Chris Oostenbrink

List of Publications by Year
in descending order

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214 papers	13,797 citations	47 h-index	110 g-index
226 all docs	226 docs citations	226 times ranked	14281 citing authors

#	Article	IF	Citations
1	A biomolecular force field based on the free enthalpy of hydration and solvation: The GROMOS force-field parameter sets 53A5 and 53A6. Journal of Computational Chemistry, 2004, 25, 1656-1676.	3.3	3,309
2	An Automated Force Field Topology Builder (ATB) and Repository: Version 1.0. Journal of Chemical Theory and Computation, 2011, 7, 4026-4037.	5.3	1,425
3	The GROMOS software for biomolecular simulation: GROMOS05. Journal of Computational Chemistry, 2005, 26, 1719-1751.	3.3	592
4	Molecular dynamics simulations. Current Opinion in Structural Biology, 2002, 12, 190-196.	5.7	551
5	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	13.8	503
6	Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284.	2.2	443
7	New Interaction Parameters for Charged Amino Acid Side Chains in the GROMOS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 3705-3723.	5.3	189
8	A consistent potential energy parameter set for lipids: dipalmitoylphosphatidylcholine as a benchmark of the GROMOS96 45A3 force field. European Biophysics Journal, 2003, 32, 67-77.	2.2	181
9	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. Journal of Chemical Theory and Computation, 2011, 7, 3379-3390.	5.3	180
10	An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737.	3.3	161
11	Exploring genetic suppression interactions on a global scale. Science, 2016, 354, .	12.6	157
12	The Role of Water Molecules in Computational Drug Design. Current Topics in Medicinal Chemistry, 2010, 10, 55-66.	2.1	155
13	Estimating entropies from molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 2652-2661.	3.0	138
14	Catalytic Site Prediction and Virtual Screening of Cytochrome P450 2D6 Substrates by Consideration of Water and Rescoring in Automated Docking. Journal of Medicinal Chemistry, 2006, 49, 2417-2430.	6.4	138
15	A fast and sensitive activity assay for lytic polysaccharide monooxygenase. Biotechnology for Biofuels, 2018, 11, 79.	6.2	126
16	Impact of Plasticity and Flexibility on Docking Results for Cytochrome P450 2D6: A Combined Approach of Molecular Dynamics and Ligand Docking. Journal of Medicinal Chemistry, 2008, 51, 7469-7477.	6.4	123
17	Free energies of ligand binding for structurally diverse compounds. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6750-6754.	7.1	107
18	Improved Ligand-Protein Binding Affinity Predictions Using Multiple Binding Modes. Biophysical Journal, 2010, 98, 2682-2691.	0.5	104

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19	Identification of Critical Residues in Novel Drug Metabolizing Mutants of Cytochrome P450 BM3 Using Random Mutagenesis. Journal of Medicinal Chemistry, 2007, 50, 455-461.	6.4	101
20	Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902.	13.8	101
21	Simulations of the Estrogen Receptor Ligand-Binding Domain:â€‰ Affinity of Natural Ligands and Xenoestrogens. Journal of Medicinal Chemistry, 2000, 43, 4594-4605.	6.4	100
22	An Effective Force Field for Molecular Dynamics Simulations of Dimethyl Sulfoxide and Dimethyl Sulfoxideâ^'Water Mixtures. Journal of Physical Chemistry B, 2004, 108, 1436-1445.	2.6	97
23	Classification of Cytochrome P450 1A2 Inhibitors and Noninhibitors by Machine Learning Techniques. Drug Metabolism and Disposition, 2009, 37, 658-664.	3.3	91
24	Testing of the GROMOS Force-Field Parameter Set 54A8: Structural Properties of Electrolyte Solutions, Lipid Bilayers, and Proteins. Journal of Chemical Theory and Computation, 2013, 9, 1247-1264.	5.3	88
25	A Systematic Framework for Molecular Dynamics Simulations of Protein Post-Translational Modifications. PLoS Computational Biology, 2013, 9, e1003154.	3.2	88
