DAVID C. CHATFIELD, CURRICULUM VITAE

Department of Chemistry & Biochemistry, Florida International University, Miami, FL 33199, (305) 348-3977, David.Chatfield@fiu.edu

EDUCATION

Degree	Institution	Field	Dates
Postdoctoral	National Institutes of Health Bethesda, MD	Computational Chemistry	1992-1995
Ph.D.	University of Minnesota Minneapolis, MN	Physical Chemistry	1986-1991
M.A.	Middlebury College Middlebury, VT	German	1982-1984
B.A.	Carleton College Northfield, MN	Chemistry	1976-1980

ACADEMIC EXPERIENCE

Institution	Rank/Office	Dates
Department of Chemistry & Biochemistry, FIU	Chair	2008-present
Department of Chemistry & Biochemistry, FIU	Associate Professor	2001-present
Department of Chemistry & Biochemistry, FIU	Assistant Professor	1995-2001

PUBLICATIONS IN DISCIPLINE (FIU students underlined; superscripts u, g, p indicate undergraduate student, graduate student, postdoctoral)

30. A.N. Morozov[p], J.P. Roach[u], M. Kotzer[u], and **D.C. Chatfield**, "A possible mechanism for redox control of human neuroglobin activity," J. Chem. Inf. Model. 54(7), 1997-2003 (2014), COVER ARTICLE.
29. R. Zhang[g], Q. He, **D.C. Chatfield**, and X. Wang, "Paramagnetic NMR Relaxation and Molecular Mechanics Studies of Chloroperoxidase-Indole Complex: Insights into the Mechanism of Chloroperoxidase-Catalyzed Regioselective Oxidation of Indole," Biochem. 52 (21) 3688-3701 (2013).
28. C. D'Cunha[g], A.N. Morozov[p], and **D.C. Chatfield**, "Theoretical study of role of water in aqueous keto-enol tautomerization of b-cyclopentanedione," J. Phys. Chem. A, 117 (35), 8437-8448 (2013).
27. A.N Morozov[p] and **D.C. Chatfield**, "Chloroperoxidase-Catalyzed Epoxidation of Cis-β-Methylstyrene: Distal Pocket Flexibility Tunes Catalytic Reactivity," J. Phys. Chem. B, 116, 12905-12914 (2012).
26. A.N. Morozov[p], C. D'Cunha[g], C.A. Alvarez[g], and **D.C. Chatfield**, "Enantiospecificity of Chloroperoxidase-catalyzed Expoxidation: Biased Molecular Dynamics Study of a Cis-b-methylstyrene/Chloroperoxidase-Compound I Complex," Biophys. J., 100(4), 1066-1075 (2011).
25. J.T. Landrum, **D.C. Chatfield**, A.A. Mebel, F. Alvarez-Calderon[u], M. Fernandez[g], "The conformation of end-groups is one determinant of carotenoid topology suitable for high fidelity molecular recognition: A study of b- and e-end-groups," Archives of Biochemistry and Biophysics, 493, 169-174 (2010).

