Mihaly Mezei

List of Publications by Year
in descending order

98	4,778	172457	102487
papers	citations	29 h-index	66 g-index

102	102	102	5210
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery. Current Computer-Aided Drug Design, 2011, 7, 146-157.	1.2	1,955
2	A cavity-biased (T, V, Î¼) Monte Carlo method for the computer simulation of fluids. Molecular Physics, 1980, 40, 901-906.	1.7	227
3	Monte Carlo studies of the structure of dilute aqueous sclutions of Li+, Na+, K+, Fâ^', and Clâ^'. Journal of Chemical Physics, 1981, 74, 6902-6910.	3.0	215
4	Theoretical studies of hydrogen bonding in liquid water and dilute aqueous solutions. Journal of Chemical Physics, 1981, 74, 622-632.	3.0	213
5	Polyproline II helix is the preferred conformation for unfolded polyalanine in water. Proteins: Structure, Function and Bioinformatics, 2004, 55, 502-507.	2.6	158
6	Grand-canonical ensemble Monte Carlo study of dense liquid. Molecular Physics, 1987, 61, 565-582.	1.7	150
7	Studies on free energy calculations. I. Thermodynamic integration using a polynomial path. Journal of Chemical Physics, 1993, 99, 6052-6061.	3.0	91
8	A new method for mapping macromolecular topography. Journal of Molecular Graphics and Modelling, 2003, 21, 463-472.	2.4	89
9	Simulaid: A simulation facilitator and analysis program. Journal of Computational Chemistry, 2010, 31, 2658-2668.	3.3	85
10	Convergence characteristics of Monte Carloâ€“Metropolis computer simulations on liquid water. Journal of Chemical Physics, 1979, 71, 3366-3373.	3.0	78
11	Selective Inhibition of SIN3 Corepressor with Avermectins as a Novel Therapeutic Strategy in Triple-Negative Breast Cancer. Molecular Cancer Therapeutics, 2015, 14, 1824-1836.	4.1	65
12	Characterization of the Binding Site of Aspartame in the Human Sweet Taste Receptor. Chemical Senses, 2015, 40, 577-586.	2.0	64
13	Structure-Guided Discovery of Selective Antagonists for the Chromodomain of Polycomb Repressive Protein CBX7. ACS Medicinal Chemistry Letters, 2016, 7, 601-605.	2.8	55
14	Monte Carlo Computer Simulation of the Aqueous Hydration of the Glycine Zwitterion at 25Â°C. Journal of Biomolecular Structure and Dynamics, 1984, 2, 1-27.	3.5	51
15	Theoretical Calculation of the Liquidâ€”Vapor Coexistence Curve of Water, Chloroform and Methanol with the Cavity-Biased Monte Carlo Method in the Gibbs Ensemble. Molecular Simulation, 1992, 9, 257-267.	2.0	50
16	Grand canonical ensemble Monte Carlo simulation of a lipid bilayer using extension biased rotations. Journal of Chemical Physics, 1999, 111, 10770-10773.	3.0	49
17	Excess free energy of different water models computed by Monte Carlo methods. Molecular Physics, 1982, 47, 1307-1315.	1.7	48
18	Monte Carlo Computer Simulation Studies of the Equilibrium Properties and Structure of Liquid Water. Advances in Chemistry Series, 1983, , 297-351.	0.6	47

