Alexander D Mackerell

List of Publications by Year
in descending order

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423 papers	69,311 citations	2544 96 h-index	816 246 g-index
472 all docs	472 docs citations	472 times ranked	44257 citing authors

#	Article	IF	Citations
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
2	CHARMM general force field: A force field for drugâ€like molecules compatible with the CHARMM allâ€atom additive biological force fields. Journal of Computational Chemistry, 2010, 31, 671-690.	3.3	4,718
3	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. Nature Methods, 2017, 14, 71-73.	19.0	3,959
4	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone Ï•, Ï^ and Side-Chain Ï‡₁ and Ï‡₂ Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 3257-3273.	5.3	3,696
5	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	2.6	3,676
6	Extending the treatment of backbone energetics in protein force fields: Limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations. Journal of Computational Chemistry, 2004, 25, 1400-1415.	3.3	3,145
7	CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data. Journal of Computational Chemistry, 2013, 34, 2135-2145.	3.3	2,613
8	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2016, 12, 405-413.	5.3	2,567
9	All-atom empirical force field for nucleic acids: I. Parameter optimization based on small molecule and condensed phase macromolecular target data. Journal of Computational Chemistry, 2000, 21, 86-104.	3.3	1,460
10	Automation of the CHARMM General Force Field (CGenFF) I: Bond Perception and Atom Typing. Journal of Chemical Information and Modeling, 2012, 52, 3144-3154.	5.4	1,409
11	Automation of the CHARMM General Force Field (CGenFF) II: Assignment of Bonded Parameters and Partial Atomic Charges. Journal of Chemical Information and Modeling, 2012, 52, 3155-3168.	5.4	1,278
12	Empirical force fields for biological macromolecules: Overview and issues. Journal of Computational Chemistry, 2004, 25, 1584-1604.	3.3	1,134
13	Development and current status of the CHARMM force field for nucleic acids. Biopolymers, 2000, 56, 257-265.	2.4	923
14	Improved Treatment of the Protein Backbone in Empirical Force Fields. Journal of the American Chemical Society, 2004, 126, 698-699.	13.7	912
15	An Improved Empirical Potential Energy Function for Molecular Simulations of Phospholipids. Journal of Physical Chemistry B, 2000, 104, 7510-7515.	2.6	729
16	All-atom empirical force field for nucleic acids: II. Application to molecular dynamics simulations of DNA and RNA in solution. Journal of Computational Chemistry, 2000, 21, 105-120.	3.3	701
17	An all-atom empirical energy function for the simulation of nucleic acids. Journal of the American Chemical Society, 1995, 117, 11946-11975.	13.7	690
18	Extension of the CHARMM general force field to sulfonylâ€containing compounds and its utility in biomolecular simulations. Journal of Computational Chemistry, 2012, 33, 2451-2468.	3.3	659

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19	A simple polarizable model of water based on classical Drude oscillators. Journal of Chemical Physics, 2003, 119, 5185-5197.	3.0	635
20	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. Journal of Chemical Theory and Computation, 2009, 5, 2353-2370.	5.3	578
21	CHARMM Additive All-Atom Force Field for Carbohydrate Derivatives and Its Utility in Polysaccharide and Carbohydrateâ€“Protein Modeling. Journal of Chemical Theory and Computation, 2011, 7, 3162-3180.	5.3	559
22	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	2.6	548
23	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	3.3	483
24	Optimization of the CHARMM Additive Force Field for DNA: Improved Treatment of the BI/BII Conformational Equilibrium. Journal of Chemical Theory and Computation, 2012, 8, 348-362.	5.3	464
25	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. Chemical Reviews, 2016, 116, 4983-5013.	47.7	434
26	Polyunsaturated Fatty Acids in Lipid Bilayers:â€‰Intrinsic and Environmental Contributions to Their Unique Physical Properties. Journal of the American Chemical Society, 2002, 124, 318-326.	13.7	423
27	Molecular Dynamics Studies of Polyethylene Oxide and Polyethylene Glycol: Hydrodynamic Radius and Shape Anisotropy. Biophysical Journal, 2008, 95, 1590-1599.	0.5	415
28	CHARMM fluctuating charge force field for proteins: II Protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. Journal of Computational Chemistry, 2004, 25, 1504-1514.	3.3	410
29	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	5.3	401
30	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	47.7	386
31	Impact of 2â€²â€hydroxyl sampling on the conformational properties of RNA: Update of the CHARMM allâ€atom additive force field for RNA. Journal of Computational Chemistry, 2011, 32, 1929-1943.	3.3	341
32	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2013, 9, 5430-5449.	5.3	329
33	Importance of the CMAP Correction to the CHARMM22 Protein Force Field: Dynamics of Hen Lysozyme. Biophysical Journal, 2006, 90, L36-L38.	0.5	321
34	Computer-Aided Drug Design Methods. Methods in Molecular Biology, 2017, 1520, 85-106.	0.9	317
35	Development of the CHARMM Force Field for Lipids. Journal of Physical Chemistry Letters, 2011, 2, 1526-1532.	4.6	316
36	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	1.4	314

