

Pengyu Ren

List of Publications by Year in descending order

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142
papers

12,479
citations

41258

49
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25716

108
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175
all docs

175
docs citations

175
times ranked

9862
citing authors

#	ARTICLE	IF	CITATIONS
1	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. <i>Journal of Physical Chemistry B</i> , 2003, 107, 5933-5947.	1.2	1,270
2	The COMPASS force field: parameterization and validation for phosphazenes. <i>Computational and Theoretical Polymer Science</i> , 1998, 8, 229-246.	1.1	1,186
3	Current Status of the AMOEBA Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2549-2564.	1.2	1,093
4	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. <i>Journal of Computational Chemistry</i> , 2002, 23, 1497-1506.	1.5	545
5	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4046-4063.	2.3	524
6	Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field. <i>Journal of the American Chemical Society</i> , 2003, 125, 15671-15682.	6.6	474
7	Tinker 8: Software Tools for Molecular Design. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5273-5289.	2.3	403
8	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3143-3161.	2.3	385
9	Systematic Improvement of a Classical Molecular Model of Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9956-9972.	1.2	279
10	Polarizable Force Fields for Biomolecular Simulations: Recent Advances and Applications. <i>Annual Review of Biophysics</i> , 2019, 48, 371-394.	4.5	253
11	Simulation of Ca ²⁺ and Mg ²⁺ Solvation Using Polarizable Atomic Multipole Potential. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18553-18559.	1.2	246
12	Classical Electrostatics for Biomolecular Simulations. <i>Chemical Reviews</i> , 2014, 114, 779-814.	23.0	229
13	Calculation of protein-ligand binding free energy by using a polarizable potential. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 6290-6295.	3.3	222
14	Temperature and Pressure Dependence of the AMOEBA Water Model. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13427-13437.	1.2	191
15	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. <i>Chemical Science</i> , 2018, 9, 956-972.	3.7	190
16	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2084-2108.	2.3	178
17	Virtual screening using molecular simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1940-1951.	1.5	171
18	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. <i>Journal of Chemical Physics</i> , 2006, 125, 054511.	1.2	169

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19	Calculating protein–ligand binding affinities with MMPBSA: Method and error analysis. <i>Journal of Computational Chemistry</i> , 2016, 37, 2436-2446.	1.5	169
20	Biomolecular electrostatics and solvation: a computational perspective. <i>Quarterly Reviews of Biophysics</i> , 2012, 45, 427-491.	2.4	152
21	Polarizable Molecular Dynamics Simulation of Zn(II) in Water Using the AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2059-2070.	2.3	137
22	Automation of AMOEBA polarizable force field parameterization for small molecules. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1138.	0.5	134
23	Modeling Structural Coordination and Ligand Binding in Zinc Proteins with a Polarizable Potential. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1314-1324.	2.3	100
24	Trypsin–ligand binding free energies from explicit and implicit solvent simulations with polarizable potential. <i>Journal of Computational Chemistry</i> , 2009, 30, 1701-1711.	1.5	96
25	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2609-2618.	2.3	93
26	Tinker–OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. <i>Journal of Computational Chemistry</i> , 2017, 38, 2047-2055.	1.5	89
27	AMOEBA+ Classical Potential for Modeling Molecular Interactions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4122-4139.	2.3	89
28	Generalized coarse-grained model based on point multipole and Gay-Berne potentials. <i>Journal of Chemical Physics</i> , 2006, 125, 064103.	1.2	86
29	Coarse-Grained Model for Simulation of RNA Three-Dimensional Structures. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13497-13506.	1.2	83
30	Calculations of the Electric Fields in Liquid Solutions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16236-16248.	1.2	83
31	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1390-1395.	1.0	81
32	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. <i>Journal of Chemical Physics</i> , 2007, 126, 124114.	1.2	79
33	Experimental and Computational Studies Reveal an Alternative Supramolecular Structure for Fmoc-Dipeptide Self-Assembly. <i>Biomacromolecules</i> , 2012, 13, 3562-3571.	2.6	79
34	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1721-1736.	2.3	77
35	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: I. Toward Massively Parallel Direct Space Computations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1638-1651.	2.3	76
36	RNA 3D Structure Prediction by Using a Coarse-Grained Model and Experimental Data. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3135-3144.	1.2	74

