

List of Publications of Gerrit Schüürmann

Status: February 2022

Total Number = 316 (without scientific reports and abstracts):

- 245 Articles in journals with peer review (pp. 1-20)
- 44 Articles in books/proceedings (pp. 21-26)
- 23 Articles in journals without peer review (pp. 27-29)
- 4 Books and proceedings edited/co-edited (p. 30)

A) Articles in Journals with Peer Review

2022

245. Scholz S, Nichols JW, Escher BI, Ankley GT, Altenburger R, Blackwell B, Brack W, Burkhard L, Collette TW, Doering JA, Ekman D, Fay K, Fischer F, Hackermüller J, Hoffman JC, Lai C, Leuthold D, Martinovic-Weigelt D, Reemtsma T, Pollesch N, Schroeder A, Schüürmann G, von Bergen M 2022. The Eco-Exposome Concept: Supporting an Integrated Assessment of Mixtures of Environmental Chemicals. *Environ. Toxicol. Chem.* 41: 30-45.

2021

244. Zhang S, Adrian L, Schüürmann G 2021. Outer-sphere electron transfer does not underpin B₁₂-dependent olefinic reductive dehalogenation in anaerobes. *Phys. Chem. Chem. Phys.* 23: 27520-27524.

243. Böhme A, Moldrickx J, Schüürmann G 2021. Amino Reactivity of Glutardialdehyde and Monoaldehydes – Chemoassay Profile vs Skin Sensitization Potency. *Chem. Res. Toxicol.* 34: 2353-2365.

242. Liess M, Liebmann L, Vormeier P, Weisner O, Altenburger R, Borchardt D, Brack W, Chatzinotas A, Escher B, Foit K, Gunold R, Hens S, Hitzfeld KL, Schmitt-Jansen M, Kamjunke N, Kaske O, Knillmann S, Krauss M, Küster E, Link M, Lück M, Möder M, Müller A, Paschke A, Schäfer RB, Schneeweiss A, Schreiner VC, Schulze T, Schüürmann G, von Tümpling W, Weitere M, Wogram J, Reemtsma T 2021. Pesticides are the dominant stressors for vulnerable insects in lowland streams. *Wat. Res.* 201: 117262.

241. Grodtke M, Paschke A, Harzdorf J, Krauss M, Schüürmann G 2021. Calibration and field application of the Atlantic HLB Disk containing Chemcatcher® passive sampler – Quantitative monitoring of herbicides, other pesticides, and transformation products in German streams. *J. Haz. Mat.* 410, 124538 (10pp).

2020

240. Arunrungvichian K, Chongruchoj S, Sarasamkan J, Schüürmann G, Brust P,

Vajragupta O 2020. In Silico Finding of Key Interaction Mediated $\alpha 3\beta 4$ and $\alpha 7$ Nicotinic Acetylcholine Receptor Ligand Selectivity of Quinuclidine-Triazole Chemotype. *Int. J. Mol. Sci.* 21: 6189 (18 pp).

239. Chepchirchir BS, Zhou X, Paschke A, Schüürmann G 2020. Polyethersulfone as suitable passive sampler for waterborne hydrophobic organic compounds – Laboratory calibration and field test in the Sosiani river, Kenya. *Sci. Total Environ.* 699: 134056 (8 pp).

238. Holbech H, Matthiessen P, Hansen M, Schüürmann G, Knapen D, Reuver M, Flamant F, Sachs L, Kloas W, Hilscherova K, Leonard M, Arning J, Strauss V, Iguchi T, Baumann L 2020. ERGO: Breaking Down the Wall between Human Health and Environmental Testing of Endocrine Disruptors. *Int. J. Mol. Sci.* 21: 2954 (18 pp).

237. Sadeghzadeh M, Wenzel B, Gündel D, Deuther-Conrad W, Toussaint M, Moldovan R-P, Fischer S, Ludwig F-A, Teodoro R, Jonnalagadda S, Jonnalagadda SK, Schüürmann G, Meredy VR, Drewes LR, Brust P 2020. Development of Novel Analogs of the Monocarboxylate Transporter Ligand FACH and Biological Validation of One Potential Radiotracer for Positron Emission Tomography (PET) Imaging. *Molecules* 25: 2309 (21 pp).

