

# Yu-Shan Lin

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## APPOINTMENT

**Associate Professor with Tenure, Department of Chemistry, Tufts University, 2018–present**  
**Assistant Professor, Department of Chemistry, Tufts University, 2012–2018**

## EDUCATION

**Bio-X Postdoctoral Fellow, Department of Chemistry, Stanford University, 2009–2012**

Advisor: Professor Vijay S. Pande

**Ph.D., Chemistry, University of Wisconsin – Madison, 2009**

Thesis title: Theoretical vibrational spectroscopy of water and peptides

Advisor: Professor James L. Skinner

**M.S., Chemistry, University of Wisconsin – Madison, 2007**

Advisor: Professor James L. Skinner

**B.S., Chemistry, National Taiwan University, 2004**

Advisor: Professor Pi-Tai Chou

## SELECTED FELLOWSHIPS AND AWARDS

- Machine Learning in the Chemical Sciences & Engineering Award, Camille and Henry Dreyfus Foundation, 2020
- ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry, American Chemical Society, 2015
- Achievement Award, Department of Chemistry, Tufts University, 2015
- Knez Family Faculty Investment Fund, Tufts University, 2012
- Bio-X Postdoctoral Fellowship, Stanford University, 2009–2011

## CURRENT FUNDING

- R01GM124160 (PI: Lin) 9/1/2017–8/31/2022  
NIH/NIGMS \$1,479,840 (total award)  
Understanding and designing cyclic peptides
- Program for Machine Learning in the Chemical Sciences & Engineering (PI: Lin)  
Camille and Henry Dreyfus Foundation \$120,000 (total award)  
Low-supervision machine learning for automated analysis of molecular dynamics simulations
- DISC SEED grant (PI: Lin) 11/1/2021–10/31/2022  
Tufts University \$20,000 (total award)

Unsupervised clustering for molecular dynamics: Internal distance geometry and manifold dictionary learning

- R01GM125856 (co-I: Lin; PI: Kritzer) 9/1/2018–8/31/2022

NIH/NIGMS \$137,892 (total sub-award)

Translation of hot loops into macrocyclic inhibitors of protein–protein interactions

## PUBLICATIONS

- X. Ye, Y.-C. Lee, Z. Gates, Y. Ling, J. Mortensen, F.-S. Yang, **Y.-S. Lin**, B. L. Pentelute, “Deep alanine scanning reveals potent multi-alanine-substituted proteinprotein interaction inhibitors,” submitted.
- J. Yoon, E. E. Nekongo, J. E. Patrick, A. M. Phillips, A. I. Ponomarenko, S. J. Hendel, V. L. Butty, C. B. Ogbunugafor, **Y.-S. Lin**, M. D. Shoulders, “The host cell’s endoplasmic reticulum proteostasis network profoundly shapes the protein sequence space accessible to HIV envelope,” in revision.
- J. Miao, M. Descoteaux, **Y.-S. Lin**, “Structure prediction of cyclic peptides by molecular dynamics + machine learning,” *Chem. Sci.* accepted (2021).
- J. Damjanovic, J. Murphy,\* **Y.-S. Lin**,\* “CATBOSS: Cluster analysis of trajectories based on segment splitting,” *J. Chem. Inf. Model.* in press (2021).

\*Co-corresponding authors.

- J. Damjanovic,<sup>†</sup> J. Miao,<sup>†</sup> H. Huang,<sup>†</sup> **Y.-S. Lin**, “Elucidating solution structures of cyclic peptides using molecular dynamics simulation,” *Chem. Rev.* **121**, 2292–2324 (2021).

<sup>†</sup> Equal contributions.

- H. Huang,<sup>†</sup> J. Damjanovic,<sup>†</sup> J. Miao, **Y.-S. Lin**, “Cyclic peptides: Backbone rigidification and capability of mimicking motifs at protein–protein interfaces,” *Phys. Chem. Chem. Phys.* **23**, 607–616 (2021).

<sup>†</sup> Equal contributions.