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37	An ab Initio Study on the Torsional Surface of Alkanes and Its Effect on Molecular Simulations of Alkanes and a DPPC Bilayer. Journal of Physical Chemistry B, 2005, 109, 5300-5311.	2.6	303
38	Decoding the Signaling of a GPCR Heteromeric Complex Reveals a Unifying Mechanism of Action of Antipsychotic Drugs. Cell, 2011, 147, 1011-1023.	28.9	271
39	A Small-Molecule Inhibitor of BCL6 Kills DLBCL Cells In Vitro and In Vivo. Cancer Cell, 2010, 17, 400-411.	16.8	263
40	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2005, 1, 153-168.	5.3	260
41	Molecular Dynamics Simulation Analysis of a Sodium Dodecyl Sulfate Micelle in Aqueous Solution: Decreased Fluidity of the Micelle Hydrocarbon Interior. The Journal of Physical Chemistry, 1995, 99, 1846-1855.	2.9	253
42	The Structure of Aqueous Guanidinium Chloride Solutions. Journal of the American Chemical Society, 2004, 126, 11462-11470.	13.7	245
43	Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers. Journal of Chemical Theory and Computation, 2007, 3, 1120-1133.	5.3	233
44	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. Journal of Physical Chemistry Letters, 2011, 2, 87-92.	4.6	233
45	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	3.3	224
46	CHARMM additive and polarizable force fields for biophysics and computer-aided drug design. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 861-871.	2.4	223
47	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	2.3	214
48	Recent Advances in Ligand-Based Drug Design: Relevance and Utility of the Conformationally Sampled Pharmacophore Approach. Current Computer-Aided Drug Design, 2011, 7, 10-22.	1.2	210
49	Development of an Empirical Force Field for Silica. Application to the Quartzâ^'Water Interface. Journal of Physical Chemistry B, 2006, 110, 2782-2792.	2.6	209
50	Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation. PLoS Computational Biology, 2009, 5, e1000435.	3.2	208
51	Force Field Influence on the Observation of Ï€-Helical Protein Structures in Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 2831-2836.	2.6	204
52	Polarizable Empirical Force Field for Alkanes Based on the Classical Drude Oscillator Model. Journal of Physical Chemistry B, 2005, 109, 18988-18999.	2.6	193
53	CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. Biophysical Journal, 2014, 107, 134-145.	0.5	192
54	An Empirical Potential Energy Function for Phospholipids: Criteria for Parameter Optimization and Applications. , 1996, , 31-81.		183

