Ravinder Abrol

Research Scientist II Faculty (Professorial), **Email:** abrolr@csmc.edu

Department of Medicine and Department of BioMedical Sciences, Cedars-Sinai Medical Center
Los Angeles, CA 90048; **Phone:** 1-(310)-423-0124 (Work); 1-(626)-320-4987 (Cell)

EDUCATION

Postdoctoral Fellow	**California Institute of technology, Pasadena, CA** Division of Chemistry and Chemical Engineering	2005-2006
	IBM Thomas J. Watson Research Center, NY Theory and Computation Group	2003-2005
Ph.D. Chemistry	**California Institute of technology, Pasadena, CA** Division of Chemistry and Chemical Engineering	2003
M.Sc. Chemistry	**Indian Institute of Technology, Kanpur, India** Department of Chemistry	1995
B.Sc. (Honors) Chemistry	**Hans Raj College, University of Delhi, India** Department of Chemistry	1993

AWARDS & HONORS

Travel Fellowship for the 3rd Annual NIH Roadmap Membrane Protein Production and Technologies Meeting at La Jolla, CA	2010
Mariwala Trust Travel Scholarship for studying abroad	1995
Best Research Thesis Award for M.Sc. Chemistry from IIT Kanpur	1995
Jawahar Lal Nehru Summer Research Fellowship of the J. N. Center for Advanced Scientific Research for research work at Indian Institute of Science, Bangalore	1993-1995
Academic Proficiency Award from IIT Kanpur	1994
Science Academic Award from University of Delhi	1992
Swaroop Ratan Memorial Scholarship for Academic Excellence	1992

PROFESSIONAL & RESEARCH EXPERIENCE

Research Scientist II Faculty, Department of Medicine and Department of BioMedical Sciences, Cedars-Sinai Medical Center	12/2012-Current
Director of BioMolecular Simulations Group and Senior Scientist, Caltech	2006-2012
Postdoctoral Scholar in Chemistry at California Institute of Technology	2005-2006
Postdoctoral Research Fellow at IBM Thomas J Watson Research Center	2003-2005
Ph.D. Student at California Institute of Technology	1995-2002
Research Assistant at Indian Institute of Technology Kanpur	1995
Summer Research Fellow at Indian Institute of Science	1994
Independent Research at University of Delhi	1992-1993

OTHER PROFESSIONAL ACTIVITIES

NIH Study Sections

Adhoc Reviewer for Molecular and Integrative Signal Transduction (MIST)	2014-Current
Reviewer for Biological Chemistry, Biophysics, and Drug Discovery	2012-2013

Research Journal Editorial Boards

Associate Editor for *Frontiers in Physiology*	2012-Current
Editorial Board of the Journal of Biophysics	2013-Current

Research Journal Reviewer

Acta Pharmaceutica Sinica B
Biochemical and Biophysical Research Communications
Chemical Physics Letters
Current Protein and Peptide Science
Frontiers in Physiology
International Journal of Molecular Sciences
Journal of the American Chemical Society
Journal of Molecular Graphics and Modelling
Methods
Molecular Oncology
Pancreas
PLoS One

Seminar Series

Co-Chair of the Chemical Physics Seminar Series at Caltech	1998-2000

MENTORING

I enjoy training the next generation of scientists (postdocs, graduate, undergraduates, and high school students) in research methods, computational biochemistry & molecular biology, cellular signaling, G protein-coupled receptors, and use of modeling to probe the molecular basis of disease.

PROFESSIONAL MEMBERSHIPS

American Chemical Society	2003-
Protein Society	2012-
American Pancreatic Association	2014-

COMMUNITY ACTIVITIES

Protein Society 28th Annual Symposium (San Diego) Poster Session Judge	2014
Caltech Summer Undergraduate Research Seminar Day, Biology Session Chair	2014
Intel International Science Fair, Biochemistry Judge	2014
California State Science Fair, Biochemistry and Molecular Biology Judge	2013, 2014
Caltech Summer Undergraduate Research Fellowship Proposal Reviewer	2013
Protein Society 27th Annual Symposium (Boston) Abstract Reviewer	2013
Chemistry Member of the College Science Quiz Team at University of Delhi	1992,1993
Founding Member of the Budding Chemists' Society at University of Delhi	1992

