

Table S2 Information on application and/or formation and toxicity of the organic contaminants identified in wastewaters from different units of the chemical production site

Compound	Application/Formation	Group	Toxicity for freshwater animals	Reference
Halogenated compounds				
Bromoform (No. 1)	Solvent, educt for pharmaceutical manufacturings; ingredient in fire-resistant chemicals, by-product of wastewater chlorination	U	LC ₅₀ 46 mg L ⁻¹ , 48 h, <i>Daphnia magna</i>	ENVICHEM data base A. O. Wistrom, T. Chou, D. P. Y. Chang, E. D. Schroeder, <i>Water Research</i> , 1996, 30 , 3146-3151;
1,2,3,4-Tetrachlorobutane (No. 2)	Educt for the synthesis of resins, educt for the polymer manufacturing	PR	-	
3-Chlorobicyclo[3.2.1]oct-2-ene (No. 3)	Educt for the synthesis of bicyclo[3.2.1]octan-3-one, educt for the synthesis of medications for cocaine abuse	P	-	P. C. Meltzer, P. Blundell, Z. Chen, Y. F. Yong, B. K. Madras, <i>Bioorganic & medicinal chemistry letters</i> , 1999, 9 , 857-862; C. P. Chang, C. H. Chen, G. J. Chuang, C. C. Liao, <i>Tetrahedron Letters</i> , 2009, 50 , 3414-3417;
Dichlorobenzene (No. 4)	Solvent in industry, degreasing agent for metals, leather and wool; ingredient of metal polishes, intermediate in the manufacture of dyes and agricultural chemicals	U	1,4-Dichlorobenzene EC ₅₀ 0.74 mg L ⁻¹ , 48 h, <i>Daphnia magna</i> 1,2-Dichlorobenzene EC ₅₀ 0.74 mg L ⁻¹ , 48 h, <i>Daphnia magna</i>	CCR chemical data base
Chlorophenol (No. 5) and Dichlorophenol (No. 6)	Chlorophenols are used as educts for the synthesis of agricultural chemicals, pharmaceuticals, biocides, and dyes	U	2-Chlorophenol: LC ₅₀ 2.6 mg L ⁻¹ , 48 h, <i>Daphnia magna</i> 2,4-Dichlorophenol: LC ₅₀ 0.26 mg L ⁻¹ , <i>Carassius auratus</i> , goldfish, 192 h	CCR chemical data base ENVICHEM data base
Dichloroveratrol (No. 7)	Used as fungicide		Fish toxicity LC ₅₀ 2.0 mg L ⁻¹ (as predicted by PNN)	CCR chemical data base

Trichlorobenzoic acid (No. 8)	In herbicide formulations (former use); in synthesis of antimicrobial and anti-inflammatory agents	U	-	P. Karegoudar, D.J. Prasad, M. Ashok, M. Mahalinga, B. Poojara, B.S. Holla, <i>European journal of medicinal chemistry</i> , 2008, 43 , 808-815;
Dichloroaniline (No. 9)	Intermediate in the production of plastics, dyestuffs, pesticides and pharmaceuticals	U	2,5-Dichloroaniline: LC ₅₀ 2.92 mg L ⁻¹ , 48 h, <i>Daphnia magna</i>	ENVICHEM data base
Trichloroaniline (No. 10)	Intermediate in the manufacture of chlorinated benzene derivatives, fungicides, dyestuffs, product of microbial and chemical degradation of pesticides	U	2,4,6- Trichloroaniline, LC ₅₀ 8.2 mg L ⁻¹ , 48 h, <i>Oryzias latipes</i> , orange-red killifish	W. R. Mitchell, S. H. Hoke, A. B. Rosencrance, <i>Journal of Environmental Science & Health Part A</i> , 1984, 19 , 679-696;
Chlorofluoroaniline (No. 11)	Intermediate for pharmaceuticals	P	-	e.g. R. K. Gilpin, L. A. Pachla, <i>Analytical chemistry</i> , 1997, 69 , 145-164;
Bromofluoroaniline (No. 12)	Intermediate for pharmaceuticals	P	-	G. Zareba, J. Castaner, J. Bozzo, <i>Drugs of the Future</i> , 2005, 30 , 138-146; M. T. Stone, <i>Organic Letters</i> , 2011, 13 , 2326-2329;
4-Bromo-2,6-dichloroaniline (No. 13)	Intermediate for agricultural chemicals, azodyes, and pigments and pharmaceuticals	U	-	B. Latli, M. Hrapchak, D. Krishnamurthy, C. H. Senanayake, <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 2008, 51 , 283-285;
2-Bromo-6-chloro-4-fluoroaniline (No. 14)	Intermediate for pharmaceuticals	P	-	K. Menzel, F. Machrouhi, M. Bodenstein, A. Alorati, C. Cowden, A. W. Gibson, D. E. Frantz, <i>Organic Process Research & Development</i> , 2009, 13 , 519-524;
Chloroquinolinol (No. 15)	Pharmaceutical	P	-	Z. Q. Liu, K. Han, Y. J. Lin, X. Y. Luo, <i>Biochimica et Biophysica Acta (BBA)-General Subjects</i> , 2002, 1570 , 97-103;

