Alexei A. Podtelezhnikov — Curriculum Vitæ

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Research Interests: Genomics, Genetics, RNA-Seq and DNA-Seq Data Analysis, Statistical Learning, Computational Biophysics and Biochemistry, Structural Bioinformatics, Molecular Modeling

Teaching Interests: Numerical and Computational Methods in Biophysics and Biochemistry, Statistical Methods, Advanced Monte Carlo Methods, Bioinformatics, Genetics, Genomics, Proteomics

Education

New York University
Ph.D. in Biomolecular Chemistry (2000),
Dissertation: Kinetics and thermodynamics of DNA cyclization.

Moscow Institute of Physics and Technology
M.S. in Molecular Biophysics (1994) and
B.S. in Applied Physics and Mathematics (1992),
Thesis: Testing the quality of electron microscope mapping data for DNA molecules with sequence-specific ligands.

Research Experience:

Merck & Co., Inc.
Merck Research Laboratories

West Point, PA
07/2008-present

Principal Scientist — Genetics and Pharmacogenomics

- Statistical analysis of gene expression profiling
- Development of predictive toxicity and carcinogenicity biomarkers
- Devise biomarkers for optimal bioprocess harvest
- Disease progression and target engagement biomarkers for neuroscience
- Characterization of animal disease models through mRNA profiling
- Integration of genomics and genetics of brain aging

Michigan Technological University

Houghton, MI
08/2007-06/2008

Visiting Assistant Professor — Department of Physics

- Contrastive divergence learning of protein energetics
- Bayesian modeling of residue contacts in proteins
- Monte Carlo reconstruction of protein secondary structure
- Protein structure prediction using knowledge-based potentials

Keck Graduate Institute of Applied Life Sciences

Claremont, CA
11/2003-06/2007

Postdoctoral Fellow — Wild Research Group

- Knowledge-based protein structure prediction
- Machine learning of hydrogen bonding and other protein interactions
- Data mining of domain sequences and their secondary structures
- Efficient Monte Carlo sampling of peptide conformations

Howard Hughes Medical Institute (UC San Diego)

San Diego, CA
11/2000-11/2003

Research Associate — McCammon Research Group

- Modeling tetrameric HIV-1 integrase complex with DNA
- Hydrodynamics and electrostatics of HIV-1 integrase
- Docking of small ligands to smallpox topoisomerase
- Brownian dynamics of ligand binding to acetylcholinesterase

New York University, Department of Chemistry

New York, NY
09/1995-10/2000

Graduate Assistant — Vologodskii Research Group

- Brownian dynamics and Monte Carlo simulations of DNA cyclization
- Supercoiling and knotting of long DNA molecules
- DNA topology and its implications for oncology
- Non-equilibrium transcriptional properties of DNA

Institute of Molecular Genetics of Russian Academy of Science

Moscow, Russia
09/1991-08/1995

Intern — Frank-Kamenetskii Research Group

- Brownian dynamics simulations of diffusional polymer cyclization
- Alignment of DNA images for Electron Microscopy mapping
- Electron microscopy of specific DNA-ligand binding

Teaching Experience

Visiting Assistant Professor — Michigan Technological University (2007-2008)

- Teaching and grading Statistical Mechanics and Solid State Physics
- Supervising a senior project for a Physics-major student

Graduate Supervisor — University of California, San Diego (2002-2003)

- Guided a graduate student project on solution and visualization of Poisson-Boltzmann equation for small molecule docking studies.

Teaching Assistant — New York University (1995-2000)

- Instructed laboratory and recitation sessions for College Chemistry I and II. Graded exams, homeworks, and laboratory reports.

Awards and Honors

- Merck New Jersey Reward & Recognition Awardee (2013).
- Participant in the NSF-funded Proteomics program, IPAM UCLA (2004).
- M.S. diploma with excellence, cum laude (1994).

Additional Skills

- Statistical methods and numerical methods
- C/C++ and Fortran programming, parallel programming with MPI
- Matlab and R
- Linux, UNIX, and Windows environment

Software Development

- CRANKITE: a suite for polypeptide backbone conformation sampling
- jfm2full: a calculator for DNA cyclization probability

References

- **David L. Wild**, Ph.D., Molecular Biophysics, University of Oxford; Professor, Warwick Systems Biology Centre, University of Warwick.
- **J. Andrew McCammon**, Ph.D., Chemical Physics, Harvard University; Investigator, Howard Hughes Medical Institute; Joseph E. Mayer Professor of Theoretical Chemistry, Professor of Pharmacology, UCSD.
- **Alexander V. Vologodskii**, Ph.D., Moscow Institute of Physics and Technology, D.S., Moscow State University; Research Professor, Department of Chemistry, NYU.
- **Frederic D. Bushman**, Ph.D., Cellular and Developmental Biology, Harvard University; Professor, Department of Microbiology, University of Pennsylvania School of Medicine.
- **Zoubin Ghahramani**, Ph.D., Cognitive Neuroscience, Massachusetts Institute of Technology; Professor in Information Engineering, University of Cambridge.

