## Invited Lectures

1) "The Azulene to Naphthalene Rearrangement", The University of Arkansas (Main Campus), Department of Chemistry, Jan. 1986.

2) "The Azulene to Naphthalene Rearrangement", Northern Illinois University, Department of Chemistry, Jan 1986.

3) "The Azulene to Naphthalene Rearrangement", Mississippi State University, Department of Chemistry, Jan 1986.

4) "The Azulene to Naphthalene Rearrangement", Sterling-Winthrop Inc., Department of Medicinal Chemistry, Mar. 1986.

5) The Azulene to Naphthalene Rearrangement", University of Belgrade (Yugoslavia), Department of Chemistry, July 1987.

6) The Azulene to Naphthalene Rearrangement", The Boris Kidric Institute, Vinca, (Yugoslavia), Department of Chemistry, July 1987.

7) The Mode of Action of Carbonic Anhydrase and the Inhibition of Thermolysin" The Pennsylvania State University (University Park), Dec. 1987.

8) "The Mode of Action of Carbonic Anhydrase and the Inhibition of Thermolysin", The University of Texas at Austin, Department of Pharmaceutical Chemistry, Jan. 1988.

9) "The Mode of Action of Carbonic Anhydrase and the Inhibition of Thermolysin", The University of Alabama (Main Campus), Department of Chemistry, Jan. 1988.

10) "The Mode of Action of Carbonic Anhydrase and the Inhibition of Thermolysin", The University of Missouri (Main Campus), Department of Chemistry, Jan. 1988.

11) "The Mode of Action of Carbonic Anhydrase and the Inhibition of Thermolysin", Oregon State University, Department of Chemistry, Jan. 1988.

12) "The Mode of Action of Carbonic Anhydrase and the Inhibition of Thermolysin", North Texas State University, Department of Chemistry, Feb. 1988.

13) "Computer Simulations of Zinc-Containing Enzymes", "Industrial Applications of Computational Chemistry Conference", Ithaca, New York, June 15-16, 1988.

14) "Application of the Free Energy Perturbation Method to Drug Design", "8$^{th}$ International Biotechnology Symposium", Paris, France, July 17-22, 1988.

15) "Computer-Aided Drug Design", "National Cooperative Drug Discovery and Development Meeting", Oakland, California, October 31-November 2, 1988.

16) "Drug Design in Zinc Metalloenzymes: Carbonic Anhydrase", "Fourth International Conference on Supercomputing and Third World Supercomputer Exhibition", Santa Clara, California, April 30-May 5, 1989.

17) "Substrate Binding in Carbonic Anhydrase II", University of Firenze, Firenze, Italy, June 14, 1989.

18) "Free Energy Perturbation Studies on the Inhibition of Thermolysin and Human Carbonic Anhydrase II", "From Molecular Modeling and Dynamics to Protein Structures and Drug Interactions Conference", San Miniato, Italy, June 19-20, 1989.

19) "The Binding and Hydration of Carbon Dioxide by Human Carbonic Anhydrase II", "NATO Advanced Study Institute, Summer School on Enzymatic and Model Carboxylation and Reduction Reactions for Carbon Dioxide Utilization", Riva dei Tessali, Italy, June 17-28, 1989.

20) "Computer Simulation of Human Carbonic Anhydrase II: Inhibition and Substrate Binding", "Computer Simulation of New Materials Conference", Ithaca, New York, October 3-4, 1989.

21) "Computer Simulations of Zinc Metalloenzymes", Susquehanna Regional ACS Meeting, Lycoming College, March 14, 1990.

22) "$CO_2$ Binding to HCAII", Duke University, April 12, 1990.

23) "$CO_2$ Binding to HCAII", University of Pennsylvania, October 25, 1990.

24) "Structure, Function and Dynamics of Antibiotic Ionophores", INDO-U.S. Workshop: Membrane Structure and Function. The State of The Art. Bangalore, India, January 7-18, 1991.

25) "Structure, Function and Inhibition of Human Carbonic Anhydrase II", Merck, Sharp and Dohme, West Point, Pennsylvania, March 20,1991.

26) "Molecular Design Using Free Energy Perturbation Techniques", 1991 Joint Central-Great Lakes Regional American Chemical Society Meeting, May 29-31, 1991.

27) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Carbonic Anhydrase. Symposium in the Leibniz House, Hannover, Germany, July 10-12, 1991.

28) "Theoretical Investigations of Zinc Metalloenzymes" Structure and Function of Mutated Proteins, Firenze, Italy, August 25-30, 1991.

29) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of Florida, December 3, 1991.

30) "Computer Simulation of the DLPE Lipid Bilayer", University of Cincinnati, March 5, 1992.

31) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of Cincinnati, March 6, 1992.

32) "Quantum Chemical Applications to Carbohydrates and Their Analogs", American Chemical Society Meeting, San Francisco, California, April, 5, 1992.

33) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of Umeå, Sweden, April 9, 1992.

34) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of Uppsala, Sweden, April 10, 1992.

35) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of Lund, Sweden, April 14, 1992.

36) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of FIrenze, Italy, May 15, 1992.

37) "Recent Advances in the Design of Metal Force Fields", Computational Chemistry Gordon Research Conference, New Hampton School, June 29-July 3, 1992.

39) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Enzymes, Coenzymes and Metabolic Pathways Gordon Research Conference, Kimball Union Academy, July 18-22, 1990.

40) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Merck, Sharp and Dohme, West Point, Pennsylvania, July 13, 1992.

41) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Glaxo, Reseach Triangle Park, North Carolina, August 6, 1992.

42) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Miami University, October 8, 1992.

43) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Eli Lilly & Co., Indianapolis, Indiana, October 9, 1992.

44) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", Temple University, Philadelphia, Pennsylvania, November 6, 1992.

45) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", University of North Carolina, Chapel Hill, North Carolina, March 16, 1993.

46) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", 3rd International Conference on the Carbonic Anhydrases, Oulu, Finland, July 12-15, 1993.

47) "Computer Simulation of the Lipid Bilayer Assemblies", 11th International Congress of Biophysics, Budapest, Hungary, July 25-30, 1993.

48) "Theoretical Investigations of the Structure, Function and Dynamics of HCAII", The Structure/Function Relationships in Proteins and Enzymes, State College, Pennsylvania, July 26-30, 1993.

49) "Non-Aqueous Solvation of Proteins", American Chemical Society Meeting, Chicago, Illinois, August 22-27, 1993.

50) "Structure, Function and Dynamics of the Antibiotic Ionophores Valinomycin and Nonactin", "NATO Advanced Research Workshop, "Computational Approaches to Supramolecular Chemistry", Strasbourg, France, September 1-5, 1993.

51) "Studies of Reactions Using a Combined QM/MM Methodology" ISQBP President's Meeting, "Chemical Reactions and Molecular Recognition in Drug Design" Asilomar, California, December 12-15, 1993.

52) "Interaction of Small Peptides with Lipid Bilayers: Molecular Dynamics and Free Energy Simulation Studies" Biophysical Society Meeting, New Orleans, Louisiana, March 6-10, 1993

53) "Development and Application of Quantum Mechanical/Molecular Mechanical Coupled Potentials" American Chemical Society Meeting, San Diego, California, March 13-18, 1994.

54) "Molecular Dynamics Simulations of Carbyne Network Polymers" American Chemical Society Meeting, San Diego, California, March 13-18, 1994.

55) "Protein Dynamics in Aqueous and Nonaqueous Environments" American Chemical Society Meeting, San Diego, California, March 13-18, 1994.

56) "Sugar/Surface Interactions" Molecular Interactions at Marine Interfaces, Buffalo, New York, June 8-10, 1994.

57) "Parallel Molecular Dynamics Simulations: Methodology and Application to Lipid Bilayers" American Chemical Society Meeting, Washington, DC, Auguest 21-26, 1994.

58) "Non-Aqueous Solvation of Proteins" Biomolecular Recognition at ONR, Berkeley Springs, West Virginia, October 26-30, 1994.