26	Validation of the GROMOS force-field parameter set 45A3 against nuclear magnetic resonance data of hen egg lysozyme. Journal of Biomolecular NMR, 2004, 30, 407-422.	2.8	87
27	Free energy calculations of proteinâ€“ligand interactions. Current Opinion in Chemical Biology, 2011, 15, 547-552.	6.1	83
28	Water in protein hydration and ligand recognition. Journal of Molecular Recognition, 2019, 32, e2810.	2.1	81
29	Hamiltonian replica exchange molecular dynamics using soft-core interactions. Journal of Chemical Physics, 2008, 128, 144121.	3.0	79
30	Virtual Screening and Prediction of Site of Metabolism for Cytochrome P450 1A2 Ligands. Journal of Chemical Information and Modeling, 2009, 49, 43-52.	5.4	78
31	Prediction of cytochrome P450 mediated metabolism. Advanced Drug Delivery Reviews, 2015, 86, 61-71.	13.7	78
32	Free energies of binding of polychlorinated biphenyls to the estrogen receptor from a single simulation. Proteins: Structure, Function and Bioinformatics, 2003, 54, 237-246.	2.6	77
33	Cytochrome P450 3A4 Inhibition by Ketoconazole: Tackling the Problem of Ligand Cooperativity Using Molecular Dynamics Simulations and Free-Energy Calculations. Journal of Chemical Information and Modeling, 2012, 52, 1573-1582.	5.4	77
34	Expression and glycoengineering of functionally active heteromultimeric IgM in plants. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 6263-6268.	7.1	77
35	Calculation of Relative Free Energies for Ligand-Protein Binding, Solvation, and Conformational Transitions Using the GROMOS Software. Journal of Physical Chemistry B, 2011, 115, 13570-13577.	2.6	71
36	Molecular Dynamics Simulations of the Standard Leonardite Humic Acid: Microscopic Analysis of the Structure and Dynamics. Environmental Science & Technology, 2017, 51, 5414-5424.	10.0	71

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37	Computational prediction of drug binding and rationalisation of selectivity towards cytochromes P450. Expert Opinion on Drug Metabolism and Toxicology, 2008, 4, 513-527.	3.3	67
38	Molecular dynamics simulations and free energy calculations of netropsin and distamycin binding to an AAAAA DNA binding site. Nucleic Acids Research, 2005, 33, 725-733.	14.5	66
39	Role of Water in Molecular Docking Simulations of Cytochrome P450 2D6. Journal of Chemical Information and Modeling, 2010, 50, 146-154.	5.4	66
40	Metabolic Regio- and Stereoselectivity of Cytochrome P450 2D6 towards 3,4-Methylenedioxy-N-alkylamphetamines:Â in Silico Predictions and Experimental Validation. Journal of Medicinal Chemistry, 2005, 48, 6117-6127.	6.4	64
41	Comparison of thermodynamic integration and Bennett acceptance ratio for calculating relative proteinâ€ligand binding free energies. Journal of Computational Chemistry, 2013, 34, 1024-1034.	3.3	63
42	Single-step perturbations to calculate free energy differences from unphysical reference states: Limits on size, flexibility, and character. Journal of Computational Chemistry, 2003, 24, 1730-1739.	3.3	62
43	Net charge changes in the calculation of relative ligand-binding free energies via classical atomistic molecular dynamics simulation. Journal of Computational Chemistry, 2014, 35, 227-243.	3.3	60
44	Are Automated Molecular Dynamics Simulations and Binding Free Energy Calculations Realistic Tools in Lead Optimization? An Evaluation of the Linear Interaction Energy (LIE) Method. Journal of Chemical Information and Modeling, 2006, 46, 1972-1983.	5.4	58
45	A Library of Fluorescent Peptides for Exploring the Substrate Specificities of Prolyl Isomerases. Biochemistry, 2009, 48, 10423-10436.	2.5	56
46	Methane clustering in explicit water: effect of urea on hydrophobic interactions. Physical Chemistry Chemical Physics, 2005, 7, 53.	2.8	52
47	Advances in the calculation of binding free energies. Current Opinion in Structural Biology, 2020, 61, 207-212.	5.7	52
48	Processing of complex N-glycans in IgG Fc-region is affected by core fucosylation. MAbs, 2015, 7, 863-870.	5.2	50