Chloroindole (No.16)	5-chloroindole is an intermediate for the production of pharmaceuticals	P	-	
5-Fluoroindole (No.17)	Intermediate for pharmaceuticals	P	-	W. K. Hagmann, <i>Journal of medicinal chemistry</i> , 2008, 51 , 4359-4369;
Chlorothieno[2,3-c]pyridine (No. 18)	2- Chlorothienopyridine is used as pharmaceutical, chlorothieno[2,3-c]pyridine is an intermediate for pharmaceuticals	P	-	B. S. Collier, <i>Journal of Thrombosis and Haemostasis</i> , 2011, 9(s1), 374-395;
2,3,5,6-Tetrafluorophenol (No. 19)	Component of tetrafluorophenol (TFP)-activated resins; educt for the synthesis of polyurethane polymeric compounds used for electric double-layer capacitors	PR	-	J. M. Salvino, R. E. Dolle, <i>Methods in Enzymology</i> , 2003, 369 , 151-163;
3'-(Trifluoromethyl)acetophenone (No. 20)	Intermediate for pharmaceuticals, pesticides, dyes	U	Fish toxicity LC ₅₀ 17.4 mg L ⁻¹ (as predicted by PNN)	CCR chemical data base
3,4-Dichloromethylthiobenzene (No. 21)	Chlorinated methylthiobenzenes are formed during the biotransformation of hexachlorobenzene, Educt for the synthesis of e.g. polychlorinated biphenyls		-	G. Renner, P. T. Nguyen, <i>Xenobiotica</i> , 1984, 14 , 705-710; K. Haraguch, A. Bergman, <i>Chemosphere</i> , 1991, 23 , 1837-1843;
3,4-Dichlorothiophenol (No. 22)	Educt for the synthesis of dyes	U	-	
Nitrogen-containing compounds				
Tetramethylbutanedinitrile (No. 23)	Decomposition product of 2,2'-azobisisobutyronitrile (polymerization initiator for monomers in plastic production)	PR	Fish toxicity LC ₅₀ 149 mg L ⁻¹ (as predicted by PNN)	H. Ishiwata, T. Sugita, T. Yamada, <i>Food Hygiene and Safety Science</i> , 1994, 35 , 385-389; CCR chemical data base
3,3-Diphenyl-2-propenenitrile (No. 24)	Product in the reaction of acrylonitrile with iodobenzene, used in the synthesis of intermediates in agricultural and pharmaceutical applications	U	-	A. Wali, S. Muthukumar Pillai, V. K. Kaushik, S. Satish, <i>Applied Catalysis A: General</i> , 1996, 135 , 83-93; D. J. Adams, J. H. Clark, L. B. Hansen, V. C. Sanders, S. J. Tavener, <i>Journal of fluorine chemistry</i> , 1998, 92 , 123-125;

