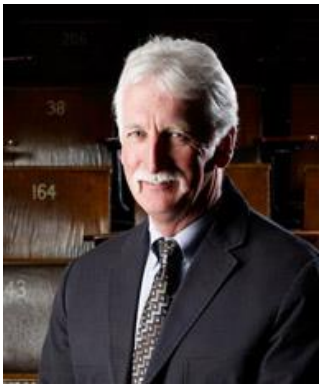
VITA OF WILLIAM L. JORGENSEN

Department of Chemistry
Yale University
225 Prospect Street
New Haven, Connecticut 06520-8107

Telephone: (203)432-6278
Fax: (203)432-6299
Email: william.jorgensen@yale.edu
Website : http://www.jorgensenresearch.com
Date of Birth: October 5, 1949 (New York, New York)



Employment

2009-	Sterling Professor of Chemistry, Yale University
2009-2012	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).

Education

1970-1975	Harvard University - Ph. D. in Chemical Physics
1967-1970	Princeton University - A. B. in Chemistry

Honors

2015	Tetrahedron Prize
2012	Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids (ACS)
2011	Member, National Academy of Sciences
2010	Member, International Academy of Quantum Molecular Science
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 (ACS)
1994	Fellow, American Association for the Advancement of Science
1990	Arthur C. Cope Scholar Award, American Chemical Society (ACS)
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 (Princeton)

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; 6th W. S. Johnson Lectures, Stanford U.; Steiglitz Memorial Lecturer, Chicago ACS; 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 Sate; Lise Meitner Lecturer, Israel; Gilda Loew Memorial Lecturer, ISQBP 2010; J. Wiley Lecturer, Scripps; Grandpierre Lecturer, Columbia U.; Molecular Physics Lecturer, Thermodynamics 2011 (Athens); MGMS Lecturer, Comput. Mol. Sci. 2012; Federico Arcamone Lecturer, IIT Genoa; Kolthoff Lecturer, U. Minnesota; Bryan E. Koehler Lecturer, UC Riverside; Bone Lecturer, Wilkes U.; Topliss Award Lecturer, U. Michigan. Plenary Lecturer, ACS Annual Meeting – San Diego, 2016. 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), 2005-2013
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
Chair, Search Committee for the Editor of the Journal of Medicinal Chemistry, 2010

Yale Committees
Fellow, Trumbull College, 1990-
Physical Sciences & Engineering Advisory Committee, 1994-96, 2004-2012
Biological Sciences Advisory Committee, 2004-2006
Scholar Awards Committee, 2005-9
Wilbur Cross Medal Committee, 2009-2012
Chemical Biology Institute Advisory Committee, 2009-
Science & Engineering Advisory Committee, 2009-2012
Cancer Biology Institute Advisory Committee, 2011-
Cooperative Research Committee, 2011-2016
Screening Core Advisory Committee, 2012-
Science Hill Building Committee, 2011-2016
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., 1991-2000
Scientific Advisory Board, CombiChem Inc., 1994-1999
Scientific Advisory Board, Schrödinger Inc., 1996-
Scientific Advisory Board & Founder, Rib-X Pharmaceutical Inc., 2001-2013
Scientific Advisory Board & Founder, Melinta Therapeutics Inc., 2013-
Scientific Advisory Board, Vitae Pharmaceuticals, 2005-2016
Scientific Advisory Board, IFM Therapeutics, 2016-
Scientific Advisory Board, Kleo Pharmaceuticals, 2016-
Scientific Advisory Board, Reo Discovery, 2017-
Expert Witness: Kaye Scholer LLP; Kirkland & Ellis LLP; Williams & Connolly; Others
Past Consultant: Agouron, Parke-Davis, Pfizer, Pharmacia, Warp Drive
AAAS Electorate Nominating Committee, 2003-2006; Chair, 2004
World Association of Theoretical & Computational Chemists (WATOC), 2003-9
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
Advisory Board, IRB-BSC-CRG Joint Program, U. Barcelona, 2008-
Advisory Committee, NCRR Resource for Integrated Glycotechnology, 2010-2013
Israeli Council on Higher Education, Chemistry Evaluation Committee, 2011
Tetrahedron Prize Committee, 2017

Editorial Advisory Boards
Bioorganic and Medicinal Chemistry Letters, 1990-
Bioorganic and Medicinal Chemistry, 1992-
Journal of Computer Aided Molecular Design, 1992-2010
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; 2009-2014
Journal of Medicinal Chemistry, 2013-16

Memberships in Professional Societies
American Chemical Society
Israeli Chemical Society (Honorary Life Member)
American Association for the Advancement of Science
International Society for Quantum Biology and Pharmacology
International AIDS Society
World Association of Theoretical & Computational Chemists
Connecticut Academy of Arts and Sciences
Connecticut Academy of Science and Engineering
International Academy of Quantum Molecular Science
American Academy of Arts and Sciences
National Academy of Sciences

Publication Statistics
425 primary publications
H-Index = 103 (ISI), 110 (Google Scholar)
Citations >67,000 (ISI), >81,000 (Google Scholar)

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, 749-753 (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, 3082-3090 (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 (l976).

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 Unsaturatively 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 6-3lG 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, 3309-3315 (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, l. 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, 341-345 (1981).

39. Simulation of Liquid Ethanol Including Internal Rotation.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 345-350 (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, l0l (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 Methods for Monte Carlo Simulations of n-Butane in Dilute Solution.
B. Bigot and W. L. Jorgensen
J. Chem. Phys., 75, l944 (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).

5l. Pressure Dependence of Hydrogen Bonding in Liquid Methanol.
W. L. Jorgensen and M. Ibrahim
J. Am. Chem. Soc., 104, 373 (l982).

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 (l982).

53. Pressure Dependence of the Mixing of Enantiomeric Liquids, l,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. Wattley, 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. S_N2 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 (l985).

81. Magnitude and Origin of the ß-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., l08, 2517 (l986).

9l. 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 (l986).

92. Computer-Assisted Mechanistic Evaluation of Organic Reactions, l2. pK_a Predictions for Organic Compounds in DMSO.
A. J. Gushurst and W. L. Jorgensen
J. Org. Chem., 5l, 3513 (l986).

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 (l986).

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 (l986).

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 CH_3Cl.
J. D. Evanseck, J. F. Blake, and W. L. Jorgensen
J. Am. Chem. Soc., 109, 2349 (l987).

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 $(CH_3)_3CCl$ 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, 6857-6858 (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, 1657-1666 (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).

113. Efficient Computation of Absolute Free Energies of Binding by Computer Simulations. Application to the Methane Dimer in Water.
W. L. Jorgensen, J. K. Buckner, S. Boudon and J. Tirado-Rives
J. Chem. Phys., 89, 3742 (1988).

114. Free Energy of TIP4P Water and the Free Energies of Hydration of CH_4 and Cl- from Statistical Perturbation Theory.
W. L. Jorgensen, J. F. Blake and J. K. Buckner
Chem. Phys., 129, 193 (1989).

115. Computer-Assisted Evaluation of Oxidation Reactions.
G. D. Paderes and W. L. Jorgensen
J. Org. Chem., 54, 2058 (1989).

116. Ab Initio Investigation of the ß-Silicon Effect on Alkyl and Cyclopropyl Carbenium Ions and Radicals.
M. R. Ibrahim and W. L. Jorgensen
J. Am. Chem. Soc., 111, 819 (1989).

117. Free Energies in Solution - The Aqua Vitae of Computer Simulations.
W. L. Jorgensen
In "Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications", W. F. van Gunsteren and P. Weiner, Eds.; Escom Science Publishers: Leiden (1989), p 60.

118. Energetics and Hydration of the Constituent Ion Pairs of Tetramethylammonium Chloride.
J. K. Buckner and W. L. Jorgensen
J. Am. Chem. Soc., 111, 2507 (1989).

119. Variational Transition State for the Reaction of Cl_2C: with Ethylene and the Thermodynamics of Carbene Additions.
J. F. Blake, S. G. Wierschke and W. L. Jorgensen
J. Am. Chem. Soc., 111, 1919 (1989).

120. A Priori pK_a Calculations and the Hydration of Organic Anions.
W. L. Jorgensen and J. M. Briggs
J. Am. Chem. Soc., 111, 4190-4197 (1989).

121. Structure and Binding for Rebek's Diacid in Chloroform. A Demure Host for Pyrazine.
W. L. Jorgensen, S. Boudon, and T. B. Nguyen
J. Am. Chem. Soc., 111, 755 (1989).

122. Substituent Effects and Transition Structures for Diels-Alder Reactions of Butadiene and Cyclopentadiene with Cyanoalkenes.
K. N. Houk, R. J. Loncharich, J. F. Blake, and W. L. Jorgensen
J. Am. Chem. Soc., 111, 9172 (1989).

123. Molecular Dynamics Simulation of the Third Domain of Silver Pheasant Ovomucoid in Water.
W. L. Jorgensen and J. Tirado-Rives
In "Proceedings of the l988 Nobel Symposium", Chem. Scripta, 29A, 191-196 (1989).

124. Free Energy Calculations, A Breakthrough for Modeling Organic Chemistry in Solution.
W. L. Jorgensen
Acc. Chem. Res., 22, 184-189 (l989).

125. Interactions Between Amides in Solution and the Thermodynamics of Weak Binding.
W. L. Jorgensen
J. Am. Chem. Soc., 111, 3770 (1989).

126. Molecular Dynamics of Proteins with the OPLS Potential Functions. Simulation of the Third Domain of Silver Pheasant Ovomucoid in Water
J. Tirado-Rives and W. L. Jorgensen
J. Am. Chem. Soc., 112, 2773 (1990).

127. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 17. Free Radical Chain Reactions.
E. R. Laird and W. L. Jorgensen
J. Org. Chem., 55, 9 (1990).

128. Relative Partition Coefficients for Organic Solutes from Fluid Simulations.
W. L. Jorgensen, J. M. Briggs, and M. L. Contreras
J. Phys. Chem., 94, 1683 (1990).

129. Structure and Basicity of Silyl Ethers: A Crystallographic and Ab Initio Inquiry into the Mode of Silicon-Oxygen Interactions.
S. Shambayati, J. F. Blake, S. G. Wierschke, W. L. Jorgensen, and S. L. Schreiber
J. Am. Chem. Soc., 112, 697 (1990).

130. The Importance of Secondary Interactions in Triply Hydrogen-Bonded Complexes: Guanine-Cytosine vs. Uracil-Diaminopyridine.
W. L. Jorgensen and J. Pranata
J. Am. Chem. Soc., 112, 2008 (1990).

131. Aromatic-Aromatic Interactions: Free Energy Profiles for the Benzene Dimer in Water, Chloroform, and Liquid Benzene.
W. L. Jorgensen and D. L. Severance
J. Am. Chem. Soc., 112, 4768 (1990).

132. Monte Carlo Simulations of Liquid Alkyl Ethers with the OPLS Potential Functions.
J. M. Briggs, T. Matsui, and W. L. Jorgensen
J. Comput. Chem., 11, 958 (1990).

133. Origin of the Strong Binding of Adenine to a Molecular Tweezer.
J. F. Blake and W. L. Jorgensen
J. Am. Chem. Soc., 112, 7269 (1990).

134. Computer Assisted Analysis of Reactions Involving Organic Free Radicals and Diradicals.
E. R. Laird and W. L. Jorgensen
J. Chem. Info. Comput. Sci., 30, 458 (1990).

135. CAMEO: A Program for the Logical Prediction of the Products of Organic Reactions.
W. L. Jorgensen, E. R. Laird, A. J. Gushurst, J. M. Fleischer, S. A. Gothe, H. E. Helson, G. D. Paderes, and S. Sinclair
Pure Appl. Chem., 62, 1921 (1990).

136. OPLS Potential Functions for Nucleotide Bases. Relative Association Constants of Hydrogen-Bonded Base Pairs in Chloroform.
J. Pranata, S. G. Wierschke, and W. L. Jorgensen
J. Am. Chem. Soc., 113, 2810 (1991).

137. Monte Carlo Simulations of Liquid Acetic Acid and Methyl Acetate with the OPLS Potential Functions.
J. M. Briggs, T. B. Nguyen, and W. L. Jorgensen
J. Phys. Chem., 95, 3315 (1991).

138. Chemical Chameleons: Hydrogen Bonding with Imides and Lactams in Chloroform.
W. L. Jorgensen and D. L. Severance
J. Am. Chem. Soc., 113, 209 (1991).

139. Molecular Dynamics Simulations of the Unfolding of an α-Helical Analog of Ribonuclease-A S-Peptide in Water.
J. Tirado-Rives and W. L. Jorgensen
Biochemistry, 30, 3864-3871 (1991).

140. Monte Carlo Simulations Yield Absolute Free Energies of Binding for Guanine-Cytosine and Adenine-Uracil Base Pairs in Chloroform.
J. Pranata and W. L. Jorgensen
Tetrahedron, 47, 2491 (1991).

141. Computer-Assisted Mechanistic Evaluation of Organic Reactions. 19. Reductions with Hydrides.
G. D. Paderes, P. Metivier, and W. L. Jorgensen
J. Org. Chem., 56, 4718 (1991).

142. Proton Affinities and Gas-phase Basicities of Alkyl and Silyl Ethers.
J. F. Blake and W. L. Jorgensen
J. Org. Chem., 56, 6052 (1991).

143. Computational Insights on Intermolecular Interactions and Binding in Solution.
W. L. Jorgensen
Chemtracts - Organic Chemistry, 4, 91-119 (1991). (Feature article.)

144. Computational Studies of FK506: Conformational Search and Molecular Dynamics Simulation in Water.
J. Pranata and W. L. Jorgensen
J. Am. Chem. Soc., 113, 9483 (1991).

145. Solvent Effects on a Diels-Alder Reaction from Computer Simulations.
J. F. Blake and W. L. Jorgensen
J. Am. Chem. Soc., 113, 7430 (1991).

146. Rusting of the Lock and Key Model of Protein-Ligand Binding.
W. L. Jorgensen
Science, 254, 954 (1991).

147. Computer-Assisted Mechanistic Analysis of Organic Reactions. 20. Ene and Retro-ene Chemistry.
G. D. Paderes and W. L. Jorgensen
J. Org. Chem., 57, 1904 (1992).

