Yiannis N. Kaznessis

Assistant Professor

Department of Chemical Engineering and Materials Science, and Digital Technology Center,
University of Minnesota
421 Washington Ave. S.E., Minneapolis, MN 55455-0132
Tel: (612) 624-4197, Fax: (612) 626-7246, E-mail: yiannis@cems.umn.edu
URL: http://www.cems.umn.edu/research/kaznessis

Professor Kaznessis' research interests focus on computer modeling of biological matter, on the development of bioinformatics methods and on statistical mechanical modeling of biomolecular recognition phenomena. Professor Kaznessis teaches undergraduate "Chemical Engineering Thermodynamics", undergraduate "Process Dynamics and Control" and the graduate course "Statistical Thermodynamics and Kinetics". Professor Kaznessis is also the Director of the University of Minnesota Summer Bioinformatics Institute.

Education

- Diploma, Chemical Engineering, Aristotle University of Thessaloniki, Greece, 1994.
- Ph.D., Chemical Engineering, University of Notre Dame, 1999.
- Postdoctoral Fellowship, University of Michigan and Pfizer Global Research and Development, 05/99-08/01

Appointments

ASSOCIATE PROFESSOR, 08/01/07-
Department of Chemical Engineering and Materials Science, University of Minnesota
Digital Technology Center, University of Minnesota

ASSISTANT PROFESSOR, 08/23/01-07/31/07
Department of Chemical Engineering and Materials Science, University of Minnesota
Digital Technology Center, University of Minnesota

DIRECTOR, 01/01/03-present
University of Minnesota Summer Bioinformatics Institute

POSTDOCTORAL FELLOW, 05/99-08/01
Biomolecular Structure and Drug Design, Pfizer Global Research and Development.
Department of Chemical Engineering, University of Michigan.

RESEARCH ASSISTANT, 09/94-04/99
Department of Chemical Engineering, University of Notre Dame.

PROJECT MANAGER ASSISTANT, 12/93-08/94
Euroconsultants S.A., Thessaloniki, Greece.

RESEARCH ASSISTANT, 01/91-05/92
Chemical Process Engineering Research Institute, Thessaloniki, Greece.

Honors and Awards

- 2006, Fellow, Minnesota Supercomputing Institute
- 2004-2005, 3M non-Tenured Faculty Award
- 2003, IBM Young Faculty Award
- 2003, Young Investigator Petroleum Research Fund Award
- Postdoctoral Fellowship, University of Michigan/Pfizer GRD, 1999-2001
- 2000, SGI Computational Science and Visualization Award, University of Notre Dame
- Fulbright Award, 1994
- 1994, Technical Chamber of Greece Honor Award
- 1991-1993, Greek National Fellowship Foundation Awards

Research Publications

1. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, “Molecular Dynamics Simulations of Polar Polymer Brushes”, Macromolecules, Vol. 31, p. 3116, 1998.

2. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, “A Molecular Dynamics Study of Macromolecules in Good Solvents. Comparison with Dielectric Spectroscopy Experiments”, Journal of Chemical Physics, Vol. 109, p. 5078, 1998.

3. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, “Dielectric Relaxation of Dipole-Inverted Macromolecules Using Computer Simulations”, Macromolecules, Vol. 32, p. 6679, 1999.

4. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, “Concentration and Size Dependence of Dielectric Strength and Dielectric Relaxation of Flexible Polymers in Dilute and Semidilute Solutions of a Theta Solvent”, Macromolecules, Vol. 32, p. 1284, 1999.

5. Y. N. Kaznessis, D. A. Hill, E. J. Maginn, “Dielectric Relaxation of Concentrated Polymer Solutions via Molecular Dynamics Simulations”, Journal of Chemical Physics, Vol. 111, p. 1325, 1999.

6. Y. N. Kaznessis, L. Narashimhan, M. E. Snow, “Binding Free Energy Calculations for Benzamidine-Trypsin Complexes”, Proceedings of Foundations of Molecular Modeling and Simulation Conference, AIChE Symposium Series, p. 283, 2000.

7. Y. N. Kaznessis, M. E. Snow, C. J. Blankley, “Prediction of Blood-Brain Partitioning Using Monte-Carlo Simulations of Molecules in Water”, Journal of Computer-Aided Molecular Design, Vol. 15, p. 697, 2001.

8. Y. N. Kaznessis, S. Kim, R. G. Larson, “Simulations of Zwitterionic and Anionic Phospholipid Monolayers”, Biophysical Journal, Vol. 82, p. 1731-42, 2002.

9. Y. N. Kaznessis, S. Kim, R. G. Larson, “Specific Mode of Interaction Between Components of Model Pulmonary Surfactants Using Computer Simulations”, Journal of Molecular Biology. Vol. 322, p. 569-582, 2002.

