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Supplementary Information

MANUSCRIPT TITLE: Fecal steroids in riverine runoff of the Pearl River Delta, South China: Levels, potential sources and inputs to the coastal ocean

AUTHORS: Ji-Zhong Wang, Yu-Feng Guan, Hong-Gang Ni, Gui-Jian Liu, and Eddy Y Zeng

ADDRESS: State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou 510640,

CAS Key Laboratory of Crust-Mantle Materials and Environment, School of Earth and Space Science, University of Science and Technology of China, Hefei 230026, China

The Key Laboratory for Environmental and Urban Sciences, Shenzhen Graduate School, Peking University, Shenzhen 518055, China

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Table S1 Nomenclature, molecular formula (MF), retention times (RT), quantitation ions (QI), and reporting limits (RL) of the target analytes measured in the present study

Compound	Abbreviation	MF	RT (min)	QI (*m*/*z*)	RL
Coprostanol	COP	$C_{27}H_{48}O$	26.04	370	1.3/0.03[a]
Epicoprostanol	ECOP	$C_{27}H_{48}O$	26.53	370	1.3/0.03
β-cholestanone	bONE	$C_{27}H_{44}O$	27.42	386	1.3/0.03
Cholesterol	CHOE	$C_{27}H_{46}O$	27.79	368	1.3/0.03
Cholestanol	CHOA	$C_{27}H_{48}O$	28.05	445	1.3/0.03
α-cholestanone	aONE	$C_{27}H_{44}O$	28.34	231	1.3/0.03
Stigmasterol	STIG	$C_{29}H_{48}O$	30.71	394	1.3/0.03
Stigmastanol	STAN	$C_{29}H_{52}O$	32.64	473	1.3/0.03

[a] 1.3/0.03 represents the reporting limits for filtrate (ng L^{-1})/SPM (μg g^{-1}) samples.

Table S2 Reported maximum concentrations (C_{max}) of coprostanol ($\mu g\ L^{-1}$) in different types of water around the world

Country	Location	Type of water	N[a]	C_{max}	Ref
France	Paris	Raw	1	250	1
Japan	Tokyo	Raw	2	204[d]	2
Spain	Barcelona	Raw	7	165	3
France	Toulon	Raw	2	2400	4
France	Toulon	Raw	3	940[d]	4
France	Morlaix	Raw	2	493	4
France	Morlaix	Raw	1	1339[d]	4
France	Brest	Raw	2	2781[d]	4
Italy	northern Italy	Raw	11	36.8	5
U.S.	Ohio	Primary	[c]	750	6
U.S.	Narragansett Bay	Primary	11	475[d]	7
U.S.	JWPCP/Log Angeles	Primary	11	400	3i
U.S.	JWPCP/Log Angeles	Primary	1	29	8
U.S.	Hyperion-5/Log Angeles	Primary	4	448	3 i
U.S.	OSDOC/Los Angeles	Primary	4	437	3 i
U.S.	PCTP/Los Angeles	Primary	4	545	3 i
U.S.	South Essex/Salem Harbor	Primary	6	71	9
U.K.	Inverkip	Primary	1	620	10
U.K.	Dalmuir	Primary	2	232	10
France	Toulon	Primary	1	340	4
France	Toulon	Primary	2	220[d]	4
Japan	Nagafusa	Partial[b]	24	61.2	3 i
Canada	St. Lawrence River	Partial[b]	1	14.7	11
U.S.	Hyperion-5/Log Angeles	Primary+AS[e]	1	158	8
U.S.	CSDOC/Los Angeles	Primary+AS[e]	3	270	3 i
U.S.	Ohio	Septic tank	[c]	260	6
Spain	Barcelona	[c]	1	630[d]	12
Japan	Tokyo	Septic tank	6	71	3 i
U.S.	Ohio	TFT[f]	[c]	240	6
U.S.	Narragansett Bay	TFT[f]	8	136[d]	7
Canada	Biggar	Lagoon	4	13.8	13
Canada	Grimsby	AS[e]	4	417	13
U.S.	Narragansett Bay	AS[e]	20	45.3[d]	7
France	Morlaix	AS[e]	1	31.7	4
France	Morlaix	AS[e]	2	32.4[d]	4
France	Brest	AS[e]	2	20.6[d]	4
U.S.	Cheaspeake-Elizabeth	AS[e]	4	36	14
U.S.	Ohio	AS[e]	[c]	15	6
Canada	Burlington	AS[e]	4	3.8	13
Canada	Milton	AS[e]	5	16.55	13
Japan	Tokyo	AS[e]	2	13	3 i
Japan	Tokyo	AS[e]	6	6.8	3 i
Sweden	Stockholm	Greywater	12	14.9	15
Japan	Mastuyama	River	34	24	3 i
Canada	Quebec	River, Lake	3	22	16

