Alexander D Mackerell

List of Publications by Year in Descending Order

417 papers	51,479 citations	90 h-index	221 g-index
472 ext. papers	60,775 ext. citations	6 avg, IF	7.96 L-index

#	Paper	IF	Citations
417	Application of Site-Identification by Ligand Competitive Saturation in Computer-Aided Drug Design.. *New Journal of Chemistry*, **2022**, 46, 919-932	3.6	1
416	Cholecalciferol complexation with hydroxypropyl-□cyclodextrin (HPBCD) and its molecular dynamics simulation.. *Pharmaceutical Development and Technology*, **2022**, 1-10	3.4	0
415	Development of CHARMM Additive Potential Energy Parameters for □Methyl Amino Acids. *Journal of Physical Chemistry B*, **2021**, 125, 11687-11696	3.4	
414	Global Optimization of the Lennard-Jones Parameters for the Drude Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 7085-7095	6.4	0
413	Profiling the Tox21 Chemical Collection for Acetylcholinesterase Inhibition. *Environmental Health Perspectives*, **2021**, 129, 47008	8.4	6
412	Progress toward B-Cell Lymphoma 6 BTB Domain Inhibitors for the Treatment of Diffuse Large B-Cell Lymphoma and Beyond. *Journal of Medicinal Chemistry*, **2021**, 64, 4333-4358	8.3	6
411	Functional Group Distributions, Partition Coefficients, and Resistance Factors in Lipid Bilayers Using Site Identification by Ligand Competitive Saturation. *Journal of Chemical Theory and Computation*, **2021**, 17, 3188-3202	6.4	4
410	Insights into Glucose-6-phosphate Allosteric Activation of □Glucosidase A. *Journal of Chemical Information and Modeling*, **2021**, 61, 1931-1941	6.1	1
409	Additive CHARMM36 Force Field for Nonstandard Amino Acids. *Journal of Chemical Theory and Computation*, **2021**, 17, 3554-3570	6.4	5
408	Site-Selective Chemoenzymatic Modification on the Core Fucose of an Antibody Enhances Its Fc□ Receptor Affinity and ADCC Activity. *Journal of the American Chemical Society*, **2021**, 143, 7828-7838	16.4	6
407	Toward Biotherapeutics Formulation Composition Engineering using Site-Identification by Ligand Competitive Saturation (SILCS). *Journal of Pharmaceutical Sciences*, **2021**, 110, 1103-1110	3.9	4
406	Simple Synthesis of a Heterocyclophane Exhibiting Anti-c-Met Activity by Acting as a Hatch Blocking Access to the Active Site*. *Chemistry - A European Journal*, **2021**, 27, 1648-1654	4.8	1
405	Small molecules inhibitors of the heterogeneous ribonuclear protein A18 (hnRNP A18): a regulator of protein translation and an immune checkpoint. *Nucleic Acids Research*, **2021**, 49, 1235-1246	20.1	2
404	Specificity of Molecular Fragments Binding to S100B versus S100A1 as Identified by NMR and Site Identification by Ligand Competitive Saturation (SILCS). *Molecules*, **2021**, 26,	4.8	2
403	Stereoisomerization of human constitutive androstane receptor agonist CITCO. *Tetrahedron*, **2021**, 79, 131886	2.4	0
402	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. *Journal of Chemical Theory and Computation*, **2021**, 17, 1726-1741	6.4	7
401	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. *Journal of Chemical Theory and Computation*, **2021**, 17, 1562-1580	6.4	6

