

# Amarda Shehu

Associate Professor<sup>1</sup>  
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## EMPLOYMENT

### George Mason University

Associate Professor, Department of Computer Science	August 2014 – present
Assistant Professor, Department of Computer Science	August 2008 – 2014
Affiliate Appointment, School of Systems Biology	August 2008 – present
Affiliate Appointment, Department of Bioengineering	August 2011 – present
Faculty Member, Mason Nanotechnology Initiative	August 2012 – present

## EDUCATION

**Rice University, Houston, TX** December 2004 to July 2008

Ph.D. in Computer Science  
Thesis Title: “*Molecules in Motion: Computing Structural Flexibility*”  
Thesis Advisor: Professor Lydia E. Kavvaki

**Rice University, Houston, TX** August 2002 to December 2004

M.S. in Computer Science  
Thesis Title: “*Sampling Biomolecular Conformations with Spatial and Energetic Constraints*”  
Thesis Advisor: Professor Lydia E. Kavvaki

**Clarkson University, Potsdam, NY** January 2000 to May 2002

B.S. in Computer Science  
*Summa Cum Laude* in two majors: (1) Computer Science and (2) Mathematics  
Honor Thesis Title: “*Structural and Computational Complexity Results on Testing Dimension in Graphs*”  
Honor Thesis Advisor: Professor Christino Tamon

## RESEARCH INTERESTS

The application domain of my research is biomolecular modeling and simulation to *unravel the molecular basis of biological processes in the healthy and diseased cell*. The focus is on characterizing the relationship between sequence, structure, dynamics, and biological function in order to understand and predict function and dysfunction. Efforts on modeling biomolecular structure and dynamics at equilibrium exploit the energy landscape view. Highlights include modeling of pathogenic mutations and simulation of binding processes to understand and guide treatments of cancer, neurodegenerative disorders, and other proteinopathies. In 2013, research on addiction was featured on [newspaper](#) and [magazine](#) articles, [GMU-TV](#), and journal [front covers](#).

From an algorithmic point of view, my research focuses on design of novel and powerful optimization frameworks. These frameworks exploit effective combinations of discrete and continuous search for vast high-dimensional molecular search spaces with highly nonlinear and multimodal energy surfaces. They make heavy use of spatial reasoning, kinematics, and inverse kinematics, building on analogies between molecular systems and mechanical, multi-linkage systems operating in the presence of constraints, building on discrete kinetic models via analogies between biomolecular dynamics and robot motion planning and stochastic optimization under the umbrella of evolutionary computation. Additional work focuses on uncovering complex function-summarizing signals in DNA and RNA through efficient algorithmic frameworks that encapsulate machine learning within evolutionary computation frameworks to handle big data (billions of sequences in a few hours of CPU time).

This research is highly interdisciplinary. Due to my unique predoctoral training and continuous dedication to broaden my understanding beyond computer science, my research exploits concepts from statistical mechanics, theoretical chemistry, and protein biophysics. This broader understanding drives algorithmic design in my lab.

## AWARDS

Mason Emerging Researcher/Scholar/Creator Award<sup>2</sup>, 2014.

ACM Service Award in recognition of contributions to ACM as ACM-BCB local arrangements chair, 2013.

OSCAR Mentor Excellence Award<sup>3</sup>, GMU, 2013.

Honorable Mention, Humies Competition Award, ACM GECCO, 2012.

Young Faculty Research Award, Department of Computer Science, GMU, 2012.

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<sup>1</sup>Text appearing in blue (darker in grayscale mode) is a hyperlink.

<sup>2</sup>This Mason-wide award is given annually to young scholars judged most likely to make significant contributions in their fields.

<sup>3</sup>This is a GMU-wide award made to faculty with a record of propagating a culture of scholarship and research among the Mason undergraduate population.

Recipient of NIH Predoctoral Fellowship, Nanobiology Training Program, 2007-2005.

Recipient of NSF ADVANCE Fellowship on Negotiating Ideal Faculty Position Workshop, 2006 (ratio 55/730).

Recipient of Rice University Doctoral Fellowship, 2002.

Recipient of Presidential Scholarship, Clarkson University, 2000-2002.

Recipient of Honors Scholarship in recognition of academic excellence, Clarkson University, 2002.

Recipient of Phi-Mu-Epsilon Fellowship Award for “Best student in Computer Science and Mathematics”, Clarkson University, 2001.

Recipient of the University Recognition Day award, the Hamlin/Darraugh award, in Mathematics and Computer Science, Clarkson University, 2001.

Recipient of International Student Excellence Award, Clarkson University, 2001.

Honorable mention at the International Competition of Mathematics, Turkey, 1997.

## GRANTS

### External Funding (in reverse chronological order):

8. NSF Software Infrastructure for Sustained Innovation (Sustainable Software Elements) Collaborative Grant for “A Novel Plug-and-play Software Platform of Robotics-inspired Algorithms for Modeling Biomolecular Structures and Motions,” \$499,999, 02/01/2015 - 01/31/2018. (PIs: Shehu A, Plaku E/CUA, Roitberg A/UF).
7. NSF Computing Core Foundations (Algorithmic Foundations) Grant for “Novel Stochastic Optimization Algorithms for Advancing the Treatment of Dynamic Molecular Systems,” \$399,998, 07/1/2014 - 06/30/2017. (PI: Shehu A, co-PI: De Jong, K). (REU Supplement, \$8,000, 2016-2017)
6. NSF Information and Intelligent Systems (Robust Intelligence) CAREER Grant for “Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems,” \$549,924, 03/01/2012 - 02/28/2017. (PI: Shehu A, no co-PIs). (REU Supplements, \$8,000, 2012-2013, \$8,000, 2016-2017)
5. NSF CISE Grant for “Travel Awards for 2015 IEEE International Conference on Bioinformatics and Biomedicine (BIBM-2015)”, \$21,761, 08/01/2015 - 07/30/2016.
4. Virginia Foundation for Healthy Youth Award for “Molecular Mechanisms Underlying Menthol Cigarette Addiction,” \$27,544, 07/01/2013 - 10/31/2015. PI: Kabbani N/Neuroscience-GMU, co-PI: Shehu A).
3. Jeffress Trust Awards Program in Interdisciplinary Research Award for “Probabilistic Search Algorithms: Powerful Novel Tools for Peptide Modeling,” \$100,000, 09/15/2013 - 06/15/2015. PI: Shehu A, co-PI: Blaisten-Barojas E/Computational Materials Science-GMU).
2. NSF Computing Core Foundations (Algorithmic Foundations) Grant for “A Unified Computational Framework to Enhance the Ab-initio Sampling of Native-like Protein Conformations,” \$449,998, 9/1/2010 - 8/31/2014. (PI: Shehu A, no co-PIs).
1. NSF CISE Grant for “NSF CISE CAREER Writing Workshop,” \$73,750, 12/05/2013 - 05/31/2014. (PI: Shehu A, co-PI: Rangwala H/Computer Science-GMU).

### Internal Funding from Mason (in reverse chronological order):

7. Mason Seed Grant for “Towards A Unified Dry to Wet Laboratory Framework for Screening, Modifying, and Designing Antimicrobial Peptides,” \$10,000, 12/20/2013-05/01/2014. (PI: Shehu A, co-PI: Vidyashankar A/Statistics-GMU).
6. Mason Seed Grant for “Structural and Functional Mechanisms Underlying Menthol Addiction,” \$20,000, 07/01/2013-10/01/2013. (Co-PI: Shehu A, PI: Kabbani N/Neuroscience-GMU).
5. Mason Seed Grant for “Probabilistic Search Techniques as New Tools for Peptides Modeling,” \$4,000, 12/01/2012-06/01/2013 (PI: Shehu A, co-PI: Cortes J/Robotics-University of Toulouse, France)
4. Mason Seed Grant for “Combining Experiment and Computation to Characterize Dopamine Receptors and the Mode of Action of Antipsychotic Drugs,” \$12,000, 06/01/2010-06/01/2011 (co-PI: Shehu A, PI: Kabbani N/Neuroscience-GMU).
3. RA Support, AY 2010-2011.
2. Bioengineering Seed Grant for “Staying Ahead of Evolution: Engineering Novel Antimicrobial Peptides,” \$35,000, 01/01/2009-12/31/2010 (PI: Shehu A, co-PIs: Bishop B/Biochemistry-GMU and van Hoek M/Molecular Biology-GMU).
1. Mason Seed Grant for “In-silico Characterization and Design of Protein Complexes: Exploiting Symmetry and Redundancy,” \$8,000, 01/01/2009-12/31/2009 (PI: Shehu A, no co-PIs).

## CITATION INDICES AND STATISTICS

Per GoogleScholar as of November 27, 2016: 963 citations, 870 since 2011, h-index of 17, i10-index of 35. Interpretation: h-index is largest number h s.t. h publications have at least h citations; i10-index is number of publications with at least 10 citations.

