

# Publikationsliste von Gerrit Schüürmann

Status: Februar 2022

**Gesamtzahl = 316** (ohne wissenschaftliche Berichte und Abstracts):

- 245 Artikel in Zeitschriften mit Fachbegutachtung (S. 1-20)
- 44 Artikel in Büchern und Tagungsbänden (S. 21-26)
- 23 Artikel in Zeitschriften ohne Fachbegutachtung (S. 27-29)
- 4 Bücher und Tagungsbände herausgegeben (S. 30)

## A) Artikel in Zeitschriften mit Fachbegutachtung

### 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 B<sub>12</sub>-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,

*Artikel in Zeitschriften mit Fachbegutachtung – Gerrit Schüürmann*

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, Tluczkiwicz 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. Tluczkiwicz 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<sub>pesticides</sub> 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. 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.

## 2014

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.

## 2013

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  $\alpha,\beta$ -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.

## 2012

181. Ulrich N, Mühlenberg J, Retzbach H, Schüürmann G, Brack W 2012. Linear Solvation Energy Relationships as classifiers in non-target analysis - a gas chromatographic approach. *J. Chromatogr. A* 1262: 95-103.

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  $\alpha$ -Nitrosamino Radical as Initial Metabolite for Both the P450 Dealkylation and Denitrosation of Carcinogenic Nitrosamines. *J. Phys. Chem. B* 116: 903-912.

177. Blaschke U, Eismann K, Böhme A, Paschke A, Schüürmann G 2012. Structural Alerts for the Excess Toxicity of Acrylates, Methacrylates and Propiolates derived from Their Short-Term and Long-Term Bacterial Toxicity. *Chem. Res. Toxicol.* 25: 170-180.

## 2011

176. Yu H, Ebert R-U, Kühne R, Schüürmann G 2011. Prediction of the Dissociation Constant  $pK_a$  of Organic Acids from Local Molecular Parameters of Their Electronic Ground State. *J. Chem. Inf. Mod.* 51: 2336-2344.

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.

174. Ulrich N, Schüürmann G, Brack W 2011. Linear Solvation Energy Relationships as classifiers in non-target analysis – A capillary liquid chromatography approach. *J. Chromatogr. A* 1218: 8192-8196.

173. Schwöbel J, Ebert R-U, Kühne R, Schüürmann G 2011. Prediction Models for the Abraham Hydrogen Bond Donor Strength: Comparison of Semi-Empirical, *Ab Initio* and DFT Methods. *J. Phys. Org. Chem.* 24: 1072-1080.

172. Schüürmann G, Ebert R-U, Kühne R 2011. Quantitative Read-across for Predicting the Acute Fish Toxicity of Organic Compounds. *Environ. Sci. Technol.* 45: 4616-4622.
171. Schramm F, Müller A, Hammer H, Paschke A, Schüürmann G 2011. Epoxide and Thiirane Toxicity *In vitro* with the Ciliates *Tetrahymena pyriformis* – Structural Alerts Indicating Excess Toxicity. *Environ. Sci. Technol.* 45: 5812-5819.
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.
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.
167. Caicedo P, Schröder A, Ulrich N, Schröter U, Paschke A, Schüürmann G, Ahumada I, Richter P 2011. Determination of lindane leachability in soil-biosolid systems and its bioavailability in wheat plants. *Chemosphere* 84: 397-402.

## 2010

166. Yu H, Kühne R, Ebert R-U, Schüürmann G 2010. Comparative Analysis of QSAR Models for Predicting  $pK_a$  of Organic Oxygen Acids and Nitrogen Bases from Molecular Structure. *J. Chem. Inf. Model.* 50: 1949-1960.
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.
164. Thalheim T, Vollmer A, Ebert R-U, Kühne R, Schüürmann G 2010. Tautomer Identification and Tautomer Structure Generation Based on InCHI Code. *J. Chem. Inf. Model.* 50: 1223-1232.
163. Schwöbel JAH, Wondrousch D, Koleva YK, Madden JC, Cronin MTD, Schüürmann G 2010. Prediction of Michael-type Acceptor Reactivity toward Glutathione. *Chem. Res. Toxicol.* 23: 1576-1585.
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.
161. Fjodorova N, Vračko M, Tušar M, Jezierska A, Novič M, Kühne R, Schüürmann G 2010. Quantitative and qualitative models for carcinogenicity prediction for non-congeneric chemicals using CP ANN method for regulatory uses. *Mol. Divers.* 14: 581-594.
160. Böhnhardt A, Kühne R, Ebert R-U, Schüürmann G 2010. Predicting Rate Constants of OH Radical Reactions with Organic Substances – Advances for Oxygenated Organics through a Molecular Orbital HF/6-31G\*\* Approach. *Theor. Chem. Acc.* 127: 355-367.

159. Böhme A, Thaens D, Schramm F, Paschke A, Schüürmann G 2010. Thiol Reactivity and its Impact on the Ciliate Toxicity of  $\alpha,\beta$ -Unsaturated Aldehydes, Ketones and Esters. *Chem. Res. Toxicol.* 23: 1905-1912.

158. Blaschke U, Paschke A, Rensch I, Schüürmann G 2010. Acute and Chronic Toxicity towards the Bacteria *Vibrio fischeri* of Organic Narcotics and Epoxides – Structural Alerts for Epoxide Excess Toxicity. *Chem. Res. Toxicol.* 23: 1936-1946.

## 2009

157. Wang B, Chen J, Li X., Wang Y, Chen L, Zhu M, Yu H, Kühne R, Schüürmann G 2009. Estimation of Soil Organic Carbon Normalized Sorption Coefficient ( $K_{oc}$ ) Using Least Squares-Support Vector Machine. *QSAR & Comb. Sci.* 28: 561-567.

156. Kühne R, Ebert R-U, Schüürmann G 2009. Chemical Domain of QSAR Models from Atom-Centered Fragments. *J. Chem. Inf. Model.* 49: 2660-2669.

155. Schwöbel J, Ebert R-U, Kühne R, Schüürmann G 2009. Prediction of the Intrinsic Hydrogen Bond Acceptor Strength of Chemical Substances from Molecular Structure. *J. Phys. Chem. A* 113: 10104-10112.

154. Schwöbel J, Ebert R-U, Kühne R, Schüürmann G 2009. Prediction of the Intrinsic Hydrogen Bond Acceptor Strength of Organic Compounds by Local Molecular Parameters. *J. Chem. Inf. Model.* 49: 956-962.

153. Schwöbel J, Ebert R-U, Kühne R, Schüürmann G 2009. Modeling the H Bond Donor Strength of –OH, –NH, and –CH Sites by Local Molecular Parameters. *J. Comput. Chem.* 30: 1454-1464.

152. Schreiber R, Altenburger R, Paschke A, Schüürmann G, Küster E 2009. A novel *in vitro* system for the determination of bioconcentration factors and the internal dose in zebrafish (*Danio rerio*) eggs. *Chemosphere* 77: 928-933.

151. Böhme A, Thaens D, Paschke A, Schüürmann G 2009. Kinetic Glutathione Chemoassay to Quantify Thiol Reactivity of Organic Electrophiles – Application to  $\alpha,\beta$ -Unsaturated Ketones, Acrylates, and Propiolates. *Chem. Res. Toxicol.* 22: 742-750.

## 2008

150. Szymoszek A, Wenzel B, Scheunemann M, Steinbach J, Schüürmann G 2008. First CoMFA characterization of vesamicol analogs as ligands for the vesicular acetylcholine transporter. *J. Med. Chem.* 51: 2128-2136.

149. Schüürmann G, Ebert R-U, Chen J, Wang B, Kühne R 2008. External Validation and Prediction Employing the Predictive Squared Correlation Coefficient – Test Set Activity Mean vs Training Set Activity Mean. *J. Chem. Inf. Model.* 48: 2140-2145.

148. Gunold R, Schäfer RB, Paschke A, Schüürmann G, Liess M 2008. Calibration of the Chemcatcher passive sampler for monitoring selected polar and semi-polar pesticides in surface water. *Environ. Pollut.* 155: 52-60.

147. Böhnhardt A, Kühne R, Ebert R-U, Schüürmann G 2008. Indirect Photolysis of Organic Compounds: Prediction of OH Reaction Rate Constants through Molecular Orbital Cal-

culations. *J. Phys. Chem. A* **112**: 11391-11399.

146. Böhme A, Paschke A, Vrbka P, Dohnal V, Schüürmann G 2008. Determination of Temperature-Dependent Henry's Law Constant of Four Oxygenated Solutes in Water Using Headspace Solid-Phase Microextraction Technique. *J. Chem. Eng. Data* **53**: 2873-2877.

## 2007

145. Von der Ohe PC, Kühne R, Ebert R-U, Schüürmann G 2007. Comment on "Discriminating toxicant classes by mode of action: 3. Substructure indicators" (M. Nendza, M. Müller, *SAR QSAR Environ. Res.*, **18**, 155 (2007)). *SAR QSAR Environ. Res.* **18**: 621-624.

144. Paschke A, Brümmer J, Schüürmann G 2007. Silicone rod extraction of pharmaceuticals from water. *Anal. Bioanal. Chem.* **387**: 1417-1421.