400	Insights into substrate recognition and specificity for IgG by Endoglycosidase S2. *PLoS Computational Biology*, **2021**, 17, e1009103	5	1
399	Species-Specific Endotoxin Stimulus Determines Toll-Like Receptor 4- and Caspase 11-Mediated Pathway Activation Characteristics. *MSystems*, **2021**, 6, e0030621	7.6	2
398	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. *PLoS ONE*, **2021**, 16, e0244967	3.7	7
397	Rapid and accurate estimation of protein-ligand relative binding affinities using site-identification by ligand competitive saturation. *Chemical Science*, **2021**, 12, 8844-8858	9.4	5
396	CHARMM-GUI Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. *Journal of Computational Chemistry*, **2021**,	3.5	4
395	p Calculations with the Polarizable Drude Force Field and Poisson-Boltzmann Solvation Model. *Journal of Chemical Theory and Computation*, **2020**, 16, 4655-4668	6.4	7
394	Impact of electronic polarizability on protein-functional group interactions. *Physical Chemistry Chemical Physics*, **2020**, 22, 6848-6860	3.6	7
393	Rationally Designed Polypharmacology: Helix Mimetics as Dual Inhibitors of the Oncoproteins Mcl-1 and HDM2. *ChemMedChem*, **2020**, 15, 1691-1698	3.7	1
392	Optimization of a Benzothiazole Indolene Scaffold Targeting Bacterial Cell Wall Assembly. *Drug Design, Development and Therapy*, **2020**, 14, 567-574	4.4	4
391	Mg Impacts the Twister Ribozyme through Push-Pull Stabilization of Nonsequential Phosphate Pairs. *Biophysical Journal*, **2020**, 118, 1424-1437	2.9	3
390	Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLES-Fatty Acid Micellar System. *Journal of Physical Chemistry B*, **2020**, 124, 1653-1664	3.4	2
389	Structure of the cell-binding component of the binary toxin reveals a di-heptamer macromolecular assembly. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 1049-1058	11.5	12
388	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. *Journal of Chemical Theory and Computation*, **2020**, 16, 3221-3239	6.4	22
387	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches **2020**, 81-108		
386	Balanced polarizable Drude force field parameters for molecular anions: phosphates, sulfates, sulfamates, and oxides. *Journal of Molecular Modeling*, **2020**, 26, 152	2	5
385	Identification and characterization of fragment binding sites for allosteric ligand design using the site identification by ligand competitive saturation hotspots approach (SILCS-Hotspots). *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129519	4	15
384	FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules. *Journal of Computational Chemistry*, **2020**, 41, 958-970	3.5	19
383	Computational Characterization of Antibody-Excipient Interactions for Rational Excipient Selection Using the Site Identification by Ligand Competitive Saturation-Biologics Approach. *Molecular Pharmaceutics*, **2020**, 17, 4323-4333	5.6	7

382	The SKI complex is a broad-spectrum, host-directed antiviral drug target for coronaviruses, influenza, and filoviruses. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 30687-30698	11.5	7
381	Assessing hERG1 Blockade from Bayesian Machine-Learning-Optimized Site Identification by Ligand Competitive Saturation Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 6489-6501	6.1	4
380	Contributions and competition of Mg and K in folding and stabilization of the Twister ribozyme. *Rna*, **2020**, 26, 1704-1715	5.8	1
379	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. *Journal of Chemical Physics*, **2020**, 153, 114108	3.9	6
378	Improved Modeling of Cation-π and Anion-Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins. *Journal of Computational Chemistry*, **2020**, 41, 439-448	3.5	19
377	Ions Everywhere? Mg in the δ-Opioid GPCR and Atomic Details of Their Impact on Function. *Biophysical Journal*, **2020**, 118, 783-784	2.9	3
376	Force Fields for Small Molecules. *Methods in Molecular Biology*, **2019**, 2022, 21-54	1.4	15
375	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
374	Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization. *Journal of Chemical Information and Modeling*, **2019**, 59, 3018-3035	6.1	27
373	Impact of branching on the conformational heterogeneity of the lipopolysaccharide from Klebsiella pneumoniae: Implications for vaccine design. *Carbohydrate Research*, **2019**, 475, 39-47	2.9	4
372	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. *Journal of Chemical Theory and Computation*, **2019**, 15, 2460-2469	6.4	10
371	Drude Polarizable Force Field Parametrization of Carboxylate and -Acetyl Amine Carbohydrate Derivatives. *Journal of Chemical Theory and Computation*, **2019**, 15, 4982-5000	6.4	9
370	Second harmonic generation detection of Ras conformational changes and discovery of a small molecule binder. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 17290-17297	11.5	11
369	Solvation dynamics: improved reproduction of the time-dependent Stokes shift with polarizable empirical force field chromophore models. *Physical Chemistry Chemical Physics*, **2019**, 21, 17703-17710	3.6	9
368	An activating mutation of the NSD2 histone methyltransferase drives oncogenic reprogramming in acute lymphocytic leukemia. *Oncogene*, **2019**, 38, 671-686	9.2	23
367	Exploring protein-protein interactions using the site-identification by ligand competitive saturation methodology. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 289-301	4.2	10
366	Cation-π Interactions between Methylated Ammonium Groups and Tryptophan in the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 7-12	6.4	25
365	Improved Modeling of Halogenated Ligand-Protein Interactions Using the Drude Polarizable and CHARMM Additive Empirical Force Fields. *Journal of Chemical Information and Modeling*, **2019**, 59, 215-228	6.1	13

