John Terhorst / Curriculum Vitae

Adjunct Professor of Chemistry / Vanguard University of Southern California

SUMMARY OF EXPERIENCE

Fifteen years of experience in instruction of chemistry, including organic chemistry and spectroscopy lecture and lab courses, as a teaching assistant, private tutor, graduate teaching fellow including curriculum development, and university professor.

Research in applications of Monte Carlo statistical perturbation theory in computing free-energy binding affinities using implicit solvent models, including software design and implementation.

Development of next-generation force fields including explicit treatment of polarization effects, directed towards efforts in computer-aided drug design of therapeutic agents targeting infectious, inflammatory, and hyperproliferative diseases.

EDUCATION

Ph.D. in Chemistry, Yale University, 2006-2011
Chemical theory and computation.

M.S. in Chemistry, Yale University, 2006-2008
Physical organic chemistry.

B.S. in Chemistry, University of Redlands, 2002-2006
Departmental Honors, organic chemistry.

B.S. in Biology, University of Redlands, 2002-2006
Biochemistry track.

TEACHING EXPERIENCE

P, Professor / **F**, Teaching Fellow / **A**, Teaching Assistant / **T**, Tutor / **G**, Group Tutor / **D**, Director

Vanguard University of Southern California

CHEM 485: Research Topics in Chemistry. Computational, theoretical, and physical organic chemistry. Summer, 2013-2016. **P**,**D**

CHEM 455: Chemistry Teaching Internship. Oversight of students planning and conducting a lecture, recitation, and/or laboratory course. Fall and Spring, 2016-2018. **P**

CHEM 308: Introduction to Spectroscopy. Includes IR spectroscopy, 1D and 2D ^{1}H and ^{13}C NMR spectroscopy, mass spectrometry, and UV/vis spectrophotometry. Spring, 2014. **P**

CHEM 304/305/R: Organic Chemistry I/II/Recitation. Functional groups, nomenclature, stereochemistry, aromaticity, reaction mechanisms, and molecular orbital theory. Historical context. Summer, 2012-2018, and Spring, 2013 and 2016. **P**

CHEM 120/121/R: General Chemistry I/II/Recitation. Atomic structure, bonding, stoichiometry, and reactions; kinetics, equilibrium, thermodynamics, and electrochemistry. Spring, 2012 and 2016-2018, and Fall, 2015-2017. **P**

CHEM 113: Fundamentals of General, Organic, and Biochemistry II. Functional groups, basic organic reactions, carbohydrates, amino acids, protein synthesis, and nucleic acids. Spring, 2013-2015. **P**

CHEM 112C: Fundamentals of General, Organic, and Biochemistry I. Atomic theory, periodic trends, measurements, stoichiometry, chemical reactions and equilibrium, and acids and bases. Fall, 2013-2014. **P**

TEACHING EXPERIENCE (CONT.)

WyzAnt Tutoring

Introductory, Honors, A.P., General, and Organic Chemistry: Stanford University, UC Irvine, UC Riverside, University of Southern California, La Sierra University, Chapman University, Cal State Fullerton, Saddleback College, Irvine Valley College, University High School, Newport Beach High School, Woodbridge High School, San Juan Hills High School, Corona del Mar High School, Yorba Linda High School, Mater Dei High School, Troy High School, Cornelia Connelly School, Sage Hill School, Deerfield Academy. 2012-2017. **T**,**G**

Chemistry of Natural and Engineered Aquatic Systems: Hydrogen bonding, structure, molecular dynamics, solubility, equilibrium, and kinetics of microscopic and bulk aqueous solutions. Spring, 2013. **T**

Public Profile: https://www.wyzant.com/match/tutor/80301850

Yale University

CHEM 222/223: Organic Chemistry Lab I/II. Reflux, TLC, recrystallization, column chromatography, extraction, Grignard chemistry, Williamson ether synthesis, aldol and Claisen condensations, and sodium borohydride reduction. Fall, 2006 and Spring, 2007. **F**

CHEM 221: Organic Chemistry of Life Processes. A continuation of Introductory Organic Chemistry, covering reactivity and mechanisms in organic chemistry with an emphasis in their various roles in biological processes. Fall, 2009 and Spring, 2010. **T**

