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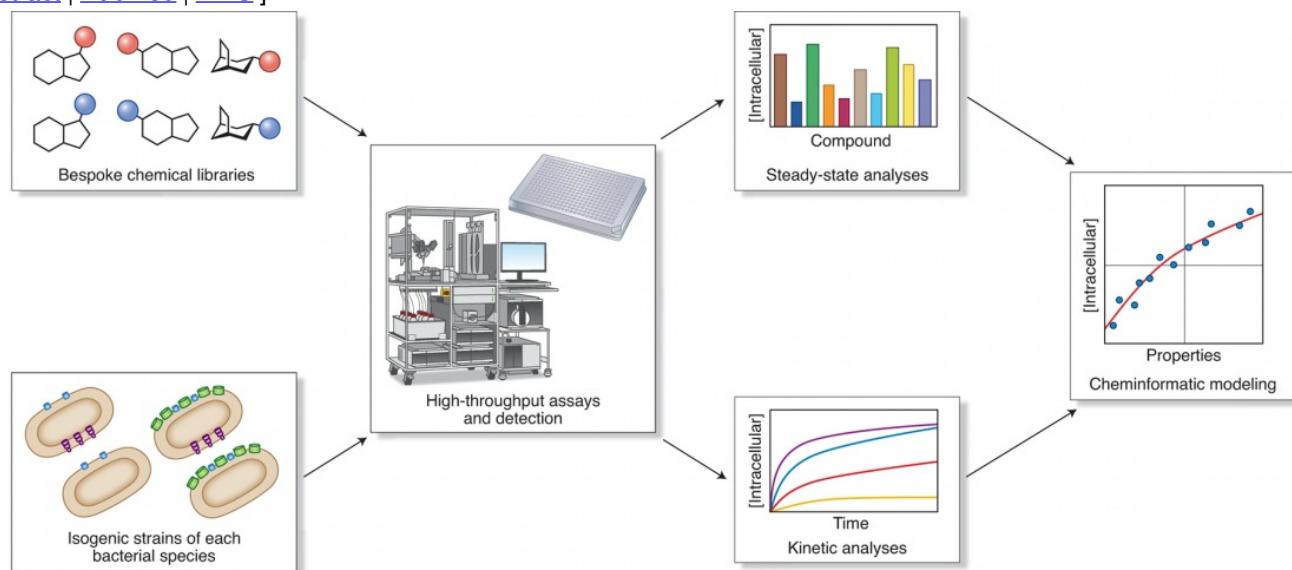
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## Tan Lab Publications

60. Defining new chemical space for drug penetration into Gram-negative bacteria.

Zhao, S.; Adamiak, J. W.; Bonifay, V.; Mehla, J.; Zgurskaya, H. I.; Tan, D. S.\* *Nat Chem Biol* 2020, **16**, 1293–1302.

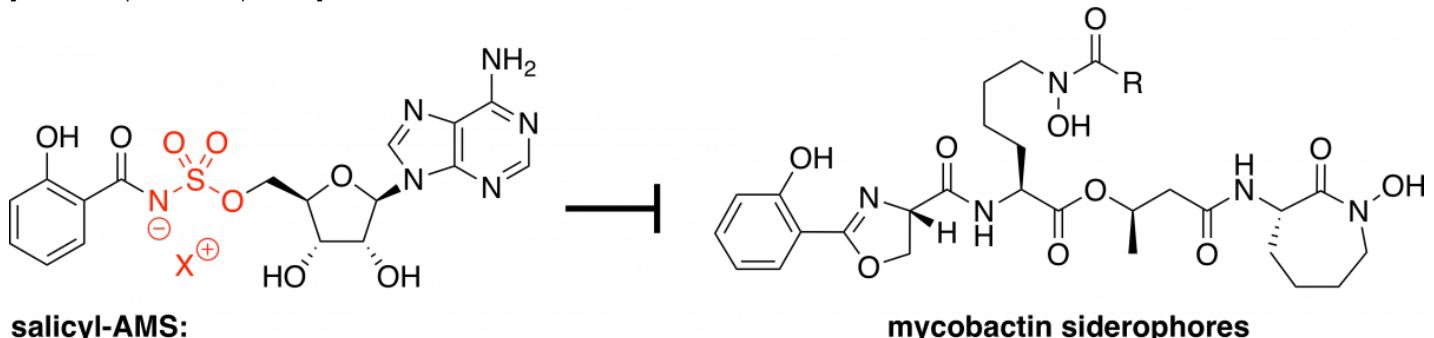
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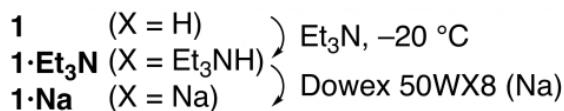
59. Gram-scale preparation of the antibiotic lead compound salicyl-AMS, a potent inhibitor of bacterial salicylate adenyltransferases.

Kinarivala, N; Standke, L. C; Guney, T.; Cheng, J.; Naoyoshi, N.; Yasutomi, A.; Tan, D. S.\* *Method Enzymol.* 2020, 638, 69–87.

[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



**salicyl-AMS:**

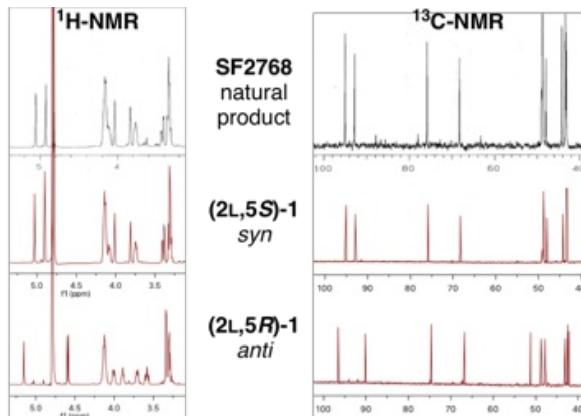
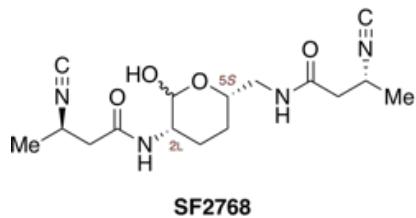


**mycobactin siderophores**

58. Total synthesis of the bacterial diisonitrile chalkophore SF2768.

Xu, Y.; Tan, D. S.\* *Org. Lett.* 2019, 21, 8731–8735.

