

Research Objective

Develop chemical technologies and computational approaches to enable the step-efficient synthesis of structurally complex natural products with potential applications to neuroscience.

Appointments

Professor of Chemistry, Member Interdepartmental Neuroscience Program, Wu Tsai Institute
Yale University, New Haven, CT, 2023

Associate Professor of Chemistry, Member Interdepartmental Neuroscience Program
Yale University, New Haven, CT, 2018

Assistant Professor of Chemistry, Member Interdepartmental Neuroscience Program
Yale University, New Haven, CT, 2013

Education

Postdoctoral Research Fellow, Harvard University, Cambridge, MA, 2010-13
Enantioselective organometallic methods development with E.J. Corey

Ph.D., Organic Chemistry, The Scripps Research Institute, La Jolla, CA, 2006-10
Natural product synthesis with Phil S. Baran
Reaction mechanism investigation with Donna G. Blackmond

B.A., Chemistry with Honors, *summa cum laude*, Colby College, Waterville, ME, 2001-05
Study of reactive intermediates with Dasan M. Thamattoor

Awards and Honors

2022	Boehringer Ingelheim Collaborative Research Award
2021	Boehringer Ingelheim Scientific Advancement Grant
2020	Genentech Research Innovation Award
2019	Arthur C. Cope Scholar Early Career Award, American Chemical Society
2019	PRF New Directions, American Chemical Society
2019	Camille Dreyfus Teacher-Scholar Award
2018	Amgen Young Investigator Award
2018	Dylan Hixon '88 Prize for Teaching Excellence
2017	Academic Young Investigator, American Chemical Society
2017	Sloan Research Fellowship
2017	NSF CAREER
2015	Rosenkranz Award
2015	Thieme Chemistry Journal Award

Awards and Honors (cont.)

2014	Anderson Award
2010-13	Bristol Myers Squibb Postdoctoral Fellowship
2012	Harvard Postdoctoral Award for Professional Development
2011	Reaxys PhD Prize Finalist
2008	Bristol Myers Squibb Graduate Fellowship
2008	Scripps Best Talk Award, Graduate Retreat, Chemistry
2005	The “Sarge” Award in Chemistry for departmental leadership
2005	Phi Beta Kappa Society member
2004	Wayne L. Smith Inorganic Chemistry Award
2003	Bradford P. Mundy Organic Chemistry Award
2003	Merck/AAAS Undergraduate Research Scholar

Independent Publications

58. W. Lu, Haote Li, J. P. Menzel, A. E. Cuomo, A. M. Nikolic, H. Ray Kelly, Y. Shee, S. Sreekumar, F. Buono, J. J. Song, R. H. Crabtree,* V. S. Batista,* and T. R. Newhouse.* Methodical Ligand Selection by Generative Modeling with Latent-Space Sampling: Application to the Mizoroki-Heck Reaction [*Submission planned for Science*]
57. A. K. Bodnar, S. M. Szywczyk, Y. Sun, Y. Chen, A. Huang, T. R. Newhouse.* “A Comparative Mechanistic Analysis of Palladium- and Nickel-Catalyzed α,β -Dehydrogenation of Carbonyls via Organozinc Intermediates” [*Under Review at J. Org. Chem.*]
56. A. K. Bodnar, T. R. Newhouse.* “Z-Selective Co-Catalyzed Propargylic Dehydrogenation.” [*Under Review at Angew. Chem. Int. Ed.*]
55. P. Zhang, T. R. Newhouse. “Pd-Catalyzed Carbonylative Difunctionalization of Unactivated Alkenes Initiated by Unstabilized Enolates.” *Angew. Chem. Int. Ed.* **2023**, 62, e202307455
54. A. Cuomo, S. Ibarraran, S. Sreekumar, H. Li, J. Eun, J. P. Menzel, P. Zhang, F. Buono, J. Song, R. H. Crabtree, V. Batista,* T. Newhouse.* “Feed Forward Neural Network for Predicting Enantioselectivity of the Asymmetric Negishi Reaction.” *ACS Cent. Sci.* **2023**, 9, 1768.
53. D. E. Kim, Y. Zhu, I. Aguilar, S. Harada, M. Wang and T. R. Newhouse.* “Total Synthesis of (+)-Shearilicine.” *J. Am. Chem. Soc.* **2023**, 145, 4394.
52. P. Zhang, J. Eun, M. Elkin, Y. Zhao, R. L. Cantrell, and T. R. Newhouse.* “A Neural Network Model Informs Total Synthesis of Clovane Sesquiterpenoids” *Nature Synth.* **2023**, 2, 527.
51. A. W. Schuppe, Y. Liu, Y. Zhao, S. Ibarraran, D. Huang, E. Wang, J. Lee, P. Loria, T. R. Newhouse.* “Strategies for the De Novo Synthesis of Highly Substituted Pyridine Scaffolds: Unified Total Synthesis of the Limonoid Alkaloids.” *Chem* **2022**, 10, 2856.
50. J. Eun, T. R. Newhouse* “Computational decoding” *Nat. Rev. Chem.* **2022**, 6, 168–169.