Japan	Tamagawa River	River	2	14.5	[3][i]
Japan	Minamiasakawa River	River	18	12.2	[3][i]
France	Morlaix River	River	5	6.23[d]	[17]
Japan	Fukuoka	River	32	5.2	[3][i]
U.S.	Ohio	River	8	5.0	[6]
Japan	Tamagawa River	River	2	4.0[d]	[2]
U.S.	Narragansett	River	20	3.8[d]	[7]
U.S.	Great Lakes	River, Lake	26	2.05	[18]
U.S.	Santa Ana River	River	54	0.026	[19]
Japan	Tamagawa River	River	3	1.8	[3][i]
Japan	Tsurumigawa River	River	7	1.4	[3][i]
Indonesia	Solo River	River	7	0.68[d]	[20]
Spain	Ebre	River	4	0.5[d]	[12]
Australia	Tuggerah Lake	River, Lake	6	0.11	[3][i]
Canada	St. Lawrence River	River	2	0.038	[11]
Italy	Po river	River	11	9	[5]
Finland	Lake Vanajavesi	Lake	19	4.1	[21]
Australia	Newcastle	Catchment water	1	15.8[d]	[22]
Australia	Newcastle	Catchment water[g]	38	0.19	[23]
Australia	Newcastle	Catchment water[h]	172	0.163	[23]
Australia	Newcastle	Catchment water[m]	63	0.014	[23]
Australia	Newcastle	Catchment water[e]	23	1.693	[23]
U.S.	northern America	surface water	19	0.294[d]	[24]
U.K.	Clyde estuary	Estuary	14	47.5	[10]
France	Morlaix estuary	Estuary	13	15.4	[17]
U.K.	Mersey	Estuary	24	7.7	[25]
U.K.	Firth of Clyde	Estuary	13	2.44	[10]
Canada	Fraser	Estuary	48	2.7	[26]
Canada	Fraser	Estuary	72	0.71	[26]
Croatia	Krka River	Estuary	5	1.05	[27]
Australia	Derwent estuary	Estuary	22	0.95	[28]
Belgium	Scheldt estuary	Estuary	8	0.28	[29]
Japan	Tokyo Bay	Coastal	18	6.6	[3][i]
Japan	Seto Inland Sea	Coastal	11	6.3	[3][i]
Australia	Off Sydney	Coastal	16	3.81[d]	[30]
Japan	Ariake Sea	Coastal	8	1.05	[3][i]
U.S.	Narragansett Bay	Coastal	64	0.66	[7]
Spain	Barcelona	Coastal	1	0.29[d]	[12]
China	Pearl River Delta	Outlets	96	0.52	This study

[a] N = the number of sample; [b] Type of water: partial = mixture of primary effluent, activated sludge effluent, and septic tank effluent; [c] no information available; [d] only particulate phase included; [e] activated sludge treatment, [f] Trickling filter treatment; [g] potentially impacted by septic tanks; [h] potentially impacted by cattle, [m] potentially impacted by sewage treatment plant; and h natural forests, [i] original texts were not found and the data was cited from the ref [3]

