Supporting Information

Effect-Directed Analysis of contaminated sediments with partition-based dosing using green algae cell multiplication inhibition

Nicole Bandow†, Rolf Altenburger‡, Georg Streck†, Werner Brack†*

†UFZ – Helmholtz Centre for Environmental Research, Department of Effect-Directed Analysis, Permoserstraße 15, 04315 Leipzig, Germany

‡ UFZ – Helmholtz Centre for Environmental Research, Department of Bioanalytical Ecotoxicology, Permoserstraße 15, 04315 Leipzig, Germany

*Corresponding author. E-mail address: werner.brack@ufz.de

Phone: +493412351531 fax: +493412351785

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Table S1: identified compounds, supplier, used column for separation during the GC-MS analysis and used SPME-fibres for concentration measurements in aqueous samples.

compound	CAS number	supplier	column	SPME – fibre[1]
hexadecanol	36653-82-4	Aldrich	VF200MS	-
triclosan	3380-34-5	Merck	DB-17 MS	PA
benz[*c*]acridine	225-11-6	Chiron	VF200MS	PA
diphenylsulfone	127-63-9	Alfa Aesar	DB-17 MS	PA
N-butylbenzensulfonamid	3622-84-2	Ehrenstorfer	DB-17 MS	Mix
palmitic acid	629-73-2	Aldrich	VF200MS	-
pentadecanol	629-76-5	Merck	VF200MS	-
2-methylanthraquinone	84-54-8	TCI	DB-17 MS	PA
7-H-benzo[*de*]-anthracen-7-one	82-05-3	Fluka	DB-17 MS	PA
cyclopenta[*def*]phenanthren-4-one	5737-13-3	Chiron	DB-17 MS	PA
fluoranthene	206-44-0	Fluka	DB-17 MS	-
benzo[*b*]fluoranthene	205-99-2	Promochem	DB-17 MS	-
benzo[*e*]pyrene	192-97-2	Aldrich	DB-17 MS	-
benzo[*j*]fluoranthene	205-82-3	Promochem	DB-17 MS	-
benzo[*k*]fluoranthene	207-08-9	Promochem	DB-17 MS	-
benzo[*a*]fluoranthene	56-55-3	Promochem	DB-17 MS	-
perylene	198-55-0	Fluka	DB-17 MS	-
benzo[*a*]pyrene	50-32-8	Aldrich	DB-17 MS	-
indeno[123,*cd*]fluoranthene	193-43-1	Promochem	DB-17 MS	-
indeno[123,*cd*]pyrene	193-39-5	BCR	DB-17 MS	-
benzo[*ghi*]perylene	191-24-2	Aldrich	DB-17 MS	-
dibenzo[*ah*]anthracene	53-70-3	Fluka	DB-17 MS	-

[1]PA: polyacrylate fibre, Mix: divinylbenzene/carbowax/polydimethylsiloxane fibre

Table S2: Description of the gradients of the RP HPLC-method. The ratio ACN/H_2O (v/v) is given at specified times.

fraction	t (min)	ratio ACN/H_2O
F8, F10	0	40/60
	59	100/0
F11	0	50/50
	49	100/0
F14	0	30/70
	70	70/30
	90	100/0
F15, F16	0	20/80
	90	60/40
	110	100/0

Table S3: Compounds and their log K_{OW} values used to determine the log K_{OW} windows of the RP HPLC.

compound	log K_{OW}*
thiocarbamate	-1.31
1,2-benzenediol	1.03
nitrobenzene	1.81
chlorobenzene	2.90
biphenyl	3.76
fluoranthene	4.93
hexachlorobenzene	5.86
PCB153	7.62
PCB 209	9.60

* predicted values, Epi Suite v.3.20, 2007, U.S. Environmental Protection Agency.

Table S4: Tentatively identified compounds in fractions 15-6, log K_{OW} values and expected log K_{OW} range from RP HPLC for sub-fraction 15-6.

log K_{OW} expected	compound	log K_{OW}*
2.93-3.37	p-tert-butyl-phenol	3.42
	1,1'-(1,2-ethanediyl)bisbenzene	4.74
	dihydro-5-pentyl-2(3H)furanone,	2.08
	benzophenone	3.15
	1(2H)acenaphthylenone	2.79
	2,3-dihydro-1-oxo-1H-phenalene	3.28
	N-butyl-benzenesulfonamide	2.31
	anthrone	3.81
	diphenylsulfone	2.61
	7H-Benz[*de*]anthracen-7-one	4.73

* predicted values, Epi Suite v.3.20, 2007, U.S. Environmental Protection Agency.

