Judith C Madden

List of Publications by Year in Descending Order

46 papers	882 citations	20 h-index	28 g-index
64 ext. papers	1,064 ext. citations	4.1 avg, IF	4.54 L-index

#	Paper	IF	Citations
46	A review of in silico toxicology approaches to support the safety assessment of cosmetics-related materials. *Computational Toxicology*, **2022**, 21, 100213	3.1	1
45	A matter of trust: Learning lessons about causality will make qAOPs credible.. *Computational Toxicology*, **2022**, 21, 100205	3.1	1
44	Pharmacokinetic Tools and Applications.. *Methods in Molecular Biology*, **2022**, 2425, 57-83	1.4	
43	Probabilistic modelling of developmental neurotoxicity based on a simplified adverse outcome pathway network.. *Computational Toxicology*, **2022**, 21, 100206	3.1	1
42	A Systematic Review of Published Physiologically-based Kinetic Models and an Assessment of their Chemical Space Coverage. *ATLA Alternatives To Laboratory Animals*, **2021**, 49, 197-208	2.1	2
41	Assessment of the predictive capacity of a physiologically based kinetic model using a read-across approach. *Computational Toxicology*, **2021**, 18, 100159	3.1	5
40	Determination of "fitness-for-purpose" of quantitative structure-activity relationship (QSAR) models to predict (eco-)toxicological endpoints for regulatory use. *Regulatory Toxicology and Pharmacology*, **2021**, 123, 104956	3.4	3
39	A mechanistic model to study the kinetics and toxicity of salicylic acid in the kidney of four virtual individuals. *Computational Toxicology*, **2021**, 19, 100172	3.1	2
38	Quantitative adverse outcome pathway (qAOP) models for toxicity prediction. *Archives of Toxicology*, **2020**, 94, 1497-1510	5.8	38
37	Key read across framework components and biology based improvements. *Mutation Research - Genetic Toxicology and Environmental Mutagenesis*, **2020**, 853, 503172	3	9
36	A Review of Tools as Alternatives to Animal Testing: Principles, Resources and Applications. *ATLA Alternatives To Laboratory Animals*, **2020**, 48, 146-172	2.1	37
35	Development of Baseline Quantitative Structure-Activity Relationships (QSARs) for the Effects of Active Pharmaceutical Ingredients (APIs) to Aquatic Species. *Methods in Pharmacology and Toxicology*, **2020**, 331-356	1.1	1
34	Development and analysis of an adverse outcome pathway network for human neurotoxicity. *Archives of Toxicology*, **2019**, 93, 2759-2772	5.8	33
33	Predicting protein-ligand binding affinity and correcting crystal structures with quantum mechanical calculations: lactate dehydrogenase A. *Chemical Science*, **2019**, 10, 2218-2227	9.4	7
32	Unlocking the potential of chemical safety assessment - A report on a cross-sector symposium on current opportunities and future challenges. *Computational Toxicology*, **2019**, 10, 38-43	3.1	16
31	In silico resources to assist in the development and evaluation of physiologically-based kinetic models. *Computational Toxicology*, **2019**, 11, 33-49	3.1	28
30	Toxicology Data Resources to Support Read-Across and (Q)SAR. *Frontiers in Pharmacology*, **2019**, 10, 561	5.6	38