N-Formylmorpholine (No. 25)	Used as selective solvent by the petroleum industry for the extraction of high-purity aromatic compounds, anticorrosive agent in fuel oil, used for the cleaning of technical gases		EC ₅₀ >500 mg L ⁻¹ , 48 h, <i>Daphnia magna</i>	ECHA Chem database
Sulphur-containing compounds				
Dimercaptomethane (No. 26)	Intermediate in manufacturing of flavour concentrates, product in the synthesis of azaphospholines (intermediates for pharmaceuticals), additive for the production of synthetic rubber, formed during decomposition of organic material		Fish toxicity LC ₅₀ 5.9 mg L ⁻¹ (as predicted by PNN)	FAO JECFA, Compendium of food additive specifications. 68 th meeting. Food and Agriculture Organization of the United Nations, 2007, Rome; R. M. Kamalov, G. S. Stepanov, I. A. Litvinov, M. A. Pudovik, <i>Heteroatom Chemistry</i> , 1994, 5 , 469-477; CCR chemical data base
1,2-Dimercaptoethane (No. 27)	Complexing agent, used for the stabilization of polymers, additive for the production of synthetic rubber, educt for chemical synthesis, formed during decomposition of organic material		Fish toxicity LC ₅₀ 9.3 mg L ⁻¹ (as predicted by PNN)	CCR chemical data base
2-(Methylthio)acetic acid (No. 28)	Constituent of plants		-	
Mercaptoacetic acid (No. 28)	Raw material for pharmaceuticals and agricultural chemicals	U	Fish toxicity LC ₅₀ 383 mg L ⁻¹ (as predicted by PNN)	
Phosphorus-containing compounds				
TCPP (No. 29), TEP (No. 30), TBP (No. 31)	Flame retardants and plasticizers	M	TCPP: Fish toxicity LC ₅₀ 9.1 mg L ⁻¹ (as predicted by PNN) TEP: LC ₅₀ 500 mg L ⁻¹ , 48h, <i>Oryzias latipes</i> , orange-red killifish TBP: Fish toxicity LC ₅₀ 4.3 mg L ⁻¹ , 96h, <i>Oncorhynchus mykiss</i> , rainbow trout	CCR chemical data base ECHA CHEM database ENVICHEM database

DBMP (No. 32)	Educt for the manufacturing of organo-phosphorus peroxide compounds which are used as initiators of polymerization reactions or as intermediates in the production of pesticides and bleaching agents	PR	-	
BEHP (No. 33)	Complexing agent for rare earth elements, educt for the synthesis of polymers	PR	LC ₅₀ 148 mg L ⁻¹ , <i>Oryzias latipes</i> , orange-red killifish	e.g. A. Proń, J. Laska, J. E. Österholm, P. Smith, <i>Polymer</i> , 1993, 34 , 4235-4240; CCR chemical data base
Oxygen-containing compounds				
Bisphenol A (No. 34)	Used for the production of polycarbonates, epoxy resins and thermal paper	M	LC ₅₀ 4.6 mg L ⁻¹ , 96h, <i>Pimephales promelas</i> , fathead minnow	CCID database
TXIB (No. 35)	Plasticizer for PVC and vinyl plastics	M	LC ₅₀ 300 mg L ⁻¹ , 24 h, <i>Daphnia magna</i>	I. Skjevraak, A. Due, K. O. Gjerstad, H. Herikstad, <i>Water Research</i> , 2003, 37 , 1912-1920;
Benzoic acid (No. 36)	Occurs in plants, used as educt for many industrial syntheses		LC ₅₀ 180 mg L ⁻¹ , 96 h, <i>Gambusia affinis</i> , mosquitofish	ENVICHEM database
Phenylacetic acid (No. 37)	Used for production of pharmaceuticals, occurs in plants and animals		EC ₅₀ 802 mg L ⁻¹ , 96h, <i>Xenopus laevis</i> , clawed toad	CCR chemical data base
4- <i>tert</i> -Butylbenzoic acid (No. 38)	Used for the manufacture of alkyd resins	M	LC ₅₀ 70 mg L ⁻¹ , 96 h, <i>Oryzias latipes</i> , orange-red killifish	ECHA CHEM database
Polycyclic aromatic compounds				
DIPN (No. 39)	Dye solvent, constituent of coating agents, adhesives, heat transfer and insulating oils		LC ₅₀ 4.5 mg L ⁻¹ , <i>Oryzias latipes</i> , orange-red killifish	CCR chemical data base

EC₅₀: Concentration of a chemical which induces a defined response of 50% of the members of a tested population after a specified test duration

LC₅₀: Concentration of a chemical required to kill 50% of the members of a tested population after a specified test duration

Information from chemical data bases were obtained from: <http://www.echemportal.org>

Compound numbers refer to Table 2, full chemical names of the compounds are given in Table 1

Groups:

U: **Unspecific** educts or intermediates in the industrial production of many agricultural chemicals, pharmaceuticals and dyes

P: Specific **pharmaceuticals** or intermediates in the production of **pharmaceuticals**

PR: Educts for the synthesis of **polymers** and **resins**

M: Known as typical constituents of **municipal sewage**