143. Kühne R, Ebert R-U, Schüürmann G 2007. Estimation of compartmental half-lives of organic compounds – structural similarity vs. EPI-suite. *QSAR & Comb. Sci.* **26**: 542-549.

## 2006

142. Wenzel K-D, Hubert A, Weissflog L, Kühne R, Popp P, Kindler A, Schüürmann G 2006. The influence of different emission sources on atmospheric organochlorine patterns in Germany. *Atmos. Environm.* **40**: 943-957.

141. Schüürmann G, Ebert R-U, Kühne R 2006. Prediction of physicochemical properties of organic compounds from 2D molecular structure – Fragment methods vs. LFER models. *Chimia* **60**: 691-698.

140. Schüürmann G, Ebert R-U, Kühne R 2006. Prediction of the sorption of organic compounds into soil organic matter from molecular structure. *Environ. Sci. Technol.* **40**: 7005-7011.

139. Paschke A, Vrana B, Popp P, Schüürmann G 2006. Comparative application of solid-phase microextraction fibre assemblies and semipermeable membrane devices as passive air samplers for semivolatile chlorinated organic compounds – A case study on the landfill 'Grube Antonie' in Bitterfeld. *Environ. Pollut.* **144**: 414-422.

138. Paschke A, Schwab K, Brümmer J, Schüürmann G, Paschke H, Popp P 2006. Rapid semi-continuous calibration and field test of membrane-enclosed silicone collector as passive water sampling. *J. Chromatogr. A* **1124**: 187-195.

137. Kühne R, Ebert R-U, Schüürmann G 2006. Model selection based on structural similarity – Method description and application to water solubility prediction. *J. Chem. Inf. Model.* **46**: 636-641.

136. Ahlers J, Riedhammer C, Vogliano M, Ebert R-U, Kühne R, Schüürmann G 2006. Acute/chronic ratios in aquatic toxicity – Variation across trophic levels and relationship with chemical structure. *Environ. Toxicol. Chem.* **25**: 2937-2945.

## 2005

135. Vrana B, Paschke H, Paschke A, Popp P, Schüürmann G 2005. Performance of semi-permeable membrane devices for sampling of organic contaminations in groundwater. *J.*

*Environ. Monitor. Z.* 500-508.

134. Von der Ohe PC, Kühne R, Ebert R-U, Altenburger R, Liess M, Schüürmann G 2005. Structural alerts - A new classification model to discriminate excess toxicity from narcotic effect levels of organic compounds in the acute daphnid assay. *Chem. Res. Toxicol.* 18: 536-555.

133. Paschke A, Schröter U, Schüürmann G 2005. Indirect determination of low vapour pressures using solid-phase microextraction – Application to tetrachlorobenzenes and tetrachlorotoluenes. *J. Chromatogr. A* 1072: 93-97.

132. Netzeva TI, Aptula AO, Benfenati E, Cronin MTD, Gini G, Lessigiarska I, Maran U, Vračko M, Schüürmann G 2005. Description of the Electronic Structure of Organic Chemicals Using Semiempirical and *Ab initio* Methods for Development of Toxicological QSARs. *J. Chem. Inf. Model.* 45: 106-114.

131. Kühne R, Ebert R-U, Schüürmann G 2005. Prediction of the temperature dependence of Henry's law constant from chemical structure. *Environ. Sci. Technol.* 39: 6705-6711.

130. Grote M, Schüürmann G, Altenburger R 2005. Modelling photoinduced algal toxicity of polycyclic aromatic hydrocarbons. *Environ. Sci. Technol.* 39: 4141-4149.

129. Grote M, Altenburger R, Brack W, Moschütz S, Mothes S, Michael C, Narten G-B, Paschke A, Schirmer K, Walter H, Wennrich R, Wenzel K-D, Schüürmann G 2005. Ecotoxicological Profiling of Transect River Elbe Sediments. *Acta Hydrochim. Hydrobiol.* 33: 555-569.

128. Altenburger R, Schmitt H, Schüürmann G 2005. Algal toxicity of nitrobenzenes – Combined effect analysis as a pharmacological probe for similar modes of interaction. *Environ. Toxicol. Chem.* 24: 324-333.

## 2004

127. Wenzel K-D, Vrana B, Hubert A, Schüürmann G 2004. Dialysis of persistent organic pollutants and polycyclic aromatic hydrocarbons from semipermeable membranes. A procedure using an accelerated solvent extraction device. *Anal. Chem.* 76: 5503-5509.

126. Suzuki T, Yoshida K, Onizuka H, Iwai Y, Arai Y, Aptula AO, Kühne R, Ebert R-U, Schüürmann G 2004. Categorical Modeling of the Flow Pattern of Liquid Organic Compounds between Blade Electrodes using Semiempirical and *Ab Initio* Quantum Chemical Descriptors. *Croatica Chemica Acta.* 77: 377-398.

125. Paschke A, Neitzel PL, Walther W, Schüürmann G 2004. Octanol/water partition coefficients of selected herbicides: Determination using shake-flask method and reversed-phase high-performance liquid chromatography. *J. Chem. Eng. Data* 49: 1639-1642.

124. Hanisch B, Abbas B, Kratz W, Schüürmann G 2004. Humanarzneimittel im aquatischen Ökosystem. Bewertungsansatz zur Abschätzung des ökotoxikologischen Risikos von Arzneimittelrückständen. *UWSF - Z. Umweltchem. Ökotox.* 16: 223-238.

## 2003

123. Tribskorn R, Adam S, Behrens A, Beier S, Böhmer J, Braunbeck T, Casper H, Dietze U, Gernhöfer M, Honnen W, Köhler H-R, Körner W, Konradt J, Lehmann R, Luckenback T, Oberemm A, Schwaiger J, Segner H, Strmac M, Schüürmann G, Siligato S, Traunspurger W 2003. Establishing causality between pollution and effects at different levels of biological

organization: The VALIMAR project. *Hum. Ecol. Risk Assess.* **9**: 171-194.

122. Schüürmann G, Funar-Timofei S 2003. Multilinear regression and comparative molecular field analysis (CoMFA) of azo dye-fibre affinities. II. Inclusion of solution-phase molecular orbital descriptors. *J. Chem. Inf. Comput. Sci.* **43**: 1502-1512.

121. Schüürmann G, Aptula AO, Kühne R, Ebert R-U 2003. Stepwise discrimination between four modes of toxic action of phenols in the *Tetrahymena pyriformis* assay. *Chem. Res. Toxicol.* **16**: 974-987.

120. Netzeva TI, Aptula AO, Chaudhury SH, Duffy JC, Schultz TW, Schüürmann G, Cronin MTD 2003. Structure-activity relationships for the toxicity of substituted poly-hydroxylated phenols to *Tetrahymena pyriformis*: Influence of free radical formation. *QSAR Comb. Sci.* **22**: 575-582.

119. Hubert A, Popp P, Wenzel K-D, Schüürmann G 2003. One-step cleanup for PAH residue analysis from plant matrices using size exclusion chromatography. *Anal. Bioanal. Chem.* **376**: 53-60.

118. Dearden JD, Schüürmann G 2003. Quantitative structure-property relationships for predicting Henry's law constant from molecular structure. *Environ. Toxicol. Chem.* **22**: 1755-1770.

117. Brack W, Kind T, Schrader S, Möder M, Schüürmann G 2003. Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld. *Environ. Pollut.* **121**: 81-85.

116. Brack W, Altenburger R, Küster E, Meissner B, Wenzel K-D, Schüürmann G 2003. Identification of toxic products of anthracene photomodification in simulated sunlight. *Environ. Toxicol. Chem.* **22**: 2228-2237.

115. Aptula AO, Kühne R, Ebert R-U, Cronin MTD, Netzeva TI, Schüürmann G 2003. Modeling discrimination between antibacterial and non-antibacterial activity based on 3D molecular descriptors. *QSAR Comb. Sci.* **22**: 113-128.

114. Altenburger R, Nendza M, Schüürmann G 2003. Mixture toxicity and its modeling by quantitative structure-activity relationships. *Environ. Toxicol. Chem.* **22**: 1900-1915.

113. Ahlers J, Filser J, Frank H, Gies A, Klein W, Nagel R, Schüürmann G 2003. Ökotoxikologie soll endlich ein wissenschaftliches Fach werden. *UWSF - Z. Umweltchem. Ökotox.* **15**: 3-4.

## 2002

112. Wenzel K-D, Manz M, Hubert A, Schüürmann G 2002. Fate of POPs (DDX, HCHs, PCBs) in upper soil layers of pine forests. *Sci. Total Environ.* **286**: 143-154.

111. Vrana B, Schüürmann G 2002. Calibrating the uptake kinetics of semipermeable membrane devices in water: The impact of hydrodynamics. *Environ. Sci. Technol.* **36**: 290-296.

110. Tolls J, van Dijk J, Verbruggen EJM, Hermens JLM, Loeprecht B, Schüürmann G 2002. Aqueous solubility-molecular size relationships - A mechanistic case study using C<sub>10</sub>- to C<sub>19</sub>-alkanes. *J. Phys. Chem. A* **106**: 2760-2765.

