

Peer-reviewed papers in scientific journals

1. S. Wiese, T. Teutenberg, T. C. Schmidt:
A general strategy for performing temperature-programming in high performance liquid chromatography - Prediction of segmented temperature gradients
J. Chromatogr. A (2011), submitted
2. L. Zhang, D. M. Kujawinski, M. A. Jochmann, T. C. Schmidt:
High Temperature Liquid Chromatography Coupled to Isotope Ratio Mass Spectrometry
Rapid Commun. Mass Spectrom. (2011), accepted for publication
3. A. Akinlua, M. A. Jochmann, J. Laaks, A. Ewert, T. C. Schmidt:
Microwave-Assisted Nonionic Surfactant Extraction of Aliphatic Hydrocarbons from Petroleum Source Rock
Anal. Chim. Acta **691** (2011), 48–55
doi:10.1016/j.aca.2011.02.018
4. S. Wiese, T. Teutenberg, T. C. Schmidt:
A general strategy for performing temperature programming in high performance liquid chromatography – Prediction of linear temperature gradients
Anal. Chem. **83** (6) (2011), 2227–2233
DOI: 10.1021/ac103113m
5. Y. Qian, T. Posch, T. C. Schmidt*:
Sorption of polycyclic aromatic hydrocarbons (PAHs) on glass surfaces
Chemosphere **82** (2011), 859–865
doi:10.1016/j.chemosphere.2010.11.002
6. M. Zedda, J. Tuerk, S. Peil, T. C. Schmidt:
Determination of polymer electrolyte membrane (PEM) degradation products in fuel cell water using electrospray ionization tandem mass spectrometry
Rapid Commun. Mass Spectrom. **24** (2010), 3531–3538
DOI: 10.1002/rcm.4808
7. J. P. Pocostales, M. M. Sein, W. Knolle, C. von Sonntag, T. C. Schmidt:
Degradation of Ozone-Refractory Organic Phosphates in Wastewater by Ozone and Ozone/Hydrogen Peroxide (Peroxone): The Role of Ozone Consumption by Dissolved Organic Matter
Environ. Sci. Technol. **44** (2010), 8248–8253
doi: 10.1021/es1018288
8. J. Laaks, M. A. Jochmann, B. Schilling, T. C. Schmidt:
In-tube Extraction of volatile organic compounds from aqueous samples: an economical alternative to purge and trap enrichment
Anal. Chem. **82** (2010), 7641–7648
doi: 10.1021/ac101414t
9. E. Bi, S. B. Haderlein, T. C. Schmidt:
Practical issues relating to soil column chromatography for sorption parameter determination
Chemosphere **89** (7) (2010), 787–793
doi:10.1016/j.chemosphere.2010.05.006
10. B. Li, Y. Qian, E. Bi, H. Chen, T. C. Schmidt*:
Sorption behavior of phthalic acid esters on reference soils evaluated by soil column