49. Y. Liu, A. W. Schuppe, Y. Zhao, J. Lee, T. R. Newhouse* “Synthesis of melazolide B, a degraded limonoid, from a natural terpene precursor.” *Tetrahedron Chem.* **2022**, *1*, 100011.
48. E. A. deRamon, V. R. Sabbasani, M. D. Streeter, Y. Liu, T. R. Newhouse, D. M. McDonald, D. A. Spiegel*. “Pentosinane, a Post-Translational Modification of Human Proteins with Underappreciated Stability” *J. Am. Chem. Soc.* **2022**, *144*, 21843.
47. P. Zhang, J. Wang, Z. R. Robertson, T. R. Newhouse.* “Coordination-Controlled Nickel-Catalyzed Benzylic Allylation of Unactivated Electron-Deficient Heterocycles.” *Angew. Chem. Int. Ed.* **2022**, 9493.
46. C.-Y. Shi, J. Eun, T. R. Newhouse*, Liang Yin* “Copper(I)-Catalyzed Asymmetric Conjugate 1,6-, 1,8-, and 1,10-Borylation” *Angew. Chem. Int. Ed.* **2021**, 9493.
45. A. K. Bodnar, A. Turlik, D. Huang, W. Butcher, J. K. Lew, T. R. Newhouse.* “Preparation of Hindered Aniline CyanH and Application in the Allyl-Ni-Catalyzed α,β -Dehydrogenation of Carbonyls” *Org. Synth.* **2021**, *98*, 263.
44. D. Huang, T. R. Newhouse.* “Dehydrogenative Pd and Ni Catalysis for Total Synthesis” *Acc. Chem. Res.* **2021**, *54*, 1118. [cover]
43. P. Zhang, T. R. Newhouse.* “Thiophene, 2-bromo-5-methyl-” *Encyclopedia for Reagents in Organic Synthesis.* **2020**, RNO2366.
42. D. Olivieri, D. Huang, A. K. Bodnar, S. Yu, T. R. Newhouse.* “Zinc-mediated anionic cyclization of unstabilized ketone enolates with unactivated alkenes” *Tetrahedron.* **2020**, *76*, 131417.
41. A. W. Schuppe, Y. Liu, T. R. Newhouse.* “An Invocation for Computational Evaluation of Isomerization Transforms: Cationic Skeletal Reorganizations as a Case Study” *Nat. Prod. Rep.* **2020**, *38*, 510.
40. Y. Liu, T. A. Holt, A. Kutateladze, T. R. Newhouse.* “Stereochemical Revision of Xylogranatin F by GIAO and DU8+ NMR Calculations” *Chirality.* **2020**, *32*, 515.
39. P. Zhang, D. Huang, T. R. Newhouse.* “Aryl-Nickel-Catalyzed Benzylic Dehydrogenation of Electron-Deficient Heteroarenes” *J. Am. Chem. Soc.* **2020**, *142*, 1757.
38. D. Huang, D. Olivieri, Y. Sun, P. Zhang, T. R. Newhouse.* “Nickel-Catalyzed Difunctionalization of Unactivated Alkenes Initiated by Unstabilized Enolates.” *J. Am. Chem. Soc.* **2019**, *141*, 16249.
37. P. Zhang, T. R. Newhouse.* “Oxidation Stepping Stones: α -Oxytriflation Enables Asymmetric Arylation of Amides.” *Chem* **2019**, *5*, 1883.
36. A. W. Schuppe, Y. Zhao, Y. Liu, T. R. Newhouse.* “Total Synthesis of (+)-Granatumine A and Related Bis lactone Limonoid Alkaloids via a Pyran to Pyridine Interconversion.” *J. Am. Chem. Soc.* **2019**, *141*, 919.

