Tom Kurtzman, Ph.D.
Assistant Professor
Department of Chemistry
Lehman College
City University of New York
ACS COMP Member # 2404296

Education and Research

- **Stanford University**
  Ph.D. in Chemistry (2002)
  Thesis Title: *A scaling principle for the dynamics of density fluctuations in atomic liquids*
- **University of California, Santa Cruz**
  B.A. in Chemistry (1994)

Academic and Research Positions

- **Lehman College, City University of New York**
  Assistant Professor, Department of Chemistry (2010-Present)
- **The Graduate Center of the City University of New York**
  Assistant Professor, Doctoral Program in Chemistry (2011-Present)
  Assistant Professor, Doctoral Program in Biochemistry (2011-Present)
  Deputy Executive Officer, Doctoral Program in Chemistry (2015-Present)
- **San José State University**
  Assistant Professor, Department of Chemistry (2008-2010)
- **Yeshiva University**
  Visiting Assistant Professor, Department of Chemistry (2007-2008)
- **Columbia University**
  Postdoctoral Research Scientist (2004-2007)
- **Technion, Israel Institute of Technology**
  Postdoctoral Research Scientist (2002-2003)

Publications (2010-2016) @ Lehman College

1. Madapa, S., Gadhiya S, **Kurtzman T.**, Alberts, I.L., Ramsey, S., Reith, M.E., Harding W.W., Synthesis and Evaluation of C9 Alkoxy Analogues of (-) Stepholidine as Dopamine Receptor Ligands, *European Journal of Medicinal Chemistry* (Accepted September 10, 2016)
2. Pal, R.K., Haider, K., Kaur, Divya, Flynn, W. Xia, J., Levy, R.M., Taran, T., Wickstrom, L., **Kurtzman, T.**, Gallicchio, E. A Combined Treatment of Hydration and Dynamical Effects for the Modeling of Host-Guest Binding Thermodynamics: The SAMPL5 Blinded Challenge, *Journal of Computer-Aided Molecular Design* (Accepted August 24, 2016)
3. *Ramsey, S., Nguyen, C., Salomon-Ferrer, R., Walker, R.C., Gilson, M.K. & **Kurtzman T.** Solvation Thermodynamic Mapping of Molecular Surfaces in AmberTools: GIST, *J. Comp. Chem.* (June 18, 2016)
4. *Haider, K., Wickstrom, L., Ramsey, S., Gilson, M. K. & **Kurtzman, T.** Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. *J. Phys. Chem. B* (May 25, 2016).

5. Gadhiya, S., Madapa, S., **Kurtzman, T.,** Alberts, I.L., Ramsey, S., Nagavara-Kishore, P., Kalidindi, T., Harding, W.W. Tetrahydroprotoberberine alkaloids with dopamine and σ receptor affinity, *Bioorg. Med. Chem.* (May 21, 2016)
6. Nguyen, C. N., **Kurtzman, T.** & Gilson, M. K. Spatial Decomposition of Translational Water–Water Correlation Entropy in Binding Pockets. *J. Chem. Theory Comput.* **12,** 414–429 (Jan. 12, 2016)
7. *Velez-Vega, C., Mckay, D.J.J., Kurtzman, T., Aravamuthan, V., Pearltesin, R., Duca, J. Estimation of solvation entropy and enthalpy via analysis of water oxygen-hydrogen correlations, *J. Chem. Theory Comput.* **11,** 5090–5102 (October 7, 2015)
8. Wickstrom, L., Deng N., He, P., Mentes, A., Nguyen, C., Gilson, M.K., **Kurtzman, T.**, Gallicchio, E., Levy, R.M. Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. *J. Mol. Recognit.* **29**, 10-12 (August 10, 2015)
9. *Nguyen, C. N., Cruz, A., Gilson, M. K. & **Kurtzman, T.** Thermodynamics of Water in an Enzyme Active Site: Grid-Based Hydration Analysis of Coagulation Factor Xa. *J. Chem. Theory Comput.* (April 3, 2014).
10. Armaiz-Pena, G. N., .. **Young, T.** , … *et al.* Src activation by β-adrenoreceptors is a key switch for tumour metastasis. *Nat. Commun.* **4,** 1403 (January 29, 2013).
11. *Nguyen, C. N., **Kurtzman Young, T.** & Gilson, M. K. Grid inhomogeneous solvation theory: Hydration structure and thermodynamics of the miniature receptor cucurbit[7]uril. *J. Chem. Phys.* **137,** 044101–044101–17 (July 28, 2012)
12. *Nguyen, C., Gilson, M. K. & **Young, T.** Structure and Thermodynamics of Molecular Hydration via Grid Inhomogeneous Solvation Theory. *arXiv:1108.4876* (August 4, 2011)