- K. Makwana, M. Sarnowski, J. Miao, **Y.-S. Lin**, J. Del Valle, “From aggregation to inhibition: N-amination converts amyloidogenic tau peptides into soluble antagonists of cellular seeding,” *ACS Chem. Neurosci.* **12**, 3928–3938 (2021).
- J. Pace, C. Abakah, A. Moyer, J. Miao, K. Deprey, R. Cerulli, **Y.-S. Lin**, J. Baleja, D. Baker, J. Kritzer, “Stapled beta-hairpins using 4-mercaptoproline,” *J. Am. Chem. Soc.* **143**, 15039–15044 (2021).
- J. Y.-K. Wong, R. Mukherjee, J. Miao, O. Bilyk, V. Triana, M. Miskolzie, A. Henninot, J. J. Dwyer, A. Iampolska, S. Kharchenko, D. Voluchnyuk, **Y.-S. Lin**, L.-M. Postovit, R. Derda, “Genetically-encoded discovery of proteolytically stable bicyclic inhibitors for morphogen NODAL,” *Chem. Sci.* **12**, 9694–9703 (2021).

- T. Balema, J. Miao, N. Wasio, C. Murphy, A. Larson, D. Patel, **Y.-S. Lin**,\* E. C. Sykes,\* “Visualizing and understanding ordered surface phases during the Ullmann coupling reaction” *J. Phys. Chem. C* **125**, 7675–7685 (2021).

\*Co-corresponding authors.

- A. E. Cummings,<sup>†</sup> J. Miao,<sup>†</sup> D. P. Slough, S. M. McHugh, J. A. Kritzer,\* **Y.-S. Lin**,\* “Beta-branched amino acids stabilize specific conformations of cyclic hexapeptides,” *Biophys. J.* **116**, 433–444 (2019).

<sup>†</sup> Equal contributions. \*Co-corresponding authors.

- E. A. Chen and **Y.-S. Lin**, “Using synthetic peptides and recombinant collagen to understand DDR-collagen interactions,” *Biochim. Biophys. Acta Mol. Cell Res.* **1866**, 118458 (2019).

- T. Balema, N. Ulumuddin, C. Murphy, D. Slough, Z. Smith, R. Hannagan, N. Wasio, A. Larson, D. Patel, K. Groden, J.-S. McEwen,\* **Y.-S. Lin**,\* E. C. Sykes,\* “Controlling molecular switching via chemical functionality; ethyl vs. methoxy rotors,” *J. Phys. Chem. C* **123**, 23738–23746 (2019).  
\*Co-corresponding authors.
- C. Tobon, L. C. Palacio, B. Chidipi, D. P. Slough, T. Tran, N. Tran, M. Reiser, **Y.-S. Lin**, B. Herweg, D. Sayad, J. Saiz, S. Noujaim, “The antimalarial chloroquine reduces the burden of persistent atrial fibrillation,” *Front. Pharmacol.* **10**, 1392 (2019).
- D. P. Slough,<sup>†</sup> S. M. McHugh,<sup>†</sup> A. E. Cummings, P. Dai, B. L. Pentelute, J. A. Kritzer, **Y.-S. Lin**, “Designing well-structured cyclic pentapeptides based on sequence–structure relationships,” *J. Phys. Chem. B* **122**, 3908–3919 (2018).  
<sup>†</sup> Equal contributions.
