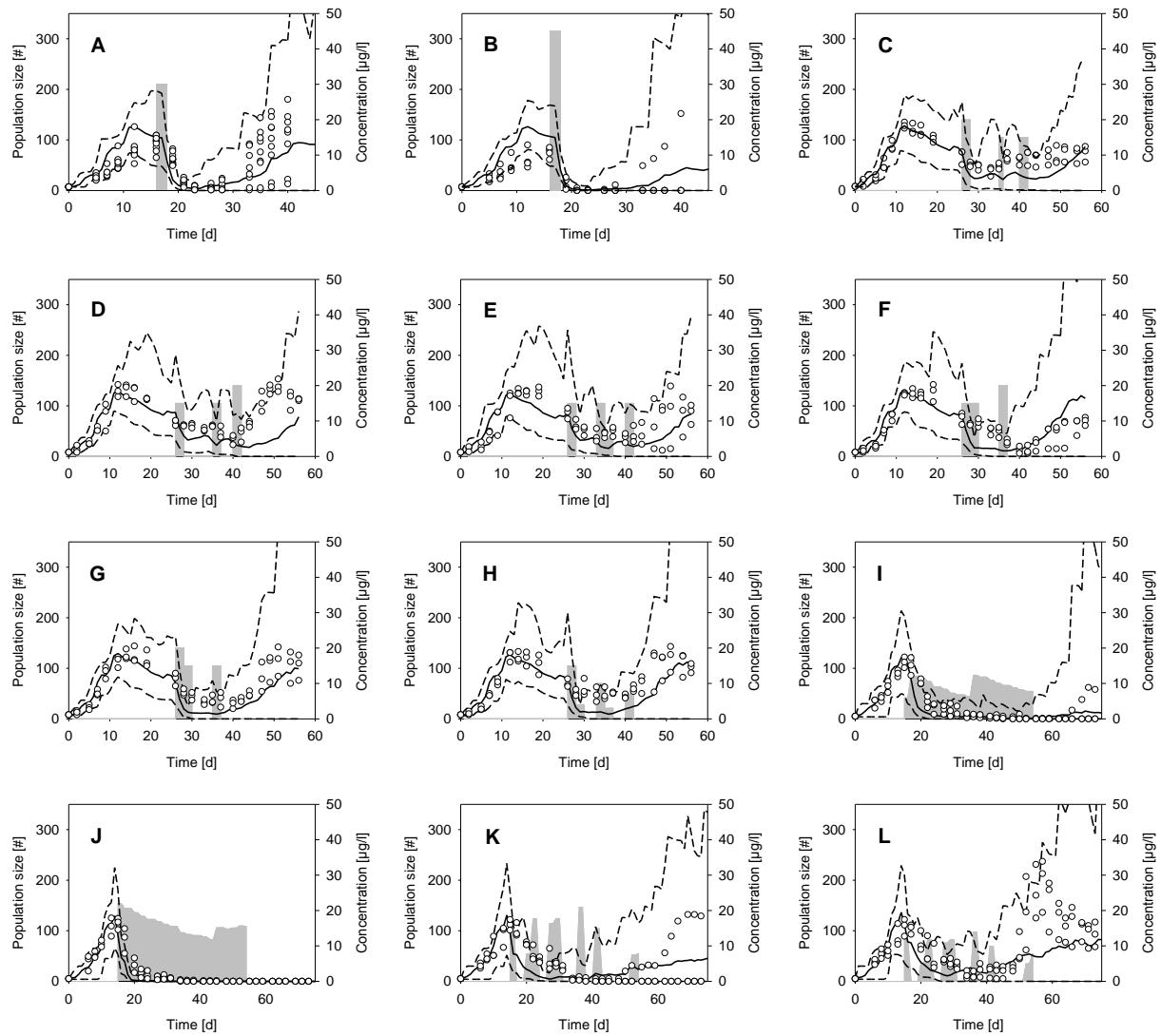


Figure S10: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the tk-td assumptions of **scaled internal concentration under consideration of body sizes** and **stochastic death** (for explanations see main text). Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.

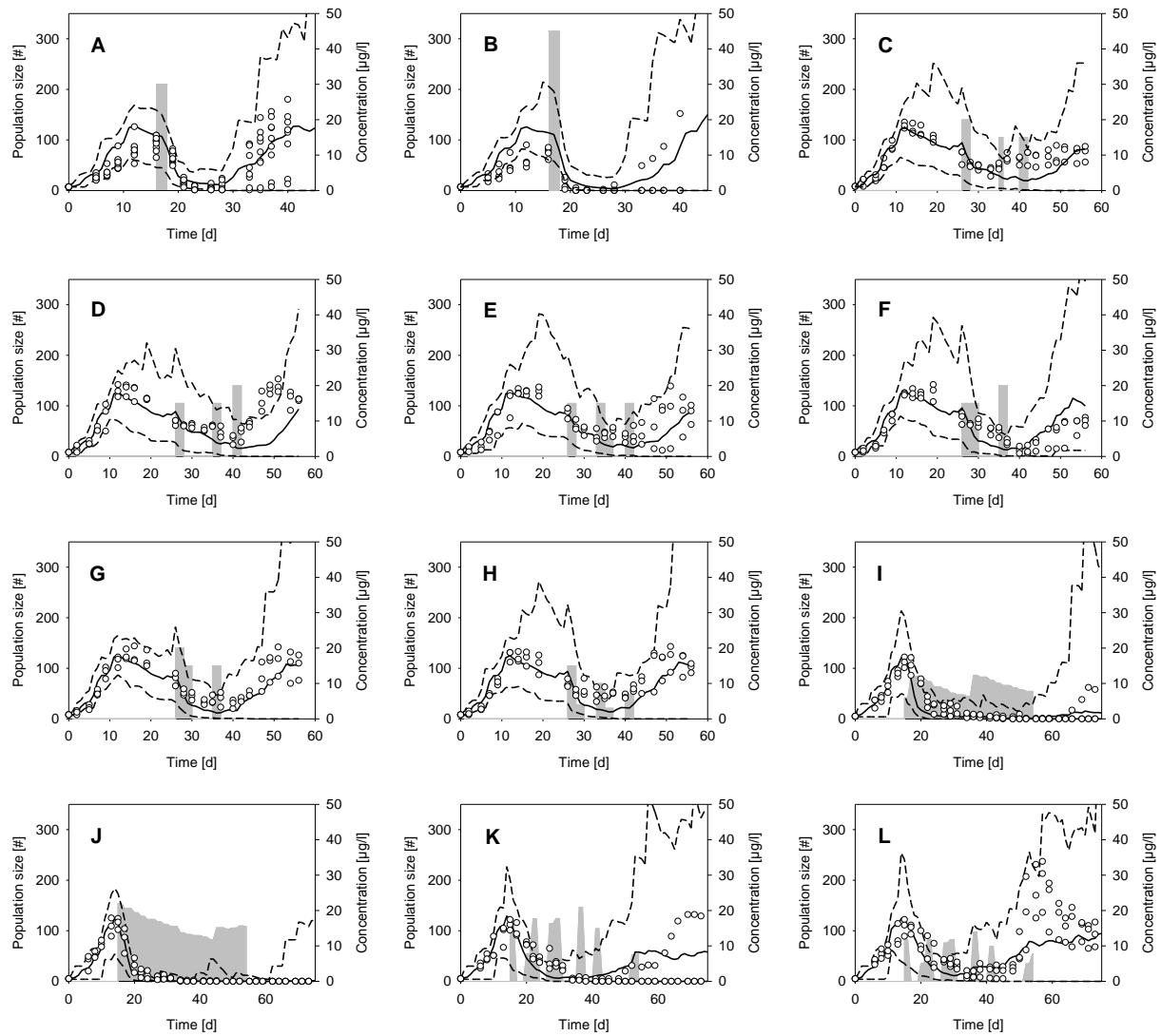


Figure S11: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the tk-td assumptions of **scaled damage under consideration of body size dependent second order kinetics** as well as **stochastic death** (for explanations see main text). Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.

