Supplemental Data

TITLE: Ecological Risk of Galaxolide and Its Transformation Product Galaxolidone: Evidence from the Literature and A Case Study in Guangzhou Waterways

AUTHORS: Yanrong Su, Faxu Li, Xiangxiang Xiao, Huizhen Li, Dali Wang*, Jing You

ADDRESS: Guangdong Key Laboratory of Environmental Pollution and Health, School of Environment, Jinan University, Guangzhou 511443, China

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*Corresponding author.

Tel: 0086-20-3733-6629, Email: wdali2018@jnu.edu.cn

Content:

Text S1. Chemicals and reagents

Galaxolide (HHCB) was purchased from Dr. Ehrenstorfer GmbH (Augsburg, Germany). Galaxolidone (HHCB-lac) was obtained from Toronto Research Chemicals (Toronto, Ontario, Canada). Tonalide-d_3 (AHTN-D3) was used as the internal standard, which was acquired from Dr. Ehrenstofer GmbH. 4,4'-Dibromooctafluorobiphenyl (DBOFB) as surrogate standards was purchased from Aladdin (Shanghai, China).

Text S2. Samples collection and preparation

Four litters of the surface water were collected at each sampling site and transported back to the laboratory immediately. The water samples were then filtered using glass fiber filters with 0.7 μm pore size. The DBOFB was added to each sample at a concentration of 50 ng/mL as the surrogate. Then the sample was loaded to a solid phase extraction (SPE) cartridge containing 200 mg of mixture adsorbents (HLB:WAX:WCX, 2:1:1, w/w/w). After extraction, the SPE cartridge was washed using 5 mL of methanol, 5 mL of methanol with 0.5% ammonia, and 5 mL of methanol with 0.5% acetic acid in sequence. Afterwards, the SPE cartridge was eluted using 5 mL of acetone, 5 mL of dichloromethane, and 5 mL of hexane. The elution was then concentrated with nitrogen blowing evaporation, resolved in 1 mL of hexane, and analyzed for musks on GC-MS/MS after adding the corresponding internal standards (50 ng/mL).

Text S3. Instrumental analysis of HHCB and HHCB-lac

The concentrations of HHCB and HHCB-lac were analyzed by GC-MS/MS (Shimadzu

TQ8040) in in electron impact ionization mode. An SH-RXi-5Sil-MS column (30 m × 0.25 mm, 0.25 μm film thickness) was used to separate the target compounds. The carrier gas (helium) was maintained at a flow rate of 1.0 mL/min. The initial column temperature was 60 ℃, which was ramped up to 180 ℃ at a rate of 20 ℃/min, finally increased to 280 °C at 10 °C/min and held at 280 °C for 5 min. The injector, ion source and transfer line temperatures were 250 ℃, 230 ℃ and 250 ℃, respectively. The injection mode is splitless, and the injection volume is 1 μL. MS-detector acquired in the selected ion monitoring mode (SIM) at an electron impact energy of 70 eV.

Text S4. Quality assurance and quality control

To ensure the stability of the instrument, a calibration standard was analyzed every 10 samples, and variations of individual compounds were within 20%. Recoveries of the analytes based on the isotopic internal standard correction ranged from 82.4% to 112.0%, with relative standard deviations less than 20.0%. The calibration standards were prepared ranging from 1 to 1000 μg/L with 50 μg/L of internal standard, resulting in acceptable linearities for all compounds (correlation coefficients of $r^2 > 0.99$). Special precautions were taken to prevent intra-laboratory contamination that could occur from perfumes, deodorants, etc. The chemists involved in this analysis were asked not to use any cosmetic during the extraction and cleaning procedure.