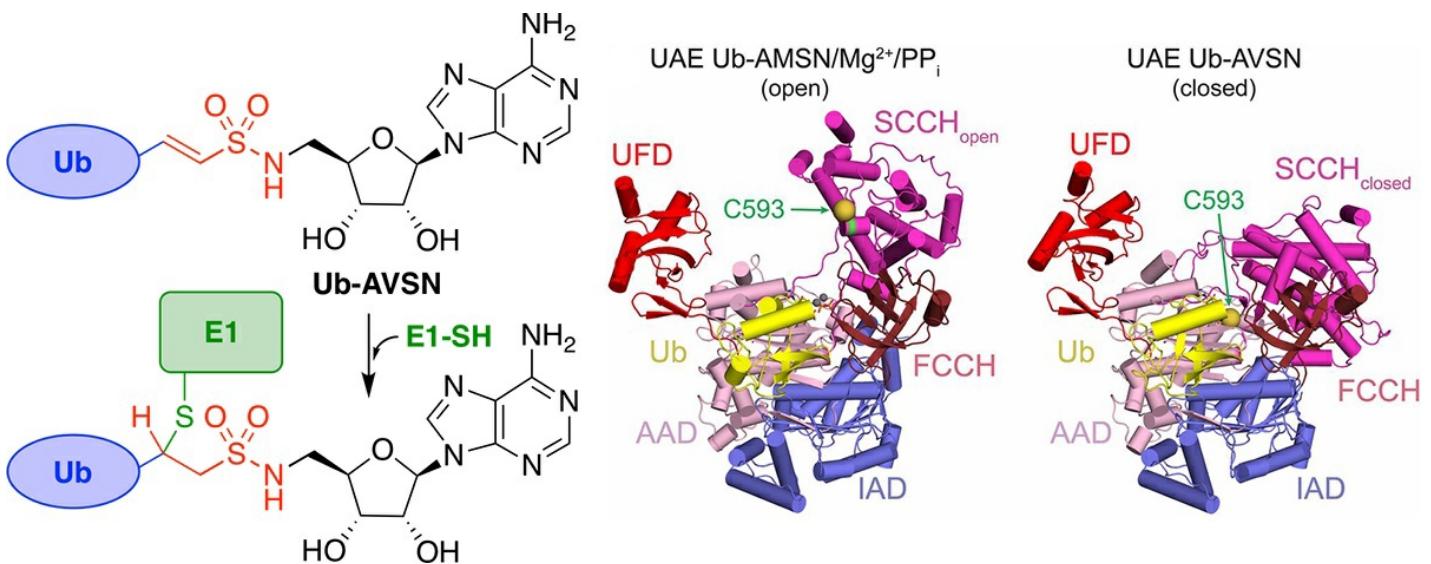
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



57. Structural basis for adenylation and thioester bond formation in the ubiquitin E1.

Hann, Z. S.; Ji, C.; Olsen, S. K.; Lu, X.; Lux, M. C.; Tan, D. S.\*; Lima, C. D.\* *Proc. Natl. Acad. Sci. U.S.A.* 2019, 15475–15484.

[ [Abstract](#) | [PubMed](#) | [PMC](#) ]

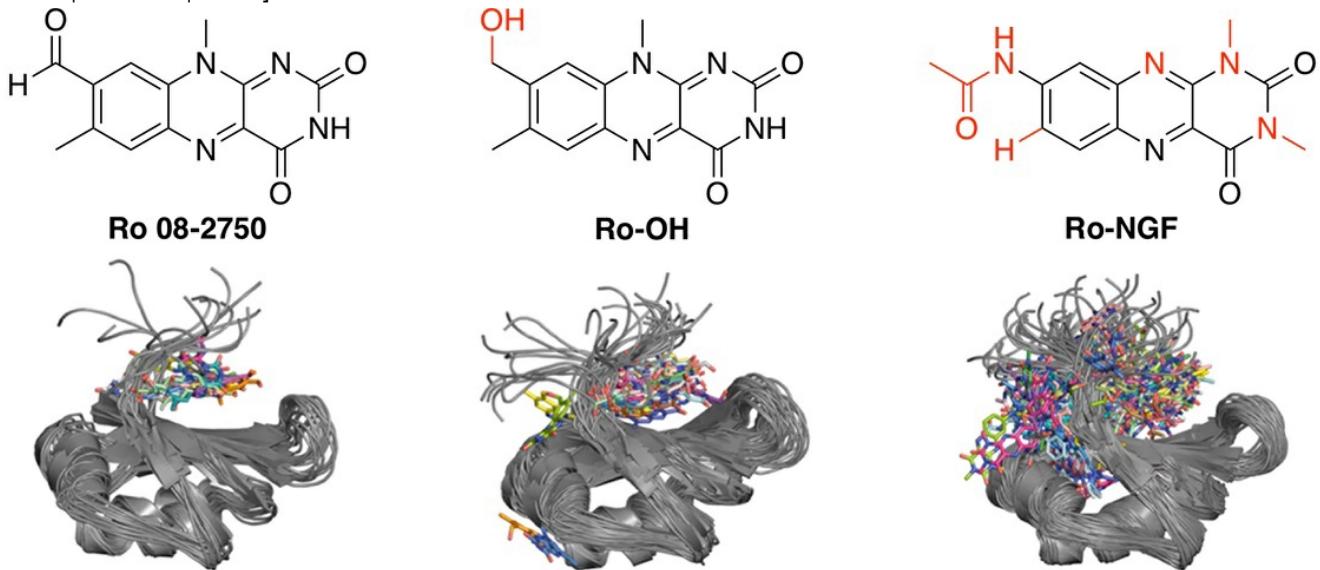


(Highlighted in [Proc. Natl. Acad. Sci. USA](#) )

56. Small-molecule targeting of MUSASHI RNA-binding activity in acute myeloid leukemia.

Minuesa, G.; Albanese, S. K.; Xie, W.; Kazansky, Y.; Worroll, D.; Chow, A.; Schurer, A.; Park, S. M.; Rotsides, C. Z.; Taggart, J.; Rizzi, A.; Naden, L. N.; Chou, T.; Gourkanti, S.; Cappel, D.; Passarelli, M. C.; Fairchild, L.; Adura, C.; Glickman, J. F.; Schulman, J.; Famulare, C.; Patel, M.; Eibl, J. K.; Ross, G. M.; Bhattacharya, S.; Tan, D. S.; Leslie, C. S.; Beuming, T.; Patel, D. J.; Goldgur, Y.; Chodera, J. D.; Kharas, M. G.\* *Nat Commun* 2019, **10**, 2691.

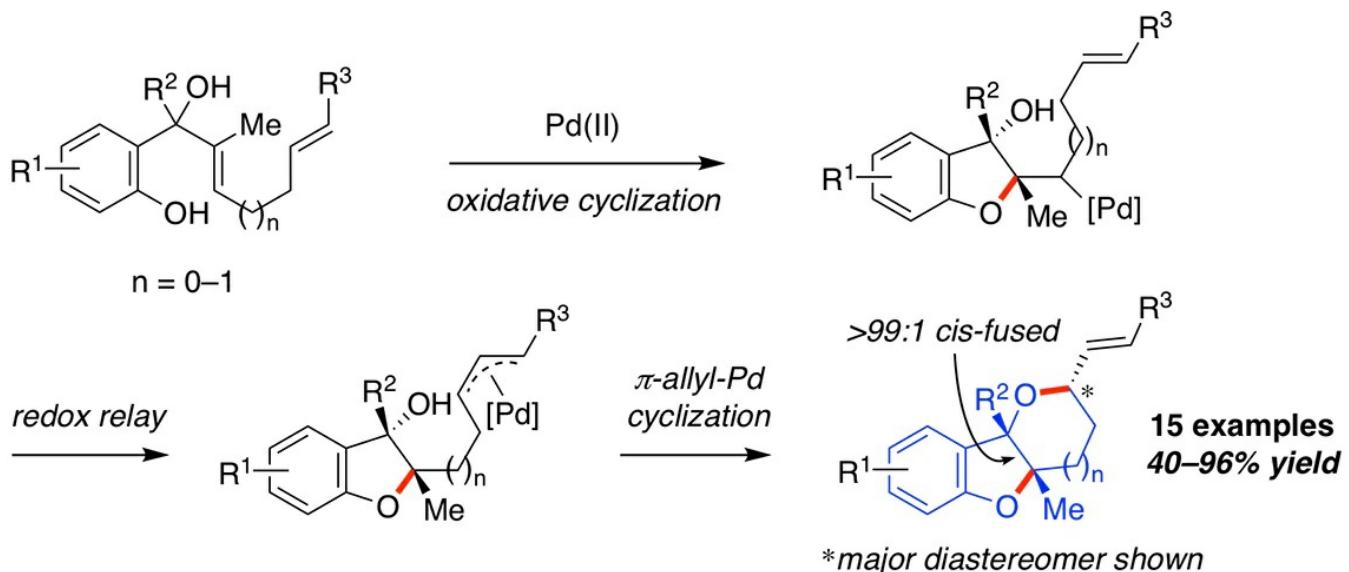
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



55. Synthesis of bicyclic ethers by a palladium-catalyzed oxidative cyclization-redox relay- $\pi$ -allyl-Pd cyclization cascade reaction.