109. Hafner C, Jung K, Schüürmann G 2002. Effects of trichloroacetic acid on the nitrogen metabolism of *Pinus sylvestris* - A <sup>13</sup>C/<sup>15</sup>N tracer study. *Chemosphere* **46**: 259-266.

108. Funar-Timofei S, Schüürmann G 2002. Comparative molecular field analysis (CoMFA) of anionic azo dye-fiber affinities. I. Gas-phase molecular orbital descriptors. *J. Chem. Inf. Comput. Sci.* 42: 788-795.
107. Cronin MTD, Aptula AO, Dearden JC, Duffy JC, Netzeva TI, Patel H, Rowe PH, Schultz TW, Worth AP, Voutzoulidis K, Schüürmann G 2002. Structure-based classification of antibacterial activity. *J. Chem. Inf. Comput. Sci.* 42: 869-878.
106. Brack W, Schirmer K, Kind T, Schrader S, Schüürmann G 2002. Effect-directed fractionation and identification of cytochrome P450-inducing halogenated aromatic hydrocarbons in a contaminated sediment. *Environ. Toxicol. Chem.* 21: 2654-2662.
105. Brack W, Altenburger R, Dorusch F, Hubert A, Möder M, Morgenstern P, Moschütz S, Mothes S, Schirmer K, Wennrich R, Wenzel K-D, Schüürmann G 2002. Hochwasser 2002 - Chemische und toxische Belastung überschwemmter Gemeinden im Raum Bitterfeld. *UWSF - Z. Umweltchem. Ökotox.* 14: 213-220.
104. Boháč M, Loeprecht B, Damborský J, Schüürmann G 2002. Impact of orthogonal signal correction (OSC) on the predictive ability of CoMFA models for the ciliate toxicity of nitrobenzenes. *Quant. Struct.-Act. Relat.* 21: 3-11.
103. Aptula AO, Netzeva TI, Valkova IV, Cronin MTD, Schultz TW, Kühne R, Schüürmann G 2002. Multivariate discrimination between modes of toxic action of phenols. *Quant. Struct.-Act. Relat.* 21: 12-22.

## 2001

102. Vrana B, Popp P, Paschke A, Schüürmann G 2001. Membrane-enclosed sorptive coating. An integrative passive sampler for monitoring organic contaminants in water. *Anal. Chem.* 73: 5191-5200.
101. Vrana B, Paschke A, Popp P, Schüürmann G 2001. Use of semipermeable membrane devices (SPMDs). Determination of bioavailable, organic, waterborne contaminants in the industrial region of Bitterfeld, Saxony-Anhalt, Germany. *ESPR - Environ. Sci. & Pollut. Res.* 8: 27-34.
100. Tribskorn R, Böhmer J, Braunbeck T, Honnen W, Köhler H-R, Lehmann R, Oberemm A, Schwaiger J, Segner H, Schüürmann G, Traunspurger W 2001. The project VALIMAR (VALidation of bioMARKers for the assessment of small stream pollution with environmental chemicals): Aims and scope, experimental design, summary of project results, and recommendations for the application of biomarkers in risk assessment. *J. Aquat. Ecosyst. Stress Recov.* 8: 161-178.
99. Suzuki T, Timofei S, Kurunczi L, Dietze U, Schüürmann G 2001. Correlation of aerobic biodegradability of sulfonated azo dyes with the chemical structure. *Chemosphere* 45: 1-9.
98. Suzuki T, Ebert R-U, Schüürmann G 2001. Application of neural networks to modeling and estimating temperature-dependent liquid viscosity of organic compounds. *J. Chem. Inf. Comput. Sci.* 41: 776-790.
97. Smith BJ, Branson K, Schüürmann G 2001. Gaussian-theory predictions of proton transfer to water of phenol and 3-chlorophenol: Resolution of an apparent difficulty. *Chem. Phys. Lett.* 342: 402-404.
96. Paschke A, Manz M, Treutler H-C, Wennrich R, Morgenstern P, Popp P, Schüürmann

G 2001. Schadstoffmobilisierbarkeit, ökotoxisches Gefährdungspotential und Pufferkapazität von potentiell Baggergut aus der Saale. *Nova Acta Leopoldina NF* 84: 65-81.

95. Paschke A, Manz M, Schüürmann G 2001. Application of different RP-HPLC methods for the determination of octanol/water partition coefficients of selected tetrachlorobenzyltoluenes. *Chemosphere* 45: 721-728.

94. Manz M, Wenzel K-D, Dietze U, Schüürmann G 2001. Persistent organic pollutants in agricultural soils of Central Germany. *Sci. Total Environ.* 277: 187-198.

93. Hubert A, Wenzel K-D, Engewald W, Schüürmann G 2001. Accelerated solvent extraction - More efficient extraction of POPs and PAHs from real contaminated plant and soil samples. *Rev. Anal. Chem.* 20: 101-144.

92. Dietze U, Braunbeck T, Honnen W, Köhler H-R, Schwaiger J, Segner H, Triebkorn R, Schüürmann G 2001. Chemometric discrimination between streams based on chemical, limnological and biological data taken from freshwater fishes and their interrelationships. *J. Aquat. Ecosyst. Stress Recov.* 8: 319-336.

91. Dimov D, Nedyalkova Z, Haladjova S, Schüürmann G, Mekenyan O 2001. QSAR modeling of antimycobacterial activity and activity against other bacteria of 3-formyl rifamycin SV derivatives. *Quant. Struct.-Act. Relat.* 20: 298-318.

## 2000

90. Wenzel K-D, Weißflog L, Manz M, Hubert A, Schüürmann G 2000. Differences in time-dependent accumulation of POPs in pine needles. *Fresenius Environ. Bull.* 9: 47-55.

89. Schweizer A, Hafner C, Jung K, Hurler K, Schüürmann G 2000. <sup>15</sup>N-Tracerstudien zur Untersuchung des Einflusses von atmosphärischen Herbizid-Konzentrationen auf den pflanzlichen N-Metabolismus. *Z. PflKrankh. PflSchutz Sonderh.* 17: 799-809.

88. Schüürmann G 2000. Prediction of Henry's law constant of benzene derivatives using quantum chemical continuum-solvation models. *J. Comput. Chem.* 21: 17-34.

87. Schmitt H, Altenburger R, Jastorff B, Schüürmann G 2000. Quantitative structure-activity analysis of the algae toxicity of nitroaromatic compounds. *Chem. Res. Toxicol.* 13: 441-450.

86. Paschke A, Schüürmann G 2000. Concentration dependence of octanol/water partition coefficients of the hexachlorocyclohexane isomers at 25 °C. *Chem. Eng. & Technol.* 23: 666-670.

85. Paschke A, Schüürmann G 2000. Die Konzentrationsabhängigkeit des Oktanol/Wasser-Verteilungskoeffizienten der Hexachlorcyclohexan-Isomere bei 25 °C. *Chem. Ing. Techn.* 72: 84-87.

84. Katritzky A, Chen K, Wang Y, Karelson M, Lucic B, Trinajstić N, Suzuki T, Schüürmann G 2000. Prediction of liquid viscosity for organic compounds by a quantitative structure-property relationship. *J. Phys. Org. Chem.* 13: 80-86.

83. Iwai Y, Yoshida K, Arai Y, Schüürmann G, Loeprecht B, Fabian WMF, Suzuki T 2000. Analysis of the flow patterns of liquid organic compounds between blade electrodes by classification models. *J. Chem. Inf. Comput. Sci.* 40: 988-993.

82. Hubert A, Wenzel K-D, Manz M, Weißflog L, Engewald W, Schüürmann G 2000. High extraction efficiency of POPs in real contaminated soil samples using accelerated solvent extraction. *Anal. Chem.* 72: 1294-1300.
81. Hafner C, Erdmenger E, Jung K, Gehre M, Schüürmann G 2000. Stable isotope tracer technique as a tool to increase the sensitivity of plant growth bioassays B investigations with pentachlorophenol and trichloroacetic acid. *Fresenius Environ. Bull.* 9: 225-231.
80. Elansky NP, Arabov AY, Olshansky DI, Weißflog L, Manz M, Popp P, Schüürmann G, Putz E, Pfirster G, Folberth G 2000. Oxidation of volatile organic compounds and generation of trichloroacetic acid in the atmosphere over the European Russia. *Doklady Akademii Nauk* 371: 109-113.
79. Breitkopf C, Kühne R, Schüürmann G 2000. Multimedia Level-III Partitioning and residence times of xenobiotics in water-rich and water-poor environments. *Environ. Toxicol. Chem.* 19: 1430-1440.
78. Brack W, Segner H, Möder M, Schüürmann G 2000. Fixed-effect-level toxicity equivalents - A suitable parameter for assessing ethoxyresorufin-O-deethylase induction potency in complex environmental samples. *Environ. Toxicol. Chem.* 19: 2493-2501.
77. Brack W, Paschke A, Segner H, Wennrich R, Schüürmann G 2000. Urease inhibition: A tool for toxicity identification in sediment elutriates. *Chemosphere* 40: 829-834.

