

Nils Weskamp

List of Publications by Year in descending order

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15
papers

694
citations

759055

12
h-index

996849

15
g-index

17
all docs

17
docs citations

17
times ranked

641
citing authors

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