236. Shamsara J, Schüürmann G 2020. A machine learning approach to discriminate MR1 binders: The importance of the phenol and carbonyl fragments. *J. Mol. Struct.* 1217: 128459 (7 pp).

235. Van Gils J, Posthuma L, Cousins IT, Brack W, Altenburger R, Baveco H, Focks A, Greskowiak J, Kühne R, Kutsarova S, Lindim C, Markus A, van de Meent D, Munthe J, Schueder R, Schüürmann G, Slobodnik J, de Zwart D, van Wenzel A 2020. Computational material flow analysis for thousands of chemicals of emerging concern in European waters. *J. Haz. Mat.* 397: 122655 (12pp).

234. Zhang S, Adrian L, Schüürmann G 2020. Dehalococoides-Mediated B12-Dependent Reductive Dehalogenation of Aromatics Does Not Proceed through Outer-Sphere Electron Transfer. *Environ. Sci. Technol.* 54: 15751-15758.

2019

233. Junker Th, Coors A, Schüürmann G 2019. Compartment-Specific Screening Tools for Persistence: Potential Role and Application in the Regulatory Context. *Integr. Environ. Assess. Managem.* 15: 470-481.

232. Lindim C, de Zwart D, Cousins IT, Kutsarova S, Kühne R, Schüürmann G 2019. Exposure and ecotoxicological risk assessment of mixtures of top prescribed pharmaceuticals in Swedish freshwaters. *Chemosphere* 220: 344-352.

2018

231. Jahreis S, Trump S, Bauer M, Bauer T, Thürmann L, Feltens R, Wang Q, Gu L, Grützmann K, Röder S, Averbek M, Weichenhahn D, Plass C, Sack U, Borte M, Schüürmann G, Simon JC, von Bergen, Hackermüller J, Eils R, Lehmann I, Polte T 2018. Maternal phthalate exposure promotes allergic airway inflammation over two generations via epigenetic modifications. *J. Allergy Clin. Immunol.* 141: 741-753.

230. Ma G, Yu H, Wei X, Chen J, Lin H, Schüürmann G 2018. Computational insight into the activation mechanism of carcinogenic N'-nitrosonornicotine (NNN) catalyzed by cytochrome P450. *Environ. Sci. Technol.* 52: 11838-11847.

229. Nendza M, Kühne R, Lombardo A, Stempel S, Schüürmann G 2018. PBT assessment under REACH: Screening for low aquatic bioaccumulation with QSAR classifications based on physicochemical properties to replace BCF in vivo testing on fish. *Sci. Total Environ.* 616-617: 97-196.

228. Zhang S, Adrian L, Schüürmann G 2018. Interaction Mode and Regioselectivity in Vitamin B12-Dependent Dehalogenation of Aryl Halides by *Dehalococcoides mccartyi* Strain CBDB1. *Environ. Sci. Technol.* 52: 1834-1843.

227. Zhang Q, Ji S, Chai L, Yang F, Zhao M, Liu W, Schüürmann G, Ji L 2018. Metabolic mechanism of aryl phosphorus flame retardants by cytochromes P450: A combined experimental and computational study on triphenyl phosphate. *Environ. Sci. Technol.* 52: 14411-14421.

2017

226. Chepchirchir BS, Paschke A, Schüürmann G 2017. Passive sampling for spatial and temporal monitoring of organic pollutants in surface water of a rural-urban river in Kenya. *Sci. Total Environ.* 601-602: 453-460.

225. Escher BI, Hackermüller J, Polte T, Scholz S, Aigner A, Altenburger R, Böhme A, Bopp SK, Brack W, Busch W, Chadeau-Hyam M, Covaci A, Eisenträger A, Galligan JJ, Garcia-Reyero N, Hartung T, Hein M, Herberth G, Jahnke A, Kleinjans J, Klüver N, Krauss M, Lamoree M, Lehmann I, Luckenbach T, Miller GW, Müller A, Phillips DH, Reemtsma T, Rolle-Kampczyk U, Schüürmann G, Schwikowski B, Tan Y-M, Trump S, Walter-Rohde S, Wambaugh JF 2017. From the exposome to mechanistic understanding of chemical-induced adverse effects. *Environ. Int.* 99: 97-106.

