Sunhwan Jo

Leadership Computing Facility, Argonne National Laboratory
9700S, Cass Ave, Lemont, IL, 60439
Tel. 630-252-5030
http://www.sunhwanj.com
sunhwanj@gmail.com

I. EDUCATIONS AND POSITIONS

2014 July	-	Current	Postdoctoral Researcher Leadership Computing Facility Argonne National Lab, Lemont, IL, USA
2013 July	-	2014 July	Postdoctoral Scholar Benoit Roux Lab The University of Chicago, Chicago, Il, USA
2008 August	-	2013 June	The University of Kansas, Lawrence, KS, USA Ph. D. in Molecular Bioscience, Biochemistry Advisors: Dr. Wonpil Im and Dr. Roberto De. Guzman
2006 August	-	2008 July	The University of Kansas, Lawrence, KS, USA B.S. in Chemistry
2005 August	-	2006 June	Hanyang University, Seoul, South Korea
2001 June	-	2005 May	GBI Consulting, Seoul, South Korea Alternative military service as a programmer
1999 March	-	2001 June	Hanyang University, Seoul, South Korea

II. RESEARCH EXPERIENCE

- CHARMM-GUI Development
- Glycan Structure Modeling
- CHARMM Development / NAMD Development in High Performance Computers
- Protein-Protein Interaction Using Free Energy MD simulations
- Membrane Protein Structure Refinement Using Solid-state Ensemble Dynamics
- Molecular Dynamics Simulation of Membrane Protein
- NMR Experiment

III. HONORS AND AWARDS

1. Philip and Marjorie Newmark Award 2013
Molecular Biosciences Department, The University of Kansas, Lawrence, KS, USA

2.Twomey Travel Award 2013
Molecular Biosciences Department, The University of Kansas, Lawrence, KS, USA

3.Sigma Xi Research Presentation Competition (2nd place; adv. graduate students) 2012
Sigma Xi, The University of Kansas Chapter, Lawrence, KS, USA

4. Sigma Xi Research Presentation Competition (1st place; early graduate students) 2008
Sigma Xi, The University of Kansas Chapter, Lawrence, KS, USA

5. Rollin Sterling Wade Memorial Scholarship 2007
The University of Kansas, Lawrence, KS, USA

4. College Top Honors Scholarship 1999
Natural Science College, Hanyang University, Seoul, South Korea

IV. PUBLICATIONS

Google Scholar Statistics: http://goo.gl/Ei82D

h-index: 10 / i10-index: 11 / first author: 11 / published or in press: 23 / in preparation: 2

1. Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model
   Avisek Das, Mert Gur, Mary Hongying Cheng, **Sunhwan Jo**, Ivet Bahar, and Benoit Roux (2014) PLoS Comput. Biol. 10(4):e1003521 DOI
2. ST-analyzer: A web-based user interface for simulation trajectory analysis
   Jong Cheol Jeong, **Sunhwan Jo**, Emilia L Wu, Yifei Qi, Viviana Monje-Galvan, Min Sun Yeom, Lev Gorenstein, Feng Chen, Jeffery B Klauda, Wonpil Im (2014) J. Comput. Chem. 35(12):957-963 DOI
3. CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations
   Yifei Qi, Xi Cheng, Wei Han, **Sunhwan Jo**, Klaus Schulten, and Wonpil Im (2014) J. Chem. Inf. Model. 54(3):1003-1009 DOI
4. CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems
   Xi Cheng, **Sunhwan Jo**, Hui Sun Lee, Jeffery B. Klauda, and Wonpil Im (2013) J. Chem. Inf. Model. 53(8):2171-2180 DOI
5. Molecular Dynamics and NMR Spectroscopy Studies of E. coli Lipopolysaccharide Structure and Dynamics
   Emilia Wu, Olof Engström, **Sunhwan Jo**, Dani Stuhlsatz, Min Sun Yeom, Jeffrey B. Klauda, Göram Widmalm, and Wonpil Im (2013) Biophys. J. 105(6):1444-1455 DOI
6. NMR-Based Simulation Studies of Pf1 Coat Protein in Explicit Membranes
   Xi Cheng, **Sunhwan Jo** Francessca Marassi, and Wonpil Im (2013) Biophys. J. 105(3):691-698 DOI
7. Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling.