- D. P. Slough,<sup>†</sup> S. M. McHugh,<sup>†</sup> **Y.-S. Lin**, “Understanding and designing head-to-tail cyclic peptides,” *Biopolymers* **109**, e23113 (2018).  
<sup>†</sup> Equal contributions.
- A. Mekkat,<sup>†</sup> E. Poppleton,<sup>†</sup> B. An, R. Visse, H. Nagase, D. L. Kaplan, B. Brodsky,\* **Y.-S. Lin**,\* “Effects of flexibility of the  $\alpha 2$  chain of type I collagen on collagenase cleavage,” *J. Struct. Biol.* **203**, 247–254 (2018).  
<sup>†</sup> Equal contributions. \*Co-corresponding authors.
- Y. Qiu, A. Mekkat, H. Yu, S. Yigit, S. Hamaia, R. W. Farndale, D. L. Kaplan, **Y.-S. Lin**,\* B. Brodsky,\* “Collagen Gly missense mutations: Effect of residue identity on collagen structure and integrin binding,” *J. Struct. Biol.* **203**, 255–262 (2018).  
\*Co-corresponding authors.
- Y. Qiu, E. Poppleton, A. Mekkat, H. Yu, S. Banerjee, S. E. Wiley, J. E. Dixon, D. L. Kaplan, **Y.-S. Lin**, and B. Brodsky “Enzymatic phosphorylation of Ser in a type I collagen peptide,” *Biophys. J.* **115**, 2327–2335 (2018).
- A. M. Phillips, A. I. Ponomarenko, K. Chen, O. Ashenberg, J. Miao, S. M. McHugh, V. L. Butty, C. A. Whittaker, C. L. Moore, J. D. Bloom, **Y.-S. Lin**, M. D. Shoulders, “Destabilized adaptive influenza variants critical for innate immune system escape are potentiated by host chaperones,” *PLoS Biology* **17**, e3000008 (2018).
- A. M. Phillips, M. B. Doud, L. O. Gonzalez, V. L. Butty, **Y.-S. Lin**, J. D. Bloom, M. D. Shoulders, “Enhanced ER proteostasis and temperature differentially impact the mutational tolerance of influenza hemagglutinin,” *eLife* **7**, e38795 (2018).
- M. Jafari, H. Yu, J. Wickware, **Y.-S. Lin**, R. Derda, “Light-responsive bicyclic peptides,” *Org. Biomol. Chem.* **16**, 7588–7594 (2018).
- Y. Takemoto,<sup>†</sup> D. P. Slough,<sup>†</sup> G. Meinke, C. Katnik, Z. A. Graziano, M. M. Alhadidy, M. Reiser, C. Bujjibabou, R. Ramirez, O. Salvador-Montanes, S. Ennis, G. Gurrero, M. Haburcak, C. Diehl, J. Cuevas, J. Jalife, A. Bohm, **Y.-S. Lin**, S. F. Noujaim, “Structural basis for the antiarrhythmic blockade of a potassium channel with a small molecule,” *FASEB J.* **32**, 1778–1793 (2018).  
<sup>†</sup> Equal contributions.
- J. R. Rogers, S. M. McHugh, **Y.-S. Lin**, “Predictions for  $\alpha$ -helical glycopeptide design from structural bioinformatics analysis,” *J. Chem. Inf. Model.* **57**, 2598–2611 (2017).
- D. P. Slough, H. Yu, S. M. McHugh, **Y.-S. Lin**, “Toward accurately modeling *N*-methylated cyclic peptides,” *Phys. Chem. Chem. Phys.* **19**, 5377–5388 (2017).