224. Le TDH, Scharmüller A, Kattwinkel M, Kühne R, Schüürmann G, Schäfer RB 2017. Contribution of waste water treatment plants to pesticide toxicity in agriculture catchments. *Ecotoxicol. Environ. Saf.* 145: 135-141.

223. Muz M, Ost O, Kühne R, Schüürmann G, Brack W, Krauss M 2017. Nontargeted detection and identification of (aromatic) amines in environmental samples based on diagnostic derivatization and LC-high resolution mass spectrometry. *Chemosphere* 166: 300-310.

222. Shafique U, Dorn V, Paschke A, Schüürmann G 2017. Adsorption of perfluorocarboxylic acids at the silica surface. *Chem. Commun.* 53: 589-592.

221. Shafique U, Schulze S, Slawik C, Kunz S, Paschke A, Schüürmann G 2017. Gas chromatographic determination of perfluorocarboxylic acids in aqueous samples. A tutorial review. *Anal. Chim. Acta* 949: 8-22.

220. Shafique U, Schulze S, Slawik C, Chepchirchir BS, Böhme A, Paschke A, Schüürmann G 2017. Perfluoroalkyl acids in aqueous samples from Germany and Kenya. *ESPR – Environ. Sci. Pollut. Res.* 24: 11031-11043; Erratum: 11044.

219. Slawik C, Rickmeyer C, Brehm M, Böhme A, Schüürmann G 2017. Glutathione Adduct Patterns of Michael-Acceptor Carbonyls. *Environ. Sci. Technol.* 51: 4018-4026.

218. Winter M, Thürmann L, Zugang G, Schüürmann G, Herberth G, von Bergen M, Harms H, Olek S, Röder S, Eils R, Lehmann I, Trump S 2017. The benzene metabolite 1,4-benzoquinone reduces regulatory T-cell function: A potential mechanism for tobacco smoke-associated atopic dermatitis. *J. Allergy Clin. Immunol.* 140: 603-605.

217. Zhang S, Wondrousch D, Cooper M, Zinder SH, Schüürmann G, Adrian L 2017. Anaerobic Dehalogenation of Chloroanilines by Dehalococcoides mccartyi Strain CBDB1 and Dehalobacter Strain 14DCB1 via Different Pathways as Related to Molecular Electronic Structure. *Environ. Sci. Technol.* 51: 3714-3724.

2016

216. Böhme A, Laqua A, Schüürmann G 2016. Chemoavailability of organic electrophiles – Impact of hydrophobicity and reactivity on their aquatic excess toxicity. *Chem. Res. Toxicol.* 29: 952-962.

215. Eremina N, Paschke A, Mazlova EA, Schüürmann G 2016. Distribution of polychlorinated biphenyls, phthalic acid esters, polycyclic aromatic hydrocarbons and organochlorine substances in the Moscow River, Russia. *Environ. Pollut.* 210: 409-418.

214. Hirte K, Seiwert B, Schüürmann G, Reemtsma T 2016. New hydrolysis products of the beta-lactam antibiotic amoxicillin, their pH-dependent formation and search in municipal wastewater. *Water Res.* 88: 880-888.

213. Junker T, Coors A, Schüürmann G 2016. Development and application of screening tools for biodegradation in water-sediment systems and soil. *Sci. Total Environ.* 544: 1020-1030.

212. Salmina E, Wondrousch D, Kühne R, Potemkin VA, Schüürmann G 2016. Variation in predicted internal concentrations in relation to PBPK model complexity for rainbow trout. *Sci. Total Environ.* 550: 586–597.

211. Sarasamkan J, Scheunemann M, Apaijai N, Palee S, Parichatikanond W, Arunrungvichian K, Fischer S, Chattipakorn S, Deuther-Conrad W, Schüürmann G, Brust P, Vajragupta O 2016. Varying Chirality Across Nicotinic Acetylcholine Receptor Subtypes: Selective Binding of Quinuclidine Triazole Compounds. *ACS Med. Chem. Lett.* 7: 890-895.

210. Schüürmann G, Ebert R-U, Tluczkiewicz I, Escher SE, Kühne R 2016. Inhalation threshold of toxicological concern (TTC) – Structural alerts discriminate high from low repeated-dose inhalation toxicity. *Environ. Int.* 88: 123-132.

