Maria M Miteva

List of Publications by Year
in descending order

100 papers	4,812 citations	94433 37 h-index	102487 66 g-index
106 all docs	106 docs citations	106 times ranked	6630 citing authors

#	Article	IF	Citations
1	Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. Drug Discovery Today, 2010, 15, 656-667.	6.4	249
2	FAF-Drugs3: a web server for compound property calculation and chemical library design. Nucleic Acids Research, 2015, 43, W200-W207.	14.5	237
3	FAF-Drugs4: free ADME-tox filtering computations for chemical biology and early stages drug discovery. Bioinformatics, 2017, 33, 3658-3660.	4.1	230
4	Frog2: Efficient 3D conformation ensemble generator for small compounds. Nucleic Acids Research, 2010, 38, W622-W627.	14.5	224
5	FAF-Drugs2: Free ADME/tox filtering tool to assist drug discovery and chemical biology projects. BMC Bioinformatics, 2008, 9, 396.	2.6	221
6	Toward in silico structure-based ADMET prediction in drug discovery. Drug Discovery Today, 2012, 17, 44-55.	6.4	220
7	MTiOpenScreen: a web server for structure-based virtual screening. Nucleic Acids Research, 2015, 43, W448-W454.	14.5	159
8	Computational analysis of calculated physicochemical and ADMET properties of protein-protein interaction inhibitors. Scientific Reports, 2017, 7, 46277.	3.3	128
9	FAF-Drugs: free ADME/tox filtering of compound collections. Nucleic Acids Research, 2006, 34, W738-W744.	14.5	115
10	Structure-Based Virtual Ligand Screening: Recent Success Stories. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 1000-1016.	1.1	114
11	Analyzing Effects of Naturally Occurring Missense Mutations. Computational and Mathematical Methods in Medicine, 2012, 2012, 1-15.	1.3	111
12	Fast Structure-Based Virtual Ligand Screening Combining FRED, DOCK, and Surflex. Journal of Medicinal Chemistry, 2005, 48, 6012-6022.	6.4	106
13	Free Resources to Assist Structure-Based Virtual Ligand Screening Experiments. Current Protein and Peptide Science, 2007, 8, 381-411.	1.4	104
14	Molecular electroporation: a unifying concept for the description of membrane pore formation by antibacterial peptides, exemplified with NKâ€lysin. FEBS Letters, 1999, 462, 155-158.	2.8	103
15	MS-DOCK: Accurate multiple conformation generator and rigid docking protocol for multi-step virtual ligand screening. BMC Bioinformatics, 2008, 9, 184.	2.6	102
16	Drugâ€Like Proteinï£¿Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. Molecular Informatics, 2014, 33, 414-437.	2.5	93
17	Reduced phosphatase activity of SHPâ€2 in LEOPARD syndrome: Consequences for PI3K binding on Gab1. FEBS Letters, 2006, 580, 2477-2482.	2.8	91
18	New machine learning and physics-based scoring functions for drug discovery. Scientific Reports, 2021, 11, 3198.	3.3	91