Table S5: Parameters for dose-response curves fitted to fractions (F) and corresponding artificial mixtures (Mix). A three parameter sigmoid model was used for fitting ($y = a/(1+\exp((x-x_0)/b))$).

Sample	a	b	x_0
F10-6	75.93	3.77	21.51
Mix 10-6	60.75	4.73	18.53
F10-5	59.79	3.49	18.32
Mix 10-5	55.87	5.78	11.12
F11	67.22	2.98	10.03
Mix 11	45.54	4.15	18.75
F 8-7	75.34	32.56	90.42
Mix 8-7	92.50	16.08	70.85
F15-16	56.77	61.68	493.97
Mix 15-16	73*	76.00	365
F14-7	71.60	2.05	11.29
Mix14-7	92*	1.59	9.74
F15 RS	58.82	2.60	15.58
Mix 15 RS	48.91	5.10	17.51
F15-15	29.26	2.70	7.24
Mix 15-15	57.94	41.96	109.59

* These values have been fixed for the fitting, because otherwise no meaningful fits were achieved.

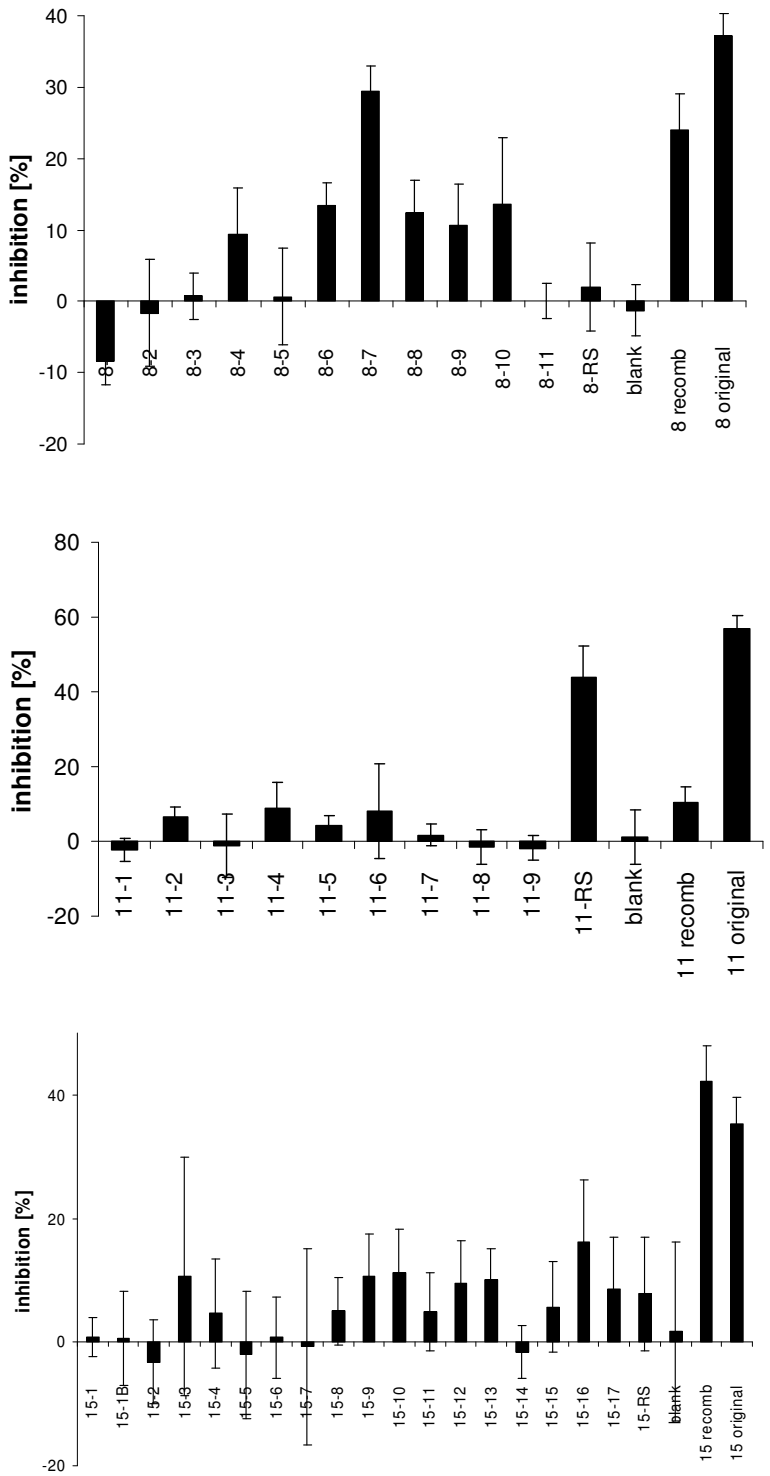

Figure S1: Growth inhibition of the green algae *Scenedesmus vacuolatus* exposed for 24 h to sub-fractions of Bílina sediment extract dosed with DMSO to the test system (c = 40 g SEQ/L). Recombination of all sub-fractions (recomb) and original fraction (c = 20 g SEQ/L). The sediment extract was first fractionated with NP HPLC and then with RP HPLC as second fractionation step.