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37	Many-body effect determines the selectivity for Ca ²⁺ and Mg ²⁺ in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7495-E7501.	3.3	73
38	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	1.5	69
39	Modeling Organochlorine Compounds and the Ĩf-Hole Effect Using a Polarizable Multipole Force Field. Journal of Physical Chemistry B, 2014, 118, 6456-6465.	1.2	69
40	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	1.3	65
41	Biocompatible and blood- brain barrier permeable carbon dots for inhibition of A β 2 fibrillation and toxicity, and BACE1 activity. Nanoscale, 2017, 9, 12862-12866.	2.8	64
42	Molecular dynamics simulations of Ago silencing complexes reveal a large repertoire of admissible -seed-less- targets. Scientific Reports, 2012, 2, 569.	1.6	62
43	Toward accurate solvation dynamics of lanthanides and actinides in water using polarizable force fields: from gas-phase energetics to hydration free energies. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	62
44	The atomistic simulation of the gas permeability of poly(organophosphazenes). Part 1. Poly(dibutoxyphosphazenes). Computational and Theoretical Polymer Science, 2000, 10, 447-463.	1.1	60
45	Molecular simulation of the glass transition of polyphosphazenes. Computational and Theoretical Polymer Science, 1999, 9, 111-116.	1.1	55
46	Synthesis and biological evaluation of pyrido[2,3-d]pyrimidine-2,4-dione derivatives as eEF-2K inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 4910-4916.	1.4	55
47	Ĩ2 Sheets Not Required: Combined Experimental and Computational Studies of Self-Assembly and Gelation of the Ester-Containing Analogue of an Fmoc-Dipeptide Hydrogelator. Langmuir, 2014, 30, 5287-5296.	1.6	53
48	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II. Toward Massively Parallel Computations Using Smooth Particle Mesh Ewald. Journal of Chemical Theory and Computation, 2015, 11, 2589-2599.	2.3	53
49	Helical antimicrobial peptides assemble into protofibril scaffolds that present ordered dsDNA to TLR9. Nature Communications, 2019, 10, 1012.	5.8	53
50	Study of interactions between metal ions and protein model compounds by energy decomposition analyses and the AMOEBA force field. Journal of Chemical Physics, 2017, 147, 161733.	1.2	48
51	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. Journal of Chemical Theory and Computation, 2015, 11, 623-634.	2.3	45
52	Anisotropic Coarse-Grained Model for Proteins Based On Gay-Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2014, 10, 731-750.	2.3	44
53	Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics, 2016, 18, 30261-30269.	1.3	44
54	Implementation of Geometry-Dependent Charge Flux into the Polarizable AMOEBA+ Potential. Journal of Physical Chemistry Letters, 2020, 11, 419-426.	2.1	43

