

VITA OF WILLIAM L. JORGENSEN

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Date of Birth: October 5, 1949 Place of Birth: New York, New York

Education

A.B. in Chemistry, 1970: Princeton University, Princeton, New Jersey
Ph.D. in Chemical Physics, 1975: Harvard University, Cambridge, Massachusetts

Employment

2009- Sterling Professor of Chemistry, Yale University
2009- Director, Division of Physical Sciences and Engineering, Yale University
1990-2009 Whitehead Professor of Chemistry, Yale University
1989 Visiting Professor, Harvard University.
1985-1990 Herbert C. Brown Professor of Chemistry, Purdue University.
1984-1987 Head, Organic Chemistry Division, Purdue University.
1982-1990 Professor, Department of Chemistry, Purdue University.
1979-1982 Associate Professor, Department of Chemistry, Purdue University.
1975-1979 Assistant Professor, Department of Chemistry, Purdue University.
1970-1975 Graduate student, Harvard University (Advisor: E. J. Corey).
1968-1970 Research Assistant, Princeton University.

Honors

2009 Fellow, American Chemical Society
2007 Member, American Academy of Arts and Sciences
2004 Sato Memorial International Award - Pharmaceutical Society of Japan
2004 Award in Computational Biology – Intl. Society for Quantum Biology and Pharmacology
1998 Award for Computers in Chemical and Pharmaceutical Research – Amer. Chem. Soc.
1994 Fellow, American Association for the Advancement of Science
1990 Arthur C. Cope Scholar Award, American Chemical Society
1990 Special Creativity Award, National Science Foundation
1989 Special Creativity Award, National Science Foundation
1986 Annual Medal of the International Academy of Quantum Molecular Sciences
1979 Alfred P. Sloan Foundation Fellow
1978 Camille and Henry Dreyfus Foundation Teacher-Scholar
1970 A.B. summa cum laude; McCay Prize in Chemistry

Invited Lectures

Dr. Jorgensen has presented more than 600 invited lectures including such distinguished lectureships as 7th Marvel Symposium, U. Arizona; 15th Leermakers Symposium, Wesleyan U.; 1988 Nobel Symposium; Organic Synthesis Distinguished Lecturer, U. Colorado - Syntex Symposium; 6th W. S. Johnson Lectures, Stanford U.; Steiglitz Memorial Lecturer; Research Scholar Lecturer, Drew U.; Royal Society Faraday and Perkin Lectures; Visiting Lecturer, ETH Zürich; 34th National Organic Symposium; Tetrahedron Symposium 2004 & 2008; Tanabe Lecturer, Scripps; Hirschmann Lecturer, Oberlin; Gunning Lecturer, U. Alberta; H. C. Brown Lecturer, Purdue U.; Schleyer Lecturer, U. Georgia; Gerhard Closs Lecturer; U. Chicago; ISQBP Plenary Lecturer; BMS Lecturer, Scripps; 3eme Cycle Lecturer, Switzerland; Olsen Lecturer, Utah State; Lise Meitner Lecturer, Israel. A complete list of recent invited lectures is at the end of this document.

Editor

Journal of Chemical Theory and Computation, 2005-
Journal of Chemical Information and Modeling (formerly JCICS), 2005-
Journal of Chemical Information and Computer Sciences (JCICS), 2004
Encyclopedia of Computational Chemistry, 2001-2005
Journal of Computational Chemistry, 2002 –2003

Member or Officer

National Institutes of Health, Medicinal Chemistry A Study Section, 2001-2004
American Chemical Society -
 Chairman-Elect, Computers in Chemistry Division, 2001; Chairman, 2002
International Society for Quantum Biology and Pharmacology -
 Vice President, 2000; President, 2001-2002

American Chemical Society Committees

W. Gibbs Medal Nominating Committee, 2001-2004
Board of Editors, 2004-
ACS Executive Director's 2010 Committee, 2004-2009
ACS Executive Director's 2020 Committee, 2009-
ACS Assessing the IT Future Committee, 2006
Search Committee for the Publications Division President, 2007
Task Force to Recommend Appointments to the Governing Board of Publishing, 2009
Chair, Search Committee for the Editor of ACS Medicinal Chemistry Letters, 2009
Task Force on Author Rights and Obligations, 2009

Yale Committees

Physical Sciences & Engineering Advisory Committee, 1994-96, 2004-
Biological Sciences Advisory Committee, 2004-2006
Scholar Awards Committee, 2005-9
Chemical Biology Institute Advisory Committee, 2009-
Fellow, Trumbull College, 1990-
Chemistry Dept.: Advisory, Planning, Building, Hiring, Awards

Memberships on Advisory Boards

Analyst for Data Trace, Inc. (Chemtracts) 1986-98
Advisory Committee, NIH Regional NMR Center (Columbia U.), 1986-90
Scientific Advisory Board, Evans & Sutherland Inc., 1987-92
Scientific Advisory Board, Ariad Pharmaceuticals Inc., 1991-
Scientific Advisory Board, CombiChem Inc., 1994-1999
Scientific Advisory Board, Schrödinger Inc., 1996-
Scientific Advisory Board & Founder, Rib-X Pharmaceutical Inc., 2001-
Current Consultant: Pfizer Global Research
Past Consultant: Agouron Pharmaceuticals, Parke-Davis, Pharmacia
AAAS Electorate Nominating Committee, 2003-2006; Chair, 2004
World Association of Theoretical & Computational Chemists (WATOC), 2003-
J. Allyn Taylor International Prize in Medicine Committee, 2006
NIH, Centers for Chemical Informatics Advisory Board, 2006
NSF, Mathematical & Physical Sciences Advisory Committee, 2006-9

Editorial Advisory Boards

Bioorganic and Medicinal Chemistry Letters, 1990-
Bioorganic and Medicinal Chemistry, 1992-
Journal of Computer Aided Molecular Design, 1992-
Supramolecular Chemistry, 1992-2009
Journal of the American Chemical Society, 1987-93
CRC Critical Reviews in Theoretical Chemistry and Biophysics, 1987-93
Journal of Physical Organic Chemistry, 1987-94
Journal of Computational Chemistry, 1989-2003
Theoretica Chimica Acta, 1990-94
Theoretical Chemistry Accounts, 1997-2002
Chemistry and Biology, 1994-2004
Accounts of Chemical Research, 2001-2004; 2009-2011

