Alexander Predeus

NGS bioinformatics, systems biology, immunology

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OBJECTIVE

My scope of interests includes next-generation sequencing, bioinformatics, systems biology, and immunology. I am experienced in analysis of RNA-seq and ChIP-seq experiments, as well as integrative approaches and biological interpretation of sequencing data.

EDUCATION

Ph.D. in Chemistry 2009

Michigan State University
Advisor: Professor William D. Wulff
Dissertation: Studies of Cyclization Reactions of Chromium (0) Complexes

Diploma in Chemistry 2003

Moscow State University
Advisor: Prof. Alexander Z. Voskoboynikov
Title: New Sterically Hindered Metallocene Complexes with Bulky Indenyl Type Ligands.

EXPERIENCE

Washington University in St. Louis, School of Medicine 7.12 – 7.15
Postdoctoral Research Associate

- Responsible for computational processing of NGS experiments: quality control, alignment, and analysis of over 100 RNA-Seq and ChIP-Seq experiments
- Whole genome segmentation analysis to identify active enhancer and promoter regions of AGR loci using hidden Markov models
- Analysis of genetic and epigenetic factors influencing the repertoire of murine T-cells
- Development of massive gene co-expression database based on the published expression experiments, implemented as a web tool (GeneQuery)
- Discovery of new non-coding RNA molecules involved in immune response regulation
- Analysis of expression changes in adipose tissue upon calorie restriction, assessed by RNA sequencing
- Numerous collaborative projects with experimental biologists, interpreting both human and murine expression data

Michigan State University 4.10 – 7.12
Department of Biochemistry & Molecular biology
Visiting Research Associate

- Parameterization of non-bonded interactions in PRIMO coarse-grained protein model
- Studied crowding effects of globular proteins on conformational sampling of small peptides using all-atom/coarse-grained multiscale simulations
- Studied of RNA polymerase II by molecular dynamics and enhanced sampling methods
- Developed a new method of enhanced sampling and implemented it in NAMD molecular dynamics package
- Studied the energetics of mismatch-containing DNA bending
- Performed full setup and molecular dynamics simulation of human MSH2-MSH3 mismatch repair complex

Michigan State University 9.03 – 10.09
Department of Chemistry
Graduate Student

- Developed a new, general method of homocalixarene synthesis
- Improved existing methods of Fischer bis-carbene complex preparation
- Discovered a novel trimethylenemethane (TMM) complex [3+2] cycloaddition

AREAS OF EXPERTISE

- Extensive experience with next-generation sequencing processing and quality control pipelines and software packages, including multiple platforms (Illumina, SOLiD) and custom method modifications (barcoding, single cell)
- Gene expression analysis, including gene set analysis, pathway enrichment, and network construction
- Analysis of ChIP-seq and DNase-seq, including integrative whole-genome segmentations
- Extensive experience with molecular dynamics simulation and analysis software packages (CHARMM, NAMD, MMTSB Toolset, X3DNA, Curves+, PyMol, VMD)
- Extensive experience with setting up, running, and analyzing simulations on various supercomputers, as well as on local performance clusters
- Solid working knowledge of Perl, C, C++, R, Fortran 90/95 programming languages, and have implemented numerous programs, both standalone and as parts of large program packages
- Extensive experience in design and application of multistep organic synthesis
- Experienced in the use of Schlenk and dry box techniques for the manipulation of air- and moisture-sensitive compounds under argon and at low temperatures
- Proficient in the manipulation of gases (oxygen, hydrogen, nitrogen) for synthesis
- Experienced in the purification and characterization of new compounds: Thin-layer and column chromatography, multinuclear 1D- and 2D-NMR spectroscopy including 1H, 13C, 19F NMR; GC, GC-MS, HPLC-MS; UV-Vis and IR spectroscopy
- Experienced user of Linux (Gentoo, Ubuntu), Mac, Sun operating systems

