Alex M Clark

List of Publications by Year
in descending order

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Version: 2024-02-01

53 papers	2,237 citations	218381 26 h-index	233125 45 g-index
60 all docs	60 docs citations	60 times ranked	2279 citing authors

#	Article	IF	Citations
1	Exploiting machine learning for end-to-end drug discovery and development. Nature Materials, 2019, 18, 435-441.	13.3	334
2	2D Depiction of Proteinâ"Ligand Complexes. Journal of Chemical Information and Modeling, 2007, 47, 1933-1944.	2.5	137
3	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. Molecular Pharmaceutics, 2018, 15, 4361-4370.	2.3	120
4	Open Source Bayesian Models. 1. Application to ADME/Tox and Drug Discovery Datasets. Journal of Chemical Information and Modeling, 2015, 55, 1231-1245.	2.5	95
5	Electrophilic Substitution Reactions at the Phenyl Ring of the Chelated 2-(2â€˜-Pyridyl)phenyl Ligand Bound to Ruthenium(II) or Osmium(II). Organometallics, 1999, 18, 2813-2820.	1.1	93
6	Comparing and Validating Machine Learning Models for Mycobacterium tuberculosis Drug Discovery. Molecular Pharmaceutics, 2018, 15, 4346-4360.	2.3	83
7	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 2015, 4, 1091.	0.8	80
8	Assessment of Substrate-Dependent Ligand Interactions at the Organic Cation Transporter OCT2 Using Six Model Substrates. Molecular Pharmacology, 2018, 94, 1057-1068.	1.0	77
9	Open Source Bayesian Models. 2. Mining a â€œBig Datasetâ€•To Create and Validate Models with ChEMBL. Journal of Chemical Information and Modeling, 2015, 55, 1246-1260.	2.5	73
10	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
11	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 2015, 4, 1091.	0.8	56
12	2D Structure Depiction. Journal of Chemical Information and Modeling, 2006, 46, 1107-1123.	2.5	53
13	Ebola Virus Bayesian Machine Learning Models Enable New in Vitro Leads. ACS Omega, 2019, 4, 2353-2361.	1.6	49
14	Multiple Machine Learning Comparisons of HIV Cell-based and Reverse Transcriptase Data Sets. Molecular Pharmaceutics, 2019, 16, 1620-1632.	2.3	49
15	Bromination and nitration reactions of metallated (Ru and Os) multiaromatic ligands and crystal structures of selected products. Journal of Organometallic Chemistry, 2000, 598, 262-275.	0.8	48
16	Flexible 3D pharmacophores as descriptors of dynamic biological space. Journal of Molecular Graphics and Modelling, 2007, 26, 622-633.	1.3	47
17	Detection and Assignment of Common Scaffolds in Project Databases of Lead Molecules. Journal of Medicinal Chemistry, 2009, 52, 469-483.	2.9	45
18	Mobile apps for chemistry in the world of drug discovery. Drug Discovery Today, 2011, 16, 928-939.	3.2	44