24. D. Simovic[g], M. Di[g], V. Marks, **D.C. Chatfield**, K.S. Rein, "1,3-Dipolar Cycloadditions of Trimethylsilyldiazonomethane Revisited: Steric Demand of the Dipolarophile and the Influence on Product Distribution," J. Org. Chem. 72, 650-653 (2007).
23. E. Lewandowska, **D.C. Chatfield**, "Regioselectivity of Michael Additions to 3-(Pyridin-3-yl or Pyrimidin-2-yl)-propenoates and Their N-Oxides – Experimental and Theoretical Studies," Eur. J. Org. Chem. 3297-3303 (2005).
22. **D.C. Chatfield**, A. Augsten[u], and C. D'Cunha[g], "Correlation Times and Adiabatic Barriers for Methyl Rotation in SNase," J. Biomol. NMR 29, 377-385 (2004).
21. **D.C. Chatfield**, A. Augsten[u], C. D'Cunha[g], E. Lewandowska, and S. F. Wnuk, "Theoretical and Experimental Study of the Regioselectivity of Michael Additions," Eur. J. Org. Chem. 313-322 (2004).
20. **D.C. Chatfield**, A. Augsten[u], C. D'Cunha[g], and S.E. Wong[u], "Methyl Dynamics in Crystalline Amino Acids: MD and NMR," J. Comp. Chem. 24, 1052-1058 (2003).
19. D. Das, K.P. Eurenius, E.M. Billings, P. Sherwood, **D.C. Chatfield**, M. Hodoscek, and B.R. Brooks, "Optimimization of Quantum Mechanical Molecular Mechanical Partitioning Schemes: Gaussian Delocalization of Molecular Mechanical Charges and the Double Link Atom Method," J. Chem. Phys., 117, 10534-10547 (2002).
18. **D.C. Chatfield** and S.E. Wong, "Methyl Motional Parameters in Crystalline L-Alanine: MD Simulation and NMR," J. Phys. Chem.B 47, 11342-11348 (2000).
17. **D.C. Chatfield**, S.L. Mielke, T.C. Allison, and D.G. Truhlar, "Quantized Dynamical Bottlenecks and Transition State Control of the Reaction of D with H2: Effect of Varying the Total Angular Momentum," J. Chem. Phys. 112, 8387-8408 (2000).
16. **D.C. Chatfield**, A. Szabo, and B.R. Brooks, "Molecular Dynamics of Staphylococcal Nuclease: Comparison of Simulation with 15N and 13C NMR Relaxation Data," J. Am. Chem. Soc. 120, 5301-5311 (1998).
15. **D.C. Chatfield**, K.P. Eurenius, and B.R. Brooks, "HIV-1 Protease Cleavage Mechanism: A Theoretical Investigation Based on Classical MD Simulation and Reaction Path Calculations using a Hybrid QM/MM Potential," Theochem 423, 79-92 (1998).
14. K.P. Eurenius, **D.C. Chatfield**, M. Hodoscek, and B.R. Brooks, "Studying Enzyme Mechanism with Hybrid Quantum Mechanical and Molecular Potentials. I. Theoretical Considerations," Int. J. Quant. Chem. 60, 1189-1200 (1996).
13. **D.C. Chatfield**, R. S. Friedman, S.L. Mielke, G.C. Lynch, T.C. Allison, and D.G. Truhlar, "Computational Spectroscopy of the Transition State," in Dynamics of Molecules and Chemical Reactions, R.E. Wyatt and J.Z.H. Zhang, Eds. (Marcel Dekker: New York, 1996)
12. **D.C. Chatfield** and B.R. Brooks, "HIV-1 Protease Cleavage Mechanism Elucidated with Molecular Dynamics Simulation," J. Am. Chem. Soc. 117, 5561-5572 (1995).
11. D.G. Truhlar, D.W. Schwenke, S.L. Mielke, M.S. Reeves, R.W. Numrich, D.M. Briesemeister, **D.C. Chatfield**, R. S. Friedman, M. Kalke, G.J. Tawa, and M.J. Unekis, "Large-Scale Calculations of the Quantum Dynamics of Molecular Collisions and Reactions," in Toward Teraflop Computing and New Grand Challenge Applications, R.K. Kalia and P. Vashishta, Eds. (Nova Science: New York, 1994)