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55	Probing the Effect of Conformational Constraint on Phosphorylated Ligand Binding to an SH2 Domain Using Polarizable Force Field Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1716-1727.	1.2	42
56	Capturing RNA Folding Free Energy with Coarse-Grained Molecular Dynamics Simulations. <i>Scientific Reports</i> , 2017, 7, 45812.	1.6	42
57	Accurate immune repertoire sequencing reveals malaria infection driven antibody lineage diversification in young children. <i>Nature Communications</i> , 2017, 8, 531.	5.8	41
58	Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields Using GPUs and Multi-GPU Systems. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2034-2053.	2.3	40
59	Solution NMR Insights into Docking Interactions Involving Inactive ERK2. <i>Biochemistry</i> , 2011, 50, 3660-3672.	1.2	39
60	A transferable coarse-grained model for hydrogen-bonding liquids. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2050.	1.3	37
61	A combined molecular dynamics and experimental study of doped polypyrrole. <i>Polymer</i> , 2010, 51, 4985-4993.	1.8	36
62	Gay-Berne and electrostatic multipole based coarse-grain potential in implicit solvent. <i>Journal of Chemical Physics</i> , 2011, 135, 155104.	1.2	36
63	United polarizable multipole water model for molecular mechanics simulation. <i>Journal of Chemical Physics</i> , 2015, 143, 014504.	1.2	36
64	Polarizable Multipole-Based Force Field for Aromatic Molecules and Nucleobases. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 666-678.	2.3	36
65	Distinct Mechanisms of Nuclease-Directed DNA-Structure-Induced Genetic Instability in Cancer Genomes. <i>Cell Reports</i> , 2018, 22, 1200-1210.	2.9	36
66	Hydration gibbs free energies of open and closed shell trivalent lanthanide and actinide cations from polarizable molecular dynamics. <i>Journal of Molecular Modeling</i> , 2014, 20, 2471.	0.8	35
67	The impact of physiological crowding on the diffusivity of membrane bound proteins. <i>Soft Matter</i> , 2016, 12, 2127-2134.	1.2	35
68	Substrate specificity of human kallikreins 1 and 6 determined by phage display. <i>Protein Science</i> , 2008, 17, 664-672.	3.1	34
69	Examining Docking Interactions on ERK2 with Modular Peptide Substrates. <i>Biochemistry</i> , 2011, 50, 9500-9510.	1.2	34
70	Understanding the Specificity of a Docking Interaction between JNK1 and the Scaffolding Protein JIP1. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1491-1502.	1.2	34
71	Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 180-190.	2.3	34
72	The Molecular Mechanism of Eukaryotic Elongation Factor 2 Kinase Activation. <i>Journal of Biological Chemistry</i> , 2014, 289, 23901-23916.	1.6	32

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73	High-resolution mining of the SARS-CoV-2 main protease conformational space: supercomputer-driven unsupervised adaptive sampling. <i>Chemical Science</i> , 2021, 12, 4889-4907.	3.7	31
74	General van der Waals potential for common organic molecules. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4911-4919.	1.4	30
75	Design of intrinsically disordered proteins that undergo phase transitions with lower critical solution temperatures. <i>APL Materials</i> , 2021, 9, .	2.2	29
76	Molecular Docking Simulations for Macromolecularly Imprinted Polymers. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 13877-13884.	1.8	28
77	Design and Characterization of Nucleopeptides for Hydrogel Self-Assembly. <i>ACS Applied Bio Materials</i> , 2019, 2, 2812-2821.	2.3	28
78	Phosphorylation of the Transcription Factor Ets-1 by ERK2: Rapid Dissociation of ADP and Phospho-Ets-1. <i>Biochemistry</i> , 2010, 49, 3619-3630.	1.2	26
79	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5326-5339.	2.3	26
80	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. <i>Journal of Computational Chemistry</i> , 2016, 37, 494-506.	1.5	26
81	Capturing Many-Body Interactions with Classical Dipole Induction Models. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2751-2761.	2.3	26
82	Discovery of a potent inhibitor of MELK that inhibits expression of the anti-apoptotic protein Mcl-1 and TNBC cell growth. <i>Bioorganic and Medicinal Chemistry</i> , 2017, 25, 2609-2616.	1.4	26
83	From in Silico Discovery to Intracellular Activity: Targeting JNK-Protein Interactions with Small Molecules. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 721-725.	1.3	25
84	Thermodynamics of ion binding and occupancy in potassium channels. <i>Chemical Science</i> , 2021, 12, 8920-8930.	3.7	25
85	Temperature-induced unfolding of epidermal growth factor (EGF): Insight from molecular dynamics simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 2-12.	1.3	24
86	Correlation of RNA Secondary Structure Statistics with Thermodynamic Stability and Applications to Folding. <i>Journal of Molecular Biology</i> , 2009, 391, 769-783.	2.0	23
87	Reversible Covalent Inhibition of eEF2K by Carbonitriles. <i>ChemBioChem</i> , 2014, 15, 2435-2442.	1.3	23
88	Estimating and modeling charge transfer from the SAPT induction energy. <i>Journal of Computational Chemistry</i> , 2017, 38, 2222-2231.	1.5	21
89	Computationally driven discovery of SARS-CoV-2 M ^{pro} inhibitors: from design to experimental validation. <i>Chemical Science</i> , 2022, 13, 3674-3687.	3.7	21
90	Manipulating JNK Signaling with (â ⁺)-Zuonin A. <i>ACS Chemical Biology</i> , 2012, 7, 1873-1883.	1.6	20