RESEARCH PUBLICATIONS

Community-Wide Effort Papers

48. "Low-frequency and rare exome chip variants associate with fasting glucose and type 2 diabetes susceptibility"; Wessel J et al. (**2015**). *Nature Commun,* **6**:5897. **[PMID: 25631608]**

47. "Advances in GPCR modeling evaluated by the GPCR Dock 2013 assessment: meeting new challenges"; Kufareva I, et al. (**2014**). *Structure*, **22**(8):1120-39. **[PMID: 25066135]**

46. "Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment"; Kufareva I et al. (**2011**). *Structure*, **19**(8):1108-26. **[PMID: 21827947]**

45. "Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008"; Michino M et al. (**2009**). *Nature Rev Drug Discov*, **8**(6):455-63. **[PMID: 19461661]**

Journal Articles and Invited Chapters

44. "The Predicted Ensemble of Low Energy Conformations of Human Somatostatin Receptor Subtype 5 and the Binding of Antagonists"; Dong S, **Abrol R**, Goddard WA 3rd (**2015**). *ChemMedChem*, **Accepted for publication**.

43. "The interaction of N-glycans in Fcγ receptor I α-chain with Escherichia coli K1 outer membrane protein A for entry into macrophages: experimental and computational analysis"; Krishnan S, Liu F, **Abrol R**, Hodges J, Goddard WA 3rd, Prasadarao NV (**2014**). *J Biol Chem*, **289**(45):30937-49. **[PMID: 25231998]**

***42.** "Ligand- and mutation-induced conformational selection in the CCR5 chemokine G protein-coupled receptor"; **Abrol R**, Trzaskowski B, Goddard WA 3rd, Nesterov A, Olave I, Irons C. (**2014**). *Proc Natl Acad Sci U S A*, **111**(36):13040-5. **[PMID: 25157173]**

41. "Down-regulation of pancreatic and duodenal homeobox-1 by somatostatin receptor subtype 5: a novel mechanism for inhibition of cellular proliferation and insulin secretion by somatostatin"; Zhou G, Sinnett-Smith J, Liu SH, Yu J, Wu J, Sanchez R, Pandol SJ, **Abrol R**, Nemunaitis J, Rozengurt E, Brunicardi FC (**2014**). *Front Physiol.* **5**:226. **[PMID: 25009500]**

***40.** "SuperBiHelix method for predicting the pleiotropic ensemble of G-protein-coupled receptor conformations"; Bray JK, **Abrol R**, Goddard WA 3rd, Trzaskowski B, Scott CE (**2014**). *Proc Natl Acad Sci U S A*, **111**(1):E72-8. **[PMID: 24344284]**

39. "The Glove-like Structure of the Conserved Membrane Protein TatC Provides Insight into Signal Sequence Recognition in Twin-Arginine Translocation"; Ramasamy S, **Abrol R**, Suloway CJ, Clemons WM Jr (2013). *Structure*, 21(5):777-88. **[PMID: 23583035]**

38. "Use of G-protein coupled and uncoupled CCR5 receptors by CCR5 inhibitor-resistant and -sensitive human immunodeficiency virus type 1 variants"; Berro R, Yasmeen A, **Abrol R**, Trzaskowski B, Abi-Habib S, Grunbeck A, Lascano D, Goddard WA 3rd, Klasse PJ, Sakmar TP, Moore JP (**2013**). *J Virology*, **87**(12):6569-81. **[PMID: 23468486]**

37. "Computationally-predicted CB1 cannabinoid receptor mutants show distinct patterns of salt-bridges that correlate with their level of constitutive activity reflected in G protein coupling levels, thermal stability, and ligand binding"; Ahn KH, Scott CE, **Abrol R**, Goddard WA 3rd, Kendall DA (**2013**). *Proteins: Struc Func Bioinf*, **81**(8):1304-17. **[PMID: 23408552]**

***36.** "Conformational Ensemble View of G Protein-Coupled Receptors and the Effect of Mutations and Ligand Binding"; **Abrol R**, Kim SK, Bray JK, Trzaskowski B, Goddard WA 3rd (**2013**). *G Protein-Coupled Receptors (Methods in Enzymology)*, Ed. Conn PM (Elsevier, Oxford), **Vol.520**, pp. 31-48.