Memberships in Professional Societies

American Chemical Society
American Physical Society
American Association for the Advancement of Science
International Society for Quantum Biology and Pharmacology
World Association of Theoretical & Computational Chemists
Connecticut Academy of Arts and Sciences
American Academy of Arts and Sciences
Israeli Chemical Society (Honorary Life Member)

Publications - W. L. Jorgensen

1. Structural and Energetic Predictions for Simple Hydrocarbons from the NDDO and CNDO Semiempirical Molecular Orbital Methods.
R. B. Davidson, W. L. Jorgensen, and L. C. Allen
J. Am. Chem. Soc., 92, 749 (1970).
2. Charge Distribution Characteristics of Attractive Dominant Barriers.
W. L. Jorgensen and L. C. Allen
Chem. Phys. Letts., 7, 483 (1970).
3. Charge Density Analysis of Rotational Barriers.
W. L. Jorgensen and L. C. Allen
J. Am. Chem. Soc., 93, 567 (1971).
4. Chemical Consequences of Orbital Interactions in Hydrocarbons Containing Unsaturatively Bridged Small Rings.
W. L. Jorgensen and W. T. Borden
J. Am. Chem. Soc., 95, 6649 (1973).
5. "The Organic Chemist's Book of Orbitals".
W. L. Jorgensen and L. Salem
Academic Press, New York, 1973.

In German, "Orbitale Organischer Molekule", Verlag Chemie. Weinheim/Bergstr., 1974.
6. Orbital Interactions in Molecules Containing Unsaturatively Bridged Cyclobutane and Bicyclobutane Rings.
W. L. Jorgensen and W. T. Borden
Tetrahedron Letters, 223 (1975).
7. Chemical Consequences of Orbital Interactions. II. Ethylene and Butadiene Bridged Polycyclic Hydrocarbons Contain Three- and Four-Membered Rings.
W. L. Jorgensen
J. Am. Chem. Soc., 97, 3082 (1975).
8. Computer-Assisted Synthetic Analysis. Synthetic Strategies Based on Appendages and the Use of Reconnective Transforms.
E. J. Corey and W. L. Jorgensen
J. Am. Chem. Soc., 98, 189 (1976).

9. Computer-Assisted Synthetic Analysis. Generation of Synthetic Sequences Involving Sequential Functional Group Interchanges.
E. J. Corey and W. L. Jorgensen
J. Am. Chem. Soc., 98, 203 (1976).
10. The Energetic Impact of Monohomoaromaticity.
W. L. Jorgensen
J. Am. Chem. Soc., 98, 6784 (1976).
11. The Behavior of Trishomocyclopropenyl Cations.
W. L. Jorgensen
Tetrahedron Letters, 3027 (1976).
12. The Structure and Stability of Coates' Cations.
W. L. Jorgensen
Tetrahedron Letters, 3033 (1976).
13. The Cyclic Structure of Monomeric Dilithioacetylene.
Y. Apeloig, P. v. R. Schleyer, J. S. Binkley, J. A. Pople, and W. L. Jorgensen
Tetrahedron Letters, 3923 (1976).
14. The Similarity of Solvent Effects on Carbocations.
W. L. Jorgensen
J. Am. Chem. Soc., 99, 280 (1977).
15. The Influence of Increasing Solvation on the Relative Energies of Bisected and Bridged Ethyl Cations.
W. L. Jorgensen and J. E. Munroe
Tetrahedron Letters, 581 (1977).
16. The Importance of the Counter Ion. The Structures and Relative Energies of Homocubyl Cations and Ion Pairs.
W. L. Jorgensen
J. Am. Chem. Soc., 99, 4272 (1977).
17. Simple Prediction of Substituent Sensitivity for Carbocations.
W. L. Jorgensen
J. Am. Chem. Soc., 99, 3840 (1977).

18. Cycloaddition Reactions of 1,2,5,6-Tetramethyl-3,4,7,8-tetramethylenetricyclo[3.3.0.0(2,6)]octane. Evidence for Chemical Consequences of Orbital Interactions in Molecules Containing Unsaturation in 1,3-Bridged Cyclobutane Rings.
W. T. Borden, A. Gold, and W. L. Jorgensen
J. Org. Chem., 43, 491 (1978).
19. Proton Affinity Correlations for Alkyl Chlorides.
W. L. Jorgensen
Chem. Phys. Letts., 53, 525 (1978).
20. The Electronic Structure and Protonation of Alkyl Chlorides.
W. L. Jorgensen
J. Am. Chem. Soc., 100, 1049 (1978).
21. Stereoelectronic Effects on the Protonation and Properties of 2-Norbornyl Chlorides.
W. L. Jorgensen and J. E. Munroe
J. Am. Chem. Soc., 100, 1511 (1978).
22. Ab Initio Molecular Orbital Study of the Geometries, Properties and Protonation of Alkyl Chlorides.
W. L. Jorgensen
J. Am. Chem. Soc., 100, 1057 (1978).
23. MINDO/3 Calculation of the Potential Energy Surface for $C_3H_5^+ \rightarrow C_3H_3^+ + H_2$ as Applied to Understanding Energy Partitioning Accompanying Fragmentation.
D. A. Krause, R. J. Day, W. L. Jorgensen, and R. G. Cooks
Int. J. Mass Spectrom. Ion Phys., 27, 227 (1978).
24. An Intermolecular Potential Function for the HF Dimer from Ab Initio 6-31G Computations.
W. L. Jorgensen and M. E. Cournoyer
J. Am. Chem. Soc., 100, 4942 (1978).
25. Ab Initio Molecular Orbital Study of the Geometries, Properties, and Protonation of Simple Organofluorides.
W. L. Jorgensen and M. E. Cournoyer
J. Am. Chem. Soc., 100, 5278 (1978).
26. The Photoelectron Spectra of the 1,2,5,6-Tetramethyl-3,4,7,8-tetramethylene Derivatives of Tricyclo[3.3.0.0(2,6)]octane and Tricyclo[4.2.0.0(2,5)]octane.
W. T. Borden, S. D. Young, D. C. Frost, N.P.C. Westwood, and W. L. Jorgensen
J. Org. Chem., 44, 737 (1979).
27. Monte Carlo Simulations of Liquid Hydrogen Fluoride.