CHEM 220: Introductory Organic Chemistry. The first semester in a two-semester sequence offers a comprehensive look at the fundamental principles of organic chemistry. Offered off-sequence for students on an accelerated track. Spring, 2010. **F**,**T**

CHEM 114: General Chemistry I. A survey of modern descriptive, inorganic, and physical chemistry. Topics included atomic theory, stoichiometry, thermochemistry, chemical periodicity, concepts in chemical bonding, and the shapes of molecules. Fall, 2007. **F**

University of Redlands

CHEM 231/232: Organic Chemistry I/II. A two-semester sequence offering a comprehensive survey of the chemistry of carbon-containing compounds, their structure, nomenclature, physical properties, spectroscopy (IR, GC-MS, NMR), stereochemistry, chemical reactivities, mechanisms of reaction, and synthesis. Fall, 2004 through Spring, 2006. **T**,**G**,**A**

CHEM 131/132: General Chemistry I/II. A two-semester sequence covering stoichiometry and modern views of the properties, structure, and reactivity of atoms and molecules. Fall, 2003 and Spring, 2004. **T**

INVITED GUEST LECTURES

Terhorst, J.; Castaldi, D. Chemistry Through Computers. Guest Speaker, 7th Grade Science. Blessed Sacrament Parish School, San Diego, California. January, 2015.

Terhorst, J.; Murillo, H. Chemistry: College, Grad School, and Beyond. Guest Science Lecture. Citrus Valley High School, Redlands, California. May, 2012.

Terhorst, J.; Jorgensen, W. L. Using Computers in Drug Discovery. University of Redlands Seminar. Department of Chemistry, University of Redlands, Redlands, California. January, 2011.

Terhorst, J.; Castaldi, D. Chemistry Through Computers. Guest Speaker, 7th Grade Science. St. John Middle School, Encinitas, California. October, 2009.

HONORS, AWARDS, AND FELLOWSHIPS

Dox Research Fellowship, Yale University, 2009
The Dox Fellowship was established to provide stipend support to graduate students in the field of organic chemistry, given in recognition of excellence in academics and research.

Distinguished Chemistry Fellowship, Yale University, 2006-2011
Graduate students of exceptional promise are awarded the Distinguished Chemistry Fellowship for five years of stipend support while conducting research towards the completion of a doctorate in chemistry.

Departmental Honors, Chemistry, University of Redlands, 2006
Given in recognition of academic excellence and outstanding achievement in undergraduate research.

Phi Beta Kappa, Xi Chapter of Southern California, 2006
Graduating seniors at the University of Redlands are inducted into PBK in recognition of excellence in the liberal arts and sciences.

Robert D. Engel Award, University of Redlands, 2006
The Robert D. Engel award is given to the outstanding senior science major at the University of Redlands.

Edmund C. Jaeger Award, University of Redlands, 2005
The Edmund C. Jaeger award is given by the University of Redlands for exceptional scholarship to a junior male biology student planning a career in teaching or research.

RESEARCH EXPERIENCE

Director, Summer Undergraduate Research Program, Vanguard University, 2015

Research Advisor, Computational Chemistry, Vanguard University, 2013-2016
Studies of pure liquids, conformational dynamics and molecular design of anti-HIV agents. Advisees: Chris Bridges (B.S., **2014**), Justin Pugh (B.S., **2014**), Josiah Morales (B.S., **2014**), Brennan Gregory (B.S., **2016**), Chalane Records (B.S., **2015**), Ashley Harris (B.S., **2016**), Israel Sanchez (B.S., **2016**), Emily Eggleston (B.S., **2018**), Mia Kilekas (B.S., **2018**)

Graduate Student, Chemical Theory and Computation, Yale University, 2007-2011
Conformational dynamics, molecular mechanical force field parameters, and new methods for computing free energies of binding using continuum solvent models in a Monte Carlo manifold. Advisor: William L. Jorgensen.

Undergraduate Researcher, Organic Chemistry, University of Redlands, 2004-2006
The [3+2] cycloaddition of carbonyl oxides in the synthesis of 1,2-dioxolanes, preparation of carbonyl oxides from precursors other than primary ozonides, and total synthesis of jasmine ketolactone. Advisor: David P. Soulsby.