JOURNAL PUBLICATIONS (PEER-REVIEWED)<sup>4</sup>

- J39. Shehu A\* and Plaku E\*. *A Survey of Computational Treatments of Biomolecules by Robotics-inspired Methods Modeling Equilibrium Structure and Dynamics*, *J Artif Intel Res* 2016, in press. [IF: 0.91]
- J38. Sapin E<sup>p</sup>, De Jong K\*, and Shehu A\*. *From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes*, *IEEE/ACM Trans Comput Bio and Bioinf* 2016, in press. [IF: 1.54]
- J37. Sapin E<sup>p</sup>, Carr DB, De Jong K\*, and Shehu A\*. *Computing energy landscape maps and structural excursions of proteins*, *BMC Genomics* 17(Suppl 4): 546, 2016. [IF: 3.99] [Citations: 1]
- J36. Maximova T<sup>p</sup>, Plaku E\*, and Shehu A\*. *Structure-guided Protein Transition Modeling with a Probabilistic Roadmap Algorithm*, *IEEE/ACM Trans Comput Bio and Bioinf* 13(5): 1-14, 2016. [IF: 1.54]
- J35. Molloy K<sup>g</sup>, Clausen R<sup>g</sup>, and Shehu A\*. *A Stochastic Roadmap Method to Model Protein Structural Transitions*, *Robotica* 34(8): 1705-1733 (featured on issue front cover), 2016. [IF: 0.89] [Citations: 4]
- J34. Molloy K<sup>g</sup> and Shehu A\*. *A General, Adaptive, Roadmap-based Algorithm for Protein Motion Computation*, *IEEE Trans NanoBioScience* 15(2): 158-165, 2016. [IF: 1.77] [Citations: 2]
- J33. Maximova T<sup>p</sup>, Moffat R<sup>g</sup>, Ma B, Nussinov R, and Shehu A\*. *Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics*, *PLoS Comput Biol* 12(4): e1004619, 2016, (selected for April issue front cover. Also featured in the PLoS Comp Biol blog), 2016. [IF: 4.83] [Citations: 6]
- J32. Shehu A\* and Nussinov R\*. *Computational Methods for Exploration and Analysis of Macromolecular Structure and Dynamics*, *PLoS Comput Biol* 11(10): e1004585, 2015 (editorial). [IF: 4.83] [Citations: 4]
- J31. Devaurs D, Molloy K<sup>g</sup>, Vaisset M, Shehu A, Simeon T, and Cortes J\*. *Characterizing Energy Landscapes of Peptides using a Combination of Stochastic Algorithms*, *IEEE Trans NanoBioScience* 14(5): 545-552, 2015. [IF: 1.77] [Citations: 6]
- J30. Veltri D<sup>g</sup>, Kamath U, and Shehu A\*. *Improving Recognition of Antimicrobial Peptides and Target Selectivity through Machine Learning and Genetic Programming*, *IEEE/ACM Trans Comput Biol and Bioinf* 2015. [IF: 1.54] [Citations: 1]
- J29. Hashmi I<sup>g</sup> and Shehu A\*. *idDock+: Integrating Machine Learning in Probabilistic Search for Protein-protein Docking*, *J Comput Biol* 22(9): 806-822. [IF: 1.67] [Citations: 2]
- J28. Clausen R<sup>g</sup> and Shehu A\*. *A Data-driven Evolutionary Algorithm for Mapping Multi-basin Protein Energy Landscape*, *J Comput Biol* 22(9): 844-860. [IF: 1.67] [Citations: 9]
- J27. Clausen R<sup>g</sup>, Ma B, Nussinov R\*, and Shehu A\*. *Mapping the Conformation Space of Wildtype and Mutant Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm*, *PLoS Comput Biol* 11(9): e1004470, 2015. [IF: 4.83] [Citations: 14]
- J26. Kamath U<sup>g</sup>, De Jong KA\*, and Shehu A\*. *Effective Automated Feature Construction and Selection for Classification of Biological Sequences*, *PLoS One* 9(7): e99982, 2014. [IF: 5.2] [Citations: 10]
- J25. Molloy K<sup>g</sup>, Van JM<sup>u</sup>, Barbara D, and Shehu A\*. *Exploring Representations of Protein Structure for Automated Remote Homology Detection and Mapping of Protein Structure Space*, *BMC Bioinf*, 15(Suppl 8): S4, 2014. [IF: 3.02] [Citations: 4]
- J24. Kabbani, N\*, Nordman JC, Corgiat B, Veltri D<sup>g</sup>, Shehu A, and Adams DJ. *Are Nicotinic Receptors Coupled to G Proteins?* *Bioessays*, 35(12):1025-1034, 2013 ([video abstract](#)). [IF: 5.42] [Citations: 18]
- J23. Ashoor A, Nordman JC, Veltri D<sup>g</sup>, Yang KS, Al Kury L, Shuba Y, Mahgoub M, Howarth FC, Lupica C, Shehu A, Kabbani N, and Oz M\*. *Menthol Inhibits 5-HT<sub>3</sub> Receptor-mediated Currents*, *J of Pharmacology and Experimental Therapeutics* 347(20):398-409, 2013 ([issue front cover](#)). [IF: 4.31] [Citations: 15]

<sup>4</sup>Articles are listed in reverse chronological order. Shehu's advisees are indicated by (p) for postdocotoral, (g) for graduate, (u) for undergraduate, and (h) for high-school students. Corresponding authors are indicated by (\*). Impact factors (IF) reported for journal publications are those at the year of publication. If not available, 5-year average or most recent values are reported. Acceptance Rates (AR) are reported for conference and workshop papers where available, whether obtained online or as reported in published proceedings.

- J22. Ashoor A, Nordman JC, Veltri D<sup>g</sup>, Yang KS, Al Kury L, Shuba Y, Mahgoub M, Howarth FC, Sadek B, **Shehu A**, Kabbani N, and Oz M\*. *Menthol Binding and Inhibition of Alpha7-nicotinic Acetylcholine Receptors*, *PLoS One* (8)7:e67674, 2013. [IF: 4.09] [Citations: 17]
- J21. Molloy M<sup>g</sup>, Saleh S<sup>u</sup>, and **Shehu A**\*. *Probabilistic Search and Energy Guidance for Biased Decoy Sampling in Ab-initio Protein Structure Prediction*, *IEEE/ACM Trans Comput Biol and Bioinf*, 10(5):1162-1175, 2013. [IF: 2.25] [Citations: 13]
- J20. Hashmi I<sup>g</sup> and **Shehu A**\*. *HopDock: A Probabilistic Search Algorithm for Decoy Sampling in Protein-protein Docking*, *Proteome Sci* 11(Suppl 1):S6, 2013. [IF: 2.42] [Citations: 10]
- J19. Saleh S<sup>u</sup>, Olson B<sup>g</sup>, and **Shehu A**\*. *A population-based Evolutionary Search Approach to the Multiple Minima Problem in de novo Protein Structure Prediction*, *BMC Struct Biol* 13(Suppl 1): S4, 2013. [IF: 2.10] [Citations: 12]
- J18. Olson B<sup>g</sup> and **Shehu A**\*. *Rapid Sampling of Local Minima in Protein Energy Surface and Effective Reduction through a Multi-objective Filter*, *Proteome Sci* 11(Suppl 1):S12, 2013. [IF: 2.42] [Citations: 10]
- J17. Molloy M<sup>g</sup> and **Shehu, A**\*. *Elucidating the Ensemble of Functionally-relevant Transitions in Protein Systems with a Robotics-inspired Method*, *BMC Struct Biol* 13(Suppl 1):S8, 2013. [IF: 2.09] [Citations: 14]
- J16. Olson B<sup>g</sup>, Hashmi I<sup>g</sup>, Molloy K<sup>g</sup> and **Shehu, A**\*. *Basin Hopping as a General and Versatile Optimization Framework for the Characterization of Biological Macromolecules*, *Advances in Artificial Intelligence J*, 674832, 2012 (special issue1 on applications in biomedicine). [Citations: 16]
- J15. Olson B<sup>g</sup> and **Shehu A**\*. *Evolutionary-inspired Probabilistic Search for Enhancing Sampling of Local Minima in the Protein Energy Surface*, *Proteome Sci*, 10(Suppl1): S5, 2012. [IF: 2.42] [Citations: 29]
- J14. Hashmi I<sup>g</sup>, Akbal B, Haspel N, and **Shehu A**\*. *Guiding Protein Docking with Geometric and Evolutionary Information*, *J Bioinf and Comp Biol*, 10(3): 1242008, 2012. [IF: 1.06] [Citations: 10]
- J13. Akbal B, Hashmi I<sup>g</sup>, **Shehu A**, and Haspel N\*. *An Evolutionary Conservation Based Method for Refining and Reranking Protein Complex Structures*, *J Bioinf and Comp Biol*, 10(3): 12420024, 2012. [IF: 1.06] [Citations: 15]
- J12. Olson B<sup>g</sup>, Molloy<sup>g</sup>, K, Hendi S-F<sup>g</sup>, and **Shehu A**\*. *Guiding Probabilistic Search of the Protein Conformational Space with Structural Profiles*, *J Bioinf and Comp Biol*, 10(3): 1242005, 2012. [IF: 1.06] [Citations: 20]
- J11. **Shehu A**\* and Kavraki LE\*. *Modeling Structures and Motions of Loops in Protein Molecules*, *Entropy J*, 14(2):252-290, 2012 (invited review article). [IF: 1.11] [Citations: 19]
- J10. Kamath U<sup>g</sup>, Compton J<sup>u</sup>, Islamaj-Dogan R, De Jong KA\*, and **Shehu A**\*. *An Evolutionary Algorithm Approach for Feature Generation from Sequence Data and its Application to DNA Splice-Site Prediction*, *IEEE Trans Comput Biol and Bioinf*, 9(5):1387-1398, 2012. [IF: 2.25] [Citations: 33]
- J9. Kamath U<sup>g</sup>, **Shehu A**\*, and De Jong KA\*. *A Two-Stage Evolutionary Approach for Effective Classification of Hypersensitive DNA Sequences*, *J Bioinf and Comp Biol*, 9(3):399-413, 2011. [IF: 1.06] [Citations: 7]
- J8. Olson B<sup>g</sup>, Molloy K<sup>g</sup> and **Shehu A**\*. *In Search of the Protein Native State with a Probabilistic Sampling Approach*, *J Bioinf and Comp Biol*, 9(3):383-398, 2011. [IF: 1.06] [Citations: 30]
- J7. **Shehu A**\* and Olson B<sup>g</sup>. *Guiding the Search for Native-like Protein Conformations with an Ab-initio Tree-based Exploration*, *Intl J of Robot Res*, 29(8):1106-1127, 2010. [IF: 4.93] [Citations: 45]
- J6. Hegler JA, Laetzer J, **Shehu A**, Clementi C, and Wolynes, PG\*. *Restriction vs. Guidance: Fragment Assembly and Associative Memory Hamiltonians for Protein Structure Prediction*, *Proc Natl Acad Sci USA*, 106(36):15302-15307, 2009. [IF: 9.54] [Citations: 38]
- J5. **Shehu A**, Clementi C\*, and Kavraki LE\*. *Multiscale Characterization of Protein Conformational Ensembles*, *Proteins: Struct Funct Bioinf*, 76(4):837-851, 2009. [IF: 3.03] [Citations: 61]
- J4. **Shehu A**, Kavraki LE, and Clementi C\*. *Unfolding the Fold of Cyclic Cysteine-rich Peptides*, *Protein Sci* 17(3):482-493, 2008. [IF: 3.11] [Citations: 24]
- J3. **Shehu A**, Clementi C, and Kavraki LE\*. *Sampling Conformation Space to Model Equilibrium Fluctuations in Proteins*, *Algorithmica* 48(4):303-327, 2007. [IF: 0.89] [Citations: 14]
- J2. **Shehu A**, Kavraki LE, and Clementi C\*. *On the Characterization of Protein Native State Ensembles*, *Biophys J* 92(5):1503-1511, 2007. [IF: 4.53] [Citations: 30]

- J1. **Shehu A**, Clementi C\*, and Kaviraki LE\*. *Modeling Protein Conformational Ensembles: From Missing Loops to Equilibrium Fluctuations*, *Proteins: Struct Funct Bioinf* 65(1):164-179, 2006. [IF: 3.88] [Citations: 71]

