# Sunhwan Jo

List of Publications by Year
in descending order

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|---|---|---|---|
| 45<br>papers | 14,662<br>citations | 186265<br>28<br>h-index | 233421<br>45<br>g-index |
| 45<br>all docs | 45<br>docs citations | 45<br>times ranked | 13040<br>citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Application of site-identification by ligand competitive saturation in computer-aided drug design. New Journal of Chemistry, 2022, 46, 919-932. | 2.8 | 8 |
| 2 | Toward Biotherapeutics Formulation Composition Engineering using Site-Identification by Ligand Competitive Saturation (SILCS). Journal of Pharmaceutical Sciences, 2021, 110, 1103-1110. | 3.3 | 9 |
| 3 | Simple Synthesis of a Heterocyclophane Exhibiting Antiâ€câ€Met Activity by Acting as a Hatch Blocking Access to the Active Site**. Chemistry - A European Journal, 2021, 27, 1648-1654. | 3.3 | 1 |
| 4 | Rapid and accurate estimation of proteinâ€“ligand relative binding affinities using site-identification by ligand competitive saturation. Chemical Science, 2021, 12, 8844-8858. | 7.4 | 18 |
| 5 | 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. | 2.4 | 34 |
| 6 | Computational Characterization of Antibodyâ€“Excipient Interactions for Rational Excipient Selection Using the Site Identification by Ligand Competitive Saturation-Biologics Approach. Molecular Pharmaceutics, 2020, 17, 4323-4333. | 4.6 | 20 |
| 7 | String Method for Proteinâ€“Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844. | 5.3 | 33 |
| 8 | CHARMM-GUIGlycan Modelerfor modeling and simulation of carbohydrates and glycoconjugates. Glycobiology, 2019, 29, 320-331. | 2.5 | 222 |
| 9 | 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. | 5.4 | 47 |
| 10 | Exploring proteinâ€protein interactions using the siteâ€identification by ligand competitive saturation methodology. Proteins: Structure, Function and Bioinformatics, 2019, 87, 289-301. | 2.6 | 21 |
| 11 | Multiple Conformational States Contribute to the 3D Structure of a Glucan Decasaccharide: A Combined SAXS and MD Simulation Study. Journal of Physical Chemistry B, 2018, 122, 1169-1175. | 2.6 | 9 |
| 12 | Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. Journal of Physical Chemistry B, 2018, 122, 9435-9442. | 2.6 | 33 |
| 13 | 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. | 5.3 | 17 |
| 14 | CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. Journal of Computational Chemistry, 2017, 38, 1879-1886. | 3.3 | 311 |
| 15 | Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944. | 5.3 | 139 |
| 16 | CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124. | 3.3 | 224 |
| 17 | Preferred conformations ofN-glycan core pentasaccharide in solution and in glycoproteins. Glycobiology, 2016, 26, cwv083. | 2.5 | 34 |
| 18 | Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742. | 2.6 | 14 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. Glycobiology, 2015, 26, cwv101. | 2.5 | 15 |
| 21 | Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. Biophysical Journal, 2015, 108, 1954-1962. | 0.5 | 11 |
| 22 | Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244. | 5.3 | 11 |
| 23 | A generic implementation of replica exchange with solute tempering (REST2) algorithm in NAMD for complex biophysical simulations. Computer Physics Communications, 2015, 197, 304-311. | 7.5 | 54 |
| 24 | Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. PLoS Computational Biology, 2014, 10, e1003521. | 3.2 | 112 |
| 25 | STâ€analyzer: A webâ€based user interface for simulation trajectory analysis. Journal of Computational Chemistry, 2014, 35, 957-963. | 3.3 | 12 |
| 26 | Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. Biophysical Journal, 2014, 107, 1885-1895. | 0.5 | 21 |
| 27 | CHARMM-GUIMembrane Buildertoward realistic biological membrane simulations. Journal of Computational Chemistry, 2014, 35, 1997-2004. | 3.3 | 1,802 |
| 28 | 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 |
| 29 | CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations. Journal of Chemical Information and Modeling, 2014, 54, 1003-1009. | 5.4 | 47 |
| 30 | Molecular Dynamics and NMR Spectroscopy Studies of E.Âcoli Lipopolysaccharide Structure and Dynamics. Biophysical Journal, 2013, 105, 1444-1455. | 0.5 | 153 |
| 31 | CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems. Journal of Chemical Information and Modeling, 2013, 53, 2171-2180. | 5.4 | 99 |
| 32 | CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application. Journal of Chemical Information and Modeling, 2013, 53, 267-277. | 5.4 | 71 |
| 33 | NMR-Based Simulation Studies of Pf1 Coat Protein in Explicit Membranes. Biophysical Journal, 2013, 105, 691-698. | 0.5 | 18 |
| 34 | Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling. PLoS Computational Biology, 2013, 9, e1002946. | 3.2 | 29 |
| 35 | The Salmonella Type III Secretion System Inner Rod Protein PrgJ Is Partially Folded. Journal of Biological Chemistry, 2012, 287, 25303-25311. | 3.4 | 28 |
| 36 | Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into Voltage-Dependent Loop-Gating. Biophysical Journal, 2012, 102, 1341-1351. | 0.5 | 35 |

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|---|---|---|---|
| 37 | Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339. | 3.3 | 43 |
| 38 | Solid-State NMR Ensemble Dynamics as a Mediator between Experiment and Simulation. Biophysical Journal, 2011, 100, 2922-2928. | 0.5 | 17 |
| 39 | Transmembrane Helix Orientation and Dynamics: Insights from Ensemble Dynamics with Solid-State NMR Observables. Biophysical Journal, 2011, 100, 2913-2921. | 0.5 | 29 |
| 40 | Novel Pyrrolopyrimidine-Based Î±-Helix Mimetics: Cell-Permeable Inhibitors of Proteinâ^'Protein Interactions. Journal of the American Chemical Society, 2011, 133, 676-679. | 13.7 | 121 |
| 41 | Glycan reader: Automated sugar identification and simulation preparation for carbohydrates and glycoproteins. Journal of Computational Chemistry, 2011, 32, 3135-3141. | 3.3 | 172 |
| 42 | Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. Journal of Physical Chemistry B, 2010, 114, 13342-13348. | 2.6 | 109 |
| 43 | CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. Biophysical Journal, 2009, 97, 50-58. | 0.5 | 1,346 |
| 44 | CHARMMâ€GUI: A webâ€based graphical user interface for CHARMM. Journal of Computational Chemistry, 2008, 29, 1859-1865. | 3.3 | 5,402 |
| 45 | Automated Builder and Database of Protein/Membrane Complexes for Molecular Dynamics Simulations. PLoS ONE, 2007, 2, e880. | 2.5 | 930 |