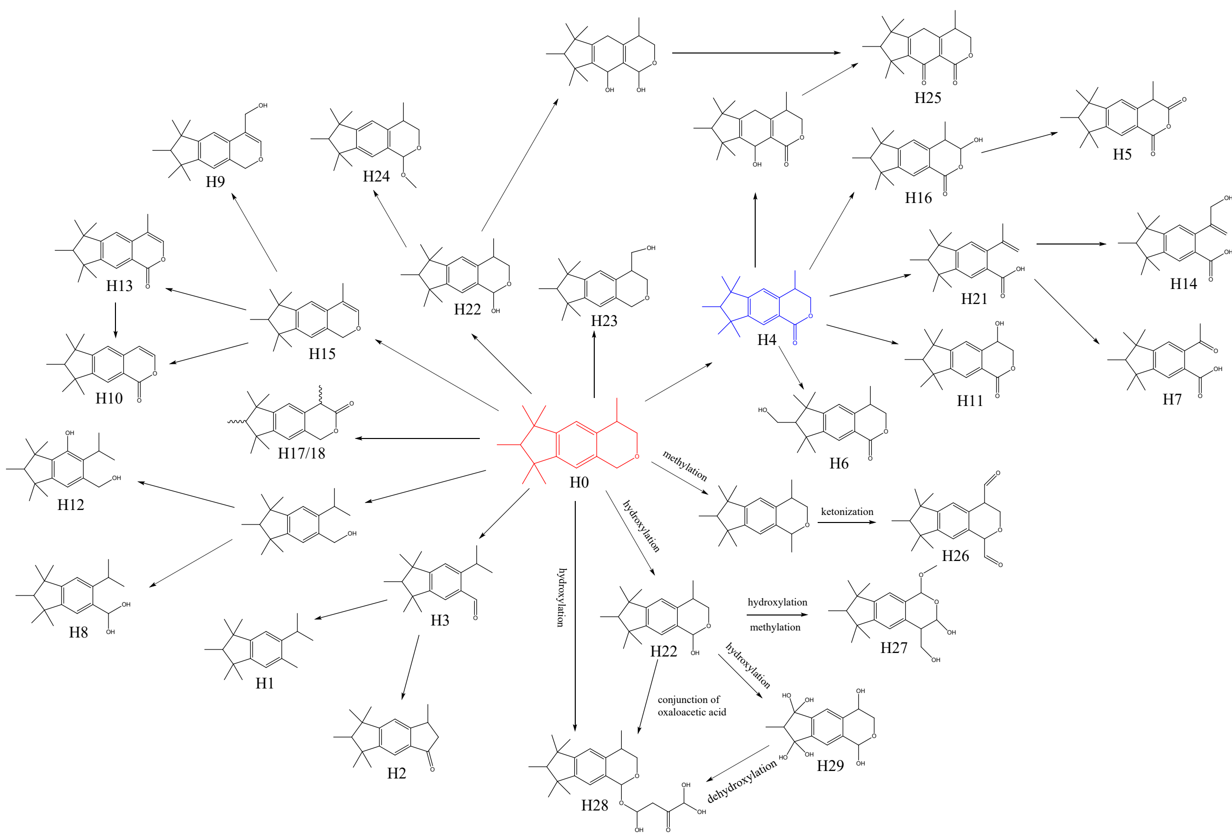

Fig. S1. Probable transformation products of galaxolide (HHCB). H0 is the parent molecule of HHCB and H4 is the galaxolidone. Detailed information is available in the below references.

Ding, T.; Li, W.; Cai, M.; Jia, X.; Yang, M.; Yang, B.; Li, J., Algal toxicity, accumulation and metabolic pathways of galaxolide. *Journal of Hazardous Materials* 2020, 384, 121360.

Herrera López, S.; Hernando, M. D.; Gómez, M. J.; Santiago-Morales, J.; Rosal, R.; Fernández-Alba, A., Investigation of Galaxolide degradation products generated under oxidative and irradiation processes by liquid chromatography/hybrid quadrupole time-of-flight mass spectrometry and comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry. *Rapid Communications in Mass Spectrometry* 2013, 27, (11), 1237-1250.

Martin, C.; Moeder, M.; Daniel, X.; Krauss, G.; Schlosser, D., Biotransformation of the polycyclic musks HHCB and AHTN and metabolite formation by fungi occurring in freshwater environments. *Environmental Science & Technology* 2007, 41, (15), 5395-5402.

Sanchez-Prado, L.; Lourido, M.; Lores, M.; Llompart, M.; Garcia-Jares, C.; Cela, R., Study of the photoinduced degradation of polycyclic musk compounds by solid-phase microextraction and gas chromatography/mass spectrometry. *Rapid Communications in Mass Spectrometry* 2004, 18, (11), 1186-1192.

