

Aleksandra A. Zagulyaeva

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Education

Ph.D. in Chemical Biology 2019 University of Florida, Department of Chemistry, Gainesville, FL

Dissertation: “Towards Elucidating the Mechanism of Action of MbtH-like Proteins: A Comprehensive Approach”

M.S. in Organic Chemistry 2010 University of Minnesota Duluth, Duluth, MN

B.S. in Chemistry 2007 M. V. Lomonosov Moscow State University, Moscow, Russia

Research Experience

Novartis Institutes for Biomedical Research, Global Discovery Chemistry

Synthetic Biology, Pathway Engineering for Microbial Biosynthesis of Natural Products

Postdoctoral Scholar (January 2020-Current)

- Developing platform for rational synthetic pathway refactoring to produce novel scaffolds for various downstream biomedical applications
- Participating in the collaborative project to advance a recombinant organism towards industrial production of biopharmaceuticals
- Establishing tools for seamless genetic manipulations of *Streptomyces* species to promote applications in industrial processes

University of Florida, Department of Chemistry

Interdisciplinary Research, Chemical Biology, Structural Biology, Protein-Protein Interactions

Graduate Student/Research Assistant (2010-2015, 2017-2019)

Supervisor: Dr. Steven D. Bruner

- Led and coordinated 2 research projects aimed at understanding protein-protein interactions in nonribosomal peptide biosynthesis of natural products for downstream engineering of hybrid systems, generating nearly \$500,000 in grant funding
- Investigated mechanism of modulation of nonribosomal peptide synthetases (NRPSs) by MbtH like proteins (MLPs) using biochemical and structural approaches as well as modern biophysical methods
- Participated in the collaborative project to investigate the role of MLP in biosynthesis of phytotoxin in potato scab pathogen *S. scabies*

- Designed and chemically/chemoenzymatically synthesized bioorthogonal probes for cross coupling reactions to decipher structural and stereochemical requirements of NRPS condensation domain binding sites for downstream directed bioengineering
- Engineered, expressed, purified, chemoenzymatically modified, and crystallized proteins (excised domains or multi-domain entities) and protein complexes to study aspects of inter- and intradomain as well as intermodular communication within NRPS systems. Deposited 4 high resolution structures to RCSB PDB protein data bank

University of Minnesota Duluth, Department of Chemistry and Biochemistry

Organic Synthesis, Synthetic Methodology Development

Graduate Student/Research Assistant (2008-2010)

Supervisor: Dr. Viktor V. Zhdankin

- Involved in the international collaboration investigating the application of hypervalent iodine compounds in organic synthesis
- Studied and developed hypervalent iodine-based synthetic methodologies, resulting in 2 first author publications (115 citations) in peer-reviewed journals
- Analyzed small molecules and monitored organic reactions using GC-MS
- Characterized perfluorinated compounds using ^{19}F NMR

M. V. Lomonosov Moscow State University, Department of Chemistry

Organic Synthesis

Undergraduate Student/Junior Researcher (2005-2007)

Supervisor: Dr. Konstantin V. Kudryavtsev

- Studied, developed, and optimized the methodology for asymmetric organo-Brønsted acid catalyzed 1,3-dipolar cycloaddition reaction of azomethine ylides and electron-deficient alkenes - Routinely performed multistep synthesis and NMR characterization of target compounds and intermediates
- Mastered crystallization of small molecules for X-ray analysis

Skills

Technical

Molecular biology: subcloning and molecular cloning (from PCR primer design to a complete expression vector, GC-rich); DNA fragment and plasmid (up to 250 kb) purification; site-directed mutagenesis

Protein biochemistry: recombinant protein construct engineering, expression (*E. coli* host), and purification (precipitation, affinity); enzyme assays; protein-protein interaction (PPI) analysis; chemoenzymatic site-specific protein modification; design of experiments to study PPIs

Protein crystallography: proteins and protein complexes (free, substrate-bound, or chemoenzymatically modified); optimization from the initial hit (sitting drop vapor diffusion) to a diffraction quality crystal (hanging drop vapor diffusion, seeding); X-ray data collection (on-site, remote) and processing; structure determination, analysis, deposition (RCSB PDB), and visualization

Biophysical methods: CD; ITC; NMR; UV-Vis and fluorescence spectroscopy; X-ray diffraction

