Vojtech Spiwok

List of Publications by Year in descending order

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73 papers	2,423 citations	257450 24 h-index	223800 46 g-index
89 all docs	89 docs citations	89 times ranked	3309 citing authors

#	Article	IF	Citations
1	Property Map Collective Variable as a Useful Tool for a Force Field Correction. Journal of Chemical Information and Modeling, 2022, 62, 567-576.	5.4	2
2	The first structureâ€“function study of GH151 Î±â€<scp>l</scp>â€fucosidase uncovers new oligomerization pattern, active site complementation, and selective substrate specificity. FEBS Journal, 2022, 289, 4998-5020.	4.7	3
3	An Early Stage Researcher's Primer on Systems Medicine Terminology. Network and Systems Medicine, 2021, 4, 2-50.	2.5	9
4	Arabinogalactanâ€like Glycoproteins from Ulva lactuca (Chlorophyta) Show Unique Features Compared to Land Plants AGPs. Journal of Phycology, 2021, 57, 619-635.	2.3	13
5	Transglycosylation abilities of Î²-d-galactosidases from GH family 2. 3 Biotech, 2021, 11, 168.	2.2	3
6	Na+/K+-ATPase Revisited: On Its Mechanism of Action, Role in Cancer, and Activity Modulation. Molecules, 2021, 26, 1905.	3.8	40
7	Quo vadis Cardiac Glycoside Research?. Toxins, 2021, 13, 344.	3.4	20
8	Structural Basis of the Function of Yariv Reagentâ€”An Important Tool to Study Arabinogalactan Proteins. Frontiers in Molecular Biosciences, 2021, 8, 682858.	3.5	7
9	Prediction of pKa in a system with high orthogonal barriers: Alchemical flying Gaussian method. Chemical Physics Letters, 2020, 760, 138012.	2.6	3
10	Time-Lagged t-Distributed Stochastic Neighbor Embedding (t-SNE) of Molecular Simulation Trajectories. Frontiers in Molecular Biosciences, 2020, 7, 132.	3.5	37
11	A framework to assess the quality and impact of bioinformatics training across ELIXIR. PLoS Computational Biology, 2020, 16, e1007976.	3.2	7
12	Regioselective 3â€Oâ€Substitution of Unprotected Thiodigalactosides: Direct Route to Galectin Inhibitors. Chemistry - A European Journal, 2020, 26, 9620-9631.	3.3	20
13	Active site complementation and hexameric arrangement in the GH family 29; a structureâ€“function study of Î±-l-fucosidase isoenzyme 1 from Paenibacillus thiaminolyticus. Glycobiology, 2019, 29, 59-73.	2.5	12
14	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
15	Editorial: Machine Learning in Biomolecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 76.	3.5	4
16	Archangelolide: A sesquiterpene lactone with immunobiological potential from Laserpitium archangelica. Beilstein Journal of Organic Chemistry, 2019, 15, 1933-1944.	2.2	4
17	Anncolvar: Approximation of Complex Collective Variables by Artificial Neural Networks for Analysis and Biasing of Molecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 25.	3.5	24
18	Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain. Scientific Reports, 2019, 9, 18918.	3.3	6

