E. Prabhu Raman prabram@gmail.com

Education

- **George Mason University** — Fairfax, VA, USA
  Ph.D., Computational Biology (Advisor: Dmitri Klimov) — *Aug. 2002 - Oct 2008*
- **Birla Institute of Technology and Science** — Pilani, India
  M.Sc.(Hons.), Mathematics — *Aug. 1998 - May 2002*

Research Interests

- Computational study of biomolecular recognition
- Method development for computer-aided drug design
- Molecular mechanics force-field development
- Cheminformatics, Bioinformatics

Research Experience

- **Univ. of Maryland** — Baltimore, MD, USA
  Postdoctoral Research with Alexander D. MacKerell, Jr. — *Nov 2008 – present*
  - Developed statistical thermodynamics based methods to model molecular recognition and solvation [Papers 1, 9]
  - Developed efficient methods for computer aided drug design (CADD) and fragment based drug design (FBDD) [Papers 8,12,15] which also contributed to setup a start-up company (SilcsBio http://silcsbio.com/)
  - Developed and deployed CADD software for novel methods in academic and industrial settings
  - Worked with multiple teams from small and large pharmaceutical companies in CADD projects (papers in preparation)
  - Optimized lead small molecule inhibitors in multiple academic drug discovery projects [Papers 3,11]
  - Developed Molecular mechanics force-fields for biomolecules and pharmaceuticals [Papers 10,13,18]
- **George Mason Univ.** — Fairfax, VA, USA
  Doctoral Research with Dmitri K. Klimov — *Jan 2005 – Oct 2008*
  - Investigated peptide aggregation and its inhibition [Papers 21,22]
  - Investigated multi-domain protein folding. Developed coarse grained models for proteins [Paper 23]
  - Developed molecular simulation software (molecular dynamics and Monte Carlo method)
- **George Mason Univ.** — Fairfax, VA, USA
  Graduate Research with John J. Grefenstette — *May 2006 – Aug 2008*
  - Implemented machine learning and bioinformatics methods (Perl) to interpret biological sequence related patent documents. A knowledgebase called 'Patomics' was created
- **George Mason Univ.** — Fairfax, VA, USA
  Graduate Research with Iosif I. Vaisman — *Jan 2004 – Dec 2004*
  - Applied structural bioinformatics methods to study structures of proteins and protein-protein interfaces.
- **George Mason Univ.** — Fairfax, VA, USA
  Graduate Research with Curtis Jamison — *Aug 2002 – May 2004*
  - Analyzed DNA microarray data using statistical methods to identify differentially expressed genes in Osteoarthritis
- **Birla Institute of Technology and Science** — Pilani, India
  Undergraduate thesis with Ashis K. Das — *Jan 2002 – May 2002*
  - Thesis title: Finding genes using machine learning methods in the P. falciparum genome
- **Center for DNA Fingerprinting and Diagnostics** — Hyderabad, India
  Summer intern with H. A. Nagarajaram — *May 2001 – July 2001*
  - Designed and implemented a PCR primer generation algorithm in Java

Publications

1. **Raman EP*** and MacKerell AD Jr., "Spatial Analysis and Quantification of the Thermodynamic Driving Forces in Protein-Ligand Binding: Binding Site Variability", *J. Am. Chem. Soc. 2015 (in-press)* [***Corresponding Author**]

2. Lakkaraju SK, Yu W, **Raman EP**, Hershfeld A, Fang L, Deshpande, D, and MacKerell AD Jr., "Mapping Functional Group Free Energy Patterns at Protein Occluded Sites: Nuclear Receptors and G-Protein Coupled Receptors", *J. Chem. Inf. Model. 2015 (in-press)*

3. Samadani R, Zhang J, Brophy A, Oashi T, Priyakumar UD, **Raman EP**, St John FJ, Jung K-Y, Fletcher S, Pozharski E, MacKerell AD Jr., and Shapiro P, "Small Molecule Inhibitors of ERK-mediated Immediate Early Gene Expression and Proliferation of Melanoma Cells Expressing Mutated BRaf", *Biochemical Journal* 2015 (in-press)

4. Yu W, Lakkaraju SK, **Raman EP**, Fang L, and MacKerell AD Jr., "Pharmacophore modeling using Site-Identification by Ligand Competitive Saturation (SILCS) with multiple probe molecules", *J. Chem. Inf. Model. 2015 (in-press)*