148. Free Energy Profiles for Na^+ Adsorption on a Metal Electrode.
T. Matsui and W. L. Jorgensen
J. Am. Chem. Soc., 114, 3220-3226 (1992).

149. Structure and Binding for Cyclophane-Arene Complexes in Water from Monte Carlo Simulations.
W. L. Jorgensen and T. B. Nguyen
NATO ASI Series C, 371, 383 (1992).

150. Enhanced View of Structure and Binding for Cyclophane-Arene Complexes through Joint Theoretical and Experimental Study.
W. L. Jorgensen, T. B. Nguyen, E. M. Sanford, I. Chao, K. N. Houk, and F. Diederich
J. Am. Chem. Soc., 114, 4003-4004 (1992).

151. Solvent Effects on the Barrier to Isomerization for a Tertiary Amide from Ab Initio and Monte Carlo Calculations.
E. M. Duffy, D. L. Severance, and W. L. Jorgensen
J. Am. Chem. Soc., 114, 7535 (1992).

152. Effects of Hydration on the Claisen Rearrangement of Allyl Vinyl Ether from Computer Simulations.
D. L. Severance and W. L. Jorgensen

J. Am. Chem. Soc., 114, 10966 (1992).

153. Solvent Effects on the Diels-Alder Reaction of Methyl Vinyl Ketone and Cyclopentadiene from Computer Simulations.
W. L. Jorgensen, D. Lim, and J. F. Blake
in Elementary Reaction Steps in Heterogeneous Catalysis, R. W. Joyner and R. A. van Santen (eds.), Kluwer Academic Publishers (1993), p 377-387.

154. Monte Carlo Simulations of the Hydration of Substituted Benzenes with OPLS Potential Functions.
W. L. Jorgensen and T. B. Nguyen
J. Comput. Chem., 13, 195 (1993).

155. Monte Carlo Simulations of Pure Liquid Substituted Benzenes with OPLS Potential Functions.
W. L. Jorgensen, E. R. Laird, T. B. Nguyen, amd J. Tirado-Rives
J. Comput. Chem., 13, 206 (1993).

156. Modeling the Complexation of Substituted Benzenes by a Cyclophane Host in Water.
W. L. Jorgensen and T. B. Nguyen
Proc. Nat. Acad. Sci. USA, 90, 1194 (1993).

157. Ab Initio Study of Diels-Alder Reactions of Cyclopentadiene with Ethylene, Isoprene, Cyclopentadiene, Acrylonitrile, and Methyl Vinyl Ketone.
W. L. Jorgensen, D. Lim, and J. F. Blake
J. Am. Chem. Soc., 115, 2936 (1993).

158. Molecular Dynamics Simulations of the Unfolding of Apomyoglobin in Water.
J. Tirado-Rives and W. L. Jorgensen
Biochemistry, 32, 4175 (1993).

159. Supramolecular Chemistry. (Invited editorial.)
W. L. Jorgensen
Proc. Nat. Acad. Sci. USA, 90, 1635 (1993).

160. Urea: Potential Functions, log P, and Free Energy of Hydration.
E. M. Duffy, D. L. Severance, and W. L. Jorgensen
Isr. J. Chem., 33, 323 (1993). (Pople issue.)

161. Limited Effects of Polarization for $Cl^-(H_2O)_n$ and $Na^+(H_2O)_n$ Clusters.
W. L. Jorgensen and D. L. Severance
J. Chem. Phys., 99, 4233 (1993).

162. Accuracy of Free Energies of Hydration for Organic Molecules from 6-31G* Derived

Partial Charges.
H. A. Carlson, T. B. Nguyen, M. Orozco, and W. L. Jorgensen
J. Comput. Chem., 14, 1240 (1993).

163. Molecular Dynamics and Monte Carlo Simulations Favor the α-Helical Form for Alanine-based Peptides in Water.
J. Tirado-Rives, D. S. Maxwell, and W. L. Jorgensen
J. Am. Chem. Soc., 115, 11590 (1993).

164. Computer Assisted Mechanistic Evaluation of Organic Reactions. 22. The Generation and Use of Three-Dimensional Structures.
S. A. Gothe, H. E. Helson, I. Houdaverdis, I. Lagerstedt, S. Sinclair, and W. L. Jorgensen
J. Org. Chem., 58, 5081 (1993).

165. Comparison of 6-31G* Based MST/SCRF and FEP Evaluations of the Free Energies of Hydration for Small Neutral Molecules.
M. Orozco, W. L. Jorgensen, and F. J. Luque
J. Comput. Chem., 14, 1498 (1993).

166. Computational Investigations of Protein Denaturation: Apomyoglobin and Chaotrope-Arene Interactions.
W. L. Jorgensen, E. M. Duffy, and J. Tirado-Rives
Phil. Trans. Roy. Soc. London A, 345, 87-96 (1993).

167. Mechanism for the Rotamase Activity of FK506 Binding Protein from Molecular Dynamics Simulations.
M. Orozco, J. Tirado-Rives, and W. L. Jorgensen
Biochemistry, 32, 12864-12874 (1993).

168. Quantification of Solvent Effects on the Acidities of Z and E Esters from Fluid Simulations.
J. D. Evanseck, K. N. Houk, J. M. Briggs, and W. L. Jorgensen
J. Am. Chem. Soc., 116, 10630-10638 (1994).

169. Do Denaturants Interact with Aromatic Hydrocarbons in Water?
E. M. Duffy, P. J. Kowalczyk, and W. L. Jorgensen
J. Am. Chem. Soc., 115, 9271 (1993).

170. Enhanced Hydrogen Bonding of Water to Diels-Alder Transition States - Ab Initio Evidence.
J. F. Blake, D. Lim, and W. L. Jorgensen
J. Org. Chem., 59, 803-805 (1994).

171. Synthesis and Investigations of Enetetraynes.
D. Elbaum, T. B. Nguyen, W. L. Jorgensen, and S. L. Schreiber
Tetrahedron, 50, 1503-1518 (1994).

172. Modeling Interactions with Benzene: Aryl-Aryl, Cation-π, and Chaotrope-π.
W. L. Jorgensen, D. L. Severance, and E. M. Duffy
in Computational Approaches in Supramolecular Chemistry,
G. Wipff (ed.), Kluwer Academic Publishers (1994), p 161-173.

173. Solvent Effects on the Ring Opening of Cyclopropanones to Oxyallyls - A Combined Ab Initio and Monte Carlo Study.
D. Lim, D. A. Hrovat, W. T. Borden, and W. L. Jorgensen
J. Am. Chem. Soc., 116, 3494-3499 (1994).

174. Computer Assisted Mechanistic Evaluation of Organic Reactions. 23. Dissolving Metal Reductions with Lithium in Liquid Ammonia Including the Birch Reduction.
S. Sinclair and W. L. Jorgensen
J. Org. Chem., 59, 762-772 (1994).

175. Investigation of Solvent Effects on Pericyclic Reactions by Computer Simulations.
W. L. Jorgensen, J. F. Blake, D. Lim, and D. L. Severance
Trans. Faraday Soc., 90, 1727-1732 (1994).

176. Monte Carlo Results for the Effect of Solvation on the Anomeric Equilibrium for 2-Methoxytetrahydropyran.
W. L. Jorgensen, P. I. Morales de Tirado, and D. L. Severance
J. Am. Chem. Soc. 116, 2199-2200 (1994).

177. Computer Assisted Mechanistic Evaluation of Organic Reactions, 24. Carbene Chemistry.
H. E. Helson and W. L. Jorgensen
J. Org. Chem., 59, 3841-3856 (1994).

178. Computer Assisted Mechanistic Evaluation of Organic Reactions, 25. Structure Diagram Positioning.
H. E. Helson and W. L. Jorgensen
J. Chem. Info. Comput. Sci., 34, 962-971 (1994).

179. Effects of Hydration and Multiple Reactant Conformers on the Claisen Rearrangement of Allyl Vinyl Ether from Computer Simulations.
D. L. Severance and W. L. Jorgensen
ACS Symposium Ser., 568, 243-259 (1994).

180. Structure and Binding for Complexes of Rebek's Acridine Diacid with Pyrazine,

Quinoxaline, and Pyridine from Monte Carlo Simulations with an All-Atom Force Field.
E. M. Duffy and W. L. Jorgensen
J. Am. Chem. Soc., 116, 6337-6343 (1994).

181. Free Energies of Hydration and Pure Liquid Properties of Hydrocarbons from the OPLS All-Atom Model.
G. Kaminski, E. M. Duffy, T. Matsui, and W. L. Jorgensen
J. Phys. Chem., 98, 13077-13081 (1994).

182. Generalized Alteration of Structure and Parameters (GASP); a New Method for Free Energy Perturbations in Systems Containing Flexible and/or Fixed Degrees of Freedom.
D. L. Severance, J. W. Essex, and W. L. Jorgensen
J. Comput. Chem., 16, 311-327 (1995).

183. An Empirical Boundary Potential for Water Droplet Simulations.
J. W. Essex and W. L. Jorgensen
J. Comput. Chem., 16, 951-972 (1995).

184. A Comprehensive Study of the Rotational Profiles of Some Organic Systems by Ab Initio MO Theory, Forming a Basis for Peptide Torsional Parameters.
D. S. Maxwell, J. Tirado-Rives, and W. L. Jorgensen
J. Comput. Chem., 16, 984-1010 (1995).

185. Investigations into the Stereochemistry of Steroid-Cyclophane Complexes via Monte Carlo Simulations.
H. A. Carlson and W. L. Jorgensen
Tetrahedron (Symposium in Print), 51, 449-472 (1995).

186. Computer Assisted Mechanistic Evaluation of Organic Reactions, 26. Diastereoselective Additions: Cram's Rule.
J. M. Fleischer, A. J. Gushurst, and W. L. Jorgensen
J. Org. Chem., 60, 490-498 (1995).

187. The Energy Difference Between the Classical and the Nonclassical 2-Norbornyl Cation in Solution. A Combined Ab Initio - Monte Carlo Study.P. R. Schreiner, D. L. Severance, W. L. Jorgensen, P. v.R. Schleyer, and H. F. Schaefer III
J. Am. Chem. Soc., 117, 2663-2664 (1995).

188. An Extended Linear Response Method for Determining Free Energies of Hydration.
H. A. Carlson and W. L. Jorgensen,
J. Phys. Chem., 99, 10667-10673 (1995).

189. Free Energies of Hydration for Organic Molecules from Monte Carlo Simulations.
W. L. Jorgensen and J. Tirado-Rives,

Perspectives in Drug Discovery and Design, 3, 123-138(1995).

190. Elucidation of Transition States and Solvent Effects for the Mislow-Evans Rearrangement of Allylic Sulfoxides.
D. K. Jones-Hertzog and W. L. Jorgensen,
J. Am. Chem. Soc., 117, 9077-9078 (1995).

191. Dielectric Constants of Formamide and Dimethylformamide via Computer Simulations.
J. W. Essex and W. L. Jorgensen,
J. Phys. Chem., 99, 17956-17962 (1995).

192. Regioselective Synthesis of Allylic Alcohols Using the Mislow-Evans Rearrangement: A Theoretical Rationalization.
D. K. Jones-Hertzog and W. L. Jorgensen,
J. Org. Chem., 60, 6682-6683 (1995).

193. The Importance of Polarization for Dipolar Solutes in Low-Dielectric Media: 1,2-Dichloroethane and Water in Cyclohexane.
W. L. Jorgensen, N. A. McDonald, M. Selmi, and P. R. Rablen,
J. Am. Chem. Soc., 117, 11809-11810 (1995).

194. SCRF/Monte Carlo Study of Solvent Effects on a Polar (2 + 2] Cycloaddition.
D. Lim and W. L. Jorgensen,
J. Phys. Chem., 100, 17490-17500 (1996).

195. Molecular Recognition of Carbohydrates: Interaction of Diols with Acetate Ion.
W. L. Jorgensen, W. Damm, A. Frontera, and M. L. Lamb,
NATO ASI Ser., Ser. C, 485, 115-126 (1996).

196. Monte Carlo vs. Molecular Dynamics for Conformational Sampling.
W. L. Jorgensen and J. Tirado-Rives,
J. Phys. Chem., 100, 14508-14513 (1996).

197. The Origin of Self-Assembling Ternary Complex Stabilities and Template Ratios in Carceplex Formation.
K. Nakamura, C. Sheu, A. E. Constable, K. N. Houk, J. C. Sherman, R. G. Chapman, and W. L. Jorgensen,
J. Am. Chem. Soc., 119, 4321-4322 (1997).

198. Viability of Molecular Modeling with Pentium-Based PC's.
J. Tirado-Rives and W. L. Jorgensen,
J. Comput. Chem., 17, 1385-1386 (1996).

199. Monte Carlo Investigations of Solvent Effects on the Chorismate to Prephenate

Rearrangement.
H. A. Carlson and W. L. Jorgensen,
J. Am. Chem. Soc., 118, 8475-8484 (1996).

200. Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids.
W. L. Jorgensen, D. S. Maxwell, and J. Tirado-Rives,
J. Am. Chem. Soc., 118, 11225-11236 (1996).

201. Performance of the AMBER94, MMFF94, and OPLS-AA Force Fields for Modeling Organic Liquids.
G. Kaminski and W. L. Jorgensen,
J. Phys. Chem., 100, 18010-18013 (1996).

202. Binding Affinities for Sulfonamide Inhibitors with HumanThrombin using Monte Carlo Simulations with a Linear Response Method.
D. K. Jones-Hertzog and W. L. Jorgensen,
J. Med. Chem., 40, 1539-1549 (1997).