10. M.S. Reeves, **D.C. Chatfield**, and D.G. Truhlar, "Preconditioned Complex Generalized Minimal Residual Algorithm for Dense Algebraic Variational Equations in Quantum Reactive Scattering," J. Chem. Phys. 99, 2739-2751 (1993).
9. **D.C. Chatfield**, R.S. Friedman, G.C. Lynch, and D.G. Truhlar, and D.W. Schwenke, "The Nature and Role of Quantized Transition States in the Accurate Quantum Dynamics of the Reaction $O + H_2 \rightarrow OH + H$," J. Chem. Phys. 98, 342-362 (1993).
8. **D.C. Chatfield**, M.S. Reeves, C. Duneczky, and D.G. Truhlar, "Complex GMRes Algorithm for Iterative Solution of Quantum Mechanical Reactive Scattering Equations," J. Chem. Phys. 97, 8322-8333 (1992).
7. **D.C. Chatfield**, D.G. Truhlar, and D.W. Schwenke, "State-Selected Chemical Reaction Dynamics at the S Matrix Level: Final-State Specificities of Near-Threshold Processes at Low and High Energies," J. Chem. Phys. 96, 4313-4323 (1992).
6. **D.C. Chatfield**, R.S. Friedman, D.G. Truhlar, and D.W. Schwenke, "Control of Chemical Reactivity by Quantized Transition States," J. Phys. Chem. 96, 2414-2421 (1992). (Feature Article)
5. **D.C. Chatfield**, R.S. Friedman, G.C. Lynch, and D.G. Truhlar, "Quantized Transition State Structure in the Cumulative Reaction Probabilities for the Cl + HCl, I + HI, and I + DI Reactions," J. Phys. Chem. 96, 57-63 (1992).
4. **D.C. Chatfield**, R.S. Friedman, D.G. Truhlar, and D.W. Schwenke, "Quantum Dynamical Characterization of Reactive Transition States," Faraday Discuss. Chem. Soc. 91, 289 (1991). [See pages 398-403 for a Faraday Discussion contribution in same issue.]
3. **D.C. Chatfield**, D.G. Truhlar, and D.W. Schwenke, "Benchmark Calculations of Thermal Reaction Rates. I. Quantal Scattering Theory," J. Chem. Phys. 94, 2040-2044 (1991**).**
2. **D.C. Chatfield**, R.S. Friedman, D.G. Truhlar, B.C. Garrett, and D.W. Schwenke, "Global Control of Suprathreshold Reactivity by Quantized Transition States," J. Am. Chem. Soc. 113, 486-494 (1991).
1. C. Duneczky, R.E. Wyatt, **D.C. Chatfield**, K. Haug, D.W. Schwenke, D.G. Truhlar, Y. Sun, and D.J. Kouri, "Iterative Methods for Solving the Non-Sparse Equations of Quantum Mechanical Reactive Scattering," Comp. Phys. Comm. 53, 357-380 (1989).

PRESENTATIONS (presenting author given first, other authors indicated as defined above)

50. Armando D. Pardillo[g], Alexander N. Morozov[p], and **David C. Chatfield**, "DFT study shows distal-pocket hydrogen bonds significantly influence mechanism of compound I formation in chloroperoxidase," ACS National Meeting, Dallas, March 2014.
49. Konstantinos Kavallieratos, Jaroslava Miksovska and **David C. Chatfield**, "Establishing a new REU Site at a large department: Challenges, rewards, and lessons learned. Presented at the 247th ACS National Meeting, Dallas, March 2014.
48. **David C. Chatfield**, Armando D. Pardillo[g], Alexander N. Morozov[p], "Reactivity of chloroperoxidase, a promising bioengineering target, revealed through simulation," ACS National Meeting, Dallas, April 2014.
47. **David C. Chatfield**, "Computational Approaches to Studying the Functions of Enzymes: Methods and Examples," CAMBIO Interest Group, FIU, February 21, 2014.