49	Calculation of the Redox Potential of the Protein Azurin and Some Mutants. ChemBioChem, 2005, 6, 738-746.	2.6	49
50	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. ChemMedChem, 2009, 4, 2070-2079.	3.2	46
51	Transiently Produced Hypochlorite Is Responsible for the Irreversible Inhibition of Chlorite Dismutase. Biochemistry, 2014, 53, 3145-3157.	2.5	46
52	Configurational Entropy Change of Netropsin and Distamycin upon DNA Minor-Groove Binding. Biophysical Journal, 2006, 91, 1460-1470.	0.5	45
53	Molecular Modeling-Guided Site-Directed Mutagenesis of Cytochrome P450 2D6. Current Drug Metabolism, 2007, 8, 59-77.	1.2	45
54	Conformationally Constrained Lipid A Mimetics for Exploration of Structural Basis of TLR4/MD-2 Activation by Lipopolysaccharide. ACS Chemical Biology, 2013, 8, 2423-2432.	3.4	45

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55	Update on phosphate and charged postâ€translationally modified amino acid parameters in the GROMOS force field. Journal of Computational Chemistry, 2017, 38, 714-720.	3.3	45
56	Identification of lectin receptors for conserved SARSâ€CoVâ€2 glycosylation sites. EMBO Journal, 2021, 40, e108375.	7.8	44
57	Two-Dimensional Heterospectral Correlation Analysis of the Redox-Induced Conformational Transition in Cytochrome c Using Surface-Enhanced Raman and Infrared Absorption Spectroscopies on a Two-Layer Gold Surface. Journal of Physical Chemistry B, 2013, 117, 9606-9614.	2.6	43
58	Efficient Free Energy Calculations for Compounds with Multiple Stable Conformations Separated by High Energy Barriers. Journal of Physical Chemistry B, 2009, 113, 12711-12720.	2.6	42
59	ACE2 is the critical in vivo receptor for SARS-CoV-2 in a novel COVID-19 mouse model with TNF- and IFNÎ³-driven immunopathology. ELife, 2022, 11, .	6.0	42
60	Molecular dynamics simulations give insight into the conformational change, complex formation, and electron transfer pathway for cytochrome P450 reductase. Protein Science, 2013, 22, 1183-1195.	7.6	41
61	Influence of Lytic Polysaccharide Monooxygenase Active Site Segments on Activity and Affinity. International Journal of Molecular Sciences, 2019, 20, 6219.	4.1	41
62	Cooperative Binding of Aflatoxin B₁ by Cytochrome P450 3A4: A Computational Study. Chemical Research in Toxicology, 2014, 27, 2136-2147.	3.3	40
63	Structural rationalization of novel drug metabolizing mutants of cytochrome P450 BM3. Proteins: Structure, Function and Bioinformatics, 2008, 71, 336-352.	2.6	39
64	Dihedral-Based Segment Identification and Classification of Biopolymers I: Proteins. Journal of Chemical Information and Modeling, 2014, 54, 266-277.	5.4	39
65	Structure of human promyeloperoxidase (proMPO) and the role of the propeptide in processing and maturation. Journal of Biological Chemistry, 2017, 292, 8244-8261.	3.4	38
66	Simulation of Reversible Proteinâ€“Protein Binding and Calculation of Binding Free Energies Using Perturbed Distance Restraints. Journal of Chemical Theory and Computation, 2017, 13, 5697-5708.	5.3	36
67	Calculating zeros: Non-equilibrium free energy calculations. Chemical Physics, 2006, 323, 102-108.	1.9	35
68	Clinical grade <scp>ACE2</scp> as a universal agent to block <scp>SARSâ€CoV</scp> â€2 variants. EMBO Molecular Medicine, 2022, 14, .	6.9	35
69	Efficient and Accurate Free Energy Calculations on Trypsin Inhibitors. Journal of Chemical Theory and Computation, 2012, 8, 3686-3695.	5.3	34
70	Efficient Calculation of Many Stacking and Pairing Free Energies in DNA from a Few Molecular Dynamics Simulations. Chemistry - A European Journal, 2005, 11, 4340-4348.	3.3	33
71	Computational Prediction of Binding Affinity for CYP1A2-Ligand Complexes Using Empirical Free Energy Calculations. Drug Metabolism and Disposition, 2010, 38, 1347-1354.	3.3	33
72	Vienna Soil-Organic-Matter Modelerâ€"Generating condensed-phase models of humic substances. Journal of Molecular Graphics and Modelling, 2015, 62, 253-261.	2.4	33