203. Energetics of Cation-Olefin Addition in the Gas Phase and in Solution.
C. Jenson and W. L. Jorgensen,
Synlett, 518-520 (1997). (E. J. Corey Issue)

204. Free Energies of Solvation in Chloroform and Water from a Linear Response Approach.
N. A. McDonald, H. A. Carlson, and W. L. Jorgensen
J. Phys. Org. Chem., 10, 563-576 (1997). (F. G. Bordwell Issue)

205. Approaches to Protein-Ligand Binding from Computer Simulations.
W. L. Jorgensen, E. M. Duffy, J. W. Essex, D. L. Severance, J. F. Blake, D. K. Jones-Hertzog, M. L. Lamb, and J. Tirado-Rives
NATO ASI Ser., Ser. E, 342, 21-34 (1997).

206. Computational Binding Studies of Orthogonal Cyclosporin-Cyclophilin Pairs.
A. C. Pierce and W. L. Jorgensen
Angew. Chem., 109, 1595-1598 (1997).
Angew. Chem. Int. Ed. Engl., 36, 1466-1469 (1997).

207. Molecular Dynamics of the Unfolding of Barnase in Water and 8M Aqueous Urea.
J. Tirado-Rives, M. Orozco, and W. L. Jorgensen
Biochemistry, 36, 7313-7329 (1997).

208. The OPLS All-Atom Force Field for Carbohydrates.
W. Damm, A. Frontera, J. Tirado-Rives, and W. L. Jorgensen
J. Comput. Chem., 18 , 1955-1970 (1997).

209. Development of an All-Atom Force Field for Heterocycles. Properties of Liquid Pyridine and Diazenes.
W. L. Jorgensen and N. A. McDonald
J. Mol. Struct. (Theochem.), 424, 145-155 (1998). (L. Salem Issue.)

210. Monte Carlo Simulations for Proteins: Binding Affinities for Trypsin-Benzamidine Complexes via Free Energy Perturbations.
J. W. Essex, D. L. Severance, J. Tirado-Rives, and W. L. Jorgensen,
J. Phys. Chem., 101, 9663-9669 (1997).

211. Computational Investigations of Carbenium Ion Reactions Relevant to Sterol Biosynthesis.
C. Jenson and W. L. Jorgensen,
J. Am. Chem. Soc., 118, 10846-10854 (1997).

212. Elucidation of Transition Structures and Solvent Effects for Epoxidations by Dimethyldioxirane.
C. Jenson, J. Liu, K. N. Houk, and W. L. Jorgensen,
J. Am. Chem. Soc., 119, 12982-12983 (1997).

213. Computational Approaches to Molecular Recognition.
M. L. Lamb and W. L. Jorgensen,
Curr. Opinion Chem. Biol., 1, 449-457 (1997).

214. BOSS - Biochemical and Organic Simulation System.
W. L. Jorgensen,
Encyclopedia of Computational Chemistry, P. v.R. Schleyer, Ed.;
Wiley: New York, 1998; Vol. 5, p 3281-3285.

215. ChemEdit - An Interactive Editor for Chemists.
D. Lim and W. L. Jorgensen,
Encyclopedia of Computational Chemistry, P. v.R. Schleyer, Ed.;
Wiley: New York, 1998; Vol. 5, p 3295-3302.

216. OPLS Force Fields.
W. L. Jorgensen,
Encyclopedia of Computational Chemistry, P. v.R. Schleyer, Ed.;
Wiley: New York, 1998; Vol. 3, p 1986-1989.

217. Monte Carlo Simulations of Liquids.
W. L. Jorgensen,
Encyclopedia of Computational Chemistry, P. v.R. Schleyer, Ed.;
Wiley: New York, 1998; Vol. 3, p 1754-1763.

218. Temperature Dependence of TIP3P, SPC, and TIP4P Water from NPT Monte Carlo Simulations: Seeking a Temperature of Maximum Density.
W. L. Jorgensen and C. Jenson,
J. Comput. Chem., 19 , 1179-1186 (1998). (N. L. Allinger Issue.)

219. Computation of Free Energy Changes in Solution.
W. L. Jorgensen,
Encyclopedia of Computational Chemistry, P. v.R. Schleyer, Ed.;
Wiley: New York, 1998; Vol. 2, p 1061-1070.

220. A QM/MM Method Based on CM1A Charges: Applications to Solvent Effects on Organic Equilibria and Reactions.
G. A. Kaminski and W. L. Jorgensen,
J. Phys. Chem. B, 102, 1787-1796 (1998).

221. Preorganized Metallomacrocycles: Improved Binding and Selectivity of Ammonia over Primary Amines.
F. C. J. M. van Veggel, H. G. Noorlander-Bunt, W. L. Jorgensen and D. N. Reinhoudt,
J. Org. Chem., 63, 3554-3559 (1998).

222. Ab Initio Calculations on Hydrogen-Bonded Complexes of Small Organic Molecules with Water.
P. R. Rablen, J. W. Lockman, and W. L. Jorgensen,
J. Phys. Chem. A, 102, 3782-3797 (1998).

223. Monte Carlo Investigations of Selective Anion Complexation by a Bis(phenylurea)-*p*-*tert*-Butylcalix(4]arene.
N. A. McDonald, E. M. Duffy, and W. L. Jorgensen,
J. Am. Chem. Soc., 120, 5104-5111 (1998).

224. Investigations of Neurotrophic Inhibitors of FK506 Binding Protein via Monte Carlo Simulations.
M. L. Lamb and W. L. Jorgensen,
J. Med. Chem., 41, 3928-3939 (1998).

225. Conformational Complexity of Succinic Acid and Its Monoanion in the Gas Phase and in Solution: Ab Initio Calculations and Monte Carlo Simulations.
D. J. Price, J. D. Roberts, and W. L. Jorgensen,
J. Am. Chem. Soc., 120, 9672-9679 (1998).

226. Development of an All-Atom Force Field for Heterocycles. Properties of Liquid Pyrrole, Furan, Diazoles, and Oxazoles.
W. L. Jorgensen and N. A. McDonald,

J. Phys. Chem. B, 102, 8049-8059 (1998).

227. Ab Initio and Monte Carlo Study of Solvent Effects on a 1,3-Dipolar Cycloaddition.
M. P. Repasky and W. L. Jorgensen,
J. Chem. Soc., Faraday Discuss., 110, 379-389 (1998).

228. Prediction of Binding Affinities for TIBO Inhibitors of HIV-1 Reverse Transcriptase Using Monte Carlo Simulations in a Linear Response Method.
R. H. Smith, Jr., W. L. Jorgensen, J. Tirado-Rives, M. L. Lamb, P. A. J. Janssen, C. J. Michejda, and M. B. Kroeger Smith,
J. Med. Chem., 41, 5272-5286 (1998).

229. Solvent as Catalyst - Computational Studies of Organic Chemistry in Solution.
D. Lim, C. Jenson, M. P. Repasky, and W. L. Jorgensen,
In *Transition State Modeling for Catalysis*, D. Truhlar and K. Morokuma, Eds.,
ACS Symposium Ser., 721, 74-85 (1999).

230. Computational Studies of Molecular Recognition from Alkane Dimers to Protein-Ligand Binding.
W. L. Jorgensen, E. M. Duffy, J. W. Essex, D. L. Severance, J. F. Blake, N. A. McDonald, and J. Tirado-Rives,
In "*Crystal Engineering*", K. R. Seddon & M. Zaworotko, Eds.; Kluwer: Amsterdam, 1999; p 113-125.

231. Estimation of the Binding Affinities of FKBP12 Inhibitors Using a Linear Response Method.
M. L. Lamb, J. Tirado-Rives, and W. L. Jorgensen,
Bioorg. Med. Chem., 7, 851-860 (1999). (D. Barton memorial.)

232. Computational Studies of the Molecular Recognition of Halide Anions by Calix[4]Aromatics.
N. A. McDonald, W. P. van Hoorn, E. M. Duffy, and W. L. Jorgensen,
NATO ASI Ser., Ser. C, 527, 147-156 (1999).

233. OPLS All-Atom Model for Amines: Resolution of the Amine Hydration Problem.
R. C. Rizzo and W. L. Jorgensen,
J. Am. Chem. Soc., 121, 4827-4836 (1999).

234. Selective Anion Complexation by a Calix[4]pyrrole Investigated by Monte Carlo Simulations.
W. P. van Hoorn and W. L. Jorgensen,
J. Org. Chem., 64, 7439-7444 (1999).

235. Host-Guest Chemistry of Rotaxanes and Catenanes: Application of a Polarizable All-

Atom Force Field to Cyclobis(paraquat-*p*-phenylene) Complexes with Disubstituted Benzenes and Biphenyls.
G. A. Kaminski and W. L. Jorgensen,
Perkin Trans. 2, 2365-2376 (1999). (R. Squires memorial.)

236. Perspective on "Equation of State Calculations by Fast Computing Machines".
W. L. Jorgensen
Theor. Chem. Acc., 103, 225-227 (2000). (New Century Issue)

237. Developing a Dynamic Pharmacaphore Model for HIV-1 Integrase.
H. A. Carlson, K. M. Masukawa, K. Rubins, F. D. Bushman, W. L. Jorgensen, R. D. Lins, J. M. Briggs, and J. A. McCammon,
J. Med. Chem., 43, 2100-2114 (2000).

238. Prediction of Properties from Simulations: Free Energies of Solvation in Hexadecane, Octanol, and Water.
E. M. Duffy and W. L. Jorgensen,
J. Am. Chem. Soc., 122, 2878-2888 (2000).

239. Monte Carlo Calculations on HIV-1 Reverse Transcriptase Complexed with the Nonnucleoside Inhibitor 8-Cl TIBO: Contribution of the L100I and Y181C Variants to Protein Stability and Biological Activity.
M. B. Kroeger Smith, M. L. Lamb, J. Tirado-Rives, W. L. Jorgensen, C. J. Michejda, S. K. Ruby, and R. H. Smith, Jr.,
Protein Engin., 13, 413-421 (2000).

240. A five-site model for liquid water and the reproduction of the density anomaly by rigid, non-polarizable models.
M. W. Mahoney and W. L. Jorgensen,
J. Chem. Phys., 112, 8910-8922 (2000).

241. Origin of the Inversion of the Acidity Order for Haloacetic Acids on Going from the Gas Phase to Solution.
K. B. Wiberg, S. Clifford, W. L. Jorgensen, and M. J. Frisch,
J. Phys. Chem. A, 104, 7625-7628 (2000).

242. Prediction of Drug Solubility from Monte Carlo Simulations.
W. L. Jorgensen and E. M. Duffy,
Bioorg. Med. Chem. Lett., 10, 1155-1158 (2000).

243. Analysis of Binding Affinities for Celecoxib Analogs with COX-1 and COX-2 from Docking and Monte Carlo Simulations and Insight into COX-2/COX-1 Selectivity.
M. L. Plount Price and W. L. Jorgensen,
J. Am. Chem. Soc., 122, 9455-9466 (2000).

244. Computational Binding Studies of Human pp60$^{c\text{-}src}$ SH2 Domain with a Series of Nonpeptide, Phosphophenyl-Containing Ligands.
Daniel J. Price and W. L. Jorgensen,
Bioorg. Med. Chem. Lett., 10, 2067-2070 (2000).

245. Validation of a Model for the Complex of HIV-1 Reverse Transcriptase with Sustiva through Computation of Resistance Profiles.
R. C. Rizzo, De-Ping Wang, J. Tirado-Rives, and W. L. Jorgensen,
J. Am. Chem. Soc., 122, 12898-12900 (2000).

246. Estimation of Binding Affinities for HEPT and Nevirapine Analogs with HIV-1 Reverse Transcriptase via Monte Carlo Simulations.
R. C. Rizzo, J. Tirado-Rives, and W. L. Jorgensen,
J. Med. Chem., 44, 145-154 (2001).

247. Diffusion constant of the TIP5P model of liquid water.
M. W. Mahoney and W. L. Jorgensen,
J. Chem. Phys., 114, 363-366 (2001).

248. Rapid Estimation of Electronic Degrees of Freedom in Monte Carlo Calculations for Polarizable Models of Liquid Water.
M. W. Mahoney and W. L. Jorgensen,
J. Chem. Phys., 114, 9337-9349 (2001).

249. Rationale for the Observed COX-2/COX-1 Selectivity of Celecoxib from Monte Carlo Simulations.
M. L. P. Price and W. L. Jorgensen,
Bioorg. Med. Chem. Lett., 11, 1541-1544 (2001).

250. Efficient Exploration of Conformational Space Using the Stochastic Search Method: Application to β-Peptide Oligomers.
J. Chandrasekhar, M. Saunders, and W. L. Jorgensen,
J. Comput. Chem., 22, 1646-1654 (2001).

251. Gas-Phase and Liquid-State Properties of Esters, Nitriles, and Nitro Compounds with the OPLS-AA Force Field.
M. L. P. Price, D. Ostrovsky, and W. L. Jorgensen,
J. Comput. Chem., 22, 1340-1352 (2001).

252. Improved Convergence of Binding Affinities with Free Energy Perturbation: Application to Nonpeptide Ligands with pp60^{src} SH2 Domain.
D. L. Price and W. L. Jorgensen,

J. Comp. Aided Mol. Design, 15, 681-695 (2001).

253. Estimation of Binding Affinities for Selective Thrombin Inhibitors via Monte Carlo Simulations.
A. C. Pierce and W. L. Jorgensen,
J. Med. Chem., 44, 1043-1050 (2001).

254. Evaluation and Reparameterization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptides.
G. Kaminski, R. A. Friesner, J. Tirado-Rives and W. L. Jorgensen,
J. Phys. Chem. B, 105, 6474-6487 (2001).

255. Protein Structure Calculation Based on NMR Data: An Enhanced Monte Carlo Approach.
A. C. Pierce and W. L. Jorgensen,
J. Biomol. NMR, 00, 0000-0000 (2001). Submitted.

256. Perfluoroalkanes: Conformational Analysis and Liquid-State Properties from Ab Initio and Monte Carlo Calculations.
E. K. Watkins and W. L. Jorgensen,
J. Phys. Chem. A, 105, 4118-4125 (2001).

257. COX-2, Src SH2 Domain, HIV Reverse Transcriptase, and Thrombin: Computational Approaches to Drug Design.
W. L. Jorgensen, M. L. P. Price, D. J. Price, R. C. Rizzo, D. Wang, A. C. Pierce, and J. Tirado-Rives,
In *Free Energy Calculations in Rational Drug Design*, M. R. Reddy and M. D. Elion, Eds.; Kluwer: New York, 2001; p 299-316.