## CONFERENCE PUBLICATIONS (PEER-REVIEWED)

- C31. Maximova T<sup>p</sup>, Carr DB, Plaku E, and **Shehu A**\*. *Sample-based Models of Protein Structural Transitions*, ACM Conf on Bioinf and Comp Biol (BCB), Seattle, WA, 2016. [AR: 20%]
- C30. Sapin E<sup>p</sup>, De Jong KA, and **Shehu A**\*. *A Novel EA-based Memetic Approach for Efficiently Mapping Complex Fitness Landscapes*, Genet and Evol Comp Conf (GECCO), Denver, CO, 2016, pg. 85-92. [AR: 40%] [Citations: 1]
- C29. Pandit R<sup>h</sup> and **Shehu A**\*. *A Principled Comparative Analysis of Dimensionality Reduction Techniques on Protein Structure Decoy Data*, Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2016, pg. 43-48. [AR: 40%] [Citations: 1]
- C28. Maximova T<sup>g</sup>, Plaku E\*, and **Shehu A**\*. *Computing Transition Paths in Multiple-Basin Proteins with a Probabilistic Roadmap Algorithm Guided by Structure Data*, IEEE Intl Conf on Bioinf and Biomed (BIBM), Washington, D.C., 2015, pg. 35-42 [AR: 19%] [Citations: 3]
- C27. Sapin E<sup>g</sup>, De Jong KA, and **Shehu A**\*. *Evolutionary Search Strategies for Efficient Sample-based Representations of Multiple-basin Protein Energy Landscapes*, IEEE Intl Conf on Bioinf and Biomed (BIBM), Washington, D.C., 2015, pg. 13-20. [AR: 19%] [Citations: 3]
- C26. Molloy K<sup>g</sup> and **Shehu A**\*. *Interleaving Global and Local Search for Protein Motion Computation*, LNCS: Bioinformatics Research and Applications, vol. 9096, pg. 175-186 (Proc. of 11th International Symposium on Bioinformatics Research and Applications – ISBRA) Norfolk, VA, 2015, vol 9096, pg. 175-186. [AR: 30%] [Citations: 2]
- C25. Clausen R<sup>g</sup>, Sapin E<sup>p</sup>, De Jong KA, and **Shehu A**\*. *Evolution Strategies for Exploring Protein Energy Landscapes*, Genet and Evol Comp Conf (GECCO), Madrid, Spain, 2014, pg. 217-224. [AR: 50%] [Citations: 2]
- C24. Veltri D<sup>g</sup>, Kamath U, and **Shehu A**\*. *A Novel Method to Improve Recognition of Antimicrobial Peptides through Distal Sequence-based Features*, IEEE Intl Conf on Bioinf and Biomed (BIBM), Belfast, UK, 2014, (*best student paper award*). [AR: 19%] [Citations: 2]
- C23. Devaurs D, **Shehu A**\*, Simeon T and Cortes S. *Sampling-based Methods for a Full Characterization of Energy Landscapes of Small Peptides*, IEEE Intl Conf on Bioinf and Biomed (BIBM), Belfast, UK, 2014. [AR: 19%] [Citations: 4]
- C22. Clausen R<sup>g</sup> and **Shehu A**\*. *A Multiscale Hybrid Evolutionary Algorithm to Obtain Sample-based Representations of Multi-basin Protein Energy Landscapes*, ACM Conf on Bioinf and Comp Biol (BCB), Newport Beach, CA, 2014. [AR: 25%] [Citations: 8]
- C21. Hashmi I<sup>g</sup>, Veltri D<sup>g</sup>, Kabbani N, and **Shehu A**\*. *Knowledge-based Search and Multiobjective Filters: Proposed Structural Models of GPCR Dimerization*, ACM Conf on Bioinf and Comp Biol (BCB), Newport Beach, CA, 2014. [AR: 25%] [Citations: 1]
- C20. Olson, B and **Shehu A**\*. *Multi-Objective Optimization Techniques for Conformational Sampling in Template-Free Protein Structure Prediction*, Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2014. [AR: 40%] [Citations: 9]
- C19. Molloy, K<sup>g</sup> and **Shehu A**\*. *A Probabilistic Roadmap-based Method to Model Conformational Switching of a Protein Among Many Functionally-relevant Structures*, Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2014 (*finalist for best paper award*). [AR: 40%] [Citations: 2]
- C18. Randou E, Veltri D<sup>g</sup>, and **Shehu A**\*. *Binary Response Models for Recognition of Antimicrobial Peptides*, ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C. 2013, pg. 76-85. [AR: 20%] [Citations: 3]
- C17. Olson B<sup>g</sup>, and **Shehu A**\*. *Multi-Objective Stochastic Search for Sampling Local Minima in the Protein Energy Surface*, ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C. 2013, pg. 430-439. [AR: 20%] [Citations: 16]
- C16. Randou E, Veltri D<sup>g</sup>, and **Shehu A**\*. *Systematic Analysis of Global Features and Model Building for Recognition of Antimicrobial Peptides*, IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), New Orleans, LA, 2013. [AR: 42%] [Citations: 5]

- C15. Molloy K<sup>g</sup>, Van JM<sup>u</sup>, Barbara D, and **Shehu A\***. *Higher-order Representations for Automated Organization of Protein Structure Space*, IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), New Orleans, LA, 2013. [AR: 42%] [Citations: 1]
- C14. Olson B<sup>g</sup>, De Jong KA, and **Shehu A\***. *Off-Lattice Protein Structure Prediction with Homologous Crossover*, Genet and Evol Comp Conf (GECCO), Amsterdam, Netherlands, 2013. [AR: 36%] [Citations: 18]
- C13. Veltri D<sup>g</sup> and **Shehu A\***. *Physicochemical Determinants of Antimicrobial Activity*, Intl Conf on Bioinf and Comput Biol, (BICoB), Hawaii, 2013. [AR: 20%] [Citations: 6]
- C12. Hashmi I<sup>g</sup> and **Shehu A\***. *A Basin Hopping Algorithm for Protein-Protein Docking*, IEEE Intl Conference on Bioinformatics and Biomedicine (BIBM) 2012, Philadelphia, PA, pg. 466-469. [AR: 20%] [Citations: 9]
- C11. Molloy K<sup>g</sup> and **Shehu A\***. *Biased Decoy Sampling to Aid the Selection of Near-Native Protein Conformations*, ACM Bioinf and Comp Biol (BCB), Orlando, FL, 2012, pg. 131-138. [AR: 21%] [Citations: 6]
- C10. Olson B<sup>g</sup> and **Shehu A\***. *Efficient Basin Hopping in the Protein Energy Surface*, IEEE Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, 2012, pg. 119-124. [AR: 20%] [Citations: 17]
- C9. Kamath U<sup>g</sup>, Kaers J, **Shehu A** and De Jong KA\*. *A Spatial EA Framework for Parallelizing Machine Learning Methods*, Intl Conf on Parallel Problem Solving From Nature (PPSN), Taormina, Italy, 2012, LNCS vol. 7491, pg. 206-215. [AR: 47%] [Citations: 6]
- C8. Olson B<sup>g</sup> and **Shehu A\***. *Populating Local Minima in the Protein Conformational Space*, IEEE Intl Conference on Bioinformatics and Biomedicine (BIBM), Atlanta, GA, 2011, pg. 114-117. [AR: 20%] [Citations: 14]
- C7. Kamath U<sup>g</sup>, De Jong KA\*, and **Shehu A\***. *An Evolutionary-based Approach for Feature Generation: Eukaryotic Promoter Recognition*, IEEE Congress on Evolutionary Computation (CEC), New Orleans, LA, 2011, pg. 277-284. [AR: 51%] [Citations: 6]
- C6. Olson B<sup>g</sup>, Molloy K<sup>g</sup>, and **Shehu A\***. *Enhancing Sampling of the Conformational Space Near the Protein Native State*, Intl. Conference on Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS), Boston, MA, 2010, LNICST (Springer), vol. 87, pg. 249-263, (*best student paper award*). [AR: 24%] [Citations: 14]
- C5. Kamath U<sup>g</sup>, **Shehu A\***, and De Jong KA\*. *Feature and Kernel Evolution for Recognition of Hypersensitive Sites in DNA Sequences*, Intl. Conference on Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS), Boston, MA, 2010, LNICST (Springer), vol. 87, pg. 213-238. [AR: 24%] [Citations: 4]
- C4. Kamath U<sup>g</sup>, **Shehu A\***, and De Jong KA\*. *Using Evolutionary Computation to Improve SVM Classification*, IEEE World Congress on Computational Intelligence (WCCI), Barcelona, Spain, 2010. [AR: 67%] [Citations: 12]
- C3. Kamath U<sup>g</sup>, De Jong KA\*, and **Shehu A\***. *Selecting Predictive Features for Recognition of Hypersensitive Sites of Regulatory Genomic Sequences with an Evolutionary Algorithm*, Genet and Evol Comp Conf (GECCO), Portland, Oregon, 2010, pg. 179-186. [AR: 45%] [Citations: 9]
- C2. Richardson SM, Olson B<sup>g</sup>, Dymond JS, Burns S, Chandrasegaran S, Boeke JD, **Shehu A**, and Bader JS\*. *Automated Design of Assemblable, Modular, Synthetic Chromosomes*, Lecture Notes in Computer Science: Parallel Processing and Applied Mathematics (PPAM), 2009, vol. 6068, pg. 280-289. [AR: 36%] [Citations: 1]
- C1. **Shehu A\***. *An Ab-initio Tree-based Exploration to Enhance Sampling of Low-energy Protein Conformations*, Robotics: Science and Systems (RSS), 2009, pg. 31-39. [AR: 25%] [Citations: 25]

## WORKSHOP PUBLICATIONS (PEER-REVIEWED)

- W11. Sapin K<sup>p</sup>, De Jong KA, and **Shehu A\***. *Path-based Guidance of an Evolutionary Algorithm in Mapping a Fitness Landscape and its Connectivity*, Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Workshops, Denver, CO, 2016, pg. 1293-1298.
- W11. Sapin K<sup>p</sup>, De Jong KA, and **Shehu A\***. *Mapping Multiple Minima in Protein Energy Landscapes with Evolutionary Algorithms*, Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Workshops, Madrid, Spain, 2015, pg. 923-927. [Citations: 4]
- W10. Molloy K<sup>g</sup>, Clausen R<sup>g</sup>, and **Shehu A\***. *On the Stochastic Roadmap to Model Functionally-related Structural Transitions in Wildtype and Variant Proteins*, Workshop on Robotics Methods for Structural and Dynamic

