

VITA OF WILLIAM L. JORGENSEN

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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

2021 Clarivate Citation Laureate
2015 Tetrahedron Prize
2014 John G. Topliss Award in Medicinal Chemistry, University of Michigan
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 ca. 700 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 State; 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; AATACC Distinguished Lecturer; Cavill Lecturer, U. New South Wales. 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, 2009-2018
Science & Engineering Advisory Committee, 2009-2012
Cancer Biology Institute Advisory Committee, 2011-14, 2018-
Cooperative Research Committee, 2011-2016
Screening Core Advisory Committee, 2012-2018
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-
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, NCCR Resource for Integrated Glycotechnology, 2010-2013
Israeli Council on Higher Education, Chemistry Evaluation Committee, 2011

Tetrahedron Prize Committee, 2017
RESPOND³ Advisory Board – Univ. of Bergen, 2020-2023
Advisory Board, SciPost, 2021-

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

>450 primary publications
H-Index = 110 (ISI), 126 (Google Scholar)
Citations >85,000 (ISI), >111,000 (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 (1976).
13. The Cyclic Structure of Monomeric Dilithioacetylene.
Y. Apeloig, P. v. R. Schleyer, J. S. Binkley, J. A. Pople, and W. L. Jorgensen
Tetrahedron Letters, 3923 (1976).
14. The Similarity of Solvent Effects on Carbocations.
W. L. Jorgensen
J. Am. Chem. Soc., 99, 280 (1977).
15. The Influence of Increasing Solvation on the Relative Energies of Bisected and Bridged Ethyl Cations.
W. L. Jorgensen and J. E. Munroe
Tetrahedron Letters, 581 (1977).
16. The Importance of the Counter Ion. The Structures and Relative Energies of Homocubyl Cations and Ion Pairs.
W. L. Jorgensen
J. Am. Chem. Soc., 99, 4272 (1977).
17. Simple Prediction of Substituent Sensitivity for Carbocations.
W. L. Jorgensen
J. Am. Chem. Soc., 99, 3840 (1977).

18. Cycloaddition Reactions of
1,2,5,6-Tetramethyl-3,4,7,8-tetramethylenetricyclo(3.3.0.0(2,6)]octane. Evidence for
Chemical Consequences of Orbital Interactions in Molecules Containing 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 6-31G
Computations.
W. L. Jorgensen and M. E. Cournoyer
J. Am. Chem. Soc., 100, 4942 (1978).
25. Ab Initio Molecular Orbital Study of the Geometries, Properties, and Protonation of
Simple Organofluorides.
W. L. Jorgensen and M. E. Cournoyer
J. Am. Chem. Soc., 100, 5278 (1978).
26. The Photoelectron Spectra of the 1,2,5,6-Tetramethyl-3,4,7,8-tetramethylene Derivatives
of Tricyclo(3.3.0.0(2,6)]octane and Tricyclo(4.2.0.0(2,5)]octane.
W. T. Borden, S. D. Young, D. C. Frost, N.P.C. Westwood, and W. L. Jorgensen
J. Org. Chem., 44, 737 (1979).

27. Monte Carlo Simulations of Liquid Hydrogen Fluoride.
W. L. Jorgensen
J. Am. Chem. Soc., 100, 7824 (1978).
28. Deriving Intermolecular Potential Functions for the Water Dimer from Ab Initio Calculations.
W. L. Jorgensen
J. Am. Chem. Soc., 101, 2011 (1979).
29. Minimal Basis Set Description of the Structure and Properties of Liquid Water.
W. L. Jorgensen
J. Am. Chem. Soc., 101, 2016 (1979).
30. Basis Set Dependence in Monte Carlo Simulations of Liquid Hydrogen Fluoride.
W. L. Jorgensen
J. Chem. Phys., 70, 5888 (1979).
31. Energy Partitioning Accompanying Fragmentation of Protonated Methanol.
R. J. Day, D. A. Krause, W. L. Jorgensen, and R. G. Cooks
Int. J. Mass Spectrom. Ion Phys., 30, 83 (1979).
32. An Intermolecular Potential Function for the Methanol Dimer from Ab Initio Calculations.
W. L. Jorgensen
J. Chem. Phys., 71, 5034 (1979).
33. The Structure and Properties of Liquid Methanol.
W. L. Jorgensen
J. Am. Chem. Soc., 102, 543 (1980).
34. The Structure and Properties of Liquid Ammonia.
W. L. Jorgensen and M. Ibrahim
J. Am. Chem. Soc., 102, 3309-3315 (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, I. Overview.
T. D. Salatin and W. L. Jorgensen
J. Org. Chem., 45, 2043 (1980).
37. Transferable Intermolecular Potential Functions for Water, Alcohols, and Ethers. Application to Liquid Water.