258. New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model.
R. Zhou, R. A. Friesner, A. Ghosh, R. C. Rizzo, W. L. Jorgensen, and R. M. Levy,
J. Phys. Chem. B, 105, 10388-10397 (2001).

259. Antiviral Drug Design: Computational Analyses of the Effects of the L100I Mutation for HIV-RT on the Binding of NNRTIs.
D.-P. Wang, R. C. Rizzo, J. Tirado-Rives, and W. L. Jorgensen,
Bioorg. Med. Chem. Lett., 11, 2799-2802 (2001).

260. Quantum, intramolecular flexibility, and polarizability effects on the reproduction of the density anomaly of liquid water by simple potential functions.
M. W. Mahoney and W. L. Jorgensen,
J. Chem. Phys., 115, 10758-10768 (2001).

261. Improved Semiempirical Heats of Formation through the Use of Bond and Group Equivalents.
M. P. Repasky, J. Chandrasekhar, and W. L. Jorgensen,
J. Comput. Chem., 23, 498-510 (2002).

262. Prediction of Drug Solubility from Structure.
W. L. Jorgensen and E. M. Duffy,
Adv. Drug Delivery Reviews, 54, 355-366 (2002).

263. Three- vs. Four-Coordinate Phosphorus in the Gas Phase and in Solution: Treacherous Relative Energies for Phosphine Oxide and Phosphinous Acid.
S. S. Wesolowski, N. R. Brinkmann, E. F. Valeev, H. F. Schaefer III, M. P. Repasky, and W. L. Jorgensen,
J. Chem. Phys., 116, 112-122 (2002).

264. QM/MM Simulations of Cycloaddition Reactions in Water: Contribution of Enhanced Hydrogen Bonding at the Transition State to the Solvent Effects.
J. Chandrasekhar, S. Shariffskul, and W. L. Jorgensen,
J. Phys. Chem. B, 106, 8078-8085 (2002). (Tully Issue)

265. Estimation of Binding Affinities for Celecoxib Analogues with COX-2 via Monte Carlo – Extended Linear Response.
S. S. Wesolowski and W. L. Jorgensen,
Bioorg. Med. Chem. Lett., 12, 267-270 (2002).

266. Prediction of Activity for Non-nucleoside Inhibitors with HIV Reverse Transcriptase Based on Monte Carlo Simulations.
R. C. Rizzo, M. Udier Blagovic, D.-P. Wang, E. K. Watkins, M. B. Kroeger Smith, R. H. Smith, Jr., J. Tirado-Rives, and W. L. Jorgensen,
J. Med. Chem., 45, 2970-2987 (2002).

267. PDDG/PM3 and PDDG/MNDO: Improved Semiempirical Methods.
M. P. Repasky, J. Chandrasekhar, and W. L. Jorgensen,
J. Comput. Chem., **23**, 1601-1622 (2002).

268. Molecular Modeling Calculations of HIV-1 Reverse Transcriptase Nonnucleoside Inhibitors: Correlation of Binding Energy with Biological Activity for Novel 2-Aryl-Substituted Benzimidazole Analogs.
Kroeger Smith, M. B.; Hose, B. M.; Hawkins, A.; Lipchock, J.; Farnsworth, D. W.; Rizzo, R. C.; Tirado-Rives, J.; Arnold, A.; Zhang, W.; Hughes, S. H.; Jorgensen, W. L.; Michejda, C. J.; and Smith, R. H., Jr., *J. Med. Chem*. **2003**, *46*, 1940-1947.

269. Monte Carlo backbone sampling for polypeptides with variable bond angles and dihedral angles using concerted rotations and a Gaussian bias.

Ulmschneider, J.; Jorgensen, W. L. *J. Chem. Phys.* **2003,** *118*, 4261-4271.

270. Investigation of Solvent Effects for the Claisen Rearrangement of Chorismate to Prephenate: Mechanistic Interpretation via Near Attack Conformations.
Repasky, M. P.; Guimaraes, C. R. W.; Chandrasekhar, J.; Tirado-Rives, J.; Jorgensen, W. L. *J. Am. Chem. Soc*. **2003**, *125*, 6663-6672. DOI: 10.1021/ja021423z

271. Contributions of Conformational Compression and Preferential Transition State Stabilization to the Rate Enhancement by Chorismate Mutase.
Guimaraes, C. R. W.; Repasky, M. P.; Chandrasekhar, J.; Tirado-Rives, J.; Jorgensen, W. L. *J. Am. Chem. Soc*. **2003**, *125*, 6892-6899. DOI: 10.1021/ja021424r

272. Activity Predictions for Efavirenz Analogues with the K103N Mutant of HIV Reverse Transcriptase.
Blagović, M. U.; Watkins, E. K.; Tirado-Rives, J.; Jorgensen, W. L., *Bioorg. Med. Chem. Lett*. **2003**, ***13***, 3337-3340.

273. Validation of a Model for the Complex of HIV-1 Reverse Transcriptase with the Novel Non-nucleoside Inhibitor TMC125.
Blagović, M. U.; Tirado-Rives, J.; Jorgensen, W. L., *J. Am. Chem. Soc*. **2003**, *125*, 6016-6017. DOI: 10.1021/ja034308c

274. Analyses of Activity for Factor Xa Inhibitors Based on Monte Carlo Simulations.
Ostrovsky, D.; Blagović, M. U.; Jorgensen, W. L., *J. Med. Chem.* **2003,** *46*, 5691-5699.

275. Extension of the PDDG/PM3 and PDDG/MNDO Semiempirical Molecular Orbital Methods to the Halogens.
Tubert-Brohman, I.; Guimaraes, C. R. W; Repasky, M. P.; Jorgensen, W. L., *J. Comput. Chem*. **2004**, *25*, 138-150.

276. Structural and Energetic Analyses for the Effects of the K103N Mutation of HIV-1 Reverse Transcriptase on Efavirenz Analogs.
Blagović, M. U.; Tirado-Rives, J.; Jorgensen, W. L., *J. Med. Chem.* **2004,** *46*, 2389-2392.

277. Steric Retardation of S_N2 Reactions in the Gas Phase and Solution.
Vayner, G.; Houk, K. N.; Jorgensen, W. L.; Brauman, J. I., *J. Am. Chem. Soc.* **2004**, *126*, 9054-9058. DOI: 10.1021/ja049070m

278. Polypeptide Folding using Monte Carlo Sampling, Concerted Rotation, and Continuum Solvation.
Ulmschneider, J. P.; Jorgensen, W. L., *J. Am. Chem. Soc*. **2004**, *126*, 1849-1857. DOI: 10.1021/ja0378862

279. General Model for Estimation of the Inhibition of Protein Kinases Using Monte Carlo Simulations.
Tominaga, Y. & Jorgensen, W. L., *J. Med. Chem*. **2004**, *47*, 2534-2549.

280. Accuracy of Free Energies of Hydration from CM1 and CM3 Atomic Charges.
Blagović, M. U.; Morales de Tirado, P.; Pearlman, S. A.; Jorgensen, W. L., *J. Comput. Chem.* **2004,** *25*, 1322-1332.

281. HIV-1 Reverse Transcriptase Variants: Molecular Modeling of Y181C, V106A, L100I, and K103N Mutations with Non-Nucleoside Inhibitors.
Marilyn B. Kroeger Smith, Sandra Ruby, Stanislav Horouzhenko, Bryan Buckingham, Julia Richardson, Ina Puleri, Emily Potts, William L. Jorgensen, Edward Arnold, Wanyi Zhang, Stephen H. Hughes, Christopher J. Michejda, and Richard H. Smith, Jr. *Drug Design Disc.* **2003**, *18*, 151-163

282. The Many Roles of Computation in Drug Discovery.
Jorgensen, W. L., *Science* **2004**, *303*, 1813-1818. PMID: 15031495

283. Free Energies of Hydration from a Generalized Born Model and an All-Atom Force Field.
Jorgensen, W. L.; Ulmschneider, J. P.; Tirado-Rives, J. *J. Phys. Chem. B* **2004**, *108*, 16264-16270.

284. Energetic Preferences for α, β- versus β, γ-Unsaturation.
Lee, P. S.; Du, W.; Boger, D. L.; Jorgensen, W. L. *J. Org. Chem.* **2004**, *69*, 5448-5453.

285. Solvent Effects and Mechanism for a Nucleophilic Aromatic Substitution from QM/MM Simulations.
Acevedo, O.; Jorgensen, W. L. *Org. Lett.* **2004**, *6*, 2881-2884.

286. Monte Carlo Backbone Sampling for Nucleic Acids using Concerted Rotations including Variable Bond Angles.
Ulmschneider, J. P.; Jorgensen, W. L. *J. Phys. Chem. B* **2004**, *108*, 16883-16892.

287. Relationship between side chain structure and 14-helix stability of β^3-peptides in water.
Kritzer, J. A.; Tirado-Rives, J.; Hart, S. A.; Lear, J. D.; Jorgensen, W. L.; Schepartz, A. *J. Am. Chem. Soc*. **2005**, *127*, 167-178.

288. Discovery of a Potent, Selective, and Efficacious Class of Reversible α-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesics.
Boger, D. L.; Miyauchi, H.; Du, W.; Hardouin, C.; Fecik, R. A.; Cheng, H.; Hwang, I.; Hedrick, M. P.; Leung, D.; Acevedo, O.; Guimaraes, C. R. W.; Jorgensen, W. L.;

Cravatt, B. F. *J. Med. Chem.* **2005**, *48*, 1849-1856.

289. Macrophomate Synthase: QM/MM Simulations Address the Diels-Alder versus Michael-Aldol Reaction Mechanism.
Guimarães, C. R. W ; Blagović, M. U.; Jorgensen, W. L., *J. Am. Chem. Soc.* **2005,** *127*, 3577-3588.

290. Potential energy functions for atomic-level simulations of water, and organic and biomolecular systems.
Jorgensen, W. L.; Tirado-Rives, J. *Proc. Nat. Acad. Sci. USA* **2005**, *102*, 6665-6670.

291. Molecular Modeling of Organic and Biomolecular Systems Using BOSS and MCPRO.
Jorgensen, W. L.; Tirado-Rives, J. *J. Comput. Chem.* **2005**, *26*, 1689-1700.

292. Extension of the PDDG/PM3 semiempirical molecular orbital method to sulfur, silicon, and phosphorus.
Tubert-Brohman, I.; Guimarães, C. R. W; Jorgensen, W. L.,
J. Chem. Theory Comput. **2005**, *1*, 817-823.

293. Influence of Inter- and Intramolecular Hydrogen Bonding on Kemp Decarboxylations from QM/MM Simulations.
O. Acevedo, W. L. Jorgensen, *J. Am. Chem. Soc.* **2005**, *127*, 8829-8834.

294. Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate.
Guimarães, C. R. W ; Blagović, M. U.; Tubert-Brohman, I.; Jorgensen, W. L., *J. Chem. Theory Comput.* **2005,** *1*, 617-625.

295. Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent α-Ketoheterocycle Derivatives from Monte Carlo Simulations.
Guimarães, C. R. W ; Boger, D. L.; Jorgensen, W. L., *J. Am. Chem. Soc.* **2005,** *127*, 17377-17384.

296. Assault on Resistance: The Use of Computational Chemistry in the Development of Anti-HIV Drugs.
Kroeger Smith, M. B.; Smith, R. H., Jr.; Jorgensen, W. L., *Perspec. Drug Disc. Design* **2006**, *12*, 1843-1856.

297. NO-MNDO: Reintroduction of the Overlap Matrix into MNDO.
Sattelmeyer, K. W.; Tubert-Brohman, I.; Jorgensen, W. L.,
J. Chem. Theory Comput. **2006**, *2*, 413-419.

298. Computer-Aided Design of Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase.
Jorgensen, W. L.; Ruiz-Caro, J.; Tirado-Rives, J.; Basavapathruni, A.; Anderson, K.

S.; Hamilton, A. D. *Bioorg. Med. Chem. Lett.* **2006**, *16*, 663-667. "BMCL - Top-50 most cited articles, 2006-2009." PMID: 16263277

299. Optimization of Diarylamines as Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase.
Ruiz-Caro, J.; Basavapathruni, A.; Kim, J. T.; Wang, L.; Bailey, C. M.; Anderson, K. S.; Hamilton, A. D.; Jorgensen, W. L. *Bioorg. Med. Chem. Lett.* **2006**, *16*, 668-671.

300. Solvent Effects on the Rates of Organic Reactions from QM/MM Simulations.
Acevedo, O.; Jorgensen, W. L. *Ann. Rep. Comput. Chem.* **2006**, *2*, 263-278.

301. Cope Elimination: Elucidation of Solvent Effects from QM/MM Simulations.
Acevedo, O.; Jorgensen, W. L. *J. Am. Chem. Soc.* **2006**, *128*, 6141-6146.

302. Medium Effects on the Decarboxylation of a Biotin Model in Pure and Mixed Solvents from QM/MM Simulations.
Acevedo, O.; Jorgensen, W. L.
J. Org. Chem. **2006**, *71*, 4896-4902.

303. Optimization of Pyrimidinyl- and Triazinyl-amines as Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase.
Thakur, V.; Kim, J. T.; Hamilton, A. D.; Bailey, C. M.; Domaoal, R. A.;Wang, L.; Anderson, K. S.; Jorgensen, W. L. *Bioorg. Med. Chem. Lett.* **2006**, *16*, 5664-5667.

304. Contribution of Conformer Focusing to the Uncertainty in Predicting Free Energies for Protein-Ligand Binding.
Tirado-Rives, J.; Jorgensen, W. L. *J. Med. Chem.* **2006**, *49*, 5880-5884.

305. Comparison of SCC-DFTB and NDDO-Based Semiempirical Molecular Orbital Methods for Organic Molecules.
Sattelmeyer, K. W.; Tirado-Rives, J.; Jorgensen, W. L. *J. Phys. Chem. A* **2006**, *110*, 13551-13559.

