Ansgar Schuffenhauer

List of Publications by Year
in descending order

49 papers	4,355 citations	172457 29 h-index	197818 49 g-index
60 all docs	60 docs citations	60 times ranked	3726 citing authors

#	Article	IF	Citations
1	Splitting chemical structure data sets for federated privacy-preserving machine learning. Journal of Cheminformatics, 2021, 13, 96.	6.1	16
2	Discovery of Potent, Highly Selective, and In Vivo Efficacious, Allosteric MALT1 Inhibitors by Iterative Scaffold Morphing. Journal of Medicinal Chemistry, 2020, 63, 14576-14593.	6.4	17
3	Systematic Chemogenetic Library Assembly. Cell Chemical Biology, 2020, 27, 1124-1129.	5.2	37
4	Evolution of Novartisâ€™ Small Molecule Screening Deck Design. Journal of Medicinal Chemistry, 2020, 63, 14425-14447.	6.4	31
5	N-aryl-piperidine-4-carboxamides as a novel class of potent inhibitors of MALT1 proteolytic activity. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 2153-2158.	2.2	19
6	Identification of SPPL2a Inhibitors by Multiparametric Analysis of a High-Content Ultra-High-Throughput Screen. SLAS Discovery, 2017, 22, 1106-1119.	2.7	10
7	High-Throughput Screening Using iPSC-Derived Neuronal Progenitors to Identify Compounds Counteracting Epigenetic Gene Silencing in Fragile X Syndrome. Journal of Biomolecular Screening, 2015, 20, 1101-1111.	2.6	78
8	Dark chemical matter as a promising starting point for drug lead discovery. Nature Chemical Biology, 2015, 11, 958-966.	8.0	110
9	Glucocorticoid Receptor Ligands ModulateCardiovirus encephalomyocarditis virusInternal Ribosome Entry Site Activity. Assay and Drug Development Technologies, 2013, 11, 355-366.	1.2	0
10	Identification of Cardiac Glycoside Molecules as Inhibitors of c-Myc IRES-Mediated Translation. Journal of Biomolecular Screening, 2013, 18, 407-419.	2.6	26
11	Latent Hit Series Hidden in High-Throughput Screening Data. Journal of Medicinal Chemistry, 2012, 55, 1161-1170.	6.4	16
12	Computational methods for scaffold hopping. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 842-867.	14.6	20
13	MultiMCS: A Fast Algorithm for the Maximum Common Substructure Problem on Multiple Molecules. Journal of Chemical Information and Modeling, 2011, 51, 788-806.	5.4	31
14	Mining for Bioactive Scaffolds with Scaffold Networks: Improved Compound Set Enrichment from Primary Screening Data. Journal of Chemical Information and Modeling, 2011, 51, 1528-1538.	5.4	70
15	Ruleâ€Based Classification of Chemical Structures by Scaffold. Molecular Informatics, 2011, 30, 646-664.	2.5	25
16	Recent trends and observations in the design of high-quality screening collections. Future Medicinal Chemistry, 2011, 3, 751-766.	2.3	55
17	The Scaffold Tree: An Efficient Navigation in the Scaffold Universe. Methods in Molecular Biology, 2010, 672, 245-260.	0.9	21
18	Compound Set Enrichment: A Novel Approach to Analysis of Primary HTS Data. Journal of Chemical Information and Modeling, 2010, 50, 2067-2078.	5.4	48