    * indicates corresponding author

Publications (Prior to joining Lehman)

13. **Young, T**., Hua, L., Huang, X., Abel, R., Friesner, R.A., Berne, B.J. Dewetting transitions in protein cavities. *Proteins Struct. Funct. Bioinforma.* **78,** 1856–1869 (2010).
14. Abel, R., **Young, T**., Farid, R., Berne, B. J. & Friesner, R. A. The role of the active site solvent in the thermodynamics of factor Xa-ligand binding. *J. Am. Chem. Soc.* **130,** 2817–2831 (2008)
15. **Young, T**., Abel, R., Kim, B., Berne, B. J. & Friesner, R. A. Motifs for molecular recognition exploiting hydrophobic enclosure in protein–ligand binding. *Proc. Natl. Acad. Sci.* **104,** 808 –813 (2007).
16. Kim, B., **Young, T.,** Harder, E., Friesner, R. A. & Berne, B. J. Structure and dynamics of the solvation of bovine pancreatic trypsin inhibitor in explicit water: a comparative study of the effects of solvent and protein polarizability. *J. Phys. Chem. B* **109,** 16529–16538 (2005)
17. **Young, T.** & Andersen, H. C. Tests of an approximate scaling principle for dynamics of classical fluids. *J. Phys. Chem. B* **109,** 2985–2994 (2005)
18. **Young, T.** & Andersen, H. C. A scaling principle for the dynamics of density fluctuations in atomic liquids. *J. Chem. Phys.* **118,** 3447 (2003).
19. Pitts, S. J., **Young, T**. & Andersen, H. C. Facilitated spin models, mode coupling theory, and ergodic–nonergodic transitions. *J. Chem. Phys.* **113,** 8671 (2000).

Patents

1) U.S. Patent Application, *Method of Using a Water-Based Pharmacophore*, **Kurtzman**, et al. (PCT/US14/59456), **Filed October 28, 2014**

2) Divisional U.S. Patent 7,970,580. **Young**, et al. *Methods of calculating differences of binding affinities between congeneric pairs of ligands by way of a displaced solvent functional.* **Granted June 28,2011** (Divisional)
3) Divisional U.S. Patent 7,970,581. **Young**, et al. *Methods of calculating differences of binding affinities between congeneric pairs of ligands by way of a displaced solvent functional*. **Granted June 28, 2011**
4) U.S. Patent 7,756,674 – **Young**, et al. *Methods of calculating differences of binding affinities between congeneric pairs of ligands by way of a displaced solvent functional*. **Granted July 13, 2010**
5) U.S. Provisional Patent. Gilson, Nguyen, & **Young**, *Computational Analysis of Solvent Structure and Thermodynamics to Support Drug Design and Molecular Design*, **Filed August 21, 2012, 61/691,097 (lapsed)**

Research Support

NIH SC3 GM095417 PI: Tom Kurtzman 1/31/2012-01/31/2016

Solvation Directed Design of Flavonoid Derivatives for Caspase Inhibition

Amount: $456,000

This project seeks to rationally design modifications to the flavonoids that result in enhanced affinity and specificity to members of the caspase family of proteins. A key focus is the use of WaterMap type calculations to guide the modification.

NIH R01 GM100946 PI: Michael K. Gilson 09/01/2013-04/30/2017

Accounting for Water Structure and Thermodynamics in Computer-Aided Drug Design
Role: Key Person Amount: $484,000 (amount of sub-contract)

This project aims to develop new computational tools that will speed structure-based drug-discovery by providing a detailed analysis of hydration structure and thermodynamics of water in targeted protein binding pockets.