306. Conformation of Alkanes in the Gas Phase and Pure Liquids.
Thomas, L. L.; Christakis, T. J.; Jorgensen, W. L. *J. Phys. Chem. B* **2006**, *110*, 21198-21204.

307. Halide, Ammonium, and Alkali Metal Ion Parameters for Modeling Aqueous Solutions.
Jensen, K. P.; Jorgensen, W. L. *J. Chem. Theory Comput.* **2006**, *2*, 1499-1509.

308. Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant.
Tubert-Brohman, I.; Acevedo, O.; Jorgensen, W. L. *J. Am. Chem. Soc.* **2006**, *128*, 16904-16913.

309. FEP-Guided Selection of Bicyclic Heterocycles in Lead Optimization for Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase
Kim, J. T.; Hamilton, A. D.; Bailey, C. M.; Domaoal, R. A.;Wang, L.; Anderson, K. S.; Jorgensen, W. L. *J. Am. Chem. Soc.* **2006**, *128*, 15372-15373. PMID: 17131993

310. Why Urea Eliminates Ammonia Rather Than Hydrolyzes in Aqueous Solution.
Alexandrova, A.; Jorgensen, W. L. *J. Phys. Chem. B* **2007**, *111*, 720-730.

311. Computation of Accurate Activation Barriers for Methyl Transfer Reactions of Sulfonium and Ammonium Salts in Aqueous Solution.
Gunaydin, H.; Acevedo, O.; Jorgensen, W. L.; Houk, K. N.
J. Chem. Theory Comput. **2007**, *3*, 1028-1035.

312. Elucidation of Rate Variations for a Diels-Alder Reaction in Ionic Liquids from QM/MM Simulations.
Acevedo, O.; Jorgensen, W. L.; Evanseck, J. D.
J. Chem. Theory Comput. **2007**, *3*, 132-138.

313. Understanding Rate Accelerations for Diels-Alder Reactions in Solution using Enhanced QM/MM Methodology.
Acevedo, O.; Jorgensen, W. L.
J. Chem. Theory Comput. **2007**, *3*, 1412-1419.

314. From Docking False-Positive to Active Anti-HIV Agent.
Barreiro, G.; Kim, J. T.; Guimaraes, C. R. W.; Bailey, C. M.; Domaoal, R. A.; Wang, L.; Anderson, K. S..; Jorgensen, W. L.
J. Med. Chem. **2007**, *50*, 5324-5329. PMID:17918923

315. Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water and Chloride Ion.
Jorgensen, W. L.; Jensen, K. P.; Alexandrova, A.
J. Chem. Theory Comput. **2007**, *3*, 1987-1992.

316. Search for Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase using Chemical Similarity, Molecular Docking, and MM-GB/SA Scoring.
Barreiro, G.; Guimaraes, C. R. W.; Tubert-Brohman, I.; Lyons, T. M.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Inf. Model. **2007**, *47*, 2416-2428. PMID:17949071

317. Optical Rotatory Dispersion of 2,3-Hexadiene and 2,3-Pentadiene.
Wiberg, K. B.; Wang, Y. G.; Wilson, S. M.; Vaccaro, P. H.; Jorgensen, W. L.; Crawford, T. D.; Abrams, M. L.; Cheeseman, J. R.; Luderer, M.
J. Phys. Chem. A **2008**, *112*, 2415-2422.

318. Performance of the B3LYP Density Functional Method for a Large Set of Organic Molecules.
Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2008**, *4*, 297-306.

319. Energetic effects for observed and unobserved HIV-1 reverse transcriptase mutations of residues L100, V106, and Y181 in the presence of nevirapine and efavirenz.
Smith, M. B. K.; Rader, L. H.; Franklin, A. M.; Taylor, E. V.; Smith, K. D.: Smith, R. H.; Tirado-Rives, J.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2008**, *18*, 969-972. PMID:18166457

320. Perspective on Free-Energy Perturbation Calculations for Chemical Equilibria.
Jorgensen, W. L.; Thomas, L. L.
J. Chem. Theory Comput. **2008**, *4*, 869-876. PMID:19936324

321. Optimization of Azoles as Anti-HIV Agents Guided by Free-Energy Calculations.
Zeevaart, J. G.; Wang, L.; Thakur, V. V.; Leung, C. S.; Tirado-Rives, J.; Bailey, C. M.; Domaoal, R. A.; Anderson, K. S.; Jorgensen, W. L.
J. Am. Chem. Soc. **2008**, *130*, 9492-9499. PMID:18588301

322. Catalytic Mechanism and Performance of Computationally Designed Enzymes for Kemp Elimination.
Alexandrova, A.; Röthlisberger, D.; Baker, D.; Jorgensen, W. L. *J. Am. Chem. Soc.* **2008**, *130*, 15907-15915. PMID:18975945

323. Exploiting structural analysis, in silico screening, and serendipity to identify novel inhibitors of drug-resistant falciparum malaria.
Dasgupta, T.; Chitnumsub, P.; Maneeruttanarungroj, C.; Kamchonwongpaisan, S.; Nichols, S. N.; Lyons, T. M.; Tirado-Rives, J.; Jorgensen, W. L.; Yuthavong, Y.; Anderson, K. S. *ACS Chem. Biol.* **2009**, *4*, 29-40. PMID:19146480

324. Origin of the Activity Drop with the E50D Variant of Catalytic Antibody 34E4 for Kemp Elimination.
Alexandrova, A.; Jorgensen, W. L. *J. Phys. Chem. B* **2009**, *113*, 497-504. PMID:19132861

325. Discovery of Human Macrophage Migration Inhibitory Factor (MIF)-CD74 Antagonists via Virtual Screening.
Cournia, Z.; Leng, L.; Gandavadi, S.; Du, X.; Bucala, R.; Jorgensen, W. L.
J. Med. Chem. **2009**, *52*, 416-424. PMID:19090668

326. Novel Non-Active Site Inhibitor of Cryptosporidium hominis TS-DHFR Identified by a Virtual Screen.
Martucci, W. E.; Udier-Blagovic, M.; Atreya, C.; Babatunde, O.; Vargo, M. A.; Jorgensen, W. L.; Anderson, K. S. *Bioorg. Med. Chem. Lett.* **2009**, *19*, 418-423. PMID:19059777

327. Efficient Drug Lead Discovery and Optimization.
Jorgensen, W. L. *Acc. Chem. Res.* **2009**, *42*, 724-733. PMCID:PMC2727934

328. Vancomycin Resistance: Modeling Backbone Variants with D-Ala-D-Ala and D-Ala-D-Lac Peptides.
Leung, S. S. F.; Tirado-Rives, J.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2009**, *19*, 1236-1239. PMID:19128968

329. Discovery of Wild-type and Y181C Mutant Non-nucleoside HIV-1 Reverse Transcriptase Inhibitors Using Virtual Screening with Multiple Protein Structures.
Nichols, S. E.; Domaoal, 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. PMID:19374380

330. 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. PMID:19415930

331. Vancomycin Analogs: Seeking Improved Binding of D-Ala-D-Ala and D-Ala-D-Lac Peptides by Side-Chain and Backbone Modifications.
Leung, S. S. F.; Tirado-Rives, J.; Jorgensen, W. L.
Bioorg. Med. Chem. **2009**, *17*, 5874-5886. PMID:19620008

332. 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. PMID:19754086
Received the *Emerging Technology Award* at the August 2009 Nat'l ACS Meeting.

333. 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

334. 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. PMID:19778066

335. 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. PMID:19888723

336. Progress and Issues for Computationally-Guided Lead Discovery and Optimization.
Jorgensen, W. L. in "Drug Design: Structure and Ligand-Based Approaches", Merz, K.; Reynolds, C.; Ringe, D., Eds.; Cambridge Univ. Press, Cambridge, UK, **2010**. ISBN 9780521887236

337. Advances in QM/MM Simulations for Organic and Enzymatic Reactions.
Acevedo, O.; Jorgensen, W. L.
Acc. Chem. Res. **2010**, *43*, 142-151. PMID:19728702

338. 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. **2010**, *53*, 1662-1672. PMID:20121196

339. Eastern extension of azoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase; cyano group alternatives.
Leung, C. S.; Zeevaart, J. G.; Domaoal, R. A.; Bollini, M.; Thakur, V. V.; Spasov, K.; Anderson, K. S.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2010**, *20*, 2485-2488. PMID:20304641

340. 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*, 3097-3104. PMID:20148559

341. Exploring Solvent Effects on the Menshutkin Reaction using a Polarizable Force Field.
Acevedo, O.; Jorgensen, W. L. *J. Phys. Chem. B* **2010**, *114*, 8425-8430. PMCID: PMC2903038

342. Thorpe-Ingold Acceleration of Oxirane Formation is Mostly a Solvent Effect.
Kostal, J.; Jorgensen, W. L.
J. Am. Chem. Soc. **2010**, *132*, 8766-8773. PMID:20524660

343. A Remote Arene Binding Site on Prostate Specific Membrane Antigen Revealed by Antibody-Recruiting Small Molecules.
Zhang, A. X.; Murelli, R. P. ; Barinka, C. ; Michel, J.; Cocleaza, A.; Jorgensen, W. L.; Lubkowski, J.; Spiegel, D. A.
J. Am. Chem. Soc. **2010**, *132*, 12711-12716. PMID:20726553

344. Optimization of *N*-benzyl-benzoxazol-2-ones as receptor antagonists of macrophage migration inhibitory factor (MIF).
Hare, A. A.; Leng, L.; Gandavadi, S.; Du, X.; Cournia, Z. ; Bucala, R. ; Jorgensen, W. L. *Bioorg. Med. Chem. Lett.* **2010**, *20*, 5811-5814. PMID:20728358; PMCID: PMC2939296

345. Pulled from a protein's embrace.
Jorgensen, W. L. *Nature* **2010**, *466*, 42-43. PMID:20596009

346. *E/Z* Energetics for Molecular Modeling and Design.
Terhorst, J. P.; Jorgensen, W. L.
J. Chem. Theory Comput. **2010**, *6*, 2762-2769. PMID:20871784

347. Synthesis and Evaluation of Selected Key Methyl Ether Derivatives of Vancomycin Aglycon.
Crane, C. M.; Pierce, J. G.; Leung, S. S. F. ; Tirado-Rives, J. ; Jorgensen, W. L. ; Boger, D. L. *J. Med. Chem*. **2010**, *53*, 7229-7235. PMID:20853900

348. Receptor agonists of macrophage migration inhibitory factor.
Jorgensen, W. L.; Gandavadi, S.; Du, X.; Hare, A. A.; Trofimov, A.; Leng, L.; Bucala, R. *Bioorg. Med. Chem. Lett.* **2010**, *20*, 7033-7036. PMID:20971005; PMCID: PMC2989669

349. Effects of Water Placement on Predictions of Binding Affinities for p38α MAP Kinase Inhibitors.
Luccarelli, J.; Michel, J.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2010**, *6*, 3850-3856. PMID: 21278915

350. Limiting Cardiac Ischemic Injury by Augmenting the MIF-AMPK Signaling Cascade with a Novel Class of MIF Receptor Agonists.
Wang, J.; Yan,, X.; Yeung, E.; Gandavadi, S.; Hare, A. H.; Du, X.; Leng, L.; Jorgensen, W. L.; Li, J.; Bucala, R. *Circulation* **2010**, *122*: A15835.

351. Aryl Extensions of Thienopyrimidinones as Fibroblast Growth Factor Receptor 1 Kinase Inhibitors.
Ekkati, A. R.; Mandiyan, V.; Ravindranathan, K. P.; Bae, J. H.; Schlessinger, J.; Jorgensen, W. L.
Tetrahedron Lett. **2011**, *52*, 2228-2231. H. H. Wasserman 90th birthday issue.

352. Benzisothiazolones as modulators of macrophage migration inhibitory factor.
Jorgensen, W. L.; Trofimov, A.; Leng, L.; Hare, A. A.; Du, X. ; Bucala, R.
Bioorg. Med. Chem. Lett. **2011**, *21*, 4545-4549. PMID: 21719283; PMCID: PMC3139435

353. Efficient Discovery of Potent Anti-HIV Agents Especially Targeting the Tyr181Cys Variant of HIV Reverse Transcriptase.
Jorgensen, W. L., Bollini, M.; Thakur, V. V.; Domaoal, R. A.; Spasov, K. A.; Anderson, K. A.
J. Am. Chem. Soc. **2011**, *133*, 15686-15696. PMCID:PMC3183387

354. Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model.
Ravindranathan, K.; Tirado-Rives, J.; Jorgensen, W. L.; Guimarães, C. R. W.
J. Chem. Theory Comput. **2011**, *7*, 3859-3866.

355. Computationally-Guided Optimization of a Docking Hit to Yield Catechol Diethers as Potent Anti-HIV Agents.
Bollini, M.; Domaoal, R. A.; Thakur, V. V.; Gallardo-Macias, R.; Spasov, K. A.; Anderson, K. A.; Jorgensen, W. L.
J. Med. Chem. **2011**, *54*, 8582-8591. PMCID:PMC3258498
News of the Week – C&E News, Dec. 5, 2011 – page 10.