Lux, M. C.; Boby, M. L.; Brooks, J. L.; Tan, D. S.\* *Chem. Commun.* 2019, **55**, 7013–7016.

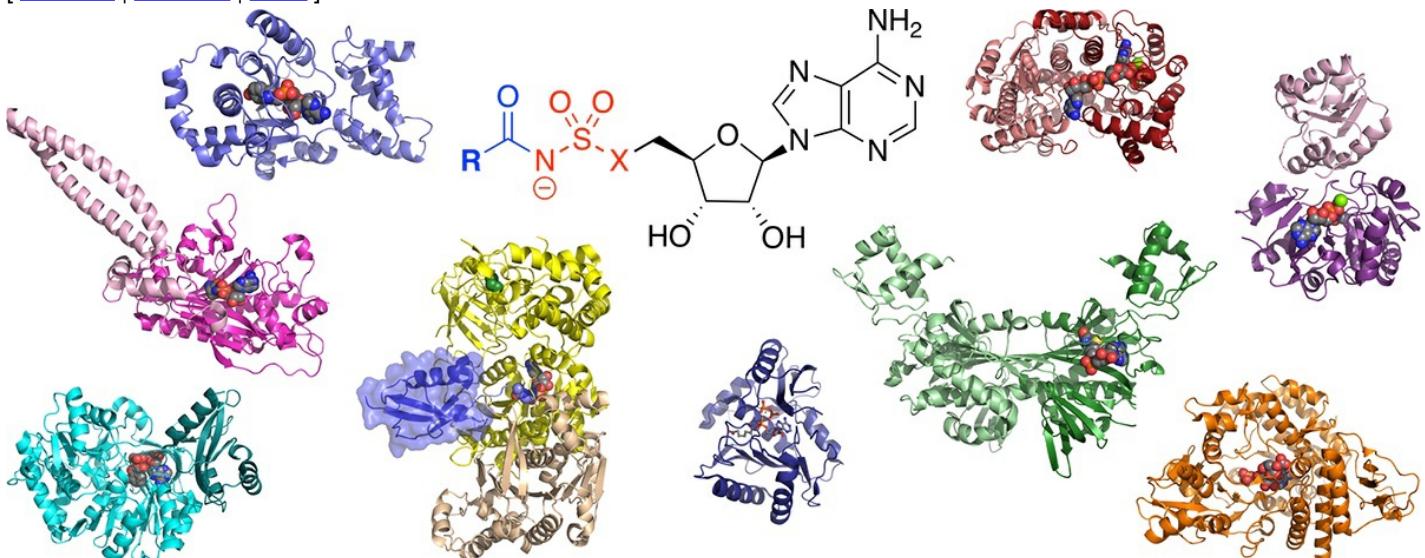
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



54. Targeting adenylate-forming enzymes with designed sulfonyladenosine inhibitors.

Lux, M. C.; Standke, L. C.; Tan, D. S.\* *J. Antibiot.* 2019, 72, 325–349.

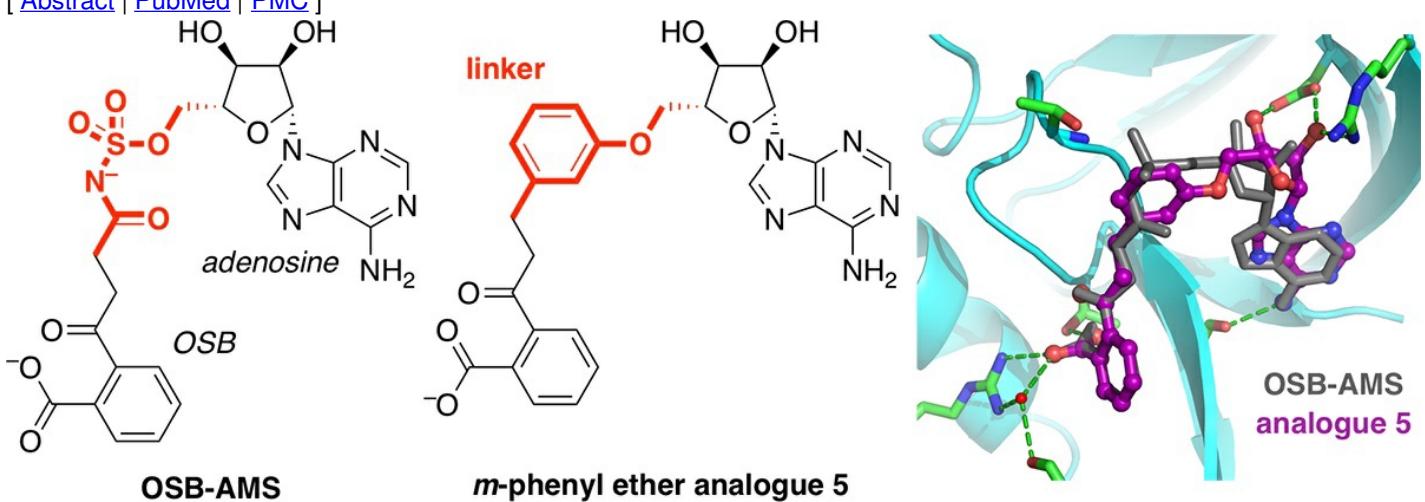
[ Abstract | PubMed | PMC ]



53. Structure-based design, synthesis, and biological evaluation of non-acyl sulfamate inhibitors of the adenylate-forming enzyme MenE.

Evans, C. E.; Si, Y.; Matarlo, J. S.; Yin, Y.; French, J. B.; Tonge, P. J.\*; Tan, D. S.\* *Biochemistry* 2019, 58, 1918–1930.

