Dusanka Janezic

List of Publications by Year
in descending order

38 papers	1,073 citations	471509 17 h-index	414414 32 g-index
38 all docs	38 docs citations	38 times ranked	1347 citing authors

#	Article	IF	Citations
1	ProBiS algorithm for detection of structurally similar protein binding sites by local structural alignment. Bioinformatics, 2010, 26, 1160-1168.	4.1	228
2	ProBiS-2012: web server and web services for detection of structurally similar binding sites in proteins. Nucleic Acids Research, 2012, 40, W214-W221.	14.5	79
3	ProBiS: a web server for detection of structurally similar protein binding sites. Nucleic Acids Research, 2010, 38, W436-W440.	14.5	71
4	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.	5.4	70
5	ProBiS-ligands: a web server for prediction of ligands by examination of protein binding sites. Nucleic Acids Research, 2014, 42, W215-W220.	14.5	61
6	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. Journal of Chemical Information and Modeling, 2015, 55, 2308-2314.	5.4	54
7	ProBiS-Database: Precalculated Binding Site Similarities and Local Pairwise Alignments of PDB Structures. Journal of Chemical Information and Modeling, 2012, 52, 604-612.	5.4	50
8	Binding site comparison for function prediction and pharmaceutical discovery. Current Opinion in Structural Biology, 2014, 25, 34-39.	5.7	48
9	Structure-Based Function Prediction of Uncharacterized Protein Using Binding Sites Comparison. PLoS Computational Biology, 2013, 9, e1003341.	3.2	38
10	Nonpeptidic Selective Inhibitors of the Chymotrypsinâ€Like (Î²5â€‰i) Subunit of the Immunoproteasome. Angewandte Chemie - International Edition, 2016, 55, 5745-5748.	13.8	38
11	Discovery of Novel Potential Human Targets of Resveratrol by Inverse Molecular Docking. Journal of Chemical Information and Modeling, 2019, 59, 2467-2478.	5.4	35
12	Identification of Conserved Water Sites in Protein Structures for Drug Design. Journal of Chemical Information and Modeling, 2017, 57, 3094-3103.	5.4	34
13	Ensemble Docking Coupled to Linear Interaction Energy Calculations for Identification of Coronavirus Main Protease (3CLpro) Non-Covalent Small-Molecule Inhibitors. Molecules, 2020, 25, 5808.	3.8	30
14	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. Journal of Medicinal Chemistry, 2016, 59, 11069-11078.	6.4	26
15	Discovery of new MurA inhibitors using induced-fit simulation and docking. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 944-949.	2.2	24
16	Modeling enzyme-ligand binding in drug discovery. Journal of Cheminformatics, 2015, 7, 48.	6.1	22
17	ProBiS tools (algorithm, database, and web servers) for predicting and modeling of biologically interesting proteins. Progress in Biophysics and Molecular Biology, 2017, 128, 24-32.	2.9	18
18	H274Yâ€™s Effect on Oseltamivir Resistance: What Happens Before the Drug Enters the Binding Site. Journal of Chemical Information and Modeling, 2016, 56, 82-100.	5.4	17

#	Article	IF	Citations
19	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.	5.4	16
20	GenProBiS: web server for mapping of sequence variants to protein binding sites. Nucleic Acids Research, 2017, 45, W253-W259.	14.5	14
21	ProBiS H2O MD Approach for Identification of Conserved Water Sites in Protein Structures for Drug Design. ACS Medicinal Chemistry Letters, 2020, 11, 877-882.	2.8	14
22	BoBER: web interface to the base of bioisosterically exchangeable replacements. Journal of Cheminformatics, 2017, 9, 62.	6.1	12
23	Potential Novel Thioether-Amide or Guanidine-Linker Class of SARS-CoV-2 Virus RNA-Dependent RNA Polymerase Inhibitors Identified by High-Throughput Virtual Screening Coupled to Free-Energy Calculations. International Journal of Molecular Sciences, 2021, 22, 11143.	4.1	11
24	Repurposing of Drugs for SARS-CoV-2 Using Inverse Docking Fingerprints. Frontiers in Chemistry, 2021, 9, 757826.	3.6	11
25	Ligand-based virtual screening interface between PyMOL and LiSiCA. Journal of Cheminformatics, 2016, 8, 46.	6.1	9
26	Omega Polynomial in Diamond-like Networks. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 236-243.	2.1	8
27	Role of magnesium ions in the reaction mechanism at the interface between Tm1631 protein and its DNA ligand. Chemistry Central Journal, 2016, 10, 41.	2.6	7
28	Exact Maximum Clique Algorithm for Different Graph Types Using Machine Learning. Mathematics, 2022, 10, 97.	2.2	5
29	Global organization of a binding site network gives insight into evolution and structure-function relationships of proteins. Scientific Reports, 2017, 7, 11652.	3.3	4
30	Molecular Dynamics Simulations Reveal Interactions of an IgG1 Antibody With Selected Fc Receptors. Frontiers in Chemistry, 2021, 9, 705931.	3.6	4
31	CROW for large scale macromolecular simulations. Cellular and Molecular Biology Letters, 2002, 7, 118-9.	7.0	4
32	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.	5.4	4
33	Sugars and Sweeteners: Structure, Properties and In Silico Modeling. Current Medicinal Chemistry, 2020, 27, 5-22.	2.4	3
34	Scaffold Hopping and Bioisosteric Replacements Based on Binding Site Alignments. Croatica Chemica Acta, 2016, 89, .	0.4	2
35	Docking study with biological validation on bacterial enzyme MurD. Chemical Data Collections, 2018, 13-14, 139-155.	2.3	1
36	Molecular Docking Studies of Flavonoids Derivatives on the Flavonoid 3- O-Glucosyltransferase. Current Computer-Aided Drug Design, 2016, 11, 353-360.	1.2	1

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37	Interactions of Indomethacin with Functionalized Rhombellanes â€“ a Molecular Docking Study. Croatica Chemica Acta, 2020, 92, 503-509.	0.4	0
38	Automatic Assembly and Calibration of Models of Enzymatic Reactions Based on Ordinary Differential Equations. Methods in Molecular Biology, 2022, 2385, 141-152.	0.9	0