[PMID: 23332694]

***35.** "Molecular basis for dramatic changes in cannabinoid CB1 G protein-coupled receptor activation upon single and double point mutations"; Scott CE, **Abrol R**, Ahn KH, Kendall DA, Goddard WA 3rd (**2013**). *Protein Science*, **22**(1):101-13. **[PMID: 23184890]**

***34.** "Predicted Structure of Agonist-Bound Glucagon-Like Peptide 1 Receptor, a Class B G Protein-Coupled Receptor"; Kirkpatrick A, Heo J, **Abrol R**, Goddard WA 3rd (**2012**). *Proc Nat Acad Sci*, **109**(49):19988-93. **[PMID: 23169631]**

***33.** "Structure Prediction of G Protein-Coupled Receptors and Their Ensemble of Functionally Important Conformations"; **Abrol R**, Griffith AR, Bray JK, Goddard WA 3rd (**2012**). *Membrane Protein Structure: Methods and Protocols (Methods in Molecular Biology)*, Eds. Vaidehi N and Klein-Seetharaman J (Humana, New York), **Vol.914**, pp. 237-254. **[PMID: 22976032]**

32. "Identification and Characterization of an Activating F229V Substitution in the V2 Vasopressin Receptor in an Infant with NSIAD"; Carpentier E, Greenbaum LA, Rochdi D, **Abrol R**, Goddard WA 3rd, Bichet DG, Bouvier M. (**2012**). *J Am Soc Nephrol*, **23**(10):1635-40. **[PMID: 22956819]**

31. "The 3D structure prediction of TAS2R38 bitter receptors bound to agonists phenylthiocarbamide (PTC) and 6-n-Propylthiouracil (PROP)"; Tan J, **Abrol R**, Trzaskowski B, Goddard WA 3rd (**2012**). *J Chem Inf Model*, **52**:1875-85. **[PMID: 22656649]**

***30.** "Molecular basis for the interplay of apoptosis and proliferation mediated by Bcl-xL:Bim interactions in pancreatic cancer cells"; **Abrol R**, Edderkaoui M, Goddard WA 3rd, Pandol SJ (**2012**). *Biochem Biophys Res Commun*, **422**(4):596-601. **[PMID: 22609401]**

29. "Genetically Encoded Photo-cross-linkers Map the Binding Site of an Allosteric Drug on a G Protein-Coupled Receptor": Grunbeck A, Huber T, **Abrol R**, Trzaskowski B, Goddard WA 3rd, Sakmar TP (**2012**). *ACS Chem Biol*, **7**(6):967-72. **[PMID: 22455376]**

28. "First-Principles-Based Multiscale, Multiparadigm Molecular Mechanics and Dynamics Methods for Describing Complex Chemical Processes"; Jaramillo-Botero A, Nielsen R, **Abrol R**, Su J, Pascal TA, Mueller J, Goddard WA 3rd (**2012**). *Top Curr Chem.*, **307**:1-42. **[PMID: 21243466]**

***27.** "Characterizing and Predicting the Functional and Conformational Diversity of Seven-Transmembrane Proteins"; **Abrol R**, Kim SK, Bray JK, Griffith AR, Goddard WA 3rd (**2011**). *Methods*, **55**(4):405-14. **[PMID: 22197575]** (**Invited Article**)

***26.** "BiHelix: Towards de novo Structure Prediction of an Ensemble of G-Protein Coupled Receptor Conformations"; **Abrol R**, Bray JK, Goddard WA 3rd (**2012**). *Proteins: Struct Funct Bioinf*, **80**(2):505-18. **[PMID: 22173949]**

***25.** "G Protein-Coupled Receptors: Conformational *Gatekeepers* of Transmembrane Signal Transduction and Diversification"; **Abrol R**, Goddard WA 3rd (**2011**), in *Extracellular and Intracellular Signaling*, Eds. JD Adams and KK Parker; pp.188-229 (RSC).