PUBLICATIONS AS AN INDEPENDENT FACULTY MEMBER

10. L.M. Gordon, P.W. Mobley, W. Lee, S. Eskandari, Y. Kaznessis, M.A. Sherman, A.J. Waring, "Conformational mapping of the N-terminal peptide of HIV-1 GP41 in lipid detergent and aqueous environments using 13C-enhanced Fourier transform infrared spectroscopy" Protein Science, Vol. 13, p. 1012-30, 2004.

11. H. Wei, Y. Kaznessis, ‘Inferring gene regulatory relationships by combining target-target pattern recognition and regulator-specific motif examination” Biotechnology and Bioengineering, Vol. 89(1), p. 52-77, 2005.

12. N. Ostberg , H. Khandelia, Y. Kaznessis, “Protegrin structure activity relationships: Using homology models of synthetic sequences to determine structural characteristics important for activity” Peptides, Vol. 26(2), p. 297-306, 2005.

13. A. Langham, Y. Kaznessis, "Molecular dynamics simulations of the N-terminus of HIV GP-41 fusion peptide in SDS micelles" Journal of Peptide Science, Vol. 14(2), p. 316-328, 2005.

14. S. Vicatos, V.B. Reddy, Y. Kaznessis, "Prediction of distant residue contacts with the use of evolutionary information" Proteins, Bioinformatics, Structure and Genetics, Vol. 58 (4): 935-49, 2005.

15. H. Salis, Y. Kaznessis, “Accurate Hybrid Stochastic Simulation of a System of Coupled Chemical or Biochemical Reactions”, Journal of Chemical Physics, Vol. 122, p. 054103 1-13, 2005.

16. H. Salis, Y. Kaznessis, "Numerical simulation of stochastic gene circuits" Computers & Chemical Engineering, Vol 29(3), p. 577-588, 2005.

17. Y. Duan, V. Reddy, Y. Kaznessis, "Physicochemical and residue conservation calculations to improve the ranking of protein-protein docking solutions" Protein Science, Vol. 14 (2), p.316-328, 2005.

18. H. Khandelia, Y. Kaznessis, "Molecular dynamics simulations of the helical antimicrobial peptide ovispirin-1 in zwitterionic dodecylphoshocholine micelles: Insights into host-cell toxicity" Journal of Physical Chemistry B, Vol. 109(26) p. 12990 – 12996, 2005.

19. V. Reddy, Y. Kaznessis, "Quantitative analysis of interfacial amino acid conservation in protein-protein hetero complexes" Journal of Bioinformatics and Computational Biology, Vol. 3(5), p.1137-50, 2005.

20. H. Khandelia, Y. Kaznessis, "Molecular dynamics simulations of helical antimicrobial peptides in SDS micelles: What do point mutations achieve?" Peptides, Vol. 26 (11), p. 2037-2049, 2005.

21. H. Salis, Y. Kaznessis “An equation-free probabilistic steady state approximation: Dynamic application to the stochastic simulation of biochemical reaction networks”, Journal of Chemical Physics, Vol. 123(21), p. 214106, 2005.

22. A. Langham, H. Khandelia, Y. Kaznessis, "How can protegrin-1 be both a potent antimicrobial and harmfully toxic?: Molecular dynamics simulations of a beta-sheet antimicrobial peptide in micelles" Biopolymers: Peptide Science, Vol. 84 (2), p.219-231, 2006.

23. L. Tuttle, H. Salis, J. Tomshine, Y. Kaznessis, “Model-Driven Design Principles of Gene Networks: the Oscillator”, Biophysical Journal, Vol. 89(6), p. 3873-83, 2005.

24. Y. Kaznessis, “Multi-Scale Models for Gene Network Engineering”, Chemical Engineering Science, Vol. 61(3), p. 940-953, 2006.

25. Y. Kaznessis, "A review of methods in computational prediction of blood-brain partitioning" Current Medicinal Chemistry, Central Nervous System Agents, Vol. 5, (3), p.185-191, 2005.

26. H. Salis, V. Sotiropoulos, Y. Kaznessis “Multiscale Hy3S: Hybrid Stochastic Simulations for Supercomputers”, BMC Bioinformatics, (highly accessed), Vol. 7:93, 2006.

27. H. Khandelia, Y. Kaznessis, " Molecular Dynamics Investigation of the Influence of Anionic and Zwitterionic Interfaces on Antimicrobial Peptides' Structure: Implications on Peptide Toxicity and Activity" Peptides, Vol. 27(6), p.1192-1200, 2006.

28. Y. Duan, B. Reddy, Y. Kaznessis "Residue conservation information for generating near-native structures in protein-protein docking" Journal of Bioinformatics and Computational Biology, 4:793-806, 2006.