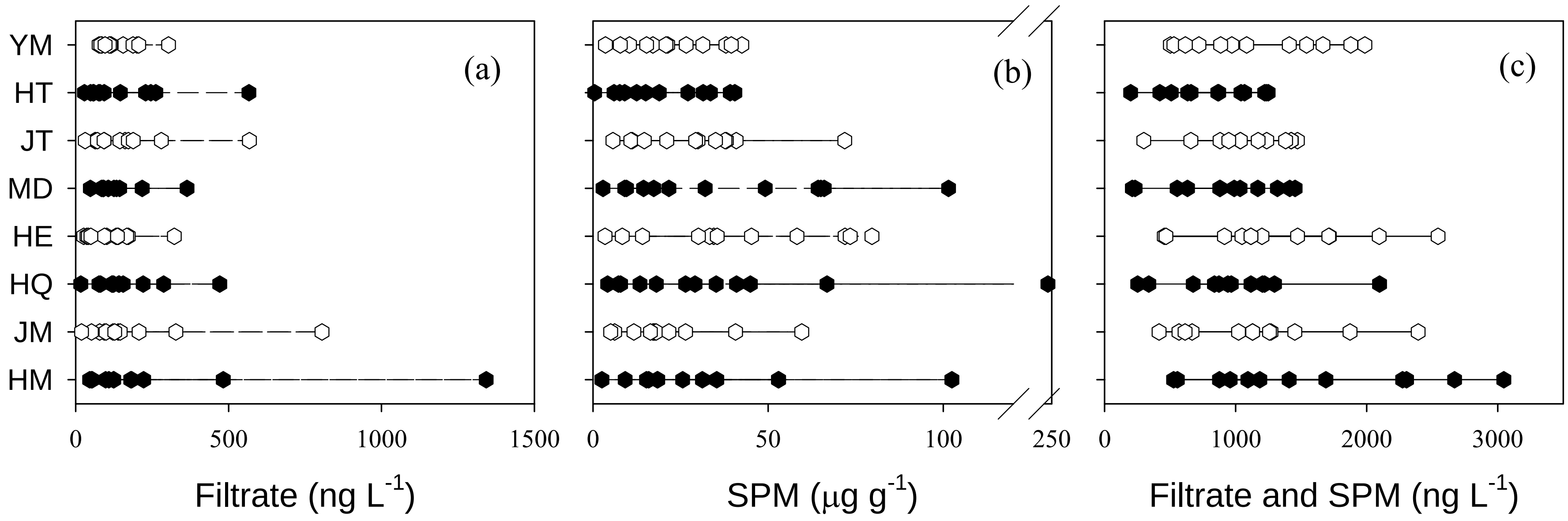

Figure S1. Concentrations of $\Sigma_8$steroid in (a) filtrate samples (ng L^{-1}); (b) suspended particulate matter (SPM) samples (µg g^{-1}); and (c) combined filtrate and SPM samples (ng L^{-1}) from riverine runoff discharged through the eight major runoff outlets in the Pearl River Delta, South China: Yamen (YM), Hutiaomen (HT), Jitimen (JT), Modaomen (MD), Hengmen (HE), Hongqilimen (HQ), Jiaomen (JM), and Humen (HM).