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73	The Impact of Using Single Atomistic Long-Range Cutoff Schemes with the GROMOS 54A7 Force Field. Journal of Chemical Theory and Computation, 2018, 14, 5823-5833.	5.3	33
74	Interaction between Cellobiose Dehydrogenase and Lytic Polysaccharide Monooxygenase. Biochemistry, 2019, 58, 1226-1235.	2.5	32
75	Improved spectrophotometric assay for lytic polysaccharide monooxygenase. Biotechnology for Biofuels, 2019, 12, 283.	6.2	31
76	Optimization of replica exchange molecular dynamics by fast mimicking. Journal of Chemical Physics, 2007, 127, 204104.	3.0	30
77	Redox Thermodynamics of High-Spin and Low-Spin Forms of Chlorite Dismutases with Diverse Subunit and Oligomeric Structures. Biochemistry, 2012, 51, 9501-9512.	2.5	30
78	Construction of pHâ€sensitive Her2â€binding IgG1â€Fc by directed evolution. Biotechnology Journal, 2014, 9, 1013-1022.	3.5	30
79	Direct Electron-Transfer Anisotropy of a Site-Specifically Immobilized Cellobiose Dehydrogenase. ACS Catalysis, 2019, 9, 7607-7615.	11.2	30
80	Efficient free energy calculations on small molecule hostâ€guest systemsâ€”A combined linear interaction energy/oneâ€step perturbation approach. Journal of Computational Chemistry, 2009, 30, 212-221.	3.3	29
81	Molecular dynamics simulations give insight into d-glucose dioxidation at C2 and C3 by Agaricus meleagris pyranose dehydrogenase. Journal of Computer-Aided Molecular Design, 2013, 27, 295-304.	2.9	29
82	Proteinâ€“Ligand Binding from Distancefield Distances and Hamiltonian Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2013, 9, 883-892.	5.3	29
83	Lipid a from lipopolysaccharide recognition: Structure, dynamics and cooperativity by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2013, 81, 658-674.	2.6	29
84	Antibody humanization by molecular dynamics simulationsâ€”inâ€silico guided selection of critical backmutations. Journal of Molecular Recognition, 2016, 29, 266-275.	2.1	29
85	Distinct FcÎ± receptor N-glycans modulate the binding affinity to immunoglobulin A (IgA) antibodies. Journal of Biological Chemistry, 2019, 294, 13995-14008.	3.4	29
86	Structure-guided glyco-engineering of ACE2 for improved potency as soluble SARS-CoV-2 decoy receptor. ELife, 2021, 10, .	6.0	29
87	CYP 2D6 Binding Affinity Predictions Using Multiple Ligand and Protein Conformations. International Journal of Molecular Sciences, 2013, 14, 24514-24530.	4.1	28
88	Redox Cofactor Rotates during Its Stepwise Decarboxylation: Molecular Mechanism of Conversion of Coproheme to Heme b. ACS Catalysis, 2019, 9, 6766-6782.	11.2	28
89	Binding free energy, energy and entropy calculations using simple model systems. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	27
90	Modeling of Oligosaccharides within Glycoproteins from Free-Energy Landscapes. Journal of Chemical Information and Modeling, 2017, 57, 2222-2236.	5.4	26

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91	Amine Hydration: A United-Atom Force-Field Solution. ChemPhysChem, 2005, 6, 1800-1804.	2.1	25
92	Extended Thermodynamic Integration: Efficient Prediction of Lambda Derivatives at Nonsimulated Points. Journal of Chemical Theory and Computation, 2016, 12, 4476-4486.	5.3	25
93	Calculation of Relative Binding Free Energy in the Water-Filled Active Site of Oligopeptide-Binding Protein A. Molecules, 2016, 21, 499.	3.8	24
94	Chemistry and Molecular Dynamics Simulations of Heme b-HemQ and Coproheme-HemQ. Biochemistry, 2016, 55, 5398-5412.	2.5	24
95	Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010.	13.8	24
96	Accelerated Enveloping Distribution Sampling: Enabling Sampling of Multiple End States while Preserving Local Energy Minima. Journal of Physical Chemistry B, 2018, 122, 5030-5037.	2.6	24
97	Correcting electrostatic artifacts due to netâ€charge changes in the calculation of ligand binding free energies. Journal of Computational Chemistry, 2020, 41, 986-999.	3.3	24