- W. L. Jorgensen
J. Am. Chem. Soc., 103, 335-340 (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, 101 (1981).
41. Ab Initio Studies of RO⁻...HOR' Complexes. Solvent Effects on the Relative Acidities of Water and Methanol.
W. L. Jorgensen and M. Ibrahim
J. Comput. Chem., 2, 7 (1981).
42. On the Existence of Homoaromaticity and Bicycloaromaticity in Carbanions.
J. B. Grutzner and W. L. Jorgensen
J. Am. Chem. Soc., 103, 1372 (1981).
43. Internal Rotation in Liquid 1,2-Dichloroethane and n-Butane.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 677-679 (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, 4393-4399 (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, 3976-3985 (1981).

46. Sampling Methods for Monte Carlo Simulations of *n*-Butane in Dilute Solution.
B. Bigot and W. L. Jorgensen
J. Chem. Phys., 75, 1944 (1981).
47. Pressure Dependence of the Structure and Properties of Liquid *n*-Butane.
W. L. Jorgensen
J. Am. Chem. Soc., 103, 4721 (1981).
48. PULSAR: A Personalized Microcomputer-Based System for Keyword Search and Retrieval of Literature Information.
S. F. Smith, W. L. Jorgensen, and P. L. Fuchs
J. Chem. Info. Comput. Sci., 21, 209 (1981).
49. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 3. Ylid Chemistry and the Organometallic Chemistry of Li, Mg, and Lithium Cuprates.
T. D. Salatin, D. McLaughlin, and W. L. Jorgensen
J. Org. Chem., 46, 5284 (1981).
50. Comment on Simulations of Liquid Ammonia Based on Quantum Mechanical Potential Functions.
W. L. Jorgensen
J. Chem. Phys., 75, 2026 (1981).
51. Pressure Dependence of Hydrogen Bonding in Liquid Methanol.
W. L. Jorgensen and M. Ibrahim
J. Am. Chem. Soc., 104, 373 (1982).
52. The Nature of Dilute Solutions of Sodium and Methoxide Ions in Methanol.
W. L. Jorgensen, B. Bigot, and J. Chandrasekhar
J. Am. Chem. Soc., 104, 4584 (1982).
53. Pressure Dependence of the Mixing of Enantiomeric Liquids, 1,2-Dichloropropane.
W. L. Jorgensen and B. Bigot
J. Phys. Chem., 86, 2867 (1982).
54. Ab Initio Study of Acid-Base Interactions. Proton, Lithium and Sodium Affinities of First and Second Row Bases.
S. F. Smith, J. Chandrasekhar, and W. L. Jorgensen
J. Phys. Chem., 86, 3308 (1982).
55. Fluoranthene: Synthesis and Biological Testing of Four Diol Epoxides.
W. H. Rastetter, R. B. Nachbar, S. Russo-Rodriguez, R. V. 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. $\text{S}_{\text{N}}2$ Reaction Profiles in the Gas Phase and Aqueous Solution.
J. Chandrasekhar, S. F. Smith, and W. L. Jorgensen
J. Am. Chem. Soc., 106, 3049 (1984).
75. Optimized Intermolecular Potential Functions for Liquid Hydrocarbons.
W. L. Jorgensen, J. D. Madura, and C. J. Swenson
J. Am. Chem. Soc., 106, 6638-6646 (1984).