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19	Lucanthone and Its Derivative Hycanthone Inhibit Apurinic Endonuclease-1 (APE1) by Direct Protein Binding. PLoS ONE, 2011, 6, e23679.	2.5	45
20	Convergence acceleration in Monte Carlo computer simulation on water and aqueous solutions. Journal of Chemical Physics, 1983, 78, 3156-3166.	3.0	43
21	Optimal position of solute for simulations. Journal of Computational Chemistry, 1997, 18, 812-815.	3.3	42
22	An NR2F1-specific agonist suppresses metastasis by inducing cancer cell dormancy. Journal of Experimental Medicine, 2022, 219, .	8.5	42
23	Prediction of protein loop structures using a local move Monte Carlo approach and a grid-based force field. Protein Engineering, Design and Selection, 2008, 21, 729-735.	2.1	35
24	TRAJELIX: A Computational Tool for the Geometric Characterization of Protein Helices During Molecular Dynamics Simulations. Journal of Computer-Aided Molecular Design, 2006, 20, 97-107.	2.9	34
25	TSH Receptor Signaling Abrogation by a Novel Small Molecule. Frontiers in Endocrinology, 2016, 7, 130.	3.5	34
26	Studies on free energy calculations. II. A theoretical approach to molecular solvation. Journal of Chemical Physics, 1994, 101, 6126-6140.	3.0	32
27	New Small Molecule Agonists to the Thyrotropin Receptor. Thyroid, 2015, 25, 51-62.	4.5	32
28	Direct Calculation of the Excess Free Energy of the Dense Lennard-Jones Fluid. Molecular Simulation, 1989, 2, 201-207.	2.0	31
29	Further quasicomponent distribution function analysis of liquid water. Temperature dependence of the results. Journal of Chemical Physics, 1982, 76, 593-600.	3.0	29
30	Evaluation of the Adaptive Umbrella Sampling Method. Molecular Simulation, 1989, 3, 301-313.	2.0	29
31	Monte Carlo Studies on Water in the dCpG/Proflavin Crystal Hydrate. Journal of Biomolecular Structure and Dynamics, 1983, 1, 287-297.	3.5	28
32	Computer simulation study of liquid CH2F2 with a new effective pair potential model. Journal of Chemical Physics, 1999, 110, 2991-3002.	3.0	27
33	Identification of a small-molecule ligand that activates the neuropeptide receptor GPR171 and increases food intake. Science Signaling, 2016, 9, ra55.	3.6	26
34	Calculation of Solvation Free-Energy Differences for Large Solute Change from Computer Simulations with Quadrature-Based Nearly Linear Thermodynamic Integration. Molecular Simulation, 1993, 10, 225-239.	2.0	24
35	Modified Proximity Criteria for the Analysis of the Solvation of a Polyfunctional Solute. Molecular Simulation, 1988, 1, 327-332.	2.0	23
36	Efficient Monte Carlo sampling for long molecular chains using local moves, tested on a solvated lipid bilayer. Journal of Chemical Physics, 2003, 118, 3874-3879.	3.0	23

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37	Identifying a Small Molecule Blocking Antigen Presentation in Autoimmune Thyroiditis. Journal of Biological Chemistry, 2016, 291, 4079-4090.	3.4	23
38	The BigLEN-GPR171 Peptide Receptor System Within the Basolateral Amygdala Regulates Anxiety-Like Behavior and Contextual Fear Conditioning. Neuropsychopharmacology, 2017, 42, 2527-2536.	5.4	23
39	Monte Carlo loop refinement and virtual screening of the thyroid-stimulating hormone receptor transmembrane domain. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1140-1152.	3.5	22
40	Virial-bias Monte Carlo methods. Molecular Physics, 1983, 48, 1075-1082.	1.7	21
41	MC-PHS: A Monte Carlo Implementation of the Primary Hydration Shell for Protein Folding and Design. Biophysical Journal, 2003, 84, 805-815.	0.5	21
42	Assessing the binding of cholinesterase inhibitors by docking and molecular dynamics studies. Journal of Molecular Graphics and Modelling, 2017, 76, 36-42.	2.4	21
43	Computer Aided Identification of Small Molecules Disrupting uPAR/Î±5Î²1- Integrin Interaction: A New Paradigm for Metastasis Prevention. PLoS ONE, 2009, 4, e4617.	2.5	20
44	A cooperative calculation and analysis of electric fields, induced dipole vectors and lattice energies for rotationally ordered ices IX, II and disordered Ih. Molecular Physics, 1980, 41, 883-905.	1.7	19
45	Homology Modeling and Site-Directed Mutagenesis To Identify Selective Inhibitors of Endothelin-Converting Enzyme-2. Journal of Medicinal Chemistry, 2008, 51, 3378-3387.	6.4	17
46	Dockres: a computer program that analyzes the output of virtual screening of small molecules. Source Code for Biology and Medicine, 2010, 5, 2.	1.7	17
47	Generic solvent sites in a crystal. Journal of Computational Chemistry, 1984, 5, 523-527.	3.3	16
48	Transmembrane Domains of Attraction on the TSH Receptor. Endocrinology, 2015, 156, 488-498.	2.8	16
49	Monte Carlo analysis of conformational transitions in superhelical DNA. Journal of Chemical Physics, 1995, 103, 8653-8665.	3.0	15
50	Conformational Space Comparison of GnRH and lGnRH-III using Molecular Dynamics, Cluster Analysis and Monte Carlo Thermodynamic Integration. Journal of Biomolecular Structure and Dynamics, 2001, 18, 733-748.	3.5	15
51	Computer Simulation Studies of the Fully Solvated Wild-type and Mutated GnRH in Extended and Î²turn Conformations. Journal of Biomolecular Structure and Dynamics, 1998, 16, 723-732.	3.5	14
52	Automatic Control of Solvent Density in Grand Canonical Ensemble Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1429-1434.	5.3	14
53	A Gq Biased Small Molecule Active at the TSH Receptor. Frontiers in Endocrinology, 2020, 11, 372.	3.5	13
54	Statistical Properties of Protein-Protein Interfaces. Algorithms, 2015, 8, 92-99.	2.1	12