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91	Development of an AMOEBA water model using GEM distributed multipoles. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	20
92	Elucidating the Phosphate Binding Mode of Phosphate-Binding Protein: The Critical Effect of Buffer Solution. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6371-6376.	1.2	20
93	A Model of a MAPK-Substrate Complex in an Active Conformation: A Computational and Experimental Approach. <i>PLoS ONE</i> , 2011, 6, e18594.	1.1	20
94	Computational Insights for the Discovery of Non-ATP Competitive Inhibitors of MAP Kinases. <i>Current Pharmaceutical Design</i> , 2012, 18, 1173-1185.	0.9	19
95	A Review of Physics-Based Coarse-Grained Potentials for the Simulations of Protein Structure and Dynamics. <i>Annual Reports in Computational Chemistry</i> , 2012, 8, 129-148.	0.9	19
96	Self-assembled nucleo-tripeptide hydrogels provide local and sustained doxorubicin release. <i>Biomaterials Science</i> , 2020, 8, 3130-3137.	2.6	19
97	A physically grounded damped dispersion model with particle mesh Ewald summation. <i>Journal of Chemical Physics</i> , 2018, 149, 084115.	1.2	18
98	Automation of AMOEBA polarizable force field for small molecules: Poltype 2. <i>Journal of Computational Chemistry</i> , 2022, 43, 1530-1542.	1.5	18
99	Statistical Potentials for Hairpin and Internal Loops Improve the Accuracy of the Predicted RNA Structure. <i>Journal of Molecular Biology</i> , 2011, 413, 473-483.	2.0	17
100	Molecular Dynamics Study of the Hybridization between RNA and Modified Oligonucleotides. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6422-6432.	2.3	17
101	Modulating multi-functional ERK complexes by covalent targeting of a recruitment site in vivo. <i>Nature Communications</i> , 2019, 10, 5232.	5.8	17
102	Large Domain Motions in Ago Protein Controlled by the Guide DNA-Strand Seed Region Determine the Ago-DNA-mRNA Complex Recognition Process. <i>PLoS ONE</i> , 2013, 8, e54620.	1.1	16
103	Using docking and alchemical free energy approach to determine the binding mechanism of eEF2K inhibitors and prioritizing the compound synthesis. <i>Frontiers in Molecular Biosciences</i> , 2015, 2, 9.	1.6	15
104	Measuring DNA Hybridization Kinetics in Live Cells Using a Time-Resolved 3D Single-Molecule Tracking Method. <i>Journal of the American Chemical Society</i> , 2019, 141, 15747-15750.	6.6	15
105	Recent progress in general force fields of small molecules. <i>Current Opinion in Structural Biology</i> , 2022, 72, 187-193.	2.6	15
106	Quantification of a Pharmacodynamic ERK End Point in Melanoma Cell Lysates: Toward Personalized Precision Medicine. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 47-52.	1.3	14
107	LNA Thymidine Monomer Enables Differentiation of the Four Single-Nucleotide Variants by Melting Temperature. <i>Journal of the American Chemical Society</i> , 2017, 139, 7110-7116.	6.6	14
108	Molecular Modeling of Conformational Properties of Oligodepsipeptides. <i>Biomacromolecules</i> , 2007, 8, 3015-3024.	2.6	13