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55	Combinedab initio/empirical approach for optimization of Lennard-Jones parameters. Journal of Computational Chemistry, 1998, 19, 334-348.	3.3	181
56	Recent developments and applications of the CHARMM force fields. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 167-185.	14.6	173
57	Glycan reader: Automated sugar identification and simulation preparation for carbohydrates and glycoproteins. Journal of Computational Chemistry, 2011, 32, 3135-3141.	3.3	172
58	Comparison of Protein Force Fields for Molecular Dynamics Simulations. Methods in Molecular Biology, 2008, 443, 63-88.	0.9	171
59	CHARMM Additive All-Atom Force Field for Glycosidic Linkages in Carbohydrates Involving Furanoses. Journal of Physical Chemistry B, 2010, 114, 12981-12994.	2.6	170
60	A molecular mechanics force field for NAD+ NADH, and the pyrophosphate groups of nucleotides. Journal of Computational Chemistry, 1997, 18, 221-239.	3.3	168
61	Molecular-Level Organization of Saturated and Polyunsaturated Fatty Acids in a Phosphatidylcholine Bilayer Containing Cholesterolâ€. Biochemistry, 2004, 43, 15318-15328.	2.5	168
62	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligandâ€“protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	3.0	168
63	A Hybrid Mechanism of Action for BCL6 in B Cells Defined by Formation of Functionally Distinct Complexes at Enhancers and Promoters. Cell Reports, 2013, 4, 578-588.	6.4	161
64	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	2.6	159
65	Molecular dynamics simulations of nucleic acidâ€“protein complexes. Current Opinion in Structural Biology, 2008, 18, 194-199.	5.7	157
66	Free Energy and Structural Pathways of Base Flipping in a DNA GCGC Containing Sequence. Journal of Molecular Biology, 2002, 319, 141-160.	4.2	151
67	Rational Design of Human DNA Ligase Inhibitors that Target Cellular DNA Replication and Repair. Cancer Research, 2008, 68, 3169-3177.	0.9	151
68	Consideration of Molecular Weight during Compound Selection in Virtual Target-Based Database Screening. Journal of Chemical Information and Computer Sciences, 2003, 43, 267-272.	2.8	150
69	CHARMM Additive All-Atom Force Field for Acyclic Polyalcohols, Acyclic Carbohydrates, and Inositol. Journal of Chemical Theory and Computation, 2009, 5, 1315-1327.	5.3	150
70	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	2.6	149
71	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2006, 2, 1587-1597.	5.3	142
72	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. Journal of Physical Chemistry Letters, 2014, 5, 3144-3150.	4.6	139

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73	Current Status of Protein Force Fields for Molecular Dynamics Simulations. Methods in Molecular Biology, 2015, 1215, 47-71.	0.9	139
74	Force field development and simulations of intrinsically disordered proteins. Current Opinion in Structural Biology, 2018, 48, 40-48.	5.7	139
75	Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. Journal of Chemical Theory and Computation, 2007, 3, 1927-1946.	5.3	136
76	Allâ€atom polarizable force field for DNA based on the classical drude oscillator model. Journal of Computational Chemistry, 2014, 35, 1219-1239.	3.3	136
77	The Expanding Role of the BCL6 Oncoprotein as a Cancer Therapeutic Target. Clinical Cancer Research, 2017, 23, 885-893.	7.0	133
78	Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma. Journal of Clinical Investigation, 2016, 126, 3351-3362.	8.2	133
79	Accurate Calculation of Hydration Free Energies using Pair-Specific Lennard-Jones Parameters in the CHARMM Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 1181-1198.	5.3	131
80	Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of Î±-Helix and Î²-Hairpin Formation. Biophysical Journal, 2012, 103, 1045-1051.	0.5	130
81	Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 68-73.	7.1	128
82	CHARMM Additive All-Atom Force Field for Aldopentofuranoses, Methyl-aldopentofuranosides, and Fructofuranose. Journal of Physical Chemistry B, 2009, 113, 12466-12476.	2.6	128
83	Intrinsic Conformational Properties of Deoxyribonucleosides: Implicated Role for Cytosine in the Equilibrium Among the A, B, and Z Forms of DNA. Biophysical Journal, 1999, 76, 3206-3218.	0.5	125
84	Inhibition of TLR2 signaling by small molecule inhibitors targeting a pocket within the TLR2 TIR domain. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5455-5460.	7.1	124
85	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	2.6	122
86	Point mutation E1099K in MMSET/NSD2 enhances its methyltranferase activity and leads to altered global chromatin methylation in lymphoid malignancies. Leukemia, 2014, 28, 198-201.	7.2	122
87	Development of CHARMM Polarizable Force Field for Nucleic Acid Bases Based on the Classical Drude Oscillator Model. Journal of Physical Chemistry B, 2011, 115, 580-596.	2.6	121
88	Identification of Novel Extracellular Signal-Regulated Kinase Docking Domain Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 4586-4595.	6.4	112
89	Intrinsic Conformational Energetics Associated with the Glycosyl Torsion in DNA: A Quantum Mechanical Study. Biophysical Journal, 2002, 82, 1554-1569.	0.5	111
90	Development of a Polarizable Intermolecular Potential Function (PIPF) for Liquid Amides and Alkanes. Journal of Chemical Theory and Computation, 2007, 3, 1878-1889.	5.3	107