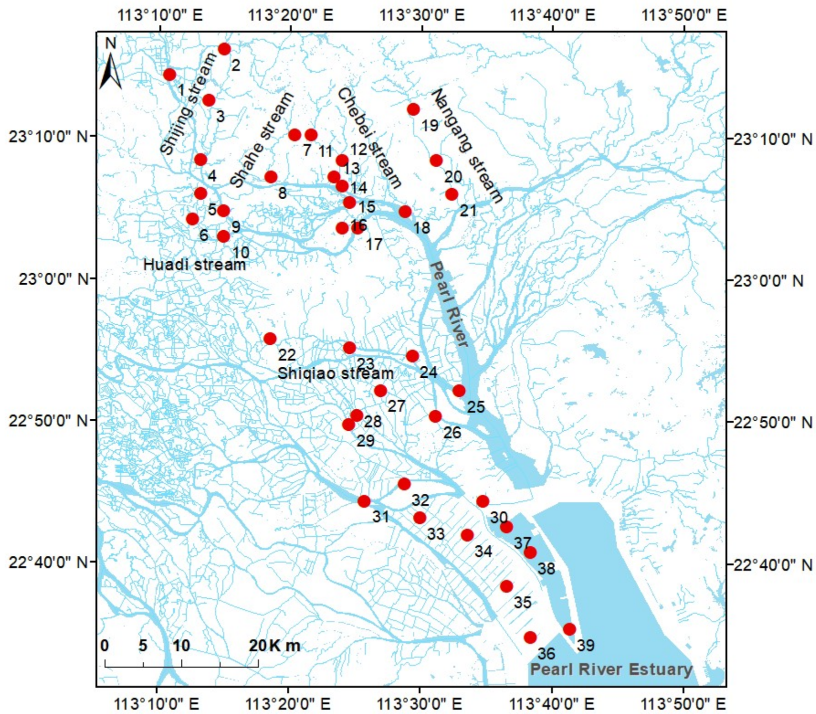

Fig. S2 Location of sampling sites

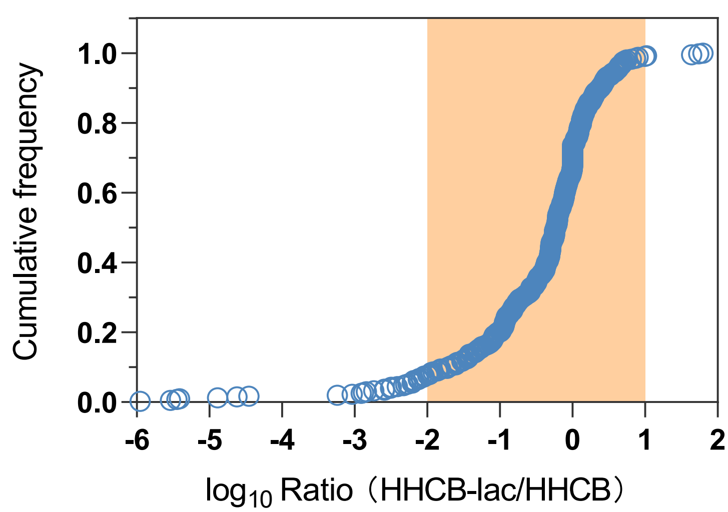

Fig. S3 Cumulative frequency of the ratios for HHCB-lac and HHCB in different environmental media reported in the literature

Table S1. Concentrations (ng/L) of HHCB and HHCB-lac in surface water samples collected from the Pearl River, South China and their concentration ratio at individual sites.

Site	HHCB	HHCB-lac	Ratio
L1	215	67.5	0.314
L2	2620	740	0.283
L3	835	260	0.311
L4	352	130	0.370
L5	235	71.3	0.304
L6	211	56.6	0.269
L7	904	312	0.345
L8	483	260	0.539
L9	241	83.3	0.346
L10	250	43.5	0.174
L11	214	43.2	0.202
L12	348	110	0.315
L13	308	108	0.351
L14	184	83.5	0.454
L15	110	58.8	0.534
L16	118	44.3	0.376
L17	124	55.5	0.449
L18	139	66.4	0.478
L19	106	38.2	0.359
L20	498	199	0.399
L21	564	229	0.406
L22	94.9	24.5	0.258
L23	208	32.5	0.156

Site	HHCB	HHCB-lac	Ratio
L24	96.6	24.7	0.255
L25	60.0	24.5	0.408
L26	39.0	21.6	0.553
L27	62.7	10.4	0.166
L28	44.1	11.3	0.256
L29	34.9	7.28	0.209
L30	38.9	7.90	0.203
L31	29.7	6.82	0.230
L32	33.4	8.13	0.243
L33	42.4	8.91	0.211
L34	35.0	22.7	0.647
L35	36.9	7.58	0.205
L36	27.8	4.20	0.151
L37	20.0	3.18	0.159
L38	24.8	8.60	0.347
L39	24.7	8.40	0.341

Table S2. Concentrations (ng/g) of HHCB and HHCB-lac and their concentration ratio (HHCB-lac/HHCB) in personal care products reported in the literature.

Country	Product	HHCB	HHCB-lac	Raito	Reference
America	Body splash	4.99×10^{6}	2.9×10^{3}	5.81×10^{-4}	1
	Body oil	1.45×10^{6}	6.81×10^{3}	4.70×10^{-3}	
	Perfume	1.01×10^{6}	3.04×10^{4}	3.01×10^{-2}	
	Eau de toilette	2.06×10^{5}	9.39×10^{3}	4.56×10^{-2}	
	Body mist	4.01×10^{2}	2.50	6.23×10^{-3}	
	Eau de toilette	6.00	2.50	0.417	
	Body mist	2.50	1.38×10^{2}	55.2	
	Body lotion	3.74×10^{6}	9.60×10^{3}	2.57×10^{-3}	
	Body cream	2.07×10^{6}	2.17×10^{5}	0.105	
	Body lotion	6.98×10^{5}	8.61×10^{2}	1.23×10^{-3}	
	Body lotion	4.95×10^{5}	7.19×10^{2}	1.45×10^{-3}	
	Body lotion	2.98×10^{5}	1.90×10^{3}	6.38×10^{-3}	
	Body lotion	7.28×10^{2}	3.20×10^{4}	44.0	
	After sun lotion	2.50	2.50	1.00	
	Antiperspirant	2.25×10^{6}	2.50	1.11×10^{-6}	
	Antiperspirant/deodorant	7.03×10^{5}	2.50	3.56×10^{-6}	
	Antiperspirant	2.71×10^{3}	2.50	9.23×10^{-4}	
	Antiperspirant	8.01×10^{2}	2.50	3.12×10^{-3}	
	Shaving cream	1.23×10^{6}	1.12×10^{4}	9.11×10^{-3}	
	Bath soap	4.56×10^{5}	5.16×10^{3}	1.13×10^{-2}	
	Bath soap	1.93×10^{5}	2.50	1.30×10^{-5}	
	Body wash	1.04×10^{5}	2.50	2.40×10^{-5}	
	Shaving cream	7.12×10^{4}	2.50	3.51×10^{-5}	
	Bash soap	6.46×10^{2}	2.50	3.87×10^{-3}	
	Facial soap	3.30×10^{2}	2.50	7.58×10^{-3}	
	Bath soap	1.71×10^{2}	2.50	1.46×10^{-2}	
	Shaving gel	36.0	2.50	6.94×10^{-2}	
	Shaving cream	2.50	2.50	1.00	
	Shower gel	2.50	2.50	1.00	
	Shaving cream	2.50	2.50	1.00	
	Shower gel	2.50	2.50	1.00	
	Shower gel	2.50	2.50	1.00	
	Hair cream	8.55×10^{5}	2.50	2.92×10^{-6}	
	Shampoo	1.22×10^{5}	1.68×10^{3}	1.38×10^{-2}	
	Conditioner	9.75×10^{4}	4.95×10^{2}	5.08×10^{-3}	
	Hair gel	6.14×10^{4}	6.24×10^{2}	1.02×10^{-2}	
	Conditioner	6.00×10^{4}	3.91×10^{2}	6.52×10^{-3}	
	Conditioner	3.31×10^{4}	5.70×10^{3}	0.172	