364	Prediction of Membrane Permeation of Drug Molecules by Combining an Implicit Membrane Model with Machine Learning. *Journal of Chemical Information and Modeling*, **2019**, 59, 1147-1162	6.1	14
363	Proper balance of solvent-solute and solute-solute interactions in the treatment of the diffusion of glucose using the Drude polarizable force field. *Carbohydrate Research*, **2018**, 457, 41-50	2.9	12
362	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. *Journal of Chemical Information and Modeling*, **2018**, 58, 993-1004	6.1	27
361	Characterization of Conformational Ensembles of Protonated N-glycans in the Gas-Phase. *Scientific Reports*, **2018**, 8, 1644	4.9	9
360	Polarizable Empirical Force Field for Halogen-Containing Compounds Based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2018**, 14, 1083-1098	6.4	30
359	CHARMM Drude Polarizable Force Field for Glycosidic Linkages Involving Pyranoses and Furanoses. *Journal of Chemical Theory and Computation*, **2018**, 14, 3132-3143	6.4	17
358	Optimized Lennard-Jones Parameters for Druglike Small Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 3121-3131	6.4	26
357	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg. *Journal of Physical Chemistry A*, **2018**, 122, 6147-6155	2.8	15
356	Combining the polarizable Drude force field with a continuum electrostatic Poisson-Boltzmann implicit solvation model. *Journal of Computational Chemistry*, **2018**, 39, 1707-1719	3.5	13
355	Force field development and simulations of intrinsically disordered proteins. *Current Opinion in Structural Biology*, **2018**, 48, 40-48	8.1	98
354	Polarizable force field for RNA based on the classical drude oscillator. *Journal of Computational Chemistry*, **2018**, 39, 2624-2646	3.5	43
353	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. *Molecules*, **2018**, 23,	4.8	23
352	Determination of Ionic Hydration Free Energies with Grand Canonical Monte Carlo/Molecular Dynamics Simulations in Explicit Water. *Journal of Chemical Theory and Computation*, **2018**, 14, 5290-5302	6.4	10
351	Identification of Thiourea-Based Inhibitors of the B-Cell Lymphoma 6 BTB Domain via NMR-Based Fragment Screening and Computer-Aided Drug Design. *Journal of Medicinal Chemistry*, **2018**, 61, 7573-7588	6.3	22
350	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 679-695	6.4	14
349	Iodobenzene-Catalyzed Synthesis of Phenanthridinones via Oxidative C-H Amidation. *Journal of Organic Chemistry*, **2017**, 82, 3589-3596	4.2	36
348	Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 349-363	4.2	13
347	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	6.4	47