209. Tluczkiewicz I, Kühne R, Ebert R-U, Batke M, Schüürmann G, Mangelsdorf I, Escher SE 2016. Inhalation TTC values: A new integrative grouping approach based on structural, toxicological and mechanistic features. *Regul. Toxicol. Pharm.* 78: 8-23.

2015

208. Barthel C, Sorger D, Deuther-Conrad W, Scheunemann M, Schweiger S, Jäckel P, Roghani A, Steinbach J, Schüürmann G, Sabri O, Brust P, Wenzel B 2015. New systematically modified vesamicol analogs and their affinity and selectivity for the vesicular acetylcholine transporter – A critical examination of the lead structure. *Eur. J. Med. Chem.* 100: 50-67.

207. Berggren E, Amcoff P, Benigni R, Blackburn K, Carney E, Cronin M, Deluyker H, Gauthier F, Judson RS, Kass GEN, Keller D, Knight D, Lilienblum W, Mahony C, Rusyn I, Schultz T, Schwarz M, Schüürmann G, White A, Burton J, Lostia A, Munn S, Worth A 2015. Chemical Safety Assessment Using Read-Across: Assessing the Use of Novel Testing Methods to Strengthen the Evidence Base for Decision-Making. *Environ. Health Perspect.* 123: 1232–1240.

206. Brack W, Altenburger R, Schüürmann G, Krauss M, López Herráez D, van Gils J, Slobodnik J, Munthe J, Gawlik BM, van Wezel A, Schriks M, Hollender J, Tollefsen KE, Mekenyan O, Dimitrov S, Bunke D, Cousins I, Posthuma L, van den Brink PJ, López de Alda M, Barceló D, Faust M, Kortenkamp A, Scrimshaw M, Ignatova S, Engelen G, Massmann G, Lemkine G, Teodorovic I, Walz K-H, Dulio V, Jonker MTO, Jäger F, Chipman K, Falciani F, Liska I, Rooke D, Zhang X, Hollert H, Vrana B, Hilscherova K, Kramer K, Neumann S, Hammerbacher R, Backhaus T, Mack J, Segner H, Escher B, de Aragão Umbuzeiro G 2015. The SOLUTIONS project: Challenges and responses for present and future emerging pollutants in land and water resources management. *Sci. Total Environ.* 503-504: 22-31.

205. Cooper M, Wagner A, Wondrousch D, Sonntag F, Sonnabend A, Brehm M, Schüürmann G, Adrian L 2015. Anaerobic Microbial Transformation of Halogenated Aromatics and Fate Prediction Using Electron Density Modeling. *Environ. Sci. Technol.* 49, 10: 6018-6028.

204. Ji L, Schüürmann G 2015. Computational biotransformation profile of paracetamol catalyzed by cytochrome P450. *Chem. Res. Toxicol.* 28: 585-596.

203. Münze R, Orlinskiy P, Gunold R, Paschke A, Kaske O, Beketov MA, Hundt M, Bauer C, Schüürmann G, Möder M, Liess M 2015. Pesticide impact on aquatic invertebrates identified with Chemcatcher® passive samplers and the SPEAR_{pesticides} index. *Sci. Total Environ.* 537: 69-80.

202. Petersen J, Paschke A, Gunold R, Schüürmann G 2015. Calibration of Chemcatcher® passive sampler for selected highly hydrophobic organic substances under fresh and sea water conditions. *Environ. Sci.: Water Res. Technol.* 1: 218-226.

201. Thalheim T, Wagner B, Kühne R, Middendorf M, Schüürmann G 2015. A Branch-and-Bound Approach for Tautomer Enumeration. *Mol. Inf.* 34, 5: 263-275.

200. Roviada C, Alépée N, Api AM, Basketter DA, Bois FY, Caloni F, Corsini E, Daneshian M, Eskes C, Ezendam J, Fuchs H, Hayden P, Hegele-Hartung C, Hoffmann S, Hubesch B, Jacobs MN, Jaworska J, Kleensang A, Kleinstreuer N, Lalko J, Landsiedel R, Lebreux F, Luechtefeld T, Locatelli M, Mehling A, Natsch A, Pitchford JW, Prater D, Prieto P, Schepky A, Schüürmann G, Smirnova L, Toole C, van Vliet E, Weisensee D, Hartung T 2015. T4 Report. Integrated Testing Strategies (ITS) for Safety Assessment. *ALTEX* 32, 1: 25-40.