5. Faller CE, **Raman EP**, MacKerell AD Jr. and Guvench O, "Site Identification by Ligand Competitive Saturation (SILCS) Simulations for Fragment-Based Drug Design", *Methods in Molecular Biology 2015 (in-press)*

6. Lakkaraju SK, **Raman EP**, Yu W, and MacKerell AD Jr., "Sampling of Organic Solutes in Aqueous and Heterogeneous Environments using Oscillating Excess Chemical Potentials in Grand Canonical-Like Monte Carlo-Molecular Dynamics Simulations", *J. Chem. Theor. Comput. 2014, 10(6), 2281*

7. Yu W, Lakkaraju SK, **Raman EP**, and MacKerell AD Jr., "Site-Identification by Ligand Competitive Saturation (SILCS) Assisted Pharmacophore Modeling", *J. Comput. Aided. Mol. Des. 2014, 28(5), 491*

8. **Raman EP**, Yu W, Lakkaraju SK, and MacKerell AD Jr., "Inclusion of multiple fragment types in the Site Identification by Ligand Competitive Saturation (SILCS) approach", *J. Chem. Inf. Model. 2013, 53(12), 3384*

9. **Raman EP*** and MacKerell AD Jr., "Rapid estimation of hydration thermodynamics of macromolecular regions", *J. Chem. Phys. 2013, 139(6), 055105* [***Corresponding Author**]

10. Vanommeslaeghe K, **Raman EP**, MacKerell AD Jr., "Automation of the CHARMM General Force Field (CGenFF) II: Assignment of bonded parameters and partial atomic charges", *J. Chem. Inf. Model. 2012, 52(12), 3155*

11. McKnight LE, **Raman EP**, Bezawada P, Kudrimoti S, Wilder PT, Hartman KG, Toth EA, Coop A, MacKerell AD Jr., Weber DJ "Structure-based discovery of a novel Pentamidine-related inhibitor of the calcium binding protein S100B", *ACS Med. Chem. Lett. 2012, 3(12), 975*

12. **Raman EP**, Vanommeslaeghe K, MacKerell AD Jr., "Site-Specific fragment identification guided by single-step free energy perturbation calculations", *J. Chem. Theor. Comput. 2012, 8(10), 3513*

13. Guvench O, Mallajosyula SS, **Raman EP**, Hatcher E, Vanommeslaeghe K, Foster TJ, Jamison FW 2nd, Mackerell AD Jr. "CHARMM additive all-atom force field for carbohydrate derivatives and its utility in polysaccharide and carbohydrate-protein modeling", *J. Chem. Theor. Comput. 2011, 7(10), 3162*

14. Abel S, Dupradeau FY, **Raman EP**, MacKerell AD Jr., Marchi M. "Molecular simulations of dodecyl-β-maltoside micelles in water: influence of the headgroup conformation and force field parameters", *J. Phys. Chem. B 2011, 115(3), 487*

15. **Raman EP**, Yu W, Guvench O, Mackerell AD Jr., "Reproducing crystal binding modes of ligand functional groups using Site-Identification by Ligand Competitive Saturation (SILCS) simulations", *J. Chem. Inf. Model. 2011, 51(4), 877*

16. Oashi T, Ringer AL, **Raman EP**, MacKerell AD Jr. "Automated selection of compounds with physicochemical properties to maximize bioavailability and druglikeness", *J. Chem. Inf. Model. 2011, 51(1), 148*

17. Takeda T, Kumar R, **Raman EP**, Klimov DK "Nonsteroidal anti-inflammatory drug naproxen destabilizes A amyloid fibrils: a molecular dynamics investigation", *J. Phys. Chem. B 2010, 114(46), 15394*

18. **Raman EP**, Guvench O, Mackerell AD Jr., "CHARMM additive all-atom force field for glycosidic linkages in carbohydrates involving furanoses", *J. Phys. Chem. B 2010, 114(40), 12981*

19. Takeda T, Chang WE, **Raman EP**, Klimov DK "Binding of nonsteroidal anti-inflammatory drugs to Abeta fibril", *Proteins 2010, 78(13), 2849*

20. Chang WE, Takeda T, **Raman EP**, Klimov DK "Molecular dynamics simulations of anti-aggregation effect of ibuprofen", *Biophys. J. 2010, 98(11), 2662*