346	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	6.4	46
345	Novel Noncatalytic Substrate-Selective p38α-Specific MAPK Inhibitors with Endothelial-Stabilizing and Anti-Inflammatory Activity. *Journal of Immunology*, **2017**, 198, 3296-3306	5.3	19
344	Development of a glycoconjugate vaccine to prevent invasive Salmonella Typhimurium infections in sub-Saharan Africa. *PLoS Neglected Tropical Diseases*, **2017**, 11, e0005493	4.8	24
343	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. *Journal of Chemical Physics*, **2017**, 147, 161727	3.9	57
342	Structure and Dynamics of FosA-Mediated Fosfomycin Resistance in Klebsiella pneumoniae and Escherichia coli. *Antimicrobial Agents and Chemotherapy*, **2017**, 61,	5.9	18
341	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. *Journal of Chemical Theory and Computation*, **2017**, 13, 4535-4552	6.4	63
340	Mapping the Drude polarizable force field onto a multipole and induced dipole model. *Journal of Chemical Physics*, **2017**, 147, 161702	3.9	32
339	Do Halogen-Hydrogen Bond Donor Interactions Dominate the Favorable Contribution of Halogens to Ligand-Protein Binding?. *Journal of Physical Chemistry B*, **2017**, 121, 6813-6821	3.4	63
338	Conformational Heterogeneity of the HIV Envelope Glycan Shield. *Scientific Reports*, **2017**, 7, 4435	4.9	22
337	Computer-Aided Drug Design Methods. *Methods in Molecular Biology*, **2017**, 1520, 85-106	1.4	160
336	Estimation of relative free energies of binding using pre-computed ensembles based on the single-step free energy perturbation and the site-identification by Ligand competitive saturation approaches. *Journal of Computational Chemistry*, **2017**, 38, 1238-1251	3.5	22
335	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. *Nature Methods*, **2017**, 14, 71-73	21.6	1819
334	The Expanding Role of the BCL6 Oncoprotein as a Cancer Therapeutic Target. *Clinical Cancer Research*, **2017**, 23, 885-893	12.9	85
333	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
332	Conformational Preference of Serogroup B Salmonella O Polysaccharide in Presence and Absence of the Monoclonal Antibody Se155-4. *Journal of Physical Chemistry B*, **2017**, 121, 3412-3423	3.4	7
331	Characterization of Mg Distributions around RNA in Solution. *ACS Omega*, **2016**, 1, 680-688	3.9	24
330	Balancing the Interactions of Mg in Aqueous Solution and with Nucleic Acid Moieties For a Polarizable Force Field Based on the Classical Drude Oscillator Model. *Journal of Physical Chemistry B*, **2016**, 120, 11436-11448	3.4	28
329	Conformational Heterogeneity of Intracellular Loop 3 of the δ-opioid G-protein Coupled Receptor. *Journal of Physical Chemistry B*, **2016**, 120, 11897-11904	3.4	8

328	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4812-4825	3.4	95
327	Structural effects of modified ribonucleotides and magnesium in transfer RNAs. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4826-4834	3.4	5
326	Novel protein-inhibitor interactions in site 3 of Ca(2+)-bound S100B as discovered by X-ray crystallography. *Acta Crystallographica Section D: Structural Biology*, **2016**, 72, 753-60	5.5	10
325	Structure of Penta-Alanine Investigated by Two-Dimensional Infrared Spectroscopy and Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 5325-39	3.4	13
324	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. *Chemical Reviews*, **2016**, 116, 4983-5013	68.1	299
323	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, 405-13	6.4	1303
322	Additive CHARMM force field for naturally occurring modified ribonucleotides. *Journal of Computational Chemistry*, **2016**, 37, 896-912	3.5	36
321	Ribosome-Templated Azide-Alkyne Cycloadditions: Synthesis of Potent Macrolide Antibiotics by In Situ Click Chemistry. *Journal of the American Chemical Society*, **2016**, 138, 3136-44	16.4	43
320	Structure-based design of N-substituted 1-hydroxy-4-sulfamoyl-2-naphthoates as selective inhibitors of the Mcl-1 oncoprotein. *European Journal of Medicinal Chemistry*, **2016**, 113, 273-92	6.8	34
319	Small Molecule Inhibitors of Ca(2+)-S100B Reveal Two Protein Conformations. *Journal of Medicinal Chemistry*, **2016**, 59, 592-608	8.3	12
318	Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma. *Journal of Clinical Investigation*, **2016**, 126, 3351-62	15.9	92
317	Towards Development of Small Molecule Lipid II Inhibitors as Novel Antibiotics. *PLoS ONE*, **2016**, 11, e0164515	3.7	7
316	Iminoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of Pseudomonas aeruginosa. *Journal of Medicinal Chemistry*, **2016**, 59, 6929-42	8.3	26
315	DIRECT-ID: An automated method to identify and quantify conformational variations--application to β2-adrenergic GPCR. *Journal of Computational Chemistry*, **2016**, 37, 416-25	3.5	12
314	The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis. *Cancer Research*, **2016**, 76, 3593-603	10.1	38
313	Improving the Force Field Description of Tyrosine-Choline Cation-π Interactions: QM Investigation of Phenol-N(Me) Interactions. *Journal of Chemical Theory and Computation*, **2016**, 12, 5585-5595	6.4	29
312	Estimating glycosaminoglycan-protein interaction affinity: water dominates the specific antithrombin-heparin interaction. *Glycobiology*, **2016**, 26, 1041-1047	5.8	17
311	Delineating the conformational flexibility of trisaccharides from NMR spectroscopy experiments and computer simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 18776-94	3.6	28