59) "Computer Simulation of Reactive Processes Using Coupled Quantum Mechanical/Molecular Mechanical Methods" International Symposium on Computational

Molecular Dynamics, University of Minnesota Supercomputer Institute, Minneapolis, Minnesota, October 24-26, 1994.

60) "Computer Simulation of Peptide/Lipid Interactions" University of Virginia, Charlottesville, Virginia, October 13, 1994.

61) "Computer Simulation of Reactive Processes Using Coupled Quantum Mechanical/Molecular Mechanical Methods" Indiana University Purdue University Indianapolis, Indianapolis, Indiana, November 9, 1994.

62) "Theoretical Investigation of the Structure, Function and Dynamics of Human Carbonic Anhydrase II" University of Montreal, Montreal, Canada, February 28, 1995.

63) "Computer Simulation of Bilayer/Peptide Interactions" Wyeth-Ayerst Research, Princeton, New Jersey, March 10, 1995.

64) "Theoretical Studies of Peptide/Lipid Interactions" Villanova University, Villanova, Pennsylvania, March 21, 1995.

65) "Theoretical Studies of Peptide/Lipid Interactions" American Chemical Society Meeting, Anaheim, California, April 2-7, 1995.

66) "Development of a Quantum Free Energy Perturbation Methodology" American Chemical Society Meeting, Anaheim, California, April 2-7, 1995.

67) "Development of a Quantum Free Energy Perturbation Methodology" CECAM Meeting, Lyon, France, May 9-11, 1995.

68) "Theoretical Investigation of the Structure, Function and Dynamics of Human Carbonic Anhydrase II" 4$^{th}$ International Conference on the Carbonic Anhydrases, Oxford, England, July 26-30, 1995.

69) "Computer Simulation of Bilayer/Peptide Interactions" High Performance Computing Conference (HPCC), Pleasanton, California, August 13-16, 1995.

70) "Computer Simulation of Saccharide/Surface Interactions" American Chemical Society Meeting, Chicago, Illinois, August 20-24, 1995.

71) "Computer Simulation of Bilayer/Peptide Interactions" American Chemical Society Meeting, Chicago, Illinois, August 20-24, 1995.

72) "Theoretical Investigation of the Structure, Function and Dynamics of Human Carbonic Anhydrase II" Fox Chase Cancer Center, Philadelphia, Pennsylvania, November 9, 1995.

73) "Application of Combined Quantum Mechanical/Molecular Mechanical Methodologies to Chemistry" Rohm and Haas Co. Philadelphia, Pennsylvania, November 16, 1995.

74) "Development and Application of Quantum Free Energy Perturbation Methodologies" Pacific Symposium on Biocomputing, Hawaii, January 3-6, 1996.

75) "Mechanism of Action of Fusion Inhibiting Peptides" Biophysical Society Meeting, Baltimore, Maryland, February 18-22, 1996.

76) "Application of Coupled Potentials to Chemical Problems" Georgetown University, Washington DC, April 17, 1996.

77) "Application of Coupled Potentials to Enzyme Solvation" Theoretical Methods for the Study of Solvation", Barcelona, Spain, June 16-18, 1996.

78) "Application of Coupled Potentials to Chemical Problems" WATOC '96 Conference, Jerusalem, Israel, July 7-12, 1996.

79) "Mechanism of Action of Fusion and Fusion Inhibiting Peptides" FASEB Summer Conference on the Molecular Biophysics of Cellular Membranes, Saxton's River, Vermont, July 20-25, 1996.

80) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" HyperCem User Group Meeting, September 8-11, 1996.

81) "Sugar/Surface Interactions" Molecular Interactions at Marine Interfaces, Atlantic Beach, Florida, September 23-25, 1996.

82) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" University of Florida Quantum Theory Project, September 26, 1996.

83) "Mechanism of Action of Fusion and Fusion Inhibiting Peptides" The International Symposium on Molecular Dynamics of Biomembranes, University of North Carolina, Chapel Hill, North Carolina, October 24-26, 1996.

84) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" NASA-Ames Research Center, Moffett Field, California, November 20, 1996.

85) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" University of Southern California, Los Angles, California, December 2, 1996.

86) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" California Institute of Technology , Pasadena, California December 4, 1996.

87) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" University of California, Los Angles, Los Angles, California, December 5, 1996.

88) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" University of California, San Barbara, Santa Barbara, California, December 9, 1996.

89) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" University of California, San Diego, San Diego California, December 11, 1996.

90) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" Scripps Research Clinic, San Diego, California, December 12, 1996.

91) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" Pacific Symposium on Biocomputing, Hawaii, January 3-6, 1996.

92) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" University of California, Berkeley, Berkeley, California, January 14, 1997.

93) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" University of Virginia, Charlottesville, Virginia, January 16, 1997.

94) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" ETH, Zurich, Switzerland, January 30, 1997.

95) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" NATO Advanced Workshop: Molecular Modeling and Dynamics of Biological Molecules Containing Metal Ions, San Miniato, Pisa, Italy, March 15-21, 1997.

96)"Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" State University of Groningen, Groningen, The Netherlands, March 26, 1997.

97) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" University of Louis Pasteur, Strasbourg, France, April 1, 1997.

98) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" University of Zurich, Zurich, Switzerland, April 15, 1997.

99) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" Theoretical Chemistry in Biology: From Molecular Structure to Functional Mechanisms, Savannah, Georgia, June 3-7, 1997.

100) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" Model(l)ing '97, Erlangen, Germany, September 2-5, 1997.

101) "Linear-Scaling Quantum Mechanical Calculations of Biomacromolecules" American Chemical Society Meeting, Las Vegas, Nevada, September 7-11, 1997.

102) "Combined QM/MM Methodologies: Strategies and Applications" University of Geneva , Geneva, Switzerland October 6, 1997.

103) "Linear-Scaling QM Methodologies: Strategies and Applications" University of Geneva , Geneva, Switzerland October 7, 1997.

104) "Strategies Towards Modeling Enzyme Catalysis Using QM/MM Methods" University of Basel , Basel, Switzerland October 8, 1997.

105) "Quantum Mechanical and Molecular Mechanical Methods" University of Fribourg , Fribourg, Switzerland October 9, 1997.

106) "Divide and Conquer Semiempirical Quantum Calculations" University of Fribourg , Fribourg, Switzerland October 10, 1997.

107) "Towards All-Electron Modeling of Biological Molecules" University of Utah , Salt Lake City, Utah November 3, 1997.

108) "Application of Linear-Scaling Quantum Mechanical Calculations to Biological Systems" California Institute of Technology , Pasadena, California November 4, 1997.

109) "ChargeTransfer Effects in Biomolecular Systems" Southern Illinois University, Carbondale, Illinois January 23, 1998.

110) "Towards All-Electron Modeling in Biomolecular Systems" State University of Groningen, Groningen, The Netherlands, March 9, 1998.

111) "ChargeTransfer Effects in Biomolecular Systems" American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

112) "Towards All-Electron Modeling in Biomolecular Systems" American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

113) "Towards All-Electron Modeling in Biomolecular Systems" XXXIII ICCC, Florence, Italy, August 30, - September 4, 1998.

114) "Towards All-Electron Modeling in Biomolecular Systems" 34th Symposium for Theoretical Chemistry, Gwatt-Zentrum am Thunersee, Switzerland, September 20-24, 1998.

115) "Towards All-Electron Modeling in Biomolecular Systems" DARPA BioInformatics Workshop, Washington, DC, January 19-20, 1999.

116) "Property Estimation Tools to Facilitate Library Design" Computational Technologies for Library Design and Analysis, Princeton, New Jersey, May 26, 1999.

117) "Property Estimation Tools to Facilitate Library Design" Techniques for Library Design, Analysis, Profiling and Data Utilization, Cambridge, MA, May 27, 1999.

118) "Towards All-Electron Modeling in Biomolecular Systems" SFB Congress, Jena, Germany, September 12-16, 1998.

