Niel M Henriksen

List of Publications by Year
in descending order

25 papers	1,297 citations	361045 20 h-index	580395 25 g-index
26 all docs	26 docs citations	26 times ranked	1531 citing authors

#	Article	IF	Citations
1	Overview of the SAMPL5 hostâ€“guest challenge: Are we doing better?. Journal of Computer-Aided Molecular Design, 2017, 31, 1-19.	1.3	140
2	Highly sampled tetranucleotide and tetraloop motifs enable evaluation of common RNA force fields. Rna, 2015, 21, 1578-1590.	1.6	123
3	Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. Journal of Chemical Theory and Computation, 2014, 10, 492-499.	2.3	120
4	Computational Calorimetry: High-Precision Calculation of Hostâ€“Guest Binding Thermodynamics. Journal of Chemical Theory and Computation, 2015, 11, 4377-4394.	2.3	96
5	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	1.3	86
6	Bridging Calorimetry and Simulation through Precise Calculations of Cucurbiturilâ€“Guest Binding Enthalpies. Journal of Chemical Theory and Computation, 2014, 10, 4069-4078.	2.3	83
7	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€“Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. Journal of Physical Chemistry B, 2017, 121, 11144-11162.	1.2	62
8	Antitumor Activity of 1,18-Octadecanedioic Acid-Paclitaxel Complexed with Human Serum Albumin. Journal of the American Chemical Society, 2019, 141, 11765-11769.	6.6	61
9	Reliable Oligonucleotide Conformational Ensemble Generation in Explicit Solvent for Force Field Assessment Using Reservoir Replica Exchange Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 4014-4027.	1.2	60
10	Evaluating Force Field Performance in Thermodynamic Calculations of Cyclodextrin Hostâ€“Guest Binding: Water Models, Partial Charges, and Host Force Field Parameters. Journal of Chemical Theory and Computation, 2017, 13, 4253-4269.	2.3	51
11	Attach-Pull-Release Calculations of Ligand Binding and Conformational Changes on the First BRD4 Bromodomain. Journal of Chemical Theory and Computation, 2017, 13, 3260-3275.	2.3	49
12	Evaluation and Minimization of Uncertainty in ITC Binding Measurements: Heat Error, Concentration Error, Saturation, and Stoichiometry. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 485-498.	1.1	45
13	Araiosamines Aâ€“D: Tris-bromoindole Cyclic Guanidine Alkaloids from the Marine Sponge Clathria (Thalysias) araiosa. Journal of Organic Chemistry, 2011, 76, 5515-5523.	1.7	36
14	Binding Enthalpy Calculations for a Neutral Hostâ€“Guest Pair Yield Widely Divergent Salt Effects across Water Models. Journal of Chemical Theory and Computation, 2015, 11, 4555-4564.	2.3	36
15	The SAMPL5 hostâ€“guest challenge: computing binding free energies andÂenthalpies from explicit solvent simulations by the attach-pull-release (APR) method. Journal of Computer-Aided Molecular Design, 2017, 31, 133-145.	1.3	33
16	Totopotensamides, Polyketideâ€“Cyclic Peptide Hybrids from a Mollusk-Associated Bacterium Streptomyces sp.. Journal of Natural Products, 2012, 75, 644-649.	1.5	30
17	Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics. Journal of Physical Chemistry B, 2015, 119, 10145-10155.	1.2	30
18	Molecular dynamics re-refinement of two different small RNA loop structures using the original NMR data suggest a common structure. Journal of Biomolecular NMR, 2012, 53, 321-339.	1.6	26

#	Article	IF	Citations
19	Bind3P: Optimization of a Water Model Based on Hostâ€“Guest Binding Data. Journal of Chemical Theory and Computation, 2018, 14, 3621-3632.	2.3	23
20	Accounting for apparent deviations between calorimetric and van't Hoff enthalpies. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 692-704.	1.1	22
21	Consensus Conformations of Dinucleoside Monophosphates Described with Well-Converged Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 1456-1470.	2.3	21
22	Binding Thermodynamics of Hostâ€“Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. Journal of Chemical Theory and Computation, 2019, 15, 6225-6242.	2.3	21
23	Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters. Journal of Chemical Theory and Computation, 2020, 16, 1115-1127.	2.3	15
24	Structural and Energetic Analysis of 2-Aminobenzimidazole Inhibitors in Complex with the Hepatitis C Virus IRES RNA Using Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2014, 54, 1758-1772.	2.5	12
25	Probing the orientation of inhibitor and epoxy-eicosatrienoic acid binding in the active site of soluble epoxide hydrolase. Archives of Biochemistry and Biophysics, 2017, 613, 1-11.	1.4	9