CUNY CIRG 23: PI: Emilio Gallicchio 09/01/2016-06/30/2017

A Combined Treatment of Hydration and Dynamical Effects for the Modeling of Protein-Ligand Binding Thermodynamics
Role: CO-PI Amount: $9,850 (to each PI)
Other CO-PIs: Lauren Wickstrom - BMCC, Wayne Harding - Hunter

Pending Research Support

NIH SC3-GM095417 : PI: Tom Kurtzman Submitted: 05/25/2016

Exploiting Solvation Structure and Thermodynamics for Prospective Drug Discovery and Rational Design
Renewal 2nd submission

NIH R01 : PI: Wayne Harding Submitted: 06/05/2016

Dopamine multireceptor ligands for cocaine antagonism.
Role: Consultant

Unfunded External Grant Submissions

NSF RUI : PI: Lauren Wickstrom Submitted: 11/14/2015
Quantifying the role of water on conformational selectivity and reorganization in protein-ligand binding
Role: Key Person

NIH SC3-GM095417 : PI: Tom Kurtzman Submitted: 05/25/2015
Renewal
Exploiting Solvation Structure and Thermodynamics for Prospective Drug Discovery and Rational Design

NSF-13-573 (NSF-BSF) PI: Tom Kurtzman Submitted: 09/09/2013
Incorporating NMR and solvation thermodynamics into traditional structure based drug discovery and the application towards finding new protein-protein inhibitors
CO-PIs: Itai Bloch, Maayan Gal

Unfunded Internal Grant Submissions

PSC CUNY: PI: Tom Kurtzman Submitted: 01/11/2012
A Computational Approach to the Design of Flavonoid Analogues for Caspase Inhibition

CUNY CIRG Round 19 : PI: Tom Kurtzman Submitted: 02/15/2012
Acquisition of Suitable Inhibitory Agents of Never In Mitosis A Related Kinase-2 (Nek2), A Molecular Target of Breast Cancer Therapeutics
CO-PI: Sanjai Kumar

CUNY CIRG Rounds 21: PI: Tom Kurtzman Submitted: 03/15/2014
New chemical tools for the dopamine D3 receptor: synthetic, biological and computational studies
CO-PIs: Wayne Harding, Ian Alberts

Presentations (2011-2016**)**

Bold *indicates presenting author*

1) *Frustrated Water Networks on Protein Active Site Surfaces*, **Kamran Haider**, Michael Gilson, Tom Kurtzman, (ACS National Meeting Philadelphia - August 24, 2016 - COMP 360)
2) *Water in Dopamine Receptors: Using Solvation Thermodynamics to Modify a Lead Compound for Specificity*, **Steven Ramsey**, Tom Kurtzman, Wayne Harding, Ian Alberts (ACS National Meeting Philadelphia - August 24, 2016 - COMP 361)
3) *Making a Splash in Implicit Solvent: Application of Inhomogeneous Solvation Theory and Continuum Solvation to Host-Guest Bindina Affinity Predictions*, (**Lauren Wickstrom**, Rajat Pal, Kamran Haider, Junchao Xia, William Flynn, Tom Kurtzman, Ronald Levy, Emilio Gallicchio, ACS National Meeting Philadelphia - August 24, 2016 - COMP 362)
4) *Exploiting Active-site Water Structure and Thermodynamics for Drug Discovery and Design*, **Tom Kurtzman** (Department of Molecular Biology and Biochemistry – Faculty of Life Sciences, Tel Aviv University – August 7, 2016)
5) *Exploiting Active-site Water Structure and Thermodynamics for Drug Discovery and Design*, **Tom Kurtzman** (The Fritz Haber Reseach Center for Molecular Dynamics, Chemistry Institute, The Hebrew University, Givat-Ram Campus, Jerusalem, Israel – August 4, 2016)