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

- Aromatic Substitution.
M. G. Bures, B. L. Roos-Kozel, and W. L. Jorgensen
J. Org. Chem., 50, 4490 (1985).
86. Monte Carlo Simulation of Differences in Free Energies of Hydration.
W. L. Jorgensen and C. Ravimohan
J. Chem. Phys., 83, 3050-3054 (1985).
87. Temperature and Size Dependence for Monte Carlo Simulations of TIP4P Water.
W. L. Jorgensen and J. D. Madura
Mol. Phys., 56, 1381 (1985).
88. Monte Carlo Simulations of the Hydration of Ammonium and Carboxylate Ions.
W. L. Jorgensen and J. Gao
J. Phys. Chem., 90, 2174 (1986).
89. Optimized Intermolecular Potential Functions for Liquid Alcohols.
W. L. Jorgensen
J. Phys. Chem., 90, 1276 (1986).
90. Ab Initio and Monte Carlo Calculations for a Nucleophilic Addition Reaction in the Gas Phase and in Aqueous Solution.
J. D. Madura and W. L. Jorgensen
J. Am. Chem. Soc., 108, 2517 (1986).
91. Computer Simulations of Organic Reactions in Solution.
W. L. Jorgensen, J. Chandrasekhar, J. K. Buckner, and J. D. Madura
Ann. N. Y. Acad. Sci., 482, 198 (1986).
92. Computer-Assisted Mechanistic Evaluation of Organic Reactions, 12. pK_a Predictions for Organic Compounds in DMSO.
A. J. Gushurst and W. L. Jorgensen
J. Org. Chem., 51, 3513 (1986).
93. Effect of Hydration on the Structure of an S_N2 Transition State.
W. L. Jorgensen and J. K. Buckner
J. Phys. Chem., 90, 4651 (1986).
94. Ab Initio Study of the Structures and Binding Energies of Anion-Water Complexes.
J. Gao, D. S. Garner, and W. L. Jorgensen
J. Am. Chem. Soc., 108, 4784 (1986).
95. Intermolecular Potential Functions and Monte Carlo Simulations for Liquid Sulfur Compounds.

- W. L. Jorgensen
J. Phys. Chem., 90, 6379 (1986).
96. Computer Simulation of Chemical and Biomolecular Systems.
D. L. Beveridge and W. L. Jorgensen, Eds.
Annals of the New York Academy of Sciences, Vol. 482 (1986).
97. Ab Initio Study of the S_N2 Reactions of OH⁻ and OOH⁻ with CH₃Cl.
J. D. Evanseck, J. F. Blake, and W. L. Jorgensen
J. Am. Chem. Soc., 109, 2349 (1987).
98. Network Topology in Simulated Water.
R. J. Speedy, J. D. Madura, and W. L. Jorgensen
J. Phys. Chem., 91, 909 (1987).
99. Energy Profiles for (CH₃)₃CCl Ion Pairs in Aqueous Solution.
W. L. Jorgensen, J. K. Buckner, S. E. Huston, and P. J. Rossky
J. Am. Chem. Soc., 109, 1891 (1987).
100. Ab Initio Study of the Displacement Reactions of Chloride Ion with Formyl and Acetyl Chloride.
J. F. Blake and W. L. Jorgensen
J. Am. Chem. Soc., 109, 3856 (1987).
101. A General Treatment of Nucleophilic Chemistry.
P. Metivier, A. J. Gushurst, and W. L. Jorgensen
J. Org. Chem., 52, 3724 (1987).
102. Computational Investigations of Organic Reaction Mechanisms: Nucleophilic Reactions of Carbonyl Compounds.
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Patents and Applications

Aniline derivatives as antiviral and anticancer agents, their preparation, pharmaceutical compositions, and use in therapy.

Jorgensen, William L.; Ruiz-Caro, Juliana; Hamilton, Andrew D. PCT Int. Appl. (2007), 93 pp. CODEN: PIXXD2 WO 2007038387 A2 20070405 CAN 146:401679 AN 2007:385257

Novel Compositions and Methods of Treating HIV-1 Infections Using Same

WL Jorgensen, KS Anderson - US Patent 20140378443 (2014)

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 Publ. No. 20140356322 (2014); US Patent 10730862 (2020)

Compounds and methods for the treatment of viruses and cancer.

WL Jorgensen, J Ruiz-Caro, Juliana, AD Hamilton, Andrew D. US Patent 9,018,209 (2015)

Preparation of heterocycloxyphenoxyethyl substituted pyrimidine-2,4(1H,3H)-diones for treating HIV infections.

WL Jorgensen, KS Anderson - U.S. Pat. Appl. Publ. (2015), US 20150105351 A1 20150416

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)

Novel azoles and related derivatives as non-nucleoside reverse transcriptase inhibitors (NNRTIs) in antiviral therapy (HIV).

Jorgensen, William L. PCT Int. Appl. (2009), 68pp. CODEN: PIXXD2 WO 2009005811 A1 20090108 CAN 150:114237 AN 2009:20165

Preparation of benzylbenzoxazolone derivatives and analogs for use as MIF modulators.

Jorgensen, William; Bucala, Richard J. PCT Int. Appl. (2010), 67 pp. CODEN: PIXXD2 WO 2010021693 A2 20100225 CAN 152:287368 AN 2010:235888

Preparation of azole derivatives as MIF modulators.