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109	Hydration Free Energy from Orthogonal Space Random Walk and Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2792-2801.	2.3	13
110	Interfacial Water Many-Body Effects Drive Structural Dynamics and Allosteric Interactions in SARS-CoV-2 Main Protease Dimerization Interface. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6218-6226.	2.1	13
111	Identification and Validation of Novel PERK Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1467-1475.	2.5	12
112	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3607-3621.	2.3	12
113	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2323-2341.	2.3	10
114	Trypsin-ligand binding free energy calculation with AMOEBA. , 2009, 2009, 2328-31.		9
115	Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11169-11179.	1.2	9
116	Investigating the Association Mechanism between Rafoxanide and Povidone. <i>Langmuir</i> , 2018, 34, 13971-13978.	1.6	9
117	Computational and Experimental Studies of Inhibitor Design for Aldolase A. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6034-6041.	1.2	9
118	Molecular dynamics free energy simulations of ATP:Mg ²⁺ and ADP:Mg ²⁺ using the polarisable force field AMOEBA. <i>Molecular Simulation</i> , 2021, 47, 439-448.	0.9	8
119	E2EDNA: Simulation Protocol for DNA Aptamers with Ligands. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4139-4144.	2.5	8
120	Imaging sub-diffuse optical properties of cancerous and normal skin tissue using machine learning-aided spatial frequency domain imaging. <i>Journal of Biomedical Optics</i> , 2021, 26, .	1.4	8
121	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	2.2	8
122	Atomic Polarizabilities for Interactive Dipole Induction Models. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 79-87.	2.5	8
123	Advanced Electrostatic Model for Monovalent Ions Based on Ab Initio Energy Decomposition. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2806-2817.	2.5	7
124	Accurate description of molecular dipole surface with charge flux implemented for molecular mechanics. <i>Journal of Chemical Physics</i> , 2020, 153, .	1.2	6
125	Virial-based Berendsen barostat on GPUs using AMOEBA in Tinker-OpenMM. <i>Results in Chemistry</i> , 2019, 1, 100004.	0.9	5
126	Computational insights into the binding of IN17 inhibitors to MELK. <i>Journal of Molecular Modeling</i> , 2019, 25, 151.	0.8	5

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127	Some insights into the binding mechanism of Aurora B kinase gained by molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2012, 18, 4591-4601.	0.8	4
128	Reconciling NMR Structures of the HIV-1 Nucleocapsid Protein NCp7 Using Extensive Polarizable Force Field Free-Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2013-2020.	2.3	4
129	Prediction and Coarse-Grained Modeling of RNA Structures. , 2013, , 53-68.		4
130	Hydration of divalent lanthanides, Sm ²⁺ and Eu ²⁺ : A molecular dynamics study with polarizable AMOEBA force field. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	4
131	Three-site and five-site fixed-charge water models compatible with AMOEBA force field. <i>Journal of Computational Chemistry</i> , 2020, 41, 1034-1044.	1.5	3
132	Conformational preference of ChaK1 binding peptides: a molecular dynamics study. <i>PMC Biophysics</i> , 2010, 3, 2.	2.2	2
133	Elucidating binding modes of zuonin A enantiomers to JNK1 via in silico methods. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 45, 38-44.	1.3	2
134	High-Order Ab Initio Valence Force Field with Chemical Pattern-Based Parameter Assignment. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 431-447.	1.0	2
135	Exploring the Relationship between Sequences, Structures, Dynamical Behaviors and Functions of New Type Protein Drugs: DARPinS. <i>Current Pharmaceutical Design</i> , 2013, 19, 2308-2317.	0.9	1
136	Computational Insights for the Discovery of Non-ATP Competitive Inhibitors of MAP Kinases. <i>Current Drug Metabolism</i> , 2012, 18, 1173-1185.	0.7	1
137	Role of Bivalent Cations in Structural Stabilities of New Drug Targets "Vacciniarelated Kinases (VRK) from Molecular Dynamics Simulations. <i>Current Pharmaceutical Design</i> , 2013, 19, 2269-2281.	0.9	1
138	Pharmaceutical Applications of the Polarizable Amoeba Potential, Including Protein-Ligand Binding Affinity and Drug Solubility, using the Force Field X Software. <i>Biophysical Journal</i> , 2012, 102, 409a-410a.	0.2	0
139	Investigation of the Mechanism of Antimicrobial Lipopeptides using Coarse-Grained Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2013, 104, 602a.	0.2	0
140	Multiscale modeling of RNA 3D structures. , 2013, , .		0
141	Abstract 4542: Towards the identification of PKR-like endoplasmic reticulum kinase (PERK) inhibitors.. , 2013, , .		0
142	Trapping Ca ⁺ inside a Molecular Cavity: Computational study of the potential energy surfaces for Ca ⁺ -[n]cycloparaphenylene, n=5-12. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	0