Daniel Reker

List of Publications by Year
in descending order

40 papers	2,649 citations	236612 25 h-index	243296 44 g-index
47 all docs	47 docs citations	47 times ranked	3559 citing authors

#	Article	IF	Citations
1	Oral mRNA delivery using capsule-mediated gastrointestinal tissue injections. Matter, 2022, 5, 975-987.	5.0	48
2	Computationally guided high-throughput design of self-assembling drug nanoparticles. Nature Nanotechnology, 2021, 16, 725-733.	15.6	64
3	Combating small-molecule aggregation with machine learning. Cell Reports Physical Science, 2021, 2, 100573.	2.8	11
4	Adaptive Optimization of Chemical Reactions with Minimal Experimental Information. Cell Reports Physical Science, 2020, 1, 100247.	2.8	42
5	Historical Evolution and Provider Awareness of Inactive Ingredients in Oral Medications. Pharmaceutical Research, 2020, 37, 234.	1.7	0
6	Artificial intelligence in chemistry and drug design. Journal of Computer-Aided Molecular Design, 2020, 34, 709-715.	1.3	79
7	Machine Learning Uncovers Food- and Excipient-Drug Interactions. Cell Reports, 2020, 30, 3710-3716.e4.	2.9	37
8	Robotically handled whole-tissue culture system for the screening of oral drug formulations. Nature Biomedical Engineering, 2020, 4, 544-559.	11.6	35
9	Predicting protein-ligand interactions based on bow-pharmacological space and Bayesian additive regression trees. Scientific Reports, 2019, 9, 7703.	1.6	37
10	Computational advances in combating colloidal aggregation in drug discovery. Nature Chemistry, 2019, 11, 402-418.	6.6	51
11	â€œInactiveâ€•ingredients in oral medications. Science Translational Medicine, 2019, 11, .	5.8	68
12	Practical considerations for active machine learning in drug discovery. Drug Discovery Today: Technologies, 2019, 32-33, 73-79.	4.0	46
13	Advanced Editorial to announce a JCAMD Special Issue on Artificial Intelligence and Machine Learning. Journal of Computer-Aided Molecular Design, 2019, 33, 941-941.	1.3	0
14	Cheminformatic Analysis of Natural Product Fragments. Progress in the Chemistry of Organic Natural Products, 2019, 110, 143-175.	0.8	1
15	Selection of Informative Examples in Chemogenomic Datasets. Methods in Molecular Biology, 2018, 1825, 369-410.	0.4	9
16	Active learning for computational chemogenomics. Future Medicinal Chemistry, 2017, 9, 381-402.	1.1	75
17	Matrixâ€based Molecular Descriptors for Prospective Virtual Compound Screening. Molecular Informatics, 2017, 36, 1600091.	1.4	18
18	Small Random Forest Models for Effective Chemogenomic Active Learning. Journal of Computer Aided Chemistry, 2017, 18, 124-142.	0.3	14

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19	New use of an old drug: inhibition of breast cancer stem cells by benztropine mesylate. Oncotarget, 2017, 8, 1007-1022.	0.8	22
20	Counting on natural products for drug design. Nature Chemistry, 2016, 8, 531-541.	6.6	879
21	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. Angewandte Chemie - International Edition, 2016, 55, 12408-12411.	7.2	31
22	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. Angewandte Chemie, 2016, 128, 12596-12599.	1.6	3
23	Multi-objective active machine learning rapidly improves structureâ€“activity models and reveals new proteinâ€“protein interaction inhibitors. Chemical Science, 2016, 7, 3919-3927.	3.7	55
24	Spotting and designing promiscuous ligands for drug discovery. Chemical Communications, 2016, 52, 1135-1138.	2.2	33
25	De Novo Fragment Design for Drug Discovery and Chemical Biology. Angewandte Chemie - International Edition, 2015, 54, 15079-15083.	7.2	30
26	Fragmentâ€Based Deâ€...Novo Design Reveals a Smallâ€Molecule Inhibitor of Helicobacter Pylori HtrA. Angewandte Chemie - International Edition, 2015, 54, 10244-10248.	7.2	37
27	Revealing the Macromolecular Targets of Fragmentâ€Like Natural Products. Angewandte Chemie - International Edition, 2015, 54, 10516-10520.	7.2	54
28	Multidimensional Deâ€...Novo Design Reveals 5â€HT_{2B} Receptorâ€Selective Ligands. Angewandte Chemie - International Edition, 2015, 54, 1551-1555.	7.2	39
29	Chemography of Natural Product Space. Planta Medica, 2015, 81, 429-435.	0.7	23
30	Active-learning strategies in computer-assisted drug discovery. Drug Discovery Today, 2015, 20, 458-465.	3.2	169
31	Coping with Polypharmacology by Computational Medicinal Chemistry. Chimia, 2014, 68, 648.	0.3	6
32	Identifying the macromolecular targets of de novo-designed chemical entities through self-organizing map consensus. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 4067-4072.	3.3	196
33	Revealing the macromolecular targets of complex natural products. Nature Chemistry, 2014, 6, 1072-1078.	6.6	114
34	Target prediction by cascaded self-organizing maps for ligand de-orphaning and side-effect investigation. Journal of Cheminformatics, 2014, 6, .	2.8	1
35	Deorphaning Pyrrolopyrazines as Potent Multiâ€Target Antimalarial Agents. Angewandte Chemie - International Edition, 2014, 53, 7079-7084.	7.2	30
36	Common non-epigenetic drugs as epigenetic modulators. Trends in Molecular Medicine, 2013, 19, 742-753.	3.5	68

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37	De novo design and optimization of Aurora A kinase inhibitors. Chemical Science, 2013, 4, 1229.	3.7	23
38	Chemically Advanced Template Search (CATS) for Scaffoldâ€Hopping and Prospective Target Prediction for â€˜Orphanâ€™ Molecules. Molecular Informatics, 2013, 32, 133-138.	1.4	132
39	Bioinformatic Challenges in Targeted Proteomics. Journal of Proteome Research, 2012, 11, 4393-4402.	1.8	20
40	Computation of mutual information from Hidden Markov Models. Computational Biology and Chemistry, 2010, 34, 328-333.	1.1	4