Emma L. Schymanski

List of Publications by Year
in descending order

67 papers	9,201 citations	87401 40 h-index	116156 66 g-index
78 all docs	78 docs citations	78 times ranked	9410 citing authors

#	Article	IF	Citations
1	Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence. Environmental Science & Technology, 2014, 48, 2097-2098.	4.6	2,300
2	MetFrag relaunched: incorporating strategies beyond in silico fragmentation. Journal of Cheminformatics, 2016, 8, 3.	2.8	665
3	The exposome and health: Where chemistry meets biology. Science, 2020, 367, 392-396.	6.0	499
4	Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. Analytical and Bioanalytical Chemistry, 2015, 407, 6237-6255.	1.9	489
5	Nontarget Screening with High Resolution Mass Spectrometry in the Environment: Ready to Go?. Environmental Science & Technology, 2017, 51, 11505-11512.	4.6	453
6	Mass spectral databases for LC/MS- and GC/MS-based metabolomics: State of the field and future prospects. TrAC - Trends in Analytical Chemistry, 2016, 78, 23-35.	5.8	404
7	Tracking complex mixtures of chemicals in our changing environment. Science, 2020, 367, 388-392.	6.0	390
8	Strategies to Characterize Polar Organic Contamination in Wastewater: Exploring the Capability of High Resolution Mass Spectrometry. Environmental Science & Technology, 2014, 48, 1811-1818.	4.6	333
9	Effect-directed analysis supporting monitoring of aquatic environments â€" An in-depth overview. Science of the Total Environment, 2016, 544, 1073-1118.	3.9	288
10	Extended Suspect and Non-Target Strategies to Characterize Emerging Polar Organic Contaminants in Raw Wastewater with LC-HRMS/MS. Environmental Science & Technology, 2015, 49, 12333-12341.	4.6	263
11	Future water quality monitoring â€" Adapting tools to deal with mixtures of pollutants in water resource management. Science of the Total Environment, 2015, 512-513, 540-551.	3.9	243
12	Metabolite identification: are you sure? And how do your peers gauge your confidence?. Metabolomics, 2014, 10, 350-353.	1.4	205
13	patRoon: open source software platform for environmental mass spectrometry based non-target screening. Journal of Cheminformatics, 2021, 13, 1.	2.8	136
14	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	2.8	122
15	Systematic Exploration of Biotransformation Reactions of Amine-Containing Micropollutants in Activated Sludge. Environmental Science & Technology, 2016, 50, 2908-2920.	4.6	111
16	Dark matter in host-microbiome metabolomics: Tackling the unknownsâ€"A review. Analytica Chimica Acta, 2018, 1037, 13-27.	2.6	108
17	Biotransformation of Benzotriazoles: Insights from Transformation Product Identification and Compound-Specific Isotope Analysis. Environmental Science & Technology, 2014, 48, 4435-4443.	4.6	101
18	Prioritizing Unknown Transformation Products from Biologically-Treated Wastewater Using High-Resolution Mass Spectrometry, Multivariate Statistics, and Metabolic Logic. Analytical Chemistry, 2015, 87, 12121-12129.	3.2	101

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19	Exploring the Potential of a Global Emerging Contaminant Early Warning Network through the Use of Retrospective Suspect Screening with High-Resolution Mass Spectrometry. Environmental Science & Technology, 2018, 52, 5135-5144.	4.6	101
20	How to confirm identified toxicants in effect-directed analysis. Analytical and Bioanalytical Chemistry, 2008, 390, 1959-1973.	1.9	91
21	Suspect and nontarget screening approaches to identify organic contaminant records in lake sediments. Analytical and Bioanalytical Chemistry, 2014, 406, 7323-7335.	1.9	91
22	Automatic recalibration and processing of tandem mass spectra using formula annotation. Journal of Mass Spectrometry, 2013, 48, 89-99.	0.7	87
23	Development and Application of Liquid Chromatographic Retention Time Indices in HRMS-Based Suspect and Nontarget Screening. Analytical Chemistry, 2021, 93, 11601-11611.	3.2	79
24	Nontarget Screening Reveals Time Trends of Polar Micropollutants in a Riverbank Filtration System. Environmental Science & Technology, 2019, 53, 7584-7594.	4.6	70
25	Identification of a phytotoxic photo-transformation product of diclofenac using effect-directed analysis. Environmental Pollution, 2010, 158, 1461-1466.	3.7	69
26	Improving Target and Suspect Screening High-Resolution Mass Spectrometry Workflows in Environmental Analysis by Ion Mobility Separation. Environmental Science & Technology, 2020, 54, 15120-15131.	4.6	69
27	Integrating ion mobility spectrometry into mass spectrometry-based exposome measurements: what can it add and how far can it go?. Bioanalysis, 2017, 9, 81-98.	0.6	66
28	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	1.3	64
29	Empowering large chemical knowledge bases for exposomics: PubChemLite meets MetFrag. Journal of Cheminformatics, 2021, 13, 19.	2.8	63
30	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
31	Communicating Confidence of Per- and Polyfluoroalkyl Substance Identification via High-Resolution Mass Spectrometry. Environmental Science and Technology Letters, 2022, 9, 473-481.	3.9	61
32	Matching Structures to Mass Spectra Using Fragmentation Patterns: Are the Results As Good As They Look?. Analytical Chemistry, 2009, 81, 3608-3617.	3.2	60
33	The use of MS classifiers and structure generation to assist in the identification of unknowns in effect-directed analysis. Analytica Chimica Acta, 2008, 615, 136-147.	2.6	58
34	Consensus Structure Elucidation Combining GC/EI-MS, Structure Generation, and Calculated Properties. Analytical Chemistry, 2012, 84, 3287-3295.	3.2	57
35	Open Science for Identifying â€œKnown Unknownâ€•Chemicals. Environmental Science & Technology, 2017, 51, 5357-5359.	4.6	53
36	A European proposal for quality control and quality assurance of tandem mass spectral libraries. Environmental Sciences Europe, 2020, 32, .	2.6	53

