Kenneth N. McGuinness, Ph.D.
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Curriculum Vitae

Mission: Tenured teaching professor of Bioinformatics at a research-intensive university to inspire and give back

SUMMARY

- Curious computational biologist, and *in vitro* molecular biophysicist passionate about molecular interactions
- Combined three years of experience as an Adjunct Professor and Teaching Assistant
- Seven years of mentoring undergraduate and high-school research in computational biology and bioinformatics
- Academic and industrial post-doctoral experience in peptide and protein design, and evolution
- Supported peptide drug discovery and protein process chemistry: engineered, implemented, deployed software
- Multiple modeling modalities from machine learning to all-atom and coarse-grained molecular dynamics
- Desire to utilize, develop, and deploy bioinformatics tools that drive hypothesis testing, and decision making

EDUCATION

Rutgers University - New Brunswick, NJ
Associate Scientist, Postdoctoral Associate in Biochemistry and Microbiology *September 2018 – **Present***
- Advisor*:* Yana Bromberg, Ph.D. Research Area: Origins of life: Microbial metabolism

Merck & Co. Inc. - Kenilworth, NJ
Associate Scientist, Postdoctoral Research Fellow in Modeling and Informatics *June 2016 – June 2018*
- Advisor*:* Alejandro Crespo, Ph.D. Research Area: Chemistry Modeling and Informatics

City University of New York, Advanced Science Research Center
Associate Scientist, Postdoctoral Research Fellow in Nanoscience *January 2016 – June 2016*
- Advisor*:* Rein Ulijn, Ph.D. Research Area: Dynamic assembly of small peptides

Rutgers University - New Brunswick, NJ
Ph.D. in Computational Biology and Molecular Biophysics *2016*
- Advisor*:* Vikas Nanda, Ph.D.
- Ph.D. Title: "The design, characterization, and utility of self-assembling hydrophobic collagen peptides"

BA in Biomathematics, Rutgers *2010*

TEACHING AND MENTORING

Adjunct Professor

Kean University, Union, NJ
Probabilistic Methods Lab *fall 2018*
- Implemented active learning techniques such as think-pair-share exercises to maintain student engagement
- Developed R modules to reinforce fundamental statistics and probability concepts
- Stressed the importance of clearly presenting data and the relevancy of statistics in real life

Stevens Institute of Technology, Hoboken, NJ
Fundamentals of Computational Biology *fall 2018*
- Taught the first class in Computational Biology offered specifically for undergraduates
- Translated a SIT graduate-level syllabus and projects into material suitable for undergraduates
- Lectured and facilitated computational labs on homology, sequence alignments, molecular phylogeny, protein design and modeling, RNAseq analysis
- Taught fundamental scientific programing techniques using Python, Biopython, R, and command-line scripting

- Hands-on mentoring of each student's individual research project on genetic diseases

Teaching Assistant

Rutgers University, New Brunswick, NJ

Quantitative Biology and Bioinformatics *2012 – 2013*

- Taught 25 students per semester fundamental scientific programing techniques using Biopython
- Lectured and facilitated computational labs on sequence alignment (ClustalW, MUSCLE) and molecular phylogeny (UPGMA, Neighbor-joining) algorithms and software (BLAST, MEGA), Biostatistics, genetics, protein design, and the structure of DNA
- Intensive hands-on bi-weekly office hour with an average of six students

Biological Research Laboratory *fall 2011*

- Taught 45 students in general biology laboratory, hands-on office hours with an average of 2 students, graded homework and lab reports
- Lectured on genetics, ecology, the cell-cycle, and taxonomy

Mentoring

Rutgers University, Center for Advanced Biotechnology and Medicine

Senior Thesis mentor *2017 – 2018*

- Developed and guided research in peptide lipid membrane mimetic interactions with membrane proteins
- Utilized sequence, rigid body, and molecular dynamics docking methods to probe energetics of interactions
- Manuscript underway highlights the role of hydrophobic mismatch when designing membrane mimetics

Summer Undergraduate Research Experience program mentor *2011 – 2015, lead 2014 – 2015*

- Co-developed engaging curricula that included journal club and lectures on Biostatistics
- Trained on average 20 students per summer in fundamental science techniques including how to read scientific literature, and present scientific information

Aresty Research Fellow mentor *2012 – 2014*

- Awarded funding from the Aresty Research Foundation to study collagen peptide self-assembly
- Developed and guided Bioinformatics research in sequence analysis of the protein family collagen for the design of collagen-like peptide sequences predicted to self-assemble into nanomaterials
- Taught fundamental programming techniques using Biopython, and biochemical laboratory protocols

City University of New York, Advanced Science Research Center

Collegiate High School Research Fellow mentor *2016 – 2017*

- Developed and guided a student's senior research thesis studying peptide-blood brain barrier interactions using MARTINI coarse-grained modeling

RESEARCH BACKGROUND

Rutgers University, New Brunswick, NJ
Marine and Coastal Sciences

Associate Scientist, Postdoctoral Research Fellow *September 2018 – **Present***

- Member of the NASA Astrobiology Institute team Evolution of Nanomachines In Geospheres and Microbial Ancestors
- Developed computational methods for linking protein structure to the evolution of redox functionality