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19	Frog: a FRee Online druG 3D conformation generator. Nucleic Acids Research, 2007, 35, W568-W572.	14.5	86
20	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. Bioinformatics, 2011, 27, 2018-2020.	4.1	81
21	One hundred thousand mouse clicks down the road: selected online resources supporting drug discovery collected over a decade. Drug Discovery Today, 2013, 18, 1081-1089.	6.4	76
22	How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 and normal mode analysis. European Biophysics Journal, 2010, 39, 1365-1372.	2.2	68
23	In Silico-In Vitro Screening of Protein-Protein Interactions: Towards the Next Generation of Therapeutics. Current Pharmaceutical Biotechnology, 2008, 9, 103-122.	1.6	59
24	Pharmacogenomics of the cytochrome P450 2C family: impacts of amino acid variations on drug metabolism. Drug Discovery Today, 2017, 22, 366-376.	6.4	58
25	In silico design of low molecular weight proteinâ€“protein interaction inhibitors: Overall concept and recent advances. Progress in Biophysics and Molecular Biology, 2015, 119, 20-32.	2.9	56
26	Genetic, molecular and functional analyses of complement factor I deficiency. European Journal of Immunology, 2009, 39, 310-323.	2.9	53
27	Design, synthesis, and biological evaluation of novel naphthoquinone derivatives with CDC25 phosphatase inhibitory activity. Bioorganic and Medicinal Chemistry, 2005, 13, 4871-4879.	3.0	51
28	PCE: web tools to compute protein continuum electrostatics. Nucleic Acids Research, 2005, 33, W372-W375.	14.5	51
29	Design of proteinâ€“membrane interaction inhibitors by virtual ligand screening, proof of concept with the C2 domain of factor V. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 12697-12702.	7.1	50
30	Anti-Factor B Antibodies and Acute Postinfectious GN in Children. Journal of the American Society of Nephrology: JASN, 2020, 31, 829-840.	6.1	50
31	iPPI-DB: an online database of modulators of proteinâ€“protein interactions. Nucleic Acids Research, 2016, 44, D542-D547.	14.5	49
32	Receptor-Based Computational Screening of Compound Databases: The Main Docking-Scoring Engines. Current Protein and Peptide Science, 2006, 7, 369-393.	1.4	47
33	Structure-based virtual ligand screening with LigandFit: Pose prediction and enrichment of compound collections. Proteins: Structure, Function and Bioinformatics, 2007, 68, 712-725.	2.6	45
34	AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening. BMC Bioinformatics, 2008, 9, 438.	2.6	44
35	Receptor-Based Virtual Ligand Screening for the Identification of Novel CDC25 Phosphatase Inhibitors. Journal of Chemical Information and Modeling, 2008, 48, 157-165.	5.4	43
36	Stabilization of proteinâ€“protein interaction complexes through small molecules. Drug Discovery Today, 2016, 21, 48-57.	6.4	41

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37	Advances in Molecular Modeling of Human Cytochrome P450 Polymorphism. Journal of Molecular Biology, 2013, 425, 3978-3992.	4.2	39
38	DG-AMMOS: A New tool to generate 3D conformation of small molecules using Distance Geometry and Automated Molecular Mechanics Optimization for in silico Screening. BMC Chemical Biology, 2009, 9, 6.	1.6	38
39	Targeting the Proangiogenic VEGF-VEGFR Protein-Protein Interface with Drug-like Compounds by In Silico and InÂVitro Screening. Chemistry and Biology, 2011, 18, 1631-1639.	6.0	38
40	Multiply-Protonated Protein Ions in the Gas Phase:Â Calculation of the Electrostatic Interactions between Charged Sites. Journal of Physical Chemistry B, 1997, 101, 9645-9650.	2.6	36
41	Discovery of novel inhibitors of vascular endothelial growth factor-Aâ€“Neuropilin-1 interaction by structure-based virtual screening. Bioorganic and Medicinal Chemistry, 2014, 22, 4042-4048.	3.0	35
42	MED-SuMoLig:â€‰ A New Ligand-Based Screening Tool for Efficient Scaffold Hopping. Journal of Chemical Information and Modeling, 2007, 47, 1097-1110.	5.4	34
43	In Silico Prediction of Aqueous Solubility: A Multimodel Protocol Based on Chemical Similarity. Molecular Pharmaceutics, 2012, 9, 3127-3135.	4.6	33
44	Factor V New Brunswick: Ala221Val associated with FV deficiency reproduced in vitro and functionally characterized. Blood, 2003, 102, 1316-1322.	1.4	31
45	Molecular models of the procoagulant Factor VIIIa-Factor IXa complex. Journal of Thrombosis and Haemostasis, 2005, 3, 2044-2056.	3.8	31
46	Fr-PPIChem: An Academic Compound Library Dedicated to Proteinâ€“Protein Interactions. ACS Chemical Biology, 2020, 15, 1566-1574.	3.4	29
47	Comparative structural and evolutionary analyses predict functional sites in the artemisinin resistance malaria protein K13. Scientific Reports, 2019, 9, 10675.	3.3	28
48	Integrated structure- and ligand-based in silico approach to predict inhibition of cytochrome P450 2D6. Bioinformatics, 2015, 31, 3930-3937.	4.1	27
49	Combining Ligand- and Structure-Based Methods in Drug Design Projects. Current Computer-Aided Drug Design, 2008, 4, 250-258.	1.2	27
50	MED-3DMC: A new tool to generate 3D conformation ensembles of small molecules with a Monte Carlo sampling of the conformational space. European Journal of Medicinal Chemistry, 2009, 44, 1405-1409.	5.5	26
51	Pan-assay interference compounds (PAINS) that may not be too painful for chemical biology projects. Drug Discovery Today, 2017, 22, 1131-1133.	6.4	26
52	1,2,4-Oxadiazoles Identified by Virtual Screening and their Non-Covalent Inhibition of the Human 20S Proteasome. Current Medicinal Chemistry, 2013, 20, 2351-2362.	2.4	25
53	Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. Oncotarget, 2018, 9, 32346-32361.	1.8	25
54	Structural Dynamics of DPP-4 and Its Influence on the Projection of Bioactive Ligands. Molecules, 2018, 23, 490.	3.8	25

