Supplementary Material

MANUSCRIPT TITLE: Sedimentary loadings and ecological significance of polycyclic aromatic hydrocarbons in a typical mariculture zone of South China

AUTHORS: Huan-Yun Yu, Lian-Jun Bao, Charles S. Wong, Yuanan Hu* and Eddy Y. Zeng

ADDRESS: State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou 510640, China,; Richardson College for the Environment, Environmental Studies Program and Department of Chemistry, University of Winnipeg, Winnipeg, Manitoba R3B 2E9, Canada; Graduate School, Chinese Academy of Sciences, Beijing 100049, China; and Guangdong Key Laboratory of Agricultural Environment Pollution Integrated Control, Guangdong Institute of Eco-Environmental and Soil Sciences, Guangzhou, China

NO. OF FIGURES: 2

NO. OF TABLES: 4

NO. OF PAGES: 9

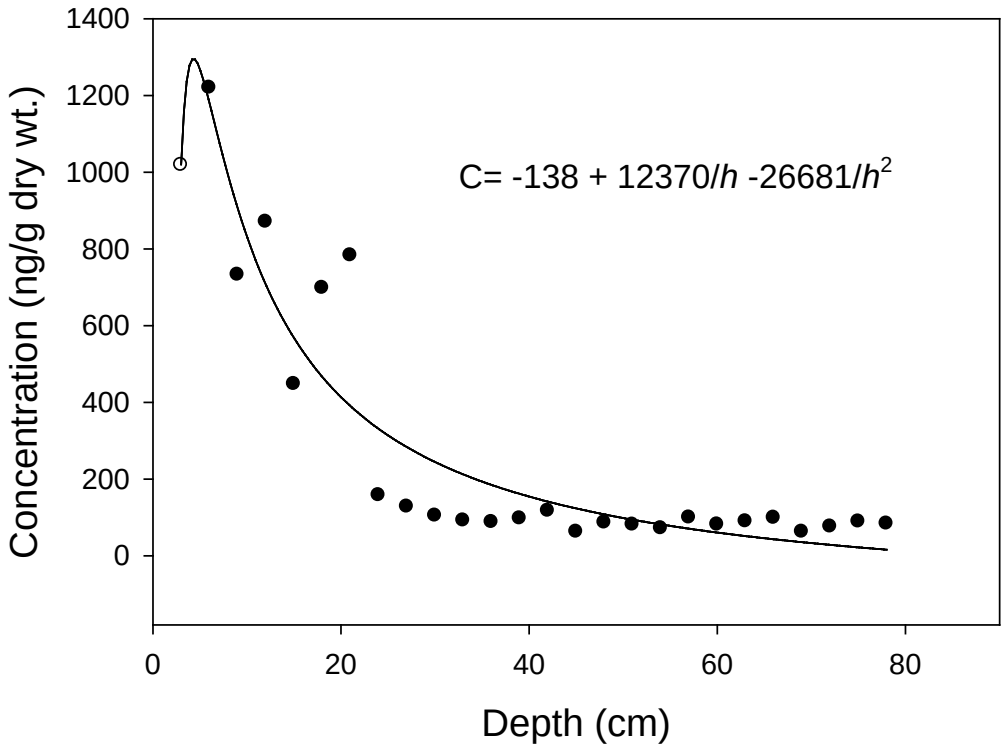

Figure S1. Variation of measured concentrations of PAHs in sediment core B with depth, and related regression curve.

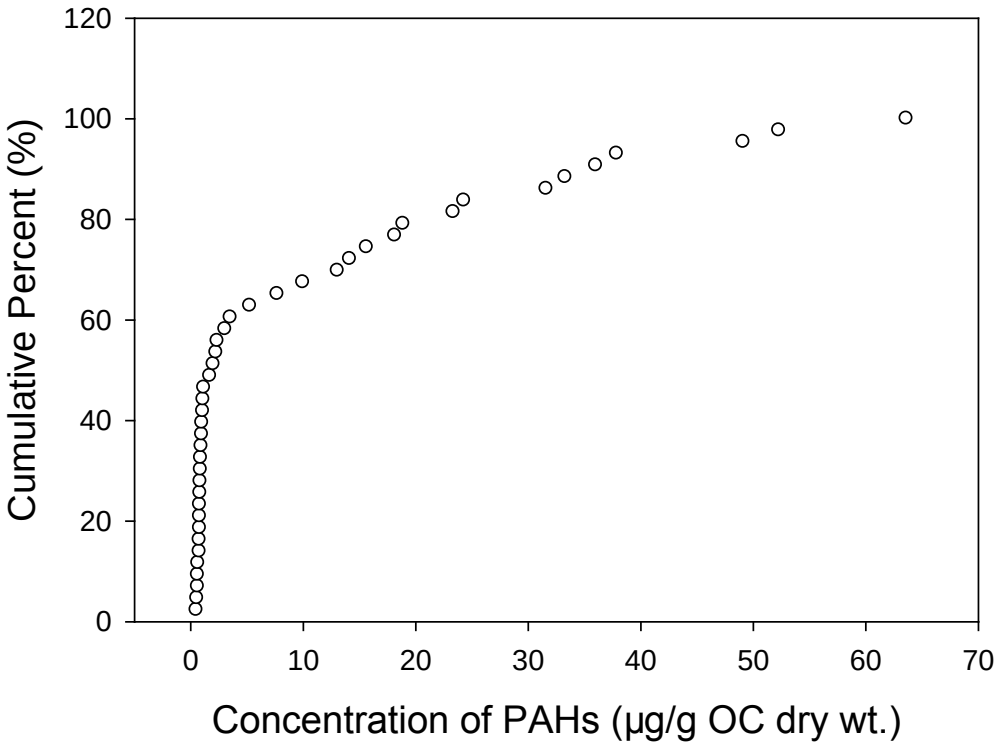

Figure S2. The cumulative percent for concentrations of 12 PAHs (AC, ACE, FL, PHT, ANT, FLU, PYR, BaA, CHR, BbF, BkF and BaP in Supplementary material, Table S4) in sediment on μg/g OC dry wt.