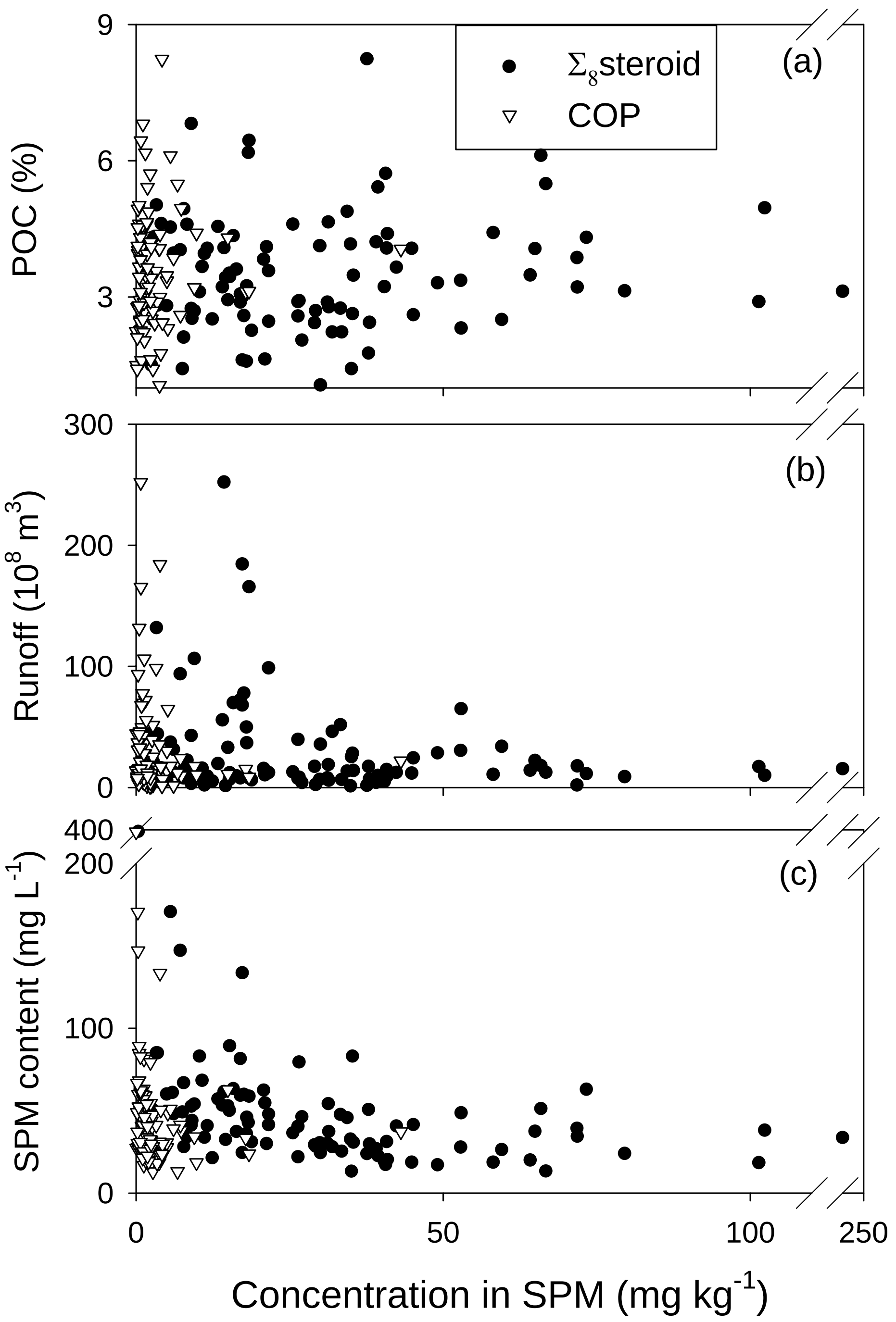

Figure S2. The correlations between the concentrations of $\Sigma_8$steroid (circles) and COP (triangles down) in suspended particulate matter (SPM) with (a) particulate organic carbon (POC), (b) riverine runoff, and (c) SPM content.