356. On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids.
Alexandrova, A.; Jorgensen, W. L.
J. Phys. Chem. B **2011**, *115*, 13624-13632. PMID: 21995727; PMCID: PMC3241013

357. Investigation of Solvent Effects on the Rate and Stereoselectivity of the Henry Reaction.
Kostal, J.; Voutchkova, A. M.; Jorgensen, W. L.
Org. Lett. **2012**, *14*, 260-263. PMID: 22168236; PMCID: PMC3258499

358. Targeting the von Hippel-Landau E_3 Ubiquitin Ligase using Small Molecules to Disrupt the VHL/HIF-1α Interaction.
Buckley, D. L.; Van Molle, I.; Gareiss, P. C.; Tae, H. S.; Michel, J.; Noblin, D. J.; Jorgensen, W. L.; Ciulli, A.; Crews, C. M.
J. Am. Chem. Soc. **2012**, *134*, 4465-4468. PMCID: PMC3448299

359. Discovery of dimeric inhibitors by extension into the entrance channel of HIV-1 reverse transcriptase.
Ekkati, A. R.; Bollini, M.; Domaoal, R. A.; Spasov, K. A.; Anderson, K. A.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2012**, *22*, 1565-1568. PMCID: PMC3278212

360. Role of macrophage migration inhibitory factor in the regulatory T-cell response of tumor-bearing mice.
Choi, S.; Kim, H.-R.; Leng, L.; Kang, I.; Jorgensen, W. L.; Cho, C.-S.; Bucala, R.; Kim, W.-U.
J. Immunol. **2012**, *189*, 3905-3913. PMCID: PMC3466372

361. Treatment of Halogen Bonding in the OPLS-AA Force Field; Application to Potent Anti-HIV Agents.
Jorgensen, W. L.; Schyman, P. *J. Chem. Theory Comput.* **2012**, *8*, 3895-3901. PMCID:PMC3544186

362. Methyl Effects on Protein-Ligand Binding.
Leung, C. S.; Leung, S. S. F.; Tirado-Rives, J.; Jorgensen, W. L.
J. Med. Chem. **2012**, *55*, 4489-4500. PMCID: PMC3353327

363. Challenges for Academic Drug Discovery.
Jorgensen, W. L. *Angew. Chem. Int. Ed*. **2012**, *51*, 11680-11684. PMID: 23097176

364. Small Molecule Inhibitors of the Interaction between the E3 Ligase VHL and HIF1α.
Buckley, D. L.; Gustafson, J. L.; Van Molle, I.; Roth, A. G.; Tae, H. S.; Gareiss, P. C.; Jorgensen, W. L.; Ciulli, A.; Crews, C. M.
Angew. Chem. Int. Ed. **2012**, *51*, 11463-11467. PMID:23065727

365. Virtual Screening and Optimization Yield Low-Nanomolar Inhibitors of the Tautomerase Activity of *Plasmodium falciparum* MIF.
Dahlgren, M. K.; Garcia, A. B.; Hare, A. A.; Tirado-Rives, J.; Leng, L.; Bucala, R.; Jorgensen, W. L. *J. Med. Chem*. **2012**, *55*, 10148-10159. PMID: 23067344

366. Crystal Structures of HIV-1 Reverse Transcriptase with Picomolar Inhibitors Reveal Key Interactions for Drug Design.
Frey, K. M.; Bollini, M.; Mislak, A. C.; Cisneros, J. A.; Gallardo-Macias, R.; Jorgensen, W. L.; Anderson, K. A.
J. Am. Chem. Soc. **2012**, *134*, 19501-19503. PMID:23163887; PMCID: PMC3518392.

367. Optimization of benzyloxazoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase to enhance Y181C potency.
Bollini, M.; Gallardo-Macias, R.; Spasov, K. A.; Tirado-Rives, J.; Anderson, K. S.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2013**, *23*, 1110-1113. PMID: 23298809; PMCID: PMC3561933.

368. Exploring Adsorption of Water and Ions on Carbon Surfaces using a Polarizable Force Field.
Schyman, P.; Jorgensen, W. L. *J. Phys. Chem. Lett.* **2013**, *4*, 468-474. PMID:23440601; PMCID: PMC3579643

369. Automated ligand- and structure-based protocol for in silico prediction of Human Serum Albumin binding.
Hall, M. L.; Jorgensen, W. L.; Whitehead L. *J. Chem. Info. Model.* **2013**, *53*, 907-922. PMID:23472823

370. Small Molecular Modulation of Macrophage Migration Inhibitory Factor (MIF) in the Hyperoxia-Induced Mouse Model of Bronchopulmonary Dysplasia.
Sun, H.; Choo-Wing, R.; Fan, J.; Leng, L.; Syed, M. A.; Hare, A. A.; Jorgensen, W. L.; Bucala, R.; Bhandari, V.
Respiratory Res.. **2013**, *14*: 27. doi: 10.1186/1465-9921-14-27 PMID:23448134; PMCID:PMC3637059

371. Bifunctional Inhibition of HIV-1 Reverse Transcriptase: Mechanism and proof-of-concept as a novel therapeutic design strategy.
Bailey, C.; Sullivan, T.; Iyidogan, P.; Tirado-Rives, J.; Chung, R.; Ruiz-Caro, J.; Mohamed, E.; Jorgensen, W. L.; Hunter, R.; Anderson, K. A. *J. Med. Chem*. **2013**, *56*, 3959-3968.

372. Limiting Cardiac Ischemia by Pharmacologic Augmentation of MIF-AMPK Signal Transduction.
Wang, J.; Yan, X.; Yeung, E.; Gandavadi, S.; Hare, A. A.; Du, X.; Chen, Y.; Xiong, H.; Leng, L.; Young, L.; Jorgensen, W. L.; Li, J.; Bucala, R.
Circulation **2013**, *128*, 225-236. PMID:23753877

373. Characterization of Biaryl Torsional Energetics and its Treatment in OPLS All-Atom Force Fields.
Dahlgren, M. K.; Schyman, P.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Inf. Model. **2013**, *53*, 1191-1199. PMID:23621692; PMCID:PMC3707137

374. Polarized Protein-Specific Charges from AIM Electron Density Partitioning.
Lee, L. P.; Cole, D. J.; Skylaris, C.-K.; Jorgensen, W. L.; Payne, M. C.
J. Chem. Theory Comput. **2013**, *9*, 2981-2991. PMID:23894231

375. Extension into the entrance channel of HIV 1 reverse transcriptase – Crystallography and enhanced solubility.
Bollini, M.; Frey, K. M.; Cisneros, J. A.; Spasov, K. A.; Das, K.; Bauman, J. D.; Arnold, E.; Anderson, K. S.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2013**, *23*, 5209-5912. PMID: 23899617; PMCID: PMC3761378

376. Optimization of diarylazines as anti-HIV agents with dramatically enhanced solubility.
Bollini, M.; Cisneros, J. A.; Spasov, K. A.; Anderson, K. S.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2013**, *23*, 5213-5216.
PMID:23937980; PMCID: PMC3759246.

377. Picomolar Inhibitors of HIV Reverse Transcriptase Featuring Bicyclic Replacement of a Cyanovinylphenyl Group.
Lee, W.-G.; Gallardo-Macias, R.; Frey, K. M.; Spasov, K. A.; Bollini, M.; Anderson, K. S.; Jorgensen, W. L.
J. Am. Chem. Soc. **2013**, *135*, 16705-16713. PMID: 24151856; PMCID:

378. Foundations of Biomolecular Modeling.
Jorgensen, W. L. *Cell* **2013**, *155*, 1199-1202.

379. Structure-Based Evaluation of C5 Derivatives in the Catechol Diether Series Targeting HIV-1 Reverse Transcriptase.
Frey, K. M.; Gray, W. T.; Spasov, K. A.; Bollini, M.; Gallardo-Macias, R.; Jorgensen, W. L.; Anderson, K. S.
Chem. Biol. Drug Des. **2014**, *83*, 541-549. doi: 10.1111/cbdd.12266

380. Virtual screening reveals allosteric inhibitors of the *Toxoplasma gondii* thymidylate synthase-dihydrofolate reductase.
Sharma, H.; Landau, M. J.; Sullivan, T. J.; Kumar, V. P.; Dahlgren, M. K.; Jorgensen, W. L.; Anderson, K. S.
Bioorg. Med. Chem. Lett. **2014**, *24*, 1232-1235.

381. Quantum and Molecular Mechanical (QM/MM) Monte Carlo Techniques for Modeling Condensed-Phase Reactions.
Acevedo, O.; Jorgensen, W. L.
WIRE Comput. Mol. Sci. **2014**, *4*, 422-435.

382. Illuminating gp120-Ligand Recognition through Computationally-Driven Optimization of Antibody-Recruiting Molecules.
Parker, C. G.; Dahlgren, M. K.; Li, D. T.; Douglass, E. F.; Jawanda, N.; Shoda, T.; Spasov, K. A.; Domaoal, R. A.; Sutton, R.; Anderson, K. S.; Jorgensen, W. L.; Spiegel, D. A. *Chem. Sci.* **2014**, *5*, 2311-2317.

383. Enhanced Monte Carlo Sampling through Replica Exchange with Solute Tempering.
Cole, D. J.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2014**, *10*, 565-571.

384. Biochemical assays for discovery of TDP1/TDP2 inhibitors.
Marchand, C.; Huang, S. N.; Dexheimer, T. S.; Lea, W. A.; Mott, B. T.; Chergui, A.; Naumova, A.; Rosenthal, A. S.; Raj, G.; Gao, R.; Maloney, D. J.; Jadhav, A.; Jorgensen, W. L.; Simeonov, A.; Pommier, Y.
Mol. Cancer. Ther. **2014**, *13*, 2116-2126.

385. A Mechanistic and Structural Investigation of Modified Derivatives of the Diaryltriazine Class of NNRTIs Targeting HIV-1 Reverse Transcriptase.
Mislak, A. C.; Frey, M.; Bollini, M.; Jorgensen, W. L.; Anderson, K. S.
Biochim. Biophys. Acta **2014**, *1840*, 2203-2211.

386. Evaluation of CM5 Charges for Condensed-Phase Modeling.
Vilseck, J. Z.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2014**, *10*, 2802-2812. PMID: 25061445

387. Cooperative Effects and Optimal Halogen Bonding Motifs for Self-Assembling Systems.
Yan, X. C.; Schyman, P.; Jorgensen, W. L.
J. Phys. Chem. A **2014**, *118*, 2820-2826.

388. The Many Faces of Halogen Bonding: A Review of Theoretical Models and Methods.
Wolters, L. P.; Schyman, P.; Pavan, J.; Jorgensen, W. L.; Bickelhaupt, F. M.; Kozuch, S.
WIRE Comput. Mol. Sci. **2014**, *6*, 523-540.

389. Crystallographic and Receptor Binding Characterization of *Plasmodium falciparum* Macrophage Migration Inhibitory Factor Complexed to Two Potent Inhibitors.
Pantouris, G.; Rajasekaran, D.; Garcia, A, B.; Ruiz, V. G.; Leng, L.; Jorgensen, W. L.; Bucala, R.; Lolis, E. J.
J. Med. Chem. **2014**, *57*, 8652-8656.

390. Structural studies provide clues for analog design of specific inhibitors of *Cryptosporidium hominis* thymidylate synthase-dihydrofolate reductase.
Kumar, V. P.; Cisneros, J. A.; Frey, K. M.; Castellanos-Gonzalez, A.; Wang, Y. Q.; Gangjee, A.; white, A. C.; Jorgensen, W. L.; Anerson, K. S.
Bioorg. Med. Chem. Lett. **2014**, *24*, 4158-4161.

391. Picomolar Inhibitors of HIV-1 Reverse Transcriptase: Design and Crystallography of Naphthyl Phenyl Ethers
Lee, W.-G.; Frey,K. M.; Gallardo-Macias, R.; Spasov, K. A.; Bollini, M.; Anderson, K. S.; Jorgensen, W. L. *ACS Med. Chem. Lett.* **2014**, *5*, 1259-1262.

392. Macrophage migration inhibitory factor (MIF) is detrimental in pneumococcal pneumonia and a target for therapeutic immunomodulation.
Weiser, J. N.; Roche, A. M.; Hergott, C. B.; LaRose, M. I.; Connolly, T.; Jorgensen, W. L.; Leng, L.; Bucala, R.; Das, R. *J. Infect. Diseases* **2015**, *212*, 1677-1682.

393. A Reflection on Paul von Ragué Schleyer.
Jorgensen, W. L. *J Chem. Theory Comput*. **2015**, *11*, 1-1.

394. Molecular Dynamics and Monte Carlo Simulations for Protein-Ligand Binding and Inhibitor Design.
Cole, D. J.; Tirado-Rives, J.; Jorgensen, W. L.
Biochim. Biophys. Acta. **2015**, *1850*, 966-971.

395. Scientific History and Recollections.
Jorgensen, W. L. *J. Phys. Chem. B* **2015**, *119*, 624-632.

396. Design, Synthesis, and Protein Crystallography of Biaryltriazoles as Potent Tautomerase Inhibitors of Macrophage Migration Inhibitory Factor.
Dziedzic, P.; Cisneros, J. A.; Robertson, M. J.; Hare, A. A.; Danford, N. E.; Baxter, R. H. G.; Jorgensen, W. L.
J. Am. Chem. Soc. **2015**, *137*, 2996-3003. PMCID: PMC4386841

397. Determination of Partial Molar Volumes from Free Energy Perturbation Theory.
Vilseck, J. Z.; Tirado-Rives, J.; Jorgensen, W. L. *Phys. Chem. Chem. Phys*. **2015**, *17*, 8407-8415. Special Issue on Solvation Science. PMID: 25589343

398. Structure-based Evaluation of Non-nucleoside Inhibitors with Improved Potency and Solubility that Target HIV Reverse Transcriptase Variants.
Frey, K. M.; Puleo, D. E.; Spasov, K. A.; Bollini, M.; Jorgensen, W. L.; Anderson, K. S. *J. Med. Chem*. **2015**, *58*, 2737-2745.

399. Endothelial CD74 mediates macrophage migration inhibitory factor protection in hyperoxic lung injury.
Sauler, M.; Zhang, Y.; Min, J. N.; Leng, L.; Shan, P. Y.; Roberts, S.; Jorgensen, W. L.; Bucala, R.; Lee, P. J. *FASEB J*. **2015**, *29*, 1940-1949.

400. Accurate and Reliable Prediction of Relative Protein-Ligand Binding Affinities via Free Energy Calculations: Validation in Prospective Drug Discovery.
Wang, L.; Wu, Y.; Deng, Y.; Kim, B.; Pierce, L.; Krilov, G.; Lupyan, D.; Robinson, S.; Dahlgren, M. K.; Greenwood, J.; Romero, D. L.; Masse, C.; Knght, J. L.; Steinbrecher, T.; Beuming, T.; Damm, W.; Harder, E.; Sherman, W.; Brewer, M.; Wester, R.; Murcko, M.; Frye, L.; Farid, R.; Lin, T. Mobley, D. L.; Jorgensen, W. L.; Berne, B. J.; Friesner, R. A.; Abel, R. *J. Am. Chem. Soc.* **2015**, *137*, 2695-2703.

