

# Maria M Miteva

## List of Publications by Year in descending order

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100  
papers

4,812  
citations

108046

37  
h-index

116156

66  
g-index

106  
all docs

106  
docs citations

106  
times ranked

7389  
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine learning-driven identification of drugs inhibiting cytochrome P450 2C9. <i>PLoS Computational Biology</i> , 2022, 18, e1009820.	1.5	11
2	New machine learning and physics-based scoring functions for drug discovery. <i>Scientific Reports</i> , 2021, 11, 3198.	1.6	91
3	Insights into the substrate binding mechanism of SULT1A1 through molecular dynamics with excited normal modes simulations. <i>Scientific Reports</i> , 2021, 11, 13129.	1.6	16
4	Computational Analysis of Chemical Space of Natural Compounds Interacting with Sulfotransferases. <i>Molecules</i> , 2021, 26, 6360.	1.7	3
5	Anti-Factor B Antibodies and Acute Postinfectious GN in Children. <i>Journal of the American Society of Nephrology: JASN</i> , 2020, 31, 829-840.	3.0	50
6	Analysis of protein missense alterations by combining sequence- and structure-based methods. <i>Molecular Genetics &amp; Genomic Medicine</i> , 2020, 8, e1166.	0.6	25
7	Fr-PPIChem: An Academic Compound Library Dedicated to Protein-Protein Interactions. <i>ACS Chemical Biology</i> , 2020, 15, 1566-1574.	1.6	29
8	Comparative structural and evolutionary analyses predict functional sites in the artemisinin resistance malaria protein K13. <i>Scientific Reports</i> , 2019, 9, 10675.	1.6	28
9	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4648.	1.8	16
10	Analysis of solvent-exposed and buried co-crystallized ligands: a case study to support the design of novel protein-protein interaction inhibitors. <i>Drug Discovery Today</i> , 2019, 24, 551-559.	3.2	20
11	Insights into molecular mechanisms of drug metabolism dysfunction of human CYP2C9*30. <i>PLoS ONE</i> , 2018, 13, e0197249.	1.1	24
12	Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. <i>Oncotarget</i> , 2018, 9, 32346-32361.	0.8	25
13	Structural Dynamics of DPP-4 and Its Influence on the Projection of Bioactive Ligands. <i>Molecules</i> , 2018, 23, 490.	1.7	25
14	Insights into the interaction of high potency inhibitor IRC083864 with phosphatase CDC25. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 593-601.	1.5	7
15	Computational Biology and Chemistry in MTi: Emphasis on the Prediction of Some ADMET Properties. <i>Molecular Informatics</i> , 2017, 36, 1700008.	1.4	3
16	Computational analysis of calculated physicochemical and ADMET properties of protein-protein interaction inhibitors. <i>Scientific Reports</i> , 2017, 7, 46277.	1.6	128
17	FAF-Drugs4: free ADME-tox filtering computations for chemical biology and early stages drug discovery. <i>Bioinformatics</i> , 2017, 33, 3658-3660.	1.8	230
18	In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening. <i>Scientific Reports</i> , 2017, 7, 7249.	1.6	15