PUBLICATIONS

- Sharma, M.; Predeus, A. V.; Kovacs, N.; Feig, M. «Differential Mismatch Recognition Specificities of Eukaryotic MutS Homologs, MutSα and MutSβ» *Biophys. J.*, **2014**, *106(11)*, 2483–2492
- Predeus, A. V.; Gopalakrishnan, S.; Huang, Y.; Tang, J.; Feeney, A. J.; Oltz, E. M.; Artyomov, M. N. «Targeted Chromatin Profiling Reveals Novel Enhancers in Ig H and Ig L Chain Loci» *J. Immunol.*, **2014**, *192(3)*, 835-836
- Gopalakrishnan, S.; Majumder, K.; Predeus, A.; Huang, Y.; Koues, O. I.; Verma-Gaur, J.; Loguercio, S.; Su, A. I.; Feeney, A. J.; Artyomov, M. N.; Oltz, E. M. «Unifying model for molecular determinants of the preselection Vβ repertoire» *Proc. Nat. Acad. Sci. USA*, **2013**, *110(34)*, E3206–E3215
- Wang, B.; Predeus, A. V.; Burton, Z. F.; Feig, M. «Energetic and Structural Details of the Trigger-Loop Closing Transition in RNA Polymerase II» *Biophys. J.*, **2013**, *105(3)*, 545–546
- Kar, P.; Gopal, S. M.; Cheng, Y.-M.; Predeus, A.; Feig, M. «PRIMO: A Transferable Coarse-Grained Force Field for Proteins» *J. Chem. Theory Comput.*, **2013**, *9(8)*, 3769–3788
- Sharma, M.; Predeus, A. V.; Mukherjee, S.; Feig, M. «DNA Bending Propensity in the Presence of Base Mismatches: Implications for DNA Repair» *J. Phys. Chem. B*, **2013**, *117 (20)*, 6194–6205
- Wang, H.; Predeus, A. V.; Wulff, W. D. «Synthesis of [m.n]Cyclophanes: Regiochemistry Transfer from Vinyl Halides to Cyclophanes via Fischer Carbene Complexes» *Chem. Eur. J.* **2013**, *19(25)*, 8261-8267
- Predeus, A. V.; Gopalsamuthiram, V.; Staples, R. J.; Wulff, W. D. «Rational Synthesis for All All-Homocalixarenes» *Angew. Chem. Int. Ed.* **2013**, *52(3)*, 911-915
- Predeus, A. V.; Gul, S.; Gopal, S. M.; Feig, M. «Conformational Sampling of Peptides in the Presence of Protein Crowders from AA/CG-Multiscale Simulations» *J. Phys. Chem. B* **2012**, *116(29)*, 8610-8620
- Gopalsamuthiram, V.; Predeus, A. V.; Huang, R. H.; Wulff, W. D. «Optically Active Calixarenes Conduced by Methylene Substitution» *J. Am. Chem. Soc.* **2009**, *131 (50)*, 18018–18019
- Newman, C. A.; Antilla, J. C.; Chen, P.; Predeus, A. V.; Fielding, L.; Wulff, W. D. «Regulation of Orthogonal Functions in a Dual Catalyst System. Subservient Role of a Nonchiral Lewis Acid in an Asymmetric Catalytic Heteroatom Diels−Alder Reaction» *J. Am. Chem. Soc.* **2007**, *129(23)*, 7216 – 7217
- Vorogushin, A. V.; Predeus, A. V.; Wulff, W. D.; Hansen, H.-J. «Diels−Alder Reaction−Aromatization Approach toward Functionalized Ring C Allocolchicinoids. Enantioselective Total Synthesis of (−)-7*S*-Allocolchicine» *J. Org. Chem.* **2003**, *68(15)*, 5826 – 5831

TEACHING EXPERIENCE

- Taught multiple chemistry courses at Michigan State University (organic chemistry, inorganic chemistry, and general chemistry labs, organic chemistry and general chemistry recitations), for a total of 13 semesters
- Organized Systems Biology Workshop in 2014 and 2015

HONORS AND AWARDS

- 30th International Chemistry Olympiad, Melbourne, Australia – Bronze Medal, 1998
- Winner of numerous Ukrainian, Russian, and international ISSEP student Olympiads: 1995 – 1998
- International Soros Science Education Program (ISSEP) Fellow: 1998, 1999, 2000
- International Lomonosov Student Conference Award, Moscow, Russia, 1999
- Award for Outstanding Diploma Work: Moscow State University, 2003

CONNECT

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