- W. L. Jorgensen
J. Am. Chem. Soc., 100, 7824 (1978).
28. Deriving Intermolecular Potential Functions for the Water Dimer from Ab Initio Calculations.
W. L. Jorgensen
J. Am. Chem. Soc., 101, 2011 (1979).
29. Minimal Basis Set Description of the Structure and Properties of Liquid Water.
W. L. Jorgensen
J. Am. Chem. Soc., 101, 2016 (1979).
30. Basis Set Dependence in Monte Carlo Simulations of Liquid Hydrogen Fluoride.
W. L. Jorgensen
J. Chem. Phys., 70, 5888 (1979).
31. Energy Partitioning Accompanying Fragmentation of Protonated Methanol.
R. J. Day, D. A. Krause, W. L. Jorgensen, and R. G. Cooks
Int. J. Mass Spectrom. Ion Phys., 30, 83 (1979).
32. An Intermolecular Potential Function for the Methanol Dimer from Ab Initio Calculations.
W. L. Jorgensen
J. Chem. Phys., 71, 5034 (1979).
33. The Structure and Properties of Liquid Methanol.
W. L. Jorgensen
J. Am. Chem. Soc., 102, 543 (1980).
34. The Structure and Properties of Liquid Ammonia.
W. L. Jorgensen and M. Ibrahim
J. Am. Chem. Soc., 102, 3309 (1980).
35. Monte Carlo Results for Hydrogen Bond Distributions in Liquid Water.
W. L. Jorgensen
Chem. Phys. Lett., 70, 326 (1980).
36. Computer Assisted Mechanistic Evaluation of Organic Reactions, I. Overview.
T. D. Salatin and W. L. Jorgensen
J. Org. Chem., 45, 2043 (1980).
37. Transferable Intermolecular Potential Functions for Water, Alcohols, and Ethers. Application to Liquid Water.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 335 (1981).

38. Transferable Intermolecular Potential Functions. Application to Liquid Methanol Including Internal Rotation.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 341 (1981).
39. Simulation of Liquid Ethanol Including Internal Rotation.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 345 (1981).
40. Computer Assisted Mechanistic Evaluation of Organic Reactions, 2. Perception of Rings, Aromaticity, and Tautomers.
B. L. Roos-Kozel and W. L. Jorgensen
J. Chem. Info. Comp. Sci., 21, 101 (1981).
41. Ab Initio Studies of RO...HOR' Complexes. Solvent Effects on the Relative Acidities of Water and Methanol.
W. L. Jorgensen and M. Ibrahim
J. Comput. Chem., 2, 7 (1981).
42. On the Existence of Homoaromaticity and Bicycloaromaticity in Carbanions.
J. B. Grutzner and W. L. Jorgensen
J. Am. Chem. Soc., 103, 1372 (1981).
43. Internal Rotation in Liquid 1,2-Dichloroethane and n-Butane.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 677 (1981).
44. Structures and Properties of Organic Liquids: n-Butane and 1,2-Dichloroethane and Their Conformational Equilibria.
W. L. Jorgensen, R. C. Binning, Jr., and B. Bigot
J. Am. Chem. Soc., 103, 4393 (1981).
45. Structures and Properties of Organic Liquids: n-Alkyl Ethers and Their Conformational Equilibria.
W. L. Jorgensen and M. Ibrahim
J. Am. Chem. Soc., 103, 3976 (1981).

46. Sampling Efficiency in Monte Carlo Simulations of *n*-Butane in Dilute Solution.
B. Bigot and W. L. Jorgensen
J. Chem. Phys., 75, 1944 (1981).
47. Pressure Dependence of the Structure and Properties of Liquid *n*-Butane.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 4721 (1981).
48. PULSAR: A Personalized Microcomputer-Based System for Keyword Search and Retrieval of Literature Information.
S. F. Smith, W. L. Jorgensen, and P. L. Fuchs
J. Chem. Info. Comput. Sci., 21, 209 (1981).
49. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 3. Ylid Chemistry and the Organometallic Chemistry of Li, Mg, and Lithium Cuprates.
T. D. Salatin, D. McLaughlin, and W. L. Jorgensen
J. Org. Chem., 46, 5284 (1981).
50. Comment on Simulations of Liquid Ammonia Based on Quantum Mechanical Potential Functions.
W. L. Jorgensen
J. Chem. Phys., 75, 2026 (1981).
51. Pressure Dependence of Hydrogen Bonding in Liquid Methanol.
W. L. Jorgensen and M. Ibrahim
J. Am. Chem. Soc., 104, 373 (1982).
52. The Nature of Dilute Solutions of Sodium and Methoxide Ions in Methanol.
W. L. Jorgensen, B. Bigot, and J. Chandrasekhar
J. Am. Chem. Soc., 104, 4584 (1982).
53. Pressure Dependence of the Mixing of Enantiomeric Liquids, 1,2-Dichloropropane.
W. L. Jorgensen and B. Bigot
J. Phys. Chem., 86, 2867 (1982).
54. Ab Initio Study of Acid-Base Interactions. Proton, Lithium and Sodium Affinities of First and Second Row Bases.
S. F. Smith, J. Chandrasekhar, and W. L. Jorgensen
J. Phys. Chem., 86, 3308 (1982).
55. Fluoranthene: Synthesis and Biological Testing of Four Diol Epoxides.
W. H. Rastetter, R. B. Nachbar, S. Russo-Rodriguez, R. V. Wattlely, W. G. Thilly, B. M. Andon, W. L. Jorgensen, and M. Ibrahim
J. Org. Chem., 47, 4873 (1982).