29. H. Khandelia, A. Langham, Y. Kaznessis, "Driving engineering of novel antimicrobial peptides from simulations of peptide-micelle interactions", BBA, Biomembranes, 1758(9):1224-34, 2006.

30. W. Wang, C. Mulakala, S.C. Ward, G. Jung, H. Luong, D. Pham , A.J. Waring, Y. Kaznessis, W. Lu, K.A. Bradley, R.I. Lehrer. "Retrocyclins kill bacilli and germinating spores of Bacillus anthracis and inactivate anthrax lethal toxin." Journal of Biological Chemistry, 281(43):32755-64, 2006.

31. J. Tomshine, Y. Kaznessis, "Optimization of a stochastically-simulated gene network model via simulated annealing," Biophysical Journal, Biophys J. 91(9):3196-205, 2006.

32. A. Langham, Y. Kaznessis "Effects of mutations on the C-terminus of protegrin-1: a molecular dynamics simulation study", Molecular Simulation, 32(3-4):193-201, 2006.

33. H. Salis, Y. Kaznessis, "Computer-aided design of modular protein devices: Boolean AND gene activation." Phys Biol. 3(4):295-310, 2006.

34. V. Sotiropoulos, Y. Kaznessis, " Synthetic tetracycline-inducible regulatory networks: computer-aided design of dynamic phenotypes" BMC Systems Biology, 1:7, 2007

35. C. Mulakala, J.D. Lambris, Y. Kaznessis, "A simple, yet highly accurate, QSAR model captures the complement inhibitory activity of compstatin", Bioorg Med Chem. 15(4):1638-44, 2007.

36. H. Khandelia, Y. Kaznessis, "Structure of the Antimicrobial β-hairpin Peptide Protegrin-1 in a DLPC Lipid Bilayer Investigated by Molecular Dynamics Simulation", BBA Biomembranes, 1768(3):509-20, 2007.

37. H. Khandelia, Y. Kaznessis, "Cation-π Interactions Stabilize the Structure of the Antimicrobial Peptide Indolicidin near Membranes: Molecular Dynamics Simulations", J. Phys. Chem. B, 111(1):242-250, 2007.

38. D. Bolintineanu, A. Langham, T.H. Davis, Y. Kaznessis, “Molecular dynamics simulations of three protegrin-type anti-microbial peptides: interplay between charges at the termini, β-sheet structure and amphiphilic interactions", Molecular Simulation, in press.

39. A. Langham, A.J. Waring, Y. Kaznessis, "Comparison of interactions between β-hairpin decapeptides and SDS/DPC micelles from experimental and simulation data", BMC Biochemistry, in press

40. S. Vicatos, Y. Kaznessis, "Separating true positive predicted residue contacts from false positive ones in mainly alpha proteins, using constrained Metropolis MC simulations." Proteins, in press

Chapters in Books

Y. N. Kaznessis, R.G. Larson, “Molecular mechanics simulations and bioinformatics calculations in the study of lung surfactants”. Invited chapter in the book “Recent Research Developments in Lung Surfactant and its Dysfunction” Edited by Kaushik Nag, Marcel-Dekker. New York, 2005.

Invited and Conference Presentations (15 invited presentations and more than 40 presentations in conferences as an independent faculty)

