Chris Oostenbrink

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4422244/publications.pdf

Version: 2024-02-01

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	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
2	Soil organic matter in molecular simulations. , 2022, , .		0
3	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
4	On the effects of induced polarizability at the waterâ€“graphene interface via classical charge-on-spring models. Physical Chemistry Chemical Physics, 2022, 24, 7748-7758.	2.8	4
5	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
6	Inhibition of the Peroxygenase Lytic Polysaccharide Monooxygenase by Carboxylic Acids and Amino Acids. Antioxidants, 2022, 11, 1096.	5.1	4
7	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
8	On glyphosateâ€“kaolinite surface interactions. A molecular dynamic study. European Journal of Soil Science, 2021, 72, 1231-1242.	3.9	11
9	Optimization of Alchemical Pathways Using Extended Thermodynamic Integration. Journal of Chemical Theory and Computation, 2021, 17, 56-65.	5.3	7
10	Efficient In Silico Saturation Mutagenesis of a Member of the Caspase Protease Family. Journal of Chemical Information and Modeling, 2021, 61, 1193-1203.	5.4	6
11	Vienna soil organic matter modeler 2 (VSOMM2). Journal of Molecular Graphics and Modelling, 2021, 103, 107817.	2.4	22
12	Exploring the structure and dynamics of proteins in soil organic matter. Proteins: Structure, Function and Bioinformatics, 2021, 89, 925-936.	2.6	11
13	Modeling soil organic matter: Changes in macroscopic properties due to microscopic changes. Geochimica Et Cosmochimica Acta, 2021, 307, 228-241.	3.9	12
14	On the use of multipleâ€timeâ€step algorithms to save computing effort in molecular dynamics simulations of proteins. Journal of Computational Chemistry, 2021, 42, 1263-1282.	3.3	3
15	Identification of lectin receptors for conserved SARSâ€CoVâ€2 glycosylation sites. EMBO Journal, 2021, 40, e108375.	7.8	44
16	Fighting Against Bacterial Lipopolysaccharide-Caused Infections through Molecular Dynamics Simulations: A Review. Journal of Chemical Information and Modeling, 2021, 61, 4839-4851.	5.4	5
17	Reaction intermediate rotation during the decarboxylation of coproheme to heme b in C.Âdiphtheriae. Biophysical Journal, 2021, 120, 3600-3614.	0.5	12
18	PROFICS: A bacterial selection system for directed evolution of proteases. Journal of Biological Chemistry, 2021, 297, 101095.	3.4	3

#	Article	IF	Citations
19	Soil organic matter stabilization at molecular scale: The role of metal cations and hydrogen bonds. Geoderma, 2021, 401, 115237.	5.1	19
20	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
21	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
22	Pembrolizumab Induces an Unexpected Conformational Change in the CCâ€²-loop of PD-1. Cancers, 2021, 13, 5.	3.7	8
23	In silico identification of noncompetitive inhibitors targeting an uncharacterized allosteric site of falcipain-2. Journal of Computer-Aided Molecular Design, 2021, 35, 1067-1079.	2.9	5
24	On the Adsorption Mechanism of Humic Substances on Kaolinite and Their Microscopic Structure. Minerals (Basel, Switzerland), 2021, 11, 1138.	2.0	5
25	Structure-guided glyco-engineering of ACE2 for improved potency as soluble SARS-CoV-2 decoy receptor. ELife, 2021, 10, .	6.0	29
26	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
27	UDP-N-acetyl-Î±-D-galactosamine:polypeptide N-acetylgalactosaminyltransferase from the snail Biomphalaria glabrata â€“ structural reflections. Glycoconjugate Journal, 2020, 37, 15-25.	2.7	5
28	An NMR and MD study of complexes of bacteriophage lambda lysozyme with tetraâ€•and hexaâ€Nâ€acetylchitohexaose. Proteins: Structure, Function and Bioinformatics, 2020, 88, 82-93.	2.6	3
29	Hamiltonian Reweighing To Refine Protein Backbone Dihedral Angle Parameters in the GROMOS Force Field. Journal of Chemical Information and Modeling, 2020, 60, 279-288.	5.4	9
30	The effect of different cutoff schemes in molecular simulations of proteins. Journal of Computational Chemistry, 2020, 41, 2740-2749.	3.3	12
31	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
32	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
33	Molecular Dynamics and In Vitro Quantification of Safrole DNA Adducts Reveal DNA Adduct Persistence Due to Limited DNA Distortion Resulting in Inefficient Repair. Chemical Research in Toxicology, 2020, 33, 2298-2309.	3.3	7
34	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
35	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
36	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