401. A nanotherapy strategy significantly enhances anticryptosporidial activity of an inhibitor of bifunctional thymidylate synthase-dihydrofolate reductase from Cryptosporidium.
Mukerjee, A.; Iyidogan, P.; Castellanos-Gonzalez, A.; Cisneros, J. A.; Czyzyk, D.; Ranjan, A.P.; Jorgensen, W. L.; White, A.C., Jr.; Vishwanatha, J.K.; Anderson, K.S.
Bioorg. Med. Chem. Lett. **2015**, *25*, 2065-2067.

402. Improved Peptide and Protein Torsional Energetics with the OPLS-AA Force Field.
Robertson, M. J.; Tirado-Rives, J.; Jorgensen, W.L.
J. Chem. Theory Comput. **2015**, *11*, 3499-3509.

403. Evaluation of CM5 Charges for Modeling Non-Aqueous Condensed Phase Systems.
Dodda, L. S.; Vilseck, J. Z.; Cutrona, K. J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2015**, *11*, 4273-4282. PMID: 4857764

404. A BOSS-Gaussian Interface for Combined QM/MM and MC/FEP Simulations.
Vilseck, J. Z.; Kostal, J.; Tirado-Rives, J.; Jorgensen, W. L.
J. Comput. Chem. **2015**, *36*, 2064-2074. Schleyer Memorial Issue. PMID:26311531

405. Discovery and crystallography of bicyclic arylaminoazines as potent inhibitors of HIV-1 reverse transcriptase.
Lee, W.-G.; Frey,K. M.; Gallardo-Macias, R.; Spasov, K. A.; Chan, A. H.; Anderson, K. S.; Jorgensen, W. L. *Bioorg. Med. Chem. Lett.* **2015**, *25*, 4824-4827.

406. Potent Inhibitors Active Against HIV Reverse Transcriptase with K101P, a Mutation Conferring Rilpivirine Resistance.
Gray, W. T.; Frey, K. M.; Laskey, S. B.; Mislak, A. C.; Spasov, K. A.; Lee, W.-G.; Bollini, M.; Siliciano, R. F.; Jorgensen, W. L.; Anderson, K. S.
ACS Med. Chem. Lett. **2015**, *6*, 1075-1079.

407. Illustrating Concepts in Physical Organic Chemistry with 3D Printed Orbitals.
Robertson, M. J.; Jorgensen, W. L. *J. Chem. Educ*. **2015**, *92*, 2113-2116.

408. OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins.
Harder, E.; Damm, W.; Maple, J.; Wu, C. J.; Reboul, M.; Xiang, J. Y.; Wang, L. L.: Lupyan, D.; Dahlgren, M. K.; Knight, J. L.; Kaus, J. W.; Cerutti, D. S.; Krilov, G.; Jorgensen, W. L.; Abel, R.; Friesner, R. A.
J. Chem. Theory Comput. **2016**, *12*, 281-296.

409. Biomolecular Force Field Parameterization via Atoms-in-Molecule Electron Density Partitioning.
Cole, D. J.; Vilseck, J. Z.; Tirado-Rives, J.; Payne, M. C.; Jorgensen, W. L.
J. Chem. Theory Comput. **2016**, *12*, 2312-2323. PMID: 27057643

410. Hydration Properties and Solvent Effects for All-Atom Solutes in Polarizable Coarse-Grained Water.
Yan, X. C.; Tirado-Rives, J.; Jorgensen, W. L.
J. Phys. Chem. B **2016**, *120*, 8102-8114. (McCammon Festschrift)

411. A Fluorescence Polarization Assay for Binding to Macrophage Migration Inhibitory Factor and Crystal Structures for Two Potent Complexes.
Cisneros, J. A.; Robertson, M. J.; Valhondo, M.; Jorgensen, W. L.
J. Am. Chem. Soc. **2016**, *138*, 8630-8638.

412. Irregularities in enzyme assays: the case of macrophage migration inhibitory factor.
Cisneros, J. A.; Robertson, M. J.; Valhondo, M.; Jorgensen, W. L.
Bioorg. Med. Chem. Lett. **2016**, *26*, 2764-2767.

413. Performance of Protein-Ligand Force Fields for the Flavodoxin - Flavin Mononucleotide Complex.
Robertson, M. G.; Tirado-Rives, J.; Jorgensen, W. L.
J. Phys. Chem. Lett. **2016**, *7*, 3032-3036.

414. Computer-Aided Discovery of Anti-HIV Agents.
Jorgensen, W. L. *Bioorg. Med. Chem*. **2016**, *24*, 4768-4788. Tetrahedron Prize paper.

415. Design, Conformation, and Crystallography of 2-Naphthyl Phenyl Ethers as Potent Anti-HIV Agents.
Lee, W.-G.; Chan, A. H.; Spasov, K.A.; Anderson, K. A.; Jorgensen, W. L.
ACS Med. Chem. Lett. **2016**, *7*, 1156-1160.

416. Systematic Study of Effects of Structural Modifications on the Aqueous Solubilities of Drug-like Molecules.
Cisneros, J. A.; Robertson, M. J.; Mercado, B. Q.; Jorgensen, W. L.
ACS Med. Chem. Lett. **2017**, *8*, 124-127.

417. Structural and Preclinical Studies of Computationally-Designed Non-nucleoside Reverse Transcriptase Inhibitors for Treating HIV Infection.
Kudalkar, S. N.; Beloor, J.; Chan, A. H.; Lee, W.-G.; Jorgensen, W. L.; Kumar, P.; Anderson, K. S.
Mol. Pharm. **2017**, *91*, 383-391.

418. Improved Treatment of Nucleosides and Nucleotides in the OPLS-AA Force Field.
Robertson, M. J.; Tirado-Rives, J.; Jorgensen, W.L.
Chem. Phys. Lett. **2017**, *683*, 276-280. Zewail Memorial Issue.

419. Localized Bond Charge Corrected CM1A Charges for Condensed-Phase Simulations.
Dodda, L. S.; Vilseck, J. Z.; Tirado-Rives, J.; Jorgensen, W. L.
J. Phys. Chem. B **2017**, *121*, 3864-3870. Schulten Memorial Issue.

420. LigParGen web server: An automatic OPLS-AA parameter generator for organic molecules.
Dodda, L. S.; Cabeza de Vaca, I.; Tirado-Rives, J.; Jorgensen, W. L.
Nucl. Acids Res. **2017**, *45*, W331-W336.

421. Identification and Characterization of Small Molecules Binding to the JAK2 Pseudokinase Domain.
Puleo, D. E.; Kucera, K.; Hammarén, H.; Ungureanu, D.; Newton, A. S.; Silvennoinen, O.; Jorgensen, W. L.; Schlessinger, J.
ACS Med. Chem. Lett. **2017**, *8*, 618-621.

422. JAK2-JH2 Fluorescence Polarization Assay and Crystal Structures for Complexes with Three Small Molecules.
Newton, A. S.; Deiana, L.; Puleo, D.; Cisneros, J. A; Cutrona, K. J.; Schlessinger, J.; Jorgensen, W. L.
ACS Med. Chem. Lett. **2017**, *8*, 614-617.

423. Improved Description of Sulfur Anisotropy in OPLS Force Fields. Model Development and Parameterization.
Yan, X. C.; Robertson, M. J.; Tirado-Rives, J.; Jorgensen, W. L.
J. Phys. Chem. B **2017**, *121*, 6626-6636.

424. Covalent inhibitors for eradication of drug-resistant HIV-1 reverse transcriptase: from design to protein crystallography.
Chan, A. H.; Lee, W.-G.; Spasov, K. A.; Cisneros, J. A.; Kudalkar, S. N.; Petrova, Z. O.; Buckingham, A. B.; Anderson, K. S.; Jorgensen, W. L.
Proc. Nat. Acad. Sci. USA. **2017**, 114, 9725-9730.

425. Computationally-Guided Optimization of Small-Molecule Inhibitors of the Aurora A Kinase – TPX2 Protein-Protein Interaction.
Cole, D. J.; Janecek, M.; Stokes, J. E.; Rossmann, M.; Faver, J. C.; McKenzie, G. J.; Venkitaraman, A. R.; Hyvönen, M.; Spring, D. R.; Huggins, D. J.; Jorgensen, W. L.
Chem. Commun. **2017**, *53*, 9372-9375.

426. Adding a Hydrogen Bond May Not Help: Naphthyridinone vs. Quinoline Inhibitors of Macrophage Migration Inhibitory Factor.
Dawson, T. K.; Dziedzic, P.; Robertson, M. J.; Cisneros, J. A.; Krimmer, S. G.; Newton, A. S.; Tiraado-Rives, J.; Jorgensen, W. L.
ACS Med. Chem. Lett. **2017**, *8*, 1287-1291.

427. From In Silico Hit to Long-Acting Late-Stage Preclinical Candidate to Combat HIV Infection.
Kudalkar, S. N.; Beloor, J.; Quijano, E.; Spasov, K. A.; Lee, W.-G.; Cisneros, J. A.; Saltzman, W. M.; Kumar, P.; Jorgensen, W. L.; Anderson, K. S.
Proc. Nat. Acad. Sci. USA. **2017**, *114*, E802-E811.

428. Development and Testing of the OPLS-AA/M Force Field for RNA.
Robertson, M. J.; Qian, Y.; Robinson, M. C.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2018**, *14*, 0000-0000. Submitted.

429. Enhanced Monte Carlo Methods for Modeling Proteins Including Computation of Absolute Free Energies of Binding.
Cabeza de Vaca, I.; Qian, Y.; Vilseck, J. Z.; Tirado-Rives, J.; Jorgensen, W. L.
J. Chem. Theory Comput. **2018**, *14*, 0000-0000. Submitted.

430. Optimization of Pyrazoles as Phenol Surrogates to Yield Potent Inhibitors of Macrophage Migration Inhibitory Factor.
Trivedi-Parmar, V.; Robertson, M. J.; Cisneros, J. A.; Krimmer, S. G.; Jorgensen, W. L. *Angew. Chem. Int. Ed.* **2018**, *000*, 0000-0000. Submitted.

Patents and Applications

Jorgensen, William L.; Ruiz-Caro, Juliana; Hamilton, Andrew D. **Aniline derivatives as antiviral and anticancer agents, their preparation, pharmaceutical compositions, and use in therapy.** PCT Int. Appl. (2007), 93 pp. CODEN: PIXXD2 WO 2007038387 A2 20070405 CAN 146:401679 AN 2007:385257

Jorgensen, William L.; Ruiz-Caro, Juliana; Hamilton, Andrew D. **Compounds and methods for the treatment of viruses and cancer.** US Patent 9,018,209. April 28, 2015.

Jorgensen, William L. **Novel azoles and related derivatives as non-nucleoside reverse transcriptase inhibitors (NNRTIs) in antiviral therapy (HIV).** PCT Int. Appl. (2009), 68pp. CODEN: PIXXD2 WO 2009005811 A1 20090108 CAN 150:114237 AN 2009:20165

Jorgensen, William; Bucala, Richard J. **Preparation of benzylbenzoxazolone derivatives and analogs for use as MIF modulators.** PCT Int. Appl. (2010), 67 pp. CODEN: PIXXD2 WO 2010021693 A2 20100225 CAN 152:287368 AN 2010:235888

Jorgensen, William L.; Bucala, Richard J. **Preparation of azole derivatives as MIF modulators.** PCT Int. Appl. (2011), WO 2011140202 A2 20111110.

Jorgensen, William L.; Bucala, Richard J. **MIF modulators.**
U.S. Pat. Appl. Publ. (2012), US 20120004261 A1 20120105. US Patent 9,540,322 (2017)

Novel Compositions and Methods of Treating HIV-1 Infections Using Same
WL Jorgensen, KS Anderson - US Patent 20140378443

Compounds and methods for treating HIV infections
WL Jorgensen, KS Anderson US Patent 9,382,245 (2016)

Catechol diethers as potent anti-HIV agents
WL Jorgensen, KS Anderson - US Patent 9,487,476 (2016)

Compounds & Methods for the Enhanced Degradation of Targeted Proteins & Other Polypeptides by an E3 Ubiquitin Ligase
CM Crews, D Buckley, A Ciulli, W Jorgensen et al. - US Patent 20140356322

Invited Lectures 2004 - present

2018
Austin Symposium ASMD@D 2018 – March 3-5
Rutgers University – CABM Seminar – March 7
Peking Univ. Shenzhen Grubbs/Houk Symposium – May 16-18
VI European Workshop on Drug Synthesis – Siena, Italy – May 20-25
ISQBP President's Meeting – Barcelona – June 19-21
Tetrahedron Symposium -Riva del Garda – June 26-29
ACS National Meeting – Boston – Madura Symposium – Aug 19-23
ACS National Meeting – Boston – Skolnik Award Symposium
22nd EuroQSAR – Thessaloniki, Greece – Sept 16-20
CECAM Workshop on Intermolecular Interactions
Berson Lecturer, Yale U. - April

2017
Scripps Research Institute – Feb 6
UC San Diego – Physical Chemistry – Feb 7
Drug Discovery Reinvented III – Fusion Conference – Cancun – Feb 21-24
XIth European Workshop on Drug Design – Siena - May 21-26
CECAM Workshop on Challenges in Drug Discovery – Lausanne, June 5-9
46th IUPAC World Congress – Med Chem & Chem Biol Symposium – Sao Paulo, July 9-14
NCI Workshop on CADD for RAS – Frederick, MD - August 17
Pfizer – Cambridge, MA – August 29
CECAM Workshop on Computational Drug Discovery – Lausanne, Sept 5-8
ACS Southwest – Symposium on S_N2 Reaction Dynamics – Lubbock, TX Oct 29
ACS Southwest Regional Meeting – Plenary Lecture – Lubbock, TX Oct 30