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19	Identification of insulin-sensitizing molecules acting by disrupting the interaction between the Insulin Receptor and Grb14. <i>Scientific Reports</i> , 2017, 7, 16901.	1.6	4
20	AMMOS2: a web server for proteinâ€“ligandâ€“water complexes refinement via molecular mechanics. <i>Nucleic Acids Research</i> , 2017, 45, W350-W355.	6.5	24
21	Pan-assay interference compounds (PAINS) that may not be too painful for chemical biology projects. <i>Drug Discovery Today</i> , 2017, 22, 1131-1133.	3.2	26
22	Pharmacogenomics of the cytochrome P450 2C family: impacts of amino acid variations on drug metabolism. <i>Drug Discovery Today</i> , 2017, 22, 366-376.	3.2	58
23	Blockade of the malignant phenotype by <i>Î²</i> -subunit selective noncovalent inhibition of immuno- and constitutive proteasomes. <i>Oncotarget</i> , 2017, 8, 10437-10449.	0.8	13
24	Discoïdin Domains as Emerging Therapeutic Targets. <i>Trends in Pharmacological Sciences</i> , 2016, 37, 641-659.	4.0	21
25	Assessment of some pesticides interactions with human cytochrome P450: CYP2C8, CYP2C9 and CYP2C19 by molecular docking approach. <i>AIP Conference Proceedings</i> , 2016, , .	0.3	0
26	Binding of phenothiazines into allosteric hydrophobic pocket of human thioredoxin 1. <i>European Biophysics Journal</i> , 2016, 45, 279-286.	1.2	3
27	iPPI-DB: an online database of modulators of proteinâ€“protein interactions. <i>Nucleic Acids Research</i> , 2016, 44, D542-D547.	6.5	49
28	Stabilization of proteinâ€“protein interaction complexes through small molecules. <i>Drug Discovery Today</i> , 2016, 21, 48-57.	3.2	41
29	In Silico Approaches Assisting the Rational Design of Low Molecular Weight Proteinâ€“Protein Interaction Modulators. , 2015, , 441-482.		0
30	FAF-Drugs3: a web server for compound property calculation and chemical library design. <i>Nucleic Acids Research</i> , 2015, 43, W200-W207.	6.5	237
31	Tampering with Cell Division by Using Smallâ€“Molecule Inhibitors of CDKâ€“CKS Protein Interactions. <i>ChemBioChem</i> , 2015, 16, 432-439.	1.3	6
32	In silico design of low molecular weight proteinâ€“protein interaction inhibitors: Overall concept and recent advances. <i>Progress in Biophysics and Molecular Biology</i> , 2015, 119, 20-32.	1.4	56
33	MTiOpenScreen: a web server for structure-based virtual screening. <i>Nucleic Acids Research</i> , 2015, 43, W448-W454.	6.5	159
34	Integrated structure- and ligand-based <i>in silico</i> approach to predict inhibition of cytochrome P450 2D6. <i>Bioinformatics</i> , 2015, 31, 3930-3937.	1.8	27
35	Sampling of conformational ensemble for virtual screening using molecular dynamics simulations and normal mode analysis. <i>Future Medicinal Chemistry</i> , 2015, 7, 2317-2331.	1.1	22
36	Rational Design of Small-Molecule Stabilizers of Spermine Synthase Dimer by Virtual Screening and Free Energy-Based Approach. <i>PLoS ONE</i> , 2014, 9, e110884.	1.1	20

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37	Drug-Like Protein-Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. <i>Molecular Informatics</i> , 2014, 33, 414-437.	1.4	93
38	Discovery of novel inhibitors of vascular endothelial growth factor-Neuropilin-1 interaction by structure-based virtual screening. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 4042-4048.	1.4	35
39	Advances in Molecular Modeling of Human Cytochrome P450 Polymorphism. <i>Journal of Molecular Biology</i> , 2013, 425, 3978-3992.	2.0	39
40	Computational analysis of protein-protein interfaces involving an alpha helix: insights for terphenyl-like molecules binding. <i>BMC Pharmacology &amp; Toxicology</i> , 2013, 14, 31.	1.0	9
41	One hundred thousand mouse clicks down the road: selected online resources supporting drug discovery collected over a decade. <i>Drug Discovery Today</i> , 2013, 18, 1081-1089.	3.2	76
42	A rational free energy-based approach to understanding and targeting disease-causing missense mutations. <i>Journal of the American Medical Informatics Association: JAMIA</i> , 2013, 20, 643-651.	2.2	18
43	Post-Docking Optimization and Analysis of Protein-Ligand Interactions of Estrogen Receptor Alpha using AMMOS Software. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 83-94.	0.8	0
44	Insights into an Original Pocket-Ligand Pair Classification: A Promising Tool for Ligand Profile Prediction. <i>PLoS ONE</i> , 2013, 8, e63730.	1.1	18
45	1,2,4-Oxadiazoles Identified by Virtual Screening and their Non-Covalent Inhibition of the Human 20S Proteasome. <i>Current Medicinal Chemistry</i> , 2013, 20, 2351-2362.	1.2	25
46	In Silico Mechanistic Profiling to Probe Small Molecule Binding to Sulfotransferases. <i>PLoS ONE</i> , 2013, 8, e73587.	1.1	23
47	Post-Docking Optimization and Analysis of Protein-Ligand Interactions of Estrogen Receptor Alpha using AMMOS Software. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 83-94.	0.8	5
48	Post-docking optimization and analysis of protein-ligand interactions of estrogen receptor alpha using AMMOS software. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 83-94.	0.8	3
49	Analyzing Effects of Naturally Occurring Missense Mutations. <i>Computational and Mathematical Methods in Medicine</i> , 2012, 2012, 1-15.	0.7	111
50	Design and synthesis of novel bis-thiazolone derivatives as micromolar CDC25 phosphatase inhibitors: Effect of dimerisation on phosphatase inhibition. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 7345-7350.	1.0	19
51	In Silico Prediction of Aqueous Solubility: A Multimodel Protocol Based on Chemical Similarity. <i>Molecular Pharmaceutics</i> , 2012, 9, 3127-3135.	2.3	33
52	Toward in silico structure-based ADMET prediction in drug discovery. <i>Drug Discovery Today</i> , 2012, 17, 44-55.	3.2	220
53	AMMOS Software: Method and Application. <i>Methods in Molecular Biology</i> , 2012, 819, 127-141.	0.4	2
54	Tyrosine Kinase Syk Non-Enzymatic Inhibitors and Potential Anti-Allergic Drug-Like Compounds Discovered by Virtual and In Vitro Screening. <i>PLoS ONE</i> , 2011, 6, e21117.	1.1	23