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19	Bioactivity-guided mapping and navigation of chemical space. Nature Chemical Biology, 2009, 5, 585-592.	8.0	129
20	Natural Product-likeness Score and Its Application for Prioritization of Compound Libraries. Journal of Chemical Information and Modeling, 2008, 48, 68-74.	5.4	271
21	Cheminformatic Analysis of Natural Products and their Chemical Space. Chimia, 2007, 61, 355-360.	0.6	109
22	The Scaffold Tree â˜' Visualization of the Scaffold Universe by Hierarchical Scaffold Classification. Journal of Chemical Information and Modeling, 2007, 47, 47-58.	5.4	322
23	Clustering and Rule-Based Classifications of Chemical Structures Evaluated in the Biological Activity Space. Journal of Chemical Information and Modeling, 2007, 47, 325-336.	5.4	50
24	Introducing the Consensus Modeling Concept in Genetic Algorithms:â€‰ Application to Interpretable Discriminant Analysis. Journal of Chemical Information and Modeling, 2006, 46, 2110-2124.	5.4	18
25	New Methods for Ligand-Based Virtual Screening:Â Use of Data Fusion and Machine Learning to Enhance the Effectiveness of Similarity Searching. Journal of Chemical Information and Modeling, 2006, 46, 462-470.	5.4	202
26	Chemical diversity and biological activity. Drug Discovery Today: Technologies, 2006, 3, 387-395.	4.0	18
27	Quest for the Rings. In Silico Exploration of Ring Universe To Identify Novel Bioactive Heteroaromatic Scaffolds. Journal of Medicinal Chemistry, 2006, 49, 4568-4573.	6.4	221
28	Relationships between Molecular Complexity, Biological Activity, and Structural Diversity. Journal of Chemical Information and Modeling, 2006, 46, 525-535.	5.4	88
29	A Chemoinformatics Analysis of Hit Lists Obtained from High-Throughput Affinity-Selection Screening. Journal of Biomolecular Screening, 2006, 11, 123-130.	2.6	33
30	Complex molecules: do they add value?. Current Opinion in Chemical Biology, 2005, 9, 310-316.	6.1	69
31	Library Design for Fragment Based Screening. Current Topics in Medicinal Chemistry, 2005, 5, 751-762.	2.1	195
32	Key Aspects of the Novartis Compound Collection Enhancement Project for the Compilation of a Comprehensive Chemogenomics Drug Discovery Screening Collection. Current Topics in Medicinal Chemistry, 2005, 5, 397-411.	2.1	81
33	Charting biologically relevant chemical space: A structural classification of natural products (SCONP). Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 17272-17277.	7.1	534
34	Enhancing the Effectiveness of Similarity-Based Virtual Screening Using Nearest-Neighbor Information. Journal of Medicinal Chemistry, 2005, 48, 7049-7054.	6.4	79
35	Comparison of topological descriptors for similarity-based virtual screening using multiple bioactive reference structures. Organic and Biomolecular Chemistry, 2004, 2, 3256.	2.8	242
36	Comparison of Fingerprint-Based Methods for Virtual Screening Using Multiple Bioactive Reference Structures. Journal of Chemical Information and Computer Sciences, 2004, 44, 1177-1185.	2.8	300

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37	Annotating and mining the ligand-target chemogenomics knowledge space. Drug Discovery Today Biosilico, 2004, 2, 190-200.	0.7	25
38	Molecular Informatics as an Enabling<I> in silico</I> Technology Platform for Drug Discovery. Chimia, 2004, 58, 577-584.	0.6	3
39	Similarity Metrics for Ligands Reflecting the Similarity of the Target Proteins. Journal of Chemical Information and Computer Sciences, 2003, 43, 391-405.	2.8	257
40	Chemogenomics knowledge-based strategies in drug discovery. Drug News and Perspectives, 2003, 16, 93.	1.5	53
41	An Ontology for Pharmaceutical Ligands and Its Application for in Silico Screening and Library Design. Journal of Chemical Information and Computer Sciences, 2002, 42, 947-955.	2.8	104
42	Stereodivergent Synthesis of Highly Substituted Tetrahydropyrans. European Journal of Organic Chemistry, 2000, 2000, 73-82.	2.4	29
43	Similarity Searching in Files of Three-Dimensional Chemical Structures:â€‰ Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors. Journal of Chemical Information and Computer Sciences, 2000, 40, 295-307.	2.8	83
44	Enantioselective Synthesis of the Chromane Moiety of Vitamin E. European Journal of Organic Chemistry, 1999, 1999, 1075-1084.	2.4	26
45	Stereoselective Synthesis of Highly Substituted Piperidines. European Journal of Organic Chemistry, 1999, 1999, 3353-3362.	2.4	15
46	Synthesis of Tetrahydro- and Dihydropyridines by Hetero Diels-Alder Reactions of Enantiopure Î±,Î²-Unsaturated Sulfinimines. European Journal of Organic Chemistry, 1998, 1998, 1629-1637.	2.4	31
47	Stereoselective Intramolecular Hetero Dielsâ€“Alder Reactions of Cyclic Benzylidenesulfoxides and DFT Calculations on the Transition Structures. European Journal of Organic Chemistry, 1998, 1998, 2733-2741.	2.4	29
48	Conformations of Chiral Î±,Î²-Unsaturated Sulfoxides and Their Complexes with Lewis Acids. An ab Initio Study. Journal of the American Chemical Society, 1998, 120, 7952-7958.	13.7	77
49	Mechanistic Investigations on the Highly Stereoselective Allylation of Aldehydes with a Norpseudoephedrine Derivative. Journal of the American Chemical Society, 1998, 120, 4276-4280.	13.7	28