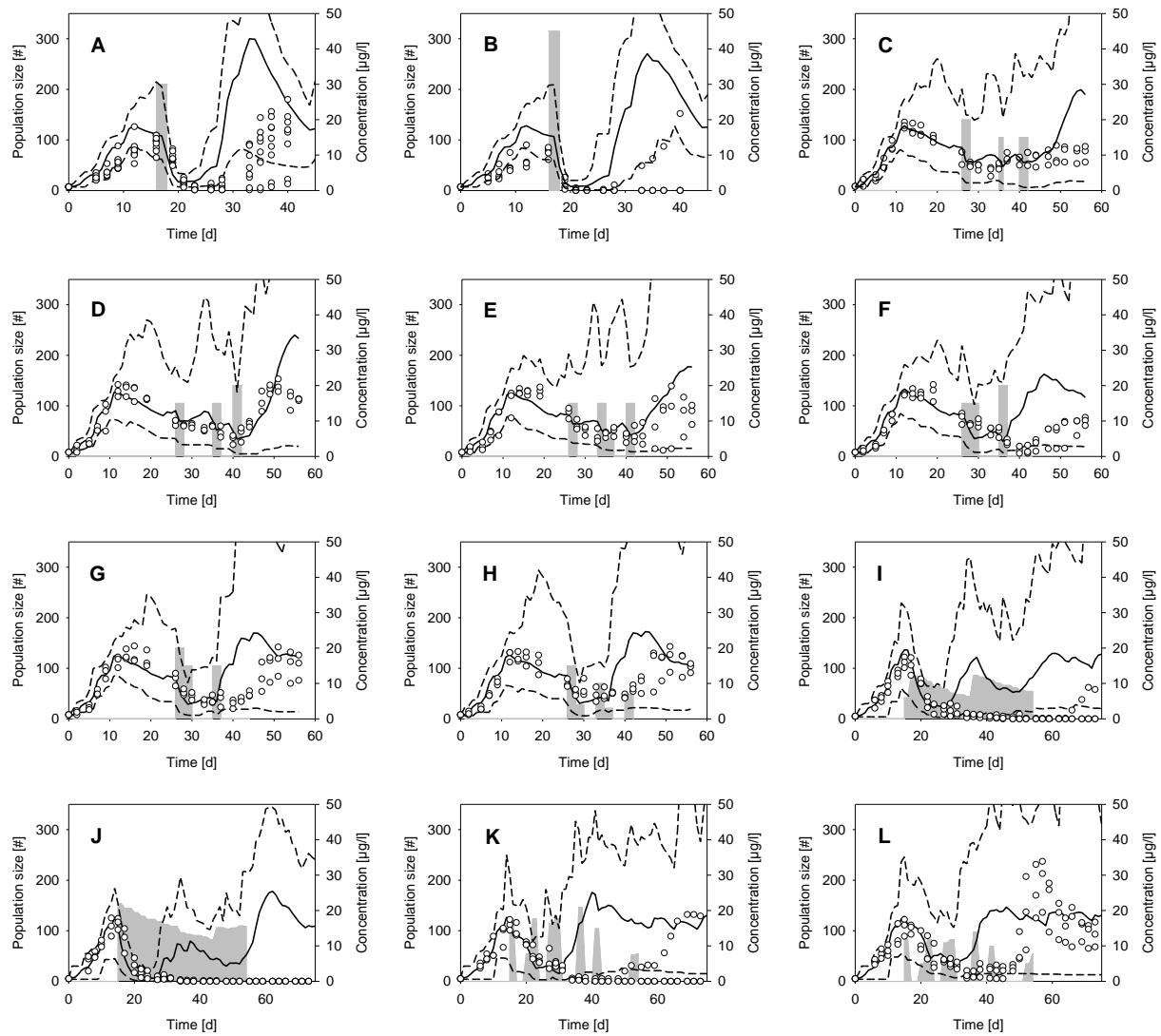


Figure S12: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the tk-td assumptions of **scaled internal concentration and **individual tolerance** (for explanations see main text). Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.**

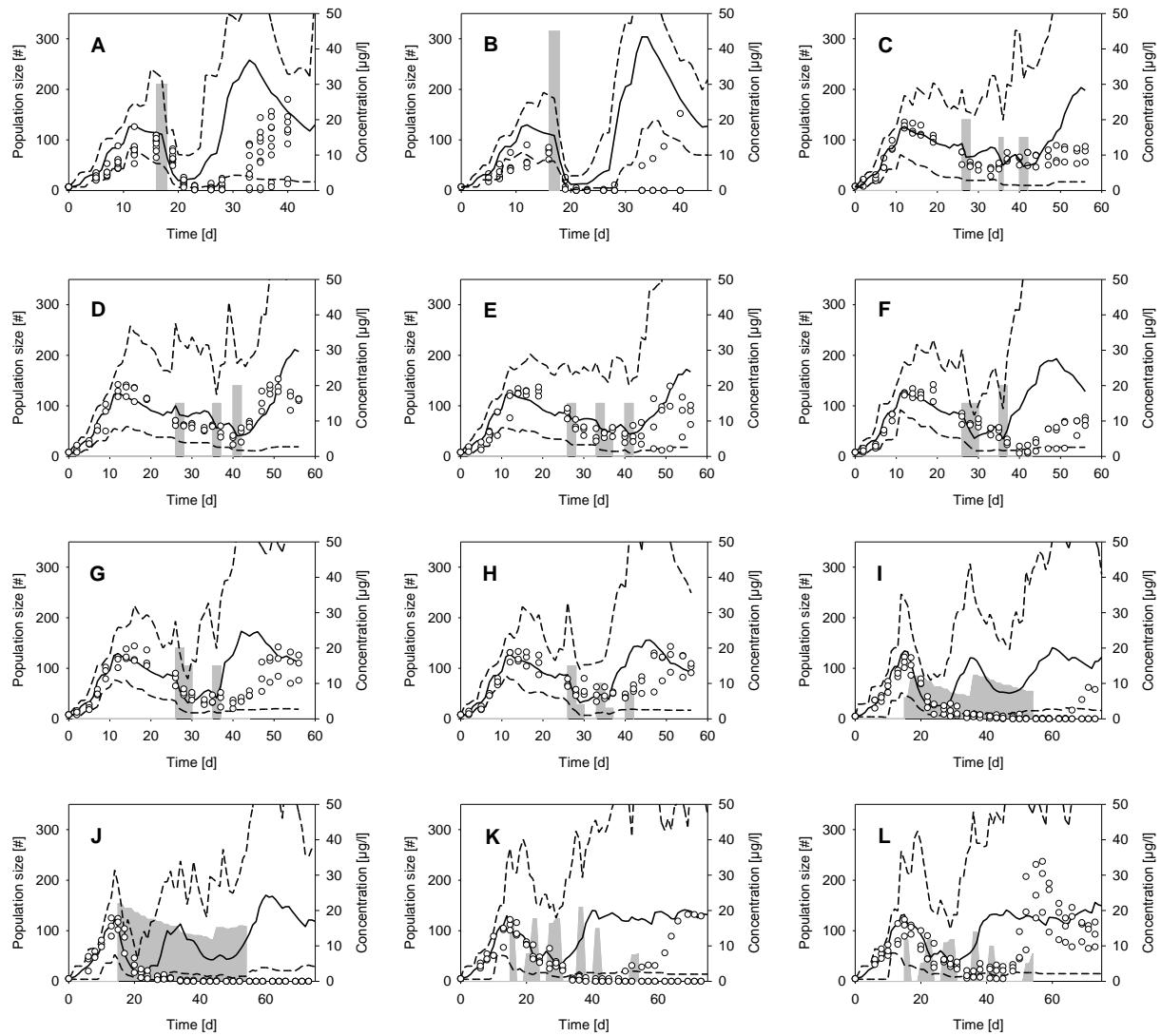


Figure S13: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the tk-td assumptions of **scaled internal concentration under consideration of body sizes and individual tolerance (for explanations see main text). Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.**