24. "Structure-based prediction of subtype-selectivity of Histamine H3 receptor selective antagonists in the clinical trials"; Kim SK, Fristrup P, **Abrol R**, Goddard WA 3rd (**2011**). *J Chem Inf Model*, **51**(12):3262-74. **[PMID: 22035233]**

23. "Novel Purine-Based Fluoroaryl-1,2,3-Triazoles as Neuroprotecting Agents: Synthesis, Neuronal Cell Culture Investigations, and CDK5 Docking Studies"; Nair N, Kudo W, Smith MA, **Abrol R**, Goddard WA 3rd, Reddy VP (**2011**). *Bioorg Med Chem Lett*, **21**:3957-61. **[PMID: 21641213]**

22. "Elucidating glycosaminoglycan-protein-protein interactions using carbohydrate microarray and computational approaches"; Rogers CJ, Clark PM, Tully SE, **Abrol R**, Garcia KC, Goddard WA 3rd, Hsieh-Wilson LC (**2011**). *Proc Natl Acad Sci U S A*, **108**(24):9747-52. **[PMID: 21628576]**

21. "Predicted structures of agonist and antagonist bound complexes of adenosine A3 receptor", Kim SK, Riley L, **Abrol R**, Jacobson KA, Goddard WA 3rd (**2011**). *Proteins: Structure, Function, and Bioinformatics*, **79**(6):1878-97. **[PMID: 21488099]**

20. "Predicted Structures and Dynamics for Agonists and Antagonists Bound to Serotonin 5-HT2B and 5- HT2C Receptors"; Kim SK, Li Y, **Abrol R**, Heo J, Goddard WA 3rd (**2011**). *J Chem Inf Model*, **51**(2):420-33. **[PMID: 21299232]**

19. "Experimental validation of the predicted binding site of Escherichia coli K1 outer membrane protein A to human brain microvascular endothelial cells: identification of critical mutations that prevent E. coli meningitis"; Pascal TA, **Abrol R**, Mittal R, Wang Y, Prasadarao NV, Goddard WA 3rd (**2010**). *J Biol Chem*, **285**(48):37753-61. **[PMID: 20851887]**

18. "Prediction of the three-dimensional Structure for the Rat Urotensin II G-Protein-Coupled Receptor and Comparison of the Antagonist Binding Sites and Binding Selectivity between Human and Rat from Atomistic Simulations"; Kim SK, Li Y, Park C, **Abrol R**, Goddard WA 3rd (**2010**). *ChemMedChem*, **5**(9):1594-608. **[PMID: 20683923]**

17. "Predicted 3D structures for adenosine receptors bound to ligands: Comparison to the crystal structure"; Goddard WA 3rd, Kim SK, Li Y, Trzaskowski B, Griffith AR, **Abrol R** (**2010**). *J Struct Biol*, **170**(1):10-20. **[PMID: 20079848]**

16. "Rottlerin Stimulates Apoptosis in Pancreatic Cancer Cells through Interactions with Proteins of the Bcl-2 Family"; Ohno I, Eibl G, Odinokova IV, Edderkaoui M, Damoiseaux RD, Yazbec M, **Abrol R**, Goddard WA 3rd, Yokosuka O, Pandol SJ, Gukovskaya AS (**2010**). *Am J Physiol Gastrointest Liver Physiol*, **298**(1):G63-73. **[PMID: 19762431]**

15. "Multiscale-Multiparadigm Modeling and Simulation of Nanometer Scale Systems and Processes for Nanomedical Applications"; Jaramillo-Botero A, **Abrol R**, van Duin A, Goddard WA 3rd (**2009**) in *Nanomedicine: A Systems Engineering Approach*, Eds. M. Zhang and N. Xi; Pan Stanford Publishing, pp. 245-300. **[PMID: 21243466]**

14. "Nonadiabatic effects in the H + H2 exchange reaction: accurate quantum dynamics calculations at a state-to-state level"; Chu TS, Han KL, Hankel M, Balint-Kurti GG, Kuppermann A, **Abrol R** (**2009**). *J Chem Phys*, **130**(14):144301. **[PMID: 19368439]**

13. "Computational studies of the structure and function of two lipid-activated GPCRs"; Niemer RK, **Abrol R**, Goddard WA 3rd (**2008**). *J Recept Sig Transd*, **28**(1-2), 138-139.