Country	Product	HHCB	HHCB-lac	Raito	Reference
	Hair gel	2.69×10^{4}	4.12×10^{2}	1.53×10^{-2}	
	Hair cream	1.29×10^{4}	7.92×10^{3}	0.614	
	Shampoo	1.36×10^{3}	2.50	1.84×10^{-3}	
	Shampoo	1.00×10^{2}	2.50	2.50×10^{-2}	
	Shampoo	95.0	2.50	2.63×10^{-2}	
	Conditioner	2.50	2.50	1.00	
	Furniture polish	6.46×10^{5}	2.50	3.87×10^{-6}	
	Laundry detergent	8.49×10^{4}	1.12×10^{2}	1.32×10^{-3}	
	Fabric softener	9.66×10^{2}	2.50	2.59×10^{-3}	
	Disinfecting wipe	7.86×10^{2}	2.50	3.18×10^{-3}	
	Liquid bleach	3.26×10^{2}	2.50	7.67×10^{-3}	
	Laundry detergent	79.0	2.50	3.16×10^{-2}	
	Fabric softener	2.50	2.50	1.00	
	Stain remover	2.50	2.50	1.00	
	Liquid dish cleaner	2.50	2.50	1.00	
	Disinfectant cleaner	2.50	2.50	1.00	
	Cleaning solvent	2.50	2.50	1.00	
	Stain remover	2.50	2.50	1.00	
	Cleaning solvent	2.50	2.50	1.00	
	Cleaning solvent	2.50	2.50	1.00	
	Bleach cleanser	2.50	2.50	1.00	
	Disinfecting wipe	2.50	2.50	1.00	
China	Hair care products	1.43×10^{5}	9.10×10^{2}	6.36×10^{-3}	[2]
	Body washes	6.96×10^{3}	3.10×10^{2}	4.45×10^{-2}	
	Toilet soaps	1.19×10^{4}	5.78×10^{3}	0.486	
	Skin lotions	3.75×10^{4}	1.10×10^{3}	2.93×10^{-2}	
	Make up	1.14×10^{4}	2.33×10^{3}	0.204	

Table S3. Concentration of HHCB and HHCB-lac and their concentration ratio (HHCB-lac/HHCB) in wastewater treatment plant reported in the literature.

Country	Location	Unit	HHCB	HHCB-lac	Ratio	Reference
Spain	Effluent	ng/mL	4.25×10^{2}	3.16×10^{2}	0.743	[3]
			2.07×10^{2}	1.46×10^{2}	0.706	
			2.19×10^{2}	1.22×10^{2}	0.556	
			8.59×10^{2}	5.75×10^{2}	0.670	
			4.06×10^{2}	5.35×10^{2}	1.32	
			3.24×10^{2}	6.56×10^{2}	2.02	
Canada	Effluent	ng/mL	0.180	0.068	0.378	[4]
			0.130	0.044	0.338	
Italy	Influent	ng/mL	4.24	0.508	0.120	[5]
			6.27	0.949	0.151	
			3.63	0.339	9.35×10^{-2}	
			6.07	0.508	8.38×10^{-2}	
Italy	Enfluent	ng/mL	4.17	2.37	0.569	[5]
			4.54	2.81	0.619	
			5.80	1.76	0.304	
			5.80	4.17	0.719	
Italy	Sludge	ng/g	9.27×10^{4}	7.22×10^{4}	0.779	[6]
			9.50×10^{4}	7.22×10^{4}	0.760	
			9.24×10^{4}	6.87×10^{4}	0.744	
			8.92×10^{4}	7.16×10^{4}	0.803	
America	Influent	ng/mL	4.76	0.741	0.156	[6]
			9.63	0.869	9.02×10^{-2}	
			7.60	0.869	0.114	
			10.4	0.855	8.22×10^{-2}	
			12.7	1.15	9.06×10^{-2}	