21. **Raman EP**, Takeda T, Klimov DK "Molecular dynamics simulations of Ibuprofen binding to Abeta peptides", *Biophys. J. 2009, 97(7), 2070*

22. **Raman EP**, Takeda T, Barsegov V, Klimov DK "Mechanical unbinding of abeta peptides from amyloid fibrils", *J. Mol. Biol. 2007, 373(3), 785*

23. **Raman EP**, Barsegov V, Klimov DK "Folding of tandem-linked domains", *Proteins 2007, 67(4), 795*

Patents

- MacKerell AD Jr., **Raman EP** "Site-Specific fragment identification guided by single-step free energy perturbation calculations", *2013, WIPO Patent Application WO 2013/142630 A1*
- MacKerell AD Jr., **Raman EP**, Lakkaraju SK "Methods and Systems for Organic Solute Sampling of Aqueous and Heterogeneous Environments", *2014, US Provisional Patent Application 61/932,890*

Prefessional Service

1. Peer-reviewer for *J. Chem. Inf. Model., PLoS Comput. Biol., PLoS One, Proteins: Struct. Func. Bioinf., J. Mol. Graph. Model., J. Mol. Model.,Int. J. Mol. Sci.* and *J. Computer-Aided Mol. Des.*

2. Presided over the session on Molecular Mechanics, *ACS national meeting*, Aug. 2012

Invited Talks and Posters

1. Quantifying the Thermodynamic Molecular Driving Forces in Protein-Ligand Binding, *Poster at Biophysical Society meeting*, Feb. 2015

2. Computer Aided Drug Design, *Talk at the Univ. of Maryland Cancer Center's Experimental Therapeutics Retreat*, Jun. 2014

3. Additive and polarizable force fields and enhanced sampling methods for MD simulations of carbohydrates, *Talk at NIH and FDA Glycosciences Research Day*, Bethesda, May 2014

4. Computational studies of Molecular Recognition and Applications in Drug Design, *Talk at the Institute of Mathematics Sciences, Chennai, India*, Dec. 2012

5. Computational studies of Molecular Recognition and Applications in Drug Design, *Talk at the Indian Institute of Chemical Technology, Hyderabad, India*, Dec. 2012

6. Use of single-step free energy perturbation to estimate binding affinity by fragment modification, *Talk at ACS national meeting*, Aug. 2012

7. Single-step free energy perturbation for estimating binding affinity by fragment modification, *Poster presentation at ACS Mid-atlantic regional meeting*, May. 2012

8. Protein affinity pattern calculations using protein-fragment site identification by ligand competitive saturation, *Talk at the 55th annual Biophysical Society meeting*, Mar. 2011

9. Search for inhibitors of the S100β-p53 interaction, *Poster presentation at the 238th national ACS meeting*, Aug. 2009

10. MD Simulations of Force-Induced Unbinding of Aβ Peptides from Amyloid Fibrils, *Poster presentation at the 52nd annual Biophysical Society meeting*, Feb. 2008

11. Does linkage of protein domains in tandems have any effect on folding?, *Poster presentation at the 21st annual Protein Society symposium*, Jul. 2007

Teaching Experience

- **Graduate level "Molecular Biophysics" course, Univ. of Maryland** Feb 2015
  Delivered 2 guest lectures
- **Graduate level "Bioinformatics" course, GMU** Aug 2007 – May 2008
  Delivered 2 guest lectures
- **Undergraduate level statistics course, GMU** Aug 2005 – May 2006
  Extensive involvement of 4 lectures per week involving problem solving
- **Computational biology course, BITS-Pilani** Jan 2002 – May 2002
  Teaching assistant

Technical Skills

Programming: Developed software in C++, Fortran and Python. Proficient in Perl, and UNIX Shell scripting. Experience working with and integrating open source APIs into custom applications (eg. OpenBabel, RDKit, OpenMM, APBS)

Educational Background: computational biophysics/chemistry, statistical mechanics, computational biology, bioinformatics, mathematics, statistics

Software: CHARMM, GROMACS, NAMD, Gaussian, VMD, UCSF Dock, Autodock, Discovery Studio, Pipeline Pilot, MOE, MODELLER, Matlab, R, MySql DB

References

Available on request.