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19	Looking Back to the Future: Predicting in Vivo Efficacy of Small Molecules versus Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2014, 54, 1070-1082.	2.5	41
20	Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses. ACS Sustainable Chemistry and Engineering, 2013, 1, 8-13.	3.2	39
21	Stepwise Conversion of an Osmium Trimethylstannyl Complex to a Triiodostannyl Complex and Nucleophilic Substitution Reactions at the Tinâ^'Iodine Bonds. Organometallics, 2000, 19, 1766-1774.	1.1	34
22	Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration. Molecular Informatics, 2012, 31, 585-597.	1.4	32
23	Four disruptive strategies for removing drug discovery bottlenecks. Drug Discovery Today, 2013, 18, 265-271.	3.2	32
24	New target prediction and visualization tools incorporating open source molecular fingerprints for TB Mobile 2.0. Journal of Cheminformatics, 2014, 6, 38.	2.8	32
25	High-throughput screening and Bayesian machine learning for copper-dependent inhibitors of Staphylococcus aureus. Metallomics, 2019, 11, 696-706.	1.0	30
26	TB Mobile: a mobile app for anti-tuberculosis molecules with known targets. Journal of Cheminformatics, 2013, 5, 13.	2.8	29
27	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
28	Parallel Worlds of Public and Commercial Bioactive Chemistry Data. Journal of Medicinal Chemistry, 2015, 58, 2068-2076.	2.9	28
29	Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data. Journal of Cheminformatics, 2015, 7, 9.	2.8	26
30	Redefining Cheminformatics with Intuitive Collaborative Mobile Apps. Molecular Informatics, 2012, 31, 569-584.	1.4	25
31	Machine Learning Model Analysis and Data Visualization with Small Molecules Tested in a Mouse Model of Mycobacterium tuberculosis Infection (2014â€“2015). Journal of Chemical Information and Modeling, 2016, 56, 1332-1343.	2.5	23
32	5-Bromination of an Î·2-8-Quinolyl Ligand Bound to Osmium(II) and Subsequent Lithiation and Derivatization of This Functionalized Ligand1. Organometallics, 1998, 17, 4535-4537.	1.1	22
33	Accurate Specification of Molecular Structures: The Case for Zero-Order Bonds and Explicit Hydrogen Counting. Journal of Chemical Information and Modeling, 2011, 51, 3149-3157.	2.5	22
34	Bigger data, collaborative tools and the future of predictive drug discovery. Journal of Computer-Aided Molecular Design, 2014, 28, 997-1008.	1.3	22
35	Cyclometallated complexes of ruthenium and osmium containing the o-C6H4PPh2 ligand. Journal of Organometallic Chemistry, 2000, 601, 299-304.	0.8	20
36	The origin of the â€˜spikeâ€™ in the EPR spectrum of C60â^'. Chemical Communications, 2000, , 1229-1230.	2.2	20

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37	Basic primitives for molecular diagram sketching. Journal of Cheminformatics, 2010, 2, 8.	2.8	19
38	2D Depiction of Fragment Hierarchies. Journal of Chemical Information and Modeling, 2010, 50, 37-46.	2.5	16
39	Osmium complexes containing either chelating or non-chelating 8-quinolyl ligands. Journal of Organometallic Chemistry, 1997, 545-546, 619-622.	0.8	15
40	Machine learning models identify molecules active against the Ebola virus in vitro. F1000Research, 0, 4, 1091.	0.8	14
41	Open Source Bayesian Models. 3. Composite Models for Prediction of Binned Responses. Journal of Chemical Information and Modeling, 2016, 56, 275-285.	2.5	14
42	Capturing mixture composition: an open machine-readable format for representing mixed substances. Journal of Cheminformatics, 2019, 11, 33.	2.8	14
43	Fast and accurate semantic annotation of bioassays exploiting a hybrid of machine learning and user confirmation. PeerJ, 2014, 2, e524.	0.9	14
44	Making Transporter Models for Drugâ€“Drug Interaction Prediction Mobile. Drug Metabolism and Disposition, 2015, 43, 1642-1645.	1.7	13
45	Collaborative drug discovery for More Medicines for Tuberculosis (MM4TB). Drug Discovery Today, 2017, 22, 555-565.	3.2	12
46	Cheminformatics workflows using mobile apps. Chem-Bio Informatics Journal, 2013, 13, 1-18.	0.1	12
47	Osmium nitrosyl complexes with osmium-tin bonds crystal structure of Os[Sn(p-tolyl)3](NO)(CO)2(PPh3). Journal of Organometallic Chemistry, 1997, 543, 111-116.	0.8	11
48	Rendering Molecular Sketches for Publication Quality Output. Molecular Informatics, 2013, 32, 291-301.	1.4	7
49	Data Mining and Computational Modeling of High-Throughput Screening Datasets. Methods in Molecular Biology, 2018, 1755, 197-221.	0.4	7
50	BioAssay Templates for the semantic web. PeerJ Computer Science, 0, 2, e61.	2.7	6
51	Using Machine Learning to Parse Chemical Mixture Descriptions. ACS Omega, 2021, 6, 22400-22409.	1.6	2
52	Cheminformatics: Mobile Workflows and Data Sources. ACS Symposium Series, 2014, , 237-253.	0.5	1
53	The Need for a Green Electronic Lab Notebook. RSC Drug Discovery Series, 2015, , 185-211.	0.2	1