

## 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

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

Assistant Professor of Chemistry, Member Interdepartmental Neuroscience Program  
Yale University, New Haven, CT, 2013-2018

## 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

2018	Amgen Young Investigator Award
2018	Dylan Hixon '88 Prize for Teaching Excellence
2017	ACS Academic Young Investigator
2017	Sloan Research Fellowship
2017	NSF CAREER
2015	Rosenkranz Award
2015	Thieme Chemistry Journal Award
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

**Awards and Honors (cont.)**

2003	Bradford P. Mundy Organic Chemistry Award
2003	Merck/AAAS Undergraduate Research Scholar

**Publications**

1. Daria E. Kim, Joshua E. Zweig, Timothy 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**, *Articles ASAP*. DOI: 10.1021/jacs.8b13127.
2. M. Elkin<sup>†</sup>, A. C. Scruse<sup>†</sup>, A. Turlik, T. R. Newhouse.\* “Computational and Synthetic Investigation of Cationic Rearrangement in the Putative Biosynthesis of Justicane Triterpenoids” *Angew. Chem. Int. Ed.* **2019**, *Accepted Article*. DOI: 10.1002/anie.201810566.
3. R. A. Coleman, C. S. Muli, Y. Zhao, A. Bhardwaj, T. R. Newhouse, Darci J. Trader. “Analysis of chain length, substitution patterns, and unsaturation of AM-404 derivatives as 20S proteasome stimulators” *Bioorganic Med. Chem. Lett.* **2019**, DOI:10.1016/j.bmcl.2018.12.030 [In Press]
4. D. E. Kim, Y. Zhu, T. R. Newhouse.\* “Vinylogous acyl triflates as an entry point to  $\alpha,\beta$ -disubstituted cyclic enones via Suzuki–Miyaura cross-coupling” *Org. Biomol. Chem.* **2019**, DOI: 10.1039/c8ob02573h.
5. M. Elkin, T. R. Newhouse.\* “Computational chemistry strategies in natural product synthesis” *Chem. Soc. Rev.* **2018**, *47*, 7830.
6. 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.
7. S. M. Szewczyk, Y. Zhao, H. Sakai, P. Dube, T. R. Newhouse.\* “ $\alpha,\beta$ -Dehydrogenation of esters with free O-H and N-H functionalities via allyl-palladium catalysis” *Tetrahedron*, **2018**, *74*, 3293.
8. 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.
9. D. Huang, Y. Zhao, T. R. Newhouse.\* “Synthesis of Cyclic Enones by Allyl-Palladium-Catalyzed  $\alpha,\beta$ -Dehydrogenation.” *Org. Lett.*, **2018**, *20*, 684.
10. Y. Zhao, Y. Chen, T. R. Newhouse.\* “Allyl-Palladium Catalyzed  $\alpha,\beta$ -Dehydrogenation of Carboxylic Acids via Enediolates” *Angew. Chem. Int. Ed.* **2017**, *56*, 13132.
11. 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.

12. 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.
13. Y. Chen, D. Huang,<sup>†</sup> Y. Zhao,<sup>†</sup> T. R. Newhouse.\* “Allyl-Palladium Catalyzed Ketone Dehydrogenation Enables Telescoping with Enone  $\alpha,\beta$ -Vicinal Difunctionalization” *Angew. Chem. Int. Ed.* **2017**, *56*, 8258.
14. J. Zweig, D. Kim, T. R. Newhouse.\* “Methods Utilizing First-Row Transition Metals in Natural Product Total Synthesis.” *Chem. Rev.* **2017**, *117*, 11680.
15. A. W. Schuppe, J. M. Cabrera, C. L. McGeoch, T. R. Newhouse.\* “Scalable synthesis of enamines utilizing Gold's reagents.” *Tetrahedron* **2017**, *73*, 3643.
16. M. Elkin, S. M. Szewczyk, A. C. Scruse, T. R. Newhouse.\* “Total Synthesis of Berkeleyone A.” *J. Am. Chem. Soc.* **2017**, *139*, 1790.
17. A. W. Schuppe, T. R. Newhouse.\* “Assembly of the Limonoid Architecture by a Divergent Approach: Total Synthesis of Andriolide N via 8 $\alpha$ -hydroxycarapin.” *J. Am. Chem. Soc.* **2017**, *139*, 631.
18. 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.
19. Y. Chen, A. Turlik, T. R. Newhouse.\* “Amide  $\alpha,\beta$ -Dehydrogenation Using Allyl-Palladium Catalysis and a Hindered Monodentate Anilide.” *J. Am. Chem. Soc.* **2016**, *138*, 1166.
20. A. Turlik, Y. Chen, T. R. Newhouse.\* “Dehydrogenation Adjacent to Carbonyls Using Pd-Allyl Intermediates.” *Synlett* **2016**, *27*, 331.
21. Y. Chen, J. P. Romaine, T. R. Newhouse.\* “Palladium-Catalyzed  $\alpha,\beta$ -Dehydrogenation of Esters and Nitriles.” *J. Am. Chem. Soc.* **2015**, *137*, 5875.
22. 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.
23. T. R. Newhouse, P. Kaib, A. Gross, E. J. Corey.\* “Versatile Approaches for the Synthesis of Chiral Fused-Ring  $\gamma$ -Lactones Utilizing Cyclopropane Intermediates.” *Org. Lett.* **2013**, *15*, 1591.
24. 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.

25. 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.
26. T. Newhouse, P. S. Baran.\* “If C-H Bonds Could Talk: Selective C-H Bond Oxidation.” *Angew. Chem. Int. Ed.* **2011**, *50*, 3362.
27. K. Foo, T. Newhouse, H. Takayama, P. S. Baran.\* “Total Synthesis – Guided Structure Elucidation of (+)-Psychotetramine.” *Angew. Chem. Int. Ed.* **2011**, *50*, 2716.
28. 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.
29. 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.
30. T. Newhouse, P. S. Baran,\* R. W. Hoffmann.\* “The Economies of Synthesis.” *Chem. Soc. Rev.* **2009**, *38*, 3010.
31. T. Newhouse, C. A. Lewis, P. S. Baran.\* “Enantiospecific Total Syntheses of Kapakahines B and F.” *J. Am. Chem. Soc.* **2009**, *131*, 6360.
32. T. Newhouse, P. S. Baran.\* “Total Synthesis of (±)-Psychotrimine.” *J. Am. Chem. Soc.* **2008**, *130*, 10886.

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