- Modeling of Molecular Systems - Robotics: Science and Systems (RSS) Workshops, Berkeley, CA, 2014, pg. 1-6. [Citations: 1]
- W9. **Shehu A\*** and De Jong KA. *Memetic, Multi-Objective, Off-Lattice, and Multiscale Evolutionary Algorithms for De-novo and Guided Protein Structure Modeling*, Workshop on Natural Computing for Protein Structure Prediction - Intl Conf on Parallel Problem Solving from nature (PPSN) Workshops, Ljubljana, Slovenia, 2014. [Citations: 1]
- W8. Clausen R<sup>g</sup> and **Shehu A\***. *Exploring the Structure Space of Wildtype Ras Guided by Experimental Data*, Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D. C., 2013, pg. 757-764. [Citations: 5]
- W7. Hashmi I<sup>g</sup> and **Shehu A\***. *Informatics-driven Protein-protein Docking*, Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D. C., 2013, pg. 772-779. [Citations: 6]
- W6. Olson B<sup>g</sup> and **Shehu A\***. *An Evolutionary Search Algorithm to Guide Stochastic Search for Near-native Protein Conformations with Multiobjective Analysis*, Workshop on Artificial Intelligence and Robotics Methods in Computational Biology - Intl Conf of Association for Advancement of Artificial Intelligence (AAAI) Workshop, Bellevue, WA, 2013. [Citations: 4]
- W5. Molloy M\* and **Shehu A\***. *A Robotics-inspired Method to Sample Conformational Paths Connecting Known Functionally-relevant Structures in Protein Systems*, Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 56-63. [AR: 33%] [Citations: 5]
- W4. Saleh S<sup>u</sup>, Olson B<sup>g</sup>, and **Shehu A\***. *A Population-based Evolutionary Algorithm for Sampling Minima in the Protein Energy Surface*, Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 48-55. [AR: 33%] [Citations: 5]
- W3. Olson B<sup>g</sup>, Hendi, S-F<sup>g</sup>, and **Shehu A\***. *Protein Conformational Search with Geometric Projections*, Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 366-373. [AR: 40%] [Citations: 1]
- W2. Akbal B, Hashmi I<sup>g</sup>, **Shehu A**, and Haspel N\*. *Refinement of Docked Protein Complex Structures Using Evolutionary Traces*, Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 400-404. [AR: 40%] [Citations: 8]
- W1. Hashmi I<sup>g</sup>, Akbal B, Haspel N, and **Shehu A\***. *Protein Docking with Information on Evolutionary Conserved Interfaces*, Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 358-365. [AR: 40%] [Citations: 9]

## BOOK CHAPTERS (PEER-REVIEWED)

- B3. **Shehu, A.\***, Barará D, and Molloy K. *A Survey of Computational Methods for Protein Function Prediction*. In Big Data Analytics in Genomics (Springer), first edition, (Editors: Wong, KC), 2016.
- B3. **Shehu, A.** *A Review of Evolutionary Algorithms for Computing Functional Conformations of Protein Molecules*. In Computer-Aided Drug Discovery (Springer Methods in Pharmacology and Toxicology Series), first edition, (Editors: Zhang W), 2015. [Citations: 1]
- B2. **Shehu, A.** *Probabilistic Search and Optimization for Protein Energy Landscapes*. In Handbook of Computational Molecular Biology, Chapman & Hall/CRC Computer & Information Series, 2nd edition (Editors: Aluru S and Singh M), 2013. [Citations: 19]
- B1. **Shehu A.** *Conformational Search for the Protein Native State*. In Protein Structure Prediction: Method and Algorithms, Wiley Book Series on Bioinformatics, 2009. [Citations: 21]

## PHD DISSERTATION

**Shehu A.** *Sampling biomolecular conformations with spatial and energetic constraints*, Rice University, June 2008. Committee: Kavradi LE (dissertation director), Clementi C, Vardi M, and Nakhleh L.

## TECHNICAL REPORTS

- T5. Pandit R<sup>h</sup> and **Shehu A\***. *A Comparative Analysis of the Performance of Linear and Non-linear Dimensionality Reduction Techniques on Protein Structure Decoy Data*. Technical Report, November 2015.
- T4. Pandit R<sup>h</sup> and **Shehu A\***. *Making Sense of Big Molecular Data: Clustering Algorithms to Identify Near-Native Protein Decoys*. Technical Report, September 2015.

- T3. Pandit R<sup>h</sup>, Singh P<sup>h</sup>, and **Shehu A\***. *Making Sense of Big Molecular Data: Dimensionality Reduction Techniques for Automated Mapping and Analysis of Molecular Structures*. Technical Report, September 2014.
- T2. Veltri D<sup>g</sup> and **Shehu A\***. *Elucidating Activity-related Physico-chemical Features in Antimicrobial Peptides*, Technical Report, GMU-CS-TR-2012-6, 2012.
- T1. Miles C<sup>g</sup>, Olson B<sup>g</sup>, and **Shehu A\***. *Geometry-based Computation of Symmetric Homo-oligomeric Protein Complexes*, Technical Report, GMU-CS-TR-2009-2, 2009.

## ABSTRACTS, POSTERS, AND EXTENDED ABSTRACTS<sup>5</sup>

- A60 Maximova T<sup>p</sup>, Plaku E, and **Shehu A\***. “Method for Extended Sampling and Transition Paths Prediction with Probabilistic Roadmap Algorithm.” 3DSig, Intelligent Systems for Molecular Biology (ISMB) Orlando, Florida, July 2016 (Poster and Extended Abstract).
- A59 Marquez M, McDermott-Roe C\*, Bukowy J, Kolander K, Kuo J, Maximova T<sup>p</sup>, **Shehu A**, Benjamin I, and Geurts A. “Modeling BAG3-associated cardiomyocyte dysfunction via genome editing in induced pluripotent stem cells.” Keystone Symposia on Molecular and Cellular Biology: Heart Failure: Genetics, Genomics and Epigenetics, Snowbird Resort, Snowbird, Utah, April 2016 (Poster and Abstract).
- A58 McDermott-Roe C\*, Mitzefeld K, Marquez M, Grzybowski M, Bukowy J, Maximova T<sup>p</sup>, **Shehu A**, Benjamin I, and Geurts A. “Modeling BAG3-associated cardiomyocyte dysfunction via genome editing in induced pluripotent stem cells.” CRISPR Precision Gene Editing Congress, Boston, Massachusetts, February 2016 (Poster and Abstract).
- A57 Mazyar K<sup>u</sup>, Hashmi I<sup>g</sup>, Neil A, and **Shehu A\***. “Platform to Support Intensive Webserver Computations on Argo.” Mason Annual Volgenau School of Engineering Undergraduate Research Celebration, Fairfax, VA, April 2015 (Poster).
- A56. Songyue H<sup>u</sup> and **Shehu A\***. “A new Distance Function for Protein Structures for the Decoy Selection Problem in De-novo Structure Prediction.” Mason Annual Volgenau School of Engineering Undergraduate Research Celebration, Fairfax, VA, April 2015 (Poster).
- A55. Clausen R<sup>g</sup>, **Shehu A\***, Ma B, and Nussinov R. “A Novel Evolutionary Algorithm to Model Energy Landscapes of Wildtype and Variant Sequences of H-Ras.” Biophysical Society Meeting, Baltimore, MD, February, 2015 (Poster).
- A54. Clausen R<sup>g</sup>, **Shehu A\***, Ma B, and Nussinov R. “Mapping the Structure Space of the Ras Protein using a Novel Hybrid Evolutionary Algorithm.” NIH Summer Poster Day, Fredericks, MD, July, 2014 (Poster).
- A53. Van MJ<sup>u</sup>, Namazi M<sup>u</sup>, Xiang R<sup>u</sup>, Blaisten-Barojas E\*, and **Shehu A\***. “Structural Analysis and Dynamics of the Met-Enkephalin Peptide.” American Chemical Society (ACS) Undergraduate Research Poster Session, Charlottesville, VA, April 2014 (Poster).
- A52. Pilapitiya H<sup>u</sup>, Kabbani N\*, and **Shehu A\***. “Modeling Binding of Amyloid beta-42 Peptide to the Alpha 7 Nicotinic Receptor.” Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).
- A51. Van MJ<sup>u</sup>, Namazi M<sup>u</sup>, Xiang R<sup>u</sup>, Blaisten-Barojas E\*, and **Shehu A\***. “Conformational Sampling and Principal Component Analysis of the Met-Enkephalin Peptide.” Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).
- A50. Namazi M<sup>u</sup>, Van MJR<sup>u</sup>, Xiang R<sup>u</sup>, **Shehu A\*** and Blaisten-Barojas E\*. “Molecular Dynamics Simulation of the Met-Enkephalin Peptide with Explicit Solvent.” Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).
- A49. Xiang R<sup>u</sup>, Van MJR<sup>u</sup>, Namazi M<sup>u</sup>, Blaisten-Barojas E\*, and **Shehu A\***. “A Clustering Algorithm for Molecular Structures: Application on the Met-Enkephalin Peptide.” Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).
- A48. Clausen R<sup>g</sup> and **Shehu A\***. “A PCA-guided Search Algorithm to Probe the Conformational Space of the Ras Protein.” ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C., September 2013 (Extended Abstract and Poster).

<sup>5</sup> Abstracts are typically 1-2 paragraph submissions that are reviewed and accepted either as poster or oral presentations at conferences and workshops. Extended abstracts are typically viewed as condensed manuscript submissions of 1-3 pages, also peer-reviewed. All extended abstracts listed in this CV are indexed by IEEE.

- A47. Hashmi I<sup>g</sup> and **Shehu A\***. “Protein-protein Docking using Information from Native Interaction Sites.” ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C., September 2013 (Extended Abstract and Poster).
- A46. Olson B<sup>g</sup> and **Shehu A\***. “A Multi-objective Guided Evolutionary Search Algorithm for Sampling Near-native Protein Conformations.” Workshop on Artificial Intelligence and Robotics Methods for Computational Biology - Conf on Association for Advancement of Artificial Intelligence Workshop, Bellevue, WA, July 2013 (Poster).
- A45. Randou EG, Veltri D<sup>g</sup>, and **Shehu A\***. “Towards Classification and Virtual Screening of Antimicrobial Peptides with Regression-based Binary Response Models.” Nonclinical Biostatistics Conference (NCB), Villanova University, PA, 2013 (Abstract and Oral Presentation).
- A44. Molloy K<sup>g</sup>, Van JM<sup>u</sup>, Barbara D, and **Shehu A\***. “Higher-order Representations for Automated Organization of Protein Structure Space.” Celebration of Undergraduate Student Scholarship, George Mason University, Fairfax, VA, May 2013 (Poster).
- A43. Saleh S<sup>u</sup>, Olson B<sup>g</sup>, and **Shehu A\***. “An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.” National Council of Undergraduate Research (NCUR), University of Wisconsin-La Crosse, La Crosse, WI, 2013 (Abstract and Poster).
- A42. Shehu A. “Probabilistic Methods for Modeling Structures and Motions of Protein Systems.” NFS Grants Conference, Fairfax, VA, 2012 (Poster).
- A41. Bohidar N<sup>h</sup> and **Shehu A\***. “From Coarse-grained Conformations to Motion Pathways in Proteins.” Thomas Jefferson Senior Research Day, Alexandria, Virginia, April 2013 (Poster).
- A40. Reinstadler B<sup>u</sup>, Van JM<sup>g</sup>, and **Shehu A\***. “Supersecondary Structure Motifs and De Novo Protein Structure Prediction.” Grace Hopper Conference Celebration of Women in Computing, Baltimore, MD, 2012 (Abstract and Poster).
- A39. Saleh S<sup>u</sup>, Olson B<sup>u</sup> and **Shehu A\***. “An evolutionary framework to sample near-native protein conformations.” CSBW at IEEE BIBM Workshops (BIBM-W), pg. 933. (Extended Abstract and Poster).
- A38. Veltri D\* and **Shehu A\***. “Physico-chemical features for recognition of antimicrobial peptides.” CSBW at IEEE BIBM Workshops (BIBM-W), pg. 942. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).
- A37. Olson B<sup>g</sup> and **Shehu A\***. “An evolutionary search framework to efficiently sample local minima in the protein conformational space.” ACM BCB, pg. 590. Orlando, FL, 2012 (Extended Abstract and Poster).
- A36. Hashmi I<sup>g</sup> and **Shehu A\***. “Sampling low-energy protein-protein configurations with basin hopping.” IEEE BIBM, pg. 947. Philadelphia, PA, October 4-7, 2012. (Extended Abstract and Poster, *Best Poster Award*).
- A35. Olson B<sup>g</sup> and **Shehu A\***. “Jumping low, jumping high: Controlling hopping in the protein energy surface.” IEEE BIBM, pg. 946. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).
- A34. Molloy K<sup>g</sup> and **Shehu A\***. “A tree-based search to bias sampling of protein decoy conformations.” IEEE BIBM, pg. 978. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).
- A33. Molloy K<sup>g</sup> and **Shehu A\***. “Mapping conformational pathways between known functional protein states.” CSBW at IEEE BIBM Workshops (BIBM-W), pg. 971. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).
- A32. Jordan S<sup>u</sup> and **Shehu A\***. “Refinement of Coarse-grained Near-native Protein Conformations Using AMBER FF99SB Force Field.” Aspiring Scientist Summer Internship Program (ASSIP) Poster Presentations, Manassas, Virginia, Summer 2012 (Poster).
- A31. Saleh S<sup>u</sup>, Olson B<sup>g</sup>, and **Shehu A\***. “An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.” Celebration of Student Scholarship, Fairfax, VA, May 2012 (Poster).
- A30. Saleh S<sup>u</sup>, Olson B<sup>g</sup>, and **Shehu A\***. “Revisiting Evolutionary Search for Effective Sampling of Near-native Conformations in the Protein Conformational Space.” Virginia Academy of Sciences, Norfolk, VA, May 2012 (Abstract and Poster).
- A29. Saleh S<sup>u</sup> and **Shehu A\***. “An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.” College of Science Symposium, George Mason University, Fairfax, VA, May 2012 (Poster).