12. "3-Dimensional Structures of G-Protein Coupled Receptors and Binding Sites of Agonists and Antagonists"; Goddard WA 3rd, **Abrol R** (**2007**). *J Nutr*, **137**(6 Suppl 1):1528S-1538S. **[PMID: 17513420]**

11. "Geometric phase effects in H3 predissociation"; Lepetit B, **Abrol R**, Kuppermann A (**2007**). *Phys Rev A*, 040702(R).

10. "Predictions of CCR1 Chemokine Receptor Structure and BX471 Antagonist Binding Followed by Experimental Validation"; Vaidehi N, Schlyer S, Trabanino RJ, Floriano WB, **Abrol R**, Sharma S, Kochanny M, Koovakat S, Dunning L, Liang M, Fox JM, de Mendonca FL, Pease JE, Goddard WA 3rd, Horuk R (**2006**). *J Biol Chem*, **281**(37):27613-20. **[PMID: 16837468]**

9. "Biological Chiral Recognition: A Substrate's Perspective"; Sundaresan V, **Abrol R** (**2005**). *Chirality*, **17**(Suppl):S30-9. **[PMID: 15736174]**

8. "Multiple potential energy surface quantum reaction dynamics"; Kuppermann A, **Abrol R** (**2004**). *Nonadiabatic Transitions in Quantum Systems*, Eds. Osherov VI and Ponomarev LI (IPCP, Chernogolovka), pp.10.

7. "Towards a general model for protein-substrate stereoselectivity"; Sundaresan V, **Abrol R** (**2002**). *Protein Sci*, **11**(6): 1330-9. **[PMID: 12021432]**

6. "Quantum reaction dynamics for multiple electronic states"; Kuppermann A, **Abrol R** (**2002**). *The Role of Degenerate States in Chemistry: A Special Volume of Advances in Chemical Physics*, Eds. Baer M and Billing GD, **124**:283-322.

5. "An optimal adiabatic to diabatic transformation of the 1^2A' and 2^2A' states of H3"; **Abrol R**,Kuppermann A (**2002**). *J Chem Phys*, **116**(3):1035-62.

4. "Accurate First-Derivative Non-adiabatic Couplings for the H3 system"; **Abrol R**, Shaw A, Yarkony DR, Kuppermann A (**2001**). *J Chem Phys*, **115**(10):4640-59.

3. "A Quantum and Semiclassical Study of Dynamical Resonances in C + NO -> CN + O Reaction"; **Abrol R**, Wiesenfeld L, Lambert B, Kuppermann A (**2001**). *J Chem Phys*, **114**(17):7461-70.

2. "Reduced Potential Energy Curves for Diatomic Molecules and their respective Cations"; **Abrol R**, Harbola M, and Sathyamurthy N (**1999**). *Chem Phys Lett*, **312**(2):341-5.

