Catrin Hasselgren

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	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	2.7	159
2	Principles and procedures for implementation of ICH M7 recommended (Q)SAR analyses. Regulatory Toxicology and Pharmacology, 2016, 77, 13-24.	2.7	83
3	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	7 5
4	Genetic toxicology in silico protocol. Regulatory Toxicology and Pharmacology, 2019, 107, 104403.	2.7	57
5	Three-Coordinate [CullX3]â^' (X=Cl, Br), Trapped in a Molecular Crystal. Chemistry - A European Journal, 2002, 8, 1269-1278.	3.3	40
6	A critical assessment of modeling safety-related drug attrition. MedChemComm, 2013, 4, 1058.	3.4	34
7	Skin sensitization in silico protocol. Regulatory Toxicology and Pharmacology, 2020, 116, 104688.	2.7	27
8	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
9	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
10	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
11	Computational Toxicology and Drug Discovery. Methods in Molecular Biology, 2018, 1800, 233-244.	0.9	15
12	Management of pharmaceutical ICH M7 (Q)SAR predictions – The impact of model updates. Regulatory Toxicology and Pharmacology, 2020, 118, 104807.	2.7	15
13	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
14	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
15	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
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	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
18	Increasing the acceptance of in silico toxicology through development of protocols and position papers. Computational Toxicology, 2022, 21, 100209.	3.3	7

#	Article	lF	CITATIONS
19	Interpretation of Conformal Prediction Classification Models. Lecture Notes in Computer Science, 2015, , 323-334.	1.3	5