## 1999

76. Weißflog L, Wenzel K-D, Manz M, Kleint F, Schüürmann G 1999. Economic upheaval in 1990-93 and the ecological situation in Central Germany. *Environ. Pollut.* 105: 341-347.
75. Weißflog L, Manz M, Popp P, Elansky N, Arabiv A, Putz E, Schüürmann G 1999. Airborne trichloroacetic acid and its deposition in the catchment area of the Caspian Sea. *Environ. Pollut.* 104: 359-364.
74. Sijm DTHM, Schüürmann G, de Vries PJ, Opperhuizen A 1999. Aqueous solubility, octanol solubility and octanol/water partition coefficient of nine hydrophobic dyes. *Environ. Toxicol. Chem.* 18: 1109-1117.
73. Schulz H, Popp P, Huhn H, Stärk HJ, Schüürmann G 1999. Biomonitoring of airborne inorganic pollutants by means of pine tree barks. *Sci. Total. Environ.* 232: 49-58.
72. Schüürmann G 1999. Gas-phase and solution-phase proton transfer to H<sub>2</sub>O analyzed by high-level ab initio quantum chemistry including complete basis set and Gaussian theory schemes. *Chem. Phys. Lett.* 302: 471-479.
71. Paschke A, Popp P, Schüürmann G 1999. Solubility and partitioning studies with polycyclic aromatic hydrocarbons using an optimized SPME procedure. *Fresenius J. Anal. Chem.* 363: 426-428.
70. Manz M, Weissflog L, Kühne R, Schüürmann G 1999. Ecotoxicological hazard and risk assessment of heavy metal contents in agricultural soils of Central Germany. *Ecotoxicol. Environ. Saf.* 42: 191-201.
69. Jung K, Kaletta K, Segner H, Schüürmann G 1999. <sup>15</sup>N metabolic test for the determination of phytotoxic effects of chemical substances and environmental samples. *ESPR - Environ. Sci. Pollut. Res.* 6: 191-201.

68. Ivanov J, Schüürmann G 1999. Simple algorithms for determining the molecular symmetry. *J. Chem. Inf. Comput. Sci.* 39: 728-737.
67. Hafner Ch, Jung K, Schüürmann G 1999. Effects of atmospheric chloroorganic compounds on nitrogen metabolism of higher plants. *Isotopes Environ. Health Stud.* 35: 297-298.
66. Brack W, Altenburger R, Ensenbach U, Möder M, Segner H, Schüürmann G 1999. Bioassay-directed identification of organic toxicants in river sediments in the industrial region of Bitterfeld (Germany) - A contribution to hazard assessment. *Arch. Environ. Contam. Toxicol.* 37: 164-174.

## 1998

65. Wenzel K-D, Hubert A, Manz M, Weißflog L, Engewald W, Schüürmann G 1998. Accelerated solvent extraction of semivolatile organic compounds from biomonitoring samples of pine needles and mosses. *Anal. Chem.* 70: 4827-4835.
64. Schüürmann G, Cossi M, Barone V, Tomasi J 1998. Prediction of the  $pK_a$  of carboxylic acids using the ab initio continuum-solvation model PCM-UAHF. *J. Phys. Chem. A* 102: 6706-6712.
63. Schüürmann G 1998. Quantum chemical analysis of the energy of proton transfer from phenol and chlorophenols to H<sub>2</sub>O in the gas phase and in aqueous solution. *J. Chem. Phys.* 109: 9523-9528.
62. Paschke A, Schüürmann G 1998. Octanol/water-partitioning of four HCH isomers at 5, 25 and 45 °C. *Fresenius Environ. Bull.* 7: 258-263.
61. Paschke A, Popp P, Schüürmann G 1998. Water solubility and octanol/water-partitioning of hydrophobic chlorinated organic substances determined by using SPME/GC. *Fresenius J. Anal. Chem.* 360: 52-57.
60. Niculescu SP, Kaiser KLE, Schüürmann G 1998. Influence of data preprocessing and kernel selection on probabilistic neural network modeling of the acute toxicity of chemicals to the fathead minnow and *Vibrio fischeri* bacteria. *Water Qual. Res. J. Canada* 33: 153-165.
59. Möcker D, Jung K, Förstel H, Schüürmann G 1998. Isotopic and enzymatic investigations into the assimilation and effect of NO<sub>2</sub> on C<sub>3</sub>, and C<sub>4</sub> plants. *J. Appl. Bot.* 72: 186-190.
58. Ivanov J, Mekenyan O, Bradbury SP, Schüürmann G 1998. A kinetic analysis of the conformational flexibility of steroid hormones. *Quant. Struct.-Act. Relat.* 17: 437-449.
57. Gabler T, Paschke A, Schüürmann G 1998. Diffusion coefficients of substituted benzenes and alcohols at high dilution in octan-1-ol. *J. Chem. Eng. Data.* 43: 413-416.

## 1997

56. Wenzel K-D, Paladini E, Gantuz M, Puliafito JL, Guerreira C, Weißflog L, Schüürmann G 1997. Immission patterns of airborne pollutants in Argentina and Germany. II. Biomonitoring of organochlorine compounds and polycyclic aromatics. *Chemosphere* 34: 2505-2518.
55. Vollmayr H, Kleint F, Schüürmann G 1997. Discrete modeling of water and pesticide movement in soil. *Water Resour. Res.* 33: 1743-1747.

54. Suzuki T, Ebert R-U, Schüürmann G 1997. Development of both linear and nonlinear methods to predict the liquid viscosity at 20 °C of organic compounds. *J. Chem. Inf. Comput. Sci.* 37: 1122-1128.
53. Segner H, Schüürmann G 1997. Cytotoxicity of MEIC chemicals to rainbow trout R1 cell line and multivariate comparison with ecotoxicity tests. *ATLA* 25: 331-338.
52. Schulz H, Huhn G, Schüürmann G, Niehus B, Liebergeld G 1997. Determination of throughfall rates on the basis of pine bark loads: results of a pilot field study. *J. Air & Waste Manage. Assoc.* 47: 510-516.
51. Schüürmann G, Segner H, Jung K 1997. Multivariate mode-of-action analysis of acute toxicity of phenols. *Aquat. Toxicol.* 38: 277-296.
50. Schüürmann G 1997. Thermodynamische Modelle für die Bioverfügbarkeit und Bioakkumulation organischer Chemikalien. *UWSF - Z. Umweltchem. Ökotox.* 9: 345-352.
49. Schüürmann G 1997. Thermodynamische Modelle für die Bioverfügbarkeit organischer Chemikalien. *UWSF - Z. Umweltchem. Ökotox.* 9: 3-5.
48. Paschke A, Wennrich R, Morgenstern P, Schumann G, Schüürmann G 1997. Modelluntersuchung zum Auslaugverhalten industrieller Reststoffe und Sonderabfälle aus Sachsen-Anhalt. Teil 1: Batch-Versuche zur Extraktion und Elution von Schwermetallen. *Chem. Techn.* 49: 157-168.
47. Kühne R, Ebert R-U, Schüürmann G 1997. Estimation of vapour pressures for hydrocarbons and halogenated hydrocarbons from chemical structure by a neural network. *Chemosphere* 34: 671-686.
46. Kühne R, Breitkopf C, Schüürmann G 1997. Error propagation in fugacity level-III models in the case of uncertain physicochemical compound properties. *Environ. Toxicol. Chem.* 16: 2067-2069.
45. Kaiser KLE, Niculescu SP, Schüürmann G 1997. Feed forward backpropagation neural networks and their use in predicting the acute toxicity of chemicals to the fathead minnow. *Water Qual. Res. J. Canada* 32: 637-657.
44. Jung K, Kristen U, Flachowsky J, Segner H, Schüürmann G 1997. Deponiesickerwässer: Bestimmung zytotoxischer Wirkungen mit dem Pollenschlauchwachstumstest. *UWSF - Z. Umweltchem. Ökotox.* 9: 317-321.
43. Jung K, Gebauer G, Gehre M, Hofmann D, Weißflog L, Schüürmann G 1997. Anthropogenic impacts on natural nitrogen isotope variations in *Pinus sylvestris* stands in an industrially polluted area. *Environ. Poll.* 97: 175-181.
42. Hofmann D, Jung K, Bender J, Gehre M, Schüürmann G 1997. Use of natural isotope variations of nitrogen in plants as an early indicator of air pollution. *J. Mass Spectrom.* 32: 855-863.

## 1996

41. Schüürmann G, Somashekar RK, Kristen U 1996. Structure-activity relationships for chloro- and nitrophenol toxicity in the pollen tube growth test. *Environ. Toxicol. Chem.* 15: 1702-1708.

40. Schüürmann G 1996. Modelling  $pK_a$  of carboxylic acids and phenols. *Quant. Struct.-Act. Relat.* 15: 121-132.

39. Gabler T, Paschke A, Schüürmann G 1996. Diffusion coefficients of substituted benzenes at high dilution in water. *J. Chem. Eng. Data* 41: 33-36.

## 1995

38. Schüürmann G, Kühne R, Ebert R-U, Kleint F 1995. Multivariate error analysis of increment methods for calculating the octanol/water partition coefficient. *Fresenius Environ. Bull.* 4: 13-18.

37. Schüürmann G 1995. Quantum chemical approach to estimate physicochemical compound properties: Application to substituted benzenes. *Environ. Toxicol. Chem.* 14: 2067-2076.

