Nils Weskamp

List of Publications by Year
in descending order

15	694	759055 12	996849 15
papers	citations	h-index	g-index

17	17	17	641
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structureâ"Activity Relationship Anatomy by Network-like Similarity Graphs and Local Structureâ"Activity Relationship Indices. Journal of Medicinal Chemistry, 2008, 51, 6075-6084.	2.9	143
2	Clustering of gene expression data using a local shape-based similarity measure. Bioinformatics, 2005, 21, 1069-1077.	1.8	96
3	From the Similarity Analysis of Protein Cavities to the Functional Classification of Protein Families Using Cavbase. Journal of Molecular Biology, 2006, 359, 1023-1044.	2.0	89
4	Functional Classification of Protein Kinase Binding Sites Using Cavbase. ChemMedChem, 2007, 2, 1432-1447.	1.6	70
5	SAR Matrices: Automated Extraction of Information-Rich SAR Tables from Large Compound Data Sets. Journal of Chemical Information and Modeling, 2012, 52, 1769-1776.	2.5	49
6	Efficient similarity search in protein structure databases by k-clique hashing. Bioinformatics, 2004, 20, 1522-1526.	1.8	46
7	Coloring Molecules with Explainable Artificial Intelligence for Preclinical Relevance Assessment. Journal of Chemical Information and Modeling, 2021, 61, 1083-1094.	2.5	45
8	Strategies to search and design stabilizers of protein-protein interactions: A feasibility study. Proteins: Structure, Function and Bioinformatics, 2007, 68, 170-186.	1.5	38
9	Merging chemical and biological space: Structural mapping of enzyme binding pocket space. Proteins: Structure, Function and Bioinformatics, 2009, 76, 317-330.	1.5	38
10	Multiple Graph Alignment for the Structural Analysis of Protein Active Sites. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2007, 4, 310-320.	1.9	30
11	Exploration of Structureâ"Activity Relationship Determinants in Analogue Series. Journal of Medicinal Chemistry, 2009, 52, 3212-3224.	2.9	28
12	Benchmarking Molecular Feature Attribution Methods with Activity Cliffs. Journal of Chemical Information and Modeling, 2022, 62, 274-283.	2.5	14
13	Matched Peptides: Tuning Matched Molecular Pair Analysis for Biopharmaceutical Applications. Journal of Chemical Information and Modeling, 2015, 55, 2315-2323.	2.5	6
14	Graph Alignment: Fuzzy Pattern Mining for the Structural Analysis of Protein Active Sites. IEEE International Conference on Fuzzy Systems, 2007, , .	0.0	1
15	Guided Iterative Substructure Search (GI-SSS) - A New Trick for an Old Dog. Molecular Informatics, 2016, 35, 286-292.	1.4	1