56. Revised TIPS for Simulations of Liquid Water and Aqueous Solutions.
W. L. Jorgensen
J. Chem. Phys., 77, 4156 (1982).
57. Solvation and Conformation of Methanol in Water.
W. L. Jorgensen and J. D. Madura
J. Am. Chem. Soc., 105, 1407 (1983).
58. Monte Carlo Simulations of Liquid Tetrahydrofuran Including Pseudorotation.
J. Chandrasekhar and W. L. Jorgensen
J. Chem. Phys., 77, 5073 (1982).
59. The Nature of Dilute Solutions of Sodium Ion in Water, Methanol, and THF.
J. Chandrasekhar and W. L. Jorgensen
J. Chem. Phys., 77, 5080 (1982).
60. Convergence of Monte Carlo Simulations of Liquid Water in the NPT Ensemble.
W. L. Jorgensen
Chem. Phys. Letts., 92, 405 (1982).
61. Monte Carlo Simulation of *n*-Butane in Water. Conformational Evidence for the Hydrophobic Effect.
W. L. Jorgensen
J. Chem. Phys., 77, 5757 (1982).
62. Ab Initio Study of the Structures and Binding Energies of Aluminum Monocation Complexes.
S. F. Smith, J. Chandrasekhar and W. L. Jorgensen
J. Phys. Chem., 87, 1898 (1983).
63. Computer-Assisted Mechanistic Evaluation of Organic Reactions. 4. Organosilicon Chemistry.
C. E. Peishoff and W. L. Jorgensen
J. Org. Chem., 48, 1970 (1983).
64. The Origin and Consequences of Alkene Pyramidalization in Ground and Triplet Excited States.
K. N. Houk, N. G. Rondan, F. Brown, J. D. Madura, D. C. Spellmeyer, and W. L. Jorgensen
J. Am. Chem. Soc., 105, 5980 (1983).
65. Comparison of Simple Potential Functions for Simulating Liquid Water.
W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey, and M. L. Klein
J. Chem. Phys., 79, 926 (1983).

66. Energy Component Analysis for the Hydration of Li^+ , Na^+ , F^- , and Cl^- .
J. Chandrasekhar, D. C. Spellmeyer, and W. L. Jorgensen
J. Am. Chem. Soc., 106, 903 (1984).
67. Computer Assisted Analysis of Organic Reactions.
W. L. Jorgensen
Kagaku, 38, 483 (1983).
68. Computer Assisted Mechanistic Evaluation of Organic Reactions. 7. Six Electron Cycloadditions.
J. A. Schmidt and W. L. Jorgensen
J. Org. Chem., 48, 3923 (1983).
69. Theoretical Studies of Medium Effects on Conformational Equilibria. (Feature Article)
W. L. Jorgensen
J. Phys. Chem., 87, 5304 (1983).
70. An Improved Intermolecular Potential Function for Simulations of Liquid Hydrogen Fluoride.
M. E. Cournoyer and W. L. Jorgensen
Mol. Phys., 51, 119 (1984).
71. Torsional Effects in the Baeyer-Villiger Oxidation.
S. N. Suryawanshi, C. Swenson, W. L. Jorgensen, and P. L. Fuchs
Tetrahedron Lett., 25, 1859 (1984).
72. Solvent Effects on the Relative Energies of Carbonium Ions. Solvation and Internal Rotation of the Allyl Cation in Liquid Hydrogen Fluoride.
M. E. Cournoyer and W. L. Jorgensen
J. Am. Chem. Soc., 106, 5104 (1984).
73. General Treatment of Periselectivity.
J. S. Burnier and W. L. Jorgensen
J. Org. Chem., 49, 3001 (1984).
74. $\text{S}_{\text{N}}2$ Reaction Profiles in the Gas Phase and Aqueous Solution.
J. Chandrasekhar, S. F. Smith, and W. L. Jorgensen
J. Am. Chem. Soc., 106, 3049 (1984).
75. Optimized Intermolecular Potential Functions for Liquid Hydrocarbons.
W. L. Jorgensen, J. D. Madura, and C. J. Swenson
J. Am. Chem. Soc., 106, 6638 (1984).
76. Delta Plots - A New Way to Visualize Electronic Excitation.
H. Morrison, W. L. Jorgensen, B. Bigot, D. Severance,

- Y. Munoz-Sola, R. Strommen, and B. Pandey
J. Chem. Educ., 62, 298 (1985).
77. Theoretical Examination of the S_N2 Reaction Involving Chloride Ion and Methyl Chloride in the Gas Phase and Aqueous Solution.
J. Chandrasekhar, S. F. Smith, and W. L. Jorgensen
J. Am. Chem. Soc., 107, 154 (1985).
78. Optimized Intermolecular Potential Functions for Amides and Peptides. Structure and Properties of Liquid Amides.
W. L. Jorgensen and C. J. Swenson
J. Am. Chem. Soc., 107, 569 (1985).
79. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 9. Reactions of Unsaturated Electrophiles Including Nucleophilic Aromatic Substitution.
C. E. Peishoff and W. L. Jorgensen
J. Org. Chem., 50, 1056 (1985).
80. Optimized Intermolecular Potential Functions for Amides and Peptides. Hydration of Amides.
W. L. Jorgensen and C. J. Swenson
J. Am. Chem. Soc., 107, 1489, 5025 (1985).
81. Magnitude and Origin of the β-Silicon Effect on Carbenium Ions.
S. G. Wierschke, J. Chandrasekhar, and W. L. Jorgensen
J. Am. Chem. Soc., 107, 1496 (1985).
82. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 10. Stereochemistry.
C. E. Peishoff and W. L. Jorgensen
J. Org. Chem., 50, 3174 (1985).
83. Energy Profile for a Non-Concerted S_N2 Reaction in Solution.
J. Chandrasekhar and W. L. Jorgensen
J. Am. Chem. Soc., 107, 2974 (1985).
84. Monte Carlo Simulations of Alkanes in Water: Hydration Numbers and the Hydrophobic Effect.
W. L. Jorgensen, J. Gao, and C. Ravimohan
J. Phys. Chem., 89, 3470 (1985).
85. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 11. Electrophilic Aromatic Substitution.
M. G. Bures, B. L. Roos-Kozel, and W. L. Jorgensen
J. Org. Chem., 50, 4490 (1985).

