

Emma L. Schymanski

List of Publications by Year in descending order

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Version: 2024-02-01

67
papers

9,201
citations

76326

40
h-index

102487

66
g-index

78
all docs

78
docs citations

78
times ranked

8560
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovering pesticides and their TPs in Luxembourg waters using open cheminformatics approaches. <i>Environment International</i> , 2022, 158, 106885.	10.0	21
2	patRoön 2.0: Improved non-target analysis workflows including automated transformation product screening. <i>Journal of Open Source Software</i> , 2022, 7, 4029.	4.6	10
3	FAIRifying the exposome journal: Templates for chemical structures and transformations. <i>Exposome</i> , 2022, 2, .	2.8	10
4	Development and Application of an LC-MS/MS Untargeted Exposomics Method with a Separated Pooled Quality Control Strategy. <i>Molecules</i> , 2022, 27, 2580.	3.8	4
5	The Next Frontier of Environmental Unknowns: Substances of Unknown or Variable Composition, Complex Reaction Products, or Biological Materials (UVCBs). <i>Environmental Science & Technology</i> , 2022, 56, 7448-7466.	10.0	29
6	Extraction of chemical structures from literature and patent documents using open access chemistry toolkits: a case study with PFAS. , 2022, 1, 490-501.		11
7	Communicating Confidence of Per- and Polyfluoroalkyl Substance Identification via High-Resolution Mass Spectrometry. <i>Environmental Science and Technology Letters</i> , 2022, 9, 473-481.	8.7	61
8	Studying the Parkinsonâ€™s disease metabolome and exposome in biological samples through different analytical and cheminformatics approaches: a pilot study. <i>Analytical and Bioanalytical Chemistry</i> , 2022, 414, 7399-7419.	3.7	12
9	Studying Charge Migration Fragmentation of Sodiated Precursor Ions in Collision-Induced Dissociation at the Library Scale. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 180-186.	2.8	4
10	Empowering large chemical knowledge bases for exposomics: PubChemLite meets MetFrag. <i>Journal of Cheminformatics</i> , 2021, 13, 19.	6.1	63
11	Retrospective non-target analysis to support regulatory water monitoring: from masses of interest to recommendations via in silico workflows. <i>Environmental Sciences Europe</i> , 2021, 33, .	5.5	18
12	FAIR chemical structures in the Journal of Cheminformatics. <i>Journal of Cheminformatics</i> , 2021, 13, 50.	6.1	19
13	Occurrence and Distribution of Pharmaceuticals and Their Transformation Products in Luxembourgish Surface Waters. <i>ACS Environmental Au</i> , 2021, 1, 58-70.	7.0	13
14	Development and Application of Liquid Chromatographic Retention Time Indices in HRMS-Based Suspect and Nontarget Screening. <i>Analytical Chemistry</i> , 2021, 93, 11601-11611.	6.5	79
15	patRoön: open source software platform for environmental mass spectrometry based non-target screening. <i>Journal of Cheminformatics</i> , 2021, 13, 1.	6.1	136
16	Historical exposomics and high resolution mass spectrometry. <i>Exposome</i> , 2021, 1, .	2.8	11
17	Evaluation of reverse osmosis drinking water treatment of riverbank filtrate using bioanalytical tools and non-target screening. <i>Environmental Science: Water Research and Technology</i> , 2020, 6, 103-116.	2.4	21
18	Improving Target and Suspect Screening High-Resolution Mass Spectrometry Workflows in Environmental Analysis by Ion Mobility Separation. <i>Environmental Science & Technology</i> , 2020, 54, 15120-15131.	10.0	69