119) "Towards All-Electron Modeling in Biomolecular Systems" Sanibel Symposium, Sanibel, Florida, February 26- March 3, 2000.

120) "Predicting ADMET Properties" Department of Medicinal Chemistry, University of Minnesota, Minneapolis, Minnesota, March 21, 2000.

121) "Computing ADMET Properties" InfoTech Pharma, Philadelphia, PA, June 22-23.

122) "Modeling Metal Ions in Biological Systems" Metal Ions In Biology, NIH Washington, DC June 28-30.

123) "Mechanism of Action of β-Lactamaes" ISQBP Meeting, New Orleans, Louisiana August 17-19.

124) "Computing ADMET Properties" CombiChem Consortium Meetings, Paris, France, September 11-13 May 2000.

125) " New Approaches to Modeling ADMET Properties" International Workshop: New Approaches in Drug Design and Discovery", Marburg, Germany March 19-22, 2001

126) "Towards All-Electron Modeling in Biomolecular Systems" American Chemical Society Meeting, San Diego, California, April 1-5, 2001.

127) "In Silico Library Design Tools" American Chemical Society Meeting, San Diego, California, April 1-5, 2001.

128) "Mechanism of Action of β-Lactamaes" American Chemical Society Meeting, San Diego, California, April 1-5, 2001.

129) "Quantum Bioinformatics: Methods and Applications" , Emerging Methods in Computational Chemistry and Materials Science, Aberdeen, Maryland, May 31-June 1, 2001.

130) "Towards All-Electron Modeling in Biomolecular Systems", 14th Canadian Symposium on Theoretical Chemistry, Ottawa, Canada, August 4-9, 2001.

131) "Quantum Bioinformatics: Methods and Applications" American Chemical Society Meeting, Chicago, Illinois, August 26-31, 2001.

132) "One-Dimensional Molecular Representations: Methodology and Validation Studies" Model(l)ing 2001, Erlangen, Germany, September 17-21, 2001. (Missed due to events of Sept. 11, 2001).

133) "Quantum Bioinformatics" 4th. Advanced Seminars on Molecular Design and Bioinformatics, Havana, Cuba, February 3-9, 2002.

134) "Towards All-electron Modeling of Biological Systems" Molcular Simulations in Structural Biology and Drug Discovery - Symposium in Remembrance of Peter A. Kollman, American Chemical Society Meeting, Orlando, Florida, February 21-22, 2002.

135) "Towards All-electron Modeling of Biological Systems" MGMS Annual Meeting, Bristol, UK, April 3-5, 2002.

136) "Towards All-electron Modeling of Biological Systems" ACS COMP Division Symposium in Remembrance of Peter A. Kollman, American Chemical Society Meeting, Orlando, Florida, April 7-11, 2002.

137) "Quantum Bioinformatics" Blue Gene Seminar, IBM T. J. Watson Research Center, Yorktown Heights, NY, March 1, 2002.

138) "Towards All-electron Modeling of Biological Systems" University of Florida, Gainesville, Florida, June 10, 2002.

139) “Structure and Function of Zinc-β-lactamases” Quantum Bioinorganic Chemistry (QBIC-2), Lund, Sweden, July 27-29, 2002.

140) “Structure and Function of Zinc-β-lactamases” Metal Mediated Reactions Modelled after Nature, Jena, Germany, September 15-19, 2002.

141) “Towards All-electron Modeling of Biological Systems” RIKEN Japan, September 18-20, 2002.

142) “Towards All-electron Modeling of Biological Systems” SUNY Stony Brook, Stony Brook, NY, November 7, 2002.

143) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery/Design” ISQBP President’s Meeting, Snowbird, Utah, December 13-14, 2002.

144) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery/Design” Pfizer, San Diego, January 14, 2003.

145) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery/Design” Concurrent Pharmaceuticals, Philadelphia, January 27, 2003.

146) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery/Design” DuPont Ag, Newark, January 29, 2003.

147) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery/Design” Wyeth, Boston, January 30, 2003.

148) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery” Sanibel Symposium, Sanibel, Florida, February 22- March 1, 2003.

149) “Quantum Mechanical Scoring Function” CHARMM/AMBER Meeting, San Diego, California, July 10-12, 2003

150) “Towards All-electron Modeling of Biological Systems” XI International Congress of Quantum Chemistry, Bonn, Germany, July 20-26, 2003.

151) “Quantum Mechanics in Drug Discovery and Design” Computer-Aided Drug Design Gordon Conference, Tilton School, NH, July 20-25, 2003.

152) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery” MERCURY Conference, Hamilton College, New York, July 31- August 1, 2003.

153) “Towards All-electron Modeling of Biological Systems: Applications to Drug Discovery” University of Florida, Gainesville, Florida, September 23, 2003.

154) “Semiempirical Density Functional Theory” University of Florida, Gainesville, Florida, September 24, 2003.

155) “Quantum Mechanics in Drug Discovery and Design” Syrrx, Inc., San Diego, California, October 15, 2003.

156) “Quantum Mechanics in Drug Discovery and Design” 5AM Ventures, Palo Alto, California, October 16, 2003.

157) “Quantum Mechanics in Drug Discovery and Design” University of Michigan, Ann Arbor, California, November 20, 2003.

158) “Quantum Mechanics in Drug Discovery and Design” Millenium Pharmaceuticals., Boston, Massachusetts, December 5, 2003.

159) “Quantum Mechanics in Drug Discovery and Design” New Jersey Technology Council, Mt Laurel, New Jersey, December 10, 2003.

160) “Quantum Mechanics in Drug Discovery and Design” Schering-Plough, Kennilworth, New Jersey, December 10, 2003.

161) “Quantum Mechanics in Drug Discovery and Design” Targacept, Winston-Salem, North Carolina, December 16, 2003.

162) “The Impact of Semiempirical Quantum Mechanics in Biology” American Chemical Society Meeting, Anaheim, California, March 28, 2004.

163) “Quantum Mechanics in Drug Discovery and Design” University of Maryland, College Park, Maryland, April 7, 2004.

164) “The Impact of Semiempirical Quantum Mechanics on Structure-Based Design” Glaxo Smith Kline, Philadelphia, Pennsylvania, May 20, 2004.

165) “Pose Scoring by NMR” University of Milano, Milano, Italy, June 9, 2004.

166) “Pose Scoring by NMR” University of Firenze, Firenze, Italy, June 15, 2004.

167) “The Impact of Semiempirical Quantum Mechanics on Structure-Based Design” Pharmacopeia, Inc. Princeton, New Jersey, July 16, 2004.

168) “The Impact of Semiempirical Quantum Mechanics on Structure-Based Design” Eli Lilly & Co., Indianapolis, Indiana, August 3, 2004.

169) “Pose Scoring by NMR” American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

170) “Pose Scoring by NMR” Johnson & Johnson, Philadelphia, Pennsylvania, September 10, 2004.

171) “The Impact of Semiempirical Quantum Mechanics on Structure-Based Design” BMS Princeton, New Jersey, September 22, 2004.

172) "The Role of Quantum Mechanics in Structure-Based Drug Design" Frontiers in Computational Biophysics and Drug Design, Washington, DC, October 21-22, 2004.

173) "The Role of Quantum Mechanics in Structure-Based Drug Design" Cornell Weill Medical College, New York, New York, November 11, 2004.

174) "The Role of Quantum Mechanics in Structure-Based Drug Design" CUNY, Hunter College, New York, New York, November 12, 2004.

175) "Using NMR Spectroscopy Combined with Quantum Mechanics to Elucidate Protein-Small Molecule Interactions" Juniata College, December 1, 2004.

176) "The Role of Quantum Mechanics in Structure-Based Drug Design" WATOC05, Capetown, South Africa, January 16-21, 2005.

177) "The Role of Quantum Mechanics in Structure-Based Drug Design" OpenEye CUP VI, Santa Fe, New Mexico, February 20-22, 2005.

178) "Quantum Mechanics in Biology: From Protein Folding to Drug Design" Max-Planck-Institute, Mülheim, Germany, November 7, 2005.