Analytical methods: ÄKTA-FPLC (affinity, ion exchange, size-exclusion); DNA electrophoresis; HPLC; LC-MS; MALDI-TOF; SDS-PAGE

Software

Microsoft Office; ChemDraw; Origin; Unicorn; HKL2000; XDS; CCP4; Phenix; PyMOL; Chimera; Geneious; SnapGene

Languages

English (full professional proficiency); Russian (native)

Other

Data analysis and reports
Internal and external seminar presentations
Multistep organic synthesis
Technical and scientific writing

Other Experience

Application and instrument training for peers
Laboratory inventory and order management
Maintenance and troubleshooting of laboratory equipment
Negotiation and solicitation of bids from vendors to ensure cost savings
Peer review
Safety compliance
Scientific consulting

Teaching

Courses taught as Graduate Teaching Assistant/Lead Teaching Assistant 2008-2015

Biochemistry/Molecular Biology Laboratory
Organic Chemistry/Biochemistry II
Organic Chemistry Laboratory I, II

Responsibilities

- Conducted laboratories for majors and non-majors
- Prepared PowerPoint presentations
- Facilitated pre-lab discussions
- Assisted with data acquisition and interpretation
- Supervised and substituted for other Teaching Assistants

Publications

Works in progress

1. Aleksandra A. Zagulyaeva, Steven D. Bruner. "Crystal Structure of FscC – Supporting

2. **Aleksandra A. Zagulyaeva**. “MbtH-Like Proteins in Nonribosomal Biosynthesis of Natural Products (Review)”. Manuscript in preparation.
3. **Aleksandra A. Zagulyaeva**. “New Insights into the Mechanism of Action of MbtH-Like Proteins.” Manuscript in preparation.

Other publications

1. **Aleksandra Zagulyaeva**, Steven D. Bruner. “Structural Biology of Nonribosomal Peptide Synthetases.” Accepted to *Comprehensive Natural Products III: Chemistry and Biology (ScienceDirect)* 2020, 2, 229-246.
2. **Aleksandra A. Zagulyaeva**, Christopher T. Banek, Mekhman S. Yusubov, Viktor V. Zhdankin. “Hofmann Rearrangement of Carboxamides Mediated by Hypervalent Iodine Species Generated in Situ from Iodobenzene and Oxone: Reaction Scope and Limitations.” *Org. Lett.* 2010, 12, 4644-4647.
3. **Aleksandra A. Zagulyaeva**, Mekhman S. Yusubov, Viktor V. Zhdankin. “A General and Convenient Preparation of [Bis(trifluoroacetoxy)iodo]perfluoroalkanes and [Bis(trifluoroacetoxy)-iodo]arenes by Oxidation of Organic Iodides Using Oxone and Trifluoroacetic Acid.” *J. Org. Chem.* 2010, 75, 2119-2122.
4. Mekhman S. Yusubov, **Aleksandra A. Zagulyaeva**, Viktor V. Zhdankin. “Iodine(V)/Ruthenium(III)-Cocatalyzed Oxidations: A Highly Efficient Tandem Catalytic System for the Oxidation of Alcohols and Hydrocarbons with Oxone.” *Chem. Eur. J.* 2009, 15, 11091-11094.
5. K.V. Kudryavtsev, **A. A. Zagulyaeva**. “1,3-Dipolar cycloaddition of Schiff bases and electron deficient alkenes, catalyzed by α -Amino acids.” *Russ. J. Org. Chem.* 2008, 44, 378-387.

Awards and Honors

Graduate Student Teaching Award 2013 University of Florida

Certificates of Outstanding Achievement 2011-2013 Achieved and maintained 4.0 GPA

University of Florida, UF International Center

Certificate of Outstanding Teaching Performance 2010-2011 University of Florida, Department of Chemistry

Grinter Fellowship 2010-2013 Excellence in Academic and Research Records

University of Florida, Department of Chemistry

UMD Siders Chemistry Graduate Fellowship 2010 Excellence in Academic and Research Records

University of Minnesota Duluth, Department of Chemistry and Biochemistry

Outstanding Graduate Teaching Assistant in Chemistry and Biochemistry 2010 University of

Minnesota Duluth, Swenson College of Science and Engineering