(Contact information is available upon request)

Publications

1. E. S. Arnardottir, E. V. Nikonova, K. R. Shockley, **A. A. Podtelezhnikov**, et al. Blood-gene expression reveals reduced circadian rhythmicity in individuals resistant to sleep deprivation, *Sleep* **37** 1589-1600 (2014).
2. B. Zhang, C. Gaiteri, L-G. Bodea, Zh. Wang, J. McElwee, **A. A. Podtelezhnikov**, et al. Integrated systems approach identifies genetic nodes and networks in late-onset Alzheimer's disease, *Cell* **153**, 707-720 (2013).
3. A. Bernard, L. S. Lubbers, K. Q. Tanis, R. Luo, **A. A. Podtelezhnikov**, et al. Transcriptional architecture of the primate neocortex, *Neuron* **73**, 1083-1099 (2012).
4. I. Krop, T. Demuth, T. Guthrie, et al., **A. Podtelezhnikov**, et al. Phase I pharmacologic and pharmacodynamic study of the gamma secretase (Notch) inhibitor MK-0752 in adult patients with advanced solid tumors, *JCO* **30** 2307-2313 (2012).
5. **A. A. Podtelezhnikov**, K. Q. Tanis, M. Nebozhyn, W. J. Ray, D. J. Stone and A. P. Loboda. Molecular insights into the pathogenesis of Alzheimer's disease and its relationship to normal aging, *PLoS ONE* **6** e29610 (2011).
6. A. McCampbell, K. Wessner, M. W. Marlatt, C. Wolffe, D. Toolan, **A. Podtelezhnikov**, et al. Induction of Alzheimer.s-like changes in brain of mice expressing mutant APP fed excess methionine, *J. Neurochem.* **116**, 82-92 (2011).
7. **A. A. Podtelezhnikov** and D. L. Wild. Reconstruction and stability of the secondary structure elements in the context of protein structure prediction, *Biophysical Journal* **96**, 4399-4408 (2009).

8. **A. A. Podtelezhnikov** and D. L. Wild. Comment on "Efficient Monte Carlo trial moves for polypeptide simulations" [J. Chem. Phys. 123, 174905 (2005)], *J. Chem. Phys.* **129**, 027103 (2008).
9. **A. A. Podtelezhnikov** and D. L. Wild. CRANKITE: A Fast Polypeptide Backbone Conformation Sampler, *Source Code Biol. Med.* **3**, 12 (2008).
10. **A. A. Podtelezhnikov**, Z. Ghahramani, D. L. Wild. Learning about protein hydrogen bonding by minimizing contrastive divergence, *Proteins* **66**, 588-599 (2007).
11. W. Chu, Z. Ghahramani, **A. Podtelezhnikov**, D. L. Wild. Bayesian segmental models with multiple sequence alignment profiles for protein secondary structure and contact map prediction, *IEEE/ACM Trans. Comp. Biol. Bioinformatics* **3**, 98-113 (2006).
12. **A. A. Podtelezhnikov** and D. L. Wild. Exhaustive Metropolis Monte Carlo sampling and analysis of polyalanine conformations adopted under the influence of hydrogen bonds, *Proteins* **61**, 94-104 (2005).
13. **A. A. Podtelezhnikov**, K. Gao, F. D. Bushman and J. A. McCammon. Modeling HIV-1 integrase complexes based on their hydrodynamic properties, *Biopolymers* **68**, 110-120 (2003).
14. A. V. Vologodskii, W. T. Zhang, V. V. Rybenkov, **A. A. Podtelezhnikov**, D. Subramanian, J. D. Griffith, N. R. Cozzarelli. Mechanism of topology simplification by type II DNA topoisomerases, *Proc. Natl. Acad. Sci. U.S.A.* **98**, 3045-3049 (2001).
15. **A. A. Podtelezhnikov**, C. Mao, N. C. Seeman and A. V. Vologodskii. Multimerization-cyclization of DNA fragments as a method of conformational analysis, *Biophysical Journal* **79**, 2692-2704 (2000).
16. **A. A. Podtelezhnikov** and A. V. Vologodskii. Dynamics of small loops in DNA molecules, *Macromolecules* **33**, 2767-2771 (2000).
17. **A. A. Podtelezhnikov**, N. R. Cozzarelli and A. V. Vologodskii. Equilibrium distributions of topological states in circular DNA: interplay of supercoiling and knotting, *Proc. Natl. Acad. Sci. U.S.A.* **96**, 12974-12979 (1999).
18. A. S. Krasilnikov, **A. Podtelezhnikov**, A. Vologodskii and S. M. Mirkin. Large-scale effects of transcriptional DNA supercoiling in vivo, *J. Mol. Biol.* **292**, 1149-1160 (1999).
19. **A. A. Podtelezhnikov** and A. V. Vologodskii. Simulations of polymer cyclization by Brownian Dynamics, *Macromolecules* **30**, 6668-6673 (1997).
20. **A. A. Podtelezhnikov**, A. V. Kurakin, A. V. Vologodskii and D. I. Cherny. Testing the quality of electron microscope mapping data for DNA molecules with sequence-specific ligands, *Micron* **25**, 439-446 (1994).