179) "The Role of Quantum Mechanics in Structure-Based Drug Design" eCheminfo, Basel, Switzerland, November 9-10, 2005.

180) "The Role of Quantum Mechanics in Structure-Based Drug Design" Serono Pharmaceuticals, Geneva, Switzerland, November 11, 2005.

181) "Quantum Mechanics in Biology: From Protein Folding to Drug Design" University of Oviedo, Oviedo, Spain, November 14, 2005.

182) "Quantum Mechanics in Biology: From Protein Folding to Drug Design" University of New Mexico, Albuquerque, New Mexico, December 2, 2005.

183) "Quantum Mechanics in Biology: From Protein Folding to Drug Design" University of Florida, Gainesville, Florida, December 7, 2005.

184) "Quantum Mechanics in Biology: From Protein Folding to Drug Design" Florida State University, Tallahassee, Florida, February 7, 2006.

185) "The Role of Quantum Mechanics in Structure-Based Drug Design", Validating Modeling and Experimental Methods to Enable Drug Discovery, NIST, Washington, D.C., April 19-21, 2006.

186) "The Role of Quantum Mechanics in Structure-Based Drug Design", Southeast Theoretical Chemist Association Meeting, Emory University, Atlanta, Georgia, May 19-20, 2006.

187) "The Role of Quantum Mechanics in Protein Folding and Structure-Based Drug Design", Enrico Fermi Summer School, Protein Folding and Drug Design, Varenna, Italy, July 4-14, 2006.

188) "Semiempirical Quantum Chemistry in Biology", Dewar Symposium, ACS National Meeting, San Francisco, California September 10-15, 2006.

189) “The Role of Quantum Mechanics in Structure-Based Drug Design”, Frontiers in Predictive ADMET, AAPS National Meeting, San Antonio, Texas, October 29 – November 2, 2006.

190) “The Role of Quantum Mechanics in Structure-Based Drug Design”, Conference on Current Trends in Computational Chemistry (CCTCC), Jackson, Mississippi, November 3-4, 2006.

191) “The Hydrolysis of Formamide and the Proficiency of Amidohydrolases: The Burden Borne by $k_W$”, Quantitative Computational Biophysics Workshop, Florida State University, February 18-21, 2007.

192) ”The Role of Quantum Mechanics in Structure-Based Drug Design”, University of Miami, Miami, Florida, April 13, 2007.

193) “Studying Protein Prenylation in Farnesyltransferase and Orf2 using Computational Tools”, ASBMB Meeting, Washington, DC, April 28-May 2, 2007.

194) “Structural Biology Viewed from the Perspective of Quantum Mechanics”, FAME Orlando, Florida, May 10-12, 2007.

195) “Structural Biology from the Quantum Chemical Perspective”, C4 Seminar Program, ETH, Zurich, June, 21, 2007.

196) “Structural Biology from the Quantum Chemical Perspective”, ETH, Lugano, Switzerland, June 26, 2007

197) “Structural Biology from a Quantum Chemical Perspective” CERM, University of Florence, Florence, Italy, July 17, 2007.

198) “ Quantum Mechanics in Drug Design: Structural Biology Applications”, ACSPropsectives, Advances in Structure-Based Drug Discovery, San Francisco, California, September 9 - 11, 2007.

199) “Quantum Mechanics in Structural Biology”, MPI 2007, University of Kansas, Lawrence, Kansas, September 30-October 2, 2007.

200) “Is Biology Quantum Mechanical?”, Michigan State University, East Lansing, Michigan, October 26, 2007.

201) “Is Biology Quantum Mechanical?”, St. Edwards University, Austin, Texas, November 15, 2007.

202) “Is Biology Quantum Mechanical?”, MM2007, Melbourne, Australia, November 27-30, 2007.

203) “Is Biology Quantum Mechanical?”, HKUST, Department of Chemistry, Hong Kong, China, December 3, 2007.

204) "A Quantum of Common Sense in Crystallography" OpenEye CUP IX, Santa Fe, New Mexico, March 17-19, 2008.

205) “Quantum Mechanics in Drug Discovery and Design” Computer-Aided Drug Design, Keystone Symposia, Steamboat, Colorado, March 29-April 3, 2008.

206) “The Hydrolysis of Formamide and the Proficiency of Amidohydrolases: The Burden Borne by $k_W$”, FAME, Orlando, Florida, May 9, 2008.

207) ”Quantum Mechanics in Drug Discovery and Design”, FAME, Orlando, Florida, May 9, 2008.

208) “A Quantum of Common Sense in Crystallography” Pushing the Boundaries of Biomolecular Simulations, ISQBP President’s Meeting, Ascona, Switzerland, June 8-13, 2008.

209) “Integrated Free Energy Simulations and X-ray Refinement Studies” Fall ACS Meeting, Philadelphia, Pennsylvania, August 17-21, 2008.

210) “The Past, Present and Future of the AMBER Biomolecular Modelling Package”, WATOC 2008, Sydney, Australia, September 14-19.

211) “A Quantum of Common Sense in Crystallography” TACC 2008, Shanghai, China, September 23-27, 2008.

212) “A Quantum of Common Sense in Crystallography” Fall ACS Meeting, Washington, DC, August 16-20, 2009.

213) “Quantum Mechanics in Drug Discovery and Design” Fall ACS Meeting, Washington, DC, August 16-20, 2009.

214) “Much Ado About Quantum Chemistry: Structure Refinement using Quantum Chemistry” CUPX, Santa Fe, New Mexico March 9-11, 2009.

215) “Much Ado About Quantum Chemistry: Structure Refinement using Quantum Chemistry” University of Connecticut, Storrs, Connecticut, April 20, 2009.

216) “A Quantum of Common Sense in Crystallography: Structure Refinement using Quantum Chemistry" Ecole Polytechnique, Paris, France, July 8, 2009.

217) “A Quantum of Common Sense in Crystallography: Structure Refinement using Quantum Chemistry" Model(l)ing09, Erlangen, Germany, September 7-11, 2009

218) “A Dose of Quantum Mechanics in Structural Biology: Structure Refinement using Quantum Chemistry” The University of Texas at Austin, Austin Texas, October 26, 2009.

219) “A Dose of Quantum Mechanics in Structural Biology: Structure Refinement using Quantum Chemistry” GSK, Philadelphia, Pennsylvania, November 13, 2009.

220) “A Dose of Quantum Mechanics in Structural Biology: Structure Refinement using Quantum Chemistry” Vitae Pharmaceuticals, Philadelphia, Pennsylvania, December 21, 2009.

221) “A Dose of Quantum Mechanics in Structural Biology: Structure Refinement using Quantum Chemistry” Second National Seminar and Workshop on Computer Aided Drug Design, Penang, Malaysia, December 8-11, 2009.

222) “Role of Quantum Mechanics in Protein Folding and Structure-Based Drug Design” Second National Seminar and Workshop on Computer Aided Drug Design, Penang, Malaysia, December 8-11, 2009.

223) “Computational Chemistry Challenges: Error Analysis Applied to Energy Computation” ACS Award for Computers in Chemical and Pharmaceutical Research Sponsored by ACS, ACS National Meeting, San Francisco, California, March 20-25, 2010.

224) “Quantum Chemical Insights into the Computation of Protein-Ligand Binding Free Energies” ESPA2010, Oviedo, Spain, June 30- July 2, 2010.

225) “Quantum Chemical Insights into the Computation of Absolute Energies” XXVI Meeting of the Reference Network on Theoretical and Computational Chemistry, Barcelona, Spain, July12-13, 2010.

226) "Quantum Chemical Insights into the Computation of Absolute Interaction Energies" "Bio-molecular Simulations on Future Computing Architectures" Oak Ridge, Tennessee, September 16-17, 2010.

227) "A Dose of Quantum Mechanics in Structural Biology" International CECAM-Workshop: Approximate Quantum-Methods, Bremen, Germany, September 20-24, 2010.