- S. M. McHugh,<sup>†</sup> H. Yu,<sup>†</sup> D. P. Slough, **Y.-S. Lin**, “Mapping the sequence–structure relationships of simple cyclic hexapeptides,” *Phys. Chem. Chem. Phys.* **19**, 3315–3324 (2017).  
<sup>†</sup>Equal contributions.
- N. A. Wasio, D. P. Slough, Z. C. Smith, C. J. Ivimey, S. W. Thomas III, **Y.-S. Lin**,\* E. C. H. Sykes,\* “Correlated rotational switching in 2D self-assembled molecular rotor arrays,” *Nat. Comm.* **8**, 16057 (2017).  
 \*Co-corresponding authors.
- Y. Li, N. P. Lavey, J. A. Coker, J. E. Knobbe, D. C. Truong, H. Yu, **Y.-S. Lin**, S. L. Nimmo, A. S. Duerfeldt, “Consequences of depsipeptide substitution on the ClpP activation activity of antibacterial acyldepsipeptides,” *ACS Med. Chem. Lett.* **8**, 1171–1176 (2017).
- S. Mong, F. Cochran, H. Yu, Z. A. Graziano, **Y.-S. Lin**, J. R. Cochran, B. L. Pentelute, “Heterochiral knottin protein: Folding and solution structure,” *Biochemistry* **56**, 5720–5725 (2017).
- A. M. Phillips, L. O. Gonzalez, E. E. Nekongo, A. I. Ponomarenko, S. M. McHugh, V. Butty, S. S. Levine, **Y.-S. Lin**, L. A. Mirny, M. D. Shoulders, “Host proteostasis modulates influenza evolution,” *eLife* **6**, e28652 (2017).
- L. Peraro, Z. Zou, K. M. Makwana, A. E. Cummings, H. L. Ball, H. Yu, **Y.-S. Lin**, B. Levine, J. Kritzer, “Diversity-oriented stapling yields intrinsically cell-penetrant inducers of autophagy,” *J. Am. Chem. Soc.* **139**, 7792–7802 (2017).
- S. M. McHugh,<sup>†</sup> J. R. Rogers,<sup>†</sup> H. Yu, **Y.-S. Lin**, “Insights into how cyclic peptides switch conformations,” *J. Chem. Theory Comput.* **12**, 2480–2488 (2016).  
<sup>†</sup>Equal contributions.
- S. M. McHugh,<sup>†</sup> J. R. Rogers,<sup>†</sup> S. A. Solomon,<sup>†</sup> H. Yu,<sup>†</sup> **Y.-S. Lin**, “Computational methods to design cyclic peptides,” *Curr. Opin. Chem. Biol.* **34**, 95–102 (2016).  
<sup>†</sup>Equal contributions.
- P. Chhum,<sup>†</sup> H. Yu,<sup>†</sup> B. An, B. Doyon, **Y.-S. Lin**,\* B. Brodsky,\* “Consequences of glycine mutations in the fibronectin binding sequence of collagen,” *J. Biol. Chem.* **291**, 27073–27086 (2016).  
<sup>†</sup>Equal contributions. \*Co-corresponding authors.
- S. Yigit,<sup>†</sup> H. Yu,<sup>†</sup> B. An, S. Hamaia, R. W. Farndale, D. L. Kaplan, **Y.-S. Lin**,\* B. Brodsky,\* “Mapping the effect of Gly mutations in collagen on  $\alpha2\beta1$  integrin binding,” *J. Biol. Chem.* **291**, 19196–19207 (2016).  
<sup>†</sup>Equal contributions. \*Co-corresponding authors.
- M. D. Simon, Y. Maki, A. A. Vinogradov, C. Zhang, H. Yu, **Y.-S. Lin**, Y. Kajihara, B. L. Pentelute, “D-Amino acid scan of two small proteins,” *J. Am. Chem. Soc.* **138**, 12099–12111 (2016).
- B. An, **Y.-S. Lin**, B. Brodsky, “Collagen interactions: Drug design and delivery,” *Adv. Drug Deliv. Rev.* **97**, 69–84 (2016).
- H. Yu and **Y.-S. Lin**, “Toward structure prediction of cyclic peptides,” *Phys. Chem. Chem. Phys.* **17**, 4210–4219 (2015).
- J. S. Quartararo, M. R. Eshelman, L. Peraro, H. Yu, J. D. Baleja, **Y.-S. Lin**, J. A. Kritzer, “A bicyclic peptide scaffold promotes phosphotyrosine mimicry and cellular uptake,” *Bioorg. Med. Chem.* **22**, 6387–6319 (2014).
- Y. Zou, A. M. Spokoyny, C. Zhang, M. D. Simon, H. Yu, **Y.-S. Lin**, B. L. Pentelute, “Convergent diversity-oriented side-chain macrocyclization scan for unprotected polypeptides,” *Org. Biomol. Chem.* **12**, 566–573 (2014).