Country	Location	Unit	HHCB	HHCB-lac	Ratio	Reference
			1.78	0.146	8.20×10^{-2}	
			4.37	0.535	0.122	
			4.29	0.323	7.53×10^{-2}	
			7.73	0.581	7.52×10^{-2}	
			11.5	0.942	8.19×10^{-2}	
America	Enfluent	ng/mL	2.90	1.36	0.467	[6]
			3.66	0.823	0.225	
			2.81	1.13	0.402	
			3.73	1.40	0.375	
			3.66	4.00	1.09	
			2.36	1.04	0.441	
			2.66	1.57	0.590	
			2.58	0.820	0.318	
			3.31	1.60	0.483	
			2.59	3.08	1.19	
America	Sludge	ng/g	6.34×10^{4}	2.04×10^{4}	0.322	[6]
			1.17×10^{5}	2.20×10^{4}	0.188	
			7.91×10^{4}	1.46×10^{4}	0.185	
			7.65×10^{4}	1.29×10^{4}	0.169	
			1.08×10^{5}	1.98×10^{4}	0.183	
Germany	Enfluent	ng/mL	0.254	6.70×10^{-2}	0.263	[7]
			0.265	6.99×10^{-2}	0.264	
			8.81×10^{-2}	1.46×10^{-2}	0.166	
			8.94×10^{-2}	1.46×10^{-2}	0.163	
			0.107	3.08×10^{-2}	0.287	
			9.61×10^{-2}	2.87×10^{-2}	0.299	
			4.28×10^{-2}	4.03×10^{-2}	0.942	
			5.85×10^{-2}	5.15×10^{-2}	0.880	
			0.269	0.137	0.509	
			0.652	0.278	0.427	
			0.433	0.181	0.417	
Swiss	Influent	ng/mL	6.90	0.430	0.430	[8]
Swiss	Enfluent	ng/mL	0.860	0.860	1.05	[8]
Germany	Influent	ng/mL	2.18	0.270	0.124	[9]
			2.33	0.270	0.116	
			1.93	0.230	0.119	
			1.86	0.215	0.116	
			1.41	0.170	0.121	
Germany	Enfluent	ng/mL	0.795	0.795	0.528	[9]
			0.691	0.691	0.535	
			0.652	0.652	0.567	

Country	Location	Unit	HHCB	HHCB-lac	Ratio	Reference
			0.669	0.669	0.508	
			0.669	0.669	0.501	
Guangzhou	Influent	ng/mL	1.08	0.547	0.506	[10]
Guangzhou	Enfluent	ng/mL	0.491	1.00	2.04	[10]
Thailand	Influent	ng/mL	2.51	4.53	1.80	[11]
Thailand	Enfluent	ng/mL	1.56	5.30	3.39	[11]
Tailand	Sludge	ng/g	3.56×10^{3}	5.25×10^{4}	14.7	[11]
Germany	Influent	ng/mL	2.22	0.690	0.311	[12]
			5.70×10^{-2}	0.153	2.68	
Germany	Enfluent	ng/mL	0.954	0.532	0.558	[12]
			6.40×10^{-2}	0.143	2.23	
Italy	Influent	ng/mL	5.70	0.905	0.159	[13]
Italy	Enfluent	ng/mL	7.01	5.11	0.728	[13]
America	Influent	ng/mL	4.30×10^{-2}	0.255	5.93	[14]
			7.03	0.300	4.27×10^{-2}	
			0.423	0.140	0.331	
America	Enfluent	ng/mL	6.70×10^{-2}	0.467	6.97	[14]
			1.00×10^{-2}	7.30×10^{-2}	7.30	
			5.30×10^{-2}	0.288	5.43	
			4.60×10^{-2}	8.60×10^{-2}	1.87	
America	Influent	ng/mL	0.455	0.766	1.68	[14]
			0.284	0.107	0.377	
			0.522	0.238	0.456	
America	Enfluent	ng/mL	2.80×10^{-2}	0.322	11.5	[14]
			9.80×10^{-2}	0.267	2.72	
			3.90×10^{-2}	0.545	14.0	
Switzerland	Sludge	ng/g	1.19×10^{4}	1.70×10^{3}	0.143	[15]
			1.21×10^{4}	1.90×10^{3}	0.157	
			3.60×10^{4}	2.90×10^{3}	8.06×10^{-2}	
			2.68×10^{4}	3.50×10^{3}	0.131	
			1.16×10^{4}	1.60×10^{3}	0.138	
			2.82×10^{4}	2.20×10^{3}	7.80×10^{-2}	
			2.46×10^{4}	1.80×10^{3}	7.32×10^{-2}	
			2.20×10^{4}	3.50×10^{3}	0.159	
			1.88×10^{4}	3.10×10^{3}	0.165	
			2.92×10^{4}	1.10×10^{3}	3.77×10^{-2}	
			2.41×10^{4}	1.40×10^{3}	5.81×10^{-2}	
			2.12×10^{4}	8.00×10^{2}	3.77×10^{-2}	
			1.55×10^{4}	8.00×10^{2}	5.16×10^{-2}	
			1.69×10^{4}	2.10×10^{3}	0.124	

Country	Location	Unit	HHCB	HHCB-lac	Ratio	Reference
			1.64×10^{4}	9.00×10^{2}	5.49×10^{-2}	
			2.30×10^{4}	2.30×10^{3}	0.100	
			1.90×10^{4}	9.00×10^{2}	4.74×10^{-2}	
			7.40×10^{3}	6.00×10^{2}	8.11×10^{-2}	
			1.37×10^{4}	1.40×10^{3}	0.102	
			1.30×10^{4}	8.00×10^{2}	6.15×10^{-2}	
			2.15×10^{4}	3.30×10^{3}	0.153	
			2.86×10^{4}	1.60×10^{3}	5.59×10^{-2}	

Table S4. Concentration (ng/mL) of HHCB and HHCB-lac and their concentration ratio (HHCB-lac/HHCB) in surface water reported in the literature.