6) *Exploiting Active-site Water Structure and Thermodynamics for Drug Discovery and Design*, **Tom Kurtzman** (Pfizer CADD Group, Boston Campus – Invited Talk, June 16, 2016)
7) *Exploiting Active-site Water Structure and Thermodynamics for Drug Discovery and Design*, **Tom Kurtzman** (Boston University, Biomolecular Engineering Research Center June 15, 2016)
8) *Exploiting Active-site Water Structure and Thermodynamics for Drug Discovery and Design*, Kamran Haider, Steven Ramsey & **Tom Kurtzman** (University of Maryland CADD Center, Computer Aided Drug Design Symposium, Baltimore May 25, 2016 - Invited Talk)
9) *Exploiting Active-site Water Structure and Thermodynamics for Drug Discovery and Design*, **Tom Kurtzman** (Lehman College Chemistry Seminar, May 11, 2016)
10) *Molecular Recognition of Cell Adhesion Proteins: Is Water the "Glue" That Holds Pathogens to Host Cells?*, **Theodore Hadges**, Emilio Gallicchio, Tom Kurtzman, Lauren Wickstrom (NY CSTEP Statewide Student Conference, Sagamore NY, April 8, 2016)
11) *Grid Inhomogeneous Solvation Theory (GIST),* ***Steven Ramsey*** *& Tom Kurtzman (Amber Developer's Meeting 2016, San Diego, March 19, 2016)*
12) *Computational thermodynamics of noncovalent binding,* ***M.K. Gilson****, A. Fenley, K. Gao, N.M. Henriksen, T. Kurtzman, H. Muddana, C. Nguyen, J. Yin (ACS San Diego 2016, March 16, 2016)*
13) *Exploiting Active-Site Water Structure and Thermodynamics for Drug Discovery and Design,* **Tom Kurtzman***, (Mathematical Biosciences Institute - Mathematical Challenges in Drug and Protein Design - Invited Talk December 9, 2015)*
14) *Binding affinity calculations: Benefits and limitations in drug discovery*, Camilo Velez-Vega, Robert Pearlstein, Daniel Mckay, Tom Kurtzman, **Jose Duca** ***(****ACS Boston 2015, COMP 57, Presented by Jose Duca, Novartis)*
15) *Parametrization of an effective potential for protein-ligand binding from host-guest data,* **Lauren Wickstrom**, Nanjie Deng, Peng He, Crystal Nguyen, Ahmet Mentes, Michael Gilson, Thomas Kurtzman, Emilio Gallicchio, Ronald Levy (ACS Boston 2015 - COMP 143)
16) *Investigating protein-ligand binding through the lens of local water structure,* **Kamran Haider**, Michael Gilson, Thomas Kurtzman (ACS Boston 2015 - COMP 439 – Poster)
17) *On the study of water-hydrogen correlations toward efficient calculation of solvation entropies and enthalpies in biomolecular systems,* **Camilo Velez-Vega**, Daniel McKay, Tom Kurtzman, Vibhas Aravamuthan, Robert Pearlstein, Jose Duca (ACS Boston 2015 - COMP 356 - Presented by Dr. Camilo Velez Vega, Novartis
18) *Exploiting active-site solvation structure and thermodynamics for drug discovery and design,* **Thomas Kurtzman**, Kamran Haider, Michael Gilson (ACS Boston 2015 - COMP 354)
19) *GistPP (gist post processing): Tools for solvation structural and thermodynamic analysis and visualization,* **Steven Ramsey** (ACS Boston 2015 - COMP 318 – Poster)
20) *Testing the effects of including receptor desolvation in docking calculations,* **Trent Balius**, Marcus Fischer, Crystal Nguyen, Anthony Cruz-Balberdy, Thomas Kurtzman, Michael Gilson, Brian Shoichet (ACS Boston 2015 - COMP 377)
21) *Binding affinity calculations: Benefits and limitations in drug discovery*, Camilo Velez-Vega, Robert Pearlstein, Tom Kurtzman, Daniel Mckay, **Jose Duca** (ACS Boston 2015, COMP 57)
22) *Grid Based Solvation Thermodynamic Mapping in cpptraj,* Instructor @ Amber Molecular Dynamics Workshop, Technion, Haifa (April 26-30, 2015)
23) *Exploiting Active-site Solvation Structure and Thermodynamics for Drug Discovery and Design*, OpenEye CUP XV, **Tom Kurtzman** (March 10, 2015)
24) *Exploiting Protein active site solvation for drug discovery and design,* GlaxoSmithKline (GSK), Philadelphia, **Tom Kurtzman** (October 30, 2014**)**
25) *Characterizing and exploiting the hydration of protein surfaces for applications in drug design and discovery*, ACS COMP 2014, San Francisco (August 10, 2014)

