

Publikationsliste von Gerrit Schüürmann

Status: September 2019

Gesamtzahl = 303 (ohne wissenschaftliche Berichte und Tagungsbände):

- 232 Artikel in Zeitschriften mit Fachbegutachtung (S. 1-19)
- 44 Artikel in Büchern und Tagungsbänden (S. 20-25)
- 23 Artikel in Zeitschriften ohne Fachbegutachtung (S. 26-28)
- 4 Bücher und Tagungsbände herausgegeben (S. 29)

A) Artikel in Zeitschriften mit Fachbegutachtung

2019

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, Thüürmann 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'-nitrosornicotine (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.

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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, 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, Gautier 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.

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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. Rovida 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, Tolleson 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.
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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.
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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.
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170. Schäfer RB, von der Ohe PC, Kühne R, Schüürmann G, Liess M 2011. Occurrence and Toxicity of 331 Organic Pollutants in Large Rivers of North Germany over a Decade (1994 to 2004). *Environ. Sci. Technol.* 45: 6167-6174.
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165. Wondrousch D, Böhme A, Thaens D, Ost N, Schüürmann G 2010. Local Electrophilicity Predicts the Toxicity-Relevant Reactivity of Michael Acceptors. *J. Phys. Chem. Lett.* **1**: 1605-1610.

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