Invited Presentations

1. **A. A. Podtelezhnikov**. Learning about Protein Energetics by Minimizing Contrastive Divergence. Machine learning in Structural Bioinformatics, Copenhagen Denmark, April 2008.
2. **A. A. Podtelezhnikov**. Polypeptide sampling, protein structure prediction, and contrastive divergence, presented at Proteomics Reunion Conference IPAM, Lake Arrowhead CA, December 2005.
3. **A. A. Podtelezhnikov**. Polypeptide sampling, knowledge-based potentials, and protein structure prediction, presented at Gatsby Computational Neuroscience Unit UCL, London UK, October 2005.
4. **A. A. Podtelezhnikov**. Molecular dynamics vs Brownian dynamics vs Monte Carlo methods: pros and cons, presented at Proteomics Culminating Conference IPAM, Lake Arrowhead CA, June 2004.

Conference Abstracts

1. **A. A. Podtelezhnikov**, K. Q. Tanis, D. J. Stone, A. P. Loboda. Accelerated aging and metabolic disruption in the brain provide the basis for Alzheimer's disease progression modeling. *Alzheimer's &*

Dementia 6 (Suppl.): e28 (2010) — International Conference on Alzheimer's Disease, Honolulu HI, July 10 - 15, 2010.

2. **A. A. Podtelezhnikov**, Z. Ghahramani, D. L. Wild. Learning about hydrogen bonding by minimizing contrastive divergence. An Isaac Newton Institute Workshop, Camdridge UK, October 30 - November 3, 2006.
3. **A. A. Podtelezhnikov**, Z. Ghahramani, D. L. Wild. Contrastive divergence learning of hydrogen bonding and side-chain interactions in proteins using Metropolis Monte Carlo. An Isaac Newton Institute Workshop, Camdridge UK, December 11 - December 15, 2006.
4. **A. A. Podtelezhnikov**, K. Gui, F. Bushman, J. A. McCammon. Modeling HIV-1 integrase complexes based on their electrostatic and hydrodynamic properties. *Protein Science* 11 (Suppl. 1): A541-A541 (2002) — 16th Symposium of the Protein Society, San Diego CA, August 17-21, 2002.
5. **A. Podtelezhnikov** and A. Vologodskii. Thermodynamics and kinetics of DNA loop formation studied by computer simulations. *Biophysical Journal* 76 (1): A316-A316 Part 2 (1999) — 43rd Annual Biophysical Society Meeting, Baltimore MD, February 13-17, 1999.
6. **A. A. Podtelezhnikov** and A. V. Vologodskii. Analysis of multimerization-cyclization of short bent DNA fragments. Efficient method of calculation of J-factors. — Gordon Research Conference on Biopolymers, Newport RI, June 14-19, 1998.
7. **A. A. Podtelezhnikov** and A. V. Vologodskii. Structural interpretation of the cyclization kinetics of bent DNA fragments. 1. Extraction of the J-factor. *Biophysical Journal* 74 (2): A287-A287 Part 2 (1998) — 42nd Annual Biophysical Society Meeting, Kansas City MO, February 22-26, 1998.
8. **A. Podtelezhnikov** and A. Vologodskii. Simulations of DNA Cyclization by Brownian Dynamics. *J. Biomol Struct. Dyn.* (1997) — 10th Conversation in the Discipline Biomolecular Stereodynamics, Albany NY, June 17-21, 1997.