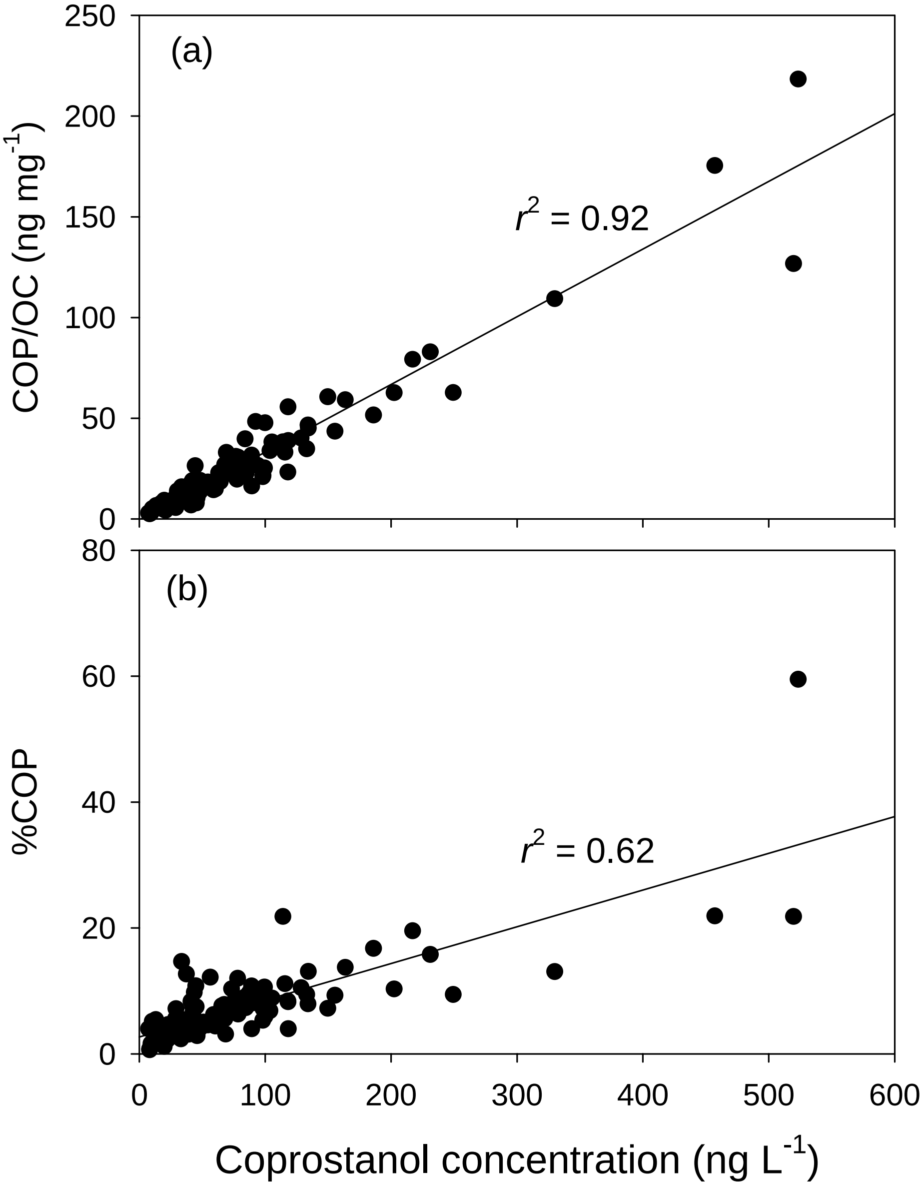

Figure S3. Correlation of the total coprostanol concentration (filtrate plus SPM) with (a) COP/OC (coprostanol concentration normalized to total organic carbon and (b) %COP (relative abundance of COP to total steroids ($\Sigma_8$steroid).