- Y. Kaznessis, “Synthetic Bio-logical AND gates”, Synthetic Biology 3.0, Zurich, Switzerland, July 2007.
- Y. Kaznessis, “Synthetic Bio-logical AND gates”, Pathways, Networks and Systems Biology, Porto Heli, Greece, July 2007.
- Y. Kaznessis, “Model-Driven Synthetic Bioengineering”, PPEPPED 2007, Crete, Greece, June 2007.
- A. Langham, “Computer-Driven Antimicrobial Peptide, Engineering”, 2007 Biophysical Meeting, Baltimore, March 2007.
- Howard Salis, Yiannis N. Kaznessis, “Bifurcation Analysis of Stochastic Gene Networks”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Vassilios Sotiropoulos, Marie-Nathalie Contou-Carrere, Prodromos Daoutidis, Yiannis N. Kaznessis, “Reduction of Multi-Scale Systems of Chemical Langevin Equations” , American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Himanshu Khandelia, Yiannis N. Kaznessis, “Molecular Dynamics Simulations to Guide the Design of Peptide Antibiotics”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Howard Salis, Yiannis N. Kaznessis, “Computer Aided Design of Modular Protein Devices: Logical "and" Gene Activation, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Abdallah Sayyed-Ahmad, Yiannis Kaznessis, “Relative Binding Free Energy Calculations of Antimicrobial Peptides in Sds/Dpc Micelles Using Molecular Dynamics/Continuum Methods”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Allison Langham, Yiannis N. Kaznessis, “The Design of New Protegrin-like Antimicrobial Peptides: a Molecular Dynamics Study”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Jonathan R. Tomshine, Yiannis N. Kaznessis, “Optimization of Stochastically-Simulated Gene Network Models”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Spyridon Vicatos, Yiannis Kaznessis, “ Separating True Positive Residue Contacts from False Positive Ones in Proteins, Using Constrained Metropolis Monte Carlo Simulations”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Vassilios Sotiropoulos, Yiannis N. Kaznessis, “In Silico Design of Synthetic Tetracycline-Inducible Regulatory Gene Networks”, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, November 2006.
- Y. Kaznessis, “The New Mathematics of Biological Engineering, “ presentation, International Conference in Bioengineering and Nanotechnology, Santa Barbara, CA, September, 2006.
- H. Salis, Y. Kaznessis, “Multi-Scale Models for Gene Network Engineering”, Raleigh, NC, August, 2006
- Y. Kaznessis, “The New Mathematics of Biological Engineering”, invited presentation, Iowa State University, April 2006.
- A. Langham, Y. Kaznessis, “Simulations of Protegrin-1, a potent antimicrobial peptide”, Biophysical Society Meeting, San Francisco, CA, 2006
- H. Khandelia, Y. Kaznessis “Molecular Dynamics Simulations of Antimicrobial Peptides” Platform presentation, American Chemical Society, Atlanta, GA, 2006
- A. Langham, Y. Kaznessis, “Simulations of Protegrin-1, a potent antimicrobial peptide”, Biophysical Society Meeting, San Francisco, CA, 2006
- H. Salis, Y. Kaznessis, “Model-Driven Designs of Gene Regulatory Networks”, Platform presentation, Biophysical Society Meeting, San Francisco, CA, 2006
- H. Khandelia, Y. Kaznessis “Molecular Dynamics Simulations of Antimicrobial Peptides” Platform presentation, Biophysical Society Meeting, San Francisco, CA, 2006
- Y. Kaznessis, “Multiscale Models for Gene Network Engineering”, invited presentation, National Technical University, Athens, Greece, January 2006

- Marie-Nathalie Contou-Carrere, P. Daoutidis, Y. Kaznessis “Model Reduction of Multi Scale Chemical Langevin Equations”, 2005 Annual AICHE Meeting, Cincinnati, OH, November 2005
- H. Salis, Y. Kaznessis, “Equation -Free Probabilistic Steady State Approximation: Dynamic Application to the Stochastic Simulation of Chemically Reacting Systems” , 2005 Annual AICHE Meeting, Cincinnati, OH, November 2005
- Y. Kaznessis, V. Sotiropoulos, “Model-Driven Engineering of Regulatable Gene Networks”, 2005 Annual AICHE Meeting, Cincinnati, OH, November 2005.
- H. Khandelia, Y. Kaznessis, “Antimicrobial Peptides and Implications on Peptide Toxicity and Activity: a Molecular Dynamics Simulation Investigation”, 2005 Annual AICHE Meeting, Cincinnati, OH, November 2005.
- Y. Kaznessis, “Computer-Aided Design of Gene Regulatory Networks: Trends and Prospects”, Invited presentation at the International Symposium on Biotechnology Trends, Past and Future, at the University of Minnesota Biotechnology Institute, Minneapolis, October, 2005
- Y. Kaznessis, “Modeling and Design of Antimicrobial Peptides”, invited presentation, UCLA, August 2005
- H. Salis, Y. Kaznessis, “Computational Design of Oscillating Gene Regulatory Networks”, Foundations of Systems Biology in Engineering, Santa Barbara, August 2005.
- H. Salis, Y. Kaznessis, “Computational Design of Oscillating Gene Regulatory Networks” XIV Bioengineering Conference, Harrison Springs, CA, July 2005
- Y. Kaznessis, “Computational Modeling and Design of Proteins” invited presentation, Beckman-Coulter, July 2005.
- H. Salis, Y. Kaznessis, “De Novo Design of Gene Regulatory Networks” Workshop in High-Performance Computational Models for Molecular Recognition and Biosensing” Santa Barbara, July 2005.
- H. Khandelia, Y. Kaznessis “Effect of Mutations on the Toxicity of Small Helical Antimicrobial Peptides: Insights from Molecular Dynamics Simulations in Zwitterionic Micelles”, Protein Society Annual Meeting, Boston, MA, July 2005
- A. Langham, Y. Kaznessis “The Effects of Mutations on Toxicity on beta-hairpin Antimicrobial Peptides: Simulations in SDS and DPC Micelles” Protein Society Annual Meeting, Boston, MA, July 2005
- Y. Kaznessis, “Multi-scale Models for Gene Network Engineering”, 2005 Midwest Thermodynamics and Statistical Mechanics Conference, West Lafayette, IN, May 2005.
- Y. Kaznessis, “Model-Driven Designs of Gene Regulatory Networks”, invited presentation, March 2005, Purdue University
- Y. Kaznessis, “Identification of Protein-Protein Interaction Sites”, invited presentation, February 2005, University of Pennsylvania.
- H. Khandelia, Y. Kaznessis, “Molecular Dynamics Simulations of Helical Antimicrobial Peptides in SDS micelles: What do Point Mutations Achieve?” Platform presentation, 2005 Biophysical Society Meeting, Long Beach, CA.
- A. Langham, Y. Kaznessis, “What Makes Protegrin Analogues Antimicrobial?”, poster presentation, 2005 Biophysical Society Meeting, Long Beach, CA.
- H. Khandelia, Y. Kaznessis, “Adding Dynamics in Structural Bioinformatics: the Case of Antimicrobial Peptides”. Presentation at the International Conference of Bioinformatics, January 2005, Singapore
- S. Vicatos Y. Kaznessis, " Correlated Mutation Analysis with protein families from PFAM database" 2004 Annual AICHE Meeting, Austin, TX, November 2004
- Y. Duan, V. Reddy, Y. Kaznessis, “Physicochemical and Residue Conservation Calculations to Improve the Ranking of Protein-Protein Docking Solutions” 2004 Annual AICHE Meeting, Austin, TX, November 2004
- H. Salis, Y. Kaznessis, "Using a Hybrid Differential/Master Equation Method to Simulate Physical or Chemical Systems" 2004 Midwest Thermodynamics and Statistical Mechanics Conference, Buffalo, NY, June 2004
- H. Salis, Y. Kaznessis, "Using Stochastic Methods to Design Gene Circuits" MIT Synthetic Biology Conference v1.0, Cambridge, MA, July 2004
- H. Salis, Y. Kaznessis, “Accurate Hybrid Stochastic Simulation of a System of Coupled Chemical or Biochemical Reactions” 2004 Annual AICHE Meeting, Austin, TX, November 2004