Country	HHCB	HHCB-lac	Ratio	Reference
Germany	1.25	1.26	1.01	[16]
	0.287	0.976	3.40	
	0.164	0.301	1.84	
	0.123	0.344	2.80	
	0.123	0.100	4.32	
	0.123	0.474	3.85	
	8.21×10^{-2}	0.158	1.92	
	0.246	1.38	5.60	
	0.174	0.746	4.28	
Germany	-	-	7.40	[16]
			6.45	
			10.5	
			8.03	
			4.75	
			1.58	
			0.997	
			1.26	
			1.68	
			4.16	
			3.48	
			1.89	
			4.69	
			2.68	
			3.58	
			1.14	
			1.35	
			2.25	
			1.61	
			2.62	
			2.93	
			4.89	
			3.93	
			3.99	
			2.51	
			1.39	
			0.87	
			1.23	
			1.34	
			2.34	
			2.45	

Country	HHCB	HHCB-lac	Ratio	Reference
			4.98	
			5.03	
			2.65	
			1.33	
			0.907	
			1.33	
			1.64	
			2.91	
			3.33	
Spain	3.24	3.24	0.100	[3]
	2.43	2.43	1.00	
	4.46	2.43	0.545	
	1.62	1.62	1.00	
	1.62	2.03	1.25	
	1.22	0.810	0.667	
	1.62	2.03	1.25	
	6.48	4.05	0.625	
	12.2	8.51	0.700	
	11.7	7.29	0.621	
	9.32	6.89	0.739	
	13.0	8.51	0.656	
	14.2	39.3	2.77	
	8.91	16.6	1.86	
	4.46	2.03	0.455	
	3.24	2.03	0.625	
	3.24	1.62	0.500	
	6.89	5.67	0.824	
	2.03	8.91	4.40	
	8.91	6.89	0.773	
Canada	7.00×10^{-3}	4.00×10^{-3}	0.571	[4]
	3.00×10^{-3}	1.00×10^{-3}	0.333	
	2.00×10^{-3}	1.00×10^{-3}	0.500	
	4.10×10^{-2}	2.50×10^{-2}	0.610	
Germany	1.62×10^{-2}	9.97×10^{-3}	9.97×10^{-3}	[7]
	9.97×10^{-3}	6.26×10^{-3}	6.26×10^{-3}	
	5.03×10^{-3}	3.79×10^{-3}	3.79×10^{-3}	
	5.46×10^{-3}	3.81×10^{-3}	3.81×10^{-3}	
	0.105	1.79×10^{-2}	1.79×10^{-2}	
	3.86×10^{-3}	4.28×10^{-3}	4.28×10^{-3}	
	4.73×10^{-2}	1.46×10^{-2}	1.46×10^{-2}	
	4.52×10^{-2}	1.46×10^{-2}	1.46×10^{-2}	

Country	HHCB	HHCB-lac	Ratio	Reference
	0.118	6.88×10^{-2}	6.88×10^{-2}	
	5.85×10^{-2}	2.54×10^{-2}	2.54×10^{-2}	
	3.00×10^{-2}	1.18×10^{-2}	1.18×10^{-2}	
	0.177	5.72×10^{-2}	5.72×10^{-2}	
	0.126	4.28×10^{-2}	4.28×10^{-2}	
	4.86×10^{-2}	2.42×10^{-2}	2.42×10^{-2}	
	7.96×10^{-2}	4.03×10^{-2}	4.03×10^{-2}	
	4.20×10^{-2}	2.05×10^{-2}	2.05×10^{-2}	
	5.65×10^{-2}	2.63×10^{-2}	2.63×10^{-2}	
	5.94×10^{-2}	2.55×10^{-2}	2.55×10^{-2}	
	8.63×10^{-2}	4.12×10^{-2}	4.12×10^{-2}	
	4.62×10^{-2}	2.47×10^{-2}	2.47×10^{-2}	
	0.133	7.43×10^{-2}	7.43×10^{-2}	
	4.95×10^{-2}	2.76×10^{-2}	2.76×10^{-2}	
	6.23×10^{-2}	4.05×10^{-2}	4.05×10^{-2}	
	6.15×10^{-2}	3.05×10^{-2}	3.05×10^{-2}	
	6.77×10^{-2}	3.39×10^{-2}	3.39×10^{-2}	
	5.41×10^{-2}	2.73×10^{-2}	2.73×10^{-2}	
	4.79×10^{-2}	2.73×10^{-2}	2.73×10^{-2}	
Italy	2.53	0.511	0.202	[17]
	3.30	1.74	0.527	
	0.952	0.442	0.464	
	0.282	7.43×10^{-2}	0.264	
	2.52	0.517	0.205	
	1.49	0.402	0.270	
	2.00	0.707	0.354	
	1.42	0.592	0.416	
	0.510	0.362	0.710	
	0.563	0.369	0.656	
	0.952	0.598	0.628	
	0.684	0.750	1.10	
	1.96	0.696	0.356	
	0.161	4.66×10^{-2}	0.290	
	0.174	8.44×10^{-2}	0.484	
Germany	1.60×10^{-2}	3.60×10^{-2}	3.60×10^{-2}	[12]

Table S5. Concentrations (ng/g) of HHCB and HHCB-lac and their concentration ratio (HHCB-

lac/HHCB) in sediment reported in the literature.