- A28. Olson B<sup>g</sup> and **Shehu A\***. “A Basin Hopping Probabilistic Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space.” 26th Annual Meeting of the Protein Society, San Diego, CA, 2012 (Abstract and Poster).
- A27. Olson B<sup>g</sup> and **Shehu A\***. “A Basin Hopping Probabilistic Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space.” Intelligent Systems for Molecular Biology (ISMB) Student Council, Long Beach, CA, 2012 (Abstract and Poster).
- A26. Molloy K<sup>g</sup> and **Shehu A\***. “Assembly of Low-Energy Protein Conformations with Heterogeneous Fragments.” IEEE BIBM, pg. 991-993. Atlanta, GA, November 12-15, 2012 (Extended Abstract and Poster).
- A25. Olson B<sup>g</sup> and **Shehu A\***. “Mapping the Protein Conformational Landscape with Adaptive Probabilistic Search.” 55th Annual Meeting of the Biophysical Society, Baltimore, Maryland, 2011 (Abstract and Poster).
- A24 : Hashmi I\*, Akbal-Delibas B, Haspel N, and **Shehu, A\***. “Protein Docking with Information on Evolutionary Conserved Interfaces.” Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshop, Atlanta, GA, November, 2011 (Abstract and Poster).
- A23 Olson B<sup>g</sup> and **Shehu, A\***. “Local Minima Hopping Along the Protein Energy Surface.” IEEE Intl Conf on Biomed and Bioinf (BIBM), Atlanta, GA, November, 2011 (Abstract and Poster).
- A22. Richardson SM, Olson B<sup>g</sup>, Dymond JS, Burns R, Chandrasegaran S, Boeke JD, **Shehu A**, and Bader JS\*. Annual RECOMB Satellite on Regulatory Genomics and Systems Biology, Boston, MA, 2009 (Abstract and Oral Presentation).
- A21. Chung R<sup>u</sup>, Jamil B<sup>u</sup>, and **Shehu A\***. “A Metropolis Monte Carlo Algorithm to compute Low-energy Structures of an RNA chain.” Grace Hopper Conference Celebration of Women in Computing, Tucson, Arizona, 2009 (Abstract and Poster).
- A20. Mostaghim A<sup>u</sup>, Veltri D<sup>g</sup>, Majul A<sup>g</sup>, and **Shehu A\***. Aspiring Scientist Summer Internship Program (ASSIP) Poster Presentations, Manassas, Virginia, 2009 (Poster).
- A19. Miles C<sup>g</sup> and **Shehu A\***. Intl Conf on Intelligent Systems for Molecular Biology & European Conf on Computational Biology (ISMB-EECB), Stockholm, Sweden, 2009 (Abstract and Poster).
- A18-A1. These posters were the result of Shehu’s research as a graduate and undergraduate student and can be found [here](#).

## OTHER PUBLICATIONS<sup>6</sup>

- O4. **Shehu A**. “Computer Scientist in Profile: Yang Zhang.” ACM SIGBIO Record 4(2), 2, 2014.
- O3. **Shehu A**. “Computer Scientist in Profile: Bruce Donald.” ACM SIGBIO Record 4(1), 5-7.
- O2. **Shehu A**. “Computational Biologist in Profile: Ruth Nussinov.” ACM SIGBIO Record 3(3), 12-14, 2013.
- O1. **Shehu A**. “Computer Scientist in Profile: Mona Singh.” ACM SIGBIO Record 3(1), 26-27, 2013.

## INVITED TALKS

- T34. *Sample-based Representations and Algorithms for Modeling Protein Structure and Dynamics*, Invited Talk, 6th Workshop on Logic and Systems Biology (LSB), 31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), July 09, 2016.
- T33. *Should Have Gone To Systems*, Invited Talk, Science Slam, Women@GECCO, Genet and Evol Comput Conf (GECCO), July 12, 2015.
- T32. *Recovering Energy Landscapes and Mapping Functionally-relevant Structural Transitions*, Highlight Talk, Computational Structural Biology Workshop (CSBW), ACM Conf on Bioinf and Comput Biol (BCB), September 20, 2014.
- T31. *Probabilistic Approaches to Unravel the Form to Function Relationship in Biomolecular Systems*, Seminar Series, Institute for Bioscience and Biotechnology Research (IBBR), Rockville, MD, March 10, 2014.
- T30. *From the Nanoscale to the Petascale: Probabilistic Algorithmic Frameworks for Characterizing Complex Biomolecular Systems in the Presence of Constraints*, Biomedical Engineering Seminar Series, University of Florida, Gainesville, FL, January 9, 2014.

<sup>6</sup>In 2013, I introduced a section to the ACM SIGBIO newsletter that features prominent computer scientists and computational biology researchers.

- T29. *Advancing Biomolecular Modeling and Simulation: A Probabilistic Approach for Characterizing Complex Systems in the Presence of Constraints*, Volgenau School of Engineering Seminar, George Mason University, Fairfax, VA, October 17, 2013.
- T28. *Probabilistic Approaches to Protein Modeling*, Mechanical Engineering Seminar Series, Johns Hopkins University, Baltimore, MD, February 14, 2013.
- T27. *Genetic Programming Based Feature Generation for Automated Functional Analysis and Annotation of DNA Sequences*, Rocky Mountain Bioinformatics Conference, Aspen/Snowmass, Colorado, December 8, 2012, accepted oral presentation.
- T26. *Probabilistic Search Frameworks for Protein Modeling*, School of Systems Biology Seminar, George Mason University, Fairfax, VA, November 20, 2012.
- T25. *Of Protein Structures and Motions: Probabilistic Search and Optimization*, Applied and Computational Math Seminar, George Mason University, Fairfax, VA, November 2, 2012.
- T24. *Probabilistic Search Frameworks for Modeling Structures and Motions of Protein Systems*, ACM BCB Invited Talk, Orlando, FL, October 8, 2012.
- T23. *Stochastic Search to Map the Space of Local Minima in the Protein Energy Surface*, Fox Chase Cancer Center, Philadelphia, PA, October 2012.
- T22. *Novel Perspectives on Exploring the Protein Conformational Space for Characterizing Structures and Motions in Protein Systems*, College of Information Science Seminar, Drexel University, Philadelphia, PA, October 2012.
- T21. *Probabilistic Methods for Structural Characterization of Protein Systems*, Computer Science Seminar, Northern Virginia Center, Virginia Tech, Falls Church, VA, March 16, 2012.
- T20. *Novel Algorithmic Frameworks for Protein Conformational Search*, Bioengineering Department Seminar, UMD, College Park, MD, February 10, 2012.
- T19. *Simplifying and Sampling the Protein Conformational Space*, Computational Materials Science Center Colloquium, George Mason University, Fairfax, VA, February 6, 2012.
- T18. *Probabilistic Frameworks for Protein Conformational Search: Characterization of Native Structures of Protein Chains and Protein-based Assemblies*, Rocky Mountain Bioinformatics Conf, Aspen/Snowmass, Colorado, December 10, 2011.
- T17. *Probabilistic Search Frameworks for Modeling Structures, Motions, and Assembly of Protein Molecules*, Computational Materials Science Center Colloquium, George Mason University, Fairfax, VA, November 28, 2011.
- T16. *Probabilistic Search Algorithms to Compute Conformations of the Protein Native State*, Chemistry Department Seminar, GMU, Fairfax, VA, September 29, 2011.
- T15. *A Probabilistic Framework for the Characterization of the Protein Native State*, Computer Science Seminar, Lehigh University, Bethlehem, PA, March 16, 2011.
- T14. *Combining Evolutionary Algorithms with Supervised Learning to Extract Signals from Biological Data*, BioLearn Workshop, BIONETICS, Boston, MA, December 02, 2010.
- T13. *Mapping Conformational Spaces of Protein Molecules*, Computer Science Seminar, University of Massachusetts at Boston, Boston, MA, December 01, 2010.
- T12. *Characterizing Biological Systems at the Molecular Level*, ACE Scholars Research Highlights Invited Talk, George Mason University, Fairfax, VA, October 13, 2010.
- T11. *Probabilistic Methods to Compute Biologically-active Protein Conformations*, Computer Science Seminar, College of William and Mary Williamsburg, VA, June 1, 2010.
- T10. *Computational Aspects of Sequence, Structure, and Function in Protein Molecules*, NCBI CBB Seminar, NIH, MD, Jun 18, 2009.
- T9. *Motions and Assembly of Biological Molecules*, ACE Scholars Program Seminar, George Mason University, VA, Mar 17, 2009.
- T8. *Geometric Algorithms for Biological Research: Everything is a Puzzle After All*, GRAND Seminar Series, George Mason University, VA, Oct 16, 2008.
- T7. *From Atoms to Molecules to Machines: Computing Protein Motions to Elucidate Function*, Bioinformatics Colloquium, George Mason University, VA, Oct 7, 2008.