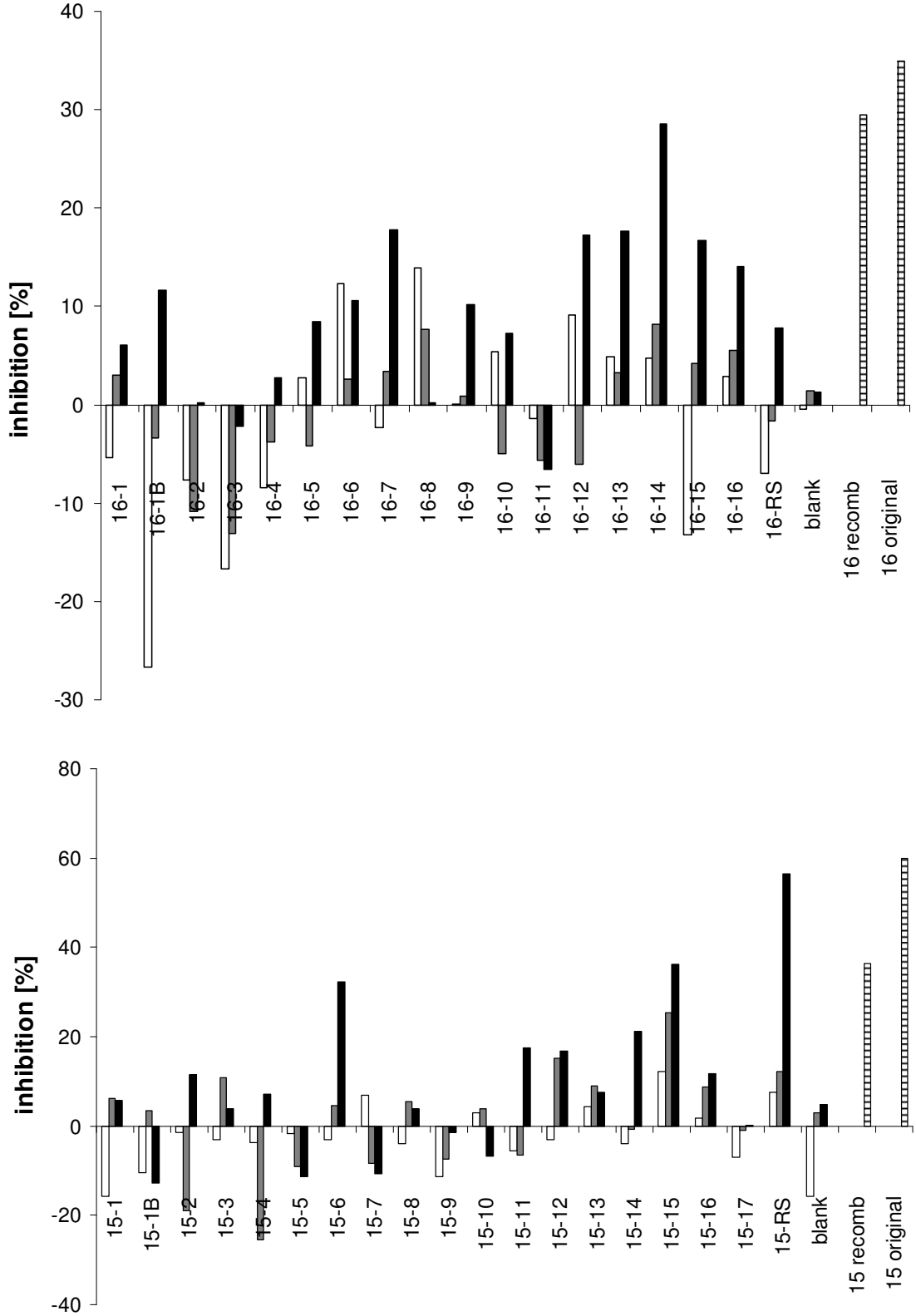

Figure S2: Growth inhibition of the green algae *Scenedesmus vacuolatus* exposed for 24 h to sub-fractions, residue (RS) and recombination of all sub-fractions (recomb) of Bílina sediment extract dosed with silicone rods (SRs) to the test system.□ 6.25 g SEQ/SR, ■ 12.5 g SEQ/SR, ■ 25 g SEQ/SR, ▤ 10 g SEQ/SR. The sediment extract was