#	Article	IF	Citations
37	Enhancing the promiscuity of a member of the Caspase protease family by rational design. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1303-1318.	2.6	6
38	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
39	Cellular levels and molecular dynamics simulations of estragole DNA adducts point at inefficient repair resulting from limited distortion of the double-stranded DNA helix. Archives of Toxicology, 2020, 94, 1349-1365.	4.2	7
40	Could Microwave Irradiation Cause Misfolding of Peptides?. Journal of Chemical Theory and Computation, 2020, 16, 2795-2802.	5.3	12
41	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
42	Advances in the calculation of binding free energies. Current Opinion in Structural Biology, 2020, 61, 207-212.	5.7	52
43	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
44	Protein Conformational Change Is Essential for Reductive Activation of Lytic Polysaccharide Monooxygenase by Cellobiose Dehydrogenase. ACS Catalysis, 2020, 10, 4842-4853.	11.2	18
45	Actinobacterial Coproheme Decarboxylases Use Histidine as a Distal Base to Promote Compound I Formation. ACS Catalysis, 2020, 10, 5405-5418.	11.2	19
46	A Suite of Advanced Tutorials for the GROMOS Biomolecular Simulation Software [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	6.4	3
47	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
48	Direct Electron-Transfer Anisotropy of a Site-Specifically Immobilized Cellobiose Dehydrogenase. ACS Catalysis, 2019, 9, 7607-7615.	11.2	30
49	Redox thermodynamics of B-class dye-decolorizing peroxidases. Journal of Inorganic Biochemistry, 2019, 199, 110761.	3.5	18
50	Germinality does not necessarily define mAb expression and thermal stability. Applied Microbiology and Biotechnology, 2019, 103, 7505-7518.	3.6	3
51	Free-Energy Calculations for Bioisosteric Modifications of A3 Adenosine Receptor Antagonists. International Journal of Molecular Sciences, 2019, 20, 3499.	4.1	2
52	Polarization Effects in Simulations of Kaoliniteâ€"Water Interfaces. Langmuir, 2019, 35, 15086-15099.	3.5	19
53	Water in protein hydration and ligand recognition. Journal of Molecular Recognition, 2019, 32, e2810.	2.1	81
54	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

#	Article	IF	Citations
55	Binding Modes and Metabolism of Caffeine. Chemical Research in Toxicology, 2019, 32, 1374-1383.	3.3	18
56	In Search of a Structural Pattern in Crazy Sugarsidentification of Conformation Clusters of the Oligosaccharides Within Glycoproteins with LEUS. Biophysical Journal, 2019, 116, 570a.	0.5	0
57	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
58	Structural Aspects of the Oâ€glycosylation Linkage in Glycopeptides via MD Simulations and Comparison with NMR Experiments. ChemPhysChem, 2019, 20, 1527-1537.	2.1	5
59	Interaction between Cellobiose Dehydrogenase and Lytic Polysaccharide Monooxygenase. Biochemistry, 2019, 58, 1226-1235.	2.5	32
60	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. , 2019, , .		2
61	Improved spectrophotometric assay for lytic polysaccharide monooxygenase. Biotechnology for Biofuels, 2019, 12, 283.	6.2	31
62	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
63	Influence of Lytic Polysaccharide Monooxygenase Active Site Segments on Activity and Affinity. International Journal of Molecular Sciences, 2019, 20, 6219.	4.1	41
64	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
65	Saturation Mutagenesis by Efficient Free-Energy Calculation. Journal of Chemical Theory and Computation, 2018, 14, 894-904.	5.3	12
66	Free energy calculations on the stability of the 14-3-3Î¶ protein. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 442-450.	2.3	9
67	Validierung von molekularen Simulationen: eine Ãœbersicht verschiedener Aspekte. Angewandte Chemie, 2018, 130, 894-915.	2.0	3
68	Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902.	13.8	101
69	Chemical Approach to Biological Safety: Molecularâ€Level Control of an Integrated Zinc Finger Nuclease. ChemBioChem, 2018, 19, 66-75.	2.6	3
70	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
71	Comparison of freeâ€energy methods using a tripeptideâ€water model system. Journal of Computational Chemistry, 2018, 39, 2226-2242.	3.3	10
72	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