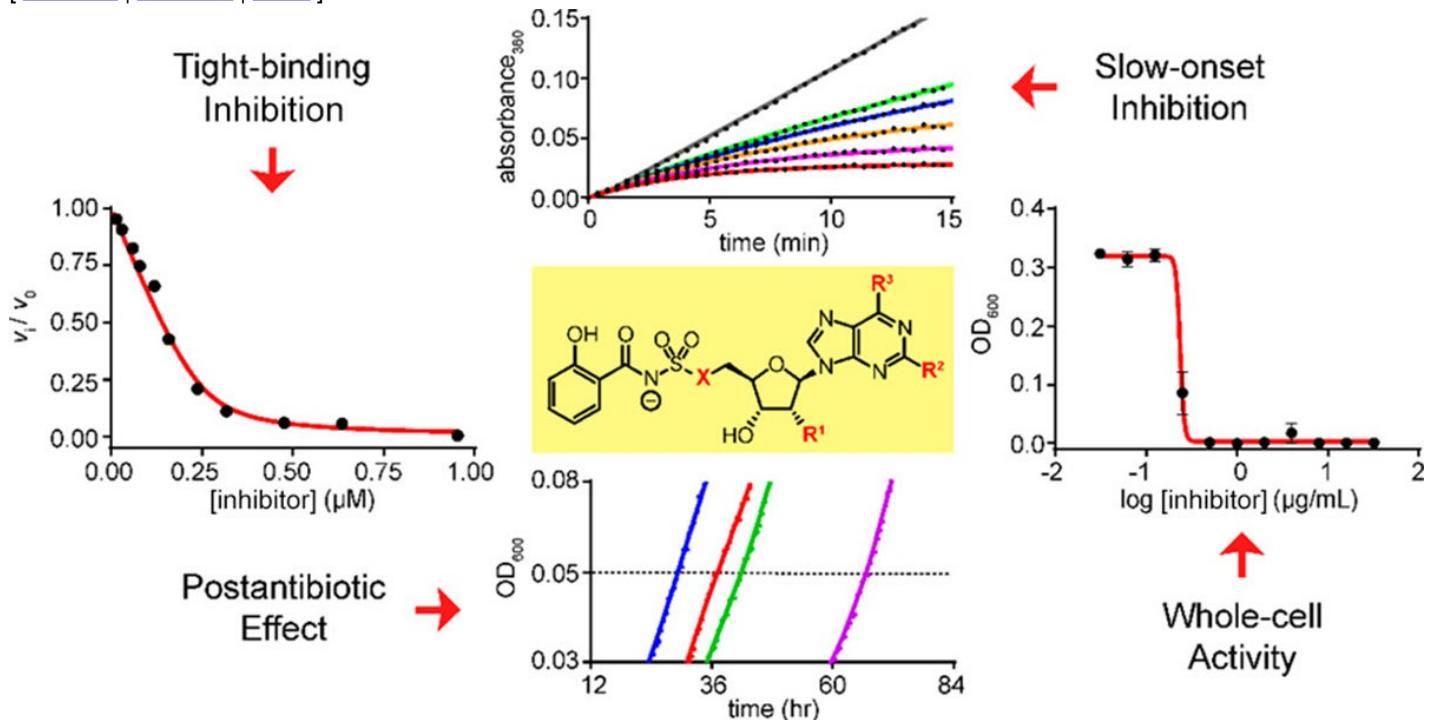
[ Abstract | PubMed | PMC ]



52. Kinetic analyses of the siderophore biosynthesis inhibitor salicyl-AMS and analogues as MbtA inhibitors and antimycobacterial agents.

Bythrow, G. V.; Mohandas, P.; Guney, T.; Standke, L. C.; Germain, G. A.; Lu, X.; Ji, C.; Levendosky, K.; Chavadi, S. S.; Tan, D. S.\*; Quadri, L. E. N.\* *Biochemistry* 2018, 883–847.

[ Abstract | PubMed | PMC ]

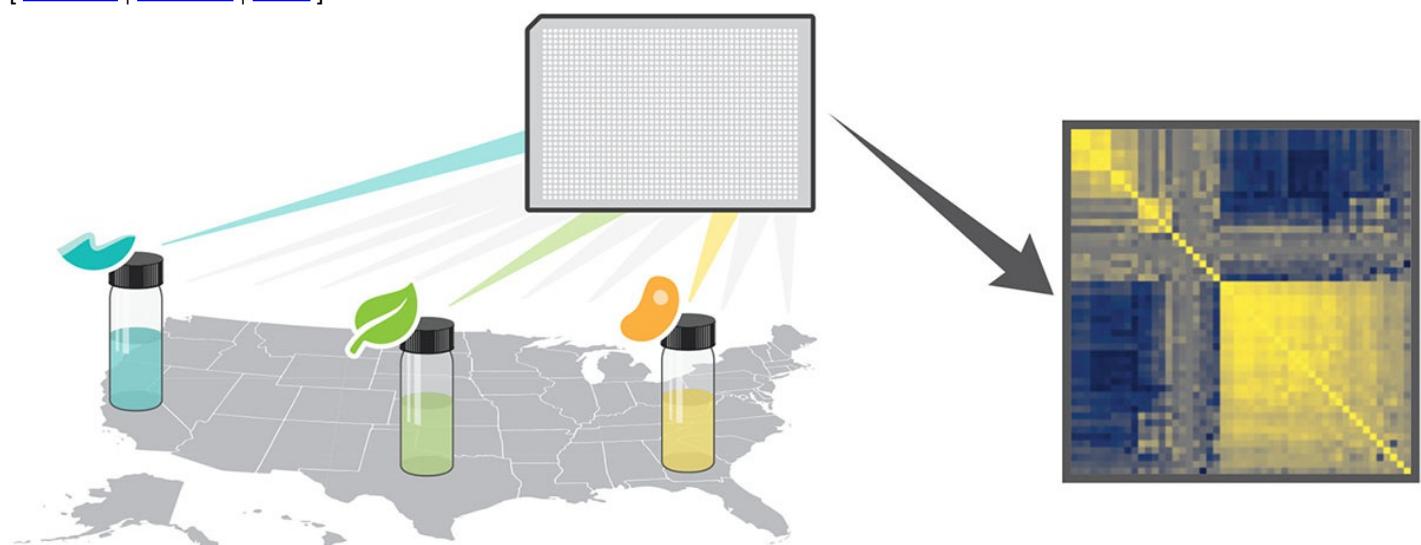


51.

Canvass: A crowd-sourced, natural-product screening library for exploring biological space.

Kearney, S. E. et al. Verano, A. L.; Tan, D. S.; Rohde, J. M.\* *ACS. Cent. Sci.* 2018, 4, 1727–1741.

[ Abstract | PubMed | PMC ]

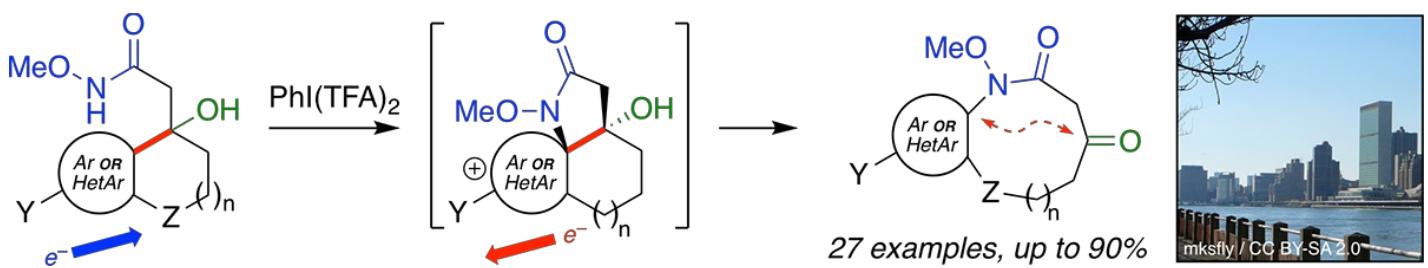


50. Synthesis of Benzannulated Medium-ring Lactams via a Tandem Oxidative Dearomatization-Ring Expansion Reaction.

Guney, T. †; Wenderski, T. A. †; Boudreau, M. W.; Tan, D. S.\* *Chem. Eur. J.* 2018, in press.