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19	PEGylated Purpurin 18 with Improved Solubility: Potent Compounds for Photodynamic Therapy of Cancer. Molecules, 2019, 24, 4477.	3.8	14
20	The C-type lectin-like receptor Nkrp1b: Structural proteomics reveals features affecting protein conformation and interactions. Journal of Proteomics, 2019, 196, 162-172.	2.4	4
21	Estradiol dimer inhibits tubulin polymerization and microtubule dynamics. Journal of Steroid Biochemistry and Molecular Biology, 2018, 183, 68-79.	2.5	16
22	The dehydration stress of couch grass is associated with its lipid metabolism, the induction of transporters and the re-programming of development coordinated by ABA. BMC Genomics, 2018, 19, 317.	2.8	3
23	Poly-N-Acetyllactosamine Neo-Glycoproteins as Nanomolar Ligands of Human Galectin-3: Binding Kinetics and Modeling. International Journal of Molecular Sciences, 2018, 19, 372.	4.1	45
24	Reducing the number of mean-square deviation calculations with floating close structure in metadynamics. Journal of Chemical Physics, 2017, 146, 115101.	3.0	3
25	Multisystem altruistic metadynamicsâ€"Well-tempered variant. Journal of Chemical Physics, 2017, 146, 125103.	3.0	5
26	Free-Energy Surface Prediction by Flying Gaussian Method: Multisystem Representation. Journal of Physical Chemistry B, 2017, 121, 10479-10483.	2.6	4
27	CH/Ï€ Interactions in Carbohydrate Recognition. Molecules, 2017, 22, 1038.	3.8	94
28	Global Scale Transcriptional Profiling of Two Contrasting Barley Genotypes Exposed to Moderate Drought Conditions: Contribution of Leaves and Crowns to Water Shortage Coping Strategies. Frontiers in Plant Science, 2016, 7, 1958.	3.6	28
29	Membrane Interactions of the Mason-Pfizer Monkey Virus Matrix Protein and Its Budding Deficient Mutants. Journal of Molecular Biology, 2016, 428, 4708-4722.	4.2	3
30	Sampling Enhancement and Free Energy Prediction by the Flying Gaussian Method. Journal of Chemical Theory and Computation, 2016, 12, 4644-4650.	5.3	8
31	<scp>M</scp>olecular aspects of the interaction between <scp>M</scp>asonâ€"<scp>P</scp>fizer monkey virus matrix protein and artificial phospholipid membrane. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1717-1727.	2.6	3
32	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
33	Altruistic Metadynamics: Multisystem Biased Simulation. Journal of Physical Chemistry B, 2016, 120, 2209-2215.	2.6	16
34	Biocatalyzed synthesis of difuranosides and their ability to trigger production of TNF-Î±. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1550-1553.	2.2	8
35	Metadyn View: Fast web-based viewer of free energy surfaces calculated by metadynamics. Computer Physics Communications, 2016, 198, 222-229.	7.5	17
36	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 3866-3877.	5.3	60

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37	Molecular simulations of hevein/(GlcNAc)3 complex with weakened OH/O and CH/Ï€ hydrogen bonds: implications for their role in complex stabilization. Carbohydrate Research, 2015, 408, 1-7.	2.3	10
38	Nonlinear vs. linear biasing in Trp-cage folding simulations. Journal of Chemical Physics, 2015, 142, 115101.	3.0	12
39	Alpha-l-Fucosidase Isoenzyme iso2 from Paenibacillus thiaminolyticus. BMC Biotechnology, 2015, 15, 36.	3.3	20
40	Enhanced sampling techniques in biomolecular simulations. Biotechnology Advances, 2015, 33, 1130-1140.	11.7	96
41	Role of Mason-Pfizer Monkey Virus CA-NC Spacer Peptide-Like Domain in Assembly of Immature Particles. Journal of Virology, 2014, 88, 14148-14160.	3.4	15
42	Effect of Chain Elongation on Biological Properties of the Toxin Paralysin Î²â€Alanylâ€tyrosine. Chemical Biology and Drug Design, 2014, 83, 418-426.	3.2	1
43	Nucleotide binding triggers a conformational change of the CBS module of the magnesium transporter CNNM2 from a twisted towards a flat structure. Biochemical Journal, 2014, 464, 23-34.	3.7	41
44	Thermodynamics of the interaction between oxytocin and its myometrial receptor in sheep: A stepwise binding mechanism. Biochemical Pharmacology, 2014, 91, 119-127.	4.4	4
45	The versatile enzyme Araf51 allowed efficient synthesis of rare pathogen-related Î²-<scp>d</scp>-galactofuranosyl-pyranoside disaccharides. Organic and Biomolecular Chemistry, 2014, 12, 3080-3089.	2.8	8
46	On the Association of the Base Pairs on the Silica Surface Based on Free Energy Biased Molecular Dynamics Simulation and Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2013, 117, 11066-11075.	3.1	10
47	Toward an Accurate Conformational Modeling of Iduronic Acid. Journal of Physical Chemistry B, 2013, 117, 1003-1009.	2.6	20
48	Enzymatic synthesis of new C-6-acylated derivatives of NAG-thiazoline and evaluation of their inhibitor activities towards fungal Î²-N-acetylhexosaminidase. Journal of Molecular Catalysis B: Enzymatic, 2013, 87, 128-134.	1.8	13
49	Conformational Free Energy Modeling of Druglike Molecules by Metadynamics in the WHIM Space. Journal of Chemical Information and Modeling, 2012, 52, 804-813.	5.4	5
50	Dispersion interactions of carbohydrates with condensate aromatic moieties: Theoretical study on the CHâ€“Ï€ interaction additive properties. Physical Chemistry Chemical Physics, 2011, 13, 14215.	2.8	29
51	Free-Energy Simulations of Hydrogen Bonding versus Stacking of Nucleobases on a Graphene Surface. Journal of Physical Chemistry C, 2011, 115, 19455-19462.	3.1	24
52	Biochemical properties of three plant nucleases with anticancer potential. Plant Science, 2011, 180, 343-351.	3.6	21
53	Editorial [Hot Topic: Computational Glycochemistry and Glycobiology (Guest Editor: Vojtech) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.8	0
54	Threeâ€Dimensional Potential Energy Surface of Selected Carbohydratesâ€™ CH/Ï€ Dispersion Interactions Calculated by Highâ€Level Quantum Mechanical Methods. Chemistry - A European Journal, 2011, 17, 5680-5690.	3.3	29