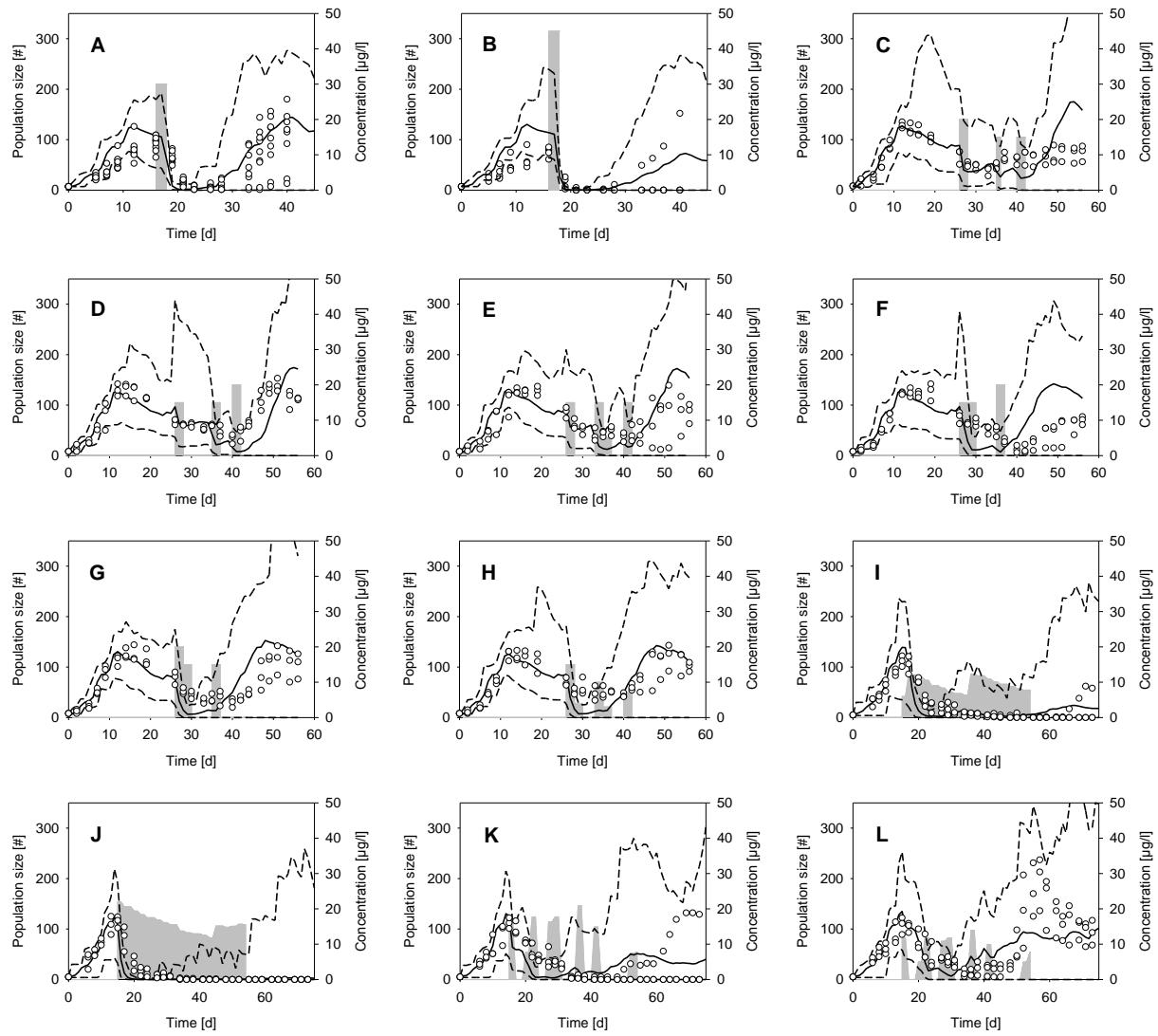


Figure S14: Responses of *Daphnia magna* populations to TPT exposure as tested for various exposure scenarios: A-B) Single pulses, C-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Dots represent measured laboratory data and lines are model predictions (mean, minimum and maximum of 100 Monte-Carlo Simulations) based on the tk-td assumptions of **scaled damage under consideration of body size dependent second order kinetics and individual tolerance (for explanations see main text). Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text.**

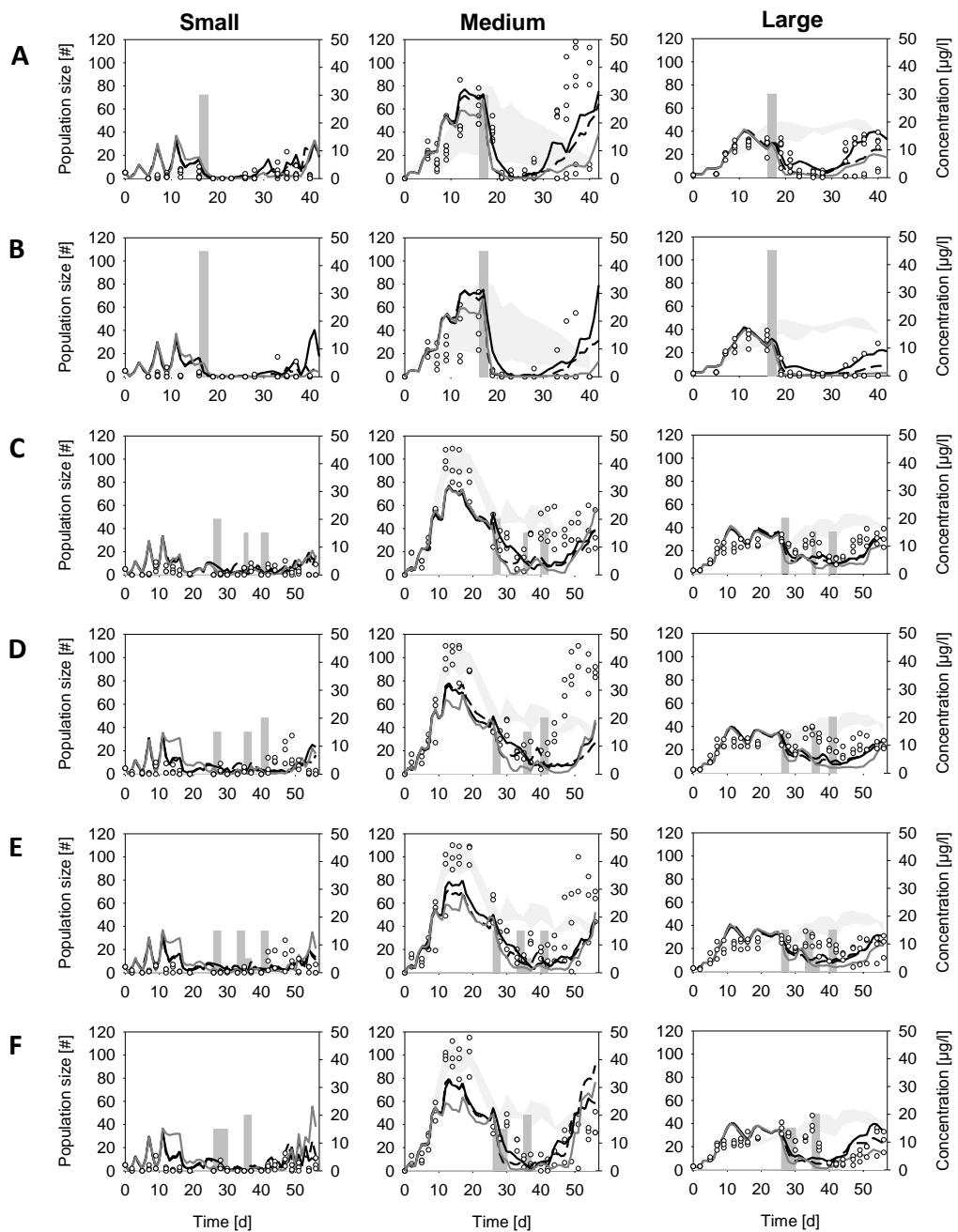


Figure S15: *Daphnia magna* population structure in TPT experiments as tested for various exposure scenarios: A-B) Single pulses, and C-F) multiple pulses. Dots represent measured abundance for each size class, dark grey bars represent exposure concentrations, and light grey shade is the empirical range of control abundance for each size class. Lines represent mean IBM predictions using different GUTS assumptions: GUTS-SIDS stochastic death size scaling (black solid line), GUTS-SICS stochastic death size scaling (black dashed line), GUTS-SIC stochastic death (grey solid line). Size classes used in model evaluation are: <1.25 mm (small), $\geq 1.25 - < 2.1$ mm (medium) and ≥ 2.1 mm (large).