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37	Integrated analytical and computer tools for structure elucidation in effect-directed analysis. TrAC - Trends in Analytical Chemistry, 2009, 28, 550-561.	5.8	52
38	Mind the Gap: Mapping Mass Spectral Databases in Genome-Scale Metabolic Networks Reveals Poorly Covered Areas. Metabolites, 2018, 8, 51.	1.3	51
39	Retention projection enables accurate calculation of liquid chromatographic retention times across labs and methods. Journal of Chromatography A, 2015, 1412, 43-51.	1.8	47
40	Expanding the Use of Spectral Libraries in Proteomics. Journal of Proteome Research, 2018, 17, 4051-4060.	1.8	47
41	The Critical Assessment of Small Molecule Identification (CASMI): Challenges and Solutions. Metabolites, 2013, 3, 517-538.	1.3	35
42	Automated Strategies To Identify Compounds on the Basis of GC/EI-MS and Calculated Properties. Analytical Chemistry, 2011, 83, 903-912.	3.2	33
43	Small Molecule Identification with MOLGEN and Mass Spectrometry. Metabolites, 2013, 3, 440-462.	1.3	32
44	Application of preparative capillary gas chromatography (pcGC), automated structure generation and mutagenicity prediction to improve effect-directed analysis of genotoxicants in a contaminated groundwater. Environmental Science and Pollution Research, 2010, 17, 885-897.	2.7	31
45	CASMI: And the Winner is . . .. Metabolites, 2013, 3, 412-439.	1.3	30
46	The Next Frontier of Environmental Unknowns: Substances of Unknown or Variable Composition, Complex Reaction Products, or Biological Materials (UVCBs). Environmental Science & Technology, 2022, 56, 7448-7466.	4.6	29
47	Exploring open cheminformatics approaches for categorizing per- and polyfluoroalkyl substances (PFASs). Environmental Sciences: Processes and Impacts, 2019, 21, 1835-1851.	1.7	25
48	Multicriteria Approach To Select Polyaromatic River Mutagen Candidates. Environmental Science & Technology, 2015, 49, 2959-2968.	4.6	24
49	Annotating Nontargeted LC-HRMS/MS Data with Two Complementary Tandem Mass Spectral Libraries. Metabolites, 2019, 9, 3.	1.3	24
50	Integrated biologicalâ€“chemical approach for the isolation and selection of polyaromatic mutagens in surface waters. Analytical and Bioanalytical Chemistry, 2013, 405, 9101-9112.	1.9	21
51	Evaluation of reverse osmosis drinking water treatment of riverbank filtrate using bioanalytical tools and non-target screening. Environmental Science: Water Research and Technology, 2020, 6, 103-116.	1.2	21
52	Discovering pesticides and their TPs in Luxembourg waters using open cheminformatics approaches. Environment International, 2022, 158, 106885.	4.8	21
53	FAIR chemical structures in the Journal of Cheminformatics. Journal of Cheminformatics, 2021, 13, 50.	2.8	19
54	Retrospective non-target analysis to support regulatory water monitoring: from masses of interest to recommendations via in silico workflows. Environmental Sciences Europe, 2021, 33, .	2.6	18

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55	Solving CASMI 2013 with MetFrag, MetFusion and MOLGEN-MS/MS. Mass Spectrometry, 2014, 3, S0036-S0036.	0.2	16
56	Exploring the Behaviour of Emerging Contaminants in the Water Cycle using the Capabilities of High Resolution Mass Spectrometry. Chimia, 2014, 68, 793.	0.3	15
57	Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. Analytical and Bioanalytical Chemistry, 2019, 411, 4683-4700.	1.9	14
58	Connecting environmental exposure and neurodegeneration using cheminformatics and high resolution mass spectrometry: potential and challenges. Environmental Sciences: Processes and Impacts, 2019, 21, 1426-1445.	1.7	13
59	Occurrence and Distribution of Pharmaceuticals and Their Transformation Products in Luxembourgish Surface Waters. ACS Environmental Au, 2021, 1, 58-70.	3.3	13
60	Studying the Parkinsonâ€™s disease metabolome and exposome in biological samples through different analytical and cheminformatics approaches: a pilot study. Analytical and Bioanalytical Chemistry, 2022, 414, 7399-7419.	1.9	12
61	Historical exposomics and high resolution mass spectrometry. Exposome, 2021, 1, .	1.2	11
62	Extraction of chemical structures from literature and patent documents using open access chemistry toolkits: a case study with PFAS. , 2022, 1, 490-501.		11
63	patRoon 2.0: Improved non-target analysis workflows including automated transformation product screening. Journal of Open Source Software, 2022, 7, 4029.	2.0	10
64	FAIRifying the exposome journal: Templates for chemical structures and transformations. Exposome, 2022, 2, .	1.2	10
65	Studying Charge Migration Fragmentation of Sodiated Precursor Ions in Collision-Induced Dissociation at the Library Scale. Journal of the American Society for Mass Spectrometry, 2021, 32, 180-186.	1.2	4
66	Development and Application of an LC-MS/MS Untargeted Exposomics Method with a Separated Pooled Quality Control Strategy. Molecules, 2022, 27, 2580.	1.7	4
67	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3