228) "How Good Do We Have to be to Compute Absolute Interaction Energies in Macromolecular Systems?" CUNY Graduate School, New York, New York October 7, 2010.

229) "Refinement Induced Stress and Strain: The Strain Energy of Protein-ligand Complexes" CUNY Hunter College, New York, New York October 8, 2010.

230) "Predicting Protein-ligand Binding Free Energies: How Good Do We Have To Be?" University of Minnesota, Minneapolis, Minnesota October, 26, 2010.

231) "How Good Do We Have to be to Compute Absolute Interaction Energies for Macromolecular Systems?" Texas A&M University, Doha, Qatar, January 20, 2011.

232) "How Good Do We Have to be to Solve the Protein Folding and Protein-ligand Scoring Problems?" Michigan State University, East Lansing, Michigan, February 21, 2011.

233) "A Little Experimental Information Goes a Long Way to Making Things Right" CUP XII Meeting, Santa Fe, New Mexico, March 6-9, 2011.

234) "How Accurate are Calculations Anyway?" 4$^{th}$ NAGC 2011, Patras, Greece, June 14-18, 2011.

235) "How Accurate are Calculations Anyway?" Free Energy Simulation: From Academic Research to Industrial Application, Telluride, Colorado, July 4-8, 2011.

236) "How Accurate are Calculations Anyway?" Innovative Approaches to Computational Drug Discovery, CECAM-HQ-EPFL, Lausanne, Switzerland, October 3-6, 2011

237) "How Accurate are Docking Calculations Anyway?" Structural & Computational Chemistry, Munich, Germany, March 13-14 2012.

238) "Making Docking/Scoring Calculations more Accurate via Error Analysis" New Approaches in Drug Design and Discovery, Rauischholzhausen, Germany, March 19-22, 2012.

239) "Making Docking/Scoring Calculations More Accurate via Error Analysis" Structure-Based Drug Design, Boston, Massachusetts, June 6-8, 2012.

240) "Exploring the ArsR/SmtB Family of Zinc Sensing Transcriptional Regulators" UCLA ICQC Satellite Symposium QM and MD of Organic and Biological Reactivity, Los Angeles, California, June 21-23, 2012.

241) "Making Docking/Scoring Calculations More Accurate via Error Analysis" 244$^{th}$ ACS National Meeting, Philadelphia, Pennsylvania, August 19-23, 2012.

242) "Novel Approaches to Study Protein-Ligand Interactions" 10$^{th}$ Chemical Physics Congress, University of Economics and Technology, Ankara, Turkey, October 10-12, 2012.

243) "Novel Approaches to Study Protein-Ligand Interactions" Boğaziçi University, Istanbul, Turkey, October 16, 2012.

244) "Allosteric Response to Transition Metal Sensing: The Case of the ArsR/SmtB Family of Transcriptional Regulators" Department of Chemistry, University of North Florida, November 15, 2012.

245) "Novel Approaches to Study Protein-Ligand Interactions" 245th ACS National Meeting, New Orleans, Louisiana, April 7-11, 2013.

246) "Using Computed Gold Standard Interaction Energies to Validate Baser Methods" 245th ACS National Meeting, New Orleans, Louisiana, April 7-11, 2013.

247) "Using computed gold standard interaction energies to validate baser methods" SETCA, Auburn, Alabama, May 9-11, 2013.

248) "Protein Structure Determination and Analysis Using Electronic Structure Based NMR Methods" Gordon conference on "Computational Aspects - Biomolecular NMR", Mount Snow Resort, West Dover, VT, June 2-7, 2013.

249) "Blurring to Bring Binding Free Energies into Focus" Structure-Based Drug Design, Boston, Massachusetts, June 19-21, 2013.

250) “Blurring to Bring Binding Free Energies into Focus” International Conference on Chemical Bonding, Kaua’i, Hawaii, July 4-8, 2013.

251) “Free Energies from a Molecular Printing Press” University of Wisconsin, September 17, 2013.

252) “Free Energies from a Molecular Printing Press” RIKEN, Tokyo, Japan, September 26, 2013.

253) “Free Energies from a Molecular Printing Press” CECAM Innovative Approaches to Drug Discovery, Lausanne, Switzerland, October 1-4, 2013.

254) “Free Energies from a Molecular Printing Press” Drug Discovery Re-Invented Conference, Scottsdale, Arizona, October 16-19, 2013.

255) “Free Energies from a Molecular Printing Press” SERMACS, Atlanta, Georgia November 12-16, 2013.

256) “Using Quantum Mechanics in Biological Structure Refinement” Biophysical Society Meeting, San Francisco, California, February 15-19, 2014.

257) “Free Energies from a Molecular Printing Press” Facility for Rare Isotope Beams (FRIB), Michigan State University, East Lansing, Michigan, April 15, 2014.

258) “Free Energies from a Molecular Printing Press” Department of Chemistry, Bowling Green State University, Bowling Green, Ohio, April 15, 2014.

259) “Free Energies from a Molecular Printing Press” Department of Chemistry, University of New Orleans, New Orleans, Louisiana, May 2, 2014.

260) “Free Energies from a Molecular Printing Press” Frontiers in Computational Chemistry International Workshop, East China Normal University, Shanghai, China, May 24-25, 2014.

261) “Free Energies from a Molecular Printing Press” Modeling the Effects of Water and Solvation in Biological Systems: Developments and Applications, 248th ACS National Meeting, San Francisco, California, August 10-14, 2014.

262) “Thermodynamic Quantities from a Molecular Printing Press” Department of Chemistry, Michigan State University, September 23, 2014.

263) “Thermodynamic Quantities from a Molecular Printing Press” Department of Chemistry, University of Michigan, September 25, 2014.

264) “Thermodynamic Quantities from a Molecular Printing Press” Big Data Analytics and Solutions, 12$^{th}$ Annual Drug Discovery on Target, October 8-9, 2014.

265) “Thermodynamic Quantities from a Molecular Printing Press” Department of Chemistry, McGill University, Montreal, Quebec, Canada, October 14, 2014.

266) “Thermodynamic Quantities from a Molecular Printing Press” The INDO-US Conference on Molecular Modeling and Informatics in Drug Design, NIPER, Mohali, India, November 3-6, 2014.

267) “Thermodynamic Quantities from a Molecular Printing Press” Dart NeuroSciences, LLC, San Diego, California, December 8, 2014,

268) “Thermodynamic Quantities from a Molecular Printing Press” RACI National Congress, Adelaide, Australia, December 7-12, 2014.

269) “Thermodynamic Quantities from a Molecular Printing Press” Wayne State University, Department of Chemistry, February 11, 2015.

270) “Thermodynamic Quantities from a Molecular Printing Press” AMBER Developer’s Meeting, University of Florida, Department of Chemistry, February 13-16, 2015.

271) “Thermodynamic Quantities from a Molecular Printing Press” 249$^{th}$ National ACS Meeting, Denver, Colorado, March 22-26, 2015.

272) “Thermodynamic Quantities from a Molecular Printing Press” X European Workshop in Drug Design, Certosa di Pontignano, Siena, Italy, May 17-22, 2015

273) “Thermodynamic Quantities from a Molecular Printing Press” Modeling and Simulation of Biological and Macromolecular Systems - Satellite Meeting of the 15$^{th}$ International Congress of Quantum Chemistry (ICQC), Changchun, Jilin Province, China, June 4-6, 2015.

274) “Thermodynamic Quantities from a Molecular Printing Press” GSK, Collegeville, Pennsylvania, May 28, 2015.

275) “Thermodynamic Quantities from a Molecular Printing Press” CERM, Florence, Italy, July 13, 2015.

276) “Thermodynamic Quantities from a Molecular Printing Press” Fondazione Istituto Italiano di Tecnologia (IIT), Genoa, Italy, July 22, 2015.

277) “Thermodynamic Quantities from a Molecular Printing Press” 250$^{th}$ ACS National Meeting, Boston, Massachusetts, August 16-20.

278) “Thermodynamic Quantities from a Molecular Printing Press” MSU Drug Discovery Seminar Series, East Lansing, Michigan, September 4, 2015.