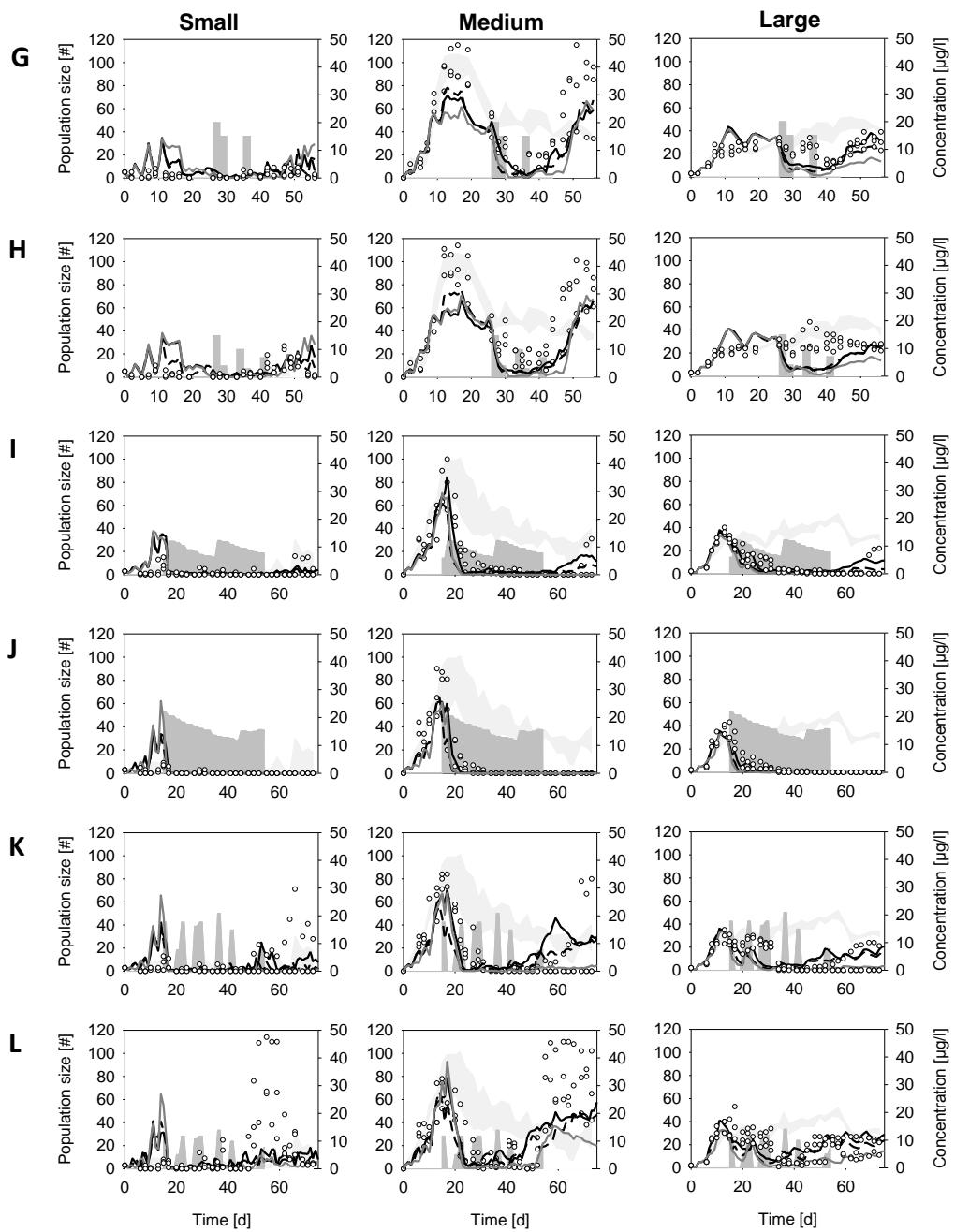


Figure S15 continued: ***Daphnia magna* population structure.** G-H) multiple pulses, I-J) lentic realistic exposure scenarios scaled by a factor of 250, and K-L) a lotic realistic exposure scenario scaled by factors of 15 and 10 respectively. Exposure scenarios A, E, G, I and L correspond to panels A, B, C, D, E of Figure 3 in the main text. Please note that a mismatch between modeled and measured size class abundances (e.g. small and medium) where total abundance is well predicted might be due to differences in the classification methods: sieving in experiments and grading individual body sizes in the IBM.

Table S1: **GUTS parameters** including mean values and confidence limits.

symbol	unit	description	Stochastic death		Individual tolerance	
			GUTS-SIC	GUTS-SIDS	GUTS-SIC	GUTS-SIDS
k_d	[h ⁻¹]	dominant rate constant	0.0029 (0.0021-0.0029)*	-	0.0016 (0.0013 - 0.0017)	-
k_{ul}	[h ⁻¹]	uptake rate constant	-	19.7021 (19.6999-34.9914)	-	19.7021 (19.6999-34.9914)
k_{el}	[h ⁻¹]	elimination rate constant	-	0.2901 (0.1558-0.2905)	-	0.2901 (0.1558-0.2905)
k_{u2}	[h ⁻¹]	uptake rate constant	-	0.0031 (0.0030-0.0126)	-	0.0031 (0.0030-0.0126)
k_{e2}	[h ⁻¹]	elimination rate constant	-	0.0008 [0-0.0009]	-	0.0008 [0-0.0009]
k_r	[h ⁻¹]	damage recovery rate constant	-	0.0002 (0.0001-0.0002)	-	0.0005 (0.0004-0.0006)
z	[$\mu\text{g L}^{-1}$]	threshold for effect	0.2102 (0-0.2104)*	0.8833 (0.4651-1.2074)	-	-
k_k	[h ⁻¹]	killing rate	0.0133 (0.0132-0.0143)*	0.0015 (0.0013-0.0016)	-	-
α	[$\mu\text{g L}^{-1}$]	median of the threshold distribution	-	-	1.5614 (0.0128 - 33.1600)	24.6613 (22.8814-26.2146)
β	[h ⁻¹]	shape parameter of the threshold distribution	-	-	2.1420 (0-1000)	3.5801 (3.1401-4.0428)

*parameter values from [2]

Table S2: Population data for the control in the single pulse exposure (**Control 1** in Figure S7). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3).

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	2	5	0	2	5	0	2
5	0	17	3	0	15	4	0	23	3
7	0	11	17	0	8	12	0	19	17
9	3	38	18	1	10	19	0	25	23
12	4	59	25	0	27	22	7	22	33
16	5	81	28	17	48	27	5	19	46
19	0	79	36	0	57	39	0	15	48
21	0	59	31	0	51	43	1	12	47
23	0	64	30	0	52	45	1	14	44
26	0	47	39	0	52	42	0	11	42
28	0	48	36	0	49	43	0	10	42
33	0	35	48	0	38	44	0	9	43
35	0	28	50	0	32	45	0	9	41
37	0	25	49	0	18	45	0	9	40
40	0	18	37	0	12	37	0	6	36

Table S3: Population data for the control in the multiple pulse experiments (**Control 2** in Figure S7). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3).