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91	Reproducing Crystal Binding Modes of Ligand Functional Groups Using Site-Identification by Ligand Competitive Saturation (SILCS) Simulations. Journal of Chemical Information and Modeling, 2011, 51, 877-896.	5.4	105
92	Automated conformational energy fitting for force-field development. Journal of Molecular Modeling, 2008, 14, 667-679.	1.8	104
93	A Small Molecule Agonist of EphA2 Receptor Tyrosine Kinase Inhibits Tumor Cell Migration In Vitro and Prostate Cancer Metastasis In Vivo. PLoS ONE, 2012, 7, e42120.	2.5	103
94	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	3.0	103
95	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. Faraday Discussions, 2013, 160, 135-149.	3.2	102
96	Active site of human liver aldehyde dehydrogenase. Biochemistry, 1987, 26, 5679-5684.	2.5	101
97	Inclusion of Multiple Fragment Types in the Site Identification by Ligand Competitive Saturation (SILCS) Approach. Journal of Chemical Information and Modeling, 2013, 53, 3384-3398.	5.4	101
98	Combinedab initio/empirical approach for optimization of Lennard-Jones parameters for polar-neutral compounds. Journal of Computational Chemistry, 2002, 23, 199-213.	3.3	100
99	CHARMM Additive All-Atom Force Field for Phosphate and Sulfate Linked to Carbohydrates. Journal of Chemical Theory and Computation, 2012, 8, 759-776.	5.3	100
100	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	13.7	98
101	Progress toward chemical accuracy in the computer simulation of condensed phase reactions.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 3698-3703.	7.1	94
102	Identification and Characterization of Small Molecule Inhibitors of the Calcium-Dependent S100Bâ^'p53 Tumor Suppressor Interaction. Journal of Medicinal Chemistry, 2004, 47, 5085-5093.	6.4	90
103	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. Journal of Chemical Theory and Computation, 2017, 13, 4535-4552.	5.3	90
104	Influence of Magnesium Ions on Duplex DNA Structural, Dynamic, and Solvation Properties. Journal of Physical Chemistry B, 1997, 101, 646-650.	2.6	88
105	A piRNA-like small RNA interacts with and modulates p-ERM proteins in human somatic cells. Nature Communications, 2015, 6, 7316.	12.8	88
106	Molecular Mechanics. Current Pharmaceutical Design, 2014, 20, 3281-3292.	1.9	87
107	Importance of attractive van der Waals contribution in empirical energy function models for the heat of vaporization of polar liquids. The Journal of Physical Chemistry, 1991, 95, 10559-10560.	2.9	86
108	Computational Identification of Inhibitors of Protein-Protein Interactions. Current Topics in Medicinal Chemistry, 2007, 7, 63-82.	2.1	86