#	Article	IF	Citations
73	A cationâ€“Ï€ interaction in a transmembrane helix of vacuolar ATPase retains the proton-transporting arginine in a hydrophobic environment. Journal of Biological Chemistry, 2018, 293, 18977-18988.	3.4	8
74	A speculation on the tandem fasciclin 1 repeat of FLA4 proteins in angiosperms. Plant Signaling and Behavior, 2018, 13, e1507403.	2.4	10
75	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
76	A fast and sensitive activity assay for lytic polysaccharide monooxygenase. Biotechnology for Biofuels, 2018, 11, 79.	6.2	126
77	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
78	Recombinant plant-derived human IgE glycoproteomics. Journal of Proteomics, 2017, 161, 81-87.	2.4	16
79	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
80	Plasmon Field-Enhanced Fluorescence Energy Transfer for Hairpin Aptamer Assay Readout. ACS Sensors, 2017, 2, 916-923.	7.8	18
81	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
82	Modeling of Oligosaccharides within Glycoproteins from Free-Energy Landscapes. Journal of Chemical Information and Modeling, 2017, 57, 2222-2236.	5.4	26
83	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
84	Reparametrisation of united-atom amine solvation in the GROMOS force field. Molecular Physics, 2017, 115, 1144-1154.	1.7	9
85	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
86	MDplot: Visualise Molecular Dynamics. R Journal, 2017, 9, 164.	1.8	19
87	MDplot: Visualise Molecular Dynamics. R Journal, 2017, 9, 164-186.	1.8	8
88	Calculation of Relative Binding Free Energy in the Water-Filled Active Site of Oligopeptide-Binding Protein A. Molecules, 2016, 21, 499.	3.8	24
89	Optimization of Protein Backbone Dihedral Angles by Means of Hamiltonian Reweighting. Journal of Chemical Information and Modeling, 2016, 56, 1823-1834.	5.4	7
90	Chemistry and Molecular Dynamics Simulations of Heme b-HemQ and Coproheme-HemQ. Biochemistry, 2016, 55, 5398-5412.	2.5	24

#	Article	IF	Citations
91	Antibody humanization by molecular dynamics simulationsâ€"inâ€silico guided selection of critical backmutations. Journal of Molecular Recognition, 2016, 29, 266-275.	2.1	29
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	Bestimmung von Strukturinformation aus experimentellen Messdaten fÃ¼r BiomolekÃ¼le. Angewandte Chemie, 2016, 128, 16222-16244.	2.0	7
94	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
95	Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010.	13.8	24
96	Exploring genetic suppression interactions on a global scale. Science, 2016, 354, .	12.6	157
97	Interaction with the Redox Cofactor MYW and Functional Role of a Mobile Arginine in Eukaryotic Catalase-Peroxidase. Biochemistry, 2016, 55, 3528-3541.	2.5	8
98	Reaction of pyranose dehydrogenase from AgaricusÂmeleagris with its carbohydrate substrates. FEBS Journal, 2015, 282, 4218-4241.	4.7	15
99	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
100	Selectivity of cytosolic phospholipase A2 type IV toward arachidonyl phospholipids. Journal of Molecular Recognition, 2015, 28, 447-457.	2.1	6
101	Eukaryotic Catalase-Peroxidase: The Role of the Trp-Tyr-Met Adduct in Protein Stability, Substrate Accessibility, and Catalysis of Hydrogen Peroxide Dismutation. Biochemistry, 2015, 54, 5425-5438.	2.5	3
102	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
103	UDP-sulfoquinovose formation by Sulfolobus acidocaldarius. Extremophiles, 2015, 19, 451-467.	2.3	10
104	Prediction of cytochrome P450 mediated metabolism. Advanced Drug Delivery Reviews, 2015, 86, 61-71.	13.7	78
105	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
106	Processing of complex N-glycans in IgG Fc-region is affected by core fucosylation. MAbs, 2015, 7, 863-870.	5.2	50
107	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
108	Cytochrome P450 Mediated Drug Metabolism. RSC Drug Discovery Series, 2015, , 66-78.	0.3	0