T6. *A Multiscale Framework for the Characterization of Protein Native States*, National Meeting of the American Chemical Society (ACS), New Orleans, LA, Apr 6, 2008.

T5. *Computing Structural Flexibility in the Protein Native State*, University of Chicago, Chicago, IL, Feb 6, 2008.

T4. *Characterizing Native Flexibility in Proteins*, Fox Chase Cancer Center, Philadelphia, PA, Jan 23, 2008.

T3-T1. These talks were during Shehu's research as a graduate student and can be found [here](#).

## OTHER RESEARCH PRODUCTS

Web servers, source code, and executables accompanying various publications are available at [Our Tools](#), including:

AMPScreen: Antimicrobial Recognition and Genome-wide Screening, 2016

SIFTER: A Structure-guided Memetic, Cellular, and Multiscale Evolutionary Algorithm for Mapping Protein Conformation Spaces, 2015

EFC-FCBF: Framework for Feature Construction and Selection for Improved Recognition of Antimicrobial Peptides, 2014

HEA-PSP: A Hybrid Evolutionary Search Framework with Various Crossover Implementations for Ab-initio Protein Structure Prediction, 2014

EFFEKT: Framework for Automated Construction and Extraction of Features for Classification of Biological Sequences, 2013

Binary Response Models for Recognition of Antimicrobial Peptides, 2013

Statistical Model Building for Antimicrobial Peptide Recognition, 2013

Novel features for Antimicrobial Peptide Recognition, 2013

Spatial EA Framework for Parallel Machine Learning, 2012

An Evolutionary Algorithm For Feature Generation from Sequence Data, 2012

An Evolutionary Algorithm For SVM Kernel Optimization, 2011

Research and educational materials, including video conference presentations and video research highlights on youtube, are also documented on [Our Computational Biology Lab Webpage](#).

## COLLABORATORS<sup>7</sup>

### CS Department, GMU:

Daniel Barbara, Kenneth De Jong, Jana Kosecka, Fei Li, Angelos Stavrou.

### Other Departments, GMU:

Barney Bishop (Biochemistry), Estela Blaisten-Barojas (Computational Materials Science), Dan Carr (Statistics), Nadine Kabbani (Neuroscience), Wanli Qiao (Statistics), Elena Randou (Mathematics, now FDA), Monique L. van Hoek (Molecular Biology), Anand Vidyashankar (Statistics).

### External:

Philip Bryan (UMD College Park, Bioengineering), Brian Chen (Lehigh University, Computer Science), John Choy (Catholic University of America), Juan Cortés (CNRS-LAAS Toulouse), Nurit Haspel (UMass Boston, Computer Science), Rezarta Islamaj-Dogan (NIH/NLM), Buyong Ma (NIH/NCI), Benjamin Matthews (USDA), Carla Mattos (Northeastern University), Anna Mitraki (Material Science, University of Crete), Lionel Mourey (IPSB, Toulouse, Structural Biophysics), Ruth Nussinov (NIH/NCI), Mourat Oz (United Arab Emirates University, Pharmacology), Kyriacos Petrakos (Institute of Molecular Biology and Biotechnology, Greece), Erion Plaku (Catholic University of America, Computer Science), Adrian Roitberg (University of Florida, Chemistry).

## TEACHING

### Curriculum Development:

*CS695 - Network Science: Principles and Applications* is a special topics graduate course I proposed and first taught in Fall 2016 in collaboration with Prof. Fei Li. The objective of this course is to introduce students to network-based treatments of complex systems and provide students with a broad but rigorous overview of network science. The course emphasizes the fundamental underpinnings of network science to graph-theoretic concepts and graph algorithms and covers a rich set of state-of-the-art algorithmic, computational, and statistical methods for diverse applications in communications, biology, ecology, brain science, sociology, economics, epidemiology, synchronization, adaptive network formation, and more.

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<sup>7</sup>This list includes only co-authors of papers published or in progress and collaborators on ongoing research projects and active and pending grant proposals. They are listed by alphabetical ordering of last names.

*CS689 - Planning Motions of Robots and Molecules* is a new graduate course I proposed as a technical elective (CS795 - Geometric Algorithms for Bioinformatics) and taught first in Fall 2009. The first offering introduced modeling and simulation of biological systems through analogies with robotic mechanisms and motion planning. After discussions with students and robotics faculty exposed the need for a graduate robot motion planning course, I redesigned the course to focus on robot motion planning and present special applications on biological molecules. The course has been approved as a regular course, CS689. I now teach CS689 every three semesters.

*CS444 - Introduction to Computational Biology* is a new undergraduate course I proposed as a technical elective (CS499 - Bioinformatics and Computational Biology I) and taught in Spring 2009-2011. The course was cross-listed as ECE401 and BINF401 to gauge student interest in new inter-departmental bioinformatics and bioengineering programs. With these goals in mind, the course provided a broad view of classic computational problems in sequence, structure, and systems biology. The course was very well received and has been approved as a regular course, CS444. I now teach CS444 every three semester.

### List of Courses Taught at Mason:

<b>CS695 Network Science: Principles and Applications</b>	Fall 2016
<b>CS485 Autonomous Robotics</b>	Fall 2016
<b>CS580 Introduction to Artificial Intelligence</b>	Spring 2016
<b>CS689 Planning Motions of Robots and Molecules</b>	Spring 2016
<b>Maternity leave</b>	Spring 2015
<b>Study leave</b>	Fall 2015
<b>CS583 Analysis of Algorithms I</b>	Fall 2014
<b>CS689 Planning Motions of Robots and Molecules</b>	Spring 2014
<b>CS485 Autonomous Robotics</b>	Fall 2013
<b>CS583 Analysis of Algorithms I</b>	Spring 2013
<b>CS444 Introduction to Computational Biology</b>	Fall 2012
<b>CS689 Planning Motions of Robots and Molecules</b>	Spring 2012
<b>Junior leave</b>	Fall 2011
<b>CS444 Introduction to Computational Biology</b> (cross-listed as BINF 401)	Spring 2011
<b>CS583 Analysis of Algorithms I</b>	Fall 2010
<b>CS483 Analysis of Algorithms I</b>	Spring 2010
<b>CS499 Bioinformatics and Computational Biology I</b> (cross-listed as BINF401, ECE499)	Spring 2010
<b>CS795 Geometric Algorithms for Bioinformatics</b>	Fall 2009
<b>CS499 Bioinformatics and Computational Biology I</b> (cross-listed as BINF401, ECE499)	Spring 2009
<b>CS583 Analysis of Algorithms I</b>	Fall 2008

### Summary of Teaching Ratings:<sup>8</sup>

Term	Number	Course		Comparison of Means			
		Title	Size	My Teaching vs. Dept.		My Course vs. Dept.	
Fall 2016	CS 580	Introduction to AI I	26	4.35	4.11	4.23	3.97
Fall 2016	CS 689	Planning Motions	9	4.33	4.11	4.33	3.97
Fall 2014	CS 583	Analysis of Algorithms I	21	4.50	4.17	4.30	3.91
Spring 2014	CS 689	Planning Motions	6	4.83	4.19	4.67	3.98
Fall 2013	CS 485	Autonomous Robotics	15	4.40	4.30	4.30	4.12
Spring 2013	CS 583	Analysis of Algorithms I	29	3.75	4.0	3.96	4.0
Fall 2012	CS444	Intro to Comp Biol	7	4.80	4.27	4.40	4.08
Spring 2012	CS689	Planning Motions	12	4.60	4.31	4.50	4.11
Spring 2011	CS444	Intro to Comp Biol	7	4.86	4.27	4.57	4.06
Fall 2010	CS583	Analysis of Algorithms I	35	4.45	4.28	4.05	4.08
Spring 2010	CS483	Analysis of Algorithms I	30	4.58	4.31	3.95	4.06
Spring 2010	CS499	Bioinf and Comp Biol	16	4.92	4.31	4.54	4.06
Fall 2009	CS795	Geom Algorithms Bioinf	5	5.00	4.27	4.80	4.03
Spring 2009	CS499	Bioinf and Comp Biol	9	4.00	4.36	3.88	4.11
Fall 2008	CS583	Analysis of Algorithms I	14	4.85	4.31	4.46	4.04

<sup>8</sup>Ratings are out of 5. Rows colored in dark gray indicate courses where both teaching and course means are above those of the department. Rows colored in light gray indicate courses where only teaching or course mean are above the corresponding departmental measure. In Spring 2013, weekly quizzes were introduced to place less weight on homeworks as a way to discourage plagiarism in CS583. Nonetheless, 5 out of 29 students were reported to the Honor Council and found guilty of cheating on homeworks.

**STUDENT ADVISING AND MENTORING****Ph.D. Theses Advised:**

4. Veltri D. *A Computational and Statistical Framework for Screening Antimicrobial Peptides*, George Mason University, July 2013. Committee: Shehu A (dissertation director), Solka J (committee chair), Vaisman I, and Matthews B.  
Daniel Veltri defended his Ph.D. on December 01, 2015 (now software engineer at USDA).  
Publication statistics: 4 journal and 5 conference papers.
3. Hashmi I. *Probabilistic Approaches to Protein-protein Docking*, George Mason University, July 2013. Committee: Shehu A (dissertation director and chair), De Jong KA, Rangwala H, Barbara D, and Kabbani N.  
Irina Hashmi defended her Ph.D. on July 27, 2015 (now postdoctoral fellow at NIH).  
Publication statistics: 5 journal, 2 conference, and 3 workshop papers.
2. Molloy K. *Probabilistic Algorithms for Modeling Protein Structure and Dynamic*, George Mason University, January 2015. Committee: Shehu A (dissertation director and chair), Barbara D, Blaisten-Barojas E, and Lien J-M.  
Kevin Molloy defended his Ph.D. on January 13, 2015 (now postdoctoral fellow at LAAS-CNRS Toulouse).  
Publication statistics: 9 journal, 4 conference and 2 workshop papers.
1. Olson B. *Evolving Local Minima in the Protein Energy Surface*, George Mason University, July 2013. Committee: Shehu A (dissertation director and chair), De Jong KA, Blaisten-Barojas E, Kosecka J, and Lien J-M.  
Brian Olson defended his Ph.D. on July 24, 2013 (now research scientist at LLNL).  
Publication statistics: 7 journal, 7 conference, and 3 workshop papers.

**M.S. Theses Advised:**

5. Majul A. *Comparative Molecular Dynamic Simulations of 2 Helical AMPs Found in Snakes ATRA-1 and ATRA-2*, George Mason University, July 2015. Committee: Bishop B (committee chair), Shehu A (thesis director), and Mikell P.
4. Veltri D. *Sequence-based Classification of Antimicrobial Peptides*, George Mason University, March 2013. Committee: Shehu A (thesis director), Vaisman I (committee chair), and Bishop B.
3. Hashmi I. *A Probabilistic Search Algorithm for Protein-Protein Docking*, George Mason University, November 2012. Committee: Shehu A (thesis director and chair), De Jong K, and Lien J-M.
2. Olson B. *Probabilistic Search Algorithms for Protein Structure Prediction*, George Mason University, November 2011. Committee: Shehu A (thesis director and chair), Kosecka J, and Lien J-M.
1. Molloy K. *Variable-Length Fragment Assembly in a Probabilistic Protein Structure Prediction Framework*, George Mason University, June 2011. Committee: Shehu A (thesis director and chair), Duric Z, and Lien J-M.