26) *De novo design of drug lead candidates towards targets involved in neurological, cancer, and autoimmune conditions, Poster* ACS COMP 2014, San Francisco (August 12, 2014)
27) *Testing the importance of receptor desolvation for docking using a model system, Poster* Fall ACS COMP 2014, San Francisco **Trent Balius**, et al.(August 11 & 12, 2014)
28) *High resolution Solvation Thermodynamic Mapping with Grid Inhomogeneous Solvation Theory (GIST)*, **Tom Kurtzman** The 2014 Workshop on the State of Free Energy Calculations in Drug Design - Poster Presentation at Vertex Pharmaceuticals, Boston (June 19, 2014)
29) *Exploiting binding site water structure and thermodynamics for drug discovery and design*, Hunter College Chemistry Seminar (February 28, 2014)
30) *Exploiting solvation for drug discovery and design*, Lehman College Biological Sciences Research Seminar (February 10, 2014)
31) *Exploiting Protein Active Site Solvation for Drug Discovery & Design*, City College of New York, Department of Chemistry Biochemistry Seminar (February 5, 2014)
32) *The role of water in protein ligand binding*, The Water Forum, Weizmann Institute of Science, Israel (December 1st, 2013)
33) *The role of water in protein ligand binding*, Migal, Galilee Research Institute (November 17, 2013)
34) *Characterizing and Exploiting the Solvation of Protein Surfaces for Applications in Drug Design and Discovery*, Cambridge Healthtech Institute and Bio-IT World's Thirteenth Annual Structure-Based Drug Design Conference, Cambridge Massachussetts (June 20, 2013)(*Invited*)
35) *Characterizing and exploiting the solvation of protein surfaces for applications in drug design and discovery,* American Chemical Society National Convention, New Orleans (April 9, 2013)
36) *The role of water in protein-ligand binding*, Queens College, CUNY (February 11, 2013)
37) The role of water in protein ligand binding, The Water Forum, Weizmann Institute of Science, Israel (December 1st, 2013)
38) *Characterizing and exploiting the solvation of protein surfaces for applications in drug design and discovery, New England Stuctural Biology Association (NESBA – Invited)* (November 15, 2012)
39) The role of water in protein-ligand binding, Albert Einstein College of Medicine, (November 3, 2012)
40) *Biomolecular Solvation Thermodynamics and Molecular Recognition*, College of Staten Island, CUNY (October 11, 2012)
41) *Localized Thermodynamics of active site solvation from Grid Inhomogeneous Solvation Theory (GIST*), ACS COMP National Conference (August 23, 2012)(*Invited*)
42) *The role of water in protein-ligand binding*, NYU Chemistry (April 18, 2012)
43) *Grid inhomogeneous Solvation Theory of Biomolecular Recognition*, ACS COMP San Diego (March 27, 2012)
44) *The role of water in molecular recognition*, Brooklyn College, CUNY, (Feb 24, 2012)
45) *The role of water in protein-ligand binding*, Rutgers Biomaps Institute, (Feb 1, 2012)
46) *The role of water in protein-ligand binding*, New York Theoretical and Computational Chemistry Conference (Jan. 23, 2012)
47) *The role of water in protein-ligand binding*, UCSD, (January 4, 2012)
48) *The role of water in protein-ligand binding*, Albert Einstein College of Medicine, (November 3, 2011)
49) *The role of water in protein-ligand binding*, Lehman College, (October 5th, 2011)
50) The role of water in protein-ligand binding, CCNY Biochemistry-Chemistry Seminar (2011)