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109	Computational Approaches for Investigating Base Flipping in Oligonucleotides. Chemical Reviews, 2006, 106, 489-505.	47.7	85
110	Do Halogenâ€“Hydrogen Bond Donor Interactions Dominate the Favorable Contribution of Halogens to Ligandâ€“Protein Binding?. Journal of Physical Chemistry B, 2017, 121, 6813-6821.	2.6	85
111	CH/Ï€ interactions involving aromatic amino acids: Refinement of the CHARMM tryptophan force field. Journal of Computational Chemistry, 2005, 26, 1452-1463.	3.3	83
112	Conformational Properties of the Deoxyribose and Ribose Moieties of Nucleic Acids:Â A Quantum Mechanical Study. Journal of Physical Chemistry B, 1998, 102, 6669-6678.	2.6	82
113	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	3.0	82
114	Is Arginine Charged in a Membrane?. Biophysical Journal, 2008, 94, L11-L13.	0.5	81
115	Competition among Li⁺, Na⁺, K⁺, and Rb⁺ Monovalent Ions for DNA in Molecular Dynamics Simulations Using the Additive CHARMM36 and Drude Polarizable Force Fields. Journal of Physical Chemistry B, 2015, 119, 4428-4440.	2.6	80
116	Implementation of extended <scp>L</scp>agrangian dynamics in <scp>GROMACS</scp> for polarizable simulations using the classical <scp>D</scp>rude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	3.3	79
117	Structure, force, and energy of a double-stranded DNA oligonucleotide under tensile loads. European Biophysics Journal, 1999, 28, 415-426.	2.2	78
118	The novel BH3 Î±-helix mimetic JY-1-106 induces apoptosis in a subset of cancer cells (lung cancer, colon) Tj ETQq0 0 0 rgBT /Overlock 1 Molecular Cancer, 2013, 12, 42.	19.2	78
119	Molecular dynamics simulations using the drude polarizable force field on GPUs with OpenMM: Implementation, validation, and benchmarks. Journal of Computational Chemistry, 2018, 39, 1682-1689.	3.3	77
120	Computational ligand-based rational design: role of conformational sampling and force fields in model development. MedChemComm, 2011, 2, 356.	3.4	76
121	Induction of Peptide Bond Dipoles Drives Cooperative Helix Formation in the (AAQAA)3 Peptide. Biophysical Journal, 2014, 107, 991-997.	0.5	76
122	Balancing the Interactions of Ions, Water, and DNA in the Drude Polarizable Force Field. Journal of Physical Chemistry B, 2014, 118, 6742-6757.	2.6	74
123	Computational evaluation of proteinâ€“small molecule binding. Current Opinion in Structural Biology, 2009, 19, 56-61.	5.7	73
124	Urea Destabilizes RNA by Forming Stacking Interactions and Multiple Hydrogen Bonds with Nucleic Acid Bases. Journal of the American Chemical Society, 2009, 131, 17759-17761.	13.7	73
125	Identification and Validation of Human DNA Ligase Inhibitors Using Computer-Aided Drug Design. Journal of Medicinal Chemistry, 2008, 51, 4553-4562.	6.4	71
126	Ab initio conformational analysis of nucleic acid components: Intrinsic energetic contributions to nucleic acid structure and dynamics. Biopolymers, 2001, 61, 61-76.	2.4	70

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127	Molecular Simulations of Dodecyl-Î²-maltoside Micelles in Water: Influence of the Headgroup Conformation and Force Field Parameters. Journal of Physical Chemistry B, 2011, 115, 487-499.	2.6	69
128	Sampling of Organic Solutes in Aqueous and Heterogeneous Environments Using Oscillating Excess Chemical Potentials in Grand Canonical-like Monte Carlo-Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2281-2290.	5.3	69
129	Polarizable Force Field for DNA Based on the Classical Drude Oscillator: II. Microsecond Molecular Dynamics Simulations of Duplex DNA. Journal of Chemical Theory and Computation, 2017, 13, 2072-2085.	5.3	69
130	Polarizable Force Field for DNA Based on the Classical Drude Oscillator: I. Refinement Using Quantum Mechanical Base Stacking and Conformational Energetics. Journal of Chemical Theory and Computation, 2017, 13, 2053-2071.	5.3	68
131	Smallâ€Molecule Inhibitors of the ERK Signaling Pathway: Towards Novel Anticancer Therapeutics. ChemMedChem, 2011, 6, 38-48.	3.2	67
132	Polarizable Empirical Force Field for Hexopyranose Monosaccharides Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2015, 119, 637-652.	2.6	67
133	Polarizable force field for RNA based on the classical drude oscillator. Journal of Computational Chemistry, 2018, 39, 2624-2646.	3.3	67
134	Novel LRRK2 GTP-binding inhibitors reduced degeneration in Parkinson's disease cell and mouse models. Human Molecular Genetics, 2014, 23, 6212-6222.	2.9	66
135	Polarizable empirical force field for nitrogenâ€containing heteroaromatic compounds based on the classical Drude oscillator. Journal of Computational Chemistry, 2009, 30, 1821-1838.	3.3	65
136	Targeting NAD Biosynthesis in Bacterial Pathogens: Structure-Based Development of Inhibitors of Nicotinate Mononucleotide Adenylyltransferase NadD. Chemistry and Biology, 2009, 16, 849-861.	6.0	63
137	Additive <scp>CHARMM</scp> force field for naturally occurring modified ribonucleotides. Journal of Computational Chemistry, 2016, 37, 896-912.	3.3	63
138	Polarizability rescaling and atom-based Thole scaling in the CHARMM Drude polarizable force field for ethers. Journal of Molecular Modeling, 2010, 16, 567-576.	1.8	62
139	Pharmacophore Modeling Using Site-Identification by Ligand Competitive Saturation (SILCS) with Multiple Probe Molecules. Journal of Chemical Information and Modeling, 2015, 55, 407-420.	5.4	62
140	2D Conformationally Sampled Pharmacophore:Â A Ligand-Based Pharmacophore To Differentiate Î´ Opioid Agonists from Antagonists. Journal of the American Chemical Society, 2003, 125, 3101-3107.	13.7	61
141	Identification of Non-Phosphate-Containing Small Molecular Weight Inhibitors of the Tyrosine Kinase p56 Lck SH2 Domain via in Silico Screening against the pY + 3 Binding Site. Journal of Medicinal Chemistry, 2004, 47, 3502-3511.	6.4	61
142	Characterization of ATP-independent ERK inhibitors identified through in silico analysis of the active ERK2 structure. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 6281-6287.	2.2	61
143	Targeting of an Interrupted Polypurine:Polypyrimidine Sequence in Mammalian Cells by a Triplex-Forming Oligonucleotide Containing a Novel Base Analogue. Biochemistry, 2010, 49, 7867-7878.	2.5	60
144	The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis. Cancer Research, 2016, 76, 3593-3603.	0.9	60