**Postdoctoral Fellow Advisor:**

2. Tatiana Maximova (June 2017 - April 2015)
1. Emmanuel Sapin (December 2016- January 2015)

**Ph.D. Student Advisor:<sup>9</sup>**

6. Erich O'Saben, CS Ph.D.
- 5.-1. Ph.D advisor of now Ph.D. alumni Daniel Veltri Irina Hashmi, Kevin Molloy, Uday Kamath, and Brian Olson.

**Ph.D. Committee Member (of students not in my lab):**

Committee Member, Achyuthan J.R., Civil, Environmental, and Infrastructure Engineering (director: David Lat-tanzi)	2017-2016
Committee Member, Christopher Siwy, School of Systems Biology (director: Dmitri Klimov)	2017-2014
Committee Member, Gregory Helmick, CSI (director: Estela Blaisten-Barojas)	2017-2014
Committee Member, Evan Behar, Computer Science, (director: Jyh-Ming Lien)	2017-2013
Committee Member, Zhonghua Xi, Computer Science (director: Jyh-Ming Lien)	2017-2015
Committee Member, Yoseph Abere, CSI (director: Estela Blaisten-Barojas)	2017-2015
Committee Member, Jose Colbes, Computer Science CICESE-Mexico, (director: Carlos Brizuela)	2015-2014
Committee Co-director, Uday Kamath, IT (director: Kenneth A De Jong)	2013
Committee Member, Yanyan Lu, Computer Science, (director: Jyh-Ming Lien)	2013-2012

<sup>9</sup>These students have earned numerous awards during their research in my lab, some of which are highlighted here.

Committee Member, Adam Cadien, SPACS, (director: Howard Sheng) 2015-2012  
 Committee Member, Nada Basit, Computer Science, (director: Harry Wechsler) 2011

### M.S. Student Advisor:

7. David Morris, CS	2016-present
6. Ryan Moffatt, CS	2016-2015
5. Rudy Clausen, CS	2015-2012
4. Arda Gumusalan, CS	2012-2015
3. Amr Majul, School of Systems Biology	2013
2. Seyed Farid Hendi, CS, now in industry	2011
1. Christopher Miles, CS, now in industry	2010

### Undergraduate Student Mentor:<sup>10</sup>

21. Erica Molinar, GMU (CS)	Spring 2017 - Fall 2016
20. Savindi Ranasinghe, GMU (CS)	Spring 2017 - Fall 2016
19. Bradley English, GMU (CSS/Neuroscience)	Spring 2017 - Fall 2016
18. Heather Hendy, GMU (CS)	Summer 2015 - Fall 2015
17. Jeffrey Horowitz, Rice University (CS)	Summer 2015
16. Mazyar Katouzian, GMU (CS)	Spring 2015 - Fall 2014
15. Songyue Huang, GMU (CS)	Spring 2015 - Fall 2014
14. Wint Hnin, CRA-W DREU student from Cornell College (CS)	Summer 2014
13. Herath Pilapitiya, GMU (CS)	Summer 2014 - Spring 2014
12. Ruxi Xiang, GMU (CS)	Spring 2015 - Fall 2013
11. Mahmoud Namazi, GMU (Math)	Spring 2015 - Fall 2013
10. Jennifer Van, GMU (CS)	Summer 2014 - Fall 2012
9. Sameh Saleh, GMU (ACS Bioinformatics)	Spring 2013 - Fall 2011
8. Bryn Reinstadler, CRAW-DREU student from Williams College (CS)	Summer 2012
7. Subeer Talapatra, UVA (Chemical Engineering)	Summer 2012
6. Talhah Zafar, GMU (CS)	Summer 2012
5. Justin Towson, GMU (Neuroscience)	Spring 2011 - Fall 2010
4. Jack Compton, GMU (CS)	Spring 2011 - Fall 2010
3. Beenish Jamil, GMU (ACS Bioinformatics)	Summer 2010 - Spring 2009
2. Rachael Chung, CRA-W DREU student from UNCC	Summer 2009
1. Anahita Mostaghim, ASSIP fellow from UVA.	Summer 2009

### High-School Student Mentor:

5. Rohan Pandit, Thomas Jefferson High School	Summer 2014-present
4. Pranay Singh, Thomas Jefferson High School	Summer 2014, 2012
4. Scott Jordan, ASSIP fellow from W. T. Woodson High School	Summer 2012
3. Niraja Bohidar, Thomas Jefferson High School	Summer-Fall 2012
2. Nakkul Sreenivas, Chantilly High School	2011-2012
1. Subeer Talapatra, Thomas Jefferson High School	Summer 2010

### Selected Student Awards (grouped by student):

21. Tatiana Maximova (CS postdoctoral fellow) Outstanding research presentation at 3DSIG/ISMB	July 2016
20. Bradley English (CSS/Neuroscience undergrad) OSCAR undergraduate apprenticeship	Fall 2016
19. Heather Hendy (CS undergrad) OSCAR undergraduate apprenticeship	Spring 2016

<sup>10</sup>Mentoring of college and pre-college students and their inclusion in my lab's research activities is an important component of my scholarship at Mason. These students have co-authored refereed articles and have earned numerous awards, some of which are listed here.

18. Mazyar Katouzian (CS undergrad, graduated May 2015)  
OSCAR undergraduate apprenticeship Spring 2015
17. Songyue Huang (CS undergrad, graduates May 2016)  
OSCAR undergraduate apprenticeship Spring 2015
16. Daniel Veltri (School of Systems Biology Ph.D., graduated 2015)  
Best student paper at IEEE BIBM in first-author capacity November 2014  
Travel Award, ICCABS June 2013  
Outstanding Oral Presentation, School of Systems Biology Student Research Day, Daniel Veltri May 2013
15. Irina Hashmi (CS Ph.D., graduated 2015)  
Best Poster Award, IEEE BIBM October 2012  
Travel Awards, IEEE BIBM, CRA-W Grad Cohort Workshop May 2011  
Research Assistant Fellowship 2010 - 2011
14. Rudy Clausen (M.S. Ph.D., graduated 2015)  
Guest (Intern) Researcher in the Cancer and Inflammation Program at the National Cancer Institute 2013-2014
13. Jennifer M. Van (CS undegrad, graduated 2015)  
Dean's Award in Physical Sciences at the College of Science Undergraduate Research Symposium 2014  
Oustanding Project Award at the Volgenau School of Engineering Undergraduate Research Celebration 2014  
Second author of a journal paper 2014  
Second author of a refereed conference paper 2013  
Princeton MOL/QCB Summer Program May 2013  
CRA-W DREU (Distributed Research Experiences for Undergraduates) May 2013  
University of Wisconsin Madison REU May 2013  
OSCAR undergraduate apprenticeship Spring 2013
12. Kevin Molloy (CS Ph.D., graduated 2015)  
Outstanding CS Graduate Student Award April 2015  
Finalist for best paper award at BiCoB March 2014  
Travel Award, ICCABS June 2013  
Outstanding Academic Achievement Award August 2011  
Dean Fellowship Fall 2011 - Spring 2012  
Best Paper award at BIONETICS in second-author capacity December 2010
11. Uday Kamath (IT Ph.D., co-advised with K. De Jong, graduated 2014)  
Honorable Mention, Humies Competition Award at GECCO June 2012
10. Herath Pilapitiya (CS undegrad, graduated 2014)  
OSCAR undergraduate apprenticeship Summer Intensive 2014
9. Brian Olson (CS Ph.D., graduated 2013)  
Mason VSE Outstanding Graduate Student Award April 2013  
Outstanding Academic Achievement Award May 2012  
Best Paper Award at BIONETICS in first-author capacity December, 2010
8. Sameh Saleh (CS undergrad, graduated May 2013)  
First author of a refereed journal and a refereed workshop paper 2013-2012  
Second author of a refereed journal paper 2013  
Author of numerous abstracts and extended abstracts 2013-2012  
Finalist, Male, CRA Outstanding Undergraduate Researcher Award May 2013  
Mason OSCAR Outstanding Undergraduate Research Award May 2013  
Selected undergraduate presenter, NCUR May 2013  
Keynote undergraduate speaker at COS Undergraduate Research Colloquium May 2012  
OSCAR undergraduate apprenticeship Fall 2011
7. Bryn Reinstadler (CS Williams College, graduated 2014)  
CRA-W DREU (Distributed Research Experiences for Undergraduates) in Shehu Lab May 2012
6. Scott Jordan (Woodson high school, now at RIT)  
ASSIP high-school fellowship June 2012
5. Justin Towson (CS undergraduate, graduated 2012)  
OSCAR undergraduate apprenticeship Fall 2010
4. Jack Compton (CS Ph.D., graduated 2011)  
Second author of a refereed journal paper 2012

3. Beenish Jamil (CS undergraduate, graduated 2011)  
*Honorable Mention, CRA Outstanding Undergraduate Research Award* May 2011  
CRA-W DREU (Distributed Research Experiences for Undergraduates) May 2011
2. Rachael Chung (CS undergradute, UNCC, now CS Ph.D.)  
CRA-W DREU (Distributed Research Experiences for Undergraduates) in Shehu Lab May 2009
1. Anahita Mostaghim  
ASSIP undergraduate fellowship June 2009

## DEPARTMENTAL AND UNIVERSITY SERVICE

### University Service:

- Member of University Scholars Selection Committee, February 20, 2016.
- Member of Cyber and Computer Mason Multidisciplinary Grants Review Panel, July 16, 2015.
- Member of Student Scholarly Activities subcommittee of the Mason Students as Scholars QEP Leadership Council, 2016-2013.

### Volgenau School of Engineering Service:

- Member of Recruitment Committee, Department of Statistics, George Mason University, 2016-2015.
- Assisted with preparations of material for SCHEV application, Department of Bioengineering, George Mason University, 2011-2012.
- Served on subcommittee to design the undergraduate curriculum, Department of Bioengineering, George Mason University, 2009-2011.
- Involved with the design of the Bioengineering program prior to it being a department, George Mason University, 2008-2010.
- Served on faculty recruitment subcommittee, Department of Bioengineering, 2008-2012.