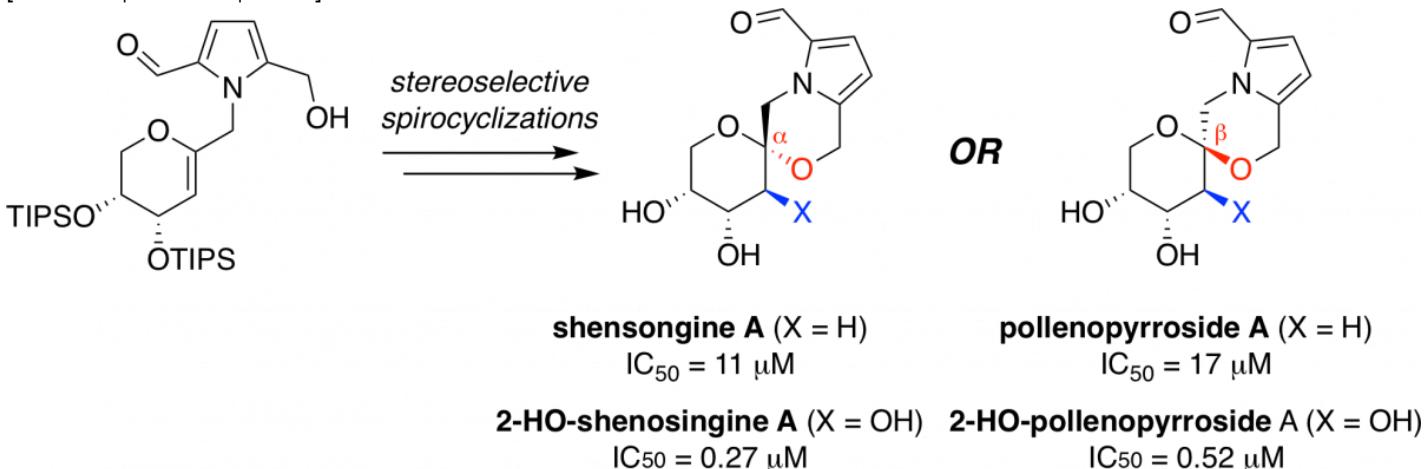
[ Abstract | PubMed ]

(Cover article in *Chem. Eur. J.*)



49. Family-level stereoselective synthesis and biological evaluation of pyrrolomorpholine spiroketal natural product antioxidants  
Verano, A. L.; Tan, D. S.\* *Chem. Sci.* 2017, 8, 3687–3693.

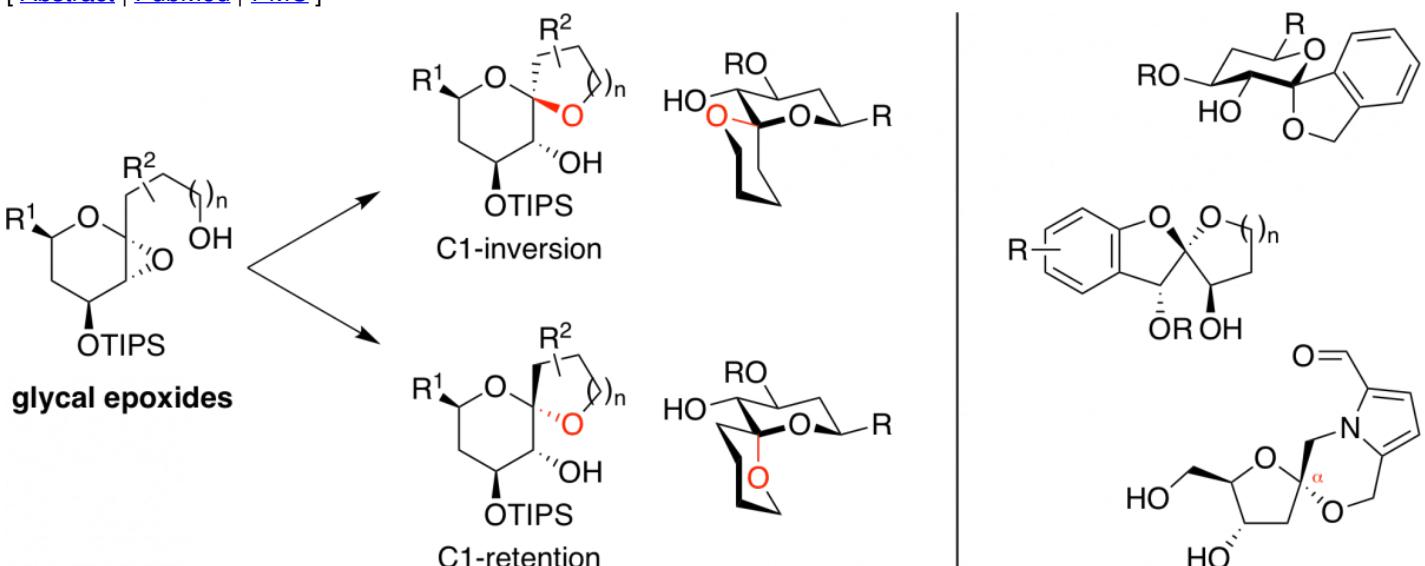
[ Abstract | PubMed | PMC ]



48. Stereocontrolled Synthesis of Spiroketsals: An Engine for Chemical and Biological Discovery

Verano, A. L.; Tan, D. S.\* *Isr. J. Chem.* 2017, 57, 279–291.

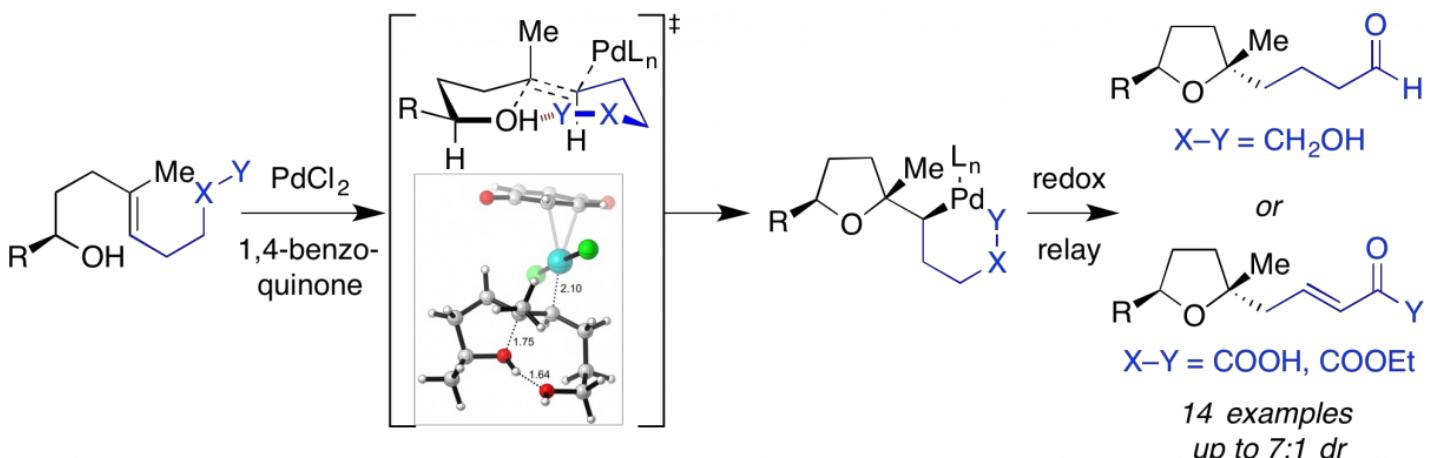
[ Abstract | PubMed | PMC ]



47. Diastereoselective synthesis of highly substituted tetrahydrofurans by Pd-catalyzed tandem oxidative cyclization-redox relay reactions controlled by intramolecular hydrogen bonding.

Brooks, J. L.; Xu, L.; Wiest, O.; Tan, D. S.\* *J. Org. Chem.* 2017, 82, 57–75.