***1.** "Computation of Vapor Pressure"; **Abrol R** (**1995**). *J Chem Ed*, **72**(12):1083-5.

* Corresponding Author

PRESENTATIONS and INVITED TALKS

1. **Poster** titled "Activation hot spot residues in GPCRs and their role in structure, function, and disease", *Molecular Pharmacology Gordon Research Conference*, Ventura, **2015**.
2. **Seminar** titled "Conformational Landscape Governing the Constitutive Activity of G Protein Coupled Receptors", *Department of Pharmacology Seminar Series*, *University of North Texas Health Sciences Campus*, Fort Worth, **2014**.
3. **Seminar** titled "Computational Chemistry and Molecular Biophysics: Modeling of Proteins, Drug Binding, and Biological Processes", *Molecular Therapeutics Interest Group Inaugural Seminar* at CSMC, Los Angeles, **2014**.
4. **Poster** titled "Conformational Landscape Governing the Constitutive Activity of GPCRs", *Protein Society 28th Annual Symposium*, San Diego, **2014**.
5. **Poster** titled "Towards a Structural Basis for the Constitutive Activity of GPCRs", *GPCR KeyStone Meeting*, Salt Lake City, **2014**.
6. **Invited Seminar** titled "A Theoretical Chemist's Gentle Foray into Biology", **Ravinder Abrol**, *Bill Goddard's 77th Birthday Symposium*, Pasadena, **2014**.
7. **Seminar** titled "Emerging role of bitter taste receptors in curing type 2 diabetes", 14th International Conference of Functional Foods Center on Functional Foods and Bioactive Compounds in the Management of Chronic Inflammation: Science and Practical Application, Los Angeles, **2013**.
8. **Seminar** titled "Advances in GPCR Structure Prediction to Understand their Signaling", *MSC Conference*, Pasadena, **2013.**
9. **Poster** titled "Designing a Constitutively Active G Protein-Coupled Receptor Mutant from an Inactive One and Vice Versa", *Protein Society 26th Annual Symposium*, San Diego, **2012**.
10. **Invited Seminar** titled "Structure Prediction of G Protein-Coupled Receptors: Methodology and Application to TAS2R38 Bitter Taste Receptor", Pancreatic Research Group Meeting, UCLA/VA, Los Angeles, **2012**.
11. **Seminar** titled "Computational molecular biology at the MSC", *MSC Conference*, Pasadena,

2012.

12. **Seminar** titled "Prediction of GPCR conformational ensembles and their role in physiological function", *MSC Conference*, Pasadena, **2012.**
13. **Seminar** titled "Probing the activation landscape of human cannabinoid CB1 receptor", *MSC Conference*, Pasadena, **2012.**
14. **Seminar** titled "Role of TAS2R38 in the bitter-sweet story of GLP1 release", *MSC Conference*, Pasadena, **2012.**
15. **Seminar** titled "Bcl-2 protein family interactions control cell proliferation and apoptosis in pancreatic cancer", *MSC Conference*, Pasadena, **2012.**
16. **Poster** titled "Molecular basis for the dramatic changes in cannabinoid CB1 GPCR activation due to single and double point mutations", *GPCR KeyStone Meeting*, Banff, **2012**.
17. **Invited Seminar** titled "Predicting the Conformational Ensemble View of GPCR Structures and Ligand Binding", *Luedtke Lab at University of North Texas*, Fort Worth, **2011**.
18. **Seminar** titled "Overview of Computational Biology at the MSC", *MSC Conference*, Pasadena, **2011**.
19. **Seminar** titled "Predicting Ensemble View of GPCR Structures and Ligand Binding", *MSC Conference*, Pasadena, **2011**.
20. **Seminar** titled "CCR5 Receptor and Ligands against HIV", *MSC Conference*, Pasadena, **2011**.
21. **Seminar** titled "Bcl-X_L interactions in Apoptosis Pathways of Pancreatic Cancer", *MSC Conference*, Pasadena, **2011**.
22. **Poster** titled "Towards the Prediction of All Physiologically Important Conformations of a GPCR", *Molecular Pharmacology Gordon Research Conference*, Ventura, **2011**.
23. **Poster** titled "Towards the Prediction of All Physiologically Important Conformations of a GPCR", *3rd Annual NIH Roadmap Meeting on Membrane Protein Technologies*, La Jolla, **2010**.
24. **Poster** titled "Towards the Prediction of All Physiologically Important GPCR Conformations", *GPCR KeyStone Meeting*, Breckenridge, **2010**.
25. **Seminar** titled "GEnSeMBLE: Structure Prediction for GPCRs", *MSC Conference*, Pasadena, **2010**.
26. **Seminar** titled "DarwinDock: Towards Complete Sampling for Docking of Ligands to Proteins", *MSC Conference*, Pasadena, **2010**.
27. **Seminar** titled "Conformational Ensemble View of CCR5 Structure Prediction, Ligand Binding, and Mutagenesis Aimed at Blocking HIV Entry", *MSC Conference*, Pasadena, **2010**.
28. **Seminar** titled "Role of Bcl-2 Family Proteins in Emerging Apoptosis Models: Implications for Rational Design of Cancer Drugs", *MSC Conference*, Pasadena, **2010**.
29. **Seminar** titled "Overview of Progress in GPCR Structure Prediction and Rational Drug Design", *MSC Conference*, Pasadena, **2009**.
30. **Invited Seminar** titled "Role of Bcl-2 Family Proteins in Emerging Apoptosis Models: Implications for Rational Design of Cancer Drugs", Pancreatic Research Group Meeting, UCLA/VA, Los Angeles, **2008**.
31. **Seminar** titled "An Ensemble Approach to GPCR Structure Prediction: Methodology and Validation", *MSC Conference*, Pasadena, **2008**.
32. **Seminar** titled "Improved Methods for Predicting the Structure and Function of G Protein-Coupled Receptors", *MSC Conference*, Pasadena, **2007**.