46. **David C. Chatfield**, "Protein Modeling to Reveal Function & The 2013 Nobel Prize in Chemistry,"Florida Gulf Coast University, January 23, 2014.
45. **David C. Chatfield**, "Protein modeling to reveal function: A matter of appropriate scale," Symposium on Computational Molecular Dynamics: From Quantum Chemistry to Molecular Biophysics to Biology, FIU, January 14, 2014.
44. Xiaotang Wang, Rui Zhang[g], **David C. Chatfield**, "Mechanism of Chloroperoxidase-Catalyzed Regioselective Oxidation of Indole based on paramagnetic NMR Relaxation and Molecular Mechanics Studies of the Chloroperoxidase-Indole Complex," Gordon Research Conference on Computational Aspects of Biomolecular NMR," West Dover, VT, June 2013.
43. **David C. Chatfield**, "Mechanistic insights into selected heme enzymes from QM and MM studies," Florida Annual Meeting and Exposition, Palm Harbor, FL, May 2013.
42. Armando D. Pardillo and David C. Chatfield, "Influence of hydrogen bonding to proximal sulfur on barrier to formation of Cpd I in Chloroperoxidase as revealed by DFT," Florida Annual Meeting and Exposition, Palm Harbor, FL, May 2013.
41. Alexander N. Morozov[p], Armando D. Pardillo[g], and **David C. Chatfield**, "Chloroperoxidase-catalyzed epoxidation of cis-b-methylstyrene: Apoenzyeme tunes reactivity of the active center," ACS National meeting, New Orleans, LA, April 2013.
40. Alexander N. Morozov[p], James P. Roach[u], and **David C. Chatfield**, "Disulfide bond in human neuroglobin determines heme-apoenzyme hydrogen bonding: a possible mechanism for redox control of neuroprotective activity," ACS National Meeting, New Orleans, LA, April 2013.
39. James P. Roach[u], Alexander N. Morozov[p], and **David C. Chatfield**, "Disulfide bond in human neuroglobin determines accessibility of active site via heme-apoenzyme hydrogen bonding: a possible mechanism for redox control of neuroprotective activity," 57th Annual Meeting of the Biophysical Society, Philadelphia, PA, February 2013.
38. **Armando D. Pardillo[g], Alexander N. Morozov[p] and David** C. Chatfield, "Comparitive Quantum Chemical Study of Thiolate, Thiol, and Hydrogen Bonded Thiol and Thiolate Proximal Heme Ligands on the Rate Determining Step of CPO Activation to Compound I," ACS National Meeting, San Diego, CA, March 2012.
37. Alexander N. Morozov[p] and **David C. Chatfield**, "Molecular dynamic study of 1S2R transition state in Chloroperoxidase-catalyzed epoxidation of Cis-β-Methylstyrene," ACS National Meeting, San Diego, CA, March 2012.
36. **David C. Chatfield**, Alexander N. Morozov[p], Cassian D'Cunha, Armando Pardillo[g] and Alejandro Padronu, "Insight from simulation into the function of three heme proteins, with emphasis on the structural basis of the enantiospecificity of chloroperoxidase-catalyzed epoxidation," Florida Annual Meeting and Exposition, May 2011.
35. Alejandro Padron[u], Armando D. Pardillo[g], Cassian D'Cunha[g] and **David C. Chatfield**, "MD study of wildtype and mutant dehaloperoxidase: Insight into halophenol ligand stabilization and allosteric role of His55," ACS National Meeting, Anaheim, CA, March 2011.
34. Alexander N. Morozov[p], Cassian D'Cunha[g] and David C. Chatfield, "Insight into the structural basis of the enantiospecificity of chloroperoxidase-catalyzed epoxidation," ACS National Meeting, Anaheim, CA, March 2011.

33. Alexander N. Morozov[p], **David C. Chatfield**, "Free energy surface of cis-b-methylstyrene/chloroperoxidase-Compound I reactive complex," ACS National Meeting, San Francisco, CA, March 2010.
32. Vanesa Mendez[g], **David C. Chatfield**, John T. Landrum, "Partial catalog of carotenoid conformer populations from semi-empirical calculations," Gordon Conference on Carotenoids, Ventura Beach, CA, January 2010.
31. **David C. Chatfield**, Carlos Alvarez[g], Xiaotang Wang, "MD study of origin of enantioselectivity in CPO-catalyzed epoxidation," ACS National Meeting, Salt Lake City, UT, March 2009.
30. Armando D. Pardillo[u], David C. Chatfield, "Molecular dynamics study of gate-keeper-residue switch in hybrid globin-peroxidase, DHP," ACS National Meeting, Salt Lake City, UT, March 2009.
29. John T. Landrum, **David C. Chatfield**, Alexander A. Mebel, Francesca Alvarez-Calderon[u], Melissa Fernandez[g], "The Conformation of End-Groups is One Determinant of Carotenoid Topology Suitable for High Fidelity Molecular Recognition: A Study of b- and e-End-Groups," 15th International Symposium on Carotenoids, Okinawa, Japan, June 2008.
28. Cassian D'Cunha[g], **David C. Chatfield**, "Hydration waters critically influence catalysis by CPO," CMM QM/MM Workshop, Philadelphia, PA, August 17-23, 2008.
27. Cassian D'Cunha[g], **David C. Chatfield**, "Hydration waters critically influence catalysis by CPO," ACS National Meeting, Philadelphia, PA, August 2008.
26. **David Chatfield**, Cassian D'Cunha[g], Carlos Alvarez[g], "Theoretical study of chloroperoxidase, a versatile enzyme and potential commercial biocatalyst: (1) Enantiospecificity of catalytic epoxidation, (2) Mechanism of catalytic halogenations," Gordon Conference on Computational Chemistry, Mount Holyoke College, South Hadley, MA, July 27-August 1, 2008.
25. **David C. Chatfield**, Cassian D'Cunha[g], Carlos Alvarez[g], "Theoretical study of chloroperoxidase, a versatile enzyme and potential commercial biocatalyst: (1) Enantiospecificity of catalytic epoxidation, (2) Mechanism of catalytic halogenations," Academia Sinica, Taipei, Taiwan, June 2008.
24. **David C. Chatfield**, "QM/MM methods," Academia Sinica, Taipei, Taiwan, June 2008.
23. **David C. Chatfield**, Cassian D'Cunha[g], Carlos Alvarezg, "Chloroperoxidase catalysis: A theoretical study," FAME, Orlando, FL, May 2008.
22. **David C. Chatfield**, "Chloroperoxidase, the most versatile heme protein: (1) Enantiospecificity of catalytic epoxidation, (2) Mechanism of catalytic halogenation," Academia Sinica, Taipei, Taiwan, June 2008.
21. **David C. Chatfield**, "QM/MM methods," Academia Sinica, Taipei, Taiwan, June 2008.
20. **David C. Chatfield**, Cassian D'Cunha[g], Carlos Alvarez[g], "Chloroperoxidase catalysis: A theoretical study," FAME, Orlando, FL, May 2008.
19. **David C. Chatfield**, "Studying macromolecular chemistry with computer simulation", Barry University, Miami, FL, Feb. 16, 2006.
18. **David C. Chatfield**, "Studying macromolecular chemistry with computer simulation", Barry University, Miami, FL, Feb. 16, 2006.