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	0	5	3	1	5	3	0	18	3
5	0	8	12	0	6	15	0	12	13
7	3	31	18	1	30	22	0	12	21
9	3	68	19	7	51	22	7	42	23
12	4	94	19	3	105	22	4	81	24
14	2	104	22	2	107	23	2	90	25
16	1	102	20	1	107	22	3	83	26
19	0	89	20	0	104	23	0	89	23
26	0	53	32	0	61	29	1	40	30
28	0	45	25	0	49	25	0	43	26
30	0	65	33	0	44	32	0	53	24
33	0	51	42	0	45	40	0	50	30
35	0	44	41	0	44	35	0	48	34
37	0	60	47	0	36	35	2	60	32
40	0	58	47	0	45	37	1	58	30
42	1	48	42	1	41	35	0	55	28
44	0	37	51	0	35	38	0	37	48
47	0	36	48	0	35	41	11	44	52
49	0	37	50	0	48	41	0	50	49
51	0	48	50	0	45	39	0	42	44
54	0	38	44	0	42	42	0	31	44
56	0	36	42	0	34	33	1	32	40

Table S4: Population data for the control in the realistic exposure scenario experiments (**Control 3** in Figure S7). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3).

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	3	0	2	3	0	2	3	0	2
6	0	26	5	0	21	5	0	8	5
8	2	32	14	0	29	20	0	26	13
10	3	45	17	9	56	27	1	42	16
13	0	66	25	9	62	36	9	64	27
15	4	77	27	2	54	29	1	92	23
17	0	77	26	1	50	29	0	99	16
20	0	78	37	2	62	36	0	99	27
22	0	70	30	2	49	35	0	101	25
24	1	51	28	0	42	34	1	88	28
27	2	33	30	2	43	24	2	81	26
29	9	34	25	7	37	24	1	64	21
31	3	32	37	10	39	29	7	71	25
34	2	36	38	5	37	34	1	54	35
36	4	26	48	11	36	36	2	55	31
38	3	33	38	7	41	38	0	59	28
41	0	31	41	1	39	35	0	56	32
43	0	28	43	0	35	37	0	42	35
45	3	25	41	2	38	38	2	40	35
48	0	26	44	0	36	44	0	49	35
50	0	26	42	1	31	46	0	36	43
52	12	22	43	3	35	45	10	39	39
55	3	30	44	0	34	49	2	37	47
57	2	31	44	0	26	43	5	25	52
59	11	26	41	4	17	38	14	31	43
62	3	32	32	0	16	22	0	28	28
64	0	29	30	0	7	26	0	28	27
66	1	26	30	30	6	29	15	27	27
69	2	30	29	18	30	33	11	23	33
71	1	24	30	21	36	31	9	21	34
73	2	22	28	18	40	32	7	16	34

Table S5: Population data for the single pulse experiment (**Scenario A** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for three replicates (R1-R3). Time variable exposure was initiated on day 16 and terminated on day 19. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	2	5	0	2	5	0	2
5	0	30	3	0	18	3	0	26	3
7	3	17	16	0	13	16	0	7	23
9	1	19	27	1	23	19	4	30	27
12	4	15	34	4	42	28	6	50	31
16	6	30	62	5	62	31	1	64	28
19	0	32	31	0	32	29	0	37	26
21	0	4	16	0	5	8	0	10	11
23	0	2	2	0	2	1	0	3	6
26	0	0	4	1	1	2	0	0	3
28	0	8	4	3	7	2	0	0	3
33	6	20	19	2	14	10	6	22	4
35	14	37	25	4	40	14	13	35	7
37	6	52	29	11	70	22	7	53	10
40	2	90	27	5	85	25	0	67	25

Table S6: Population data for the single pulse experiment (**Scenario A** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for three more replicates (R4-R6). Time variable exposure was initiated on day 16 and terminated on day 19. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R4:Cl1	R4:Cl2	R4:Cl3	R5:Cl1	R5:Cl2	R5:Cl3	R6:Cl1	R6:Cl2	R6:Cl3
0	5	0	2	5	0	2	5	0	2
5	0	24	3	0	32	3	0	17	3
7	0	6	21	0	12	21	2	30	21
9	5	28	27	3	16	25	2	54	32
12	1	44	26	5	45	30	8	85	33
16	1	47	17	2	54	29	0	78	31
19	0	34	21	0	39	30	0	41	8
21	0	4	15	0	2	15	0	0	9
23	0	7	3	0	1	1	0	0	1
26	0	3	6	0	0	1	0	3	1
28	0	3	6	0	0	1	0	3	1
33	14	54	23	0	0	1	2	53	14
35	2	79	34	0	0	1	23	51	30
37	1	118	37	2	12	1	11	80	34
40	0	154	26	3	12	7	3	100	32

Table S7: Population data for the single pulse experiment (**Scenario A** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for three more replicates (R7-R9). Time variable exposure was initiated on day 16 and terminated on day 19. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R7:Cl1	R7:Cl2	R7:Cl3	R8:Cl1	R8:Cl2	R8:Cl3	R9:Cl1	R9:Cl2	R9:Cl3
0	5	0	2	5	0	2	5	0	2
5	0	20	3	0	22	3	0	22	3
7	2	16	15	1	8	21	3	13	20
9	1	21	22	1	24	28	1	28	27
12	8	45	32	5	37	28	7	42	31
16	10	70	29	1	47	30	6	63	34
19	0	54	28	0	32	29	0	44	34
21	0	3	10	0	5	21	0	1	5
23	0	1	3	0	3	6	0	0	1
26	4	7	3	0	1	5	1	0	0
28	7	14	3	0	17	4	0	1	0
33	3	59	30	7	58	24	4	0	1
35	5	105	34	5	63	29	0	4	1
37	4	113	29	3	88	33	0	4	3
40	2	113	31	0	81	39	0	8	5

Table S8: Population data for the single pulse experiment (**Scenario B** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Time variable exposure was initiated on day 16 and terminated on day 19. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	2	5	0	2	5	0	2
5	0	30	3	0	17	3	0	22	3
7	4	29	19	2	11	20	0	18	19
9	8	35	32	3	28	20	0	14	25
12	1	50	39	1	62	23	0	18	36
16	2	52	31	1	73	22	3	23	35
19	0	3	4	0	6	3	0	1	1
21	0	0	0	0	2	1	0	0	0
23	0	0	0	0	1	1	0	0	0
26	0	0	0	0	0	0	0	0	0
28	0	0	0	0	0	0	0	0	0
33	0	0	0	0	0	0	0	0	0
35	0	0	0	0	0	0	0	0	0
37	0	0	0	0	0	0	0	0	0
40	0	0	0	0	0	0	0	0	0

Table S9: Population data for the multiple pulse experiment (**Scenario C** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Three pulses of TPT were initiated on day 26, 35 and 40 respectively. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	0	5	3	0	19	3	0	19	3
5	0	6	13	0	12	12	0	12	19
7	0	28	17	1	23	21	1	32	31
9	8	56	17	3	55	25	11	57	31
12	8	98	17	3	108	24	3	92	33
14	7	109	17	4	90	23	2	80	31
16	4	108	17	0	89	22	0	78	31
19	0	90	19	0	80	23	1	63	31
26	0	52	24	0	47	29	0	24	27
28	0	38	18	0	30	20	1	21	25
30	0	36	15	0	23	17	0	32	18
33	0	4	41	0	5	23	0	15	27
35	6	3	39	6	15	21	0	22	32
37	6	36	33	10	35	13	3	35	24
40	0	36	28	1	53	12	0	31	19
42	9	38	28	6	57	12	0	29	20
44	8	35	27	3	59	7	4	22	20
47	1	33	33	12	39	29	0	26	24
49	4	30	25	0	45	44	2	30	23
51	1	30	25	5	45	36	3	53	25
54	0	21	32	0	38	40	0	60	23
56	0	23	33	0	32	46	9	56	22

Table S10: **Population data** for the multiple pulse experiment (**Scenario D** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Three pulses of TPT were initiated on day 26, 35 and 40 respectively. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	0	10	3	2	17	3	0	5	3
5	0	9	15	2	19	10	1	15	9
7	1	28	23	1	29	29	0	34	17
9	7	59	23	10	64	29	0	27	23
12	9	110	23	1	99	29	1	90	27
14	8	110	23	2	105	30	1	94	23
16	3	110	23	0	108	27	0	78	30
19	0	89	23	0	88	27	0	89	25
26	0	45	25	0	37	24	0	36	35
28	2	37	23	9	30	23	3	25	32
30	0	47	18	0	46	16	0	33	23
33	0	20	30	0	19	38	0	14	38
35	5	18	39	2	25	33	6	13	40
37	2	10	34	2	28	30	1	10	27
40	0	8	29	0	20	21	0	4	19
42	14	17	18	1	27	28	4	6	18
44	10	44	15	14	28	23	11	34	13
47	28	81	20	9	50	30	21	67	17
49	9	105	20	12	77	34	33	84	24
51	7	110	20	4	92	32	12	121	20
54	0	103	24	3	89	27	1	69	21
56	0	87	23	3	83	28	0	92	21