310	Quantifying the Binding Interaction between the Hypoxia-Inducible Transcription Factor and the von Hippel-Lindau Suppressor. *Journal of Chemical Theory and Computation*, **2015**, 11, 3946-54	6.4	2
309	A piRNA-like small RNA interacts with and modulates p-ERM proteins in human somatic cells. *Nature Communications*, **2015**, 6, 7316	17.4	68
308	Enhanced conformational sampling using replica exchange with concurrent solute scaling and hamiltonian biasing realized in one dimension. *Journal of Chemical Theory and Computation*, **2015**, 11, 2855-67	6.4	25
307	Mapping functional group free energy patterns at protein occluded sites: nuclear receptors and G-protein coupled receptors. *Journal of Chemical Information and Modeling*, **2015**, 55, 700-8	6.1	40
306	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, 5455-60	11.5	80
305	Small-molecule inhibitors of ERK-mediated immediate early gene expression and proliferation of melanoma cells expressing mutated BRaf. *Biochemical Journal*, **2015**, 467, 425-38	3.8	22
304	Robustness in the fitting of molecular mechanics parameters. *Journal of Computational Chemistry*, **2015**, 36, 1083-101	3.5	52
303	Acyl-2-aminobenzimidazoles: a novel class of neuroprotective agents targeting mGluR5. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 2211-20	3.4	18
302	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, 4428-40	3.4	66
301	Cyclopropyl-containing positive allosteric modulators of metabotropic glutamate receptor subtype 5. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 2275-9	2.9	9
300	Differential Deformability of the DNA Minor Groove and Altered BI/BII Backbone Conformational Equilibrium by the Monovalent Ions Li(+), Na(+), K(+), and Rb(+) via Water-Mediated Hydrogen Bonding. *Journal of Chemical Theory and Computation*, **2015**, 11, 4473-85	6.4	22
299	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. *Biophysical Journal*, **2015**, 109, 2090-100	2.9	14
298	Expedient access to pre-organized □helix mimetics based on an isocinchomeronic acid core. *Tetrahedron Letters*, **2015**, 56, 6819-6822	2	1
297	Differential Impact of the Monovalent Ions Li+, Na+, K+, and Rb+ on DNA Conformational Properties. *Journal of Physical Chemistry Letters*, **2015**, 6, 212-6	6.4	39
296	Polarizable empirical force field for hexopyranose monosaccharides based on the classical Drude oscillator. *Journal of Physical Chemistry B*, **2015**, 119, 637-52	3.4	55
295	CHARMM additive and polarizable force fields for biophysics and computer-aided drug design. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 861-871	4	150
294	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. *Journal of Computational Chemistry*, **2015**, 36, 1473-9	3.5	60
293	Structure-activity exploration of a small-molecule Lipid II inhibitor. *Drug Design, Development and Therapy*, **2015**, 9, 2383-94	4.4	6