- A. M. Spokoyny, Y. Zou, J. J. Ling, H. Yu, **Y.-S. Lin**, B. L. Pentelute, “A perfluoroaryl-cysteine  $S_NAr$  chemistry approach to unprotected peptide stapling,” *J. Am. Chem. Soc.* **135**, 5946–5949 (2013).
- C. R. Baiz, **Y.-S. Lin**, C. S. Peng, K. A. Beauchamp, V. A. Voelz, V. S. Pande, A. Tokmakoff, “A molecular interpretation of 2D IR protein folding experiments with Markov state models,” *Biophys. J.* **106**, 1359–1370 (2014).
- **Y.-S. Lin** and V. S. Pande, “Effects of familial mutations on the monomer structure of  $A\beta_{42}$ ,” *Biophys. J.* **103**, L47–L49 (2012).
- K. A. Beauchamp, R. McGibbon, **Y.-S. Lin**, V. S. Pande, “Simple few-state models reveal hidden complexity in protein folding,” *Proc. Natl. Acad. Sci. U.S.A.* **109**, 17807–17813 (2012).
- K. A. Beauchamp, **Y.-S. Lin**, R. Das, V. S. Pande, “Are protein force fields getting better? A systematic benchmark on 524 diverse NMR measurements,” *J. Chem. Theory Comput.* **8**, 1409–1414 (2012).
- **Y.-S. Lin**, G. R. Bowman, K. A. Beauchamp, V. S. Pande, “Investigating how peptide length and a pathogenic mutation modify the structural ensemble of amyloid beta monomer,” *Biophys. J.* **102**, 315–324 (2012).
- C. J. Tainter, P. A. Pieniazek, **Y.-S. Lin**, J. L. Skinner, “Robust three-body water simulation model,” *J. Chem. Phys.* **134**, 184501 (2011).
- **Y.-S. Lin**, P. A. Pieniazek, M. Yang, J. L. Skinner, “On the calculation of rotational anisotropy decay, as measured by ultrafast polarization-resolved pump-probe experiments,” *J. Chem. Phys.* **132**, 174505 (2010).
- A. M. Woys, **Y.-S. Lin**, A. S. Reddy, J. J. de Pablo, J. L. Skinner, M. T. Zanni, “2D IR lineshapes probe ovispirin peptide conformation and depth in lipid bilayers,” *J. Am. Chem. Soc.* **132**, 2832–2838 (2010).
- A. S. Reddy, L. Wang, **Y.-S. Lin**, Y. L. Ling, M. T. Zanni, J. L. Skinner, J. J. de Pablo, “Solution structures of rat amylin peptide: Simulation, theory, and experiment,” *Biophys. J.* **98**, 443–451 (2010).
- P. A. Pieniazek, **Y.-S. Lin**, J. L. Skinner, “Vibrational spectroscopy and dynamics of water confined inside reverse micelles,” *J. Phys. Chem. B* **113**, 15017–15028 (2009).
- **Y.-S. Lin**, B. M. Auer, J. L. Skinner, “Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions,” *J. Chem. Phys.* **131**, 144511 (2009).
- J. Manor, P. Mukherjee, **Y.-S. Lin**, H. Leonov, J. L. Skinner, M. T. Zanni, I. T. Arkin, “Gating mechanism of the influenza A M2 channel revealed by 1D and 2D IR spectroscopies,” *Structure* **17**, 247 (2009).
- **Y.-S. Lin**, J. M. Shorb, P. Mukherjee, M. T. Zanni, J. L. Skinner, “Empirical amide I vibrational frequency map: Applications to isotope-edited membrane peptide bundles,” *J. Phys. Chem. B* **113**, 592–602 (2009).
- J. L. Skinner, B. M. Auer, **Y.-S. Lin**, “Vibrational line shapes and spectral diffusion in liquid water,” *Adv. Chem. Phys.* **142**, 59–103 (2009).
- D. E. Moilanen, E. E. Fenn, **Y.-S. Lin**, J. L. Skinner, B. Bagchi, M. D. Fayer, “Water inertial reorientation: Hydrogen bond strength and the angular potential,” *Proc. Natl. Acad. Sci. U.S.A.* **105**, 5295–5300 (2008).
- **Y.-S. Lin**, S. G. Ramesh, J. M. Shorb, E. L. Sibert III, J. L. Skinner, “Vibrational energy relaxation of the bend fundamental of dilute water in liquid chloroform and *d*-chloroform,” *J. Phys. Chem. B* **112**, 390–398 (2008).