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19	The exposome and health: Where chemistry meets biology. <i>Science</i> , 2020, 367, 392-396.	12.6	499
20	Tracking complex mixtures of chemicals in our changing environment. <i>Science</i> , 2020, 367, 388-392.	12.6	390
21	A European proposal for quality control and quality assurance of tandem mass spectral libraries. <i>Environmental Sciences Europe</i> , 2020, 32, .	5.5	53
22	Connecting environmental exposure and neurodegeneration using cheminformatics and high resolution mass spectrometry: potential and challenges. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 1426-1445.	3.5	13
23	The metaRbolomics Toolbox in Bioconductor and beyond. <i>Metabolites</i> , 2019, 9, 200.	2.9	64
24	Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 4683-4700.	3.7	14
25	Nontarget Screening Reveals Time Trends of Polar Micropollutants in a Riverbank Filtration System. <i>Environmental Science & Technology</i> , 2019, 53, 7584-7594.	10.0	70
26	Exploring open cheminformatics approaches for categorizing per- and polyfluoroalkyl substances (PFASs). <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 1835-1851.	3.5	25
27	Annotating Nontargeted LC-HRMS/MS Data with Two Complementary Tandem Mass Spectral Libraries. <i>Metabolites</i> , 2019, 9, 3.	2.9	24
28	Exploring the Potential of a Global Emerging Contaminant Early Warning Network through the Use of Retrospective Suspect Screening with High-Resolution Mass Spectrometry. <i>Environmental Science & Technology</i> , 2018, 52, 5135-5144.	10.0	101
29	Dark matter in host-microbiome metabolomics: Tackling the unknownsâ€”A review. <i>Analytica Chimica Acta</i> , 2018, 1037, 13-27.	5.4	108
30	Expanding the Use of Spectral Libraries in Proteomics. <i>Journal of Proteome Research</i> , 2018, 17, 4051-4060.	3.7	47
31	Mind the Gap: Mapping Mass Spectral Databases in Genome-Scale Metabolic Networks Reveals Poorly Covered Areas. <i>Metabolites</i> , 2018, 8, 51.	2.9	51
32	Open Science for Identifying â€œKnown Unknownâ€•Chemicals. <i>Environmental Science & Technology</i> , 2017, 51, 5357-5359.	10.0	53
33	Integrating ion mobility spectrometry into mass spectrometry-based exposome measurements: what can it add and how far can it go?. <i>Bioanalysis</i> , 2017, 9, 81-98.	1.5	66
34	Nontarget Screening with High Resolution Mass Spectrometry in the Environment: Ready to Go?. <i>Environmental Science & Technology</i> , 2017, 51, 11505-11512.	10.0	453
35	Critical Assessment of Small Molecule Identification 2016: automated methods. <i>Journal of Cheminformatics</i> , 2017, 9, 22.	6.1	122
36	SPLASH, a hashed identifier for mass spectra. <i>Nature Biotechnology</i> , 2016, 34, 1099-1101.	17.5	61