86. Monte Carlo Simulation of Differences in Free Energies of Hydration.
W. L. Jorgensen and C. Ravimohan
J. Chem. Phys., 83, 3050 (1985).
87. Temperature and Size Dependence for Monte Carlo Simulations of TIP4P Water.
W. L. Jorgensen and J. D. Madura
Mol. Phys, 56, 1381 (1985).
88. Monte Carlo Simulations of the Hydration of Ammonium and Carboxylate Ions.
W. L. Jorgensen and J. Gao
J. Phys. Chem., 90, 2174 (1986).
89. Optimized Intermolecular Potential Functions for Liquid Alcohols.
W. L. Jorgensen
J. Phys. Chem., 90, 1276 (1986).
90. Ab Initio and Monte Carlo Calculations for a Nucleophilic Addition Reaction in the Gas Phase and in Aqueous Solution.
J. D. Madura and W. L. Jorgensen
J. Am. Chem. Soc., 108, 2517 (1986).
91. Computer Simulations of Organic Reactions in Solution.
W. L. Jorgensen, J. Chandrasekhar, J. K. Buckner, and J. D. Madura
Ann. N. Y. Acad. Sci., 482, 198 (1986).
92. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 12. pK_a Predictions for Organic Compounds in DMSO.
A. J. Gushurst and W. L. Jorgensen
J. Org. Chem., 51, 3513 (1986).
93. Effect of Hydration on the Structure of an S_N2 Transition State.
W. L. Jorgensen and J. K. Buckner
J. Phys. Chem., 90, 4651 (1986).
94. Ab Initio Study of the Structures and Binding Energies of Anion-Water Complexes.
J. Gao, D. S. Garner, and W. L. Jorgensen
J. Am. Chem. Soc., 108, 4784 (1986).
95. Intermolecular Potential Functions and Monte Carlo Simulations for Liquid Sulfur Compounds.
W. L. Jorgensen
J. Phys. Chem., 90, 6379 (1986).
96. Computer Simulation of Chemical and Biomolecular Systems.
D. L. Beveridge and W. L. Jorgensen, Eds.

Annals of the New York Academy of Sciences, Vol. 482 (1986).

97. Ab Initio Study of the S_N2 Reactions of OH⁻ and OOH⁻ with CH₃Cl.
J. D. Evanseck, J. F. Blake, and W. L. Jorgensen
J. Am. Chem. Soc., 109, 2349 (1987).
98. Network Topology in Simulated Water.
R. J. Speedy, J. D. Madura, and W. L. Jorgensen
J. Phys. Chem., 91, 909 (1987).
99. Energy Profiles for (CH₃)₃CCl Ion Pairs in Aqueous Solution.
W. L. Jorgensen, J. K. Buckner, S. E. Huston, and P. J. Rossky
J. Am. Chem. Soc., 109, 1891 (1987).
100. Ab Initio Study of the Displacement Reactions of Chloride Ion with Formyl and Acetyl Chloride.
J. F. Blake and W. L. Jorgensen
J. Am. Chem. Soc., 109, 3856 (1987).
101. A General Treatment of Nucleophilic Chemistry.
P. Metivier, A. J. Gushurst, and W. L. Jorgensen
J. Org. Chem., 52, 3724 (1987).
102. Computational Investigations of Organic Reaction Mechanisms: Nucleophilic Reactions of Carbonyl Compounds.
W. L. Jorgensen, J. F. Blake, J. D. Madura, and S. G. Wierschke
ACS Symposium Ser., 353, 200 (1987).
103. A Priori Calculations of pK_a's for Organic Compounds in Water. The pK_a of Ethane.
W. L. Jorgensen, J. M. Briggs, and J. Gao
J. Am. Chem. Soc., 109, 6857 (1987).
104. Use of Statistical Perturbation Theory for Computing Solvent Effects on Molecular Conformation. Butane in Water.
W. L. Jorgensen and J. K. Buckner
J. Phys. Chem., 91, 6083 (1987).
105. Energy Profiles for Organic Reactions in Solution.
W. L. Jorgensen
Adv. Chem. Phys., Part II, 70 469 (1988).
106. The OPLS Force Field for Proteins. Energy Minimizations for Crystals of Cyclic Peptides and Crambin.
W. L. Jorgensen and J. Tirado-Rives
J. Am. Chem. Soc., 110, 1657 (1988).

107. Monte Carlo Simulations of Liquid Acetonitrile with a Three-Site Model.
W. L. Jorgensen and J. M. Briggs
Molec. Phys., 63, 547 (1988).
108. Modeling Molecular Transformations in Solution.
W. L. Jorgensen, J. K. Buckner, and J. Gao
In "Chemical Reactivity in Liquids", M. Moreau and P. Turq, Eds.; Plenum Press:
New York (1988); p 253-263.
109. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 14. Reactions of Sulfur and Phosphorus Ylides, Iminophosphoranes, and P=X-Activated Anions.
A. J. Gushurst and W. L. Jorgensen
J. Org. Chem., 53, 3397 (1988).
110. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 15. Heterocycle Synthesis.
M. G. Bures and W. L. Jorgensen
J. Org. Chem., 53, 2504 (1988).
111. Cis/Trans Energy Difference for the Peptide Bond in the Gas Phase and Aqueous Solution.
W. L. Jorgensen and J. Gao
J. Am. Chem. Soc., 110, 4212 (1988).
112. Theoretical Examination of Hexanol-Water Interfaces.
J. Gao and W. L. Jorgensen
J. Phys. Chem., 92, 5813 (1988).
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Nichols, S. E.; Domaal, R. A.; Thakur, V. V.; Bailey, C. M.; Wang, L.; Tirado-Rives, J.; Anderson, K. S.; Jorgensen, W. L. *J. Chem. Inf. Model.* **2009**, *49*, 1272-1279. NIHMS112356
331. In silico improvement of β^3 -peptide inhibitors of p53•hDM2 and p53•hDMX.
Michel, J.; Harker, E.A.; Tirado-Rives, J.; Jorgensen, W. L.; Schepartz, A. *J. Am. Chem. Soc.* **2009**, *131*, 6356-6357. NIHMS117765
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Jorgensen, W. L. in "Drug Design: Structure and Ligand-Based Approaches", Merz, K.; Reynolds, C.; Ringe, D., Eds.; Cambridge Univ. Press, Cambridge, UK, 2009. ISBN 9780521887236 In press.