### Computer Science Department Service:

- Co-organizer of “Mason Women in CS: A Networking Event,” George Mason University, November 14, 2016.
- Co-organizer of CS Ph.D. research symposium, George Mason University, 2015-present.
- Co-organizer (with Jana Kosecka) of CS Seminar, George Mason University, 2014-present
- Member of CS Graduate Studies Committee, George Mason University, 2016-present
- Member of Executive Committee, George Mason University, 2016-2014.
- Member of Strategic Vision and Planning Committee, George Mason University, 2014.
- Member of Ph.D. & IT Qualifying Exam (Foundations) Preparation Committee, 2013-present.
- Member of Ph.D. Admissions Committee, George Mason University, 2012-present.
- Member of Undergraduate Studies Committee, George Mason University, 2009-2011.
- Served on subcommittee to revise the Applied Computer Science degree in Biology into the new ACS degree in Bioinformatics, 2008-2011.

### Contributions as Invitee and Host to GMU Volgenau School of Engineering Seminars:

- |   |  |
|---|--|
| Jeremy Goecks, George Washington University     | GRAND Seminar, Fall 2014                     |
| Amina Woods, NIH                                | Bioengineering Seminar, Fall 2013            |
| Lydia Kavraki, Rice University                  | CS Distinguished Lecture Series, Spring 2013 |
| Philip Bryant, UMD College Park                 | Bioengineering Seminar, Spring 2013          |
| Silvina Matysiak, UMD College Park              | Bioengineering Seminar, Spring 2012          |
| Claire Monteleoni, George Washington University | CS GRAND Seminar, Spring 2012                |
| Brian Chen, Lehigh University                   | CS GRAND Seminar, Fall 2011                  |
| Anna Panchenko, NIH                             | CS GRAND Seminar, Fall 2009                  |
| Rezarta Islamaj-Dogan, NIH                      | CS GRAND Seminar, Fall 2009                  |

## PROFESSIONAL SERVICE

### Workshop Organization:

15. Co-organizer of “Women@GECCO” at GECCO, July 2017, Berlin, Germany.
14. Co-organizer and co-chair of “Evolutionary Computation in Computational Biology” at GECCO, July 2017, Berlin, Germany.

13. Co-organizer and co-chair of “Computational Structural Biology Workshop” at IEEE BIBM, December 15, 2016, Shenzhen, China.
12. Co-organizer of “Women@GECCO” at GECCO, July 2016, Denver, Colorado.
11. Co-organizer and co-chair of “Evolutionary Computation in Computational Biology” at GECCO, July 2016, Denver, Colorado.
10. Co-organizer and co-chair of “Computational Structural Biology Workshop” at IEEE BIBM, November 11, 2015, Washington, D.C.
9. Co-organizer and co-chair of “Evolutionary Computation in Computational Biology” at GECCO, July 11, 2015, Madrid, Spain.
8. Co-organizer and co-chair of “Computational Structural Biology Workshop” at ACM BCB, September 20, 2014, Newport Beach, LA.
7. Co-organizer and co-chair of “Robotics Methods for Biological Structures and Kinematics Modeling” Workshop at RSS, July 16, 2014 Berkeley, CA.
6. Co-organizer and co-chair of “NSF CISE CAREER Writing Workshop” March 31, 2013, Arlington, VA.
5. Co-organizer and chair of “Artificial Intelligence and Robotics Methods in Computational Biology” Workshop at AAI, July 14, 2013 Bellevue, WA.
4. Co-organizer and co-chair of “Computational Structural Biology Workshop” at ACM BCB, September 22, 2013, Washington, D.C.
3. Co-organizer and co-chair of “Computational Structural Biology Workshop” at IEEE BIBM, October 4, 2012, Philadelphia, PA.
2. Co-organizer and co-chair of “Computational Structural Biology Workshop” at IEEE BIBM, November 12, 2011, Atlanta, GA.
1. Co-organizer and chair of “Evolutionary Computation and Machine Learning in Bioinformatics Workshop” (BioLearn) at BIONETICS, Dec. 1-3, 2010, Boston, MA.

### **Tutorial Organization**

6. Co-organizer and co-chair of “Evolutionary Algorithms for Protein Structure Modeling” Tutorial at ACM BCB, July 2016, Seattle, Washington.
5. Co-organizer and co-chair of “Evolutionary Algorithms for Protein Structure Modeling” Tutorial at GECCO, July 2016, Denver, Colorado.
4. Co-organizer and co-chair of “Evolutionary Algorithms for Protein Structure Modeling” Tutorial at GECCO, July 11, 2015, Madrid, Spain.
3. Co-organizer and chair of “Robot Motion Planning Methods for Modeling Structures and Motions of Biomolecules” Tutorial at ACM BCB, September 20, 2014, Newport Beach, CA.
2. Co-organizer and co-chair of “Evolutionary Search Algorithms for Protein Modeling: From De-novo Structure Prediction to Comprehensive Maps of Functionally-relevant Structures of Protein Chains and Assemblies” Tutorial at GECCO, July 12, 2014, Vancouver, Canada.
1. Co-organizer and chair of “From Robot Motion Planning to Modeling Structures and Motions of Biological Molecules” Tutorial at ACM BCB, September 22, 2013, Washington, D.C.

### **Other Chairships:**

Program co-chair of ACM BCB 2017, Boston, MA  
Program Committee co-chair of IEEE BIBM 2015, Washington, D. C.  
Tutorial co-chair of ACM BCB 2014, Newport Beach, CA.  
Local arrangement chair of ACM BCB 2013, Washington, D.C.  
“Computer Scientist in Profile” section writer of ACM BCB newsletter, 2012-present.  
Chair of Systems Biology session, ACM BCB, October 9, 2012.  
Co-chair of Poster Session at IEEE BIBM, October 4-7, 2012.  
Organizing Committee vice-chair of BIONETICS, Dec. 1-3, 2010.  
Co-organizer of Bioinformatics track of BIONETICS, Dec. 1-3, 2010.

### **Editorial Positions:**

Editorial board member, Intl J. of Data Mining and Bioinformatics (IJDMb), 2012-present.  
Guest Co-editor of special collection on Macromolecular Structure and Dynamics of PLoS Comput Biol 2015.  
Co-editor of Robotica 2015 (special issue).  
Co-editor of IEEE/ACM Trans Comput Biol and Bioinf 2015 (special issue).  
Co-editor of J Comput Biol 2015 (special issue).  
Guest associate editor of Education Collection of PLoS Comput Biol 2014.

Co-editor of BMC Struct Biol 2013 (special issue).  
Co-editor of J Bioinf and Comp Biol 2012 (special issue).  
Co-editor of J Bioinf and Comp Biol 2011 (special issue).

**Program Committee Membership:**

PC member of ISMB, July 8-12, 2016.  
PC member of RECOMB, April 17-21, 2016.  
PC member of IEEE ICCABS, October 13-15, 2016.  
PC member of BICoB, March 24-26, 2014.  
PC member of Translational Bioinformatics section, ACM BCB, September 20-23, 2014.  
PC member of Protein Structure & Function section, ACM BCB, September 22-25, 2013.  
PC member of Protein Structure & Function section, ACM BCB, October 7-10, 2012.

**Grant Proposal Referee:**

NIH BST Study section, 2016-2015  
NIH BDMA Study Section, 2016-2015  
NSF CAREER panelist, 2015, 2013  
NSF BigDATA panelist, 2012  
NSF Sustainable Software Elements (SSE): Models of Large Systems, panelist, 2012  
NSF Comput Core Foundations (CCF): Algorithmic Foundations (AF), panelist, 2012  
NSF Macromol., Supramol. and Nano Chemistr, ad-hoc reviewer, 2012  
NSF Mol. and Cell. Biosciences, ad-hoc reviewer, 2011

**Journal Referee (in past five years):**

2016: Structure, PLoS Comput Biol, Proteins: Struct Funct Bioinf, BMC Bioinf, Mol Biol Reports, Structural Dynamics, Comput Biol and Chem, Computers in Biol and Med, F1000Research, IEEE Trans Evol Comput, J Appl Soft Comput, J Bioinf and Comput Biol.  
2015: FEBS Letters, Biophysica et Biochimica Acta, Scientific Reports, PLoS Comput Biol, Proteins: Struct Funct and Bioinf, Comput Biol and Chem J, IEEE Trans NanoBioScience, J of Artificial Intelligence Research (JAIR), IEEE Transactions on Evol Comput (TVEC), Int J Mol Sci.  
2014: BMC Genomics, Journal of the Royal Society Interface, Computers in Biology and Medicine, J of Artificial Intelligence Research (JAIR), Proteins: Struct Funct and Bioinf, IEEE/ACM Trans on Comp Biol and Bioinf (TCBB).  
2013: J of Artificial Intelligence Research (JAIR), IEEE Transactions on Robotics (T-RO), J of Applied Mathematics and Computation, IEEE/ACM Trans on Comp Biol and Bioinf (TCBB), BMC Structural Biology J, Proteome Sci.  
2012: PLoS Comp Biol, Entropy J, Computational and Mathematical Methods in Medicine, J Chem Info and Model, Comput and Struct Biotechnology J, J Bioinf and Comp Biol (JBCB).

**Conference Referee (in past five years):**

2016: ISMB, RECOMB, ACM BCB, IEEE ICCABS.  
2015: Intl Conf Res Comp Mol Biol(RECOMB), IEEE Bioinf and Biomed (BIBM).  
2014: ACM Bioinf and Comp Biol (BCB), Comput Struct Biol Workshop (CSBW), BICoB.  
2013: Symposium on Computational Geometry (SoCG)

**Professional Association Membership:**

National Council on Undergraduate Research (NCUR)  
American Association for Advancement of Science (AAAS)  
IEEE, IEEE Robotics and Automation Society, and IEEE Women in Engineering  
IEEE CIS BBTC  
ACM, SIGBIO, SIGACT, SIGART, SIGSIM, SIGEVO, SIGKDD  
International Society for Computational Biology (ICSB)  
Biophysical Society  
Protein Society  
American Chemical Society (ACS)

Mason Nanotechnology Initiative

**Selected Professional Activities:**

Judge in Computer Science Category of the (international) Undergraduate Awards, 2016-2015  
Executive Supporter of Girls Computing League, 2015-present.  
Women in Bioinformatics Panel Member at ACM BCB, 2014.  
George Mason University NSF CAREER panelist, May 20, 2014.  
State Department 3rd Young Scientist Forum, People to People Exchange, September 18, 2012.  
George Mason University NSF CAREER panelist, April 18, 2012.  
Women in Bioinformatics Panel Member at ACM BCB, 2012.  
Organizer of Chantilly High School Bioengineering Tour, June 17, 2011.  
Co-organizer of High School Bioengineering Summer Internship Program, Summer 2011.  
Two-body Problem Panel Member at Grace Hopper Conference, October 2009.  
Two-body Problem Panel Member at Grace Hopper Conference, 2009.

**Professional Development Activities:**

NIH National Centers For Systems Biology (NCSB) Annual Meeting, July 11-12, 2013  
NSF Grants Conference, October 22-23, 2012  
NSF CISE Career Writing Workshop, Norfolk, VA, April 15, 2011  
NSF Early Career Writing Workshop, Williamsburg, June 2, 2010  
AASCU Proposal Development Workshop, Washington D.C., February 25-27, 2010