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List of Publications by Year in descending order

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759233 794594 19 635 12 19 citations h-index g-index papers 21 21 21 677 docs citations times ranked citing authors all docs

#	Article	IF	Citations
1	Increasing the acceptance of in silico toxicology through development of protocols and position papers. Computational Toxicology, 2022, 21, 100209.	3.3	7
2	A cross-industry collaboration to assess if acute oral toxicity (Q)SAR models are fit-for-purpose for GHS classification and labelling. Regulatory Toxicology and Pharmacology, 2021, 120, 104843.	2.7	12
3	Management of pharmaceutical ICH M7 (Q)SAR predictions – The impact of model updates. Regulatory Toxicology and Pharmacology, 2020, 118, 104807.	2.7	15
4	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	2.7	27
5	Genetic toxicology in silico protocol. Regulatory Toxicology and Pharmacology, 2019, 107, 104403.	2.7	57
6	Extending (Q)SARs to incorporate proprietary knowledge for regulatory purposes: is aromatic <i>N</i> -oxide a structural alert for predicting DNA-reactive mutagenicity?*. Mutagenesis, 2019, 34, 67-82.	2.6	13
7	Principles and procedures for handling out-of-domain and indeterminate results as part of ICH M7 recommended (Q)SAR analyses. Regulatory Toxicology and Pharmacology, 2019, 102, 53-64.	2.7	21
8	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	2.7	159
9	Computational Toxicology and Drug Discovery. Methods in Molecular Biology, 2018, 1800, 233-244.	0.9	15
10	Principles and procedures for implementation of ICH M7 recommended (Q)SAR analyses. Regulatory Toxicology and Pharmacology, 2016, 77, 13-24.	2.7	83
11	Interpretation of Conformal Prediction Classification Models. Lecture Notes in Computer Science, 2015, , 323-334.	1.3	5
12	A critical assessment of modeling safety-related drug attrition. MedChemComm, 2013, 4, 1058.	3.4	34
13	Localized Heuristic Inverse Quantitative Structure Activity Relationship with Bulk Descriptors Using Numerical Gradients. Journal of Chemical Information and Modeling, 2013, 53, 2001-2017.	5.4	9
14	In silico methods combined with expert knowledge rule out mutagenic potential of pharmaceutical impurities: An industry survey. Regulatory Toxicology and Pharmacology, 2012, 62, 449-455.	2.7	75
15	Three-Coordinate [CullX3]â^' (X=Cl, Br), Trapped in a Molecular Crystal. Chemistry - A European Journal, 2002, 8, 1269-1278.	3.3	40
16	Halocuprates(I) crystallising with the Ph3PNPPh3+ cation: preparation and structural characterisation of (Ph3PNPPh3)2[Cu4Br6] and (Ph3PNPPh3)[CuBrCl]. Inorganica Chimica Acta, 2002, 336, 137-141.	2.4	9
17	Supramolecular Assemblies of Quaternary Ammonium Cations and Halide Anions in the Gas Phase: ESMS-FTICR Data and Computer Modelling. Chemistry - A European Journal, 2000, 6, 3671-3678.	3.3	9
18	On tuning the copper(I) coordination number in halocuprate(I) anions: new insights into cation control. Inorganica Chimica Acta, 1999, 292, 266-271.	2.4	19

#	Article	lF	CITATIONS
19	Dominant cation–cation supramolecular motifs in crystals. Hexagonal arrays of sextuple phenyl embraces in halometalate salts of MePh3P+. Journal of the Chemical Society Dalton Transactions, 1997, , 2019-2028.	1.1	20