- K.-C. Wu, **Y.-S. Lin**, Y.-S. Yeh, C.-Y. Chen, M. O. Ahmed, P.-T. Chou, Y.-S. Hon, "Design and synthesis of intramolecular hydrogen bonding systems. Their application in metal cation sensing based on excited state proton transfer reaction," *Tetrahedron* **60**, 11861–11868 (2004).
- K.-C. Wu, Y.-M. Cheng, **Y.-S. Lin**, Y.-S. Yeh, S.-C. Pu, Y.-H. Hu, J.-K. Yu, P.-T. Chou, "Competitive intramolecular hydrogen bonding formation and excited-state proton transfer reaction in 1-[(diethylamino)-methyl]-2-hydroxy-3-naphthaldehyde," *Chem. Phys. Lett.* **384**, 203–209 (2004).

### SELECTED INVITED ORAL PRESENTATIONS

- American Peptide Society, October 15, 2021
- Advancing Chemical and Materials Science through Machine Learning, Hariri Institute for Computing, Boston University, June 14, 2021
- Molecular Biophysics in the Northeast, Boston, November 9, 2019
- Boston Taiwanese Biotechnology Association Seminar Series, Cambridge, June 30, 2019
- Free Energy Calculations: Entering the Fourth Decade of Adventure in Chemistry and Biophysics, Santa Fe, June 16–21, 2019
- Stonehill College, Chemistry Departmental Seminar, November 30, 2018
- The Greater Boston Area Theoretical Chemistry Lecture Series (THEOCHEM), September 19, 2018
- Annual Meeting of the Biophysical Society of Canada, Montréal, Québec, May 24–26, 2017
- University of Washington–Seattle, Physical Chemistry Seminar, May 24, 2017
- University of California–Santa Barbara, Biomolecular Science and Engineering Seminar, May 17, 2017
- University of California–Merced, Chemistry and Chemical Biology Seminar, April 28, 2017
- University of Notre Dame, Physical/Analytical Chemistry Seminar, April 20, 2017
- Purdue University, Physical Chemistry Seminar, April 19, 2017
- American Chemical Society National Meeting, San Francisco, April 2–6, 2017
- University of Illinois at Urbana–Champaign, Chemical and Biomolecular Engineering Seminar, March 30, 2017
- Rutgers University, Proteomics/IQB@R and CABM Seminars, March 22, 2017
- Louisiana State University, LaCNS and Physical Chemistry Seminar, February 21, 2017
- Massachusetts Institute of Technology, Biophysics Seminar Series, February 8, 2017
- Trinity University, Chemistry Departmental Seminar, December 1, 2016
- Temple University, Chemistry Departmental Seminar, November 3, 2016
- Brigham Young University, Chemistry Departmental Seminar, March 25, 2016
- Boston College, Chemistry Departmental Seminar, March 22, 2016
- American Chemical Society National Meeting, San Diego, March 13–17, 2016
- Colby College, Chemistry Departmental Seminar, October 30, 2015
- University of Wisconsin – Madison, Theoretical Chemistry Institute Seminar, April 20, 2015
- Boston University, Physical Chemistry Seminar, November 19, 2014
- American Conference on Theoretical Chemistry, Telluride, July 20–24, 2014
- American Chemical Society National Meeting, New Orleans, April 7–11, 2013

## TEACHING AT TUFTS

- Chemistry 1: Chemical Fundamentals  
First-semester general chemistry with up to 180 students (SP14, SP16, SP18)
- Chemistry 31: Physical Chemistry I  
Classical thermodynamics and statistical thermodynamics for science and engineering majors (FA15, FA20)
- Chemistry 32: Physical Chemistry II  
Quantum mechanics for science and engineering majors (SP20)
- Chemistry 133: Quantum Mechanics  
Upper and graduate level quantum mechanics (FA12, FA13)
- Chemistry 135: Biophysical Chemistry  
Upper and graduate level biophysical chemistry (FA16, SP19, FA19, SP21)
- Chemistry 194: Computational Chemistry  
Special topic course with a hands-on curriculum on programming and molecular dynamics simulations (SP17)

## PROFESSIONAL SERVICE

### Peer Review

- Assorted journals, including *Chem. Sci.*, *J. Chem. Inf. Model.*, *J. Chem. Phys.*, *J. Chem. Theory Comput.*, *J. Med. Chem.*, *J. Phys. Chem. B*, *Nat. Chem.*, *Org. Lett.*, *Phys. Chem. Chem. Phys.*, *PLoS Comp. Biol.*, *RSC Advances*, and *Science*.
- Grant proposals: American Chemical Society, Beckman Foundation, National Institutes of Health, National Science Foundation.

### Departmental Committees

- Graduate Committee, 2012–2017, 2020–present  
Coordinate the graduate program; recruit and admit graduate students; advise graduate students prior to their selection of a research advisor; monitor graduate student progress, especially the timely completion of degree requirements.
- Diversity, Equity, and Inclusion Committee, 2020–present  
(Committee chair 2020–present)
- Computer Resources Committee, 2019–present
- Seminar Committee, 2016–2020  
(Committee chair 2018–2020)
- Awards Committee, 2014–2020
- Faculty Search Committee, 2012–2013, 2019–2020