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Leung, S. S. F.; Tirado-Rives, J.; Jorgensen, W. L.
Bioorg. Med. Chem. **2009**, *17*, 5874-5886.
334. Prediction of the Water Content in Protein Binding Sites.
Michel, J.; Tirado-Rives, J.; Jorgensen, W. L.
J. Phys. Chem. B **2009**, *113*, 13337-13346. Received the *Emerging Technology Award* at the August 2009 Nat'l ACS Meeting.
335. Steric and Solvation Effects in Ionic S_N2 Reactions.
Chen, X.; Regan, C. K.; Craig, S. L.; Krenske, E. H.; Houk, K. N.; Jorgensen, W. L.; Brauman, J. I.
J. Am. Chem. Soc. **2009**, *131*, 16162-16170. doi 10.1021/ja9053459
336. Energetics of Displacing Water Molecules from Protein Binding Sites: Consequences for Ligand Optimization.
Michel, J.; Tirado-Rives, J.; Jorgensen, W. L.
J. Am. Chem. Soc. **2009**, *131*, 15403-15411. doi 10.1021/ja906058w
337. Chemical Control Over Immune Recognition: A Class of Antibody-Recruiting Small Molecules (ARMs) that Target Prostate Cancer.
Murelli, R. P.; Zhang, A. X.; Michel, J.; Jorgensen, W. L., Spiegel, D. A.
J. Am. Chem. Soc. **2009**, *131*, 17090-17092.
338. Advances in QM/MM Simulations for Organic and Enzymatic Reactions.
Acevedo, O.; Jorgensen, W. L.
Acc. Chem. Res. **2010**, *43*, 142-151.
339. Discovery of Novel FGFR1 Kinase Inhibitors by Structure-Based Virtual Screening.
Ravindranathan, K. P.; Mandiyan, V.; Ekkati, A. R.; Bae, J. H.; Schlessinger, J.; Jorgensen, W. L.
J. Med. Chem. Soc. **2010**, *53*, 0000-0000. In press.
340. Optimization of azoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase.
Leung, C. S.; Zeevaart, J. G.; Domaoal, R. A.; Bollinin, M.; Thakur, V. V.; Anderson, K. S.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2010**, *20*, 0000-0000. Submitted.
341. QM/MM Modeling Finds Diels-Alder Reactions are Accelerated Less On Water than In Water.
Thomas, L.; Tirado-Rives, J.; Jorgensen, W. L.
J. Am. Chem. Soc. **2010**, *132*, 0000-0000. In press.

Recent Invited Lectures (1998-)

1998

Faraday Discussion on Chemical Reaction Theory - St. Andrews, Scotland
15th H. C. Brown Lectures - Purdue University
NATO ARW on Supramolecular Science - Lerici, Italy
Novartis Workshop on Structure-Based Drug Design - Summit, NJ
National ACS Meeting - Computers in Chem. & Pharm. Research Award - Dallas
National ACS Meeting - Symposium on Transition State Modeling - Dallas
Frederick Cancer R & D Center – Frederick, MD
University of Maryland
Glaxo-Wellcome, RTP, NC
Wyeth-Ayerst, Princeton
Agouron Pharmaceuticals - La Jolla, CA
Chemistry & Biology Symposium - Yale University
Parke-Davis Pharmaceutical Co. - Ann Arbor, MI
National ACS Meeting - Symposium on Polymers in Aq. Media - Boston
National ACS Meeting - Symposium on Force Fields - Boston
Yale Cancer Center
Wesleyan University

1999

11th Argentinian Conference on Physical Organic Chemistry - Sante Fe
WATOC-99 – London
National ACS Meeting - Symposium on Water in Chemistry & Biology - New Orleans
National ACS Meeting - Symposium on Docking & Scoring - New Orleans
University of Georgia
Schrödinger Inc.
UC San Francisco - DOCK User's Group Meeting
CombiChem Inc.
Vertex Pharmaceuticals Inc.
Gordon Conference on QSAR
Western Maryland College – Building Dedication
Pharmacopeia Inc.
8th Conf. on Trends in Computational Chemistry, Vicksburg, MS
Parke-Davis Pharmaceuticals
Pharmacia and Upjohn, Inc.

2000

National ACS Meeting - Symposium on Potential Energy Surfaces - San Francisco
National ACS Meeting – Computational Chemistry Award Symposium - San Francisco
National ACS Meeting – Symposium on Drug Design - San Francisco
Computational Chemistry Symposium Honoring P. Schleyer – Hong Kong
Computational Biophysics 2000 – Nice, France

Sanibel Conference – St. Augustine
Texas Christian University
Southern Methodist University
University of Pennsylvania
Beilstein Workshop on Chemical Data Analysis (Bozon)
CECAM Meeting on Challenges for Free Energy Calculations (Lyon)
National ACS Meeting – Frontiers in Biophysical Theory Symposium – Washington DC
IBM – Blue Gene Group – Yorktown Heights
Columbia University
Pharmacia/Upjohn – Kalamazoo
Pharmacia/Searle – Skokie, IL
Pharmacia/Monsanto – St. Louis
Gordon Conference on Computational Chemistry (Oxford)
ACS Short Course on Frontiers in Organic Chemistry, Washington DC

2001

Computational Structural Biology Symposium – Florida State U.
Retrometabolism Drug Design Conference – Amelia Is.
Gordon Conference on Physical Organic Chemistry (Holderness)
Gordon Conference on Biological Molecules in the Gas Phase (CT College)
Molecular Quantum Mechanics Conference Honoring E. Davidson – Seattle
International Conference on Cancer Research (Albany)
10th Conf. on Trends in Computational Chemistry, Jackson, MS
New York University
National ACS Meeting – Libraries for Drug Discovery Symposium - San Diego
Nemethy Symposium, Mt. Sinai School of Medicine
Schrödinger, Inc., New York
Int'l Meeting of the Molecular Graphics & Modeling Society – Erlangen *
NCI Fluid Properties Symposium
Annual Meeting -Society for Biomolecular Screening, ADME Symposium, Baltimore*
Cornell Theory Center Symposium on Protein Structure Prediction
Workshop on Polarizability for Biomolecular Simulations, Snowbird, Utah
*cancelled, 9/11