199. Wilks MF, Roth N, Aicher L, Faust M, Papadaki P, Marchis A, Calliera M, Ginebreda A, Andres S, Kühne R, Schüürmann G 2015. White Paper On The Promotion Of An Integrated Risk Assessment Concept In European Regulatory Frameworks For Chemicals. *Sci. Total Environ.* 521-522: 211-218.

198. Yu H, Wondrousch D, Yuan Q, Lin H, Chen J, Hong H, Schüürmann G 2015. Modeling and predicting pK_a values of mono-hydroxylated polychlorinated biphenyls (HO-PCBs) and polybrominated diphenyl ethers (HO-PBDEs) by local molecular descriptors. 2015. *Chemosphere* 138: 829-836.

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197. Caicedo PV, Rahman KZ, Kusch P, Blumberg B, Paschke A, Janzen W, Schüürmann G 2014. Comparison of heavy metal content in two sludge drying reed beds of different age. *Ecol. Engineer.* 74: 48-55.

196. Lombardo A, Roncaglioni A, Benfentati E, Nendza M, Segner H, Jeram S, Pauné E, Schüürmann G 2014. Optimizing the aquatic toxicity assessment under REACH through an

integrated testing strategy (ITS). *Environ. Res.* 135: 156-164.

195. Lombardo A, Roncaglioni A, Benfentati E, Nendza M, Segner H, Fernández A, Kühne R, Franco A, Pauné E, Schüürmann G 2014. Integrated testing strategy (ITS) for bioaccumulation assessment under REACH. *Environ. Int.* 69: 40-50.

194. Ren W, Paschke A, Schüürmann G 2014. Sorption of chlorimuron-ethyl on montmorillonite clays: effects of exchangeable cations, pH, and ionic strength. *ESPR – Environ. Sci. Pollut. Res.* 21:11587-11597.

193. Ulrich N, Mühlenberg J, Schüürmann G, Brack W 2014. Linear solvation energy relationships as classifier in non-target analysis – An approach for isocratic liquid chromatography. *J. Chromatogr. A* 1324: 96-103.

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192. Ulrich N, Schüürmann G, Brack W 2013. Prediction of gas chromatographic retention indices as classifier in non-target analysis of environmental samples. *J. Chromatogr. A* 1285: 139-147.

191. Tluczkiewicz I, Batke M, Kroese D, Buist H, Aldenberg T, Pauné E, Grimm H, Kühne R, Schüürmann G, Mangelsdorf I, Escher SE. The OSIRIS Weight of Evidence approach: ITS for the endpoints repeated-dose toxicity (RepDose ITS) 2013. *Regul. Toxicol. Pharmacol.* 67: 157-169.

190. Scholz S, Sela E, Blaha L, Braunbeck T, Galay-Burgos M, García-Franco M, Guinea J, Klüver N, Schirmer K, Tanneberger K, Tobor-Kapłon M, Witters H, Belanger S, Benfenati E, Creton S, Cronin MTD, Eggen RIL, Embry M, Ekman D, Gourmelon A, Halder M, Hardy B, Hartung T, Hubesch B, Jungmann D, Lampi MA, Lee L, Léonard M, Küster E, Lillicrap A, Luckenbach T, Murk AJ, Navas JM, Peijnenburg W, Repetto G, Salinas E, Schüürmann G, Spielmann H, Tollefsen KE, Walter-Rohde S, Whale G, Wheeler JR, Winter MJ 2013. A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment. *Regul. Toxicol. Pharmacol.* 67: 506-530.

189. Rorije E, Aldenberg T, Buist H, Kroese D, Schüürmann G 2013. The OSIRIS weight of evidence approach: ITS for skin sensitisation. *Regul. Toxicol. Pharmacol.* 67: 146-156.

