Samo LeÅ¡nik

List of Publications by Year in descending order

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21 papers	484 citations	758635 12 h-index	713013 21 g-index
21 all docs	21 docs citations	21 times ranked	825 citing authors

#	Article	IF	Citations
1	ProBiS-Dock: A Hybrid Multitemplate Homology Flexible Docking Algorithm Enabled by Protein Binding Site Comparison. Journal of Chemical Information and Modeling, 2022, 62, 1573-1584.	2.5	4
2	Mechanistic Insights into Biological Activities of Polyphenolic Compounds from Rosemary Obtained by Inverse Molecular Docking. Foods, 2022, 11, 67.	1.9	16
3	Rosemary (Rosmarinus officinalis L.): extraction techniques, analytical methods and health-promoting biological effects. Phytochemistry Reviews, 2021, 20, 1273-1328.	3.1	38
4	ProBiS-Dock Database: A Web Server and Interactive Web Repository of Small Ligandâ€“Protein Binding Sites for Drug Design. Journal of Chemical Information and Modeling, 2021, 61, 4097-4107.	2.5	16
5	CHARMM Force-Field Parameters for Morphine, Heroin, and Oliceridine, and Conformational Dynamics of Opioid Drugs. Journal of Chemical Information and Modeling, 2021, 61, 3964-3977.	2.5	8
6	Opioid Receptors and Protonation-Coupled Binding of Opioid Drugs. International Journal of Molecular Sciences, 2021, 22, 13353.	1.8	8
7	Stereoselective Activity of 1-Propargyl-4-styrylpiperidine-like Analogues That Can Discriminate between Monoamine Oxidase Isoforms A and B. Journal of Medicinal Chemistry, 2020, 63, 1361-1387.	2.9	33
8	Protein-water hydrogen-bond networks of G protein-coupled receptors: Graph-based analyses of static structures and molecular dynamics. Journal of Structural Biology, 2020, 212, 107634.	1.3	34
9	Loop Grafting between Similar Local Environments for Fc-Silent Antibodies. Journal of Chemical Information and Modeling, 2020, 60, 5475-5486.	2.5	3
10	Potential Energy Function for Fentanyl-Based Opioid Pain Killers. Journal of Chemical Information and Modeling, 2020, 60, 3566-3576.	2.5	13
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. European Journal of Medicinal Chemistry, 2019, 179, 109-122.	2.6	18
12	Discovery of Novel Potential Human Targets of Resveratrol by Inverse Molecular Docking. Journal of Chemical Information and Modeling, 2019, 59, 2467-2478.	2.5	35
13	Discovery of new MurA inhibitors using induced-fit simulation and docking. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 944-949.	1.0	24
14	BoBER: web interface to the base of bioisosterically exchangeable replacements. Journal of Cheminformatics, 2017, 9, 62.	2.8	12
15	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. Journal of Medicinal Chemistry, 2016, 59, 11069-11078.	2.9	26
16	Ligand-based virtual screening interface between PyMOL and LiSiCA. Journal of Cheminformatics, 2016, 8, 46.	2.8	9
17	Nonpeptidic Selective Inhibitors of the ChymotrypsinâEŁike (Î²5â€‰i) Subunit of the Immunoproteasome. Angewandte Chemie, 2016, 128, 5839-5842.	1.6	3
18	Nonpeptidic Selective Inhibitors of the ChymotrypsinâEŁike (Î²5â€‰i) Subunit of the Immunoproteasome. Angewandte Chemie - International Edition, 2016, 55, 5745-5748.	7.2	38

#	Article	IF	Citations
19	LiSiCA: A Software for Ligand-Based Virtual Screening and Its Application for the Discovery of Butyrylcholinesterase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1521-1528.	2.5	70
20	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. Journal of Chemical Information and Modeling, 2015, 55, 2308-2314.	2.5	54
21	Modeling enzyme-ligand binding in drug discovery. Journal of Cheminformatics, 2015, 7, 48.	2.8	22