Merck & Co. Inc., Kenilworth, NJ
Merck Research Laboratories, Modeling and Informatics

Associate Scientist, Postdoctoral Research Fellow *June 2016 – June 2018*

- Collaborated with chemical biologists to contribute to the peptide design pipeline by engineering and implementing software employing a novel methodology that predicts 33% more top-top down mass spectrometry fragmentation patterns of disulfide linked peptides than existing methods

- Developed, validated, and distributed, via Pipeline Pilot, machine learning models, using the random forest, xgboost and SVL methods, that correctly predicted enzyme (80%) and membrane protein (10% more than alternative methods) thermostability classification for the biocatalysis and crystallography pipelines
- Proficient in Rosetta, Bioluminate, MOE, Discovery Studio, Spotfire, Pipeline Pilot, HPC, and Git platforms

City University of New York, New York, NY
Advanced Science Research Center, Nanoscience
Associate Scientist, Postdoctoral Research Fellow *January 2016 - June 2016*

- Designed, modeled, and validated self-assembly of tripeptides in the presence of ATP
- Proficient in peptide synthesis, and atomic and coarse-grained modeling using GROMACS and MARTINI

Rutgers University, New Brunswick, NJ
Center for Advanced Biotechnology and Medicine *September 2011 – January 2016*
Graduate Research Assistant, Computational Biology and Molecular Biophysics

- Designed peptide lipid membrane mimetics that interact with light harvesting membrane proteins
- Developed, validated, and published open source code to predict collagen peptide assembly using coarse-grained molecular modeling via diffusion limited aggregation
- Extensive wet-lab training: circular dichroism, electron and atomic force microscopy, fluorescence spectroscopy

Additional research experiences

Coarse-grained assembly of peptides, Invited Guest - Lab: Siewert J.Marrink PhD, University of Groningen 2015
Synthesis and purity monitoring of polyAspirin by NMR, Lab: Kathryn Uhrich PhD, Rutgers University 2011
Monitoring the heat denaturation of collagen by NMR, Lab: Jean Baum PhD, Rutgers University 2011
Modeling diffusion limited aggregation, Lab: Vikas Nanda PhD, Rutgers University 2010
Machine learning and shape preference: consumer products, Lab: Stanley Dunn PhD, Rutgers University 2006-08

PUBLICATIONS

Role of simple descriptors and domain applicability in predicting change in protein thermostability **McGuinness K.**, Pan W., Sheridan R., Murphy G., Crespo A. *PLoS ONE* 2018: DOI: 10.1371/journal.pone.0203819

Characterization of disulfide-linked peptides using tandem mass spectrometry coupled with automated data analysis software Liang Z., **McGuinness K.**, Crespo A., Zhong W. *JASMS* 2018 DOI: 10.1007/s13361-017-1855-0

Collagen mimetic peptide discs promote assembly of a broad range of natural protein fibers through hydrophobic interactions **McGuinness K.**, and Nanda V. *Organic & Biomolecular Chemistry* 2017, DOI: 10.1039/c7ob01073g

Morphological diversity and polymorphism of self-assembling collagen peptides controlled by length of hydrophobic domain **McGuinness K.**, Khan I. J., and Nanda V. *ACS Nano* 2014 *8* (12), 12514-12523 DOI: 10.1021/nn505369d

Self-assembly of left- and right-handed molecular screws Xu F., Khan I.J. , **McGuinness K.**, Parmar A.S., Silva T., Murthy S.N., and Nanda V. *Journal of the American Chemical Society* **2013** *135* (50), 18762-18765 DOI: 10.1021/ja4106545

SELECTED PRESENTATIONS

"Developing a platform for in-silico protein design: Applications to thermostability QSAR modeling", Chemical Computing Group Users Group Meeting, Montreal CA, June 2017 (Invited talk)

"The co-assembly of collagen-mimetic peptides and natural proteins", Biophysical Society 59th Annual Meeting, Baltimore MD, Feb 2015 (Poster- Abstract published online)

"Polymorphic assembly of computationally designed hydrophobic-rich collagen peptides", Biophysical Society 57th Annual Meeting, Philadelphia Pa, Feb 2013 (Poster- Abstract published online)

"Representing multi-dimensional diffusion limited aggregation data in R", NCSI High Performance Computing Workshop: Modeling and Visualization, Stockton College, June 2011 (Talk)

AWARDS AND HONORS

Merck Post-doctoral Association Site Representative	2017-2018
Graduate Assistance in Areas of National Need (GAANN) graduate fellowship	2013-2015
President of the Quantitative Biomedicine Graduate Student Organization	2013-2015
Awarded 48 hours on the EQ-SANS Neutron Scattering beamline at Oak Ridge National Labs	2015
Education travel grant, '4th Neutrons in Structural Biology workshop' at Oak Ridge National Labs	2013
Education travel grant, Supercomputing Conference in New Orleans, LA	2010
Summer scholar innovator award**,** New York Life Insurance	2009

SERVICE AND VOLUNTEER

Bridgewater NJ Adopt-a-highway	2017-2018
Merck & Co., Inc. Bring your child to work day (Lead)	2016-2018
Rutgers Day (Lead)	2011-2015
New Brunswick homeless shelter	2011-2014
Elijah's Promise soup kitchen	2011-2013