279) “Thermodynamic Quantities from a Molecular Printing Press” Computational Advances in Drug Discovery, Lausanne, Switzerland, September 22-25.

280) ”Thermodynamic Quantities from a Molecular Printing Press” Georgia Tech, Atlanta, Georgia, October 15, 2015.

281) Adventures in Structure-based Drug Discovery" Georgia Tech, Atlanta, Georgia, October 16, 2015

282) Accurate Modeling of Metal Ions in Aqueous Solution" Pacifichem 2015, Honolulu, Hawaii, December 15-20, 2015.

283) "MT's Performance in the D3R Grand Challenge and SAMPL5" D3R Workshop, San Diego, California, March 9-12, 2016.

284) "Thermodynamics of Virus Capsid Assembly" 251st National ACS Meeting, San Diego, California, March 12-18, 2016.

285) "AMBER Related Developments in the Merz Research Group" AMBER Meeting, San Diego Supercomputer Center, San Diego, California, March 18-20, 2016.

286) "Metal Ion Homeostasis: Getting Transition Metal ions Around Cells Safely" Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments, Pisa, Italy, May 23-25, 2016.

287) "Using QM Methods to Refine Biological Structure" European Charge Density Meeting (ECDM 7), Warsaw, Poland, 26th June - 1st July, 2016.

288) "Rapid Computation of Thermodynamic Quantities for Molecular Recognition Processes" Strasbourg Summer School in Chemoinformatics, Strasbourg, France, June 27-July 1, 2016.

289) "2016 Computational Chemistry GRC Past, Present and Future" PGA Catalunya Business and Convention Centre, Girona, Spain, July 24-29 2016.

290) "Thermodynamics of Virus Capsid Assembly in Aqueous Solution" 252nd National ACS Meeting, Philadelphia, Pennsylvania, August 21-25, 2016.

291) "Rapid Estimation of Thermodynamic Quantities for Molecular Recognition Processes" EMLG/JMLG Joint Meeting, Plantanias-Chania Greece, September 11-16, 2016.

292) "Rapid Computation of Thermodynamic Quantities for Molecular Recognition Processes" Chem-Bio Informatics Society (CBI) Annual Meeting, Tokyo, Japan, October 25-27, 2016.

293) "Adventures in Structure-based Drug Discovery" 4th Annual Conference on Computation for Sciences and Technology, Langkawi, Malaysia, November 3-4, 2016.

294) "Using QM Methods to Refine Biological Structure" Approximate Quantum Methods in the ab initio World, Beijing, China, November 6-13, 2016.

295) "Allostery Driven by Metal Ions" Getting Transition Metal Ions Around Cells Safely" 251nd National ACS Meeting, San Francisco, California, April 2-6, 2017.

296) “Exploration of Molecular Recognition Processes” 11th European Workshop in Drug Design, Siena, Italy, May 21-26, 2017

297) “Exploration of Molecular Recognition Processes” Beyond Kd’s: New Computational Methods to Address Challenges in Drug Discovery , Lausanne, Switzerland, June 6-9, 2017.

298) “Using QM Methods to Refine Biological Structures” Quantum Crystallography: Current Developments and Future Perspectives, Nancy, France, June 19-20, 2017.

299) “The Role of Computation in Drug Discovery” Biomedical Research Foundation, Athens, Greece July 6, 2017.

300) “Role of Dynamics in Enzymatic Electrophilic Aromatic Substitution” 254th National ACS Meeting, Washington, DC, August 20-24, 2017.

301) “Exploration of Molecular Recognition Processes” Bar-Ilan University, Tel Aviv, Israel, September 4, 2017.

302) “Exploration of Molecular Recognition Processes” SBDD 2017: Computational Advances in Drug Discovery, Lausanne, Switzerland, September 5-8, 2017.

303) “Exploration of Molecular Recognition Processes” International Computational Science and Engineering Conference, Doha, Qatar, October 23-24, 2017.

304) “Exploration of Molecular Recognition Processes” RIKEN, Tokyo, Japan, November 29, 2017.

305) “Role of Reaction Dynamics and Surface Topology in Enzymatic Catalysis” Kyoto University, Kyoto, Japan, December 1, 2017.

306) “Exploration of Molecular Recognition Processes” Computer Aided Drug Design Seminar and Workshop, Langkawi, Malaysia, December 6-8, 2017.

307) “General Introduction to Force Fields” Computer Aided Drug Design Seminar and Workshop, Langkawi, Malaysia, December 6-8, 2017.

308) “Exploration of Molecular Recognition Processes Encountered in Structure-based Drug Design” UIUC, Champaign, Illinois, December 13, 2017.

309) “Merz Group Additions to AMBER” AMBER Developer’s Conference, Tampa, Florida, February 7-10, 2018.

310) “Exploration of Molecular Recognition Processes Encountered in Structure-based Drug Design” UNC, Chapel Hill, North Carolina, March 6, 2018.

311) “Modeling Metal Ions Using Classical Potentials: Approach and Application to Metal Ion Homeostasis” Physiological Role of Ions in the Brain: Towards a Comprehensive View by Molecular Simulation, Pisa, Italy, May 21-23, 2018

312) “Using QM Methods to Refine Biological Structures ”International School of Crystallography 52nd Course: Quantum Crystallography, Erice, Sicily, June 3-9, 2018

313) “Exploration of Intermolecular Interactions”Computational Chemistry GRC, Mount Snow, July 22-27, 2018

314) “Long term Viability of Computational Chemistry/Biology Research” ACS National Meeting, Boston, August 19-23, 2018

315) “Exploration of Molecular Recognition Processes” 22nd Euro QSAR, Thessaloniki, Greece, September 16-20, 2018

316) “Role of Dynamics and Surface Topology in Enzymatic Catalysis” Future of Enzyme Modeling, Stockholm, Sweden, September 28-29, 2018

317) Modeling Transition Metal Ions: Solvation to the Chelate Effect UIUC, Theoretical and Computational Biophysics Group, Beckman Institute, Champaign, Illinois, October 21, 2017

318) “Applying Simulations and Machine Learning to Biological Problems” CADD 2018 Bali, Indonesia, November 26-30, 2018

319) “Role of Reaction Dynamics and Surface Topology in Enzymatic Catalysis” Huazhong University of Science and Technology, Wuhan, China, December 4, 2018

320) “Exploration of Molecular Recognition Processes” Wuhan University of Technology, Wuhan, China, December 5, 2018

321) “Exploration of Molecular Recognition Processes” 4th Drug Discovery Re-Invented Conference, Nassau, Bahamas, February 21-24, 2019

322) “Simulating Coordination Chemistry” Riken, Tokyo, Japan March 6, 2019

323) “Merz Group Additions to AMBER” AMBER Developer’s Conference, Tampa, Florida, February 27-30, 2019

324) “Exploration of Molecular Recognition Processes Using Machine Learning” Twelfth European Workshop in Drug Design (XII EWDD), Siena, Italy, May 19-24, 2019

325) “Simulating Coordination Chemistry”, Challenges in modeling and simulations of nanoparticles in complex environments, Genoa, Italy, May 29-31, 2019

326) “Simulating Coordination Chemistry” Biomedical Research Foundation, Academy of Athens (BRFAA), Athens, Greece, July 3, 2019.

327) “Exploration of Molecular Recognition Processes Using Machine Learning” SBQT 2019 XX Brazilian Symposium on Theoretical Chemistry, Joao Pessoa, Brazil, November 10-14, 2019

328) “Simulating Coordination Chemistry” AMBER Developers Meeting, Tampa, Florida, February 6-8, 2020.

329) “Efficient GPU Enabled QM/MM Calculations: AMBER Coupled with GPU Enabled QUICK” NSF CSSI PI Meeting, Seattle, Washington, February 12-15 2020.