17. **David C. Chatfield**, "Catalytic mechanism of chloroperoxidase," Free University, Berlin, July, 2005," Elucidation of the halogenation mechanism of chloroperoxidase," Humboldt University, Berlin, December 8, 2004.
16. **David C. Chatfield**, "Activation of the alpha carbon of an alpha,beta-unsaturated carbonyl compound toward nucleophilic attack: an experimental and theoretical study," ACS National Meeting, Philadelphia, August, 2004.
15. **David C. Chatfield**, "Two applications of computer modeling in chemistry: (1) The Michael addition reaction and substituent effects; (2) Quantifying flexibility in proteins," Barry University, Miami, FL, November, 2002.
14. **David C. Chatfield**, "MD/NMR characterization of the internal motions of peptides and proteins," Institute of Chemistry, Ljubljana, Slovenia, June, 2000.
13. **David C. Chatfield**, "Motional parameters for alanine side-chains in crystalline peptides and in staphylococcal nuclease: MD and NMR," Florida Annual Meeting and Exposition, Orlando, FL, May, 1999.
12. **David C. Chatfield**, "Probing the internal motions of peptides with MD and NMR: From crystalline amino acids to conotoxins," University of Cincinnati, November, 1998.
11. **David C. Chatfield**, "Molecular dynamics of staphylococcal nuclease: Comparison of simulation with NMR data," Sanibel Symposium, St. Augustine, FL, February, 1998.
10. **David C. Chatfield**, Bernard R. Brooks, Atilla Szabo, "Mobility of amino acid side-chains in staphylococcal nuclease and in crystalline peptides: MD simulation and NMR," ACS National Meeting, Las Vegas, NV, September, 1997.
9. **David C. Chatfield**, "Theoretical study of the HIV-1 protease reaction mechanism using simulation with a hybrid QM/MM potential," ACS National Meeting, Orlando, FL, August, 1996.
8. **David C. Chatfield**, Bernard R. Brooks, "Theoretical study of the HIV-1 protease reaction mechanism using simulation with a hybrid QM/MM potential," Tenth Meeting of Groups Studying the Structure of AIDS-Related Systems and Their Application to Targeted Drug Design, Bethesda, MD, June, 1996.
7. **David C. Chatfield**, Bernard R. Brooks, "The HIV-1 protease cleavage mechanism: A classical molecular dynamics and hybrid QM/MM study," University of Miami, February, 1996.
6. **David C. Chatfield**, Bernard R. Brooks, "The mechanism of proteolytic cleavage by HIV-1 protease: Implications of simulation using a hybrid QM/MM potential," CECAM Workshop, Developing Hybrid Quantum and Classical Mechanical Methods for the Simulation of Biopolymers in Solution, Lyon, France, May, 1995.
5. **David C. Chatfield**, Bernard R. Brooks, " A molecular simulation study of the HIV-1 protease cleavage mechanism," Eighth Meeting of Groups Studying the Structure of AIDS-Related Systems and Their Application to Targeted Drug Design, Bethesda, MD, June, 1994.
4. **David C. Chatfield**, Bernard R. Brooks, "HIV-1 protease cleavage mechanism elucidated with MD simulation," NIH Research Festival, Bethesda, MD, 1994.
3. **David C. Chatfield**, Bernard R. Brooks, "HIV-1 protease cleavage of viral polyproteins: A molecular dynamics study of the chemical mechanism," Indiana University-Purdue University at Fort Wayne, May, 1994.