33. **Poster** titled "Towards a structural basis for bitter-tastant selectivity of bitter-taste receptors", *Chemical Senses KeyStone Meeting*, Salt Lake City, **2007**.
34. **Seminar** titled "Full Lipid-Solvent Simulations of the Prediction for the BX471-hCCR1 Complex and Experimental Verification", *MSC Conference*, Pasadena, **2006**.
35. **Poster** titled "Chiral recognition in biological systems: A general model for protein-substrate stereoselectivity", *American Chemical Society Annual Meeting*, Philadelphia, **2004**.
36. **Poster** titled "Chiral recognition in biological Systems: A topological model for protein-ligand stereoselectivity", *18th Symposium of the Protein Society: Protein Structure, Function and Disease*, San Diego, **2004**.
37. **Poster** titled "Chiral recognition in biological systems: Beyond the Easson-Stedman-Ogston model", *16th International Symposium on Chirality*, New York, **2004**.
38. **Invited Seminar** titled "Quantum theory of nonadiabatic reaction dynamics", *Atmospheric Chemistry Research Group Meeting*, Caltech, Pasadena, **2002**.
39. **Poster** titled "Optimal diabatization of the lowest two electronic states of H_3", *Workshop on Quantum Reaction Dynamics*, California Institute of Technology, Pasadena, **2001**.
40. **Invited Seminar** titled "Quantum and semiclassical analysis of the C + NO system", *Conference on Hamiltonian Dynamics and Molecular Physics: Beyond Two Degrees of Freedom*, California Institute of Technology, Pasadena, **2000**.

RESEARCH GRANTS

Title: "Brain Endothelial Cell Receptor for Escherichia Coli"

NIH R01 PI: Nemani 7/2011 - 6/2016 **Role:** Co-Investigator

Use protein structural modeling to characterize the interaction between bacterial OmpA and host gp96, which will be used in turn to design therapeutics to treat and prevent neonatal meningitis.

Title: "**Maneuvering of Macrophage Function by Escherichia Coli K1**"

NIH R01 PI: Nemani 6/2010 - 5/2015 **Role:** Co-Investigator

Model the interaction between OmpA and CD64, to design novel therapeutics aimed at disrupting this interaction for treating and preventing neonatal meningitis.

Title: "Prediction of Structures and Agonist Ligands for a Class B GPCR"

Sanofi PIs: Abrol/Goddard 8/2011 - 7/2013 **Role:** PI

Use theory and computation to design small molecule agonist ligands for a class B GPCR.

Title: "A Novel Method of Nanoparticle Delivery to Brain by Targeting Ec-gp96"

NIH R01 PI: Davis 7/2010 - 6/2013 **Role:** Co-Investigator

Use theory and computation to design ligands for Ec-gp96 with different functional outcomes.

Title: "Prediction of Structures and Ligands for GPCRs"

PharmSelex Pharma PI: Abrol/Goddard 6/2008 - 12/2009 **Role:** PI

Use theory and computation to predict structure and ligand binding sites for GPCRs.

Title: GLP1 Receptor Modeling
Allozyne Pharma PI: Goddard 1/2007 – 6/2008 **Role:** Co-PI
Use theory and computation to predict structure and ligand binding sites for GLP1R, class B GPCR.