36. Schüürmann G 1995. Quantum chemical estimation of octanol/water partition coefficient - First results with aromatic phosphorothionates. *Fresenius Environ. Bull.* 4: 238-243.

35. Schädlich G, Weißflog L, Schüürmann G 1995. Magnetic susceptibility in conifer needles as indicator of fly ash deposition. *Fresenius Environ. Bull.* 4: 7-12.

34. Kühne R, Ebert R-U, Kleint F, Schmidt G, Schüürmann G 1995. Group contribution methods to estimate water solubility of organic chemicals. *Chemosphere* 30: 2061-2077.

33. Huhn G, Schulz H, Stärk H-J, Schüürmann G 1995. Evaluation of regional heavy metal deposition by multivariate analysis of element contents in pine tree barks. *Water Air Soil Pollut.* 84: 367-383.

32. Hofmann D, Jung K, Gehre M, Schüürmann G 1995.  $^{15}\text{N}/^{14}\text{N}$  analysis of amino acids with GC-C-IRMS - methodical investigation and ecotoxicological applications. *Isotopes Environ. Health Stud.* 31: 367-375.

## 1994

31. Wenzel K-D, Mothes B, Weißflog L, Schüürmann G 1994. Bioavailability of airborne organochloro xenobiotics to conifers. *Fresenius Environ. Bull.* 3: 734-739.

30. Weißflog L, Rolle W, Wenzel K-D, Kühne R, Schüürmann G 1994. Ökologische Situation der Region Leipzig-Halle. II. Modellierung der Partikelgröße der Flugstäube. *UWSF - Z. Umweltchem. Ökotox.* 6: 135-138.

29. Weißflog L, Wienhold K, Wenzel K-D, Schüürmann G 1994. Ökologische Situation der Region Leipzig-Halle. I. Immissionsmuster luftgetragener Schwermetalle und Bioelemente. *UWSF - Z. Umweltchem. Ökotox.* 6: 75-80.

28. Weißflog L, Paladini E, Gantuz M, Puliafito JL, Puliafito S, Wenzel K-D, Schüürmann G 1994. Immission patterns of airborne pollutants in Argentina and Germany - I. First Results of a heavy metal biomonitoring. *Fresenius Environ. Bull.* 3: 728-733.

27. Verhaar HJM, Eriksson L, Sjöström M, Schüürmann G, Seinen W, Hermens J 1994. Modelling the Toxicity of Organophosphates: A Comparison of the Multiple Linear Regression and PLS Regression Methods. *Quant. Struct.-Act. Relat.* 13: 133-143.

26. Segner H, Lenz D, Hanke W, Schüürmann G 1994. Cytotoxicity of metals towards rainbow trout R1 cell line. *Environ. Toxicol. Water Qual.* 9: 237-279.
25. Schüürmann G, Wenzel K-D, Weißflog L, Wienhold K, Müller E 1994. Ökologische Situation der Region Leipzig-Halle. III. Ökotoxikologische Charakterisierung der Schwermetall-Immissionsmuster. *UWSF - Z. Umweltchem. Ökotox.* 6: 265-270.
24. Schüürmann G, Segner H 1994. Wirkungsforschung in der Chemischen Ökotoxikologie. *UWSF - Z. Umweltchem. Ökotox.* 6: 351-358.
23. Schüürmann G, Schädlich G, Kühne R 1994. Ökotoxikologische Risikoanalyse der Cadmium-Belastung im Ackerboden der Industrieregion Leipzig-Halle. *UWSF - Z. Umweltchem. Ökotox.* 6: 3-4.
22. Schüürmann G, Müller E 1994. Back-propagation neural networks - recognition vs. prediction capability. *Environ. Toxicol. Chem.* 13: 743-747.
21. Koch R, Schüürmann G 1994. Wirkungsschwellen für chemische Stoffe in Biosystemen - Eine theoretische Betrachtung. *UWSF - Z. Umweltchem. Ökotox.* 6: 28-30.
20. Jung K, Rolle W, Schlee D, Gnauck T, Schüürmann G 1994. Das stabile Stickstoffisotop <sup>15</sup>N als Indikator von Ozoneffekten bei Fichtensetzlingen (*Picea abies* L.). *Isotopenpraxis Environ. Health Stud.* 30: 184.
19. Jung K, Rolle W, Schlee D, Tintemann H, Gnauck T, Schüürmann G 1994. Ozone effects on nitrogen incorporation and superoxide dismutase activity in spruce seedlings (*Picea abies* L.). *New Phytol.* 128: 505-508.

### 1993

18. Schüürmann G, Schindler M 1993. Fish toxicity and dealkylation of aromatic phosphorothionates - QSAR analysis using NMR shifts calculated by the IGLO method. *J. Environ. Sci. Health* A28: 899-921.
17. Klamt A, Schüürmann G 1993. COSMO: A new approach to dielectric screening in solvents with explicit expressions for the screening energy and its gradient. *J. Chem. Soc. Perkin Trans. 2*: 799-805.

### 1992

16. Schüürmann G, Rothenbacher C 1992. Evaluation of estimation methods for the air-water partition coefficient. *Fresenius Environ. Bull.* 1: 10-15.

### 1991

15. Von Oepen B, Kördel W, Klein W, Schüürmann G 1991. Predictive QSPR models for estimating soil sorption coefficients: potential and limitations based on dominating processes. *Sci. Total Environ.* 109/110: 343-354.
14. Schüürmann G, Marsmann M 1991. QSARs in the chemical industry: need, scope and current limitations. *Sci. Total Environ.* 109/110: 671-675.

13. Schüürmann G 1991. First-order and pseudo-first-order elimination kinetics. *Sci. Total Environ.* 109/110: 395-405.
12. Schüürmann G 1991. Do Hammett constants model electronic properties in QSARs? *Sci. Total Environ.* 109/110: 221-235.
11. Schüürmann G, Marsmann M 1991. QSAR-Modelle - Interpretation und Prognose der Biokonzentration und aquatischen Toxizität. *UWSF - Z. Umweltchem. Ökotox.* 3: 42-47.
10. Schüürmann G 1991. Acute aquatic toxicity of alkyl phenol ethoxylates. *Ecotoxicol. Environ. Saf.* 21: 227-233.

## 1990

9. Warne MStJ, Connell DW, Hawker DW, Schüürmann G 1990. Prediction of aqueous solubility and the octanol/water partition coefficient for lipophilic organic compounds using molecular descriptors and physicochemical properties. *Chemosphere* 21: 877-888.
8. Schüürmann G 1990. QSAR analysis of the acute toxicity of oxyethylated surfactants. *Chemosphere* 21: 467-478.
7. Schüürmann G 1990. Quantitative structure-property relationships for the polarizability, solvatochromic parameters and lipophilicity. *Quant. Struct.-Act. Relat.* 9: 326-333.
6. Schüürmann G 1990. QSAR analysis of the acute toxicity of organic phosphorothioates using theoretically derived molecular descriptors. *Environ. Toxicol. Chem.* 9: 417-428.

## 1989

5. Warne MStJ, Connell DW, Hawker DW, Schüürmann G 1989. Prediction of the toxicity of mixtures of shale oil components. *Ecotoxicol. Environ. Saf.* 18: 121-128.
4. Warne MStJ, Connell DW, Hawker DW, Schüürmann G 1989. Quantitative structure-activity relationships for the toxicity of selected shale oil components to mixed marine bacteria. *Ecotoxicol. Environ. Saf.* 17: 133-148.

## 1988

3. Schüürmann G, Klein W 1988. Advances in bioconcentration prediction. *Chemosphere* 17: 1551-1574.
2. Connell DW, Schüürmann G 1988. Evaluation of various molecular parameters as predictors of bioconcentration in fish. *Ecotoxicol. Environ. Saf.* 15: 324-335.

## 1987

1. Schüürmann G, Klessinger M 1987. Interpretation of the electronic spectra of substituted naphthalenes. *Chem. Phys.* 113: 241-249.

## **B) Artikel in Büchern und Tagungsbänden**

### **2017**

44. Brehm M, Kafka A, Bamler M, Kühne R, Schüürmann G, Sikk L, Burk J, Burk P, Tamm T, Tämm K, Pokhrel S, Mädler L, Kahru A, Aruoja V, Sihtmäe M, Scott-Fordsmand J, Sorensen PB, Escorihuela L, Roca CP, Fernández A, Giral F, Rallo R 2017. An Integrated Data-Driven Strategy for Safe-by-Design Nanoparticles: The FP7 MODERN Project. In: Tran L, Bañares MA, Rallo R (eds): Modelling the Toxicity of Nanoparticles. Advances in Experimental Medicine and Biology, Springer, Vol. 947, pp. 257-301.

43. Schüürmann G 2017. Chemische Mechanismen toxikologischer Wirkung. In: Dreßler J, Maatz R, Daldrop T (Hrsg.): Toxikologie und Umfeld. Beiträge zum Symposium des Instituts für Rechtsmedizin der Universität Leipzig, 28.9.2016, Forschungszentrum des Universitätsklinikums, MOLINApres Leipzig, 04821 Brandis, S. 78-100.