### College and University Committees

- Budget and University Priorities (elected), 2020–2025
- Committee on Faculty Work/Life, 2019–2020
- Information Technology Committee, 2015–2020

## MENTORING AND ADVISING

### Current Postdoctoral Scholars

- Dr. Jiayuan Miao, 2017–present
- Dr. Jennifer Mortensen, 2020–present  
Tufts IRACDA Scholar, 2020

#### **Current Graduate Students**

- Francini Fonseca, 2017–present
- Jovan Damjanovic, 2018–present  
ACS COMP Chemical Computing Group Excellence Award for Graduate Students, 2021
- Tiffani Hui, 2020–present

#### **Current Undergraduate Students**

- Kevin Schult, 2019–present  
Beckman Scholar at Tufts, 2020–2021
- Marc Descoteaux, 2021–present  
Summer Scholar at Tufts, 2021

#### **Group Alumni**

- Yingjie (Tim) Ling, 2018–2021  
Tim was a 2019 Laidlaw Scholar at Tufts.  
Tim is currently a master student in the Department of Computer Science at Carnegie Mellon University.
- Stephanie Kearing, master student, 2019–2020 Steph is currently a senior chemist at Jordi Labs.
- Omeir Khan, undergraduate researcher, 2018–2020 (junior–senior)  
Omeir was a 2019 Summer Scholar at Tufts.  
Omeir is currently a graduate student in the Department of Chemistry at BU.
- Aidan Fike, undergraduate researcher, 2018–2020 (junior–senior)  
Aidan was a 2019 Beckman Scholar at Tufts.  
Aidan is currently a software engineer at Ab Initio Software.
- Dr. He (Agnes) Huang, postdoctoral scholar, 2018–2020  
Agnes is currently an application scientist at OpenEye Scientific Software.
- Eric Chen, undergraduate researcher, 2017–2019 (junior–senior)  
Eric was a 2018 Summer Scholar at Tufts.  
Eric is currently a graduate student in the Department of Chemistry at NYU.
- Steph Xu, undergraduate researcher, 2017–2019 (junior–senior)  
Steph is currently a software engineer at Microsoft.
- Arya Mekkat, undergraduate researcher, 2015–2018 (freshman–senior)  
Arya was a 2017 Summer Scholar at Tufts.  
Arya is currently a medical student at BU.
- Dr. Diana Slough, graduate student, 2012–2018  
Diana is currently an ORISE postdoctoral fellow at the US Army Research Institute of Environmental Medicine.
- Dr. Sean McHugh, graduate student, 2012–2018  
Sean is currently a consultant at EQUITAS Life Sciences.
- Dan McKeen, 2016–2017 (sophomore)
- Mong Mary Touch, graduate student, 2016–2017



- Dr. Hongtao Yu, postdoctoral scholar, 2012–2017  
Hongtao is currently an applied scientist at Amazon Lab126.
- Zachary Graziano, undergraduate researcher, 2015–2016 (sophomore–junior)  
Zach was a 2016 Summer Scholar at Tufts.  
Zach is currently a senior software engineer at Appcues.
- Dr. Julia Rogers, undergraduate researcher, 2014–2016 (junior–senior)  
Julia was a 2015 Beckman Scholar at Tufts.  
Julia went on to the Department of Chemistry at UC Berkeley for graduate school. She is currently a postdoctoral researcher at Columbia University.
- Sarah Solomon, master student, 2014–2016  
Sarah is currently a senior associate scientist at Alnylam Pharmaceuticals.
- Diana Gooding, master student, 2014–2015
- Joshua Levy, undergraduate researcher, 2012–2014 (junior–senior)  
Josh is currently a graduate student in the Department of Engineering Sciences and Applied Mathematics at Northwestern University.
- Owen Martin, undergraduate researcher, 2013–2014 (freshman)  
Owen is currently a graduate student in the Department of Computer Science at University of Colorado, Boulder.
- Jordan Rossen, undergraduate researcher, 2013–2014 (freshman)  
Jordan is currently an associate computational biologist at the Broad Institute of MIT and Harvard.
- Andrew Rosen, undergraduate researcher, 2013–2014 (junior)  
Andrew was a 2014 Goldwater Scholar.  
Andrew is currently a graduate student in the Department of Chemical Engineering at Northwestern University.
- Benjamin Kim, undergraduate researcher, 2012–2013 (junior)