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	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
2	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
3	Role of CH/Ï€ interactions in substrate binding by Escherichia coli Î²-galactosidase. Carbohydrate Research, 2004, 339, 2275-2280.	2.3	96
4	Enhanced sampling techniques in biomolecular simulations. Biotechnology Advances, 2015, 33, 1130-1140.	11.7	96
5	CH/Ï€ Interactions in Carbohydrate Recognition. Molecules, 2017, 22, 1038.	3.8	94
6	Metadynamics in Essential Coordinates:â€‰ Free Energy Simulation of Conformational Changes. Journal of Physical Chemistry B, 2007, 111, 3073-3076.	2.6	93
7	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
8	Metadynamics in the conformational space nonlinearly dimensionally reduced by Isomap. Journal of Chemical Physics, 2011, 135, 224504.	3.0	62
9	Modelling of Î²-d-glucopyranose ring distortion in different force fields: a metadynamics study. Carbohydrate Research, 2010, 345, 530-537.	2.3	61
10	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
11	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
12	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
13	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
14	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
15	Cold-active enzymes studied by comparative molecular dynamics simulation. Journal of Molecular Modeling, 2007, 13, 485-497.	1.8	42
16	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
17	Na+/K+-ATPase Revisited: On Its Mechanism of Action, Role in Cancer, and Activity Modulation. Molecules, 2021, 26, 1905.	3.8	40
18	Time-Lagged t-Distributed Stochastic Neighbor Embedding (t-SNE) of Molecular Simulation Trajectories. Frontiers in Molecular Biosciences, 2020, 7, 132.	3.5	37

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19	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
20	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
21	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
22	Threeâ€Ðimensional Potential Energy Surface of Selected Carbohydratesâ€™ CH/Ï€ Dispersion Interactions Calculated by Highâ€Łevel Quantum Mechanical Methods. Chemistry - A European Journal, 2011, 17, 5680-5690.	3.3	29
23	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
24	Metadynamics modelling of the solvent effect on primary hydroxyl rotamer equilibria in hexopyranosides. Carbohydrate Research, 2009, 344, 1575-1581.	2.3	25
25	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
26	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
27	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
28	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
29	Biochemical properties of three plant nucleases with anticancer potential. Plant Science, 2011, 180, 343-351.	3.6	21
30	Toward an Accurate Conformational Modeling of Iduronic Acid. Journal of Physical Chemistry B, 2013, 117, 1003-1009.	2.6	20
31	Alpha-l-Fucosidase Isoenzyme iso2 from Paenibacillus thiaminolyticus. BMC Biotechnology, 2015, 15, 36.	3.3	20
32	Regioselective 3â€Oâ€Substitution of Unprotected Thiodigalactosides: Direct Route to Galectin Inhibitors. Chemistry - A European Journal, 2020, 26, 9620-9631.	3.3	20
33	Quo vadis Cardiac Glycoside Research?. Toxins, 2021, 13, 344.	3.4	20
34	Metadyn View: Fast web-based viewer of free energy surfaces calculated by metadynamics. Computer Physics Communications, 2016, 198, 222-229.	7.5	17
35	Altruistic Metadynamics: Multisystem Biased Simulation. Journal of Physical Chemistry B, 2016, 120, 2209-2215.	2.6	16
36	Estradiol dimer inhibits tubulin polymerization and microtubule dynamics. Journal of Steroid Biochemistry and Molecular Biology, 2018, 183, 68-79.	2.5	16

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37	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
38	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
39	PEGylated Purpurin 18 with Improved Solubility: Potent Compounds for Photodynamic Therapy of Cancer. Molecules, 2019, 24, 4477.	3.8	14
40	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
41	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
42	Nonlinear vs. linear biasing in Trp-cage folding simulations. Journal of Chemical Physics, 2015, 142, 115101.	3.0	12
43	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
44	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
45	Molecular simulations of hevein/(GlcNAc)3 complex with weakened OH/O and CH/Î€ hydrogen bonds: implications for their role in complex stabilization. Carbohydrate Research, 2015, 408, 1-7.	2.3	10
46	An Early Stage Researcher's Primer on Systems Medicine Terminology. Network and Systems Medicine, 2021, 4, 2-50.	2.5	9
47	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
48	Sampling Enhancement and Free Energy Prediction by the Flying Gaussian Method. Journal of Chemical Theory and Computation, 2016, 12, 4644-4650.	5.3	8
49	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
50	A framework to assess the quality and impact of bioinformatics training across ELIXIR. PLoS Computational Biology, 2020, 16, e1007976.	3.2	7
51	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
52	Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain. Scientific Reports, 2019, 9, 18918.	3.3	6
53	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
54	Multisystem altruistic metadynamicsâ€”Well-tempered variant. Journal of Chemical Physics, 2017, 146, 125103.	3.0	5

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55	Modelling the Effect of Solvents on Carbohydrates. Mini-Reviews in Organic Chemistry, 2011, 8, 249-255.	1.3	5
56	Collective Variable for Metadynamics Derived From AlphaFold Output. Frontiers in Molecular Biosciences, 0, 9, .	3.5	5
57	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
58	Free-Energy Surface Prediction by Flying Gaussian Method: Multisystem Representation. Journal of Physical Chemistry B, 2017, 121, 10479-10483.	2.6	4
59	Editorial: Machine Learning in Biomolecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 76.	3.5	4
60	Archangelolide: A sesquiterpene lactone with immunobiological potential from Laserpitium archangelica. Beilstein Journal of Organic Chemistry, 2019, 15, 1933-1944.	2.2	4
61	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
62	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
63	<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
64	Reducing the number of mean-square deviation calculations with floating close structure in metadynamics. Journal of Chemical Physics, 2017, 146, 115101.	3.0	3
65	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
66	Prediction of pKa in a system with high orthogonal barriers: Alchemical flying Gaussian method. Chemical Physics Letters, 2020, 760, 138012.	2.6	3
67	Transglycosylation abilities of Î²-d-galactosidases from GH family 2. 3 Biotech, 2021, 11, 168.	2.2	3
68	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
69	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
70	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
71	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
72	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1

#	Article	IF	Citations
73	Editorial [Hot Topic: Computational Glycochemistry and Glycobiology (Guest Editor: Vojtech) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	1.5	0