### **2007**

42. Schüürmann G, Ebert R-U, Nendza M, Dearden JC, Paschke A, Kühne R 2007. Predicting fate-related physicochemical properties. In: Van Leeuwen K, Vermeire T (eds): Risk assessment of chemicals: An Introduction. 2<sup>nd</sup> Edition. Springer, Dordrecht, The Netherlands, Chapter 9, pp. 375-426.

41. Paschke A, Vrana B, Popp P, Wennrich R, Paschke H, Schüürmann G 2007. Membrane enclosed sorptive coating (MESCO) for monitoring organic compounds in water. In: Greenwood R, Mills GS, Vrana B (eds): Passive sampling techniques in environmental monitoring; Chapter 10. Part of the book series: Barcelo D (ed.): Wilson & Wilson's Comprehensive Analytical Chemistry. Elsevier, Amsterdam, NL, pp. 231-250.

### **2004**

40. Schüürmann G 2004. Quantum chemical descriptors in structure-activity relationships – Calculation, interpretation and comparison of methods. In: Cronin MTD, Livingstone DJ (eds) Predicting chemical toxicity and fate, Chapter 6. CRC Press, pp. 85-149.

### **2003**

39. Paschke A, Vrana B, Popp P, Wennrich L, Lorenz W, Schüürmann G 2003. Novel passive samplers for monitoring organic pollutants in surface and ground water based on membrane-enclosed silicone material. In: Namiesnik J, Chrzanowski W, Zmijewska P (eds.): New horizons and challenges in environmental analysis and monitoring. Centre of Excellence in Environmental Analysis and Monitoring, Gdansk, Poland, Chapter 24, pp. 486-492.

38. Küster E, Dorusch F, Weiss H, Schüürmann G, Altenburger R 2003. Beurteilung der Entgiftung von Grundwasser durch Sanierungsverfahren mittels kontinuierlicher biologischer Überwachung. In: Foth H (ed.) Risk assessment and management of large contamination sites. Proceedings of the workshop at Martin-Luther-Universität Halle Wittenberg, 22-24 February 2002, pp. 41-45.

## 2001

37. Wenzel K-D, Hubert A, Engewald W, Schüürmann G 2001. Optimierung der ASE für Boden und Altlastensanierung. 5. Anwendertreffen "Extraktion zur Probenvorbereitung - ASE, SPE, SBSE, SPME, SPE", Siegen 9.-10.5.2001, Tagungsband, S. 2-8.

## 2000

36. Triebkorn R, Adam S, Behrens A, Beier S, Böhmer J, Braunbeck T, Eckwert H, Frahne D, Hartig K, Honnen W, Kappus B, Klingebiel M, Köhler H-R, Konradt J, Lehmann R, Luckenbach T, Oberemm A, Pawert M, Schlegel T, Schramm M, Schüürmann G, Schwaiger J, Segner H, Siligato S, Strmac M, Traunspurger W, Müller E 2000. Das BMBF-Verbundprojekt VALIMAR: Ziele, Inhalte, Methoden, Verbundpartner. In: Fomin A, Arndt U, Elsner D, Klump A (Hrsg) Bioindikation. Biologische Testverfahren. 2. Hohenheimer Workshop zur Bioindikation am Kraftwerk Altbach-Deizisau 1998, Verlag Günther Heimbach, Ostfildern, S. 165-168.

35. Schulz H, Schulz U, Huhn G, Schüürmann G 2000. Biomonitoring of airborne inorganic and organic pollutants by means of pine tree barks. II. Deposition types and impact levels. In: International Atomic Energy Agency, IAEA (ed.): Biomonitoring of atmospheric pollution (with emphasis on trace elements) - BioMAP. Proceedings of an international workshop organized by the International Atomic Energy Agency in co-operation with the Instituto Tecnológico e Nuclear, held in Lisbon, Portugal, 21-24 September 1997. IAEA-TECDOC-1152, pp. 159-167.

34. Schulz H, Popp P, Huhn G, Stärk H-J, Schüürmann G 2000. Biomonitoring of airborne inorganic and organic pollutants by means of pine tree barks. I. Temporal and spatial variations. In: International Atomic Energy Agency, IAEA (ed.): Biomonitoring of atmospheric pollution (with emphasis on trace elements) - BioMAP. Proceedings of an international workshop organized by the International Atomic Energy Agency in co-operation with the Instituto Tecnológico e Nuclear, held in Lisbon, Portugal, 21-24 September 1997. IAEA-TECDOC-1152, pp. 149-158.

33. Müller E, Braunbeck T, Honnen W, Köhler H-R, Oberemm A, Schüürmann G, Schwaiger J, Segner H, Triebkorn R 2000. Der BMBF-Verbund Valimar: Validierung und Einsatz biologischer, chemischer und mathematischer Tests und Biomarkerstudien zur Bewertung und Belastung kleiner Fließgewässer mit Umweltchemikalien. In: Fomin A, Arndt U, Elsner D, Klump A (Hrsg) Bioindikation. Biologische Testverfahren. 2. Hohenheimer Workshop zur Bioindikation am Kraftwerk Altbach-Deizisau 1998, Verlag Günther Heimbach, Ostfildern, S. 147-155.

32. Hafner Ch, Jung K, Gehre M, Altenburger R, Schüürmann G 2000. Isotopenmassenspektrometrische  $^{13}\text{C}/^{15}\text{N}$ -Traceruntersuchungen zur Wirkung von Chlororganika auf höhere Pflanzen am Beispiel von Pentachlorphenol. In: Fomin A, Arndt U, Elsner D, Klump A (Hrsg) Bioindikation. Biologische Testverfahren. 2. Hohenheimer Workshop zur Bioindikation am Kraftwerk Altbach-Deizisau 1998, Verlag Günther Heimbach, Ostfildern, S. 199-204.

31. Brack W, Altenburger R, Ensenbach U, Nehls S, Segner H, Schüürmann G 2000. Wirkungsorientierte Identifikation toxischer organischer Inhaltsstoffe in Flußsedimenten. In: Friese K, Witter B, Miehl G, Rode M: Stoffhaushalt von Auenökosystemen B Böden und Hydrologie, Schadstoffe, Bewertungen. Springer, Berlin-Heidelberg, S. 337-346.

## 1999

30. Tribskorn R, Adam S, Behrens A, Braunbeck T, Gränzer S, Honnen W, Konradt J, Köhler H-J, Oberemm A, Pawert M, Schlegel T, Schramm M, Schüürmann G, Schwaiger J, Segner H, Strmac M, Müller E 1999. Eignung von Biomarkern zur Fließgewässerbewertung: Zwischenergebnisse aus dem Projekt "VALIMAR" (1995-1997). In: Oehlmann J, Markert B (Hrsg.) Ökotoxikologie - Ökosystemare Ansätze und Methoden. Ecomed Verlagsgesellschaft, S. 382-389.
29. Schulz H, Härtling S, Morgenstern P, Schüürmann G 1999. Nachweis ökotoxikologischer Wirkungen in Kiefernökosystemen - Ergebnisse einer langfristig angelegten Freilandstudie. In: Oehlmann J, Markert B (Hrsg.) Ökotoxikologie - Ökosystemare Ansätze und Methoden. Ecomed Verlagsgesellschaft, S. 248-267.
28. Praszczyk B, Altenburger R, Oehlmann J, Markert B, Schüürmann G 1999. Brauchen wir einen Biotest mit höheren Pflanzen in der aquatischen Toxikologie? In: Oehlmann J, Markert B (Hrsg.) Ökotoxikologie - Ökosystemare Ansätze und Methoden. Ecomed Verlagsgesellschaft, S. 138-149.
27. Luckenbach T, Adam S, Behrens A, Beier S, Böhmer J, Braunbeck T, Dietze U, Honnen W, Kappus B, Klingebiel M, Knigge T, Köhler H-R, Konradt J, Lehmann R, Müller E, Oberemm A, Schüürmann G, Schwaiger J, Segner H, Siligato S, Strmac M, Traunspurger W, Tribskorn R 1999. Das Verbundprojekt Valimar. In: Böcker R (Hrsg.) Umweltforschung im Dialog B aktuelle Beiträge aus dem mittleren Neckarraum. Hohenheimer Umwelttagung 31, S. 79-84.
26. Hafner C, Jung K, Gehre M, Schüürmann G 1999. Einsatz stabiler Isotope zum ökotoxikologischen Wirkungsnachweis chlororganischer Verbindungen. In: Oehlmann J, Markert B (Hrsg.) Ökotoxikologie - Ökosystemare Ansätze und Methoden. Ecomed Verlagsgesellschaft, S. 117-121.
25. Brack W, Altenburger R, Ensenbach U, Nehls S, Segner H, Schüürmann G 1999. Biotestorientierte Identifikation toxischer organischer Sedimentinhaltsstoffe - Ein Beitrag zur Risikoanalyse komplexer Kontaminationen am Beispiel des Spittelwassers. In: Bundesanstalt für Gewässerkunde - BFG (Hrsg.): Sedimentbewertung in europäischen Flussgebieten. Beiträge zum internationalen Symposium vom 12.-14. April 1999 in Berlin. J. Fuck, Druck und Verlag, Koblenz, S. 135-141.