References

1. D.-K. Nguyen, A. Bruchet and P. Arpino, *J. High Resolut. Chromatogr.*, 1994, **17**, 153–159.
2. N. Chalaux, H. Takada and J. M. Bayona, *Mar. Environ. Res.*, 1995, **40**, 77–92.
3. H. Takada and B. P. Eganhouse, *Molecular marker of anthropogenic waste*, John Wiley & Sons, Inc., 1998.
4. M. Quéméneur and Y. Marty, *Wat. Res.*, 1994, **28**, 1217–1226.
5. G. Gilli, R. Rovere, D. Traversi, T. Schilirò and C. Pignata, *J. Chromatogr. B*, 2006, **843**, 120–124.
6. J. J. Murtaugh and R. L. Bunch, *J. Water Pollut. Control Fed.*, 1967, **39**, 404–409.
7. L. A. LeBlanc, J. S. Latimer, J. T. Ellis and J. G. Quinn, *Estua. Coastal Shelf Sci.*, 1992, **34**, 439–458.
8. M. I. Venkatesan and I. R. Kaplan, *Environ. Sci. Technol.*, 1990, **24**, 208–214.
9. B. P. Eganhouse, *Organic Geochemistry*, The New England Aquarium, Boston, Mass., 1986.
10. R. M. Goodfellow, J. Cardoso, G. Eglinton, J. P. Dawson and G. A. Best, *Mar. Pollut. Bull.*, 1977, **8**, 272–276.
11. S. Cathum and H. Sabik, *Chromatographia*, 2001, **53**, S394–S399.
12. J. Grimalt, P. Fernandez, J. M. Bayona and J. Albaiges, *Environ. Sci. Technol.*, 1990, **24**, 357–363.
13. B. J. Dutka and A. El-Shaarawi, *Can. J. Microbiol.*, 1975, **21**, 1386–1398.
14. R. C. Brown and T. L. Wade, *Wat. Res.*, 1984, **18**, 621–632.
15. J. Ottoson and T. A. Stenström, *Wat. Res.*, 2003, **37**, 645–655.
16. J. Dougan and L. Tan, *J. Chromatogr.*, 1973, **86**, 107–116.
17. M. Quémenéur and Y. Marty, *Estua. Coastal Shelf Sci.*, 1992, **34**, 347–363.
18. B. J. Dutka, A. S. Y. Chau and J. Coburn, *Wat. Res.*, 1974, **8**, 1047–1055.
19. J. A. Noblet, D. L. Young, E. Y. Zeng and S. Ensari, *Environ. Sci. Technol.*, 2004, **38**, 6002–6008.
20. W. Li, J. Dagaut and A. Saliot, *Biogeochemistry*, 1995, **31**, 139–154.
21. S. Düreth, R. Herrmann and K. Pecher, *Water Air and Soil Pollution*, 1986, **28**, 131–149.
22. V. K. G. Shah, H. Dunstan and W. Taylor, *J. Chromatogr. A*, 2006, **1108**, 111–115.
23. V. G. Shah, R. Hugh Dunstan, P. M. Geary, P. Coombes, T. K. Roberts and T. Rothkirch, *Wat. Res.*, 2007, **41**, 3667–3674.
24. L. J. Standley, L. A. Kaplan and D. Smith, *Environ. Sci. Technol.*, 2000, **34**, 3124–3130.
25. M. F. Fitzsimons, M. K. Abdul Rashid, J. P. Riley and G. A. Wolff, *Mar. Pollut. Bull.*, 1995, **30**, 306–312.
26. L. M. Churchland, G. Kan and A. Ages, *Can. J. Microbiol.*, 1982, **28**, 239–247.
27. J. Laurcillard and A. Saliot, *Mar. Chem.*, 1993, **43**, 247–261.
28. R. Leeming and P. D. Nichols, *Wat. Res.*, 1996, **30**, 2997–3006.
29. M. Yde, E. De Wulf, S. De Maeyer-Cleempoel and D. Quaghebeur, *Bull. Environ. Contam. Toxicol.*, 1982, **28**, 129–134.
30. P. D. Nichols, R. Leeming, M. S. Rayner, V. Latham, N. J. Ashbolt and C. Turner, *J. Chromatogr.*, 1993, **643**, 189–195.