Country	HHCB	HHCB-lac	Ratio	Reference
China	2.68×10^{2}	3.04×10^{2}	1.13	[18]
	1.12×10^{2}	2.21×10^{2}	1.97	
	1.07×10^{2}	83.7	0.782	
	5.51×10^{3}	3.44×10^{3}	0.623	
	31.9	43.7	1.37	
	1.01×10^{2}	1.70×10^{2}	1.68	
	13.7	15.8	1.15	
	14.7	20.3	1.38	
	25.5	34.3	1.35	
	11.1	10.9	0.982	
	15.6	12.6	0.808	
	13.8	13.9	1.01	
	6.89	13.7	1.99	
	13.2	11.0	0.833	
	5.29	8.14	1.54	
	10.0	0.00	0.00	

Table S6. Concentrations (ng/g) of HHCB and HHCB-lac and their concentration ratio (HHCB-

lac/HHCB) in indoor dust reported in the literature.

Country	Indoor house dust type	HHCB	HHCB-lac	Ratio	Reference
China	Houses	37.9	3.16	8.34×10^{-2}	[19]
	Dormitories	31.9	3.97	0.124	
	Offices	26.6	1.00	3.76×10^{-2}	
	Laboratories	9.09	1.19	0.131	
	PC	51.9	3.47	6.69×10^{-2}	
	Aircondition	42.2	11.1	0.263	
Canada	Fresh dust	6.76×10^{2}	4.53×10^{2}	0.670	[20]
	Household vacuum dust	9.92×10^{2}	4.92×10^{2}	0.496	

Table S7. .Concentrations (ng/g) of HHCB and HHCB-lac and their concentration ratio (HHCB-lac/HHCB) in aquatic organisms reported in the literature.

Country	HHCB	HHCB-lac	Ratio	Reference
Germany	8.02×10^{2}	8.02×10^{2}	1.00	[16]
	1.18×10^{4}	2.98×10^{3}	0.251	
	9.67×10^{3}	4.27×10^{3}	0.441	
	4.99×10^{3}	2.32×10^{3}	0.464	
	2.36×10^{3}	9.35×10^{2}	0.396	
	2.41×10^{3}	3.88×10^{3}	1.61	
	2.94×10^{3}	2.94×10^{3}	1.00	
	2.41×10^{3}	1.87×10^{3}	0.778	
	2.18×10^{3}	1.11×10^{3}	0.510	
	25.5	58.1	2.28	
	27.2	75.3	2.77	
	11.6	0.00	0.00	
	20.3	0.00	0.00	
	22.4	0.00	0.00	
	22.3	0.00	0.00	
	52.4	52.1	0.994	
	19.0	0.00	0.00	
	16.9	8.20	0.485	
	19.1	9.30	0.487	
	23.7	1.25×10^{2}	5.25	
	38.0	55.8	1.47	
	58.8	8.70	0.148	
	12.8	56.6	4.42	
	25.5	58.1	2.28	[21]
	27.2	75.3	2.77	
	11.6	0.00	0.00	
	20.3	0.00	0.00	
	22.4	0.00	0.00	
	22.3	0.00	0.00	
	52.4	52.1	0.994	
	19.0	0.00	0.00	
	16.9	8.20	0.485	
	19.1	9.30	0.487	
	23.7	1.25×10^{2}	5.25	
	38.0	55.8	1.47	
	58.8	8.70	0.148	
	12.8	56.6	4.42	

Table S8. Concentrations (ng/g) of HHCB and HHCB-lac and their concentration ratio (HHCB-

lac/HHCB) in human bodies reported in the literature.

Country	Type	HHCB	HHCB-lac	Ratio	Reference
China	Umbilical cord blood	8.40	83.3	9.92	[22]
	Breast milk	7.90	8.60	1.09	
	Maternal	31.1	18.0	0.579	
	Umbilical cord blood	56.8	15.1	0.266	
	Breast milk	12.8	2.80	0.219	
China	Breast milk	4.56×10^2	2.57×10^2	0.564	[23]
		58.1	1.79×10^2	3.08	
		1.66×10^2	1.41×10^2	0.852	
		3.56×10^2	1.27×10^2	0.356	
		1.49×10^2	1.33×10^2	0.897	
		93.1	1.25×10^2	1.34	
		1.61×10^2	91.6	0.568	
		1.56×10^2	76.0	0.487	
		68.3	83.7	1.23	
		56.4	75.1	1.33	
		91.7	60.6	0.661	
		23.9	68.3	2.85	
		36.3	54.1	1.49	
		57.0	45.0	0.790	
		73.8	41.9	0.567	
		23.7	33.1	1.40	
		51.8	31.8	0.613	
		0.456	28.6	62.6	
		46.6	23.0	0.493	
		24.2	18.7	0.772	
		19.0	11.9	0.629	
		7.00	8.61	1.23	
		6.29	0.00	0.00	
		34.3	0.00	0.00	
		1.02×10^2	0.00	0.00	
		1.87×10^2	0.00	0.00	
		15.3	0.00	0.00	
		7.94	6.55	0.825	
		15.7	9.99	0.635	
		12.7	15.5	1.22	
		17.8	25.3	1.42	
		35.2	22.2	0.629	
		0.00	35.4	0.00	
		17.5	36.4	2.08	
		28.0	34.3	1.23	