#	Article	IF	Citations
109	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
110	Pyranose Dehydrogenase Ligand Promiscuity: A Generalized Approach to Simulate Monosaccharide Solvation, Binding, and Product Formation. PLoS Computational Biology, 2014, 10, e1003995.	3.2	9
111	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
112	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
113	Construction of pHâ€sensitive Her2â€binding IgG1â€Fc by directed evolution. Biotechnology Journal, 2014, 9, 1013-1022.	3.5	30
114	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
115	On the use of one-step perturbation to investigate the dependence of NOE-derived atomâ€"atom distance bound violations of peptides upon a variation of force-field parameters. European Biophysics Journal, 2014, 43, 113-119.	2.2	7
116	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
117	Transiently Produced Hypochlorite Is Responsible for the Irreversible Inhibition of Chlorite Dismutase. Biochemistry, 2014, 53, 3145-3157.	2.5	46
118	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
119	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
120	Cooperative Binding of Aflatoxin B₁ by Cytochrome P450 3A4: A Computational Study. Chemical Research in Toxicology, 2014, 27, 2136-2147.	3.3	40
121	Investigation of Ion Binding in Chlorite Dismutases by Means of Molecular Dynamics Simulations. Biochemistry, 2014, 53, 4869-4879.	2.5	17
122	Molecular dynamics simulations of the auxin-binding protein 1 in complex with indole-3-acetic acid and naphthalen-1-acetic acid. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2744-2755.	2.6	3
123	Dihedral-Based Segment Identification and Classification of Biopolymers I: Proteins. Journal of Chemical Information and Modeling, 2014, 54, 266-277.	5.4	39
124	Design of a colicin E7 based chimeric zinc-finger nuclease. Journal of Computer-Aided Molecular Design, 2014, 28, 841-850.	2.9	11
125	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
126	Dihedral-Based Segment Identification and Classification of Biopolymers II: Polynucleotides. Journal of Chemical Information and Modeling, 2014, 54, 278-288.	5.4	10

#	Article	IF	Citations
127	Creating stable stem regions for loop elongation in Fcabs â€" Insights from combining yeast surface display, in silico loop reconstruction and molecular dynamics simulations. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1530-1540.	2.3	3
128	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
129	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
130	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
131	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
132	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
133	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
134	Proteinâ€"Ligand Binding from Distancefield Distances and Hamiltonian Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2013, 9, 883-892.	5.3	29
135	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
136	Freeâ€energy differences between states with different conformational ensembles. Journal of Computational Chemistry, 2013, 34, 1398-1408.	3.3	15
137	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
138	CYP 2D6 Binding Affinity Predictions Using Multiple Ligand and Protein Conformations. International Journal of Molecular Sciences, 2013, 14, 24514-24530.	4.1	28
139	A Systematic Framework for Molecular Dynamics Simulations of Protein Post-Translational Modifications. PLoS Computational Biology, 2013, 9, e1003154.	3.2	88
140	Malleability and Versatility of Cytochrome P450 Active Sites Studied by Molecular Simulations. Current Drug Metabolism, 2012, 13, 190-196.	1.2	18
141	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
142	Efficient and Accurate Free Energy Calculations on Trypsin Inhibitors. Journal of Chemical Theory and Computation, 2012, 8, 3686-3695.	5.3	34
143	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
144	Molecular Insight into Propeptideâ€"Protein Interactions in Cathepsins L and O. Biochemistry, 2012, 51, 8636-8653.	2.5	6

#	Article	IF	Citations
145	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
146	Rationalization of stereospecific binding of propranolol to cytochrome P450 2D6 by free energy calculations. European Biophysics Journal, 2012, 41, 1065-1076.	2.2	9
147	Binding free energy, energy and entropy calculations using simple model systems. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	27
148	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
149	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
150	Calculation of the relative free energy of oxidation of azurin at pH 5 and pH 9. Journal of Computational Chemistry, 2012, 33, 1467-1477.	3.3	1
151	Free Energy Calculations from One-Step Perturbations. Methods in Molecular Biology, 2012, 819, 487-499.	0.9	18
152	Fast and Efficient Calculations of Binding Affinities for C8-Substituted GTP Analogues to the FtsZ Protein. Biophysical Journal, 2011, 100, 158a-159a.	0.5	0
153	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
154	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. Journal of Chemical Theory and Computation, 2011, 7, 3379-3390.	5.3	180
155	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
156	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
157	Identification of CYP1A2 ligands by structure-based and ligand-based virtual screening. MedChemComm, 2011, 2, 853.	3.4	8
158	Calculation of binding free energies of inhibitors to plasmepsin II. Journal of Computational Chemistry, 2011, 32, 1801-1812.	3.3	18
159	Molecular dynamics simulations and free energy calculations on the enzyme 4â€hydroxyphenylpyruvate dioxygenase. Journal of Computational Chemistry, 2011, 32, 2160-2169.	3.3	5
160	Free energy calculations of proteinâ€“ligand interactions. Current Opinion in Chemical Biology, 2011, 15, 547-552.	6.1	83
161	Molecular Simulations to Rationalize Humanized Ab2/3H6 Activity. Australian Journal of Chemistry, 2011, 64, 900.	0.9	3
162	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