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55	A Modifying Autoantigen in Gravesâ€™ Disease. Endocrinology, 2019, 160, 1008-1020.	2.8	11
56	Retro-inverso D-peptides as a novel targeted immunotherapy for Type 1 diabetes. Journal of Autoimmunity, 2020, 115, 102543.	6.5	10
57	Test of the overlap ratio method on the calculation of the aqueous hydration free energy difference between acetone and dimethylamine. Molecular Physics, 1988, 65, 219-223.	1.7	9
58	Modeling dimerizations of transmembrane proteins using Brownian dynamics simulations. Journal of Computer-Aided Molecular Design, 2008, 22, 553-561.	2.9	9
59	The energetics of the acetylation switch in p53â€mediated transcriptional activation. Proteins: Structure, Function and Bioinformatics, 2010, 78, 447-456.	2.6	9
60	Discriminatory Power of Stoichiometry-Driven Protein Folding?. Journal of Biomolecular Structure and Dynamics, 2011, 28, 625-626.	3.5	9
61	Implications of an Improved Model of the TSH Receptor Transmembrane Domain (TSHR-TMD-TRIO). Endocrinology, 2021, 162, .	2.8	9
62	Inhibitor of CBP Histone Acetyltransferase Downregulates p53 Activation and Facilitates Methylation at Lysine 27 on Histone H3. Molecules, 2018, 23, 1930.	3.8	8
63	On predicting foldability of a protein from its sequence. Proteins: Structure, Function and Bioinformatics, 2020, 88, 355-365.	2.6	8
64	Rescore protein-protein docked ensembles with an interface contact statistics. Proteins: Structure, Function and Bioinformatics, 2017, 85, 235-241.	2.6	7
65	Protein Binding Pocket Optimization for Virtual High-Throughput Screening (vHTS) Drug Discovery. ACS Omega, 2020, 5, 14297-14307.	3.5	7
66	Monte Carlo Studies of the Structure of Liquid Water and Dilute Aqueous Solutions. ACS Symposium Series, 1978, , 191-218.	0.5	6
67	Comparison of the percolation model with computer simulation results on different water models. Molecular Physics, 1984, 52, 1003-1010.	1.7	6
68	A Near-neighbour Algorithm for Metropolis Monte Carlo Simulations. Molecular Simulation, 1988, 1, 169-171.	2.0	6
69	Comment on â€œMolecular dynamics simulations in the grand canonical ensemble: Formulation of a bias potential for umbrella samplingâ€•[J. Chem. Phys. 110, 8295 (1999)]. Journal of Chemical Physics, 2000, 112, 1059-1060.	3.0	6
70	A novel fingerprint for the characterization of protein folds. Protein Engineering, Design and Selection, 2003, 16, 713-715.	2.1	6
71	Comparison of a quantum random number generator with pseudorandom number generators for their use in molecular Monte Carlo simulations. Journal of Computational Chemistry, 2017, 38, 2713-2720.	3.3	6
72	Revisiting Chameleon Sequences in the Protein Data Bank. Algorithms, 2018, 11, 114.	2.1	6