Undergraduate Researcher, Theoretical Chemistry, University of Redlands, 2003-2004
Theoretical investigations of photopumping in doubly illuminated liquid membranes containing photoactive carriers. Advisor: Teresa Longin.

PUBLICATIONS

Terhorst, J.; Jorgensen, W. L. *E/Z* Energetics for Molecular Modeling and Design. *J. Chem. Theory Comput.* **2010**, *6*, 2762-2769. doi:10.1021/ct1004017

Longin, T. L.; **Terhorst, J.**; Lang, C. Simulations of Photopumping in Doubly Illuminated Liquid Membranes Containing Photoactive Carriers. *J. Phys. Chem. B* **2010**, *114*, 15846-15856. doi:10.1021/jp106802q

THESES

Terhorst, J. Continuum Solvent Models and Force Field Development in Computer-aided Drug Design. ProQuest UMI-3496989. Ph.D. Dissertation. **2011.** Yale University, New Haven, Connecticut. 153 pages.

Terhorst, J. An Efficient Method for Calculating Born Energies with the GB/SA Solvation Model in Monte Carlo Simulations. Dissertation Prospectus. **2008.** Yale University, New Haven, Connecticut. 14 pages.

Terhorst, J. Theoretical Studies of Photopumping in Photofacilitated Liquid Membranes and The [3+2] Cycloaddition of Carbonyl Oxides in the Synthesis of 1,2-Dioxolanes. Honors Thesis. **2006.** University of Redlands, Redlands, California. 96 pages.

SCIENTIFIC PROGRAMMING

MCPRO. Jorgensen, W. L.; Tirado-Rives, J. (contributor, proprietary): Implementation of new modules for utilizing the GB/SA continuum solvent model in simulations with Monte Carlo free-energy perturbation. 2008-2011.

BOSS. Jorgensen, W. L.; Tirado-Rives, J. (contributor, proprietary): Development of new OPLS-AA parameters for functionalized heterocyles, and expansion of code for inclusion of solvent-by-solvent polarization within the OPLS-AA polarizable force field. 2008-2011.

DIHOPT. **Terhorst, J.**; Jorgensen, W. L. (chief author, open source): A Perl utility for automated discovery and optimization of dihedral torsion coefficients for the OPLS-AA force field. 2010.

SELECTED PRESENTATIONS

Terhorst, J. Computer-aided Drug Design Using Torsion Profiles and Molecular Docking. SURP Symposium. Department of Chemistry, Vanguard University, Costa Mesa, California. June, 2016.

Pugh, J.; **Terhorst, J.** Computer-aided Drug Design Concerning HIV. Southern California Undergraduate Research Conference on Chemistry and Biochemistry. Concordia University, Irvine, California. April, 2014.

Terhorst, J.; Jorgensen, W. L. Optimizing the OPLS Force Field for NNRTI Drug Design. Bristol-Meyers Squibb Research Symposium. Department of Chemistry, Yale University, New Haven, Connecticut. August, 2011.

Terhorst, J.; Jorgensen, W. L. Examining Intersubstituent Distances in Heterocycles and Evaluation of Tautomeric Equilibria. Connecticut Organic Chemistry Symposium. New Haven, Connecticut. January, 2010.

TECHNICAL SKILLS

Laboratory Skills and Expertise: Organic synthesis (total and concise routes), separation (TLC and column chromatography, extraction, recrystallization, distillation), characterization (GC-MS, HPLC, CE, NMR, IR, UV/Vis), computational chemistry (MM, QM, MC, MC/FEP, GB/SA). **Chemical Simulation and Visualization:** MCPRO, BOSS, Gaussian, MGL AutoDock/Vina, Spartan, Chimera, WebLab, PyMol, RasMol, ChemDraw. **Productivity:** Microsoft Office, OpenOffice, Apple iWork, vim, GNUplot. **Programming:** Perl, FORTRAN, HTML, bash/csh, LaTeX, GNUprof. **Operating Systems:** Mac OS X, Linux (Debian/Ubuntu, Redhat/Fedora), UNIX, Windows.