2. **David C. Chatfield**, Bernard R. Brooks, "The cleavage of viral polyproteins by HIV-1 protease: A molecular dynamics study of the chemical mechanism," Eleventh International Biophysics Conference, Budapest, Hungary, July, 1993.
1. **David C. Chatfield**, Donald G. Truhlar, "Quantized transition state control of chemical reactivity," Annual Meeting of the American Physical Society Division of Atomic, Molecular, or Optical Physics, Reno, NV, May, 1993.

WORKS IN PROGRESS

3. A.D. Pardillo[g], A.N. Morozov[p], **D.C. Chatfield**, "DFT study shows distal-pocket hydrogen bonds significantly influence mechanism of compound I formation in chloroperoxidase," *in preparation*.
2. A.N. Morozov[p], A.D. Pardillo[g], **D.C. Chatfield**, "Proximal pocket helix influences enantiospecificity of chloroperoxidase-catalytic epoxidation of cis-beta-methylstyrene," *in preparation*.
1. C. D'Cunha[p], **David C. Chatfield**, Y.-C. Tse-Dinh, "Molecular dynamics derived mechanism of Mg(II) driven shift from DNA cleavage to DNA religation by type IA DNA topoisomerases," *in preparation*.

FUNDED RESEARCH

Completed:

2008-2012 NIH/MBRS SC3GM83723; **Chloroperoxidase Catalytic Mechanism**; (PI, $400,000).
2002 NIH/MBRS; **Equipment Grant for Beowulf Computer Cluster;** (PI; $60,000).
2001-2004 NIH/ARCH S11ES11181; **MD/NMR study of internal motions of peptide toxins**; (Co-PI, Chatfield portion $120,000).
2000-2004 NIH/MBRS GM08205; **MD Interpretation of SNase Motional Parameters**; (PI; $240,000).

PROPOSALS SUBMITTED BUT NOT FUNDED (Previous five years only)

2014-2017 NIH/R15; **Mechanistic Characterization and Bioengineering of Chloroperoxidase**; (PI, $425,000).
2006-2010 NIH/MBRS/SCORE; **Chloroperoxidase-Catalylzed Halogenation and Epoxidation Reactions**; (PI, $400,000)

PROFESSIONAL HONORS, PRIZES, FELLOWSHIPS

1993: Finalist, American Physical Society Award for Outstanding Doctoral Thesis Research in Atomic, Molecular, or Optical Physics.
1991: Army High Performance Computing Research Fellow.
1984-1985: German Academic Exchange Service (DAAD) scholar at Johannes Gutenberg Universität, Mainz, Germany.

OFFICES HELD IN PROFESSIONAL SOCIETIES

Full Member:

American Chemical Society
Biophysical Society

COURSES TAUGHT
General Chemistry I (CHM 1045)
General Chemistry II (CHM 1046)
Fundamentals of Physical Chemistry (CHM 3400)
Physical Chemistry I (CHM 3410)
Physical Chemistry I Lab (CHM 3410L)
Physical Chemistry I (CHM 3411)
Physical Chemistry I Lab (CHM 3411L)
Senior Seminar (CHM 4930)
Computer Modeling of Biological Molecules (CHM 5351)
Computational Chemistry (CHM 5990)
Advanced Thermodynamics (CHM 6430)
Statistical Thermodynamics (CHM 6461)
Graduate Seminar (CHM 6935)
Chemistry Colloquium (CHM 6936)
The Idea of Origins and the Origin of Ideas (IDH 1001, IDH 1002)