Title: Human CXCR3 Receptor Modeling
Boehringer-Ingelheim Pharma PI: Goddard 2/2008– 6/2008 **Role:** Co-PI
Use theory and computation to predict structure and ligand binding sites for CXCR3 receptor.

Title: Human Serotonin 2b,2c Receptor Modeling
Boehringer-Ingelheim Pharma PI: Goddard 2/2007 – 1/2008 **Role:** Co-PI
Use theory and computation to predict structure and ligand binding sites for serotonin receptors.

Title: "Subtype Specific Agonists for D1-D5 Dopamine Receptors"
NIH R21 PI: Goddard 2/2006 – 1/2008 **Role:** Co-PI
Predict structure and ligand binding sites for five Dopamine GPCRs.

TEACHING EXPERIENCE

CALTECH

- **Co-Instructor for Freshman Chemistry (2011-2012):** Coordinated all aspects of the course mechanics that includes managing ~15 TAs in charge of recitations or grading, class demos, course website, problem sets, preparing exams, and tracking student progress.
- **Atomic Level Simulations of Materials and Molecules (2006, 2008, 2010):** Gave lectures on structure prediction of soluble/membrane proteins and ligand docking.
- **Freshman Chemistry (1999-2000):** As a "supersection" recitation teaching assistant, taught advanced General Chemistry. Also, prepared and graded challenging problem sets different from the regular Freshman Chemistry course.
- **Freshman Chemistry (1997-1999):** As a tutor at the Minority Student Affairs Office, taught and guided a group of students through General Chemistry.
- **Advanced Topics in Chemical Physics (1998, 2000):** Assisted with the course, once on Quantum Dynamics and once on Semiclassical Dynamics.
- **Chemical Dynamics (1997):** As a teaching assistant, developed and graded assignments. Developed computational projects involving a quantum reactive scattering code.
- **The Elements of Quantum Chemistry (1996, 1997, 1998):** As a teaching assistant, developed and graded assignments and examinations.

Cedars-Sinai Medical Center

- As part of the Molecular Therapeutics Interest Group Lecture Series on Research Methods, I am developing a set of lectures on Computational Biology and Chemistry methods as applied to protein structure, molecular biology, cellular signaling, and drug discovery.
- Discussions underway with the CSMC Graduate Program to provide this series of lectures to first-year graduate students as a supplemental course.

PROFESSIONAL REFERENCES

1. **Prof. William A. Goddard III** [California Institute of Technology (Pasadena, CA)]
   Charles and Mary Ferkel Professor of Chemistry and Applied Physics
   Ph: 626-395-3093
   Email: wag@wag.caltech.edu

2. **Prof. Rudy A. Marcus** [California Institute of Technology (Pasadena, CA)]
   Arthur Amos Noyes Professor of Chemistry
   Ph: 626-395-6566
   Email: ram@caltech.edu

3. **Prof. Douglas C. Rees** [California Institute of Technology (Pasadena, CA)]
   Professor of Chemistry and Investigator, Howard Hughes Medical Institute
   Ph: 626-395-8393
   Email: dcrees@caltech.edu

4. **Prof. Debra A. Kendall** [University of Connecticut (Storrs, CT)]
   Board of Trustees Distinguished Professor of Molecular and Cell Biology
   Department Head of Pharmaceutical Sciences
   Ph: 860-486-1891
   Email: debra.kendall@uconn.edu

5. **Prof. Nemani Prasadarao** [Saban Research Institute, Children's Hospital (Los Angeles)]
   Professor of Infectious Diseases
   Ph: 323- 361-5465
   Email: pnemani@chla.usc.edu

6. **Prof. Bil Clemons** [California Institute of Technology (Pasadena, CA)]
   Professor of Biochemistry
   Ph: 626-395-1796
   Email: clemons@caltech.edu

7. **Prof. Robert Luedtke** [University of North Texas (Fort Worth, TX)]
   Professor of Pharmacology and Neuroscience
   Ph: 817-735-5124
   Email: robert.luedtke@unthsc.edu