

Publications

1. "Studying ultra-complex crude oil mixtures by using High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) coupled to an ESI-LTQ-Orbitrap Mass Spectrometer", W. Schrader, Y. Xuan, A. Gaspar, *Eur. J. Mass Spectrom.* (2013) accepted for publication
2. "Direct Coupling of Normal-Phase High-Performance Liquid Chromatography to Atmospheric Pressure Laser Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for the Characterization of Crude Oil" S. Lababidi, S.K. Panda, J.T. Andersson, W. Schrader, *Anal. Chem.* (2013) 85, 9478–9485
3. "Deep Well Deposits: Effects of Extraction on Mass Spectrometric Results", S. Lababidi, S.K. Panda, J.T. Andersson, W. Schrader, *Energy Fuels* (2013) 27, 1236–1245
4. "The formation of zeolites from solution – Analysis by mass spectrometry", I.H. Lim, W. Schrader, F. Schüth, *Micropor. Mesopor. Mat.* (2013) 16620–36
5. "High-molecular weight sulfur-containing aromatics refractory to weathering as determined by Fourier transform ion cyclotron resonance mass spectrometry", A.H. Hegazi, E.M. Fathalla, S.K. Panda, W. Schrader, J.T. Andersson, *Chemosphere* (2012) 89, 205-212
6. "Characterization of Saturates, Aromatics, Resins, and Asphaltenes Heavy Crude Oil Fractions by Atmospheric Pressure Laser Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry", A. Gaspar, E. Zellermann, S. Lababidi, J. Reece, W. Schrader, *Energy Fuels* (2012) 26, 3481–3487
7. "Direct experimental observation of the aggregation of α -amino acids into 100–200 nm clusters in aqueous solution", D. Hagemeyer, J. Ruesing, T. Fenske, H.-W. Klein, C. Schmuck, W. Schrader, M.E. Minas da Piedaded, M Epple, *RSC Advances* (2012) 2, 4690–4696
8. "Impact of different ionization methods on the molecular assignments of asphaltenes by FT-ICR MS", A. Gaspar, E. Zellermann, S. Lababidi, J. Reece, W. Schrader, *Anal. Chem.* (2012) 84, 5257–5267
9. "Expanding the data depth for the analysis of complex crude oil samples by Fourier transform ion cyclotron resonance mass spectrometry using the spectral stitching method", A. Gaspar, W. Schrader, *Rapid Commun. Mass Spectrom.* (2012) 26, 1047–1052
Highlight in: Spectroscopy Now 10. Mai 2012
<http://www.spectroscopynow.com/details/ezine/137218312d4/Journal-Highlight-Expanding-the-data-depth-for-the-analysis-of-complex-crude-oil.html>
10. "Atmospheric pressure laser ionization (APLI) coupled with Fourier transform ion cyclotron resonance mass spectrometry applied to petroleum samples analysis: comparison with electrospray ionization and atmospheric pressure photoionization methods", S.K. Panda, K-J. Brockmann, T. Benter, W. Schrader, *Rapid Commun. Mass Spectrom.* (2011) 25, 2317–2326
11. "Electrospray Mass Spectrometry for Detailed Mechanistic Studies of a Complex Organocatalyzed Triple Cascade Reaction", M.W. Alachraf, P.P. Handayani, M.R.M. Hüttel, C. Grondal, D. Ender, W. Schrader, *Org. Bioorg. Chem.* (2011) 9, 1047–1053
12. "Ultrahigh resolution mass spectrometric investigations on asphaltene deposits" J.T. Andersson, S.K. Panda, W. Schrader, *Abstr. Papers of the American Chemical Society Vol: 239:43-PETR* (2010)

13. "Evidence for a Non-Concerted, Dissoziative Mechanism of the Palladium-Catalyzed "Enolate Claisen Rearrangement" of Allylic Esters", M. Braun, P. Meletis, W. Schrader, *Eur. J. Org. Chem.* (2010), 5369–5372
