Ansgar Schuffenhauer

List of Publications by Year
in descending order

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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	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
2	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
3	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
4	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
5	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
6	Comparison of topological descriptors for similarity-based virtual screening using multiple bioactive reference structures. Organic and Biomolecular Chemistry, 2004, 2, 3256.	2.8	242
7	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
8	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
9	Library Design for Fragment Based Screening. Current Topics in Medicinal Chemistry, 2005, 5, 751-762.	2.1	195
10	Bioactivity-guided mapping and navigation of chemical space. Nature Chemical Biology, 2009, 5, 585-592.	8.0	129
11	Dark chemical matter as a promising starting point for drug lead discovery. Nature Chemical Biology, 2015, 11, 958-966.	8.0	110
12	Cheminformatic Analysis of Natural Products and their Chemical Space. Chimia, 2007, 61, 355-360.	0.6	109
13	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
14	Relationships between Molecular Complexity, Biological Activity, and Structural Diversity. Journal of Chemical Information and Modeling, 2006, 46, 525-535.	5.4	88
15	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
16	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
17	Enhancing the Effectiveness of Similarity-Based Virtual Screening Using Nearest-Neighbor Information. Journal of Medicinal Chemistry, 2005, 48, 7049-7054.	6.4	79
18	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

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19	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
20	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
21	Complex molecules: do they add value?. Current Opinion in Chemical Biology, 2005, 9, 310-316.	6.1	69
22	Recent trends and observations in the design of high-quality screening collections. Future Medicinal Chemistry, 2011, 3, 751-766.	2.3	55
23	Chemogenomics knowledge-based strategies in drug discovery. Drug News and Perspectives, 2003, 16, 93.	1.5	53
24	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
25	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
26	Systematic Chemogenetic Library Assembly. Cell Chemical Biology, 2020, 27, 1124-1129.	5.2	37
27	A Chemoinformatics Analysis of Hit Lists Obtained from High-Throughput Affinity-Selection Screening. Journal of Biomolecular Screening, 2006, 11, 123-130.	2.6	33
28	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
29	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
30	Evolution of Novartisâ€™ Small Molecule Screening Deck Design. Journal of Medicinal Chemistry, 2020, 63, 14425-14447.	6.4	31
31	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
32	Stereodivergent Synthesis of Highly Substituted Tetrahydropyrans. European Journal of Organic Chemistry, 2000, 2000, 73-82.	2.4	29
33	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
34	Enantioselective Synthesis of the Chromane Moiety of Vitamin E. European Journal of Organic Chemistry, 1999, 1999, 1075-1084.	2.4	26
35	Identification of Cardiac Glycoside Molecules as Inhibitors of c-Myc IRES-Mediated Translation. Journal of Biomolecular Screening, 2013, 18, 407-419.	2.6	26
36	Annotating and mining the ligand-target chemogenomics knowledge space. Drug Discovery Today Biosilico, 2004, 2, 190-200.	0.7	25

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37	Ruleâ€Based Classification of Chemical Structures by Scaffold. Molecular Informatics, 2011, 30, 646-664.	2.5	25
38	The Scaffold Tree: An Efficient Navigation in the Scaffold Universe. Methods in Molecular Biology, 2010, 672, 245-260.	0.9	21
39	Computational methods for scaffold hopping. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 842-867.	14.6	20
40	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
41	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
42	Chemical diversity and biological activity. Drug Discovery Today: Technologies, 2006, 3, 387-395.	4.0	18
43	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
44	Latent Hit Series Hidden in High-Throughput Screening Data. Journal of Medicinal Chemistry, 2012, 55, 1161-1170.	6.4	16
45	Splitting chemical structure data sets for federated privacy-preserving machine learning. Journal of Cheminformatics, 2021, 13, 96.	6.1	16
46	Stereoselective Synthesis of Highly Substituted Piperidines. European Journal of Organic Chemistry, 1999, 1999, 3353-3362.	2.4	15
47	Identification of SPPL2a Inhibitors by Multiparametric Analysis of a High-Content Ultra-High-Throughput Screen. SLAS Discovery, 2017, 22, 1106-1119.	2.7	10
48	Molecular Informatics as an Enabling<I> in silico</I> Technology Platform for Drug Discovery. Chimia, 2004, 58, 577-584.	0.6	3
49	Glucocorticoid Receptor Ligands ModulateCardiovirus encephalomyocarditis virusInternal Ribosome Entry Site Activity. Assay and Drug Development Technologies, 2013, 11, 355-366.	1.2	0