## 1998

24. Schüürmann G 1998. Ecotoxic modes of action of chemical substances. In: Schüürmann G, Markert B (eds) Ecotoxicology. John Wiley and Spektrum Akademischer Verlag, New York (USA), pp. 665-749.
23. Ensenbach U, Altenburger R, Behrens A, Brack W, Knops M, Navas JM, Nehls S, Schrag B, Segner H, Sturm A, Walter H, Schüürmann G 1998. Ökotoxikologische Analyse komplexer Stoffgemische. Tagungsbericht 1997 der Deutschen Gesellschaft für Limnologie (DGL), Band II. Eigenverlag der DGL, Krefeld, S. 882-885.

## 1997

22. Schüürmann G, Kühne R, Kleint F, Ebert R-U, Rothenbacher C, Herth P 1997. A software system for automatic chemical property estimation from molecular structure. In: Chen F,

Schüürmann G (eds) Quantitative Structure-Activity Relationships in Environmental Sciences - VII. SETAC Press, Pensacola (FL, USA), pp. 93-114.

21. Schüürmann G, Flemmig B, Dearden JC, Cronin MTD, Schultz TW 1997. CoMFA study of acute toxicity of nitrobenzenes to *Tetrahymena pyriformis*. In: Chen F, Schüürmann G (eds) Quantitative Structure-Activity Relationships in Environmental Sciences - VII. SETAC Press, Pensacola (FL, USA), pp. 315-327.

20. Schüürmann G 1997. Assessment of semiempirical quantum chemical continuum-solvation models to estimate  $pK_a$  of organic compounds. In: Chen F, Schüürmann G (eds) Quantitative Structure-Activity Relationships in Environmental Sciences - VII. SETAC Press, Pensacola (FL, USA), pp. 225-242.

19. Kühne R, Ebert R-U, Kleint F, Schüürmann G 1997. Estimation of Henry's law constant at varying temperatures from chemical structure. In: Alef K, Brandt J, Fiedler H, Hauthal W, Hutzinger O, Mackay D, Matthies M, Morgan K, Newland L, Robitaille H, Schlummer M, Schüürmann G, Voigt K (eds) 1997. ECO-INFORMA '97, Vol. 12. Information and Communication in Environmental and Health Issues. Proceedings of ECO-INFORMA '97, October 6-9, Neuherberg (Germany). Eco-Inforna Press, Bayreuth (Germany), pp. 464-469.

18. Ensenbach U, Schüürmann G 1997. Effects of polycyclic aromatic hydrocarbons (PAHs) on the early development of Zebrafish. In: Alef K, Brandt J, Fiedler H, Hauthal W, Hutzinger O, Mackay D, Matthies M, Morgan K, Newland L, Robitaille H, Schlummer M, Schüürmann G, Voigt K (eds) 1997. ECO-INFORMA '97, Vol. 12. Information and Communication in Environmental and Health Issues. Proceedings of ECO-INFORMA '97, October 6-9, Neuherberg (Germany). Eco-Inforna Press, Bayreuth (Germany), pp. 458-463.

17. Altenburger R, Schüürmann G 1997. Instrumentarien zur Bewertung möglicher Kombinationswirkungen von Schadstoffen auf die menschliche Gesundheit. Integrierte Bewertung radiologischer und chemisch-toxischer Kontaminanten, Workshop am 24.11.1997. Materialien zu Strahlenschutz/Umweltradioaktivität 3/97, Bundesamt für Strahlenschutz, Salzgitter, S. 27-35.

16. Altenburger R, Ensenbach U, Jung K, Knops M, Popp P, Segner H, Weiß H, Schüürmann G 1997. Ecotoxicity identification for the hazard characterisation of groundwater contamination. In: Alef K, Brandt J, Fiedler H, Hauthal W, Hutzinger O, Mackay D, Matthies M, Morgan K, Newland L, Robitaille H, Schlummer M, Schüürmann G, Voigt K (eds) 1997. ECO-INFORMA '97, Vol. 12. Information and Communication in Environmental and Health Issues. Proceedings of ECO-INFORMA '97, October 6-9, Neuherberg (Germany). Eco-Inforna Press, Bayreuth (Germany), pp. 452-457.

## 1996

15. Kühne R, Kleint F, Ebert R-U, Schüürmann G 1996. Calculation of Compound Properties Using Experimental Data From Sufficiently Similar Chemicals. In: Gasteiger J (ed) Software development in chemistry 10. Proceedings of the 10th workshop "Computer in Chemistry", Hochfilzen, Österreich, 1995. PROserv Springer Produktionsgesellschaft, Berlin, S. 125-134.

14. Balzuweit G, Welk M, Der R, Schüürmann G 1996. Nonlinear partial least-squares regression. In: Bulsari AB, Kallio S, Tsaptsinos D (eds) Solving engineering problems with neural networks. Proceedings of the International Conference EANN '96, London (UK), pp. 495-498.

## 1995

13. Wenzel K-D, Kühne R, Weißflog L, Schüürmann G 1995. Uptake of airborne semivolatile organochloro compounds in pine needles. In: Flousek J, Roberts GCS (eds) Mountain National Parks and Biosphere Reserves: Monitoring and Management. Proceedings of the International Conference, September 1993, Špindlerův Mlýn, Czech Republic. Krkonoše National Park Administration Vrchlabí (Czech Republic), pp. 61-67.
12. Schulz H, Huhn G, Jung K, Härtling S, Schüürmann G 1995. Biochemical responses in needles of Scots pine (*Pinus sylvestris* L.) from air polluted field sites in eastern Germany. In: Ebel A, Moussiopoulos N (eds) Observation and simulation of air pollution 95: Results from SANA and EUMAC (EUROTAC). Air Pollution III, Vol. 4, pp. 31-42.

## 1994

11. Schüürmann G, Wenzel K-D, Weißflog L 1994. Exposition und Bioverfügbarkeit mittelflüchtiger Organika in der Umgebung von Leipzig. In: Alef K, Fiedler H, Hutzinger O (Hrsg) ECOINFORMA '94, Band 5. Umweltbundesamt Wien (Österreich) S. 183-200.
10. Schüürmann G, Segner H 1994. Struktur-Wirkungs-Analyse von Trialkylzinnverbindungen. In: Totsche K, Matthies M, Strutzenberger F, Petek W, Klöpffer W, Czedik-Eysenberg P, Meinholz H, Fiedler H, Alef K, Hutzinger O (Hrsg) ECOINFORMA '94, Band 7. Umweltbundesamt Wien (Österreich) S. 439-453.
9. Müller E, Schüürmann G 1994. Neural networks - training and prediction for biological activities of chemicals. In: Jochum C (ed) Software-Entwicklung in der Chemie 8. Proceedings of the Workshop "Computer in Chemistry". Seeheim-Jugenheim, Darmstadt (Germany) November 17-19, 1993. PRODUserv Springer Produktions-Gesellschaft, Berlin (Germany), pp. 281-291.
8. Kühne R, Rothenbacher C, Herth P, Schüürmann G 1994. Group contribution methods for physicochemical properties of compounds. In: Jochum C (ed) Software-Entwicklung in der Chemie 8. Proceedings of the Workshop "Computer in Chemistry". Seeheim-Jugenheim, Darmstadt (Germany) November 17-19, 1993. PRODUserv Springer Produktions-Gesellschaft, Berlin (FRG), pp. 207-224.

## 1993

7. Pfennigsdorff A, Wienhold K, Weißflog L, Schüürmann G 1993. Multielementanalyse von Kiefernadeln als Bioindikationssystem - Ergebnisse für Vanadium und Eisen im Raum Leipzig-Halle. In: Dittrich K, Welz B (Hrsg) CANAS '93, Colloquium Analytische Atomspektroskopie. Universität Leipzig und UFZ-Umweltforschungszentrum Leipzig-Halle, Leipzig, S. 787-792.

## 1992

6. Schüürmann G 1992. Ecotoxicology and structure-activity studies of organophosphorus compounds. In: Fujita T, Draber W (eds) Rational Approaches to Structure, Activity and Ecotoxicology of Agrochemicals. CRC Press, Boca Raton (Florida, USA), pp. 485-541.

**1991**

5. Marsmann M, Schüürmann G 1991. Chlororganische Verbindungen - Struktur-Wirkungs-Beziehungen zur Analyse ökotoxischer Eigenschaften. In: Held M (Hrsg) Leitbilder der Chemiepolitik. Stoffökologische Perspektiven der Industriegesellschaft. Campus Verlag, Frankfurt, S. 151-171.
4. Caspers N, Schüürmann G 1991. Bioconcentration of xenobiotics from the chemical industry's point of view. In: Nagel R, Loskill R (eds) Bioaccumulation in aquatic systems. VCH Verlag, Weinheim (Germany), pp. 81-98.
3. Bomhard E, Marsmann M, Rühl-Fehlert Ch, Schade-Lehn R, Schüürmann G 1991. Screening of aromatic compounds for their potency of inducing hyaline droplet accumulation in male rat kidney. In: Bach PH, Gregg NJ, Wilks MF, Delacruz L (eds) Nephrotoxicity – mechanisms, early diagnosis and therapeutic management. Marcel Dekker, New York (USA), pp. 273-277.