14. "Nucleation of ITQ-21 studied by ESI-MS", B.B. Schaack, W. Schrader, A. Corma, F. Schüth, *Chem. Mat.* (2009), **21**, 4448–4453
15. "Structural insight into germanium containing silicate species by electrospray ionization mass spectrometry (ESI-MS) and ESI-MS/MS", B.B. Schaack, W. Schrader, F. Schüth, *J. Phys. Chem. B* (2009) **113**, 11240–11246
16. "How are Heteroelements (Ga and Ge) Incorporated in Silicate Oligomers? ", B. B. Schaack, W. Schrader, F. Schüth, *Chem. Eur. J.* (2009) **15**, 5920–5925
17. "Characterization of supercomplex crude oil mixtures: What is really in there?", S.K. Panda, J.T. Andersson, W. Schrader, *Angew. Chemie Int. Ed.* (2009) **48**, 1788–1791
18. "Mass Spectrometric Characterization of Key Intermediates in a Complex Organocatalytic Cascade Reactions ", W. Schrader, P. Handayani, J. Zhou, B. List, *Angew. Chemie Int. Ed.* (2009) **48**, 1463–1466
19. "3,3'-Dihydroxyisorenieratene, a Natural Carotenoid with Superior Antioxidant and Photoprotective Properties ", H.D. Martin, S. Kock, R. Scherrers, K. Lutter, T. Wagener, C. Hundsdörfer, S. Frixel, K. Schaper, H. Ernst, W. Schrader, H. Görner, W. Stahl, *Angew. Chemie Int. Ed.*, (2009) **48**, 400–403
20. "Detection of structural elements of different zeolites in nucleating solutions by electrospray ionisation mass spectrometry (ESI-MS)", B.B. Schaack, W. Schrader, F. Schüth, *Angew. Chemie Int. Ed.*, (2008) **47**, 9092–9095
21. "Fourier transform ion cyclotron resonance mass spectrometry in the speciation of high-molecular-weight sulfur heterocycles in vacuum gas oils of different boiling ranges", S.K. Panda, W. Schrader, J.T. Andersson, (2008) *Anal. Bioanal. Chem.* (2008) 392:839–848
22. "Characterization of polyaromatic heterocycles in complex crude oil mixtures using atmospheric pressure laser ionization on a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (APLI FT-ICR MS)", W. Schrader, S.K. Panda, K.J. Brockmann, T. Benter, *Analyst* (2008) **133**, 867–869
23. "Mass-spectrometric analysis of complex volatile and non-volatile crude oil components: a challenge" S.K. Panda, J.T. Andersson, W. Schrader, *Anal. Bioanal. Chem.* (2007), **389**, 1329–1339
24. "Dynamics of silicate species in solution", S. Pelster, B. Schaack, B. Weimann, W. Schrader, F. Schüth, *Angew. Chemie Int. Ed.* (2007), **46**, 6674–6677
25. "A detailed study on the use of Electrospray Mass Spectrometry to investigate nucleation effects of highly concentrated silicate solutions", S.A. Pelster, F. Schüth, W. Schrader, *Anal. Chem.* (2007) **79**, 6005–6012
26. "Distribution of sulphur aromatics in three Saudi Arabian crude oils as determined by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry" S.K. Panda, W. Schrader, A. al-Hajji, J. Andersson, *Energy&Fuels* (2007) **21**, 1071–1077
27. "Monitoring Nucleation of Zeolites Using Mass Spectrometry", S.A. Pelster, R. Kalamajka, W. Schrader, F. Schüth, *Angew. Chemie Int. Ed.* (2007) **46**, 2299–2302
28. "Carotenylflavonoids, a novel group of potent, dual-functional antioxidants", S. Beutner, S. Frixel, H. Ernst, T. Hoffmann, I. Hernandez-Blanco, C. Hundsdorfer, N. Kiesendahl, S. Kock, H.-D. Martin, B. Mayer,

- P. Noack, A. Perez-Galvez, G. Kock, R. Scherrers, W. Schrader, S. Sell, W. Stahl, (2007) *Arkivoc* (viii) 279-295
29. "Investigating Organocatalytic Reactions: Mass Spectrometric studies of Conjugate Umpolung Reaction", W. Schrader, P.P. Handayani, C. Burstein, F. Glorius, *Chem. Commun.* (2007) (7), 716