#	Article	IF	Citations
163	Molecular mechanism of allosteric communication in the human PPARÎ±â€RXRÎ± heterodimer. Proteins: Structure, Function and Bioinformatics, 2010, 78, 873-887.	2.6	19
164	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
165	The Role of Water Molecules in Computational Drug Design. Current Topics in Medicinal Chemistry, 2010, 10, 55-66.	2.1	155
166	Improved Ligand-Protein Binding Affinity Predictions Using Multiple Binding Modes. Biophysical Journal, 2010, 98, 2682-2691.	0.5	104
167	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
168	Role of Water in Molecular Docking Simulations of Cytochrome P450 2D6. Journal of Chemical Information and Modeling, 2010, 50, 146-154.	5.4	66
169	Classification of Cytochrome P450 1A2 Inhibitors and Noninhibitors by Machine Learning Techniques. Drug Metabolism and Disposition, 2009, 37, 658-664.	3.3	91
170	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. ChemMedChem, 2009, 4, 2070-2079.	3.2	46
171	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. ChemMedChem, 2009, 4, 1965-1965.	3.2	0
172	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
173	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
174	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
175	A Library of Fluorescent Peptides for Exploring the Substrate Specificities of Prolyl Isomerases. Biochemistry, 2009, 48, 10423-10436.	2.5	56
176	Structural rationalization of novel drug metabolizing mutants of cytochrome P450 BM3. Proteins: Structure, Function and Bioinformatics, 2008, 71, 336-352.	2.6	39
177	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
178	Hamiltonian replica exchange molecular dynamics using soft-core interactions. Journal of Chemical Physics, 2008, 128, 144121.	3.0	79
179	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
180	Molecular Modeling-Guided Site-Directed Mutagenesis of Cytochrome P450 2D6. Current Drug Metabolism, 2007, 8, 59-77.	1.2	45

#	Article	IF	Citations
181	Optimization of replica exchange molecular dynamics by fast mimicking. Journal of Chemical Physics, 2007, 127, 204104.	3.0	30
182	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
183	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
184	On using oscillating time-dependent restraints in MD simulation. Journal of Biomolecular NMR, 2007, 37, 1-14.	2.8	15
185	Configurational Entropy Change of Netropsin and Distamycin upon DNA Minor-Groove Binding. Biophysical Journal, 2006, 91, 1460-1470.	0.5	45
186	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
187	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
188	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
189	Calculating zeros: Non-equilibrium free energy calculations. Chemical Physics, 2006, 323, 102-108.	1.9	35
190	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	13.8	503
191	Computational study of ground-state chiral induction in small peptides: Comparison of the relative stability of selected amino acid dimers and oligomers in homochiral and heterochiral combinations. Journal of Computational Chemistry, 2006, 27, 857-867.	3.3	8
192	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
193	An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737.	3.3	161
194	The GROMOS software for biomolecular simulation: GROMOS05. Journal of Computational Chemistry, 2005, 26, 1719-1751.	3.3	592
195	Amine Hydration: A United-Atom Force-Field Solution. ChemPhysChem, 2005, 6, 1800-1804.	2.1	25
196	Calculation of the Redox Potential of the Protein Azurin and Some Mutants. ChemBioChem, 2005, 6, 738-746.	2.6	49
197	Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284.	2.2	443
198	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

#	Article	IF	Citations
199	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
200	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
201	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
202	Methane clustering in explicit water: effect of urea on hydrophobic interactions. Physical Chemistry Chemical Physics, 2005, 7, 53.	2.8	52
203	On the transferability of the SPC/L water model to biomolecular simulation. Brazilian Journal of Physics, 2004, 34, 116-125.	1.4	5
204	Simulating the Physiological Phase of Hydrated DPPC Bilayers: The Ester Moiety. Soft Materials, 2004, 2, 27-45.	1.7	16
205	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
206	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
207	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
208	Estimating entropies from molecular dynamics simulations. Journal of Chemical Physics, 2004, 120, 2652-2661.	3.0	138
209	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
210	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
211	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
212	Molecular dynamics simulations. Current Opinion in Structural Biology, 2002, 12, 190-196.	5.7	551
213	A least squares multicenter approach to continuum wave functions. Chemical Physics, 2002, 284, 565-574.	1.9	3
214	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