98	Biophysical and physicochemical methods differentiate highly ligand-efficient human D-amino acid oxidase inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 4808-4819.	5.5	22
99	Production of Circularly Permuted Caspase-2 for Affinity Fusion-Tag Removal: Cloning, Expression in Escherichia coli, Purification, and Characterization. Biomolecules, 2020, 10, 1592.	4.0	22
100	Vienna soil organic matter modeler 2 (VSOMM2). Journal of Molecular Graphics and Modelling, 2021, 103, 107817.	2.4	22
101	Insights into structural features determining odorant affinities to honey bee odorant binding protein 14. Biochemical and Biophysical Research Communications, 2014, 446, 1042-1046.	2.1	21
102	Free energies of binding of R- and S-propranolol to wild-type and F483A mutant cytochrome P450 2D6 from molecular dynamics simulations. European Biophysics Journal, 2007, 36, 589-599.	2.2	20
103	Toward Automated Free Energy Calculation with Accelerated Enveloping Distribution Sampling (A-EDS). Journal of Chemical Information and Modeling, 2020, 60, 5395-5406.	5.4	20
104	Calculations of binding affinity between C8-substituted GTP analogs and the bacterial cell-division protein FtsZ. European Biophysics Journal, 2010, 39, 1573-1580.	2.2	19
105	Molecular mechanism of allosteric communication in the human PPARÎ±â€RXRÎ± heterodimer. Proteins: Structure, Function and Bioinformatics, 2010, 78, 873-887.	2.6	19
106	On the thermodynamics of carbon nanotube single-file water loading: free energy, energy and entropy calculations. Physical Chemistry Chemical Physics, 2014, 16, 5119-5128.	2.8	19
107	Polarization Effects in Simulations of Kaoliniteâ€“Water Interfaces. Langmuir, 2019, 35, 15086-15099.	3.5	19
108	Actinobacterial Coproheme Decarboxylases Use Histidine as a Distal Base to Promote Compound I Formation. ACS Catalysis, 2020, 10, 5405-5418.	11.2	19

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109	Soil organic matter stabilization at molecular scale: The role of metal cations and hydrogen bonds. Geoderma, 2021, 401, 115237.	5.1	19
110	Chimeric Cellobiose Dehydrogenases Reveal the Function of Cytochrome Domain Mobility for the Electron Transfer to Lytic Polysaccharide Monooxygenase. ACS Catalysis, 2021, 11, 517-532.	11.2	19
111	MDplot: Visualise Molecular Dynamics. R Journal, 2017, 9, 164.	1.8	19
112	Comparison of murine and human estrogen sulfotransferase inhibition in vitro and in silicoâ€"Implications for differences in activity, subunit dimerization and substrate inhibition. Molecular and Cellular Endocrinology, 2010, 317, 127-140.	3.2	18
113	Calculation of binding free energies of inhibitors to plasmepsin II. Journal of Computational Chemistry, 2011, 32, 1801-1812.	3.3	18
114	Malleability and Versatility of Cytochrome P450 Active Sites Studied by Molecular Simulations. Current Drug Metabolism, 2012, 13, 190-196.	1.2	18
115	Thermodynamic Characterization of New Positive Allosteric Modulators Binding to the Glutamate Receptor A2 Ligand-Binding Domain: Combining Experimental and Computational Methods Unravels Differences in Driving Forces. Journal of Chemical Information and Modeling, 2014, 54, 3404-3416.	5.4	18
116	Plasmon Field-Enhanced Fluorescence Energy Transfer for Hairpin Aptamer Assay Readout. ACS Sensors, 2017, 2, 916-923.	7.8	18
117	Redox thermodynamics of B-class dye-decolorizing peroxidases. Journal of Inorganic Biochemistry, 2019, 199, 110761.	3.5	18
118	Binding Modes and Metabolism of Caffeine. Chemical Research in Toxicology, 2019, 32, 1374-1383.	3.3	18
119	Protein Conformational Change Is Essential for Reductive Activation of Lytic Polysaccharide Monooxygenase by Cellobiose Dehydrogenase. ACS Catalysis, 2020, 10, 4842-4853.	11.2	18
120	Free Energy Calculations from One-Step Perturbations. Methods in Molecular Biology, 2012, 819, 487-499.	0.9	18