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55	Analysis of protein missense alterations by combining sequenceâ€•and structureâ€based methods. Molecular Genetics & Genomic Medicine, 2020, 8, e1166.	1.2	25
56	Post-docking virtual screening of diverse binding pockets: Comparative study using DOCK, AMMOS, X-Score and FRED scoring functions. European Journal of Medicinal Chemistry, 2010, 45, 2622-2628.	5.5	24
57	AMMOS2: a web server for proteinâ€“ligandâ€“water complexes refinement via molecular mechanics. Nucleic Acids Research, 2017, 45, W350-W355.	14.5	24
58	Insights into molecular mechanisms of drug metabolism dysfunction of human CYP2C9*30. PLoS ONE, 2018, 13, e0197249.	2.5	24
59	Calculating the Protonation States of Proteins and Small Molecules: Implications to Ligand-Receptor Interactions. Current Computer-Aided Drug Design, 2008, 4, 169-179.	1.2	24
60	Tyrosine Kinase Syk Non-Enzymatic Inhibitors and Potential Anti-Allergic Drug-Like Compounds Discovered by Virtual and In Vitro Screening. PLoS ONE, 2011, 6, e21117.	2.5	23
61	In Silico Mechanistic Profiling to Probe Small Molecule Binding to Sulfotransferases. PLoS ONE, 2013, 8, e73587.	2.5	23
62	Sampling of conformational ensemble for virtual screening using molecular dynamics simulations and normal mode analysis. Future Medicinal Chemistry, 2015, 7, 2317-2331.	2.3	22
63	Discoidin Domains as Emerging Therapeutic Targets. Trends in Pharmacological Sciences, 2016, 37, 641-659.	8.7	21
64	Rational Design of Small-Molecule Stabilizers of Spermine Synthase Dimer by Virtual Screening and Free Energy-Based Approach. PLoS ONE, 2014, 9, e110884.	2.5	20
65	Analysis of solvent-exposed and buried co-crystallized ligands: a case study to support the design of novel proteinâ€“protein interaction inhibitors. Drug Discovery Today, 2019, 24, 551-559.	6.4	20
66	Design and synthesis of novel bis-thiazolone derivatives as micromolar CDC25 phosphatase inhibitors: Effect of dimerisation on phosphatase inhibition. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7345-7350.	2.2	19
67	Theoretical and Experimental Study of the D2194G Mutation in the C2 Domain of Coagulation Factor V. Biophysical Journal, 2004, 86, 488-498.	0.5	18
68	A rational free energy-based approach to understanding and targeting disease-causing missense mutations. Journal of the American Medical Informatics Association: JAMIA, 2013, 20, 643-651.	4.4	18
69	Insights into an Original Pocket-Ligand Pair Classification: A Promising Tool for Ligand Profile Prediction. PLoS ONE, 2013, 8, e63730.	2.5	18
70	Screening Outside the Catalytic Site: Inhibition of Macromolecular Interactions Through Structure-Based Virtual Ligand Screening Experiments. The Open Biochemistry Journal, 2008, 2, 29-37.	0.5	17
71	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. International Journal of Molecular Sciences, 2019, 20, 4648.	4.1	16
72	Insights into the substrate binding mechanism of SULT1A1 through molecular dynamics with excited normal modes simulations. Scientific Reports, 2021, 11, 13129.	3.3	16