GRADUATE STUDENT MENTORING

Graduated Students:
Cassian D'Cunha, Ph.D. Chemistry, "Theoretical study of halogenation mechanism of chloroperoxidase," FIU, 2011.
Andres Alvarez, M.S. Chemistry, "Docking and simulation study of the enantiospecificity of chiral epoxidation reactions catalyzed by chloroperoxidase," FIU, 2006.
Cassian D'Cunha, M.S. Computer Science, "A molecular simulation study of the utility of methyl groups as probes of protein packing and flexibility and maintaining the computational environment for computational biomolecular research," FIU, 2003

Current Students:
Armando D. Pardillo, Ph.D. Chemistry, "Computational evaluation of two stages in the catalytic cycle of chloroperoxidase-catalyzed epoxidation reactions," FIU, in progress.
Antonija Tangar, Ph.D. Chemistry, "Structure-function relationships in hexacoordinate heme proteins: Mechanisms of cytoglobin interactions with exogenous ligands," FIU, in progress.

UNDERGRADUATE STUDENT MENTORING (title, date of report, degree given)
Vy Trinh, "Creating a homology model of a antarctic fish neuroglobin," 2014.
Marisse Padron, "Computational chemistry study of 2-(methylthio) thiophene and hydrogen peroxide," 2013.
Bryan Rivas, "Cytoglobin, a review," 2013, B.S.
James Roach, "Disulfide bond in human neuroglobin determines accessibility of active site via heme-apoenzyme hydrogen bonding: a possible mechanism for redox control of neuroprotective activity," 2012, B.S.

Margarita Kotzer, "Topology work on the disulfide bond in the CD loop in human neuroglobin," 2011, B.S.

Alejandro Padron, "The molecular dynamics of catalytically active residues in dehaloperoxdase," 2011, B.S.

Andres Alvarez, "Computational analysis of Michael additions," 2003, B.S.

Alberto Augsten, "Methyl dynamics in crystalline amino acids," 2002, B.S.

Sergio Wong, "Study of backbone hydrogen motional parameters and entropy contribution using α-conotoxin GI," 2000, B.S.

Eleonore Naydis, "The QM/MM approach in application to enzyme-catalyzed reactions: Model system study with QM method," 1998, B.S.

Orlando Acevedo, "Establishing a protocol for studying helix stability and the stabilizing effect of AIB residues," 1998, B.S.

Franklin Gutierrez, "Rotational barriers for methyl groups in crystalline cyclo-L-alanine-L-alanine," 1997, B.S.

SERVICE

TO FIU

Chair, Chairs Advisory Council, 2013-2014

iREAL Working Group on Research & PhD Production, 2013-2014

Committee on Sustained Performance Evaluation, 2014

Senator, Faculty Senate, 2008

Faculty Senate Steering Committee, 2008

Student Grievance Committee, 2008

Honors College Faculty, 2006-2009

Co-Chair of Committee on Development of PhD in Biochemistry, 2005-2008

TO DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

Department Chair, 2008-present

Chair, Human Resources Committee, 2006-2008

Chair, Public Relations/Website Committee, 2005-2006

Chair, Safety Committee, 2003-2004

Chair, Physical Chemist Search & Screen Committee, 2003-2004

TO COMMUNITY

Science Fair Judge, St. Stephen's Day School 2001, 2002, 2004

PROFESSIONAL SERVICE

Organizing Committee, 8th Electronic Computational Chemistry Conference (2003)

Organizing Committee, 9th Electronic Computational Chemistry Conference (2004)

Organizing Committee, 10th Electronic Computational Chemistry Conference (2005)

Ad hoc referee for the following scientific journals:

Biochemistry
Chemistry–A European Journal
European Journal of Organic Chemistry
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Computational Chemistry
Journal of Physical Chemistry
Proteins: Structure, Functions, and Bioinformatics

Theoretical Chemistry Accounts

Grant proposal review:

NIH/MBRS

Petroleum Research Foundatoin