- Y. Kaznessis, “Cyberinfrastructure Requirements for Systems Biology”, Invited presentation, National Science Foundation, May 2004
- Y. Kaznessis, “Computer Simulations and Bioinformatics in Protein Engineering”, Invited presentation, Tulane University, March 2004
- H. Wei, Y. Kaznessis, “Pattern Recognition in Gene Expression Data Using a Response Surface Algorithm”, 2003 Annual AIChE Meeting, San Fransisco, CA, November 2003
- H. Salis, Y. Kaznessis, “Stochastic Simulations of Gene Regulatory Networks” 2003 Annual AIChE Meeting, San Fransisco, CA, November 2003
- S. Vicatos, Y. Kaznessis, “De novo Protein Contact Map Prediction Using Evolutionary Information”, 2003 Annual AIChE Meeting, San Fransisco, CA, November 2003
- H. Khandelia, Y. Kaznessis, “Integration of Computer Simulations and Bioinformatics in Antimicrobial Peptide Engineering” 2003 Annual AIChE Meeting, San Fransisco, CA, November 2003
- S. Vicatos, Y. Kaznesis, "De novo contact map prediction using evolutionary information, derived by Correlated Mutation Analysis", 2003 Bioinformatics Symposium at the Center of excellence in Bioninformatics, University of New York at Buffalo, Buffalo, NY, June 2003
- Y. N. Kaznessis, H. Khandelia, “Lipid Monolayer Binding of NK-lysin”, 2003 Annual Biophysical Society Conference, San Antonio, TX, March 2003.
- Y. N. Kaznessis, “What is the Role of Chemical Engineers in the Revolution in Biology?” AIChE Minnesota Chapter Annual Meeting, January 2003.
- Y.N. Kaznessis, “Atomistic Simulations of Lipid Monolayers” 2002 Annual AIChE Meeting, Indianapolis, IN, November 2002.
- Y. N. Kaznessis, “Protein Fold Recognition Based on Detection of Nonlocal Interactions in Proteins”, 2002 Annual AIChE Meeting, Indianapolis, IN, November 2002.
- Y.N. Kaznessis, A. Gopal, K.Y.C. Lee, R. Larson “Computational and experimental approaches to elucidate the mechanism of action of surfactant-protein B.” 2002 Annual Biophysical Society Conference, San Francisco, CA, February 2002.
- Y. N. Kaznessis, “Synergistic computational approaches for proteinformatics”, Invited presentation, Biotechnology Institute, University of Minnesota, October, 2001.
- Y. N. Kaznessis “Determination of Lipid-Protein Interactions in Lung Surfactants Using Computer Simulations and Structural Bioinformatics”, Invited presentation at the 2001 Annual Meeting of the APS Division of Computational Physics, Boston, MA, June 2001.
- Y. N. Kaznessis “Development of Design Rules for Synthetic Lung Surfactant Analogues Using Computer Simulations and Structural Bioinformatics”, Invited presentation at the 33rd Central/Great Lakes Joint ACS Regional Meeting, Grand Rapids, MI, June 2001.
- Y. N. Kaznessis “Molecular Modeling and Bioinformatics in Drug Discovery Process”, Invited presentation at Eli Lilly, Indianapolis, IN, May 2001.
- Y.N. Kaznessis, “Development of design rules for synthetic lung surfactant analogues using computer simulations and structural bioinformatics, 2001 Midwest Conference on Thermodynamics and Statistical Mechanics, Michigan State University, May 2001.
- Mark E. Snow, James Dunbar, Lakshmi Narasimhan, Jack A. Bikker, Dan Ortwine, Christopher Whitehead, Yiannis N. Kaznessis, Dave Moreland, Christine Humblet, “Virtual Screening. How are We Doing?”, Spring 2001 ACS National Meeting, San Diego, CA, April 2001.
- Y. N. Kaznessis, Ajaykumar Gopal, KaYee Lee, Ronald G. Larson, “Effects of Pulmonary Surfactant Protein B and Calcium Ions on the Interfacial Properties of Lipid Monolayers.”, 2001 Annual Biophysical Society Meeting, Boston, MA, February 2001.
- Y. N. Kaznessis, Mark E. Snow, C. John Blankley, “Prediction of Blood-Brain Partitioning Using Monte Carlo Simulations”, 2000 Annual AIChE Meeting, Los Angeles, CA, November 2000.
- Y. N. Kaznessis, Sangtae Kim, Ronald G. Larson, “Structure and Dynamics of Lung Surfactant Monolayers”, 2000 Midwest Conference on Thermodynamics and Statistical Mechanics, Un. of Minnessota, May 2000.
- Y. N. Kaznessis, Sangtae Kim, Ronald G. Larson, “Molecular Dynamics Simulations of a DPPC/DPPG Monolayer.”, 2000 Annual Biophysical Society Meeting, New Orleans, LA, February 2000.
- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “Computer Simulations of Dipole-Inverted Polar Macromolecules”, 1999 Annual AIChE Meeting, Dallas, TX, November 1999.

- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “Statistical Mechanics of Polar Macromolecules”, Invited presentation at the National Research Centre for Physical Sciences “Demokritos”, Ag. Paraskevi, Greece, December 1998.
- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “Molecular Dynamics Study of Dielectric Strength and Relaxation of Flexible Type-A Polar Macromolecules in Good and Theta Solvents”, 1998 Annual AIChE Meeting, Miami, FL, November 1998.
- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “ Dielectric Relaxation of Flexible Type-A Polar Macromolecules in Good Solvents”, 1998 Midwest Conference on Thermodynamics and Statistical Mechanics, Notre Dame, IN, May 1998.
- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “Dynamic Behavior of Polymers Using Molecular Dynamics Simulations”, Invited presentation at the National Research Centre for Physical Sciences “Demokritos”, Ag. Paraskevi, Greece, December 1997.
- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “Dielectric Relaxation of End-Grafted Polar Polymers via Molecular Dynamics Simulations”, 1997 Annual AIChE Meeting, Los Angeles, CA, November 1997.
- Y. N. Kaznessis, E. J. Maginn, D. A. Hill, “Structure of Polar Tethered Macromolecules Using Molecular Dynamics Simulations”, 1997 Midwest Conference on Thermodynamics and Statistical Mechanics, Williams Bay, WI, May 1997.

