

Dusanka Janezic

List of Publications by Year in descending order

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38
papers

1,073
citations

471509

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times ranked

1347
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	5.4	4
2	Automatic Assembly and Calibration of Models of Enzymatic Reactions Based on Ordinary Differential Equations. <i>Methods in Molecular Biology</i> , 2022, 2385, 141-152.	0.9	0
3	Exact Maximum Clique Algorithm for Different Graph Types Using Machine Learning. <i>Mathematics</i> , 2022, 10, 97.	2.2	5
4	Molecular Dynamics Simulations Reveal Interactions of an IgG1 Antibody With Selected Fc Receptors. <i>Frontiers in Chemistry</i> , 2021, 9, 705931.	3.6	4
5	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.	5.4	16
6	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. <i>International Journal of Molecular Sciences</i> , 2021, 22, 11143.	4.1	11
7	Repurposing of Drugs for SARS-CoV-2 Using Inverse Docking Fingerprints. <i>Frontiers in Chemistry</i> , 2021, 9, 757826.	3.6	11
8	Ensemble Docking Coupled to Linear Interaction Energy Calculations for Identification of Coronavirus Main Protease (3CLpro) Non-Covalent Small-Molecule Inhibitors. <i>Molecules</i> , 2020, 25, 5808.	3.8	30
9	ProBiS H2O MD Approach for Identification of Conserved Water Sites in Protein Structures for Drug Design. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 877-882.	2.8	14
10	Interactions of Indomethacin with Functionalized Rhombellanes – a Molecular Docking Study. <i>Croatica Chemica Acta</i> , 2020, 92, 503-509.	0.4	0
11	Sugars and Sweeteners: Structure, Properties and In Silico Modeling. <i>Current Medicinal Chemistry</i> , 2020, 27, 5-22.	2.4	3
12	Discovery of Novel Potential Human Targets of Resveratrol by Inverse Molecular Docking. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2467-2478.	5.4	35
13	Docking study with biological validation on bacterial enzyme MurD. <i>Chemical Data Collections</i> , 2018, 13-14, 139-155.	2.3	1
14	Discovery of new MurA inhibitors using induced-fit simulation and docking. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 944-949.	2.2	24
15	ProBiS tools (algorithm, database, and web servers) for predicting and modeling of biologically interesting proteins. <i>Progress in Biophysics and Molecular Biology</i> , 2017, 128, 24-32.	2.9	18
16	Global organization of a binding site network gives insight into evolution and structure-function relationships of proteins. <i>Scientific Reports</i> , 2017, 7, 11652.	3.3	4
17	Identification of Conserved Water Sites in Protein Structures for Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 3094-3103.	5.4	34
18	GenProBiS: web server for mapping of sequence variants to protein binding sites. <i>Nucleic Acids Research</i> , 2017, 45, W253-W259.	14.5	14

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19	BoBER: web interface to the base of bioisosterically exchangeable replacements. <i>Journal of Cheminformatics</i> , 2017, 9, 62.	6.1	12
20	Role of magnesium ions in the reaction mechanism at the interface between Tm1631 protein and its DNA ligand. <i>Chemistry Central Journal</i> , 2016, 10, 41.	2.6	7
21	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.	6.4	26
22	Ligand-based virtual screening interface between PyMOL and LiSiCA. <i>Journal of Cheminformatics</i> , 2016, 8, 46.	6.1	9
23	Nonpeptidic Selective Inhibitors of the Chymotrypsin-Like (20S) Subunit of the Immunoproteasome. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5745-5748.	13.8	38
24	H274Y's Effect on Oseltamivir Resistance: What Happens Before the Drug Enters the Binding Site. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 82-100.	5.4	17
25	Scaffold Hopping and Bioisosteric Replacements Based on Binding Site Alignments. <i>Croatica Chemica Acta</i> , 2016, 89, .	0.4	2
26	Molecular Docking Studies of Flavonoids Derivatives on the Flavonoid 3- O-Glucosyltransferase. <i>Current Computer-Aided Drug Design</i> , 2016, 11, 353-360.	1.2	1
27	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.	5.4	70
28	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.	5.4	54
29	Modeling enzyme-ligand binding in drug discovery. <i>Journal of Cheminformatics</i> , 2015, 7, 48.	6.1	22
30	ProBiS-ligands: a web server for prediction of ligands by examination of protein binding sites. <i>Nucleic Acids Research</i> , 2014, 42, W215-W220.	14.5	61
31	Binding site comparison for function prediction and pharmaceutical discovery. <i>Current Opinion in Structural Biology</i> , 2014, 25, 34-39.	5.7	48
32	Structure-Based Function Prediction of Uncharacterized Protein Using Binding Sites Comparison. <i>PLoS Computational Biology</i> , 2013, 9, e1003341.	3.2	38
33	ProBiS-2012: web server and web services for detection of structurally similar binding sites in proteins. <i>Nucleic Acids Research</i> , 2012, 40, W214-W221.	14.5	79
34	ProBiS-Database: Precalculated Binding Site Similarities and Local Pairwise Alignments of PDB Structures. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 604-612.	5.4	50
35	Omega Polynomial in Diamond-like Networks. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2010, 18, 236-243.	2.1	8
36	ProBiS: a web server for detection of structurally similar protein binding sites. <i>Nucleic Acids Research</i> , 2010, 38, W436-W440.	14.5	71

#	ARTICLE	IF	CITATIONS
37	ProBiS algorithm for detection of structurally similar protein binding sites by local structural alignment. <i>Bioinformatics</i> , 2010, 26, 1160-1168.	4.1	228
38	CROW for large scale macromolecular simulations. <i>Cellular and Molecular Biology Letters</i> , 2002, 7, 118-9.	7.0	4