chromatography

CLEAN **38** (5-6) (2010), 425–429

11. D. M. Kujawinski, M. Stephan, M. A. Jochmann, K. Krajenke, J. Haas, T. C. Schmidt*:
Stable Carbon and Hydrogen Isotope Analysis of Methyl Tert-Butyl Ether and Tert-Amyl Methyl Ether by Purge and Trap-Gas Chromatography-Isotope Ratio Mass Spectrometry: Method Evaluation and Application
J. Environ. Monit. **12** (1) (2010), 347-354
DOI:10.1039/B914514A
12. M. A. Jochmann, D. Steinmann, M. Stephan, T. C. Schmidt:
Flow Injection Isotope Ratio Mass Spectrometry for Bulk Carbon Stable Isotope Analysis of Alcoholic Beverages
J. Agric. Food Chem. **57** (2009), 10489–10496
DOI: 10.1021/jf900506t
13. M. Zedda, J. Tuerk, T. Teutenberg, S. Peil, T. C. Schmidt:
A strategy for the systematic development of an LC-UV-MS/MS screening method for polymer electrolyte membrane degradation products using isocratic and gradient phase optimized liquid chromatography
J. Chromatogr. A **1216** (2009), 8910–8917
doi:10.1016/j.chroma.2009.10.052
14. S. Kowal, P. Balsaa, F. Werres, T. C. Schmidt*:
Determination of the polar pesticide degradation product N,N-dimethylsulfamide in aqueous matrices by UPLC-MS/MS
Anal. Bioanal. Chem. **395** (6) (2009), 1787-1794
DOI: 10.1007/s00216-009-2861-2
15. K. E. Pooley, M. Blessing, T. C. Schmidt, S. B. Haderlein, K. T. B. MacQuarrie, H. Prommer:
Aerobic biodegradation of chlorinated ethenes in a fractured bedrock aquifer: quantitative assessment by compound-specific isotope analysis (CSIA) and reactive transport modeling
Environ. Sci. Technol. **43** (19) (2009), 7458-7464
DOI: 10.1021/es900658n
16. E. Bi, L. Zhang, T. C. Schmidt, S. B. Haderlein:
Simulation of nonlinear sorption of N-heterocyclic organic contaminants in soil columns
J. Contam. Hydrol. **107** (1-2) (2009), 58-65
DOI:10.1016/j.jconhyd.2009.04.001
17. L. Liu, S. Endo, C. Eberhardt, P. Grathwohl, T. C. Schmidt*:
Partition behavior of polycyclic aromatic hydrocarbons between aged coal tar and water
Environ. Tox. Chem. **28** (8) (2009), 1578-1584
18. M. M. Sein, A. Golloch, T. C. Schmidt, C. von Sonntag:
Oxidation of Some Typical Wastewater Contaminants (Tributyltin, Clarithromycin, Metoprolol and Diclofenac) by Ozone
Water Sci. Technol. **59** (8) (2009), 1479-1485
19. S. Endo, P. Grathwohl, S. B. Haderlein, T. C. Schmidt:
Effects of Native Organic Material and Water on Sorption Properties of Reference Diesel Soot

