

Samo LeÅ¡nik

List of Publications by Year in descending order

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21
papers

484
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758635

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21
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825
citing authors

#	ARTICLE	IF	CITATIONS
1	LiSiCA: A Software for Ligand-Based Virtual Screening and Its Application for the Discovery of Butyrylcholinesterase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1521-1528.	2.5	70
2	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2308-2314.	2.5	54
3	Nonpeptidic Selective Inhibitors of the Chymotrypsin-Like (β 5 α) Subunit of the Immunoproteasome. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5745-5748.	7.2	38
4	Rosemary (<i>Rosmarinus officinalis</i> L.): extraction techniques, analytical methods and health-promoting biological effects. <i>Phytochemistry Reviews</i> , 2021, 20, 1273-1328.	3.1	38
5	Discovery of Novel Potential Human Targets of Resveratrol by Inverse Molecular Docking. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2467-2478.	2.5	35
6	Protein-water hydrogen-bond networks of G protein-coupled receptors: Graph-based analyses of static structures and molecular dynamics. <i>Journal of Structural Biology</i> , 2020, 212, 107634.	1.3	34
7	Stereoselective Activity of 1-Propargyl-4-styrylpiperidine-like Analogues That Can Discriminate between Monoamine Oxidase Isoforms A and B. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 1361-1387.	2.9	33
8	Discovery of <i>Mycobacterium tuberculosis</i> InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 11069-11078.	2.9	26
9	Discovery of new MurA inhibitors using induced-fit simulation and docking. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 944-949.	1.0	24
10	Modeling enzyme-ligand binding in drug discovery. <i>Journal of Cheminformatics</i> , 2015, 7, 48.	2.8	22
11	Selective Toll-like receptor 7 agonists with novel chromeno[3,4-d]imidazol-4(1H)-one and 2-(trifluoromethyl)quinoline/quinazoline-4-amine scaffolds. <i>European Journal of Medicinal Chemistry</i> , 2019, 179, 109-122.	2.6	18
12	ProBiS-Dock Database: A Web Server and Interactive Web Repository of Small Ligand-Protein Binding Sites for Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4097-4107.	2.5	16
13	Mechanistic Insights into Biological Activities of Polyphenolic Compounds from Rosemary Obtained by Inverse Molecular Docking. <i>Foods</i> , 2022, 11, 67.	1.9	16
14	Potential Energy Function for Fentanyl-Based Opioid Pain Killers. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3566-3576.	2.5	13
15	BoBER: web interface to the base of bioisosterically exchangeable replacements. <i>Journal of Cheminformatics</i> , 2017, 9, 62.	2.8	12
16	Ligand-based virtual screening interface between PyMOL and LiSiCA. <i>Journal of Cheminformatics</i> , 2016, 8, 46.	2.8	9
17	CHARMM Force-Field Parameters for Morphine, Heroin, and Oliceridine, and Conformational Dynamics of Opioid Drugs. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3964-3977.	2.5	8
18	Opioid Receptors and Protonation-Coupled Binding of Opioid Drugs. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13353.	1.8	8

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19	ProBiS-Dock: A Hybrid Multitemplate Homology Flexible Docking Algorithm Enabled by Protein Binding Site Comparison. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1573-1584.	2.5	4
20	Nonpeptidic Selective Inhibitors of the Chymotrypsin-Like (25%) Subunit of the Immunoproteasome. <i>Angewandte Chemie</i> , 2016, 128, 5839-5842.	1.6	3
21	Loop Grafting between Similar Local Environments for Fc-Silent Antibodies. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5475-5486.	2.5	3