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145	Induced Polarization Influences the Fundamental Forces in DNA Base Flipping. Journal of Physical Chemistry Letters, 2014, 5, 2077-2083.	4.6	59
146	Robustness in the fitting of molecular mechanics parameters. Journal of Computational Chemistry, 2015, 36, 1083-1101.	3.3	58
147	Cation-Ï€ Interactions between Methylated Ammonium Groups and Tryptophan in the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2019, 15, 7-12.	5.3	58
148	Contribution of the Phosphodiester Backbone and Glycosyl Linkage Intrinsic Torsional Energetics to DNA Structure and Dynamics. Journal of Physical Chemistry B, 1999, 103, 10955-10964.	2.6	57
149	Relaxation of the rigid backbone of an oligoamide-foldamer-based Î±-helix mimetic: identification of potent Bcl-xL inhibitors. Organic and Biomolecular Chemistry, 2012, 10, 2928.	2.8	57
150	Altered structural fluctuations in duplex RNA versus DNA: a conformational switch involving base pair opening. Nucleic Acids Research, 2003, 31, 7131-7140.	14.5	56
151	Influence of Solvent and Intramolecular Hydrogen Bonding on the Conformational Properties of O-Linked Glycopeptides. Journal of Physical Chemistry B, 2011, 115, 11215-11229.	2.6	56
152	Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling. Journal of Computer-Aided Molecular Design, 2014, 28, 491-507.	2.9	56
153	Role of the Adenine Ligand on the Stabilization of the Secondary and Tertiary Interactions in the Adenine Riboswitch. Journal of Molecular Biology, 2010, 396, 1422-1438.	4.2	55
154	Ribosome-Templated Azideâ€“Alkyne Cycloadditions: Synthesis of Potent Macrolide Antibiotics by In Situ Click Chemistry. Journal of the American Chemical Society, 2016, 138, 3136-3144.	13.7	55
155	Chapter 1 Considerations for Lipid Force Field Development. Current Topics in Membranes, 2008, , 1-48.	0.9	54
156	Conformationally Sampled Pharmacophore for Peptidic Î´ Opioid Ligands. Journal of Medicinal Chemistry, 2005, 48, 7773-7780.	6.4	53
157	Divalent Metal Ion Complexes of S100B in the Absence and Presence of Pentamidine. Journal of Molecular Biology, 2008, 382, 56-73.	4.2	53
158	Atomistic Simulation Study of Linear Alkylbenzene Sulfonates at the Water/Air Interface. Journal of Physical Chemistry B, 2010, 114, 9787-9794.	2.6	53
159	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. Journal of Chemical Theory and Computation, 2020, 16, 3221-3239.	5.3	53
160	Binding Response:â€‰ A Descriptor for Selecting Ligand Binding Site on Protein Surfaces. Journal of Chemical Information and Modeling, 2007, 47, 2303-2315.	5.4	52
161	Iodobenzene-Catalyzed Synthesis of Phenanthridinones via Oxidative Câ€“H Amidation. Journal of Organic Chemistry, 2017, 82, 3589-3596.	3.2	52
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