Sunhwan Jo, Hui Sun Lee, Jeffrey Skolnick, and Wonpil Im. (2013) PLoS Comp. Biol. 9(3):e1002946 DOI

8. CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application.
   Sunhwan Jo, Wei Jiang, Hui Sun Lee, Benoit Roux, and Wonpil Im. (2013) J. Chem. Inf. Model. 53(1):267-277 DOI

9. Glycan Fragment DB: A Database of PDB-Based Glycan 3D Structures.
   Sunhwan Jo and Wonpil Im. (2013) Nucleic Acid Res. 41(D1):D470-474 DOI

10. Application of Absolute Binding Free Energy Calculations to Prediction of Binding Modes and Affinities of MDM2 and MDMX Inhibitors.
    Hui Sun Lee, **Sunhwan Jo**, Hyun-Suk Lim, and Wonpil Im. (2012) J. Chem. Inf. Model. *52*(7): 1821-1832 DOI

11. The Salmonella Type III Secretion System Inner Rod Protein PrgJ Is Partially Folded.
    Dalian Zhong, Matthew Lefebre, Kawaljit Kaur, Melanie A McDowell, Courtney Godwski, **Sunhwan Jo**, Yu Wang, Stephen H Benedict, Susan M Lea, Jorge E Galan, and Roberto De. Guzman. (2012) J. Biol. Chem. 287(30):25303-25311 DOI

12. Molecular Dynamics Simulation of the Cx26 Hemichannel: Insight Into Voltage-Dependent Loop-Gating.
    Taekyung Kwon, Benoit Roux, **Sunhwan Jo**, Jeffery B. Klauda, Andrew L. Harris, and Thaddeus A. Bargiello. (2012) Biophys. J. 102(6):1341-1351 ***(Selected as cover)*** DOI

13. Web Interface for Brownian Dynamics Simulation of Ion Transport and Its Applications to Beta-Barrel Pores.
    Kyuil Lee, **Sunhwan Jo**, Huan Rui, Bernhard Egwolf, Benoit Roux, Richard Paster, and Wonpil Im. (2012) J. Comput. Chem. 33(3):331-339 ***(Selected as cover)*** DOI

14. An Ensemble Dynamics Approach to Decipher Solid-state NMR Observables of Membrane Proteins.
    Wonpil Im, **Sunhwan Jo**, and Taehoon Kim. (2012) Biochim. Biophys. Acta 1818(2):252-262 DOI

15. Glycan Reader: Automated Sugar Identification and Simulation Preparation for Carbohydrates and Glycoproteins.
    Sunhwan Jo, Kevin Song, Heather Desaire, Alexander D. MacKerell, Jr., and Wonpil Im. (2011) J. Comput. Chem. 32: 3135-3141 ***(Selected as cover)*** DOI

16. Transmembrane Helix Orientation and Dynamics: Insights from Ensemble Dynamics with Solid-State NMR Observables.
    Sunhwan Jo and Wonpil Im. (2011) Biophys. J. 100(12):2913-2921 DOI

17. Solid-State NMR Ensemble Dynamics as a Mediator between Experiment and Simulation.
    Taehoon Kim, **Sunhwan Jo**, Wonpil Im. (2011) Biophys. J. 100(12):2922-2928 DOI

18. Novel Pyrrolopyrimidine-Based α-Helix Mimetics: Cell-Permeable Inhibitors of Protein-Protein Interactions.

Ji Hoon Lee, Qi Zhang, **Sunhwan Jo**, Sergio Cha, Misook Oh, Wonpil Im, Hua Lu, Hyun-Suk Lim. (2011) J Am. Chem. Soc. 33(4):676-9 DOI

19. Cholesterol flip-flop: insights from free energy simulation studies.
Sunhwan Jo, Huan Rui, Joseph. B. Lim, Jeffrey B. Klauda, Wonpil Im. (2010) Phys Chem B. 114(42):13342-8 DOI

20. CHARMM-GUI Membrane Builder for Mixed Bilayers and Its application to Yeast Membrane.
Sunhwan Jo, Joseph B. Lim, Jeffery B. Klauda, and Wonpil Im. (2009) Biophys. J. 97(1):50-8 DOI