Table S11: **Population data** for the multiple pulse experiment (**Scenario E** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Two pulses of TPT were initiated on day 26 and 40 respectively. In between these two pulses exposure was 15 µg/L on days 33 and 34 and 5 µg/L on days 35 and 36. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	0	13	3	0	16	3	2	5	2
5	0	9	10	0	12	16	0	6	7
7	1	30	19	2	20	26	1	20	11
9	7	61	19	5	56	27	6	19	16
12	3	102	20	0	94	26	3	49	24
14	5	110	19	0	99	26	7	89	28
16	1	109	20	1	94	26	1	100	28
19	0	109	20	0	93	26	0	108	29
26	0	63	25	0	43	31	0	67	28
28	1	35	22	0	27	27	0	44	29
30	0	36	18	1	20	20	1	36	21
33	0	13	24	0	8	22	0	20	35
35	4	12	32	0	15	22	5	11	30
37	0	27	25	1	25	13	1	34	22
40	0	12	27	0	18	9	0	22	23
42	10	6	23	2	10	17	18	24	19
44	19	32	16	4	10	10	4	21	15
47	28	65	21	1	10	4	16	22	20
49	10	68	20	5	1	6	19	43	29
51	12	100	27	0	8	7	1	70	28
54	5	83	29	5	26	7	0	67	24
56	0	64	26	7	44	12	0	70	31

Table S12: **Population data** for the multiple pulse experiment (**Scenario F** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Three pulses of TPT were initiated on day 26, 28 and 35 respectively. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	0	5	3	0	13	3	2	6	3
5	0	7	9	0	15	9	0	9	11
7	2	32	17	5	18	23	1	30	21
9	13	52	19	2	43	25	2	59	22
12	3	102	21	0	99	25	2	96	23
14	1	112	21	1	90	25	0	97	27
16	0	105	22	1	97	24	3	79	33
19	0	115	27	0	81	27	0	103	28
26	0	49	36	0	32	31	0	38	41
28	4	29	31	9	27	29	2	28	32
30	2	39	17	0	42	25	0	49	25
33	0	17	25	0	27	28	0	27	29
35	0	3	34	0	13	38	0	10	47
37	0	6	17	0	14	20	0	4	23
40	0	6	6	1	14	5	0	0	6
42	0	2	4	6	10	6	4	0	5
44	1	5	4	8	16	9	5	17	5
47	4	7	4	15	27	12	10	35	9
49	0	8	7	5	34	13	1	39	17
51	3	2	11	0	49	20	7	40	20
54	2	27	12	0	34	36	0	37	33
56	11	51	15	5	33	33	2	33	26

Table S13: **Population data** for the multiple pulse experiment (**Scenario G** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Three pulses of TPT were initiated on day 26, 28 and 35 respectively. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	1	12	3	0	5	3	5	5	3
5	0	16	12	0	13	9	0	9	9
7	6	24	28	0	25	22	1	30	18
9	2	73	27	8	65	22	4	57	18
12	0	75	26	4	96	22	2	97	19
14	0	89	30	0	92	30	3	112	23
16	2	88	27	3	88	24	1	115	28
19	0	80	30	0	81	24	0	111	25
26	0	35	30	0	53	28	0	56	34
28	1	22	24	0	25	26	2	31	26
30	0	27	19	0	17	20	0	34	18
33	0	9	23	0	3	25	0	9	29
35	0	4	28	2	5	26	7	6	34
37	4	2	17	4	21	17	5	20	27
40	0	9	11	2	20	15	1	19	11
42	6	21	8	9	19	14	3	18	13
44	9	32	14	1	31	13	2	29	15
47	9	74	29	1	54	24	2	33	19
49	2	86	27	8	84	29	2	38	32
51	3	115	24	9	80	30	5	40	39
54	0	87	26	1	100	31	0	35	35
56	2	85	23	0	96	30	3	34	39

Table S14: **Population data** for the multiple pulse experiment (**Scenario H** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). Five pulses of TPT were initiated on day 26, 28, 33, 35 and 40 respectively. For an overview on TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	5	0	3	5	0	3	5	0	3
2	0	12	3	0	5	3	2	5	3
5	0	16	9	0	6	12	0	7	12
7	1	23	22	0	32	18	2	26	18
9	5	39	23	10	51	19	6	49	18
12	0	88	24	6	105	20	1	111	19
14	2	88	24	3	106	24	2	90	26
16	4	93	25	0	114	18	0	80	24
19	0	86	25	0	105	21	0	63	24
26	0	53	26	0	40	27	0	32	32
28	0	23	27	0	29	29	3	19	24
30	0	28	20	0	49	31	0	36	18
33	0	9	25	0	23	40	0	23	24
35	5	9	26	2	14	47	2	19	24
37	4	24	22	0	12	41	3	24	24
40	5	20	24	0	6	36	0	12	29
42	19	27	21	12	6	36	8	20	31
44	8	50	25	4	13	33	4	41	30
47	24	76	30	6	20	27	27	68	30
49	17	76	28	8	40	27	12	81	29
51	17	83	27	9	55	28	18	101	24
54	4	93	28	1	57	24	2	99	23
56	0	76	27	2	61	28	1	86	22

Table S15: Population data for the realistic exposure scenario experiment (**Scenario I** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). For TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	3	0	2	3	0	2	3	0	2
6	0	16	5	1	30	6	1	31	5
8	0	14	20	0	26	20	1	21	20
10	2	46	26	0	25	27	0	34	31
13	2	60	34	13	30	40	0	54	36
15	5	90	27	15	64	33	8	63	30
17	0	100	21	0	80	26	2	56	28
20	0	68	11	0	50	19	2	42	26
22	0	16	6	1	21	12	1	27	16
24	0	2	7	1	9	17	0	21	8
27	0	1	8	0	4	15	0	17	9
29	0	2	3	0	3	13	6	10	14
31	1	1	4	0	2	8	5	8	12
34	1	2	4	0	1	1	1	6	4
36	0	3	3	2	1	1	0	5	4
38	4	1	3	0	0	2	0	5	3
41	0	3	2	0	0	1	0	1	4
43	2	5	1	0	0	1	0	0	2
45	0	4	1	0	0	0	0	0	1
48	0	1	3	0	0	0	0	0	0
50	5	1	3	0	0	0	0	0	0
52	0	0	1	0	0	0	0	0	0
55	0	0	1	0	0	0	0	0	0
57	0	0	1	0	0	0	0	0	0
59	0	0	1	0	0	0	0	0	0
62	0	0	1	0	0	0	0	0	0
64	0	0	1	0	0	0	0	0	0
66	16	0	1	0	0	0	0	0	0
69	14	8	16	0	0	0	0	0	0
71	15	26	21	0	0	0	0	0	0
73	5	31	22	0	0	0	0	0	0