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55	Targeting the Proangiogenic VEGF-VEGFR Protein-Protein Interface with Drug-like Compounds by In Silico and In Vitro Screening. <i>Chemistry and Biology</i> , 2011, 18, 1631-1639.	6.2	38
56	Three-dimensional structure generators of drug-like compounds: DG-AMMOS, an open-source package. <i>Expert Opinion on Drug Discovery</i> , 2011, 6, 339-351.	2.5	9
57	Exploring NMR ensembles of calcium binding proteins: Perspectives to design inhibitors of protein-protein interactions. <i>BMC Structural Biology</i> , 2011, 11, 24.	2.3	15
58	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. <i>Bioinformatics</i> , 2011, 27, 2018-2020.	1.8	81
59	How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 and normal mode analysis. <i>European Biophysics Journal</i> , 2010, 39, 1365-1372.	1.2	68
60	Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. <i>Drug Discovery Today</i> , 2010, 15, 656-667.	3.2	249
61	Post-docking virtual screening of diverse binding pockets: Comparative study using DOCK, AMMOS, X-Score and FRED scoring functions. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 2622-2628.	2.6	24
62	Frog2: Efficient 3D conformation ensemble generator for small compounds. <i>Nucleic Acids Research</i> , 2010, 38, W622-W627.	6.5	224
63	Genetic, molecular and functional analyses of complement factor I deficiency. <i>European Journal of Immunology</i> , 2009, 39, 310-323.	1.6	53
64	DG-AMMOS: A New tool to generate 3D conformation of small molecules using Distance Geometry and Automated Molecular Mechanics Optimization for in silico Screening. <i>BMC Chemical Biology</i> , 2009, 9, 6.	1.6	38
65	MED-3DMC: A new tool to generate 3D conformation ensembles of small molecules with a Monte Carlo sampling of the conformational space. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 1405-1409.	2.6	26
66	Structure-Based Virtual Ligand Screening: Recent Success Stories. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009, 12, 1000-1016.	0.6	114
67	MS-DOCK: Accurate multiple conformation generator and rigid docking protocol for multi-step virtual ligand screening. <i>BMC Bioinformatics</i> , 2008, 9, 184.	1.2	102
68	FAF-Drugs2: Free ADME/tox filtering tool to assist drug discovery and chemical biology projects. <i>BMC Bioinformatics</i> , 2008, 9, 396.	1.2	221
69	AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening. <i>BMC Bioinformatics</i> , 2008, 9, 438.	1.2	44
70	Receptor-Based Virtual Ligand Screening for the Identification of Novel CDC25 Phosphatase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 157-165.	2.5	43
71	Hierarchical Structure-Based Virtual Screening for Drug Design. <i>Biotechnology and Biotechnological Equipment</i> , 2008, 22, 634-638.	0.5	9
72	In Silico-In Vitro Screening of Protein-Protein Interactions: Towards the Next Generation of Therapeutics. <i>Current Pharmaceutical Biotechnology</i> , 2008, 9, 103-122.	0.9	59