**1988**

2. Von Oepen B, Schüürmann G, Kördel W, Klein W 1988. Soil/water sorption of chemicals - relationships between adsorption coefficients and structural parameters. In: Løkke H, Tyle H, Bro-Rasmussen F (eds.): First european conference on ecotoxicology - conference proceedings. October 17-19, 1988, Copenhagen (Denmark), pp. 490-491.
1. Schüürmann G, Röderer G 1988. Acute toxicity of organotin compounds and its predictability by quantitative structure-activity relationships (QSARs). In: Astruc M and Lester JN (eds.): Heavy metals in the hydrological cycle. Selper Ltd., London (UK), pp. 433-440.

## C) Artikel in Zeitschriften ohne Fachbegutachtung

### 2011

23. Laqua A, Mulliner D, Blaschke U, Schramm F, Schüürmann G 2011. Chemie und Toxikologie – Experimentelle und theoretische Methoden zur Aufklärung molekularer Wirkmechanismen. *ACAMONTA – Zeitschrift für Freunde und Förderer der TU Bergakademie Freiberg* 18: 61-66.

### 2010

22. Böhme A, Schramm F, Wondrousch D, Schüürmann G 2010. Alternativmethoden zur toxikologischen Bewertung chemischer Stoffe. *Zeitschrift für Freunde und Förderer der Technischen Universität Bergakademie Freiberg* 17: 117-121.

### 2009

21. Paschke A, Vrana B, Popp P, Wennrich L, Paschke H, Schüürmann G 2009. MESCO – Neue Passivsammler zur zeitintegrierten Erfassung von organischen Gewässerschadstoffen. *Vom Wasser* 107: 13-18.

### 2006

20. Schüürmann G 2006. Neue Kooperation in den Umweltwissenschaften – Assoziation zwischen GDCh und UWSF. *UWSF – Z. Umweltchem. Ökotox.* 18: 78-79.

19. Hollert H, Ebke KP, Kubiak R, Lorenz W, Ratte HT, Schäffer A, Schulz R, Schüürmann G, Nagel R 2006. Postgraduale Weiterbildung mit dem zertifizierten Abschluß Fachökotoxikologin/e GDCh/SETAC. Übersicht über das Kursprogramm ab Sommer 2006. *UWSF – Z. Umweltchem. Ökotox.* 18: 138-139.

18. Hollert H, Ebke KP, Foth H, Debus R, Römbke J, Seitz A, Schüürmann G, Kubiak R, Schulz R, Nagel R 2006. Postgraduale Weiterbildung mit dem zertifizierten Abschluß Fachökotoxikologin/e GDCh/SETAC. Übersicht über das Kursprogramm 2006. *UWSF – Z. Umweltchem. Ökotox.* 18: 57-59.

### 2005

17. Hollert H, Ahlers J, Schulz R, Schüürmann G, Ratte HT, Braunbeck Th, Kubiak R, Nagel R 2005. Auf zu neuen Ufern - Postgraduale Weiterbildung mit dem zertifizierten Abschluss Fachökotoxikologin/e GDCh/SETAC. Die ersten drei Kurse starten im Oktober/November 2005. *UWSF – Z. Umweltchem. Ökotox.* 17: 129-130.

16. Schüürmann G 2005. Modellierung der Lebensdauer und Abbaubarkeit organischer Verbindungen in Luft, Boden und Wasser (Übersetzung der Publikation "Sabljic A, Peijnenburg W 2001. Modeling lifetime and degradability of organic compounds in air, soil, and water systems. *Pure Appl. Chem.* 73: 1331-1348"). *Angew. Chem.* 117: 843-845.

15. Hollert H, Ahlers J, Schulz R, Schüürmann G, Ratte HT, Nagel R 2005. Auf zu neuen Ufern - Postgraduale Weiterbildung mit dem zertifizierten Abschluss Fachökotoxikologin/e

SETAC/GDCh beginnt 2005. *UWSF – Z. Umweltchem. Ökotox.* 17: 1-2.

## 2004

14. Hollert H, Gies A, Oehlmann J, Schüürmann G, Schaefer M, Braunbeck T 2004. Podiumsdiskussion "New Blood in Ecotoxicology". Wie kann die Berliner Erklärung zur Ökotoxikologie umgesetzt werden? *UWSF – Z. Umweltchem. Ökotox.* 16: 281-282.

13. Hollender J, Roß-Nikoll M, Ratte HAT, Schäffer A, Schüürmann G, Hollert H 2004. Erfolgreiche zweite Gemeinsame Jahrestagung von SETAC-GLB und GDCh-Fachgruppe Umweltchemie und Ökotoxikologie unter dem Motto "Grenzen finden – Grenzen überwinden – Molekulare Mechanismen und ökosystemare Prozesse – am 6.-8.10.2004 in Aachen. *UWSF – Z. Umweltchem. Ökotox.* 16: 149-150.

12. Schüürmann G 2004. Rezension des Buches "Martin Scheringer: Persistence and Spatial Range of Environmental Chemicals. Wiley-VCH 2002, 294 pp.". *Angew. Chem.* 116: 1345-1346; *Angew. Chem. Int. Ed.* 43: 1323-1324.

## 2003

11. Schüürmann G, Aptula AO, Ebert R-U, Kühne R 2003. Klassifizierung von Phenolderivaten nach Toxizitätsmechanismen – Struktur-Wirkungs-Modell für Schadefekte im Ciliaten-Assay *Tetrahymena pyriformis*. *GDCh Mitteilungen der Fachgruppe Umweltchemie und Ökotoxikologie* 9: 4-5,23.

10. Schüürmann G 2003. Ist das Jahr der Chemie auch ein Jahr der Umweltchemie? *GDCh Mitteilungen der Fachgruppe Umweltchemie und Ökotoxikologie* 9: 3.

9. Küster E, Dorusch F, Meißner B, Weiss H, Schüürmann G, Altenburger R 2003. Toxizitätsreduktion durch (Grundwasser-)Sanierungen. Erfolgskontrolle von in situ Grundwasser-Sanierungsverfahren mit Hilfe von kontinuierlichen und diskontinuierlichen Biotesten. *Grundwasser - Zeitschrift der Fachsektion Hydrogeologie in der Deutschen Geologischen Gesellschaft (FH-DGG)* 8: 32-40.

8. Kördel W, Schüürmann G 2003. Kurzbericht zur Jahrestagung der GDCh-Fachgruppe Umweltchemie und Ökotoxikologie 7.-8.10. 2003 in München. *GDCh Mitteilungen der Fachgruppe Umweltchemie und Ökotoxikologie* 9: 15-16.

## 2002

7. Meene R, Schüürmann G, Altenburger R 2002. pH-abhängige Algentoxizität von Phenolderivaten. *GDCh Mitteilungen der Fachgruppe Umweltchemie und Ökotoxikologie* 8: 9-11.

6. Schüürmann G 2002. Sicherheitsvorsorge für Industriechemikalien - Eine gesamtgesellschaftliche Aufgabe. *GDCh Mitteilungen der Fachgruppe Umweltchemie und Ökotoxikologie* 8: 3,20.

## 2001

5. Wenzel K-D, Hubert A, Engewald W, Schüürmann G 2001. Effizientere Extraktion - besserer Nachweis. *Nachr. Chem. (Heft 1)*: 96-98.

**2000**

4. Schüürmann G 2000. Ökotoxikologie - Quo vadis. *Mitteilungsblatt der GDCh-Fachgruppe Umweltchemie und Ökotoxikologie* 6: 3-5.
3. Hubert A, Wenzel K-D, Engewald W, Schüürmann G 2000. ASE zur effizienteren Extraktion von POPs aus real kontaminierten Böden. *GIT (Spezial Separation 1/00)* 20: 8-10.

**1999**

2. Wenzel K-D, Hubert A, Engewald W, Schüürmann G 1999. ASE von POPs aus realen pflanzlichen Proben. *GIT (Spezial Separation 2/99)* 19: 72-74.
1. Schüürmann G, Altenburger R, Segner H 1999. Trendberichte Ökotoxikologie. *Nachr. Chem. Techn. Lab.* 47: 295-302.

## D) Herausgabe von Büchern und Tagungsbänden

### 2003

4. Breton R, Purdy R, Schüürmann G 2003. Proceedings of the 10th International Workshop on Quantitative Structure-Activity Relationships (QSARs) in Environmental Sciences. *QSAR Comb. Sci.* 22, Nos. 1-3. Preface: *QSAR Comb. Sci.* 22: 3-4.

### 1998

3. Schüürmann G, Markert B (eds) 1998. *Ecotoxicology*. John Wiley and Spektrum Akademischer Verlag, New York, USA, 900 pp.

### 1997

2. Chen F, Schüürmann G (eds) 1997. *Quantitative Structure-Activity Relationships in Environmental Sciences - VII*. SETAC Press, Pensacola (FL), USA, 470 pp.
1. Alef K, Brandt J, Fiedler H, Hauthal W, Hutzinger O, Mackay D, Matthies M, Morgan K, Newland L, Robitaille H, Schlummer M, Schüürmann G, Voigt K (eds) 1997. *ECO-INFORMA '97, Vol. 12. Information and Communication in Environmental and Health Issues. Proceedings of ECO-INFORMA '97, October 6-9, Neuherberg (Germany)*. Eco-Informa Press, Bayreuth (Germany), 620 pp.