21. PBEQ-Solver for Online Visualization of Electrostatic Potential of Biomolecules.
Sunhwan Jo, Miklos Vargyas, Judit Vasko-Szedlar, Benoît Roux, and Wonpil Im (2008) Nucleic Acids Res. 36:W270-5 DOI

22. CHARMM-GUI: Web-based Graphical User Interface for CHARMM.
Sunhwan Jo, Taehoon Kim, Vidyashankara G. Iyer, and Wonpil Im. (2008) J. Comput. Chem. 29(11):1859-1865 DOI

23. Automated Builder and Database of Protein/Membrane Complexes for Molecular Dynamics Simulations.
Sunhwan Jo, Taehoon Kim, and Wonpil Im. (2007) PLoS ONE 2(9): e880. DOI

VI. BOOK CHAPTERS

1. Lipopolysaccharide Membrane Building and Simulation.
Sunhwan Jo, Emilia Wu, Danielle Stuhlsatz, Jeffery B. Klauda, Göran Wildmalm, and Wonpil Im. (2012) Methods in Molecular Biology: Glycoinformatics. *Submitted*
2. Molecular Dynamics Simulations of Glycoproteins using CHARMM.
Sairam S. Mallajosyula, **Sunhwan Jo**, Wonpil Im, and Alexander D. MacKerell, Jr. (2012) Methods in Molecular Biology: Glycoinformatics. *Submitted*

VII. PRESENTATIONS AT MEETINGS AND SYMPOSIA

1. Glycan Builder for In Silico Glycosylation: Template-Based Structure Prediction of Carbohydrate Structures of Glycoconjugates.
Oral Presentation (2012-3-7). Graduate student research competetion, Lawrence, KS, USA.
2. Glycan Reader: Automated Sugar Identification and Simulation Preparation for Carbohydrates and Glycoproteins.
Poster Presentation (2012-2-25). Biophysical Society Meeting, San Diego, CA, USA
3. Glycan Reader: Automated Sugar Identification and Simulation Preparation for Carbohydrates and Glycoproteins.

Poster Presentation (2011-6-20). Gordon Research Conference: Carbohydrates, Waterville, ME, USA.

4. Transmembrane Helix Orientation and Dynamics Examined by Ensemble Dynamics with Solid-State NMR Observables and Potential of Mean Force Calculations.
   Poster Presentation (2011-3-5). Biophysical Society Meeting, Baltimore, MD, USA
5. Cholesterol flip-flop: insights from free energy simulation studies.
   Oral Presentation (2010-11-13). KSU-KU Physical Chemistry Symposium. Manhattan, KS, USA.
6. Transmembrane Helix Orientation and Dynamics Examined by Ensemble Dynamics with Solid-State NMR Observables and Potential of Mean Force Calculations.
   Oral Presentation (2009-9-26). GRASP NMR Symposium. Lawrence, KS, USA.
7. NMR Characterization of the Inner Rod Proteins of the Bacterial Needle Apparatus.
   Oral Presentation (2009-4-25). Sigma Xi Student Research Competition. Lawrence, KS, USA.
8. NMR Characterization of the Inner Rod Proteins of the Bacterial Needle Apparatus.
   Oral Presentation (2009-3-27). American Society for Microbiology Mo Valley Branch Meeting. Lawrence, KS, USA.
9. NMR Structure Calculation in CHARMM-GUI: A Web Server for the NMR Structure Calculation of Bio-molecules.
   Oral Presentation (2008). KU Undergraduate Honors Symposium, Lawrence, KS, USA.
10. CHARMM-GUI: Web-based Graphical User Interface for CHARMM.
    Poster Presentation (2007). American Chemical Society National Meeting, Chicago, IL, USA.

VII.INVITED TALKS

1. Quantifying protein-protein binding with greatly scalable multiple copy algorithms of NAMD
   Leadership Computing Center, Argonne National Lab, Lemont, IL, USA (2014)
2. Computational Studies of Glycan Conformations in Glycoproteins
   Illinois Institute of Technology, Chicago, IL, USA (2013)