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37	MetFrag relaunched: incorporating strategies beyond in silico fragmentation. <i>Journal of Cheminformatics</i> , 2016, 8, 3.	6.1	665
38	Systematic Exploration of Biotransformation Reactions of Amine-Containing Micropollutants in Activated Sludge. <i>Environmental Science & Technology</i> , 2016, 50, 2908-2920.	10.0	111
39	Effect-directed analysis supporting monitoring of aquatic environments – An in-depth overview. <i>Science of the Total Environment</i> , 2016, 544, 1073-1118.	8.0	288
40	Mass spectral databases for LC/MS- and GC/MS-based metabolomics: State of the field and future prospects. <i>TrAC - Trends in Analytical Chemistry</i> , 2016, 78, 23-35.	11.4	404
41	Future water quality monitoring – Adapting tools to deal with mixtures of pollutants in water resource management. <i>Science of the Total Environment</i> , 2015, 512-513, 540-551.	8.0	243
42	Multicriteria Approach To Select Polyaromatic River Mutagen Candidates. <i>Environmental Science & Technology</i> , 2015, 49, 2959-2968.	10.0	24
43	Retention projection enables accurate calculation of liquid chromatographic retention times across labs and methods. <i>Journal of Chromatography A</i> , 2015, 1412, 43-51.	3.7	47
44	Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. <i>Analytical and Bioanalytical Chemistry</i> , 2015, 407, 6237-6255.	3.7	489
45	Extended Suspect and Non-Target Strategies to Characterize Emerging Polar Organic Contaminants in Raw Wastewater with LC-HRMS/MS. <i>Environmental Science & Technology</i> , 2015, 49, 12333-12341.	10.0	263
46	Prioritizing Unknown Transformation Products from Biologically-Treated Wastewater Using High-Resolution Mass Spectrometry, Multivariate Statistics, and Metabolic Logic. <i>Analytical Chemistry</i> , 2015, 87, 12121-12129.	6.5	101
47	Solving CASMI 2013 with MetFrag, MetFusion and MOLGEN-MS/MS. <i>Mass Spectrometry</i> , 2014, 3, S0036-S0036.	0.6	16
48	Exploring the Behaviour of Emerging Contaminants in the Water Cycle using the Capabilities of High Resolution Mass Spectrometry. <i>Chimia</i> , 2014, 68, 793.	0.6	15
49	Suspect and nontarget screening approaches to identify organic contaminant records in lake sediments. <i>Analytical and Bioanalytical Chemistry</i> , 2014, 406, 7323-7335.	3.7	91
50	Metabolite identification: are you sure? And how do your peers gauge your confidence?. <i>Metabolomics</i> , 2014, 10, 350-353.	3.0	205
51	Biotransformation of Benzotriazoles: Insights from Transformation Product Identification and Compound-Specific Isotope Analysis. <i>Environmental Science & Technology</i> , 2014, 48, 4435-4443.	10.0	101
52	Strategies to Characterize Polar Organic Contamination in Wastewater: Exploring the Capability of High Resolution Mass Spectrometry. <i>Environmental Science & Technology</i> , 2014, 48, 1811-1818.	10.0	333
53	Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence. <i>Environmental Science & Technology</i> , 2014, 48, 2097-2098.	10.0	2,300
54	Integrated biological–chemical approach for the isolation and selection of polyaromatic mutagens in surface waters. <i>Analytical and Bioanalytical Chemistry</i> , 2013, 405, 9101-9112.	3.7	21

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55	Automatic recalibration and processing of tandem mass spectra using formula annotation. <i>Journal of Mass Spectrometry</i> , 2013, 48, 89-99.	1.6	87
56	Small Molecule Identification with MOLGEN and Mass Spectrometry. <i>Metabolites</i> , 2013, 3, 440-462.	2.9	32
57	The Critical Assessment of Small Molecule Identification (CASMI): Challenges and Solutions. <i>Metabolites</i> , 2013, 3, 517-538.	2.9	35
58	CASMI: And the Winner is . . . <i>Metabolites</i> , 2013, 3, 412-439.	2.9	30
59	Consensus Structure Elucidation Combining GC/EI-MS, Structure Generation, and Calculated Properties. <i>Analytical Chemistry</i> , 2012, 84, 3287-3295.	6.5	57
60	Automated Strategies To Identify Compounds on the Basis of GC/EI-MS and Calculated Properties. <i>Analytical Chemistry</i> , 2011, 83, 903-912.	6.5	33
61	Application of preparative capillary gas chromatography (pcGC), automated structure generation and mutagenicity prediction to improve effect-directed analysis of genotoxicants in a contaminated groundwater. <i>Environmental Science and Pollution Research</i> , 2010, 17, 885-897.	5.3	31
62	Identification of a phytotoxic photo-transformation product of diclofenac using effect-directed analysis. <i>Environmental Pollution</i> , 2010, 158, 1461-1466.	7.5	69
63	Matching Structures to Mass Spectra Using Fragmentation Patterns: Are the Results As Good As They Look?. <i>Analytical Chemistry</i> , 2009, 81, 3608-3617.	6.5	60
64	Integrated analytical and computer tools for structure elucidation in effect-directed analysis. <i>TrAC - Trends in Analytical Chemistry</i> , 2009, 28, 550-561.	11.4	52
65	How to confirm identified toxicants in effect-directed analysis. <i>Analytical and Bioanalytical Chemistry</i> , 2008, 390, 1959-1973.	3.7	91
66	The use of MS classifiers and structure generation to assist in the identification of unknowns in effect-directed analysis. <i>Analytica Chimica Acta</i> , 2008, 615, 136-147.	5.4	58
67	ELIXIR and Toxicology: a community in development. <i>F1000Research</i> , 0, 10, 1129.	1.6	3