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55	Metadynamics in the conformational space nonlinearly dimensionally reduced by Isomap. Journal of Chemical Physics, 2011, 135, 224504.	3.0	62
56	Modelling the Effect of Solvents on Carbohydrates. Mini-Reviews in Organic Chemistry, 2011, 8, 249-255.	1.3	5
57	Modelling of Î²-d-glucopyranose ring distortion in different force fields: a metadynamics study. Carbohydrate Research, 2010, 345, 530-537.	2.3	61
58	Cross-Talk between the Catalytic Core and the Regulatory Domain in Cystathionine Î²-Synthase: Study by Differential Covalent Labeling and Computational Modeling. Biochemistry, 2010, 49, 10526-10534.	2.5	15
59	Enzymatic synthesis of oligo-d-galactofuranosides and l-arabinofuranosides: from molecular dynamics to immunological assays. Organic and Biomolecular Chemistry, 2010, 8, 2092.	2.8	31
60	Metadynamics modelling of the solvent effect on primary hydroxyl rotamer equilibria in hexopyranosides. Carbohydrate Research, 2009, 344, 1575-1581.	2.3	25
61	Conformational Free Energy Surface of Î±-N-Acetylneuraminic Acid: An Interplay Between Hydrogen Bonding and Solvation. Journal of Physical Chemistry B, 2009, 113, 9589-9594.	2.6	32
62	Continuous metadynamics in essential coordinates as a tool for free energy modelling of conformational changes. Journal of Molecular Modeling, 2008, 14, 995-1002.	1.8	22
63	Potentialâ€Energy and Freeâ€Energy Surfaces of Glycylâ€Phenylalanylâ€Alanine (GFA) Tripeptide: Experiment and Theory. Chemistry - A European Journal, 2008, 14, 4886-4898.	3.3	47
64	Synthesis, In Vitro, and In Silico Evaluation of Organometallic Technetium and Rhenium Thymidine Complexes with Retained Substrate Activity toward Human Thymidine Kinase Type 1. Journal of Medicinal Chemistry, 2008, 51, 6689-6698.	6.4	43
65	Metadynamics in Essential Coordinates:â€‰ Free Energy Simulation of Conformational Changes. Journal of Physical Chemistry B, 2007, 111, 3073-3076.	2.6	93
66	Synthesis, in vitro and in silico assessment of organometallic Rhenium(I) and Technetium(I) thymidine complexes. Journal of Organometallic Chemistry, 2007, 692, 1255-1264.	1.8	22
67	Cold-active enzymes studied by comparative molecular dynamics simulation. Journal of Molecular Modeling, 2007, 13, 485-497.	1.8	42
68	Modelling of carbohydrateâ€“aromatic interactions: ab initio energetics and force field performance. Journal of Computer-Aided Molecular Design, 2006, 19, 887-901.	2.9	58
69	Cold-active Î²-Galactosidase from Arthrobacter sp. C2-2 Forms Compact 660kDa Hexamers: Crystal Structure at 1.9Ã... Resolution. Journal of Molecular Biology, 2005, 353, 282-294.	4.2	108
70	Crystallization and Preliminary X-ray Diffraction Analysis of Cold-Active Î²-Galactosidase from Arthrobacter sp. C2-2. Collection of Czechoslovak Chemical Communications, 2005, 70, 124-132.	1.0	3
71	Role of CH/Ï€ interactions in substrate binding by Escherichia coli Î²-galactosidase. Carbohydrate Research, 2004, 339, 2275-2280.	2.3	96
72	The cloning, purification and characterisation of a cold-active Î²-galactosidase from the psychrotolerant Antarctic bacterium Arthrobacter sp. C2-2. Enzyme and Microbial Technology, 2003, 33, 836-844.	3.2	66

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73	Collective Variable for Metadynamics Derived From AlphaFold Output. Frontiers in Molecular Biosciences, 0, 9, .	3.5	5