- Environ. Sci. Technol.* **43** (9) (2009), 3187-3193
DOI: 10.1021/es803519a
20. S. Endo, P. Grathwohl, S. B. Haderlein, T. C. Schmidt:
LFERs for Soil Organic Carbon–Water Distribution Coefficients (KOC) at Low Sorbate Concentrations
Environ. Sci. Technol. **43** (9) (2009), 3094-3100
DOI: 10.1021/es803157e
21. M. Blessing, T. C. Schmidt*, R. Dinkel, S. B. Haderlein:
Delineation of multiple chlorinated ethene sources in an industrialized area – A forensic field study using compound-specific isotope analysis
Environ. Sci. Technol. **43** (2009), 2701-2707
DOI: 10.1021/es803100p
22. F. Werres, P. Balsaa, T. C. Schmidt:
Total Concentration Analysis of Polycyclic Aromatic Hydrocarbons in Aqueous Samples with High Suspended Particulate Matter Content
J. Chromatogr. A **1216** (2009), 2235-2240
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23. S. Endo, P. Grathwohl, S. B. Haderlein, T. C. Schmidt:
Characterization of Sorbent Properties of Soil Organic Matter and Carbonaceous Geosorbents Using n-Alkanes and Cycloalkanes as Molecular Probes
Environ. Sci. Technol. **43** (2009), 393-400
DOI: 10.1021/es802277
24. S. Endo, W. Xu, K.-U. Goss, T. C. Schmidt:
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Chemosphere **73** (2008), 532-538
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25. M. M. Sein, M. Zedda, J. Türk, T. C. Schmidt, A. Golloch, C. von Sonntag:
Oxidation of Diclofenac with Ozone in Aqueous Solution
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26. S. Endo, P. Grathwohl, S. B. Haderlein, T. C. Schmidt:
Compound-Specific Factors Influencing Sorption Nonlinearity in Natural Organic Matter
Environ. Sci. Technol. **42** (16) (2008), 5897–5903.
DOI: 10.1021/es8001426
27. S. Endo, P. Grathwohl, T. C. Schmidt:
Absorption or Adsorption? Insights from Molecular Probes n-Alkanes and Cycloalkanes into Modes of Sorption by Environmental Solid Media
Environ. Sci. Technol. **42** (11) (2008), 3989-3995
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28. M. Blessing, M. A. Jochmann, T. C. Schmidt*:
Pitfalls in Compound-Specific Isotope Analysis of Environmental Samples
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29. M. A. Jochmann, X. Yuan, B. Schilling, T. C. Schmidt*:
In-tube Extraction (ITEX) for Enrichment of Volatile Organic Hydrocarbons from Aqueous Samples
J. Chromatogr. A **1179** (2) (2008), 96-105
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30. T. Gocht, J. A. C. Barth, M. Epp, M. A. Jochmann, M. Blessing, T. C. Schmidt, P. Grathwohl:
Indications for pedogenic formation of perylene in a terrestrial soil profile: depth distribution and first results from stable carbon isotope ratios
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31. M. M. Sein, A. Golloch, T. C. Schmidt, C. von Sonntag:
No Marked Kinetic Isotope Effect in the Peroxone ($\text{H}_2\text{O}_2/\text{D}_2\text{O}_2 + \text{O}_3$) Reaction – Mechanistic Consequences
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32. E. Bi, T. C. Schmidt*, S. B. Haderlein:
Environmental factors influencing sorption of heterocyclic aromatic compounds to soil
Environ. Sci. Technol. **41** (9) (2007), 3172-3178
33. M. A. Jochmann, X. Yuan, T. C. Schmidt*:
Determination of halogenated volatile organic hydrocarbons in water samples by solid-phase dynamic extraction
Anal. Bioanal. Chem. **387** (6) (2007), 2163-2174
34. M. A. Jochmann, M. Blessing, S. B. Haderlein, T. C. Schmidt*:
A new approach to determine method detection limits for compound-specific isotope analysis of volatile organic compounds
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Sorption of heterocyclic organic compounds to reference soils studied by soil column chromatography
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36. S. Endo, T. C. Schmidt*:
Partitioning Properties of Linear and Branched Ethers: Determination of Linear Solvation Energy Relationship (LSER) Descriptors
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37. K.-U. Goss, G. Bronner, T. Harner, M. Hertel, T. C. Schmidt:
The Partition Behavior of Fluorotelomer Alcohols and Olefins
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38. M. A. Jochmann, M. P. Kmiecik, T. C. Schmidt*:
Solid-phase dynamic extraction for the enrichment of polar volatile organic compounds from water
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Prediction of Partitioning between Complex Organic Mixtures and Water: Application of Polyparameter Linear Free Energy Relationships
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42. H. P. H. Arp, K. Fenner, T. C. Schmidt:
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43. L. Zwank, M. Berg, M. Elsner, T. C. Schmidt, R. P. Schwarzenbach, S. B. Haderlein:
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46. T. C. Schmidt*, M. Schirmer, H. Weiß, S. B. Haderlein:
Microbial degradation of methyl tert-butyl ether (MTBE) and tert-butyl alcohol (TBA) in the subsurface
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HPLC-MS Investigations of Acidic Contaminants in Ammunition Wastes using Volatile Ion-Pairing Reagents (VIP-LC-MS)
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In Situ Derivatization/Solid-Phase Microextraction: Determination of Polar Aromatic Amines
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Compound-specific Stable Isotope Analysis of Organic Contaminants in Natural Environments – A Critical Review of State of the Art, Prospects and Future Challenges
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Analysis of methyl tert-butyl ether (MTBE) and tert-butyl alcohol (TBA) in ground and surface water
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Invited Book Chapters

1. C. von Sonntag, T. C. Schmidt:
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R. Zellner (ed.): Chemie über den Wolken ...und darunter
Wiley-VCH, Weinheim, 2011, pp 101-103
2. M. A. Jochmann, T. C. Schmidt*:
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