first fractionated with NP HPLC and then with RP HPLC as the second fractionation step.

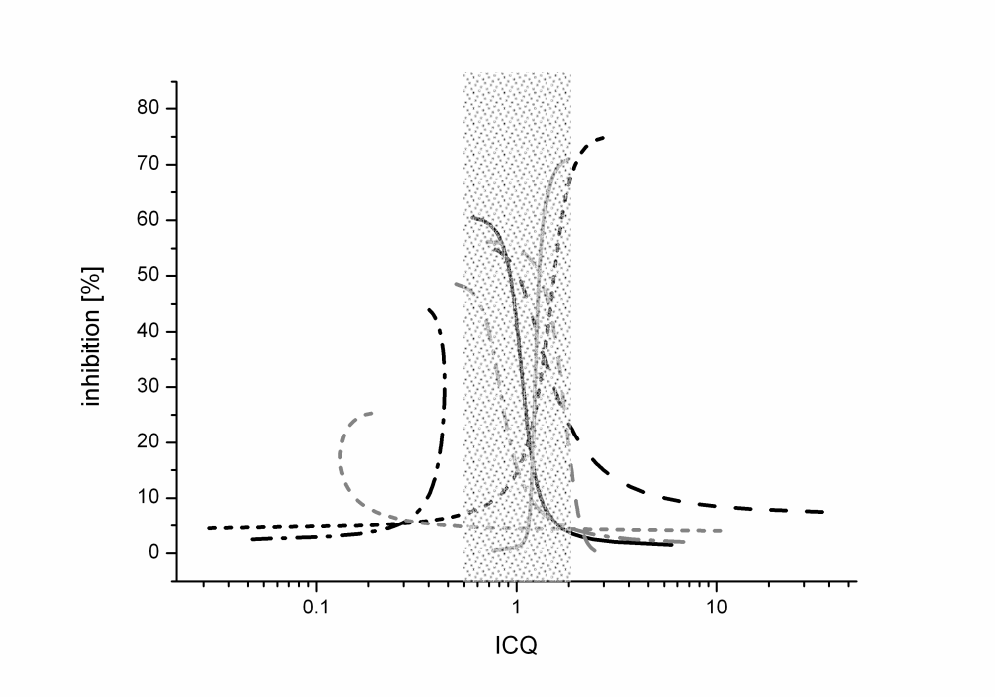

Figure S3: Index of Confirmation Quality of sub-fractions for dosing with DMSO (— F10-6, – – F10-5 – · – F11, ... F8-7 and _ _ F15-16) and for dosing with SRs (— F14-7, ... F15-15 and _ · _ F15 RS). The range of ICQ between 0.5 and 2 is shaded in grey.