29	Advances in the prediction of gastrointestinal absorption: Quantitative Structure-Activity Relationship (QSAR) modelling of PAMPA permeability. *Computational Toxicology*, **2019**, 10, 51-59	3.1	7
28	Assessment and Reproducibility of Quantitative Structure-Activity Relationship Models by the Nonexpert. *Journal of Chemical Information and Modeling*, **2018**, 58, 673-682	6.1	25
27	A critical review of adverse effects to the kidney: mechanisms, data sources, and in silico tools to assist prediction. *Expert Opinion on Drug Metabolism and Toxicology*, **2018**, 14, 1225-1253	5.5	5
26	Validation of a Fragment-Based Profiler for Thiol Reactivity for the Prediction of Toxicity: Skin Sensitization and Tetrahymena pyriformis. *Chemical Research in Toxicology*, **2017**, 30, 604-613	4	3
25	Turbocharging Matched Molecular Pair Analysis: Optimizing the Identification and Analysis of Pairs. *Journal of Chemical Information and Modeling*, **2017**, 57, 2424-2436	6.1	9
24	Prediction of Organ Level Toxicity: Linking Chemistry to Adverse Effects. *Toxicological Research*, **2017**, 33, 173-182	3.7	20
23	Linking existing in vitro dermal absorption data to physicochemical properties: Contribution to the design of a weight-of-evidence approach for the safety evaluation of cosmetic ingredients with low dermal bioavailability. *Regulatory Toxicology and Pharmacology*, **2016**, 76, 74-8	3.4	20
22	Adverse Outcome Pathway (AOP) Informed Modeling of Aquatic Toxicology: QSARs, Read-Across, and Interspecies Verification of Modes of Action. *Environmental Science & Technology*, **2016**, 50, 3995-4007	10.3	34
21	Development of a Fragment-Based in Silico Profiler for Michael Addition Thiol Reactivity. *Chemical Research in Toxicology*, **2016**, 29, 1073-81	4	12
20	Investigation of Critical Body Residues and Modes of Toxic Action Based on Injection and Aquatic Exposure in Fish. *Water, Air, and Soil Pollution*, **2015**, 226, 1	2.6	11
19	Development of computational models for the prediction of the toxicity of nanomaterials. *Perspectives in Science*, **2015**, 3, 27-29	0.8	17
18	Ensuring confidence in predictions: A scheme to assess the scientific validity of in silico models. *Advanced Drug Delivery Reviews*, **2015**, 86, 101-11	18.5	13
17	Development of an in Silico Profiler for Mitochondrial Toxicity. *Chemical Research in Toxicology*, **2015**, 28, 1891-902	4	36
16	Data Quality in the Human and Environmental Health Sciences: Using Statistical Confidence Scoring to Improve QSAR/QSPR Modeling. *Journal of Chemical Information and Modeling*, **2015**, 55, 1739-46	6.1	10
15	Investigation of the Verhaar scheme for predicting acute aquatic toxicity: improving predictions obtained from Toxtree ver. 2.6. *Chemosphere*, **2015**, 139, 146-54	8.4	31
14	Methods for assigning confidence to toxicity data with multiple values--Identifying experimental outliers. *Science of the Total Environment*, **2014**, 482-483, 358-65	10.2	13
13	Comparative metabolism as a key driver of wildlife species sensitivity to human and veterinary pharmaceuticals. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2014**, 369,	5.8	42
12	Development of an in silico profiler for respiratory sensitisation. *ATLA Alternatives To Laboratory Animals*, **2014**, 42, 367-75	2.1	8

11	Application of in silico and in vitro methods in the development of adverse outcome pathway constructs in wildlife. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2014**, 369,	5.8	20
10	Towards a Fuzzy Expert System on Toxicological Data Quality Assessment. *Molecular Informatics*, **2013**, 32, 65-78	3.8	22
9	Strategies for the optimisation of in vivo experiments in accordance with the 3Rs philosophy. *Regulatory Toxicology and Pharmacology*, **2012**, 63, 140-54	3.4	24
8	Robustness of an Immobilized Artificial Membrane High-Performance Liquid Chromatography Method for the Determination of Lipophilicity. *Journal of Chemical & Engineering Data*, **2012**, 57, 3696-3700	2.8	4
7	In Silico Approaches for Predicting Adme Properties. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 283-304	0.7	19
6	Using In Silico Tools in a Weight of Evidence Approach to Aid Toxicological Assessment. *Molecular Informatics*, **2010**, 29, 97-110	3.8	24
5	Pharmaceuticals in the environment: good practice in predicting acute ecotoxicological effects. *Toxicology Letters*, **2009**, 185, 85-101	4.4	70
4	StudentsUresponse to traditional and computer-assisted formative feedback: A comparative case study. *British Journal of Educational Technology*, **2008**, 39, 486-500	4.3	59
3	Formation of categories from structure-activity relationships to allow read-across for risk assessment: toxicity of alpha,beta-unsaturated carbonyl compounds. *Chemical Research in Toxicology*, **2008**, 21, 2300-12	4	65
2	Structure-based methods for the prediction of drug metabolism. *Expert Opinion on Drug Metabolism and Toxicology*, **2006**, 2, 545-57	5.5	30
1	(Q)SAR Models of Adverse Responses: Acute Systemic Toxicity299-314		