330) “Metabolite Structure Assignment Using *in silico* NMR and Collision Cross Section (CCS) Techniques” Symposium on “Assigning Structures to Spectra Using Density Functional Theory: Methods and Application” APS March Virtual Meeting 2021 March 15-19, 2021

331) “Evolutionary de Rham-Hodge analysis of electron densities for the prediction of molecular properties”, CECAM meeting on “Second Discussion Meeting on Quantum Crystallography: Expectations and Reality”, Virtual September 9-12, 2021.

332) “*In silico* Workflows for Metabolite Structure Elucidation” The University of Arkansas, Chemistry Department, November 8, 2021.

333) “Open-source GPU-enabled ab initio QM/MM with QUICK/AMBER including long-range electrostatics” Sanibel Symposium, St. Simon’s Island, Georgia, February 13-18.

334) “A Polarizable Cationic Dummy Metal Ion Model” PacificChem, December 18, 2021.

335) “Modeling Transition Metal Ions in Aqueous Solution A Polarizable Cationic Dummy Metal Ion Model” ACS National Meeting, San Diego, California, March 20-24, 2022.

**Contributed Presentations**

**Posters**

1) "The Catalytic Mechanism of Human Carbonic Anhydrase II", The International Symposium on Physical Organic/Theoretical Chemistry, Austin, Texas, February 25-28 1988.

2) Electrostatic Potential Derived Point Charges for Monosaccharides", Computational Chemistry Gordon Research Conference, Plymouth State College, July 18-22, 1990.

3) "$CO_2$ Binding to HCAII," Biophysical Society Meeting, San Francisco, California, February 24-28, 1991.

4) "Non-Aqueous Solvation of Proteins", Computational Chemistry Gordon Research Conference, New Hampton School, June 29-July 3, 1992.

5) "A Force Field for 1-4 Linked Polysaccharides", Biophysical Society Meeting, Washington, DC, February 14-18, 1993.

6) "Molecular Dynamics Simulation of a Lipid Bilayer-Peptide System", Biophysical Society Meeting, Washington, DC, February 14-18, 1993.

7) "Protein Dynamics in Aqueous and Nonaqueous Environments", Biophysical Society Meeting, Washington, DC, February 14-18, 1993.

8) "A Force Field for 1-4 Linked Polysaccharides", The Structure/Function Relationships in Proteins and Enzymes, State College, Pennsylvania, July 26-30, 1993.

9) "Coupled Quantum/Molecular Mechanical Simulations of Human Carbonic Anhydrase II", 11th International Congress of Biophysics, Budapest, Hungary, July 25-30, 1993.

10) "Interaction of Small Peptides with Lipid Bilayers", Biophysical Society Meeting, New Orleans, Louisiana, March 6-10, 1994.

11) "Testing of a Density Functional/Molecular Mechanical Coupled Potential", American Chemical Society Meeting, San Diego, California, March 13-18, 1994.

12) "Parallel Implementation of a Density Functional/Molecular Mechanical Coupled Potential", Computational Chemistry Gordon Research Conference, New Hampton School, New Hampshire, July 3-8, 1994.

13) "The Adsorption of Carbohydrates onto Metal Surfaces", Computational Chemistry Gordon Research Conference, New Hampton School, New Hampshire, July 3-8, 1994.

14) "Interaction of the Fusion Inhibiting Peptide Z-D-Phe-L-Phe-Gly with N-Methyl DOPE (DOPE-Me) Bilayers", FASEB Conference on Membrane Molecular Biophysics, Saxtons River, Vermont, July 16-21, 1994.

15) "Solvation and Dynamics of Chymotrypsin in Hexane" S Toba; K. M. Merz, Jr. Protein Society Meeting, San Jose, California, August 4-9, 1996.

16) "Ice-Binding Mechanism of the Anti-Freeze Protein Determined By Molecular Dynamics Simulations" A. Cheng; K. M. Merz, Jr. 12th International Biophysics Congress, Amsterdam, The Netherlands, August 11-16, 1996.

17) "Role of Active Site Water Molecules in the Mechanism of Human Carbonic Anhydrase II" S. Toba; K. M. Merz, Jr. American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

18) "Fully Quantum Mechanical Calculations on Solvated Biomolecular Systems: New Insights and Implications for QM/MM Simulation Techniques" A. van der Vaart; K. M. Merz, Jr. American Chemical Society Meeting, New Orleans, Louisiana, August 22-26, 1999.

18) "Investigation of Enzyme Reactivity Using MM, QM/MM and Linear Scaling Approaches: Human Fibroblast Collagenase" G. Monard; K. M. Merz, Jr. American Chemical Society Meeting, New Orleans, Louisiana, August 22-26, 1999.

19) "A Molecular Dynamics Simulation of Liquid water Using the Divide and Conquer Approach and a Corrected PM3 Semiempirical Method" G. Monard; M. J. Bernal-Uruchurtu; A. van der Vaart; K. M. Merz, Jr.; M. F. Ruiz-Lopez "ESCR Conference", Bellaterra, Spain, September 19-22, 2001.

20) "Pose Scoring by NMR" ISQBP President's Meeting, Como, Italy, June 6-8, 2004.

21) "QMQSAR: A semi-empirical (PM3) field-based QSAR program" Steve Dixon: K. M. Merz, Jr.: Giorgio Lauri; James Ianni; Marisa C Kozlowski American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

22) "Theoretical Study of the Electron Density Distributions in a Dipeptide Molecule" K. M. Merz, Jr.; N.Yu, American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

23) A Fast Semiemprical DivCon/Charmm QM/MM Approach for Biomolecules K. M. Merz, Jr; Xiaodong Zhang, American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

24) "Molecular Dynamics Simulations of Urea-inhibited Urease" G. L. Estiu; D. Suarez; N. Diaz; K. M. Merz, Jr., American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

25) "Effects of Grid Sizes on the Calculation of Solvation Free Energy in a Quantum Continuum Solvation Model" K. M. Merz, Jr; N. Liao, American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

26) “DFT, Molecular Dynamics, and Free Energy Calculations on the Multi-coordinate Cu(I)-Binding Protein Hah1” K. M. Merz, Jr.; B. T. Op't Holt, American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

27) “Evaluation of Semiempirical Methods for Protein Minimization and Decoy Descrimination” A. M. Wollacott; K. M. Merz, Jr., American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

28) “Refinement of Ligand Structure from a Comparison of Experimental and Calculated Chemical Shift Perturbations” B. Wang;, K. Raha; K. M. Merz, Jr., American Chemical Society Meeting, Philadelphia, Pennsylvania, August 22-26, 2004.

29)”Applicability of Semiemperical QM Methods to Study Protein Structure” D. Williams; A. Wollacot; K.M. Merz, Jr., 1st Annual SEAGEP Conference, Clemson University, Clemson, SC, USA. April, 2006.

30) ”Semiempirical Comparative Binding Energy Analysis (SE-COMBINE)”, M. B. Peters; K. M. Merz, Jr. Sanibel Symposium, St. Simon Island, Georgia, USA. Feb. 26- March 2, 2006

31) ”Semiempirical methods in structure based drug design”, M. B. Peters; K. M. Merz, Jr. American Chemical Society, 232nd National Meeting and Exposition, San Francisco, California, USA. September 2006.

32) "Farnesyltransferase, the 7Å Gap and Intermediate States" G. Cui; K. M. Merz, Jr. The 46th Sanibel Symposium, St. Simons Island, Georgia, USA. February 26, -March 2, 2006.

33) “Applicability of Semiemperical QM Methods to Study Protein Structure” D. Williams; A. Wollacot and K.M. Merz, Jr., 46th Sanibel Symposium, St. Simons Island, Georgia, USA. February 26, -March 2, 2006.
34) “Characterizing Protein-Ligand Interactions from NMR Chemical Shift Perturbations” B. Wang; K. M. Merz, Jr. American Chemical Society, The 232th National Meeting, San Francisco, California, USA. September 10-14, 2006.

35) “Characterizing Protein-Ligand Interactions from NMR Chemical Shift Perturbations” B. Wang; K. M. Merz, Jr., The 46th Sanibel Symposium, St. Simons Island, Georgia, USA. February 25 – March 3, 2006.