Table S16: Population data for the realistic exposure scenario experiment (**Scenario J** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). For TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	3	0	2	3	0	2	3	0	2
6	5	34	5	0	16	4	0	44	5
8	3	34	22	0	27	22	0	20	27
10	0	51	23	0	43	25	0	46	35
13	2	90	33	1	49	39	3	65	41
15	9	87	28	6	81	30	7	52	43
17	3	81	20	6	55	26	0	20	35
20	0	28	4	0	29	17	0	6	11
22	0	14	3	0	15	9	0	4	3
24	0	4	7	0	8	13	0	2	3
27	0	7	3	0	1	9	0	0	3
29	0	4	4	3	4	6	1	0	3
31	0	1	4	0	3	4	3	0	3
34	0	0	3	0	0	0	0	0	1
36	0	0	2	0	0	0	0	0	0
38	0	0	2	0	0	0	0	0	0
41	0	0	1	0	0	0	0	0	0
43	0	0	1	0	0	0	0	0	0
45	0	0	1	0	0	0	0	0	0
48	0	0	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0	0	0
52	0	0	0	0	0	0	0	0	0
55	0	0	0	0	0	0	0	0	0
57	0	0	0	0	0	0	0	0	0
59	0	0	0	0	0	0	0	0	0
62	0	0	0	0	0	0	0	0	0
64	0	0	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0	0	0
69	0	0	0	0	0	0	0	0	0
71	0	0	0	0	0	0	0	0	0
73	0	0	0	0	0	0	0	0	0

Table S17: Population data for the realistic exposure scenario experiment (**Scenario K** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3). For TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	3	0	2	3	0	2	3	0	2
6	0	21	5	1	30	5	0	24	6
8	0	31	23	0	25	17	0	28	16
10	1	63	25	3	25	23	3	25	23
13	1	66	35	1	43	23	3	72	30
15	1	80	31	8	71	22	13	84	25
17	3	63	25	3	73	18	11	84	21
20	0	54	24	0	52	21	0	58	14
22	0	43	29	2	20	27	0	27	17
24	0	18	30	0	12	28	3	15	19
27	1	6	27	1	2	22	1	38	26
29	0	5	24	6	10	23	0	17	19
31	0	1	24	3	8	20	0	1	20
34	0	0	6	0	3	0	0	1	1
36	0	0	3	6	3	0	0	1	1
38	0	0	1	4	0	3	0	0	0
41	0	0	0	0	4	1	0	0	0
43	0	0	0	2	3	0	0	0	0
45	0	0	0	2	1	2	0	0	0
48	0	0	0	0	2	3	0	0	0
50	0	0	0	15	2	3	0	0	0
52	0	0	0	23	4	4	0	0	0
55	0	0	0	14	9	5	0	0	0
57	0	0	0	18	6	8	0	0	0
59	0	0	0	13	8	10	0	0	0
62	0	0	0	25	15	16	0	0	0
64	0	0	0	45	23	21	0	0	0
66	0	0	0	71	26	22	0	0	0
69	0	0	0	30	78	24	0	0	0
71	0	0	0	41	67	24	0	0	0
73	0	0	0	28	80	21	0	0	0

Table S18: Population data for the realistic exposure scenario experiment (**Scenario L** in Figures S8-S15). For each census time, the TPT exposure concentration as well as the number of *Daphnia magna* individuals within three size classes (Cl1-Cl3) is given for the three replicates (R1-R3) For TPT exposure concentrations applied during the experiment see Table S19.

time [d]	R1:Cl1	R1:Cl2	R1:Cl3	R2:Cl1	R2:Cl2	R2:Cl3	R3:Cl1	R3:Cl2	R3:Cl3
0	3	0	2	3	0	2	3	0	2
6	1	31	5	0	38	5	0	28	5
8	3	27	24	0	19	26	0	39	25
10	1	24	26	0	36	36	0	30	30
13	0	40	40	0	74	40	3	40	30
15	8	52	29	6	74	42	5	78	28
17	7	51	35	1	57	53	5	77	25
20	0	46	24	0	42	21	1	68	31
22	3	11	30	0	21	23	0	56	34
24	0	7	27	0	6	21	0	40	35
27	0	8	30	1	14	27	0	25	18
29	1	4	24	14	1	19	0	14	31
31	3	7	21	9	0	15	1	3	34
34	0	5	1	0	14	7	1	2	8
36	6	1	4	0	9	11	0	2	6
38	1	4	3	25	4	6	16	3	4
41	0	2	4	0	24	4	0	20	4
43	0	1	4	0	22	10	0	19	2
45	0	1	4	0	9	20	0	6	15
48	28	0	5	0	0	27	0	0	20
50	36	3	5	20	0	27	76	2	20
52	40	17	5	109	3	25	160	27	20
55	65	33	27	67	79	24	114	97	20
57	150	37	26	38	77	21	110	109	18
59	110	58	26	26	60	11	66	103	12
62	47	80	27	13	60	9	18	110	8
64	20	62	27	9	55	13	8	110	7
65	32	72	24	12	46	10	30	108	8
69	8	79	26	4	48	26	4	102	10
71	5	80	25	4	38	23	3	86	14
73	5	65	23	4	42	22	4	102	11

Table S19: **Nominal exposure concentrations** applied during the population experiments. For scenarios also see Figures S8-S15 and resulting data for *Daphnia magna* population sizes is given in Tables S5-S18.

time [d]	exposure scenario											
	A	B	C	D	E	F	G	H	I	J	K	L
0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	6.0	21.9	17.7	11.8	
15	0	0	0	0	0	0	0	6.0	21.9	17.7	11.8	
16	30	45	0	0	0	0	0	12.1	20.6	0	0	
17	30	45	0	0	0	0	0	12.1	20.6	0	0	
18	0	0	0	0	0	0	0	12.1	20.6	0	0	
19	0	0	0	0	0	0	0	11.5	19.4	7.7	5.1	
20	0	0	0	0	0	0	0	11.5	19.4	7.7	5.1	
21	0	0	0	0	0	0	0	10.5	18.4	17.7	11.8	
22	0	0	0	0	0	0	0	10.5	18.4	17.7	11.8	
23	0	0	0	0	0	0	0	9.0	17.5	0	0	
24	0	0	0	0	0	0	0	9.0	17.5	0	0	
25	0	0	0	0	0	0	0	9.0	17.5	0	0	
26	0	0	20	15	15	15	20	15	8.4	16.8	16.3	10.8
27	0	0	20	15	15	15	20	15	8.4	16.8	16.3	10.8
28	0	0	0	0	0	15	15	4	7.3	16.1	17.7	11.8
29	0	0	0	0	0	15	15	4	7.3	16.1	17.7	11.8
30	0	0	0	0	0	0	0	6.8	15.5	0	0	
31	0	0	0	0	0	0	0	6.8	15.5	0	0	
32	0	0	0	0	0	0	0	6.8	15.5	0	0	
33	0	0	0	0	0	0	0	6.4	13.7	0	0	
34	0	0	0	0	0	0	0	6.4	13.7	0	0	
35	0	0	15	15	15	20	15	10	12.3	13.2	20.9	14.0
36	0	0	0	15	15	20	15	10	12.3	13.2	20.9	14.0
37	0	0	0	0	5	0	0	3	11.8	12.9	0	0
38	0	0	0	0	5	0	0	3	11.8	12.9	0	0
39	0	0	0	0	0	0	0	0	11.8	12.9	0	0
40	0	0	15	20	15	0	0	7	10.9	12.5	14.9	9.9
41	-	-	15	20	15	0	0	7	10.9	12.5	14.9	9.9
42	-	-	0	0	0	0	0	0	10.1	11.8	0.4	0.3
43	-	-	0	0	0	0	0	0	10.1	11.8	0.4	0.3
44	-	-	0	0	0	0	0	0	9.4	15.2	0	0
45	-	-	0	0	0	0	0	0	9.4	15.2	0	0
46	-	-	0	0	0	0	0	0	9.4	15.2	0	0
47	-	-	0	0	0	0	0	0	8.8	14.8	0	0
48	-	-	0	0	0	0	0	0	8.8	14.8	0	0
49	-	-	0	0	0	0	0	0	8.2	15.1	0	0
50	-	-	0	0	0	0	0	0	8.2	15.1	0	0
51	-	-	0	0	0	0	0	0	7.8	15.7	7.5	5.0
52	-	-	0	0	0	0	0	0	7.8	15.7	7.5	5.0
53	-	-	0	0	0	0	0	0	7.8	15.5	7.8	7.8
54	-	-	-	-	-	-	-	-	0	0	0	0

Table S20: **Survival** of large bodied *Daphnia magna* exposed to pulses of TPT.