121	BuRNN: Buffer Region Neural Network Approach for Polarizable-Embedding Neural Network/Molecular Mechanics Simulations. Journal of Physical Chemistry Letters, 2022, 13, 3812-3818.	4.6	18
122	Relative stability of homochiral and heterochiral dialanine peptides. Effects of perturbation pathways and force-field parameters on free energy calculations. Molecular Physics, 2005, 103, 1961-1969.	1.7	17
123	Investigation of Ion Binding in Chlorite Dismutases by Means of Molecular Dynamics Simulations. Biochemistry, 2014, 53, 4869-4879.	2.5	17
124	A pH Replica Exchange Scheme in the Stochastic Titration Constant-pH MD Method. Journal of Chemical Theory and Computation, 2019, 15, 3108-3116.	5.3	17
125	Exploring the binding pathways of the 14-3-3Î¶ protein: Structural and free-energy profiles revealed by Hamiltonian replica exchange molecular dynamics with distancefield distance restraints. PLoS ONE, 2017, 12, e0180633.	2.5	17
126	Simulating the Physiological Phase of Hydrated DPPC Bilayers: The Ester Moiety. Soft Materials, 2004, 2, 27-45.	1.7	16

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127	Recombinant plant-derived human IgE glycoproteomics. Journal of Proteomics, 2017, 161, 81-87.	2.4	16
128	The two cathepsin B-like proteases of Arabidopsis thaliana are closely related enzymes with discrete endopeptidase and carboxydipeptidase activities. Biological Chemistry, 2018, 399, 1223-1235.	2.5	16
129	Molecular modelling of sorption processes of a range of diverse small organic molecules in Leonardite humic acid. European Journal of Soil Science, 2020, 71, 831-844.	3.9	16
130	On using oscillating time-dependent restraints in MD simulation. Journal of Biomolecular NMR, 2007, 37, 1-14.	2.8	15
131	Freeâ€energy differences between states with different conformational ensembles. Journal of Computational Chemistry, 2013, 34, 1398-1408.	3.3	15
132	Reaction of pyranose dehydrogenase from AgaricusÂmeleagris with its carbohydrate substrates. FEBS Journal, 2015, 282, 4218-4241.	4.7	15
133	Anti-endotoxic activity and structural basis for human MD-2Â·TLR4 antagonism of tetraacylated lipid A mimetics based on Î²GlcN(1â†”1)Î±GlcN scaffold. Innate Immunity, 2015, 21, 490-503.	2.4	15
134	Free Energy Calculations Give Insight into the Stereoselective Hydroxylation of Î±-Ionones by Engineered Cytochrome P450 BM3 Mutants. Journal of Chemical Information and Modeling, 2012, 52, 2139-2148.	5.4	14
135	Multiple Binding Poses in the Hydrophobic Cavity of Bee Odorant Binding Protein AmelOBP14. Journal of Chemical Information and Modeling, 2015, 55, 2633-2643.	5.4	14
136	A contribution of molecular modeling to supramolecular structures in soil organic matter[#]. Journal of Plant Nutrition and Soil Science, 2022, 185, 44-59.	1.9	14
137	Entropic and Enthalpic Contributions to Stereospecific Ligand Binding from Enhanced Sampling Methods. Journal of Chemical Information and Modeling, 2014, 54, 151-158.	5.4	13
138	GroScore: Accurate Scoring of Proteinâ€“Protein Binding Poses Using Explicit-Solvent Free-Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 5074-5085.	5.4	13
139	Proteomics analysis of host cell proteins after immobilized metal affinity chromatography: Influence of ligand and metal ions. Journal of Chromatography A, 2020, 1633, 461649.	3.7	13
140	Charge-Changing Perturbations and Path Sampling via Classical Molecular Dynamic Simulations of Simple Guestâ€“Host Systems. Journal of Chemical Theory and Computation, 2020, 16, 7721-7734.	5.3	13
141	Binding of 7-methoxy-4-(aminomethyl)-coumarin to wild-type and W128F mutant cytochrome P450 2D6 studied by time-resolved fluorescence spectroscopy. Biochemical Journal, 2006, 393, 635-643.	3.7	12
142	A stereochemical switch in the aDrs model system, a candidate for a functional amyloid. Archives of Biochemistry and Biophysics, 2012, 522, 100-106.	3.0	12