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73	Calculating the Protonation States of Proteins and Small Molecules: Implications to Ligand-Receptor Interactions. <i>Current Computer-Aided Drug Design</i> , 2008, 4, 169-179.	0.8	24
74	Combining Ligand- and Structure-Based Methods in Drug Design Projects. <i>Current Computer-Aided Drug Design</i> , 2008, 4, 250-258.	0.8	27
75	Screening Outside the Catalytic Site: Inhibition of Macromolecular Interactions Through Structure-Based Virtual Ligand Screening Experiments. <i>The Open Biochemistry Journal</i> , 2008, 2, 29-37.	0.3	17
76	Free Resources to Assist Structure-Based Virtual Ligand Screening Experiments. <i>Current Protein and Peptide Science</i> , 2007, 8, 381-411.	0.7	104
77	Frog: a FRee Online druG 3D conformation generator. <i>Nucleic Acids Research</i> , 2007, 35, W568-W572.	6.5	86
78	Design of protein-membrane interaction inhibitors by virtual ligand screening, proof of concept with the C2 domain of factor V. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 12697-12702.	3.3	50
79	MED-SuMoLig: A New Ligand-Based Screening Tool for Efficient Scaffold Hopping. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1097-1110.	2.5	34
80	Protein Structure Analysis Online. <i>Current Protocols in Protein Science</i> , 2007, 50, Unit 2.13.	2.8	1
81	Structure-based virtual ligand screening with LigandFit: Pose prediction and enrichment of compound collections. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 712-725.	1.5	45
82	Reduced phosphatase activity of SHP-2 in LEOPARD syndrome: Consequences for PI3K binding on Gab1. <i>FEBS Letters</i> , 2006, 580, 2477-2482.	1.3	91
83	FAF-Drugs: free ADME/tox filtering of compound collections. <i>Nucleic Acids Research</i> , 2006, 34, W738-W744.	6.5	115
84	Receptor-Based Computational Screening of Compound Databases: The Main Docking-Scoring Engines. <i>Current Protein and Peptide Science</i> , 2006, 7, 369-393.	0.7	47
85	Design, synthesis, and biological evaluation of novel naphthoquinone derivatives with CDC25 phosphatase inhibitory activity. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 4871-4879.	1.4	51
86	Fast Structure-Based Virtual Ligand Screening Combining FRED, DOCK, and Surflex. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 6012-6022.	2.9	106
87	A critical role for Gly25 in the B chain of human thrombin. <i>Journal of Thrombosis and Haemostasis</i> , 2005, 3, 139-145.	1.9	9
88	Molecular models of the procoagulant Factor VIIIa-Factor IXa complex. <i>Journal of Thrombosis and Haemostasis</i> , 2005, 3, 2044-2056.	1.9	31
89	PCE: web tools to compute protein continuum electrostatics. <i>Nucleic Acids Research</i> , 2005, 33, W372-W375.	6.5	51
90	Noonan syndrome type I with PTPN11 3 bp deletion: Structure-function implications. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 58, 7-13.	1.5	15

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91	Theoretical and Experimental Study of the D2194G Mutation in the C2 Domain of Coagulation Factor V. <i>Biophysical Journal</i> , 2004, 86, 488-498.	0.2	18
92	pH-dependent stability of sperm whale myoglobin in water-guanidine hydrochloride solutions. <i>European Biophysics Journal</i> , 2003, 31, 617-625.	1.2	9
93	Factor V New Brunswick: Ala221Val associated with FV deficiency reproduced in vitro and functionally characterized. <i>Blood</i> , 2003, 102, 1316-1322.	0.6	31
94	Spectrophotometric titration of ionisable groups in proteins: a theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 2033-2041.	2.0	0
95	Molecular electroporation: a unifying concept for the description of membrane pore formation by antibacterial peptides, exemplified with NK-lysin. <i>FEBS Letters</i> , 1999, 462, 155-158.	1.3	103
96	Numerical simulation of aldolase tetramer stability. <i>European Biophysics Journal</i> , 1998, 28, 67-73.	1.2	4
97	Multiply-Protonated Protein Ions in the Gas Phase: Calculation of the Electrostatic Interactions between Charged Sites. <i>Journal of Physical Chemistry B</i> , 1997, 101, 9645-9650.	1.2	36
98	Local electrostatic potentials in pyridoxal phosphate labelled horse heart cytochrome c. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 1997, 37, 74-83.	1.7	9
99	Prediction and structural analysis of the enthalpy of ionization of proteins. <i>Thermochemica Acta</i> , 1997, 291, 141-153.	1.2	1
100	Characterization of pyridoxal phosphate as an optical label for measuring electrostatic potentials in proteins. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 1996, 32, 71-79.	1.7	6