Jorgensen, William L.; Bucala, Richard J. PCT Int. Appl. (2011), WO 2011140202 A2 20111110.

MIF modulators.

WL Jorgensen, RJ Bucala, US Patent 9,540,322 (2017)

Biaryltriazole inhibitors of macrophage migration inhibitory factor.

WL Jorgensen, P Dziedzic, J Cisneros - US Patent Publ. No. 20180179176 (2018)

Compositions and methods of treating HIV-1 infections using same.

WL Jorgensen, KS Anderson - US Patent 9,914,709 (2018)

Macrophage Migration Inhibitory Factor Inhibitors, and Methods of Making and Using Same.

WL Jorgensen - US Patent Publ. No. 20190144424 (2019)

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 Publ. No. 20190127359 (2019)

New substituted 4-phenyl-1H-pyrazole compounds are macrophage migration inhibitory factor inhibitors, useful for treating an inflammatory disease, a neurological disorder, and/or cancer. Jorgensen, W. L.; Trivedi-Parmar, V. - WO2019178480-A1 (2019)

New 7,8-Dihydro-1,7-naphthyridin-8-one compounds used for treating an inflammatory disease, autoimmune disease and cancer, and disease associated with high macrophage migration inhibitory factor expression. Jorgensen, W. L. - US2019144424-A1 (2019)

[Pyrazole-Containing Macrophage Migration Inhibitory Factor Inhibitors](#)

WL Jorgensen, V Trivedi-Parmar - US Patent App. 16/979,306 (2021)

Invited Lectures 2004 - present

2023

EWDDsy – Siena - May

ACS National Meeting – San Francisco – T. Kuntz Symposium – Aug 13-17

2022

WATOC 2020 – Vancouver, BC – July 3-8

Cecam Workshop – Genoa – Sept 20-23

2021

Virtual Winter School of Computational Chemistry – Feb 15-19

ACS National Meeting – Roles of Comp Chem in Addressing COVID-19 – April 5-16

2021 Workshop on Free Energy – June 15-17

ISQBP President's Meeting – June 29 – July 1

Univ. of Lisbon – Medicinal Chemistry Symposium – July 5-9

ACS National Meeting – Atlanta – Comp Chem of COVID-19 – Aug 22-26

ACS National Meeting – Atlanta – Symposium for D. Boger – Aug 22-26

G. Klebe Symposium – Marburg

MGMS Meeting in Memory of Frank Blaney – Belfast, Ireland

EMBO – Advances and Challenges in Biomolecular Simulations - Oct 17-20

Pacificchem 2021 – Honolulu – Dec 16-21

2020

Israel Chemical Society – Jerusalem – Feb 18-19

ACS National Meeting – Philadelphia – R. Levy Symposium – Mar 22 cancelled

Yale Cancer Center Grand Rounds – April 14 cancelled

Free Energy Workshop – Boston – May 6-8 cancelled

8th EWDS – Siena – May 18-21 cancelled

Tinker Workshop – Bethesda – June 4-6 cancelled

MGMS Meeting in Memory of Frank Blaney – Belfast, Ireland - postponed

ISQBP President's Meeting, Strasbourg – postponed

Schrodinger – NYC – Aug 6 Zoom

ACS National Meeting – San Francisco – T. Kuntz Symposium – Aug 16 - postponed

WATOC 2020 – Vancouver, BC – Aug 17-20 – postponed 2021

G. Klebe Symposium – Marburg – Sept 11-12 - postponed

EuroQSAR 2020 – Barcelona – Sept 15-19 - cancelled

BioExcel "Frontiers in Biomolecular Simulations" – Brno – Oct 18-21 postponed

Pacificchem 2020 – Honolulu – Dec 15-20 - postponed

Newcastle U. – Oct 6 Zoom

2019

Australian National University – Canberra – Feb 5

Cavill Lecturer, Univ. of New South Wales – Feb 6
University of Sydney – Feb 8
Drug Discovery Reinvented IV – Fusion Conference – Nassau – Feb 21-24
U. Georgia – Chemistry – March 14
U. Nebraska Medical Center – Pharmaceutical Sciences Seminar – Apr 12
XIIth European Workshop on Drug Design – Siena - May 19-23
Alchemical Free Energy Workshop – Göttingen – May 27-28
Zhengzhou U. – June 19
Tinker Workshop – Paris – July 18-22
SBDD 2019 – Sestri Levante – Sept 23-26
CompBioMed Conference – London – Sept 25-27
Boston University – Chemistry- Oct 29
MIT – Chemistry - Oct 30
Harvard U – Chemistry - Oct 31
Peking Univ. Shenzhen - Jorgensen Symposium – Nov 10-12