 30. "Monitoring Temporal Evolution of Silicates during Hydrolysis and Condensation of Silicates using Mass Spectrometry", S. A. Pelster, W. Schrader, F. Schüth, *J. Am. Chem. Soc.* (2006), **128**, 4310-4317
 31. " β -Cyclodextrin as a stationary phase for the group separation of polycyclic aromatic compounds in normal-phase liquid chromatography", S.K. Panda, W. Schrader, J. Andersson, *J. Chromatogr.A* (2006) **1122**, 88-96
 32. "JCAMP-DX V.6.00 for Chromatography and Mass Spectrometry hyphenated methods", J. Hau, P. Lampen, R.J. Lancashire, R.S. McDonald, P.S. McIntyre, D.N. Rutledge, W. Schrader, A.N. Davies, *Pure Appl. Chem.*
 33. "Sulfur aromatic compounds remaining in vacuum gas oils after hydrodesulfurization", J.T. Andersson, S. K. Panda, and W. Schrader, *Abstr. Pap. Am. Chem. Soc* 230: U2336-U2336 59-PETR Aug. 2005
 34. "Studies of complex reactions using modern hyphenated methods: α -pinene ozonolysis as a model reaction", W. Schrader, J. Geiger, M. Godejohann, *J. Chromatogr. A* (2005) **1075/1-2**, 185-196
 35. "Selective characterization of high-molecular weight sulfur containing aromatics in vacuum residues using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry", H. Müller, J. T. Andersson, W. Schrader, *Anal. Chem.* (2005) **77(8)**, 2536-2543
 36. "Atmosphere, a chemical reactor: formation pathways of secondary organic aerosol", W. Schrader, *Angew. Chemie* (2005) **117(10)**, 1468-1470; *Angew. Chemie Int. Ed.* (2005) **44(10)**, 1444-1446
 37. "Mass spectrometric determination of DNA adducts from a reaction with terpenoids", W. Schrader, S. Döring, W. Joppek, *Angew. Chemie* (2004) **116(48)**, 6826-6829 *Angew. Chemie Int. Ed.* **43(48)**, 6657-6660
 38. "Liquid Chromatography/Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: an early Overview" (Review), W. Schrader, H.-W. Klein *Anal. Bioanal. Chem.* (2004) **379(7-8)**, 1013-1024
 39. Synthesis of substituted 1,2,4-triazoles from reaction of nitrilimines with substituted hydrazones, A.M. Awadallah, A.R.S. Ferwanah, M.R. El-Haddad, W. Schrader, *As. J. Chem.* (2004) **16** (3-4): 1691-1698.
 40. "Characterization of high molecular weight sulfur containing aromatics in vacuum residues using Fourier transform ion cyclotron resonance mass spectrometry", H. Müller, W. Schrader, J.T. Andersson, *Abstr. Pap. Am. Chem. Soc.* 227: FUEL Part 1 Mar 28, 2004
 41. "Second-generation MS-based high-throughput screening system for enantioselective catalysts and biocatalysts", W. Schrader, A. Eipper, D. J. Pugh, and M. T. Reetz, *Can. J. Chem.* (2002) **80**, 626-632
 42. "An analytical approach for a comprehensive study of organic aerosols" "Ein analytischer Ansatz für eine detaillierte Studie des atmosphärischen organischen Aerosols", W. Schrader, J. Geiger, M. Godejohann, B. Warscheid, T. Hoffmann, *Angew. Chemie Int. Ed.*, (2001) **40** (21), 3998-4001; *Angew. Chemie*, (2001) **113** (21), 4129.
Highlight in: Frankfurter Allgemeine Zeitung FAZ 5. November 2001
Highlight in: Spectroscopy Now 2001
<http://www.spectroscopynow.com/details/ezine/sepspec591ezine/The-Blue-Ridge-chemicals-of-Virginia.html>

43. "Development of a simple gradient-LC/IR interface for the detection of terpenoids from the α -pinene / ozone reaction", J. Geiger, E.H. Korte, W. Schrader, *J. Chromatogr. A.*, (2001) **922(1-2)**, 99-110.