2002

Aventis Pharmaceuticals, Bridgewater, NJ
Mesilla Conference on Asymmetric Catalysis
Biophysical Society – Symposium on Molecular Simulations in Biology – San Francisco
National ACS Meeting – Symposium on Drug Design - Orlando
National ACS Meeting – Kollman Memorial Symposium - Orlando
Beilstein Workshop on Molecular Informatics
ISQBP President's Meeting – organizer
ACS Short Course - Philadelphia
WATOC Meeting – Lugano
SPECS Conference on New Chemistries, Delft

Volkswagen Symposium, Ulm
Gordon Conference on Computational Chemistry
University of Delaware

2003

National ACS Meeting – Comp. Chem. Award Symposium for K. N. Houk
Sigma Xi - Connecticut
Cambridge Healthtech Symposium on Drug Design – Philadelphia
AstraZeneca – Wilmington, DE
Locus Development - Philadelphia
Duquesne University
CT Quantum Chemistry Group
Schleyer Lecturer – Univ. of Georgia
UCLA
ACS Short Course – Boston
Celera Genomics
National ACS Meeting, NYC – Symposium on Drug Design
aaiPharma – Wilmington, NC
Schering-Plough – Kenilworth, NJ
DuPont – Newark, DE
US, Polish, Czech Workshop on Biomolecular Interactions - Prague

2004

National ACS Meeting – Symposium on Drug Design - Anaheim
National ACS Meeting – 1st Dewar Symposium – Anaheim
National ACS Meeting – COMP Award Symposium for G. Richards
Bristol-Myers Squibb Lecturer - Scripps Research Institute
ISQBP President's Meeting, Plenary – Como, Italy
Symposium on Computational Chemical Dynamics – U. Minn.
Computational Chemistry Symposium, Plenary – Gyeongju, Korea
3eme Cycle Lecturer – Switzerland :
 University of Basel (3 lectures)
 University of Bern
 University of Lausanne
Tetrahedron Symposium on Chemistry and Drug Discovery, New York City
Neurocrine Biosciences – San Diego, CA
Hoffmann La Roche – Nutley, NJ
Rutgers University
Merck – West Point, PA
Yale - Parallel Computing Workshop
D. E. Shaw & Co.
National ACS Meeting- Phila. – Protein Docking & Scoring Symposium
National ACS Meeting- Phila. – Skolnik Award Symposium for A. P. Johnson
MGMS Symposium on Biomolecular Recognition and Reactivity - Manchester UK
University of Arizona – Pharmacology

University of Pennsylvania – Symposium on Structure-Based Drug Design
Schrodinger Users Group – Boston
University of New Haven – Medicinal Chemistry Symposium
Johnson & Johnson – Spring House, PA
Yale - Center for Structural Biology
Soc. Royale de Chimie Belge – Medicinal Chemistry Symposium, Ghent
Wyeth-Ayerst - Cambridge

2005

WATOC Conference – Cape Town
University of Tennessee
Penn State University
Pharmaceutical Society of Japan - Tokyo - Sato Award Presentation
National ACS Meeting- San Diego – J. A. Pople Memorial Symposium
National ACS Meeting- San Diego – Drug Design Symposium
Novartis (Cambridge)
Structural Biology Symposiium - UT Medical Branch (Galveston, TX)
International AIDS Society (Rio)
Univ. Federal do Rio de Janeiro
NIH Docking Workshop
Pfizer (Groton)
ACS Prospectives Symposium on Drug Design
Pacifichem 2005 – Honolulu - Classical and QSM Solvation Symposium
Pacifichem 2005 – Honolulu - Structure, Dynamics, Function of Biomolecules Symposium

2006

Molecular Graphics & Modeling Society (Southampton, UK)
XIIth International Congress on Quantum Chemistry (Kyoto)
Biomolecular Simulation Symposium (Heraeus Found., Bad Honnef)
Texas A&M - IUCCP Pharma Symposium
Johnson & Johnson – La Jolla, CA
National ACS Meeting- Atlanta - Virtual Screening Symposium
PharmaDiscovery 2006 (Bethesda, MD)
CHI Symposium on Structure-Based Drug Design (Boston)
Ohio State University
University of Michigan
City College of New York
Schrodinger Global Users Group Meeting (New York City)
Pfizer - Ann Arbor
Boehringer-Ingelheim (Ridgefield)
Oxford University (UK) - G. Richards Symposium
National ACS Meeting- San Francisco - Drug Discovery Symposium
National ACS Meeting- San Francisco - Dewar Symposium
Medicinal Chemistry Symposium (Swedish Chemical Society) - Umeå, Sweden
CSIR Bioscience - Pretoria, SA

2007

AACR/ACS Symposium - Chemistry in Cancer Research (San Diego)
National ACS Meeting- Chicago - Rational Drug Design Symposium
National ACS Meeting- Chicago - *De Novo* Design Coupled to Synthesis Symposium
National ACS Meeting- Chicago - Measures of Accuracy in Simulations Symposium
Sanibel Conference
Computational Biology Symposium - Barcelona Supercomputer Center (Mare Nostrum)
Pulay Conference - Budapest
6th European Workshop in Drug Design, Siena, Italy
Johnson & Johnson Drug Discovery Symposium - San Diego
European Symposium on Organic Reactivity - Faro, Portugal
American Physical Society - Denver
Gordon Conference - Computer-Aided Drug Discovery - Keynote Speaker
National ACS Meeting- Boston - Quantum & Statistical Mechanics Symposium
Sacred Heart University
Wyeth-Ayerst, Princeton
Astra-Zeneca - Molndal, Sweden
ACS Symp. - Frontiers in Chemistry & Biopharmaceuticals - Keynote - San Diego
Univ. of California Los Angeles, Colloquium
Pfizer - La Jolla
Computational Biology Symposium - Rice University
Safer Chemicals Summit - Yale University