143	Calculation of substrate binding affinities for a bacterial GH78 rhamnosidase through molecular dynamics simulations. Journal of Molecular Catalysis B: Enzymatic, 2013, 92, 34-43.	1.8	12
144	Toward the correction of effective electrostatic forces in explicit-solvent molecular dynamics simulations: restraints on solvent-generated electrostatic potential and solvent polarization. Theoretical Chemistry Accounts, 2015, 134, 2.	1.4	12

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145	Freeâ€energy calculations of residue mutations in a tripeptide using various methods to overcome inefficient sampling. Journal of Computational Chemistry, 2016, 37, 2597-2605.	3.3	12
146	Saturation Mutagenesis by Efficient Free-Energy Calculation. Journal of Chemical Theory and Computation, 2018, 14, 894-904.	5.3	12
147	The effect of different cutoff schemes in molecular simulations of proteins. Journal of Computational Chemistry, 2020, 41, 2740-2749.	3.3	12
148	Could Microwave Irradiation Cause Misfolding of Peptides?. Journal of Chemical Theory and Computation, 2020, 16, 2795-2802.	5.3	12
149	Molecular Conformations of Di-, Tri-, and Tetra-Î±-(2â†'8)-Linked Sialic Acid from NMR Spectroscopy and MD Simulations. International Journal of Molecular Sciences, 2020, 21, 30.	4.1	12
150	Modeling soil organic matter: Changes in macroscopic properties due to microscopic changes. Geochimica Et Cosmochimica Acta, 2021, 307, 228-241.	3.9	12
151	Reaction intermediate rotation during the decarboxylation of coproheme to heme b in C.Âdiphtheriae. Biophysical Journal, 2021, 120, 3600-3614.	0.5	12
152	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	2.1	12
153	Molecular Dynamics Simulation of the Crystallizable Fragment of IgG1â€"Insights for the Design of Fcabs. International Journal of Molecular Sciences, 2014, 15, 438-455.	4.1	11
154	Design of a colicin E7 based chimeric zinc-finger nuclease. Journal of Computer-Aided Molecular Design, 2014, 28, 841-850.	2.9	11
155	The Effect of Using a Twin-Range Cutoff Scheme for Nonbonded Interactions: Implications for Force-Field Parametrization?. Journal of Chemical Theory and Computation, 2020, 16, 5985-5990.	5.3	11
156	On glyphosateâ€"kaolinite surface interactions. A molecular dynamic study. European Journal of Soil Science, 2021, 72, 1231-1242.	3.9	11
157	Exploring the structure and dynamics of proteins in soil organic matter. Proteins: Structure, Function and Bioinformatics, 2021, 89, 925-936.	2.6	11
158	Molecular dynamics simulation of configurational ensembles compatible with experimental FRET efficiency data through a restraint on instantaneous FRET efficiencies. Journal of Computational Chemistry, 2014, 35, 2319-2332.	3.3	10
159	Dihedral-Based Segment Identification and Classification of Biopolymers II: Polynucleotides. Journal of Chemical Information and Modeling, 2014, 54, 278-288.	5.4	10
160	UDP-sulfoquinovose formation by Sulfolobus acidocaldarius. Extremophiles, 2015, 19, 451-467.	2.3	10
161	Ion-induced modification of the sucrose network and its impact on melting of freeze-dried liposomes. DSC and molecular dynamics study. Chemistry and Physics of Lipids, 2018, 210, 38-46.	3.2	10
162	Comparison of freeâ€energy methods using a tripeptideâ€water model system. Journal of Computational Chemistry, 2018, 39, 2226-2242.	3.3	10

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163	A speculation on the tandem fasciclin 1 repeat of FLA4 proteins in angiosperms. Plant Signaling and Behavior, 2018, 13, e1507403.	2.4	10
164	Molecular dynamics of the immune checkpoint programmed cell death protein I, PD-1: conformational changes of the BC-loop upon binding of the ligand PD-L1 and the monoclonal antibody nivolumab. BMC Bioinformatics, 2020, 21, 557.	2.6	10
165	Rationalization of stereospecific binding of propranolol to cytochrome P450 2D6 by free energy calculations. European Biophysics Journal, 2012, 41, 1065-1076.	2.2	9
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