Country	Type	HHCB	HHCB-lac	Ratio	Reference
		45.4	32.2	0.709	
		40.6	40.9	1.01	
		33.0	35.2	1.07	
		18.1	29.0	1.60	
		41.0	31.0	0.756	
		25.9	23.3	0.902	
		5.51	14.5	2.63	
		18.4	15.6	0.848	
		10.5	9.98	0.954	
		7.93	5.68	0.717	
		13.5	0.00	0.00	
		10.5	0.00	0.00	
		18.3	0.00	0.00	
		5.69	5.62	0.988	
		7.77	11.2	1.44	
		7.77	15.9	2.05	
		20.2	18.8	0.932	
		30.7	21.1	0.687	
		30.4	25.6	0.844	
		15.4	27.8	1.81	
		30.4	33.4	1.10	
		11.1	0.00	0.00	
		21.3	0.00	0.00	
		2.69	2.31	0.861	
		6.11	5.88	0.962	
		14.0	9.12	0.650	
		8.78	13.5	1.54	
		19.1	15.7	0.820	
		23.2	27.6	1.19	
		33.1	32.2	0.974	
		20.1	0.00	0.00	
		7.50	4.49	0.599	
		7.50	8.98	1.20	
		12.3	18.0	1.46	
		32.4	31.2	0.963	
		3.00	0.00	0.00	
		5.24	0.00	0.00	
		8.09	0.00	0.00	
		10.3	0.00	0.00	
		12.9	0.00	0.00	
		15.6	0.00	0.00	

Country	Type	HHCB	HHCB-lac	Ratio	Reference
		18.1	0.00	0.00	
		20.8	0.00	0.00	
		240	0.00	0.00	
		5.10	0.00	0.00	
		7.50	0.00	0.00	
		9.90	0.00	0.00	
		2.24	5.56	2.48	
		2.24	4.24	1.89	
		1.95	2.12	1.09	
		5.25	0.00	0.00	
		7.94	0.00	0.00	
		10.2	0.00	0.00	
		5.24	0.00	0.00	
		2.69	5.81	2.16	
		5.24	0.00	0.00	
		8.09	0.00	0.00	
		4.80	0.00	0.00	
		5.39	0.00	0.00	
		5.10	0.00	0.00	
America	Breast milk	1.21×10^{2}	5.00	4.13×10^{-2}	[24]
		47.2	5.00	0.106	
		35.1	5.00	0.142	
		1.35×10^{2}	5.00	3.70×10^{-2}	
		35.9	5.00	0.139	
		1.99×10^{2}	5.00	2.51×10^{-2}	
		1.60×10^{2}	5.00	3.13×10^{-2}	
		1.86×10^{2}	28.6	0.154	
		1.35×10^{2}	5.00	3.70×10^{-2}	
		89.9	5.00	5.56×10^{-2}	
		1.41×10^{2}	5.00	3.55×10^{-2}	
		1.06×10^{2}	5.00	4.72×10^{-2}	
		1.32×10^{2}	5.00	3.79×10^{-2}	
		6.03×10^{2}	5.00	8.29×10^{-3}	
		4.63×10^{2}	5.00	1.08×10^{-2}	
		88.1	5.00	5.68×10^{-2}	
		1.04×10^{2}	5.00	4.81×10^{-2}	
		90.8	5.00	5.51×10^{-2}	
		9.17×10^{2}	5.00	5.45×10^{-3}	
		5.54×10^{2}	5.00	9.03×10^{-3}	
		2.50	5.00	2.00	
		7.99×10^{2}	5.00	6.26×10^{-3}	

Country	Type	HHCB	HHCB-lac	Ratio	Reference
		2.61×10^{2}	5.00	1.92×10^{-2}	
		97.9	5.00	5.11×10^{-2}	
		4.15×10^{2}	5.00	1.20×10^{-2}	
		44.1	5.00	0.113	
		1.57×10^{2}	5.00	3.18×10^{-2}	
		2.43×10^{2}	5.00	2.06×10^{-2}	
		2.02×10^{2}	5.00	2.48×10^{-2}	
		1.36×10^{2}	5.00	3.68×10^{-2}	
		4.49×10^{2}	5.00	1.11×10^{-2}	
		2.33×10^{2}	5.00	2.15×10^{-2}	
		62.9	5.00	7.95×10^{-2}	
		21.7	5.00	0.230	
		2.67×10^{2}	5.00	1.87×10^{-2}	
		68.3	5.00	7.32×10^{-2}	
		47.9	5.00	0.104	
		1.00×10^{2}	5.00	5.00×10^{-2}	
		59.4	88.0	1.48	
China	Breast milk	22.9	12.3	0.538	[25]
		28.5	8.97	0.315	
		4.42	1.75	0.396	
		11.5	10.1	0.880	
		12.8	7.28	0.567	
		17.8	5.59	0.315	
		13.3	9.52	0.718	
		11.1	8.04	0.726	
		18.7	9.30	0.497	
		18.3	13.9	0.759	
		58.2	33.4	0.574	
		11.4	8.02	0.702	
		19.1	21.4	1.12	
		15.1	10.7	0.711	
		15.9	3.08	0.194	
		8.97	3.21	0.358	
		22.8	7.10	0.311	
		22.5	6.09	0.270	
		11.6	9.09	0.787	
		12.1	9.76	0.804	
		8.62	7.75	0.899	
		14.5	12.9	0.886	
		37.5	11.7	0.311	
		15.1	9.55	0.633	

Country	Type	HHCB	HHCB-lac	Ratio	Reference
China	Breast milk	19.6	7.40	0.378	[26]
		12.7	6.90	0.543	
		31.1	18.1	0.582	

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