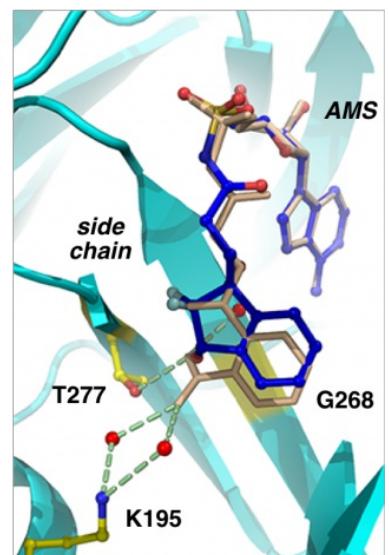
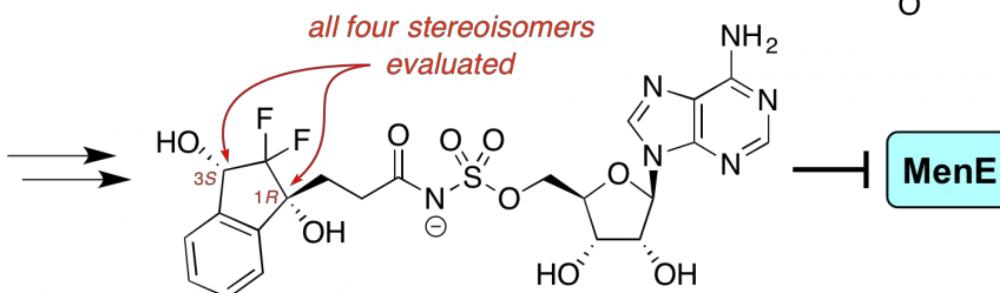
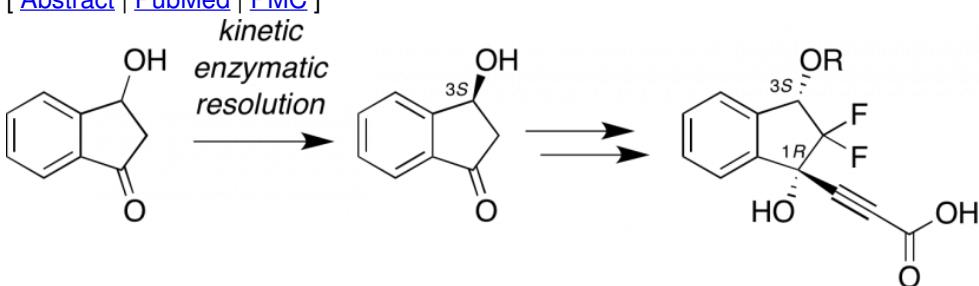
[ Abstract | PubMed | PMC ]



46. Stereoselective synthesis, docking, and biological evaluation of difluoroindanediol-based MenE inhibitors as antibiotics.

Evans, C. E.; Matarlo, J. S.; Tonge, P. J.\*; Tan, D. S.\* *Org. Lett.* 2016, **18**, 6384–6387.

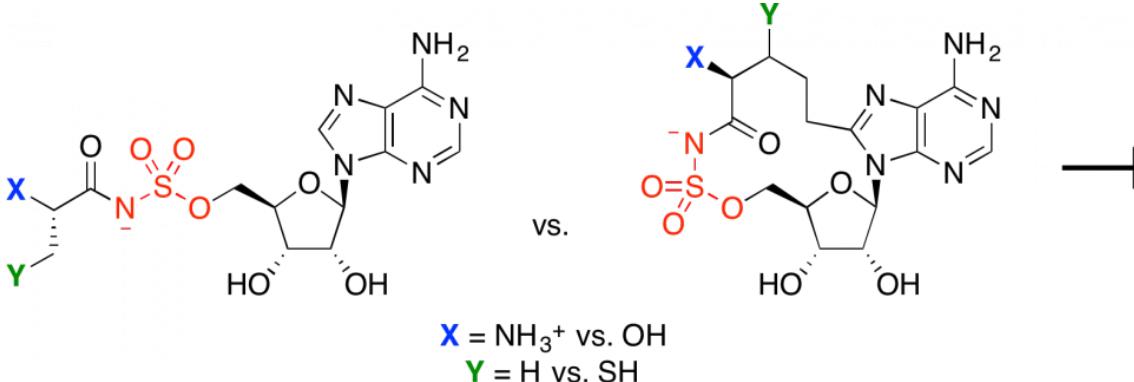
[ Abstract | PubMed | PMC ]



45. Design, synthesis, and biological evaluation of  $\alpha$ -hydroxyacyl-AMS inhibitors of amino acid adenylation enzymes.

Davis, T. D.\*; Mohandas, P. \*; Chiriac, M. I.; Bythrow, G. V.; Quadri, L. E. N.\*; Tan, D. S.\* *Bioorg. Med. Chem. Lett.* 2016, **21**, 5340–5345.

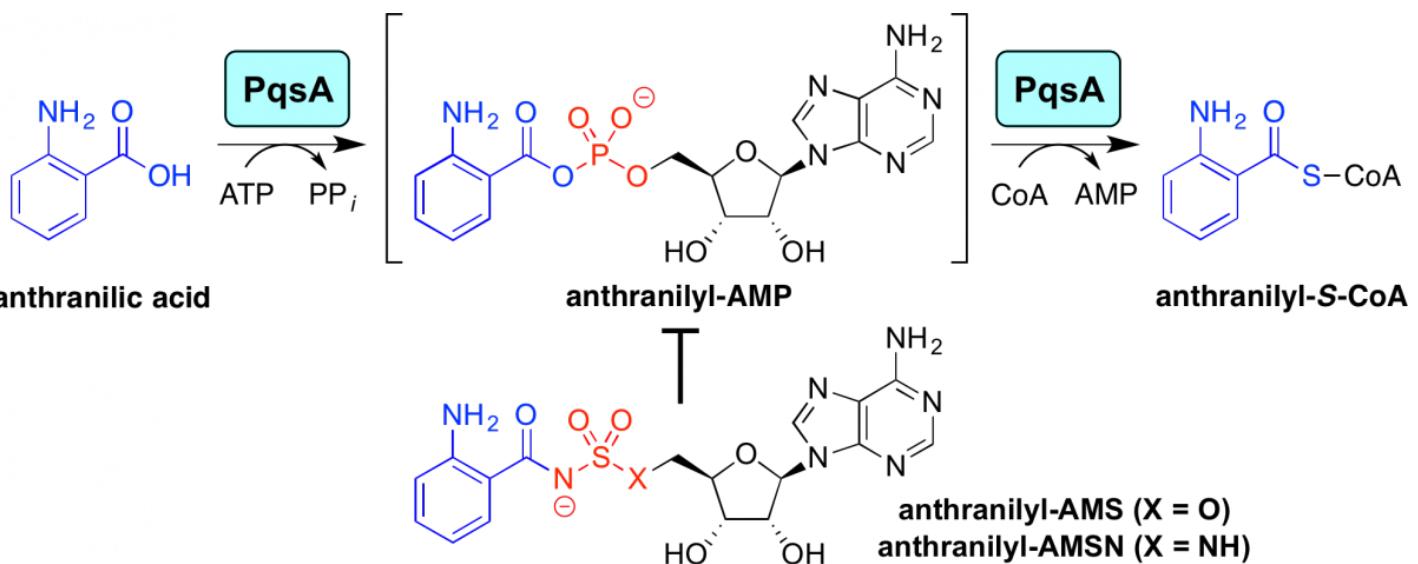
[ Abstract | PubMed | PMC ]



44. Designed small-molecule inhibitors of the anthranilyl-CoA synthetase PqsA block quinolone biosynthesis in *Pseudomonas aeruginosa*.

Ji, C.; Sharma, I.; Pratihar, I.; Hudson, L.; Maura, D.; Guney, T.; Rahme, L. G.; Pesci, E. C.; Coleman, J. P.; Tan, D. S.\* *ACS Chem. Biol.* 2016, **11**, 3061–3067.