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73	Statistical Thermodynamics Through Computer Simulation to Characterize Phospholipid Interactions in Membranes. Methods in Molecular Biology, 2007, 400, 127-144.	0.9	5
74	The Biological Significance of Targeting Acetylation-Mediated Gene Regulation for Designing New Mechanistic Tools and Potential Therapeutics. Biomolecules, 2021, 11, 455.	4.0	5
75	Computational analysis of the effects of site-specific phosphate alkylation in the DNA oligomer {d-[GGAATTCC]}2. Biopolymers, 1990, 29, 597-607.	2.4	3
76	The Effect of the Combined Volume on the Efficiency of Gibbs Ensemble Simulations. Molecular Simulation, 1993, 11, 395-397.	2.0	3
77	Iso-energy cutoff for the calculation of interionic potential of mean force in water. International Journal of Quantum Chemistry, 1994, 52, 147-152.	2.0	3
78	Results from an Early Polarization Model Based on Maxwell's Invariant Multipole Form. Journal of Chemical Theory and Computation, 2007, 3, 2138-2145.	5.3	3
79	Automatic Determination of Stepsize Parameters in Monte Carlo Simulation Tested on a Bromodomain-Binding Octapeptide. Algorithms, 2009, 2, 215-226.	2.1	3
80	The role of protein â€œStability patchesâ€•in molecular recognition: A case study of the human growth hormoneâ€•receptor complex. Journal of Computational Chemistry, 2016, 37, 913-919.	3.3	3
81	Foldability and chameleon propensity of foldâ€switching protein sequences. Proteins: Structure, Function and Bioinformatics, 2021, 89, 3-5.	2.6	3
82	The anisotropic virial-biased sampling for Monte Carlo simulations in the isothermalâ€”isobaric ensemble. Molecular Physics, 1999, 96, 293-296.	1.7	2
83	Calculating the local solvent chemical potential in crystal hydrates. Physical Review E, 2000, 62, 7077-7081.	2.1	2
84	Free Energy Simulations Over Creation/Annihilation Paths for a Flexible Solute. Molecular Simulation, 2002, 28, 39-44.	2.0	2
85	Use of circular variance to quantify the deviation of a macromolecule from the spherical shape. Journal of Mathematical Chemistry, 2015, 53, 2184-2190.	1.5	2
86	Exploiting Sparse Statistics for a Sequence-Based Prediction of the Effect of Mutations. Algorithms, 2019, 12, 214.	2.1	2
87	An algorithm for the calculation of the net induction energy and induced multipole tensors in a set of charge distributions with non-linear contributions of all potentials of external fields and both permanent and induced multipoles. Molecular Physics, 1986, 57, 1201-1218.	1.7	1
88	A novel approach to the calculation of the free energy due to molecular flexibility. Journal of Mathematical Chemistry, 2000, 27, 235-250.	1.5	1
89	Pspace: a program that assesses protein space. Source Code for Biology and Medicine, 2007, 2, 6.	1.7	1
90	In Silico Modeling of Novel Drug Ligands for Treatment of Concussion Associated Tauopathy. Journal of Cellular Biochemistry, 2016, 117, 2241-2248.	2.6	1

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91	Virtual screening of a natural compound library at orthosteric and allosteric binding sites of the neurotensin receptor. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4494-4506.	3.5	1
92	The Human TSHÎ² Subunit Proteins and Their Binding Sites on the TSH Receptor Using Molecular Dynamics Simulation. Endocrinology, 2020, 161, .	2.8	1
93	Observation of quantum signature in rivastigmine chemical bond break-up and quantum energetics, spectral studies of anti-Alzheimer inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 118-128.	3.5	1
94	Use of the Codon Table to Quantify the Evolutionary Role of Random Mutations. Algorithms, 2021, 14, 270.	2.1	1
95	Using Force-Field Grids for Sampling Translation/Rotation of Partially Rigid Macromolecules. Algorithms, 2017, 10, 6.	2.1	0
96	OR10-2 A Modifying Autoantigen in Graves' Disease. Journal of the Endocrine Society, 2019, 3, .	0.2	0
97	SAT-558 Tsh Modulation Of Bone Biology - Further Evidence From A Recombinant Tsh-Î² Variant.. Journal of the Endocrine Society, 2019, 3, .	0.2	0
98	Tools for Characterizing Proteins: Circular Variance, Mutual Proximity, Chameleon Sequences, and Subsequence Propensities. Methods in Molecular Biology, 2022, 2405, 39-61.	0.9	0