36) "Quantum-mechanics Flavored Scoring Functions for Protein Structure Evaluation" G. Cui; A. Wollacot, J. S. Yang; E. Shakhnovich, K. M. Merz, Jr., The 3rd UCSC/QB3 Symposium on Bioinformatics 2006, Santa Cruz, CA USA. December 2-3, 2006.

37) “Study of the Liquid Structure of Ethanolamine-Water Systems” E. F. da Silva; A. Hartono; H. F. Svendsen; K. M. Merz Jr., 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22-27, 2007.

38) “A Semiempirical Localized Open Shell Method” K. Ayers; B. Wang; K. M. Merz Jr., 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22-27, 2007.

39) “Combined Quantum Mechanical/Molecular Mechanical Refinement of Cytidine Deaminase Transition State Analog Complexes” X. Li; S. Hayik; K. M. Merz Jr., 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22-27, 2007.

40) “Solvation Effect in Semi-Empirical QM Protein Chemical Shift Calculation” N. Liao; K. M. Merz Jr., 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22-27, 2007.

41) “New schemes in Ligand Based QSAR Methods by Using Fourier Grid Techniques and *Ab Initio* Wavefunctions” L. Fusti-Molnar; M. Peters; K. M. Merz Jr., 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22-27, 2007.

42) “Development of new MNDO Parameters for the Prediction of Chemical Shifts of Drug-like Compounds” D. Williams; M. Peters; K.M. Merz, Jr., 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22-27, 2007.

43) “Development of new MNDO Parameters for the Prediction of Chemical Shifts of Drug-like Compounds” D. Williams, M. Peters; K.M. Merz, Jr. FGLSAMP Exposition, Tampa, Florida USA, February 22-25, 2007

44) ”Design and Development of a Large Object-Oriented Package, MTK++, and an Automated Program for Metalloprotein Force Field Parameters Generation”, M. B. Peters; K. M. Merz, Jr. The 47th Sanibel Symposium, St. Simon Island, Georgia, USA. February 22-27, 2007.

45) “The Alternative Binding in Orf2 Catalyzed Prenylation: Identification and Validation” G. Cui; X. Li,; K. M. Merz, Jr. The 47th Sanibel Symposium, St. Simon Island, Georgia, USA. February 22-27, 2007.

46) “Characterizing Protein-Ligand Interactions from NMR Chemical Shift Perturbations” B. Wang; K. M. Merz, Jr. The 47th Sanibel Symposium, St. Simons Island, Georgia, USA. February 22 – 27, 2007.

**Lectures**

1) "$CO_2$ Binding to HCAII", Biophysical Society Meeting. San Francisco, California, February 24-28, 1991

2) "Association Dynamics of $HCO_3^-$ and $CO_2$ with Human Carbonic Anhydrase II" Biophysical Society Meeting, Houston, Texas, February 9-13, 1992.

3) "Solvent Structure at the Lipid Bilayer-Solvent Interface: Comparison Between DLPE and DMPC Based Bilayers" Biophysical Society Meeting, Washington, DC, February 14-18, 1993.

4) "Mechanism of Action of Fusion Inhibiting Peptides" Biophysical Society Meeting, San Francisco, California, February 12-16, 1995.

5) "Calculation of Octanol-Water Partition Coefficients Using the GB/SA Solvation Model" C. H. Reynolds; S. A. Best; L. C. van Zant; K. M. Merz, Jr. American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

6) "Enzyme Inhibitor Interactions in Matrix Metalloproteinases: Structural and Energetic Studies" K. V. Damodaran; K. M. Merz, Jr. American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

7) "Multiple Time-Step Algorithm for Biomolecular Systems" A. Cheng; K. M. Merz, Jr. American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

8) "Computational Studies of Protein-Solvent and Protein-Ligand Interactions" Kaushik Raha; K. M. Merz, Jr. American Chemical Society Meeting, San Diego, California, March 13-17, 2005.

**Session Chairmanships**

1) "Proteins: Molecular Dynamics" Biophysical Society Meeting, Houston, Texas, February 9-13, 1992.

2) "Proteins: Predictions and Structural Motifs" Biophysical Society Meeting, Houston, Texas, February 9-13, 1992.

3) "Recent Advances in Force Fields", Computational Chemistry Gordon Research Conference, New Hampton School, June 29-July 3, 1992.

4) "Membrane Structure" Biophysical Society Meeting, Washington, DC, February 14-18, 1993.

5) "Using the Computer to Understand Biological Membranes" Biophysical Society Meeting, Baltimore, Maryland, February 18-22, 1996.

6) "Molecular Dynamics" WATOC '96 Conference, Jerusalem, Israel, July 7-12, 1996.

9) "QM/MM Methods" American Chemical Society Meeting, New Orleans, Louisiana, August 22-26, 1999.

10) "Advances in Structure-Based Drug Discovery" Charles Reynolds; K. M. Merz, Jr. ACSProspectives Meeting, Philadelphia, Pennsylvania, October 16-19, 2005.

11) “Structure-based Drug Discovery”, Keystone Symposium, Whistler, British Columbia, Canada, April 2-6, 2006.

12) “Dewar Symposium” ACS National Meeting, San Francisco, California September 10-15, 2006.

13) “Potential function uncertainty and validation” ACS National Meeting, New Orleans, Louisiana, April 7-12, 2013.

14) “Expanding Computational Chemistry with GPUs” ACS National Meeting, Indianapolis, Indiana, September 8-12, 2013.

**Conference Organizer**

1) "Large-Scale Electronic Structure Calculations" American Chemical Society Meeting, Dallas, Texas, March 23-27, 1998.

2) “Molecular Simulations in Structural Biology and Drug Discovery", in memory of Peter Kollman, San Francisco, California, February 21-22, 2002.

3) “Understanding Protein-Ligand Interactions” Charles Reynolds; K. M. Merz, Jr. American Chemical Society Meeting, San Diego, California, March 13-17, 2005.

4) “Advances in Structure-Based Drug Discovery” Charles Reynolds; K. M. Merz, Jr. ACSProspectives Meeting, Philadelphia, Pennsylvania, October 16-19, 2005.

5) “Dewar Symposium” ACS National Meeting, San Francisco, California September 10-15, 2006.

6) “Advances in Structure-Based Drug Discovery”, ACSPropsectives Meeting, San Francisco, California, September 9 - 11, 2007.

7) “Computer-Aided Drug Design”, Keystone Symposia, Steamboat Springs, Colorado, March 29 – April 3, 2008.

**Invited Workshop Lectures**

1) "Force Field Design" Molecular Mechanics and Dynamics of Biopolymers Workshop, Pittsburgh Supercomputer Center, Pittsburgh, Pennsylvania, April 7-10, 1991.

2) "Interaction Energies" Molecular Mechanics and Dynamics of Biopolymers Workshop, Pittsburgh Supercomputer Center, Pittsburgh, Pennsylvania, April 7-10, 1991.

3) "Force Field Design" Molecular Mechanics and Dynamics of Biopolymers Workshop, Pittsburgh Supercomputer Center, Pittsburgh, Pennsylvania, May 14-16, 1991.

4) "Interaction Energies" Molecular Mechanics and Dynamics of Biopolymers Workshop, Pittsburgh Supercomputer Center, Pittsburgh, Pennsylvania, May 14-16, 1991.

5) "Force Field Design"Computational Chemistry Workshop, RPI, Troy, New York, July 31-August 3, 1991.

**Visiting Professorships/Lectureships**

1) "Molecular Modelling" University of Firenze, Italy, April 18-May 15, 1992. This was a ten lecture course on molecular modeling techniques.

2) "Combined Classical/Quantum Mechanical Studies of Enzyme Structure and Function" University of Louis Pasteur, Strasbourg, France, January 25-July 28, 1997.

3) “Modern Computational Chemistry”, Computational Chemistry Lecture Series, CERM, University of Florence, Florence, Italy, June 6 – August 8, 2008. A total of five lectures were delivered to the group at CERM