time [h]	exposure concentration [µg/L]	fraction surviving [-]										
0	0	1	20	1	10	1	10	1	10	1	10	1
24	0	1	20	0.97	10	1	10	1	10	1	10	1
48	0	1	0	0.91	0	1	0	1	0	0.875	0	1
72	0	1	0	0.74	0	-	0	-	0	-	0	-
96	0	-	0	-	0	-	10	-	0	-	0	-
120	0	1	0	0.38	0	1	10	0.63	10	0.75	0	0.63
144	0	1	0	0.21	0	1	0	0.63	10	0.63	10	0.50
168	0	1	0	0.06	0	0.88	0	0.63	0	0.38	10	0.50
192	0	1	0	0	0	0.50	0	0.38	0	0.13	0	0.30
216	0	1	0	0	0	0.25	0	0.25	0	0.13	0	0.13
240	0	1	0	0	0	0.25	0	0.25	0	0.13	0	0
288	0	0.75	0	0	0	0.25	0	0.25	0	0.13	0	0

Table S21: **Bioconcentration of TPT** (mean internal concentration C_i and standard deviation sd) in three sizes classes (large, intermediate and small) of *D. magna*.

time [h]	large		intermediate		small	
	mean C_i [dpm/mg]	sd [dpm/mg]	mean C_i [dpm/mg]	sd [dpm/mg]	mean C_i [dpm/mg]	sd [dpm/mg]
uptake experiment						
6	296.25	48.24			285.13	85.23
24	404.48	77.46			738.37	140.07
48	500.31	131.16			620.23	120.33
72	370.97	139.82			806.32	275.63
elimination experiment						
0	474.48	85.09			573.7	103.27
24	406.94	92.04			563.23	214.89
72	312.34	82.91			207.5	127.37
96	295.74	53.33			176.44	50.84
168	-				100.12	105.47
					54.17	31.5

Calculation of realistic exposure scenarios

The FOCUS surface water methodology at Step 3 comprises ten scenarios that are supposed to represent realistic worst case combinations of soil, agriculture and weather across Europe [3]. These simulations were used in conjunction with a suite of models (FOCUS-MACRO, FOCUS-PRZM and FOCUS-TOXSWA) to generate predicted environmental concentrations (PECs) in surface water and sediment. In the current study, the pesticide application was assumed for potatoes few weeks after plant emergence with three applications of 320 g/ha. From the resulting exposure patterns stream R3 (Fig. S16) and pond R1 (Fig. S17) scenarios were selected as representatives for highly fluctuating and more constant exposure respectively. The scenarios were slightly changed to match the media renewal scheme of the *D. magna* population experimental design and were scaled up to induce pronounced effects on the daphnia populations: the concentrations were multiplied by factors of 10 or 15 (stream patterns) and 150 (pond patterns).

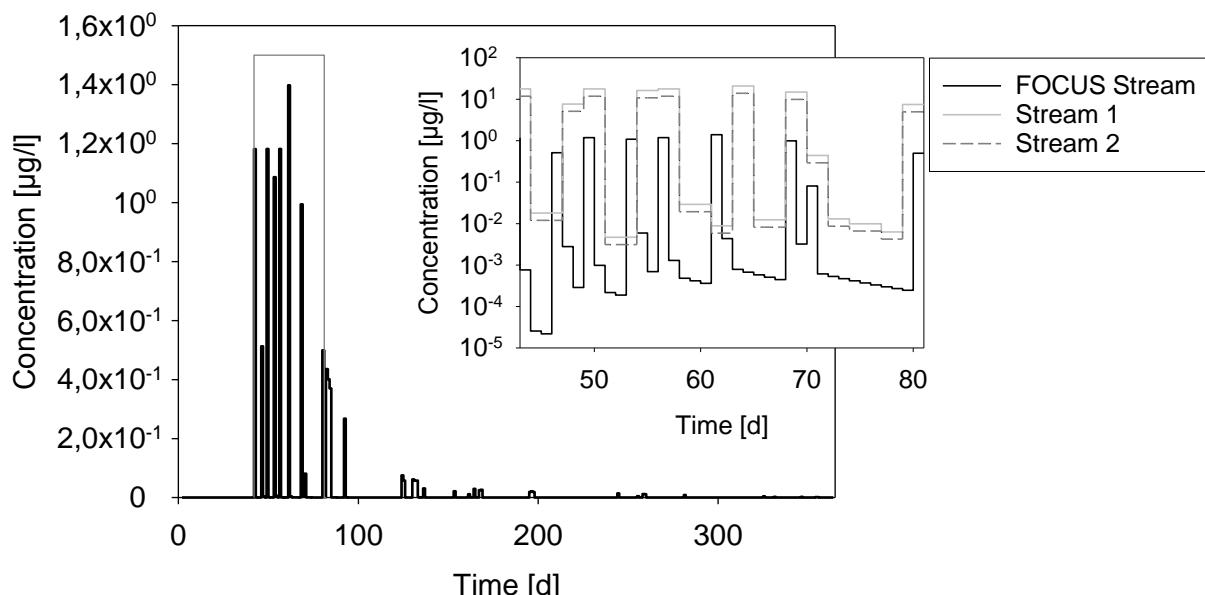


Figure S16: The calculated stream R3 scenario and the extracted exposure scenarios to be used in population experiments. A 35 day window was selected and the concentrations were adjusted to fit the media renewal interval in the population test. The concentrations were multiplied by a factors of 10 (stream1) and 15 (stream 2). The Stream 1 and Stream 2 scenarios correspond to the scenarios K and L in Table S18.

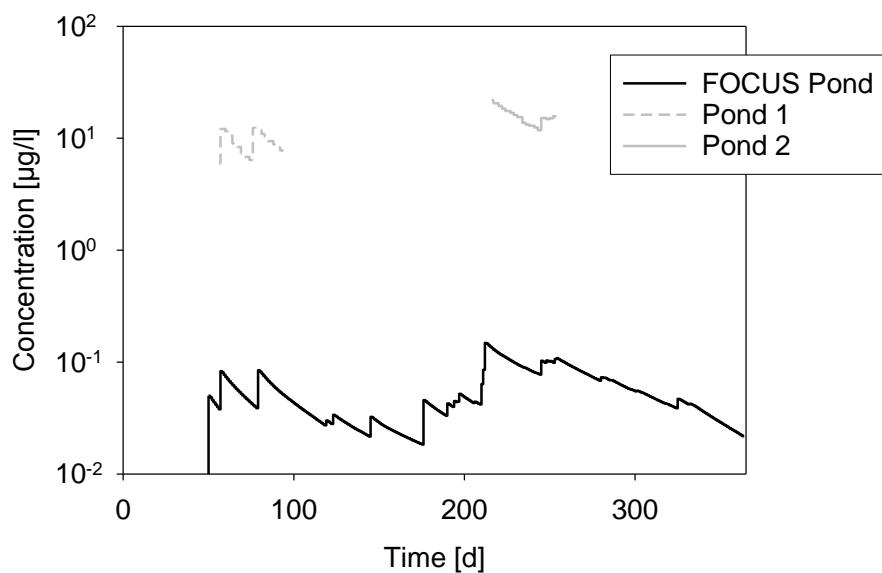


Figure S17: The calculated pond R1 scenario and the extracted exposure scenarios to be used in population experiments. A 35 day window was selected and the concentrations were adjusted fit to the media renewal interval in the population test. The concentrations were multiplied by a factor of 150. The Pond 1 and Pond 2 scenarios correspond to the scenarios I and J in Table S18.

References

- [1] Jager, T.; Albert, C.; Preuss, T.G.; Ashauer, R. General unified threshold model of survival – a toxicokinetic-toxicodynamic framework for ecotoxicology. *Environ. Sci. Technol.* **2011**, *45*, 2529–2540.
- [2] Gergs, A.; Kulkarni, D.; Preuss, T. G. Body size-dependent toxicokinetics could explain intra- and interspecies variability in toxicodynamics. *Environ. Pollut.* **2015**, *206*, 449–455.
- [3] *FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC*. Report of the FOCUS Working Group on Surface Water Scenarios, EC Document Reference SANCO/4802/2001-rev.2. 2001.