292	Facile Synthesis of Spirocyclic Lactams from Keto Carboxylic Acids. *Organic Letters*, **2015**, 17, 3070-3	6.2	17
291	CHARMM Drude Polarizable Force Field for Aldopentofuranoses and Methyl-aldopentofuranosides. *Journal of Physical Chemistry B*, **2015**, 119, 7846-59	3.4	28
290	Conformational Dynamics of Two Natively Unfolded Fragment Peptides: Comparison of the AMBER and CHARMM Force Fields. *Journal of Physical Chemistry B*, **2015**, 119, 7902-10	3.4	12
289	Induced Dipole-Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid Peptides. *Journal of Physical Chemistry B*, **2015**, 119, 15574-82	3.4	23
288	Current status of protein force fields for molecular dynamics simulations. *Methods in Molecular Biology*, **2015**, 1215, 47-71	1.4	108
287	Pharmacophore modeling using site-identification by ligand competitive saturation (SILCS) with multiple probe molecules. *Journal of Chemical Information and Modeling*, **2015**, 55, 407-20	6.1	48
286	Spatial analysis and quantification of the thermodynamic driving forces in protein-ligand binding: binding site variability. *Journal of the American Chemical Society*, **2015**, 137, 2608-21	16.4	18
285	Dispersion interactions between urea and nucleobases contribute to the destabilization of RNA by urea in aqueous solution. *Journal of Physical Chemistry B*, **2015**, 119, 3755-61	3.4	15
284	Conformational sampling of oligosaccharides using Hamiltonian replica exchange with two-dimensional dihedral biasing potentials and the weighted histogram analysis method (WHAM). *Journal of Chemical Theory and Computation*, **2015**, 11, 788-99	6.4	27
283	RUNX2 and TAZ-dependent signaling pathways regulate soluble E-Cadherin levels and tumorsphere formation in breast cancer cells. *Oncotarget*, **2015**, 6, 28132-50	3.3	25
282	Lipopolysaccharide membrane building and simulation. *Methods in Molecular Biology*, **2015**, 1273, 391-406	1.4	31
281	Molecular dynamics simulations of glycoproteins using CHARMM. *Methods in Molecular Biology*, **2015**, 1273, 407-29	1.4	18
280	Site Identification by Ligand Competitive Saturation (SILCS) simulations for fragment-based drug design. *Methods in Molecular Biology*, **2015**, 1289, 75-87	1.4	21
279	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	6.4	48
278	All-atom polarizable force field for DNA based on the classical Drude oscillator model. *Journal of Computational Chemistry*, **2014**, 35, 1219-39	3.5	115
277	Boc-protected 1-(3-oxocycloalkyl)ureas via a one-step Curtius rearrangement: mechanism and scope. *Tetrahedron Letters*, **2014**, 55, 842-844	2	10
276	Lipid-linked oligosaccharides in membranes sample conformations that facilitate binding to oligosaccharyltransferase. *Biophysical Journal*, **2014**, 107, 1885-1895	2.9	17
275	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	6.4	111

274	CHARMM-GUI PDB manipulator for advanced modeling and simulations of proteins containing nonstandard residues. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 235-65	5.3	96
273	Induction of peptide bond dipoles drives cooperative helix formation in the (AAQAA)3 peptide. *Biophysical Journal*, **2014**, 107, 991-7	2.9	60
272	Perturbation of long-range water dynamics as the mechanism for the antifreeze activity of antifreeze glycoprotein. *Journal of Physical Chemistry B*, **2014**, 118, 11696-706	3.4	25
271	CHARMM all-atom additive force field for sphingomyelin: elucidation of hydrogen bonding and of positive curvature. *Biophysical Journal*, **2014**, 107, 134-45	2.9	138
270	Desmethyl macrolides: synthesis and evaluation of 4-desmethyl telithromycin. *ACS Medicinal Chemistry Letters*, **2014**, 5, 1021-6	4.3	13
269	A Comparative Study of Transferable Aspherical Pseudoatom Databank and Classical Force Fields for Predicting Electrostatic Interactions in Molecular Dimers. *Journal of Chemical Theory and Computation*, **2014**, 10, 1652-1664	6.4	15
268	Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 491-507	4.2	46
267	Induced Polarization Influences the Fundamental Forces in DNA Base Flipping. *Journal of Physical Chemistry Letters*, **2014**, 5, 2077-2083	6.4	47
266	Conformational properties of □or □(1-6)-linked oligosaccharides: Hamiltonian replica exchange MD simulations and NMR experiments. *Journal of Physical Chemistry B*, **2014**, 118, 2851-71	3.4	38
265	Balancing the interactions of ions, water, and DNA in the Drude polarizable force field. *Journal of Physical Chemistry B*, **2014**, 118, 6742-57	3.4	62
264	Facile one-step synthesis of 2,5-diketopiperazines. *Tetrahedron Letters*, **2014**, 55, 1905-1908	2	8
263	Novel LRRK2 GTP-binding inhibitors reduced degeneration in Parkinson□s disease cell and mouse models. *Human Molecular Genetics*, **2014**, 23, 6212-22	5.6	57
262	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	10.7	95
261	Molecular mechanics. *Current Pharmaceutical Design*, **2014**, 20, 3281-92	3.3	57
260	CHARMM36 all-atom additive protein force field: validation based on comparison to NMR data. *Journal of Computational Chemistry*, **2013**, 34, 2135-45	3.5	1487
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