Table S1 Compound names, abbreviations, quantifier ion, reporting limits and ring numbers for the target analytes.

Compound name	Abbreviation[a]	Quantifier ion	RL[b]	Number of rings
2-methylnaphthalene	2-MNAP	142	20	2
1-methylnaphthalene	1-MNAP	172	20	2
biphenyl	BP	154	20	2
2,6-dimethylnaphthalene	2,6-DNAP	156	20	2
acenaphthylene	AC	152	20	3
acenaphthene	ACE	153	20	3
2,3,5-trimethylnaphthalene	2,3,5-TNAP	170	20	3
fluorene	FL	166	20	3
phenanthrene	PHE	178	20	3
anthracene	ANT	178	20	3
2-methylphenanthrene	2-MPHE	192	20	3
1-methylphenanthrene	1-MPHE	192	20	3
2,6-dimethylphenanthrene	2,6-DMPHE	206	20	3
fluoranthene	FLU	202	20	4
pyrene	PYR	202	20	4
11H-benzo[b]fluorine	11-BbF	215	20	4
benzo(a)anthracene	BaA	228	20	4
chrysene	CHR	228	20	4
benzo[b]fluoranthene	BbF	252	20	5
benzo[k]fluoranthene	BkF	252	20	5
benzo[e]pyrene	BeP	252	20	5
benzo[a]pyrene	BaP	252	20	5
perylene	PER	252	20	5
9, 10-diphenylanthracene	9, 10-DPHA	252	40	5
indeno[1,2,3-cd]pyrene	IcdP	276	40	5
dibenzo[a,h]anthrancene	DahA	278	40	6
benzo[g, h, i]perylene[a]	BghiP	276	40	6

[a] Abbreviation for compound name.

[b] Designates the reporting limit which is defined as the lowest concentration of the calibration curve for a specific analyte with the unit of ng/g dry wt.

Table S2 Pearson coefficients for PAH parent compounds (benzo[b]fluoranthene (BbF), benzo[k]fluoranthene (BkF), benzo[e]pyrene (BeP), benzo[a]pyrene (BaP), dibenzo[a,h]anthrancene (DahA), indeno[1,2,3-cd]pyrene (IcdP), benzo[g, h, i]perylene (BghiP)) and perylene in all sediment core samples.

	BbF	BkF	BeP	BaP	PER	DahA	IcdP	BghiP
BbF	1	0.99	0.95	0.95	0.037	0.97	0.98	0.97
BkF		1	0.95	0.96	0.043	0.97	0.97	0.97
BeP			1	0.97	0.069	0.96	0.99	0.99
BaP				1	0.057	0.96	0.98	0.98
PER					1	-0.022	-0.0020	0.033
DahA						1	0.99	0.98
IcdP							1	0.99
BghiP								1

Table S3 Sediment quality guidelines (SQGs) estimated by the similar method to a previous study [1] and concentration rang based on μg/g TOC in the present study.

	TEC	MEC	EEC	Concentration Range
Acenaphthylene	3.2	37	130	0–0.32
Acenaphthene	49	33	200	0–0.27
Fluorene	7.8	53	360	0–0.67
Phenanthrene	68	127	690	0–2.8
Anthracene	13	86	1300	0–0.38
Fluoranthene	101	300	3000	0–9.1
Pyrene	59	285	1600	0–8.2
Benz[a]anthracene	20	118	510	0–5.3
Chrysene	30	168	920	0–6.6
Benzo[b]fluoranthene	26	150	445	0–13
Benzo[k]fluoranthene	23	134	445	0–4.5
Benzo[a]pyrene	31	144	360	0–13
ΣPAH12	430	1636	996	0.27–64

Table S4 Estimated PAH concentrations in sediment porewater (C_{we}, ng/L), chronic toxicity values (CT, μg/L) [2] and hazard quotients(HQ) estimated by C_{we}/CT/1000. The full name of the target compounds are in Table S1.

Compound	AC	ACE	FL	PHE	ANT	FLU	PYR	BaA
C_{we}	0	38	38	174	17	73	81	9.6
CT	180	270	150	55	60	11	12	2
HQ	0	1.4E-4	2.5E-4	3.2E-3	2.8E-4	6.7E-3	6.8E-3	4.9E-3
Compound	CHR	BbF	BkF	BaP	IcdP	DahA	BghiP	
C_{we}	1	35	7.4	19	0.94	7.1	14	
CT	2.2	2.9	1.7	1.5	0.13	0.25	0.49	
HQ	6.4E-3	1.2E-2	4.4E-3	1.9E-2	7.2E-3	2.8E-2	2.9E-2	

References

1. R. C. Swartz, *Environ. Toxicol. Chem.*, 1999, **18**, 780–787.
2. J. M. Neff, S. A. Stout and D. G. Gunster, *Integrated environmental assessment and management*, 2005, **1**, 22–33.