188. Péry ARR, Schüürmann G, Ciffroy P, Faust M, Backhaus T, Aicher L, Mombelli E, Tebby C, Cronin MTD, Tissot S, Andres S, Brignon JM, Frewer L, Georgiou S, Mattas K, Vergnaud JC, Peijnenburg W, Capri E, Marchis A, Wilks MF 2013. Perspectives for integrating human and environmental risk assessment and synergies with socio-economic analysis. *Sci. Total Environ.* 456-457: 307-316.

187. Nendza M, Gabbert S, Kühne R, Lombardo A, Roncaglioni A, Benfenati E, Benigni R, Bossa C, Stempel S, Scheringer M, Fernández A, Rallo R, Giralto F, Dimitrov S, Mekenyan O, Bringezu F, Schüürmann G 2013. A comparative survey of chemistry-driven *in silico* methods to identify hazardous substances under REACH. *Regul. Toxicol. Pharmacol.* 66: 301-314.

186. Mulliner D, Schüürmann G 2013. Model suite for predicting the aquatic toxicity of α,β -unsaturated esters triggered by their chemoavailability. *Mol. Inf.* 32: 98-107.

185. Mueller A, Schlink U, Wichmann G, Bauer M, Graebisch C, Schüürmann G, Herbarth O 2013. Individual and combined effects of mycotoxins from typical indoor moulds. *Toxicol. In Vitro* 27: 1970-1978.

184. Kühne R, Ebert R-U, von der Ohe PC, Ulrich N, Brack W, Schüürmann G 2013. Read-across prediction of the acute toxicity of organic compounds toward the water flea *Daphnia magna*. *Mol. Inf.* 32: 108-120.
183. Ji L, Schüürmann G 2013. Model and Mechanism: N-hydroxylation of Primary Aromatic Amines by Cytochrome P450. *Angew. Chem. Int. Ed.* 52: 744-748; *Angew. Chem.* 125: 772-776.
182. Buist H, Aldenberg T, Batke M, Escher S, Klein Entink R, Kühne R, Marquart H, Pauné E, Rorije E, Schüürmann G, Kroese D 2013. The OSIRIS Weight of Evidence approach: ITS mutagenicity and ITS carcinogenicity. *Regul. Toxicol. Pharmacol.* 67: 170-181.

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180. Slobodnik J, Mrafkova L, Carere M, Ferrara F, Pennelli B, Schüürmann G, von der Ohe P 2012. Identification of river basin specific pollutants and derivation of environmental quality standards: a case study in the Slovak Republic. *Trends Anal. Chem.* 41: 133-154.
179. Thaens D, Heinzelmann D, Böhme A, Paschke A, Schüürmann G 2012. Chemoassay Screening of DNA-reactive Mutagenicity with 4-(4-Nitrobenzyl)pyridine – Application to Epoxides, Oxetanes and Sulfur Heterocycles. *Chem. Res. Toxicol.* 25: 2092-2102.
178. Ji L, Schüürmann G 2012. Computational Evidence for α -Nitrosamino Radical as Initial Metabolite for Both the P450 Dealkylation and Denitrosation of Carcinogenic Nitrosamines. *J. Phys. Chem. B* 116: 903-912.
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175. Von der Ohe P, Dulio V, Slobodnik J, De Deckere E, Kühne R, Ebert R-U, Ginebreda A, De Cooman W, Schüürmann G, Brack W 2011. A new risk assessment approach for the prioritization of 500 classical and emerging organic microcontaminants as potential river basin specific pollutants under the European Water Framework Directive. *Sci. Total Environ.* 409: 2064-2077.
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169. Mulliner D, Wondrousch D, Schüürmann G 2011. Predicting Michael-Acceptor Reactivity and Toxicity through Quantum Chemical Transition-State Calculations. *Org. Biomol. Chem.* 9: 8400-8412.
168. Gruber T, Eissmann F, Weber E, Schüürmann G 2011. 1-Methyl-4-(4-nitrobenzoyl)pyridinium perchlorate. *Acta Cryst. E* 67: o2542-o2543.
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162. Meinert C, Schymanski E, Küster E, Kühne R, Schüürmann G, Brack W 2010. Application of preparative capillary gas chromatography (pcGC), automated structure generation and mutagenicity prediction to improve effect-directed analysis of genotoxicants in a contaminated groundwater. *Environ. Sci. Pollut. Res.* 17: 885-897.
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