Membership

American Institute of Chemical Engineers, American Biophysical Society

Professional Activities - Service

- Director, University of Minnesota Bioinformatics Summer Institute
- Editorial Board, BMC Systems Biology
- Chair, Steering Committee, Unisys/Minnesota Supercomputing Institute Alliance
- Fellow, Minnesota Supercomputing Institute
- Member, Internal Advisory Committee, Minnesota Supercomputing Institute
- Member, NSF Partnership for Advanced Computational Infrastructure Committee
- Member, NIH Review Panel, NIH Pathway to Independence Award
- Member, Advisory Committee, University of Minnesota Digital Technology Center
- Member, Steering Committee, University of Minnesota Computational Genetic Laboratory
- Member, Graduate Admissions Committee, CEMS
- Vice Chair, Computational Genomics, 2006 AIChE Annual Meeting
- Member, Organizing Committee, 2007 Bioengineering Conference
- ***Past service*:** Member, Organizing Committee, 2005 Foundations of Systems Biology and Engineering Conference; Vice Chair, Biomedical Applications of Systems Biology Session, 2005 AIChE Annual Meeting; Member, Faculty Recruiting Committee, Department of Computer Science and Engineering; Member, Chemical Engineering Curriculum Committee (2003), CEMS; Vice Chair, Bioinformatics Topical Conference, 2001 AIChE Annual Meeting; Chair, Group T3, Bioinformatics, 2002 AIChE Annual Meeting; Member, NSF SBIR 2004 panel; Member, NSF Emerging Models and Technologies (EMT) 2004 and 2005 panels
- Reviewer of manuscripts in: Biophysical Journal, Biological Macromolecules, Biochimica & Biophysica Acta, Bioorganic and Medicinal Chemistry, BMC Bioinformatics, Biotechnology and Bioengineering, Computers and Chemical Engineering, Journal of Biotechnology, Journal of Physical Chemistry, Journal of Chemical Physics, Langmuir, Molecular Simulation, Physical Biology, Proteins.

Research Group

Graduate students: Spyros Vicatos, Allison Langham, Jonathan Tomshine, Vassilis Sotiropoulos, Dan Bolintineanu, John Barrett, Nagendra Singh, Anushree Chatterjee
Postdoctoral Fellows: Abdallah Sayyed-Ahmad, Ting-Lan Chiu, Chandrika Mulakala, Anthony Hill, Kavita Iyer

Past Group Members

Himanshu Khandelia (Ph.D. 2006) now postdoctoral fellow at the University of Southern Denmark
Howard Salis (Ph.D. 2007) now postdoctoral fellow at the University of California, San Francisco
Nathan Ostberg (M.Sc), Lisa Tuttle (BSI and M.Sc.), Yuhua Duan (postdoctoral fellow, now at DOE National Energy Technology Laboratory), Boojala Reddy (research associate, now assistant professor at CUNY), Hairong Wei (postdoctoral fellow, now research associate at the University of Alabama). Another four chemical engineering undergraduate students have worked in our group, along with seventeen Bioinformatics Summer Institute interns.

Courses taught

- 2001-2005, Fall, CHEN 4101, Chemical Engineering Thermodynamics, lectures and recitations
- 2002-2006, Spring, CHEN 8402, Statistical Thermodynamics and Kinetics, lectures
- 2007, Spring, Process Dynamics and Control, recitations

Current and Past Research Support

Modeling and Design of Antimicrobial Peptides
PI: Y.N. Kaznessis, co-PI: A. Waring (UCLA)
Source: NIH (award # 1R01GM070989)

08/01/05 - 07/31/10
Total budget: $1,147,113
Annual direct: $180,000
Annual subcontract to UCLA: $51,000

The goal of this project is to develop computer simulations methods for investigating the interactions of antimicrobial peptides with bacterial and mammalian model membranes. The first goal is to identify the molecular level interactions responsible for antimicrobial peptide activity and toxicity. A second goal is to engineer new antimicrobial peptides with therapeutic potential.

Structural Analysis of the Third Component of the Complement
PI: J. Lambris (UofPenn), co-PI: Y.N. Kaznessis
Source: NIH (award # R01 AI030040-11A1)

08/01/06 - 07/31/11
Total budget: $1,578,302
Annual direct: $326,201
Annual subcontract to University of Minnesota: $37,375

The goal of this project is to investigate the nature of protein-protein interaction cascades involved in complement activation in pathological conditions. Dr. Lambris at the University of Pennsylvania is the project's PI, conducting experimental measurements. Dr. Kaznessis is working with a postdoctoral fellow in computer-aided protein-protein docking calculations.

Computer-Aided Design of Complement Therapeutics
PI: J. Lambris (UofPenn), co-PI: Y.N. Kaznessis
Source: NIH (award # R24 BM069736)

08/01/06 - 07/31/11
Total budget:
Annual direct:
Annual subcontract to University of Minnesota: $52,325

The goal of this project is to investigate the nature of protein-protein interaction cascades involved in complement activation in pathological conditions. Dr. Lambris at the University of Pennsylvania is the project's PI, conducting experimental measurements. Dr. Kaznessis is working with a postdoctoral fellow in computer-aided protein-protein docking calculations.

Multiscale Modeling of Gene Regulatory Networks
PI: Y.N. Kaznessis, co-PI: Prodromos Daoutidis
Source: NSF (award # BES-0425882)

09/01/04 - 08/31/07
Total budget: $441,576

The major goal of this project is to develop hybrid stochastic-discrete and stochastic-continuous algorithms for modeling gene regulatory networks. The model-driven designs of circuits such as bistable switches and oscillators is a final goal.