2008

Keystone Symposium on Drug Design - Steamboat Springs, CO
University of Minnesota - Medicinal Chemistry
University of Chicago, Closs Lecturer
Michigan State University, Colloquium
Medicinal Biochemistry Symposium - UNC Greensboro
Pfizer – La Jolla
Int'l Symposium on Green Processing in Pharma - Yale U.
Symposium for K. N. Houk - UCLA
Tetrahedron Symposium - Berkeley, CA
Theoretical Biochemistry Symposium - Stockholm, Sweden
IMA Solvation Workshop - U. Minnesota
ACS National Meeting - Philadelphia - Drug Design Symposium
ACS National Meeting - Philadelphia - Free Energy Simulation Symposium
ACS National Meeting - Philadelphia - Force Field Development Symposium
ACS National Meeting - Philadelphia - Challenges in Computation Symposium
SUNY Stony Brook - Chemical Biology & Drug Discovery Symposium
DARPA Workshop - Seattle
Pfizer - Groton
Utah State U., Olsen Lecturer

2009

Univ. of Colorado - Boulder, CO
Duke University - Durham, NC
ACS National Meeting - Salt Lake City - Progress in Simulations and Force Fields Symposium
Computer-Aided Molecular Design Symposium, Royal Society of Chemistry, Antigua
7th Canadian Computational Chemistry Conference - Halifax, NS
UC San Francisco - Biophysics and CCB Seminar
Biogen - Cambridge, MA
Washington U. School of Medicine - Computational Biology
7th European Workshop on Drug Design - Siena, Italy
4th International Biophysics Symposium - Roscoff, France
Astra-Zeneca Boston Infection Seminar Series
Lise Meitner Lectureship - Technion University (Haifa)
Lise Meitner Lectureship - Jerusalem
Univ. of Cape Town, SA
AAPS Annual Meeting - Symposium on State-of-the-Art in Drug Design - Los Angeles, CA
AAPS Annual Meeting - Symposium on Role of Computational Design in Drug R&D
UC Berkeley - Biophysics & Bioengineering

2010

Symposium on "Theoretical and Computational Chemistry" at the
Max-Planck-Institut für Kohlenforschung - Mülheim
Symposium Honoring Frank Blaney, Oxford U.
ISQBP President's Meeting, Calabria, Italy
Vitae Pharmaceuticals

ACS National Meeting - Boston - Berne Symposium
ACS National Meeting - Boston - Skolnik Award Symp. for A. Hopfinger
ACS National Meeting - Boston - JCIM Anniversary Symposium - Organizer
ACS National Meeting - Boston - Water in Drug Discovery Symp.
High Performance Computing Symposium - National U. of Ireland
6th Rauschholzhausen Workshop on New Approaches to Drug Discovery
McGill University
Wesleyan University - Biophysical Symposium Honoring D. Beveridge
6th Aarhus (Denmark) Winter Meeting on Trends in Modern Chemistry
CECAM Meeting on “Approaches for Enzyme Simulations” – Bremen
University of Texas at Austin - Biophysics

Research Support

Dr. Jorgensen has had extensive research support from the National Science Foundation since 1977 and from the National Institutes of Health since 1980. He currently has research grants from the National Institute of General Medical Sciences, the National Institute of Allergy and Infectious Diseases, National Foundation for Cancer Research, and Pfizer. Dr. Jorgensen is also part of the Biophysical Training Grant at Yale. Postdoctoral fellows in his laboratory are often supported by national and industrial fellowships - recently, NIH, EMBO, Roche Research Foundation, Bayer Pharmaceuticals, Pfizer, Danish Research Council, the governments of Spain and Brazil, and the American Society for Cancer Research.

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Dr. Krishna Ravindranathan (P.D., 2006-)
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John Terhorst (Ph. D., 2011)
Jakub Kostal (Ph. D., 2011)
Dr. Julien Michel (P.D., 2007-)
Dr. Anil Ekkati (P.D., 2008-)
Dr. Alexander Trofimov (P.D., 2009-)
Dr. Mariella Bollini (P.D., 2009-)
Dr. Leyla Celik (P. D., 2009-)
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James Lucarelli (B.S., 2010)
Connie Wang (B.S., 2010)

Past Co-workers

John E. Munroe (M. S., 1977)
Timothy D. Salatin (Ph.D., 1980)
David Yang (B. S., 1981)
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Michael E. Cournoyer (Ph.D., 1983)
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Dr. C. Ravimohan (P.D., 1984-5)
Dr. Roberto Rozas (V.P., 1985-6)
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Mark Bures (Ph.D., 1987)
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Dr. Ingvar Lagerstedt (P.D., 1992-4)
Dr. Arshad Khan (Visiting Prof., 1996)
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Dr. Edward Watkins (Assoc. Res. Scientist, 1999-2001)
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Dennis Ostrovsky (Ph.D., 2003)
Dr. Yukio Tominaga (P.D., 2001-3)
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Catherine Peishoff (Ph.D., 1985)
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Dr. M. Leonor Contreras (V. P., 1985-6)
Jiali Gao (Ph.D., 1987)
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Ralph T. Mosley (M.S., 1989)
James Briggs (Ph.D., 1990)
Dr. James F. Blake (Ph.D., 1990; P.D., 90-91)
Dr. Tooru Matsui (P.D., 1989-91)
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Dr. Ellen R. Laird (Ph.D., 1990; P.D., 90-92)
Prof. Modesto Orozco (V.P., 1991-93)
Shenna Sinclair (Ph.D., 1994)
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Jonathan Essex (P.D., 1992-4)
Daqing Gao (M. S., 1995)
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Wendy Schaeffer (B.S., 1997)
Dr. Antonio Frontera (P.D., 1995-6)
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Corky Jenson (M.S., 1999)
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Dr. Jacob Zeevaart (P.D., 2007-9)

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Dr. Joseph Kim (P.D., 2005-7)
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