35. A. Turlik, Y. Chen, A. C. Scruse, and T. R. Newhouse.* “Convergent Total Synthesis of Principinol D, a Rearranged Kaurane Diterpenoid.” *J. Am. Chem. Soc.* **2019**, *141*, 8088.
34. J. E. Zweig, T. A. Ko, J. Huang, T. R. Newhouse.* “Effects of π -Extension on Pyrrole Hemithioindigo Photoswitches.” *Tetrahedron*. **2019**, *75*, 130466.
33. D. Huang, S. M. Szewczyk, P. Zhang, T. R. Newhouse.* “Allyl-Nickel Catalysis Enables Carbonyl Dehydrogenation and Oxidative Cycloalkenylation of Ketones” *J. Am. Chem. Soc.* **2019**, *141*, 5669.
32. D. E. Kim, J. E. Zweig, T. R. Newhouse.* “Total Synthesis of Paspaline A and Emindole PB Enabled by Computational Augmentation of a Transform-Guided Retrosynthetic Strategy” *J. Am. Chem. Soc.* **2019**, *141*, 1479.
31. M. Elkin, A. C. Scruse, A. Turlik, T. R. Newhouse.* “Computational and Synthetic Investigation of Cationic Rearrangement in the Putative Biosynthesis of Justicane Triterpenoids” *Angew. Chem. Int. Ed.* **2019**, *58*, 1025.
30. R. A. Coleman, C. S. Muli, Y. Zhao, A. Bhardwaj, T. R. Newhouse, D. J. Trader.* “Analysis of chain length, substitution patterns, and unsaturation of AM-404 derivatives as 20S proteasome stimulators” *Bioorganic Med. Chem. Lett.* **2019**, *29*, 420.
29. D. E. Kim, Y. Zhu, T. R. Newhouse.* “Vinylogous acyl triflates as an entry point to α,β -disubstituted cyclic enones via Suzuki–Miyaura cross-coupling.” *Org. Biomol. Chem.* **2019**, *17*, 1796.
28. M. Elkin, T. R. Newhouse.* “Computational chemistry strategies in natural product synthesis.” *Chem. Soc. Rev.* **2018**, *47*, 7830.
27. H.-J. Zhang, A. W. Schuppe, S.-T. Pan, J.-X. Chen, B.-R. Wang, T. R. Newhouse,* and L. Yin.* “Copper-Catalyzed Vinylogous Aerobic Oxidation of Unsaturated Compounds with Air.” *J. Am. Chem. Soc.* **2018**, *140*, 5300.
26. S. M. Szewczyk, Y. Zhao, H. Sakai, P. Dube, T. R. Newhouse.* “ α,β -Dehydrogenation of esters with free O-H and N-H functionalities via allyl-palladium catalysis.” *Tetrahedron*, **2018**, *74*, 3293.
25. A. W. Schuppe, D. Huang, Y. Chen, T. R. Newhouse.* “Total Synthesis of (–)-Xylogranatopyridine B via a Palladium-Catalyzed Oxidative Stannylation of Enones.” *J. Am. Chem. Soc.* **2018**, *140*, 2062.
24. D. Huang, Y. Zhao, T. R. Newhouse.* “Synthesis of Cyclic Enones by Allyl-Palladium-Catalyzed α,β -Dehydrogenation.” *Org. Lett.* **2018**, *20*, 684.
23. Y. Zhao, Y. Chen, T. R. Newhouse.* “Allyl-Palladium Catalyzed α,β -Dehydrogenation of Carboxylic Acids via Enediolates” *Angew. Chem. Int. Ed.* **2017**, *56*, 13132.
22. J. Zweig, T. R. Newhouse.* “Isomer-Specific Hydrogen Bonding as a Design Principle for Bidirectionally Quantitative and Redshifted Hemithioindigo Photoswitches” *J. Am. Chem. Soc.* **2017**, *139*, 10956.