Summer Bioinformatics Institute
P.I. Y.N. Kaznessis
Source: NSF/NIH (award #: EEC-0234112)

01/01/03 – 12/31/06
Total budget: $657,983
Annual direct: $156,796

The University of Minnesota Bioinformatics Summer Institute is bring together established senior and promising junior faculty from more than ten departments in an interlocking multidisciplinary effort to provide exceptional quality educational and research experiences in bioinformatics. Fifteen undergraduate students are attracted each year to the Institute. Professor Vipin Kumar was the PI of the project during the first year. Prof. Kaznessis has been the PI since. As the Director of the Institute and the Chair of the Institute's Executive Committee Dr. Kaznessis is

responsible for the application process, attracting students and organizing the educational and research experiences of the BSI participants.

Summer Bioinformatics Institute 01/01/07 – 12/31/09
P.I. Y.N. Kaznessis Total budget: $422,872
Source: NSF/NIH (award #: EEC-0234112) Annual direct: $132,193

We were recently awarded a renewal for BSI until 12/31/09.

Synthesis of computer modeling and bioinformatics to determine the nature of toxin formation 01/01/03 – 05/31/07
Total Budget: $300,000
P.I: Y.N. Kaznessis Annual budget: $75,000
Source: U.S. Army Research Laboratory and University of Minnesota Army Center for High Performance Computing Research Center

The major goal of this project is to determine the exact mode of protein-protein interactions in toxin formation, using smart docking calculations. Prof. Kaznessis directs a research associate in developing and employing docking calculations and developing structural bioinformatics tools that improve the accuracy and computational efficiency of docking. Funds are also available for a graduate student.

University of Minnesota – Mayo Clinic Partnership 09/01/04 - 08/31/06
PI: D. Connely (UMinn) and G. Klee (Mayo) Annual budget to Dr. Kaznessis: $5,000
Source: Minnesota State

The major goal of this project is to identify marker protein for prostate cancer. In our group we are developing algorithms for identifying antibody molecules that bind strongly to prostate cancer biomarker proteins. Dr. Kaznessis is paying a postdoctoral fellow part-time to contribute with computational tools.

Protein Fold Recognition Using Non-Local Interactions 8/01/03-07/31/05
PRF No: 38758-G7 Total budget: $35,000
PI: Y.N. Kaznessis
Source: Petroleum Research Fund – American Chemical Society

The major goals of this project are to develop and employ computational tools for efficient and accurate protein fold recognition. Yiannis Kaznessis was the PI, directing the efforts of a graduate student in the Department of Chemical Engineering and Materials Science.

Modeling and Design of Antimicrobial Peptides 09/01/03 - 08/31/06
PI: Y.N. Kaznessis Total budget: $45,000
Source: 3M

3M awarded Prof. Kaznessis the non-tenured Faculty award. The PI employs computer simulations to investigate the interactions of antimicrobial peptides with lipid bilayers.

Protein-protein Interactions Using Correlated Mutations Analysis 01/01/03 - 12/31/04
Total budget: $150,000
PI: Y.N. Kaznessis,
Source: University of Minnesota Digital Technology Center

The major goals are to develop smart docking algorithms for protein-protein interactions. One research associate and one graduate student are working on this project under the direction of the PI.

Computational Functional Genomics 01/01/03 - 12/31/04
PI: Y.N. Kaznessis, Total budget: $100,000
Source: Unisys / Minnesota Supercomputing Institute Alliance

The major goal of this project is to explore solutions driven by database design and SQL query development that leverage the architecture of the ES7000 Server (32 Intel® XeonTM processors MP), recently donated to the Minnesota Supercomputing Center by Unisys and reap the full benefits of Microsoft Windows Server 2003. A research associate built a microarray database on Microsoft SQL server 2003, and we explored a number of capabilities of Transact-SQL in mining biological patterns.

Computational Engineering of a New Class of Antibiotic Molecules: The Case of Antimicrobial Peptides: 08/01/03 - 07/31/05
Total budget: $40,000
PI: Y.N. Kaznessis
Source: IBM

The major goal of this project was to develop pattern recognition computational tools to mine the set of known antimicrobial peptide sequences, in order to identify recurring sequence features that are responsible for activity and specificity. The PI worked with Dr. Isidore Rigoutsos at IBM to develop a pattern recognition algorithm based on TEIRESIAS, a pattern recognition tool developed at IBM.

Protein engineering using structural bioinformatics: 06/01/02 - 07/31/05
PI: Y.N. Kaznessis Total budget: $30,000
Source: University of Minnesota Biotechnology Institute

The major goal of this project was to develop protein folding recognition methods.