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73	Noonan syndrome type I with PTPN11 3 bp deletion: Structureâ€“function implications. Proteins: Structure, Function and Bioinformatics, 2005, 58, 7-13.	2.6	15
74	Exploring NMR ensembles of calcium binding proteins: Perspectives to design inhibitors of protein-protein interactions. BMC Structural Biology, 2011, 11, 24.	2.3	15
75	In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening. Scientific Reports, 2017, 7, 7249.	3.3	15
76	Blockade of the malignant phenotype by Î²-subunit selective noncovalent inhibition of immuno- and constitutive proteasomes. Oncotarget, 2017, 8, 10437-10449.	1.8	13
77	Machine learning-driven identification of drugs inhibiting cytochrome P450 2C9. PLoS Computational Biology, 2022, 18, e1009820.	3.2	11
78	Local electrostatic potentials in pyridoxal phosphate labelled horse heart cytochrome c. Journal of Photochemistry and Photobiology B: Biology, 1997, 37, 74-83.	3.8	9
79	pH-dependent stability of sperm whale myoglobin in water-guanidine hydrochloride solutions. European Biophysics Journal, 2003, 31, 617-625.	2.2	9
80	A critical role for Gly25 in the B chain of human thrombin. Journal of Thrombosis and Haemostasis, 2005, 3, 139-145.	3.8	9
81	Hierarchical Structure-Based Virtual Screening for Drug Design. Biotechnology and Biotechnological Equipment, 2008, 22, 634-638.	1.3	9
82	Three-dimensional structure generators of drug-like compounds: DG-AMMOS, an open-source package. Expert Opinion on Drug Discovery, 2011, 6, 339-351.	5.0	9
83	Computational analysis of protein-protein interfaces involving an alpha helix: insights for terphenylâ€“like molecules binding. BMC Pharmacology & Toxicology, 2013, 14, 31.	2.4	9
84	Insights into the interaction of high potency inhibitor IRCâ€083864 with phosphatase CDC25. Proteins: Structure, Function and Bioinformatics, 2017, 85, 593-601.	2.6	7
85	Characterization of pyridoxal phosphate as an optical label for measuring electrostatic potentials in proteins. Journal of Photochemistry and Photobiology B: Biology, 1996, 32, 71-79.	3.8	6
86	Tampering with Cell Division by Using Smallâ€Molecule Inhibitors of CDKâ€“CKS Protein Interactions. ChemBioChem, 2015, 16, 432-439.	2.6	6
87	Post-Docking Optimization and Analysis of Protein-Ligand Interactions of Estrogen Receptor Alpha using AMMOS Software. Current Computer-Aided Drug Design, 2013, 9, 83-94.	1.2	5
88	Numerical simulation of aldolase tetramer stability. European Biophysics Journal, 1998, 28, 67-73.	2.2	4
89	Identification of insulin-sensitizing molecules acting by disrupting the interaction between the Insulin Receptor and Grb14. Scientific Reports, 2017, 7, 16901.	3.3	4
90	Binding of phenothiazines into allosteric hydrophobic pocket of human thioredoxin 1. European Biophysics Journal, 2016, 45, 279-286.	2.2	3

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91	Computational Biology and Chemistry in MTi: Emphasis on the Prediction of Some ADMET Properties. Molecular Informatics, 2017, 36, 1700008.	2.5	3
92	Computational Analysis of Chemical Space of Natural Compounds Interacting with Sulfotransferases. Molecules, 2021, 26, 6360.	3.8	3
93	Post-docking optimization and analysis of protein-ligand interactions of estrogen receptor alpha using AMMOS software. Current Computer-Aided Drug Design, 2013, 9, 83-94.	1.2	3
94	AMMOS Software: Method and Application. Methods in Molecular Biology, 2012, 819, 127-141.	0.9	2
95	Prediction and structural analysis of the enthalpy of ionization of proteins. Thermochimica Acta, 1997, 291, 141-153.	2.7	1
96	Protein Structure Analysis Online. Current Protocols in Protein Science, 2007, 50, Unit 2.13.	2.8	1
97	Spectrophotometric titration of ionisable groups in proteins: a theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2000, 56, 2033-2041.	3.9	0
98	Post-Docking Optimization and Analysis of Protein-Ligand Interactions of Estrogen Receptor Alpha using AMMOS Software. Current Computer-Aided Drug Design, 2013, 9, 83-94.	1.2	0
99	In Silico Approaches Assisting the Rational Design of Low Molecular Weight Proteinâ€“Protein Interaction Modulators. , 2015, , 441-482.		0
100	Assessment of some pesticides interactions with human cytochrome P450: CYP2C8, CYP2C9 and CYP2C19 by molecular docking approach. AIP Conference Proceedings, 2016, , .	0.4	0