2016
ACS National Meeting – San Diego – National Lecture Symposium
ACS National Meeting – San Diego – Computer Simulations of Thermodynamics Symposium
ACS National Meeting – San Diego – Status of CADD Symposium
VI European Workshop on Drug Synthesis – Siena, Italy
ACS National Meeting – Philadelphia – Tetrahedron Award Symposium
ACS National Meeting – Philadelphia – Symposium on QM/MM Simulation of Chemical and Biochemical Reaction Pathways
ISQBP President's Meeting – Bergen, Norway
Gordon Conference on Molecular Structure Elucidation
21st EuroQSAR Symposium (Verona)
SABINA Conference – Kruger Park, South Africa

2015
ACS National Meeting – Denver – Truhlar Chemical Dynamics Symposium
X European Workshop in Drug Design – Siena, Italy

University of Witwatersrand
CECAM Workshop on Computational Drug Discovery – Lausanne
University of Texas, El Paso
Pacifichem 2015 – Symposium on De Novo Drug Design – Honolulu

2014
University of Utah
Univ. Marburg – Academic Drug Discovery Symposium
Yale School of Medicine – HIV Focus Group
Telluride Conference
Gordon Conference on Computational Chemistry
CCG Annual Meeting – Montreal
Worcester Polytechnic Institute
Schrödinger User Group Meeting – Keynote - Princeton
Bone Lecturer, Wilkes University
Topliss Lecturer, Univ. of Michigan, Medicinal Chemistry
Cancelled:
SACI-ACS Organic Chemistry Conference (BOCC-2014) – Stellenbosch, SA
Techniche, Indian Institute of Technology - Guwahati, Keynote Speaker

2013
ACS National Meeting – New Orleans – Non-Covalent Interactions Symposium
ACS National Meeting – New Orleans – Protein-Ligand Interactions Symposium
Free Energy Conference – Snowmass
IX European Workshop in Drug Design – Siena, Italy
Vanderbilt University - Dept. of Biochemistry
Georgia Tech – Center for Systems Biology – Distinguished Lecturer
Drug Discovery Re-Invented Symposium – Scottsdale, AZ
CECAM Workshop on Computational Drug Discovery - Lausanne
CECAM Workshop on Coupling Protein, Water & Lipid Dynamics – Lausanne
Molecular Simulation Symposium – Ruhr U. Bochum
Merck – Medicinal Chemistry Seminar – West Point, PA
Alcon Pharmaceuticals – Fort Worth
Molecular Modeling & Drug Discovery Symposium – Northwestern U.
Seaborg Symposium – Honoring K. N. Houk – UCLA
Georgia Tech – Chemistry & Biochemistry
Genentech – San Francisco

2012
Scripps Research Institute - John Wiley & Sons Lecturer
ACS National Meeting - San Diego - McCammon Symposium
ACS National Meeting - San Diego – Rational Drug Design Symposium
ACS National Meeting - San Diego – Structure Based Design Symposium
ACS National Meeting - San Diego – PHYS Awards Symposium

4th European Workshop in Drug Synthesis - Siena
CMS 2012, Royal Agricultural College, Cirencester
ESPA (Electronic Structure Principles & Applications) 2012 – Barcelona
ISQBP President's Meeting – Stockholm
University of Miami (Florida)
University of Georgia
Italian Institute of Technology, Genoa – F. Arcamone Lecture on Medicinal Chemistry
University of Bologna
Georgia State U. – Molecular Basis of Disease Distinguished Lecture
Mercury Conference for Undergraduates – Bucknell U.
Rauischholzhausen Workshop on New Approaches in Drug Discovery
Basel Chemical Society
Syngenta (Stein, Switzerland)
Pfizer, Cambridge
Amgen, San Francisco
Princeton ACS Fall Organic Symposium
Kolthoff Lecturer - U. Minnesota (3 lectures)
Bryan E. Koehler Lecturer – UC Riverside
UC Riverside – Physical Chemistry Seminar

2011
Thermodynamics 2011 - Molecular Physics Keynote Lecturer - Athens, Greece
2011 Mesilla Chemistry Workshop - Mesilla, NM
IPAM - UCLA - Workshop on Drug Design (2 lectures)
Institute of Organic Chemistry & Biochemistry, Academy of Sciences, Prague CR
VIII European Workshop on Drug Discovery - Siena, Italy
Tsinghua University - 100th Anniversary Symposium - Bejing
Grandpierre Lecturer, Columbia U.
International MIF Symposium - Yale U.
CCTCC - 20th Meeting - Jackson, MS
Brandeis University - Chemistry
Duke University School of Medicine (Biochemistry)
University of Georgia
Chemical Biology Retreat - Yale
CECAM Workshop on Computational Drug Discovery - Lausanne

2010
Symposium on "Theoretical and Computational Chemistry" at the
Max-Planck-Institut für Kohlenforschung - Mülheim (W. Thiel 60th)
Symposium Honoring Frank Blaney, Oxford U.
ISQBP President's Meeting, Calabria, Italy - Gilda Loew Memorial Lecturer
University of 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 Symposium
High Performance Computing Symposium - National U. of Ireland
6th Rauischholzhausen Workshop on New Approaches to Drug Discovery
Vertex Pharmaceuticals - Free Energy Calculations in Drug Design Workshop
McGill University
New York Academy of Sciences - Chemical Biology - Keynote
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
IEEE Symposium on Drug Discovery - Philadelphia

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

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 Processsing 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

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

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 Meting (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

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 Sympoium - 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

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

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 and the National Institute of Allergy and Infectious Diseases. Dr. Jorgensen is also part of the Biophysical Training Grant at Yale and the Yale Cancer Center. Postdoctoral fellows in his laboratory are often supported by national and industrial fellowships.

Co-workers

Dr. Jorgensen has had more than 150 co-workers including ca. 50 graduate students, who have received Ph. D. degrees under his guidance. Almost all of his former co-workers are still employed in academia or the pharmaceutical and biotech industries. His research group normally consists of 15-20 people; roughly half are postdoctoral fellows. Dr. Tirado-Rives is Dr. Jorgensen's longtime senior associate, who oversees laboratory logistics and projects in computational biology. Ms. Morales is Dr. Jorgensen's assistant, who oversees the editorial office for *JCTC*.

Co-Workers of William L. Jorgensen (1975-2014)

John E. Munroe (M. S., 1977)
Timothy D. Salatin (Ph.D., 1980)
David Yang (B. S., 1981)
Mustafa Ibrahim (Ph.D., 1981)
David Spellmeyer (B.S., 1983)
Michael E. Cournoyer (Ph.D., 1983)
Julia A. Schmidt (Ph.D., 1984)
Carol Swenson (M.S., 1984)
Debra S. Garner (B.S., l985)
Dr. C. Ravimohan (P.D., 1984-5)
Roberto Rozas (V. P., 1985-6)
Pascal Metivier (P.D., 1985-6)
Mark Bures (Ph.D., 1987)
Alan Gushurst (Ph.D., 1988)
Stephane Boudon (VGS, 1987-9)
Kathleen A. Novak (M.S., 1989)
Weiya Yun (M.S., 1990)
Scott G. Wierschke (M.S., 1990)
Julianto Pranata (P.D., 1988-91)
Scott A. Gothe (P.D., 1989-92)
Harold Helson (Ph.D., l993) D
Toan Nguyen (Ph.D., 1993)
Vincent-Henri Peuch (VGS, 1993)
Shenna Sinclair (Ph.D., 1994)
Dean Jaegels (B. S., 1981)
Robert C. Binning (P.D., 1980)
Bernard Bigot (P.D., 1980-81)
Barbara Roos-Kozel (Ph.D., 1982)
David McLaughlin (Ph.D., 1983)
Scott Smith (B. S., 1983)
J. Chandrasekhar (V.P., 1980-84, 2001-3)
Catherine Peishoff (Ph.D., 1985)
Jeffry D. Madura (Ph.D., l985)
Jeffrey Evanseck (B. S., 1986)
M. Leonor Contreras (V. P., l985-6)
Jiali Gao (Ph.D., 1987)
Mustafa Ibrahim (V.P., 1987-8)
Cynthia MacMahon (M.S., 1989)
J. Kathleen Buckner (Ph.D., 1988)
Ralph T. Mosley (M.S., 1989)
James Briggs (Ph.D., 1990)
James F. Blake (Ph.D., 1990; P.D., 90-91)
Tooru Matsui (P.D., 1989-91)
Genevieve Paderes (Ph.D., 1988; P.D., 88-91)
Ellen R. Laird (Ph.D., 1990; P.D., 90-92)
Modesto Orozco (V.P., 1991-93)
Jan M. Fleischer (Ph.D., 1994)
Daniel L. Severance (Ph.D., 1993)

Erin M. Duffy (Ph.D., 1994)
Jonathan Essex (P.D., 1992-4)
Daqing Gao (M. S., 1995)
Heather Carlson (Ph.D., 1996)
Wendy Schaeffer (B.S., 1997)
Antonio Frontera (P.D., 1995-6)
George Kaminski (Ph.D., 1997)
Nora McDonald (Ph.D., 1998)
Edward Watkins (ARS, 1999-2001)
Iordanis Houdaverdis (Ph.D., 1998)
Corky Jenson (M.S.., 1999)
Daniel Price (Ph.D., 2000)
Michael Mahoney (Ph.D., 2000)
Shane Shariffskul (B.S., 2001)
Steven S. Wesolowski (P.D., 2000-3)
Matthew P. Repasky (Ph.D., 2001)
Dennis Ostrovsky (Ph.D., 2003)
Dr. Yukio Tominaga (P.D., 2001-3)
Marina Udier-Blagovic (Ph.D., 2004)
Juliana Ruiz-Caro (P.D., 2004-5)
Ivan Tubert-Brohman (Ph.D., 2006)
Theresa Lyons (Ph.D., 2006)
Theodore J. Christakis (B.S., 2006)
Kasper P. Jensen (P.D., 2005-6)
Joseph Kim (P.D., 2005-7)
Zheren Yang (B.S., 2007)
Nunzio Iraci (VGS, 2008)
Anastassia Alexandrova (P.D., 2005-8)
Jacob Zeevaart (P.D., 2007-9)
Zoe Cournia (P.D., 2006-9)
Cristina Tintori (V P.D, 2010)
Leyla Celik (P. D., 2009-11)
Valeria LaPietra (V.G.S., 2009-2010)
Julien Michel (P.D., 2007-10)
John Terhorst (Ph. D., 2012)
Jakub Kostal (Ph. D., 2012)
Cheryl Leung (Ph. D., 2012)
Hannes Harbrecht (VGS, 2012)
Mariella Bollini (P.D., 2009-2013)
David Steinberg (B.S., 2013)
Michelle Lynn Hall (P.D., 2011-2013)
Todd J. Sullivan (P.D., 2012-2013)
Patric Schyman (P. D., 2011-14)
Ricardo Gallardo-Macias (Ph.D., 2014)
David Maxwell (Ph.D., 1995)
Ingvar Lagerstedt (P.D., 1992-4)
Arshad Khan (V. P., 1996)
Vickie Tsui (B.S., 1997)
Rong Liu (Ph.D., 1996)
Deborah Jones-Hertzog (P.D., 1994-6)
Wolfgang Damm (P.D., 1995-7)
Paul Rablen (P.D., 1995-7)
Michelle Lamb (Ph.D., 1997)
Dongchul Lim (P.D., 1996-98)
Melissa Plount (Ph.D., 2000)
Willem P. van Hoorn (P.D., 1997-99)
Albert C. Pierce (Ph. D., 2000)
DePing Wang (P.D., 1999-2001)
Robert C. Rizzo (Ph.D., 2000)
Shoshannah Pearlman (M.S.,2001)
Fenglou Mao (P.D., 2001-3)
Oladapo Babatunde (BS, 2004)
Jakob Ulmschneider (Ph.D., 2004)
Cristiano R. W. Guimaraes (P.D., 2001-5)
Gabriela Barriero (P.D., 2004-5)
Patrick S. Lee (P.D., 2003-5)
Orlando Acevedo (P.D., 2003-6)
Kurt Sattelmeyer (P.D., 2004-6)
Birgit Albrecht (P.D., 2005-2007)
Sunilkumar Gandavadi (P.D., 2007-9)
Simone Fulle (VGS, 2008)
Siegfried S. F. Leung (Ph. D., 2009)
Sara E. Nichols (Ph. D., 2009)
Laura L. Thomas (Ph. D., 2010)
James Luccarelli (B.S., 2010)
Connie Wang (B.S., 2010)
Alexander Trofimov (P.D., 2009-11)
Huan Lu (M.S., 2011)
Vinay Thakhur (P.D.; ARS, 2005-10)
Krishna Ravindranathan (P.D., 2006-11)
Alissa A. Hare (Ph.D., 2012)
Anil Ekkati (P.D., 2008-2012)
Nadia E. Danford (B.S., 2012)
Markus K. Dahlgren (P.D., 2010-13)
Sara Kramar (VGS, 2013)
Mattia Bernetti (VGS, 2013)
Roland Huber (VGS, 2013)
Pawel Dziedzic (P.D., 2012-15)

Luca Deiana (P.D., 2014-16)
John C. Faver (P.D., 2012-5)
Won-Gil Lee (P.D., 2012-2017)
Daniel J. Cole (P.D., 2012-15)
Jonah Z. Vilseck (Ph. D., 2016)
Cindy Xin Yan (Ph. D., 2017)

Current Group Members:

Julian Tirado-Rives (PD; ARS; Senior Res. Scientist, 1985-)
Patricia Morales (Res. Asst., 1990-)
Ana Newton (P.D., 2012-)
Vinay Trivendi-Parmar (Ph.D., 2018)
Michael J. Robertson (Ph.D., 2017)
Leela Dodda (Ph. D., 2018)
Kara Cutrona (Ph.D., 2018)
Israel Cabeza (P.D., 2016-)
Maria-Elena Liosi (Ph. D., 2020)
Jose Cisneros Trigo (P.D.; ARS 2011-)
Zachary Carter (Ph. D., 2020)
Margarita Valhondo (P.D., 2015-)
Stefan G. Krimmer (P.D., 2017-)
Yue Qian (Ph. D., 2018)
Maheen Zakaria (B.S., 2017)
Thomas Dawson (P.D., 2016-)