2018

Austin Symposium ASMD@D 2018 – March 3-5
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
10th iMed.Ulissboa Postgraduate Students Meeting – July 24-25
ACS National Meeting – Boston – Madura Symposium – Aug 19-23
ACS National Meeting – Boston – Skolnik Award Symposium
22nd EuroQSAR – Thessaloniki, Greece – Sept 16-20
Conference on the Future of Enzyme Modeling – Stockholm – Sept 28-29
Rutgers University – CABM Seminar – Oct 3
Texas Tech University – Chemistry – Nov 2
ACS New Haven Section – Nov 14
Schrödinger - NYC – Nov 30
Vanderbilt University – Chemistry – Dec 3

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
Technique, 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 - Beijing
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 Meeting (New York City)
Pfizer - Ann Arbor
Boehringer-Ingelheim (Ridgefield)
Oxford University (UK) - G. Richards Symposium
National ACS Meeting- San Francisco - Drug Discovery Symposium
National ACS Meeting- San Francisco - Dewar Symposium
Medicinal Chemistry Symposium (Swedish Chemical Society) - Umeå, Sweden
CSIR Bioscience - Pretoria, SA

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 Symposium - 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 (1975-2019)

Purdue:

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., 1985)
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)

Yale:

James F. Blake (Ph.D., 1990; P.D., 90-91)
Julianto Pranata (P.D., 1988-91)
Scott A. Gothe (P.D., 1989-92)
Harold Helson (Ph.D., 1993)

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)
Catherine Peishoff (Ph.D., 1985)
Jeffrey D. Madura (Ph.D., 1985)
Jeffrey Evanseck (B. S., 1986)
M. Leonor Contreras (V. P., 1985-6)
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)

J. Chandrasekhar (V.P., 2001-3)
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)

Toan Nguyen (Ph.D., 1993)
 Vincent-Henri Peuch (VGS, 1993)
 Shenna Sinclair (Ph.D., 1994)
 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) Robert C. Rizzo (Ph.D., 2000)
 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)
 Modesto Orozco (V.P., 1991-93)
 Jan M. Fleischer (Ph.D., 1994)
 Daniel L. Severance (Ph.D., 1993)
 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)
 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 Barrierio (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)

Todd J. Sullivan (P.D., 2012-2013)
Patric Schyman (P. D., 2011-14)
Ricardo Gallardo-Macias (Ph.D., 2014)
Luca Deiana (P.D., 2014-16)
John C. Faver (P.D., 2012-5)
Won-Gil Lee (P.D., 2012-2017)
Maheen Zakaria (B.S., 2017)
Vinay Trivendi-Parmar (Ph.D., 2018)
Luca Menestrina (VGS, 2018)
Ayan Bhattacharjee (Intern, 2018)
Margarita Valhondo (P.D., 2015-2018)
Thomas Dawson (P.D., 2016-2019)
Aysegul Turupcu (PD, 2019-2020)

Mattia Bernetti (VGS, 2013)
Roland Huber (VGS, 2013)
Pawel Dziedzic (P.D., 2012-15)
Daniel J. Cole (P.D., 2012-15)
Jonah Z. Vilseck (Ph. D., 2016)
Cindy Xin Yan (Ph. D., 2017)
Michael J. Robertson (Ph.D., 2017)
Leela Dodda (Ph. D., 2018)
Giorgio Amendola (VGS, 2018)
Jose Cisneros Trigo (P.D.; ARS 2011-2019)
Brittany Simpson (B.S., 2019)
Yue Qian (Ph. D., 2019)
Rene Olivarez (B.S., 2020)

Current Group Members:

Julian Tirado-Rives (PD; ARS; Senior Res. Scientist, 1985-)
Patricia Morales (Res. Asst., 1990-) Stefan G. Krimmer (P.D., 2017-2020)
Ana Newton (PD, 2012-17; ARS 2017-2020) Zachary Carter (Ph. D., 2020)
Israel Cabeza (P.D., 2016-2020) Sean Henry (PD, 2019-)
Maria-Elena Liosi (Ph. D., 2020) Haichan Niu (P.D., 2019-)
Chun-Hui Zhang (PD, 2019-) Kara Cutrona (Ph.D., 2020; PD, 2020)
M. Ghahremanpour (PD, 2019-)