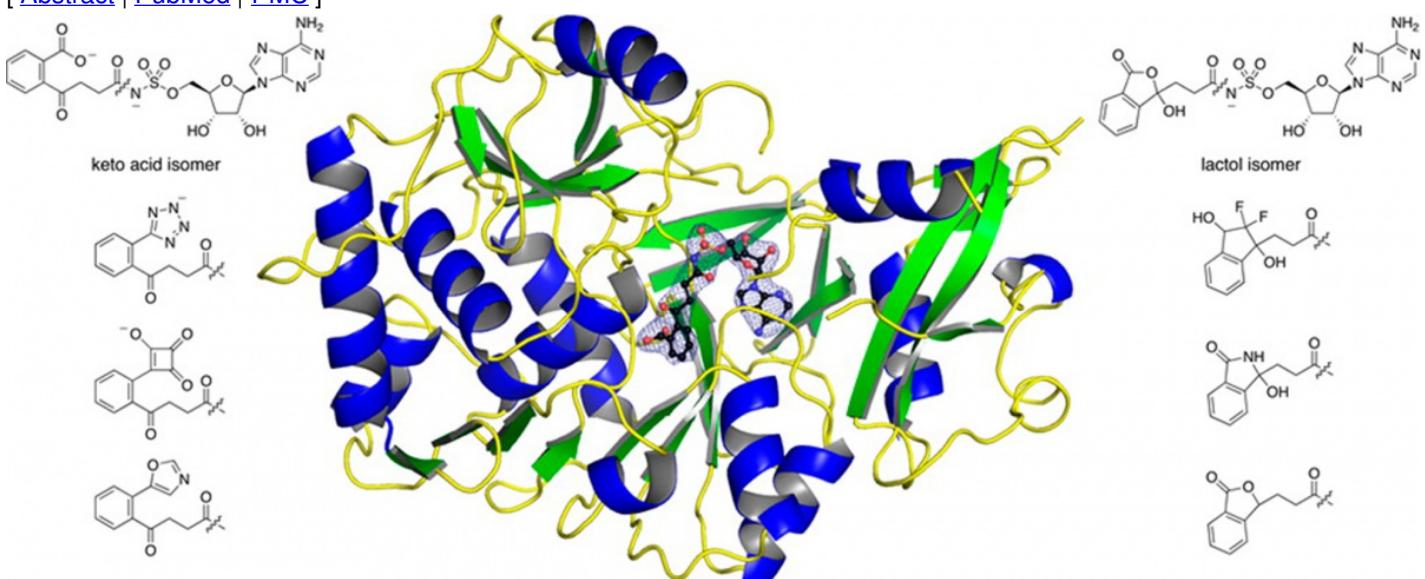
[ Abstract | PubMed | PMC ]



43. Mechanism of MenE inhibition by acyl-adenylate analogues and discovery of novel antibacterial agents.

Matarlo, J. S.<sup>†</sup>; Evans, C. E.<sup>†</sup>; Sharma, I.; Lavaud, L. J.; Ngo, S. C.; Shek, R.; Rajashankar, K. R.; French, J. B.; Tan, D. S.\*; Tonge, P. J.\* *Biochemistry* 2015, 54, 6514–6524.

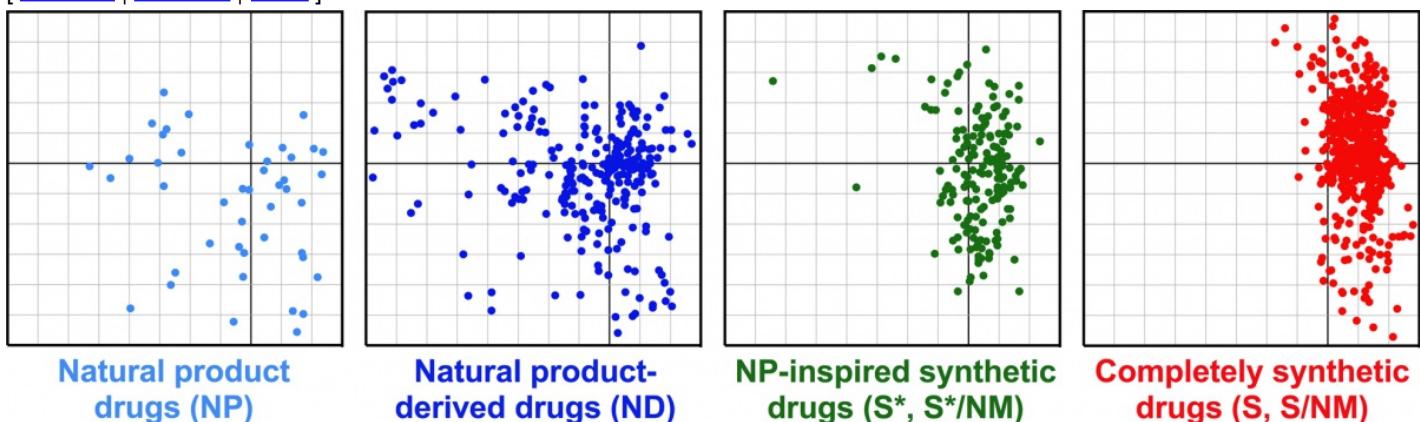
[ Abstract | PubMed | PMC ]



42. Cheminformatic comparison of approved drugs from natural product versus synthetic origins.

Stratton, C. F.; Newman, D. J.; Tan, D. S.\* *Bioorg. Med. Chem. Lett.* 2015, 25, 4802–4807.

[ Abstract | PubMed | PMC ]

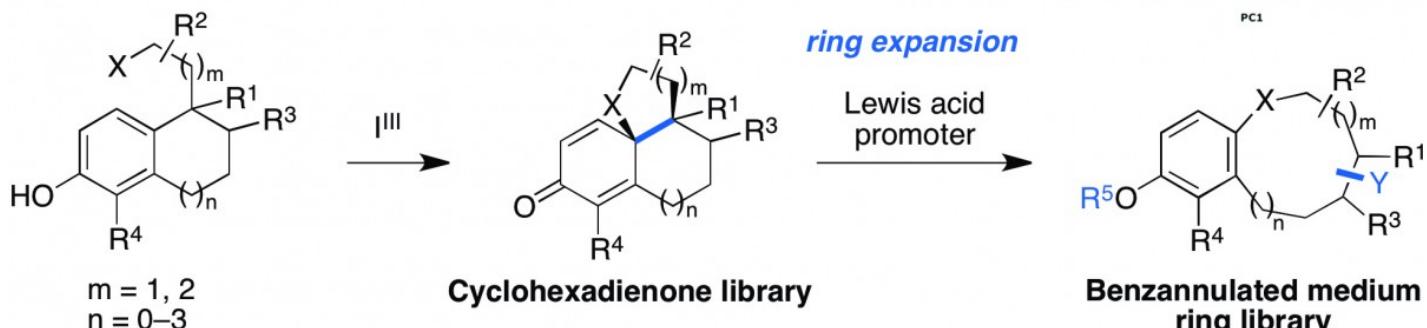
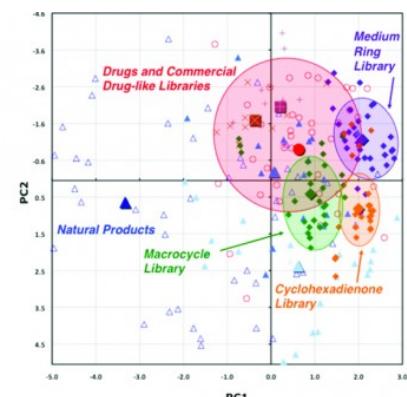


41. Principal component analysis as a tool for library design: A case study investigating natural products, brand-name drugs,

natural product-like libraries, and drug-like libraries.