21. G. Xu, M. Elkin, D. J. Tantillo, T. R. Newhouse,* T. J. Maimone.* “Traversing Biosynthetic Carbocation Landscapes in the Total Synthesis of Andrastin and Terretonin Meroterpenes.” *Angew. Chem. Int. Ed.* **2017**, *56*, 12498.
20. Y. Chen, D. Huang, Y. Zhao, T. R. Newhouse.* “Allyl-Palladium Catalyzed Ketone Dehydrogenation Enables Telescoping with Enone α,β -Vicinal Difunctionalization” *Angew. Chem. Int. Ed.* **2017**, *56*, 8258.
19. J. Zweig, D. Kim, T. R. Newhouse.* “Methods Utilizing First-Row Transition Metals in Natural Product Total Synthesis.” *Chem. Rev.* **2017**, *117*, 11680.
18. A. W. Schuppe, J. M. Cabrera, C. L. McGeoch, T. R. Newhouse.* “Scalable synthesis of enamines utilizing Gold's reagents.” *Tetrahedron*, **2017**, *73*, 3643.
17. M. Elkin, S. M. Szewczyk, A. C. Scruse, T. R. Newhouse.* “Total Synthesis of Berkeleyone A.” *J. Am. Chem. Soc.* **2017**, *139*, 1790.
16. A. W. Schuppe, T. R. Newhouse.* “Assembly of the Limonoid Architecture by a Divergent Approach: Total Synthesis of Andriolide N via 8α -hydroxycarapin.” *J. Am. Chem. Soc.* **2017**, *139*, 631.
15. D. Huang, A. W. Schuppe, M. Z. Liang, T. R. Newhouse.* “Scalable procedure for the fragmentation of hydroperoxides mediated by copper and iron tetrafluoroborate salts.” *Org. Biomol. Chem.* **2016**, *14*, 6197.
14. Y. Chen, A. Turlik, T. R. Newhouse.* “Amide α,β -Dehydrogenation Using Allyl-Palladium Catalysis and a Hindered Monodentate Anilide.” *J. Am. Chem. Soc.* **2016**, *138*, 1166.
13. A. Turlik, Y. Chen, T. R. Newhouse.* “Dehydrogenation Adjacent to Carbonyls Using Pd-Allyl Intermediates.” *Synlett*, **2016**, *27*, 331.
12. Y. Chen, J. P. Romaine, T. R. Newhouse.* “Palladium-Catalyzed α,β -Dehydrogenation of Esters and Nitriles.” *J. Am. Chem. Soc.* **2015**, *137*, 5875.
11. R. I. Goldstein, R. Guo, C. Hughes, D. P. Maurer, T. R. Newhouse, T. J. Sisto, R. R. Conry, S. L. Price, D. M. Thamattoor.* “Concomitant Conformational Dimorphism in 1,2-Bis(9-anthryl)acetylene” *CrystEngComm* **2015**, *17*, 4877.
10. T. R. Newhouse, P. Kaib, A. Gross, E. J. Corey.* “Versatile Approaches for the Synthesis of Chiral Fused-Ring γ -Lactones Utilizing Cyclopropane Intermediates.” *Org. Lett.* **2013**, *15*, 1591.
9. L. Zou, R. S. Paton,* A. Eschenmoser, T. R. Newhouse, P. S. Baran, K. N. Houk.* “Enhanced Reactivity in Dioxirane C-H Oxidations via Strain Release.” *J. Org. Chem.* **2013**, *78*, 4037.
8. T. R. Newhouse, X. Li, M. M. Blewett, C. M. C. Whitehead, E. J. Corey.* “A Tetradentate Ligand for the Enantioselective Ti(IV)-Promoted Oxidation of Sulfides to Sulfoxides: Origin of Enantioselectivity.” *J. Am. Chem. Soc.* **2012**, *134*, 17354.

7. T. Newhouse, P. S. Baran.* “If C-H Bonds Could Talk: Selective C-H Bond Oxidation.” *Angew. Chem. Int. Ed.* **2011**, *50*, 3362.
6. K. Foo, T. Newhouse, H. Takayama, P. S. Baran.* “Total Synthesis – Guided Structure Elucidation of (+)-Psychotetramine.” *Angew. Chem. Int. Ed.* **2011**, *50*, 2716.
5. T. Newhouse, C. A. Lewis, K. J. Eastman, P. S. Baran.* “Scalable Total Syntheses of *N*-Linked Tryptamine Dimers by Direct Indole-Aniline Coupling: Psychotrimine and Kapakahines B and F.” *J. Am. Chem. Soc.* **2010**, *132*, 7119.
4. M. A. Schallenberger, T. Newhouse, P. S. Baran, F. E. Romesberg.* “The Psychotrimine Natural Products Have Antibacterial Activity Against Gram-Positive Bacteria and Act Via Membrane Disruption.” *J. Antibiot.* **2010**, *63*, 685.
3. T. Newhouse, P. S. Baran,* R. W. Hoffmann.* “The Economies of Synthesis.” *Chem. Soc. Rev.* **2009**, *38*, 3010.
2. T. Newhouse, C. A. Lewis, P. S. Baran.* “Enantiospecific Total Syntheses of Kapakahines B and F.” *J. Am. Chem. Soc.* **2009**, *131*, 6360.
1. T. Newhouse, P. S. Baran.* “Total Synthesis of (±)-Psychotrimine.” *J. Am. Chem. Soc.* **2008**, *130*, 10886.

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