44. "Degradation of α -pinene on Tenax during sample storage: effects of daylight radiation and temperature", W. Schrader, J. Geiger, D. Klockow, E.H. Korte, *Env. Sci. Technol.*, (2001) **35(13)**, 2717-2720.
45. "Coupling Liquid Chromatography to Mass Spectrometry, Infrared Spectroscopy and Nuclear Magnetic Resonance for the identification of reaction products from α -Pinene ozonolysis", W. Schrader, J. Geiger, M. Godejohann, T. Hoffmann, B. Warscheid, U. Marggraf, *Abstr. Pap. Am. Chem. Soc.* 221: 129-ENVR, Part 1 APR 1 2001
46. "A hard/soft mismatch enables catalytic Friedel-Crafts Acylation", A. Fürstner, D. Voigtländer, W. Schrader, D. Giebel, M.T. Reetz, *Org. Lett.*, (2001) **3(3)**, 417-420.
47. "Speciation in Solution: Silicate Oligomers in Aqueous Solutions detected by Mass Spectrometry", P. Bussian, F. Sobott, B. Brutschy, W. Schrader, F. Schüth, *Angew. Chemie Int. Ed.*, (2000) **39 (21)**, 3901-3905; *Angew. Chemie*, (2000) **112 (21)**, 4065.
48. "The use of LC/MS, LC/IR and LC/NMR for the identification of low volatile compounds formed during the α -pinene/ozone reaction", W. Schrader, J. Geiger, M. Godejohann, T. Hoffmann, U. Marggraf, W. Nigge, Proc. 48. ASMS Conf. on Mass Spectrometry, (2000)
49. "Application of GC/Cryocondensation-FT-IR and GC/MS for the identification of gasphase reaction products from the α -pinene/ozone reaction", W. Schrader, J. Geiger, T. Hoffmann, E.H. Korte, D. Klockow, *J. Chromatogr. A.*, (1999) **864**, 299-314
50. "Using Thermodesorption-GC/Cryocondensation-FT-IR for the determination of biogenic VOC emissions", J. Geiger, T. Hoffmann, J. Kahl, D. Klockow, E.H. Korte, W. Schrader, *Fresenius J. Anal. Chem.*, (1998), **362**, 148.
51. "A new approach to identify reaction products of biogenic hydrocarbons using chromatographic separation coupled with mass spectrometric and infrared spectroscopic detection", W. Schrader, R. Bandur, J. Geiger, T. Hoffmann, E.H. Korte, D. Klockow, M. Lemke, S. Wagner, *Proc. 5. Int. Symp. on Hyphenated Techniques in Chromatography*, 11. - 13. Februar 1998 in Brügge, Belgien;
52. "Styrene oxide DNA Adducts: In vitro Reaction and Sensitive Detection of Modified Oligo-nucleotides with Capillary Zone Electrophoresis Interfaced to Electrospray Mass Spectrometry", W. Schrader, M. Linscheid, *Arch. Toxicol.*, (1997), **71**, 588-595
53. "The Determination of Styrene Oxide Adducts in DNA and DNA Components", W. Schrader, M. Linscheid, *J. Chromatogr. A*, (1995), **717**, 117-125
54. "Transport von Platin in biologischen Systemen: Neue analytische Strategien", M. Linscheid, P. Janning, W. Schrader, in: *"Mechanismen des Transports von Mineralstoffen und Spurenkomponenten"*, Hrsg. H.J. Haas, Homburg/Saar, Wissenschaftliche Verlagsgesellschaft, Stuttgart, 1995
55. "A new Mass Spectrometric Approach to detect Modifications in DNA", P. Janning, W. Schrader und M. Linscheid, *Rapid Comm. Mass Spectrometry*, (1994), **8**, 1035-1040.
56. "Continuous-Flow Fast Atom Bombardment Mass Spectrometry: A Concept to Improve the Sensitivity", J. Hau, W. Schrader, M. Linscheid, *Org. Mass Spectrom.*, 1993, **28**, 216-22.