Wenderski, T. A.; Stratton, C. F.; Bauer, R. A.; Kopp, F.; Tan, D. S.\* *Methods Mol. Biol.* 2015, 1263, 225–242.

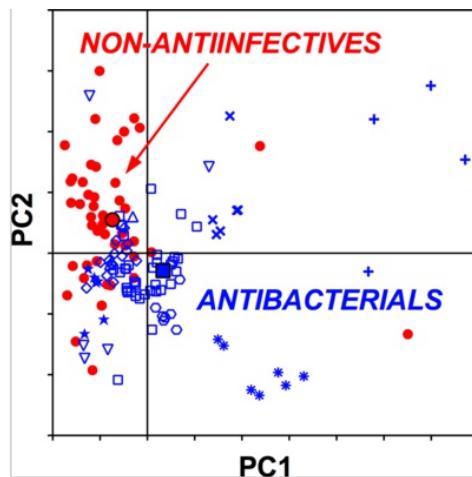
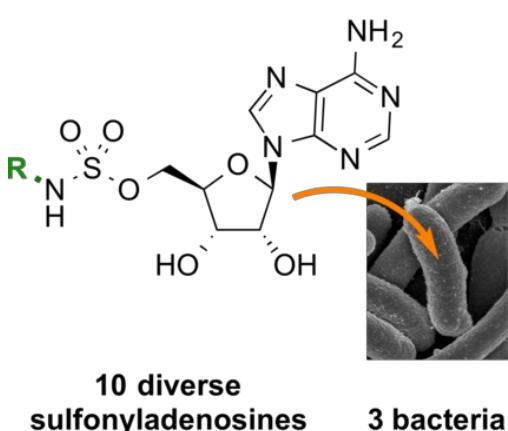
[ Abstract | PubMed | PMC ]



40. General platform for systematic quantitative evaluation of small-molecule permeability in bacteria.

Davis, T. D.; Gerry, C. J.; Tan, D. S.\* *ACS Chem. Biol.* 2014, 9, 2535–2544.

[ Abstract | PubMed | PMC ]



	Parameter	<i>E. coli</i>	<i>B. subtilis</i>	<i>M. smegmatis</i>
Size & Hydrogen Bonding	MW	0.46	0.55	0.16
	SA	0.52	<b>0.78</b>	0.01
	N	-0.38	-0.34	-0.12
	O	-0.26	0.01	-0.32
	HBD	-0.33	-0.04	0.19
Hydrophobicity & Polarity	HBA	-0.36	-0.05	-0.30
	LogD	<b>0.70</b>	0.52	0.60
	LogP	<b>0.71</b>	<b>0.67</b>	0.48
	ALogPs	<b>0.84</b>	<b>0.83</b>	0.35
	tPSA	-0.84	-0.76	-0.35
3-D Structure	nStereo	-0.24	-0.25	-0.36
	nSTMW	-0.43	-0.48	-0.34
	Fsp3	-0.27	0.31	<b>-0.74</b>
	RotB	0.20	<b>0.79</b>	-0.41
Ring Content	Rings	0.61	0.08	<b>0.75</b>
	RngAr	0.61	0.08	<b>0.75</b>
	RngSys	0.61	0.08	<b>0.75</b>
	RRSys	-0.49	-0.02	-0.70

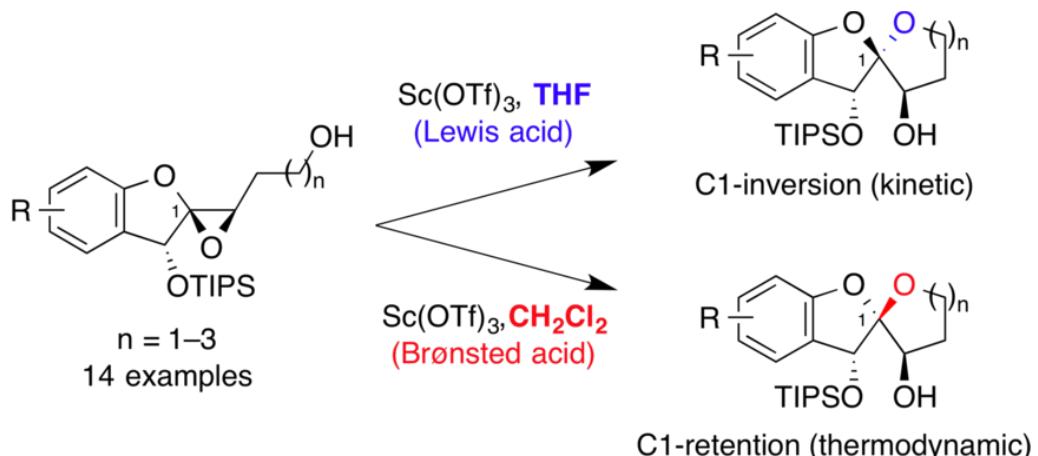
cheminformatic correlations

(Highlighted in *ACS Chem. Biol.*)

39. Solvent-dependent divergent functions of  $\text{Sc}(\text{OTf})_3$  in stereoselective epoxide-opening spiroketalizations.

Sharma, I.; Wurst, J. M.; Tan, D. S.\* *Org. Lett.* 2014, 16, 2474–2477.

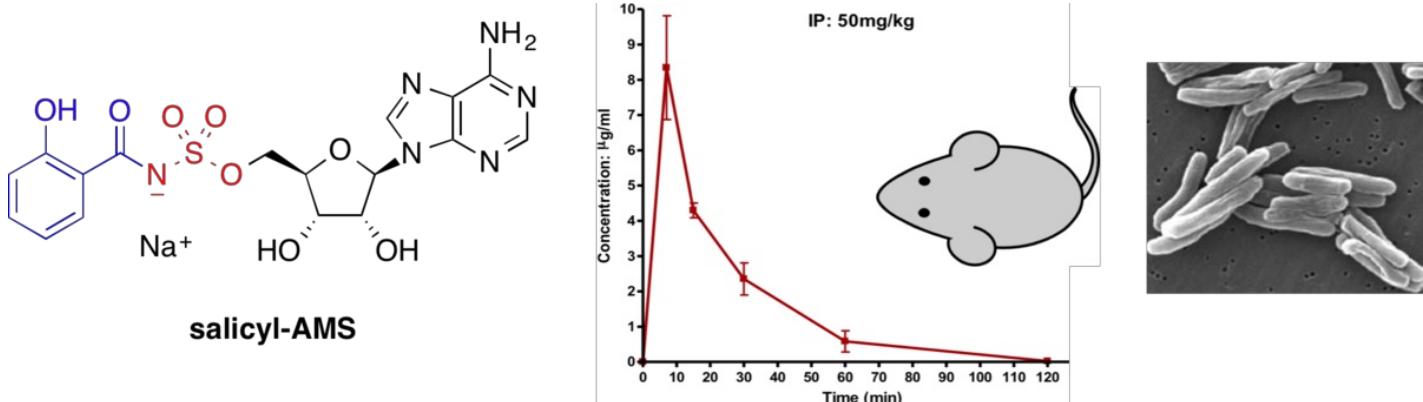
[ Abstract | PubMed | PMC ]



38. Pharmacokinetic and *in vivo* efficacy studies of the mycobactin biosynthesis inhibitor salicyl-AMS in mice.

Lun, S.; Guo, H.; Adamson, J.; Cisar, J. S.; Davis, T. D.; Sundaram Chavadi, S.; Warren, J. D.; Quadri, L. E. N.\*; Tan, D. S.\*; Bishai, W. R.\* *Antimicrob. Agents Chemother.* 2013, 57, 5138–5140.

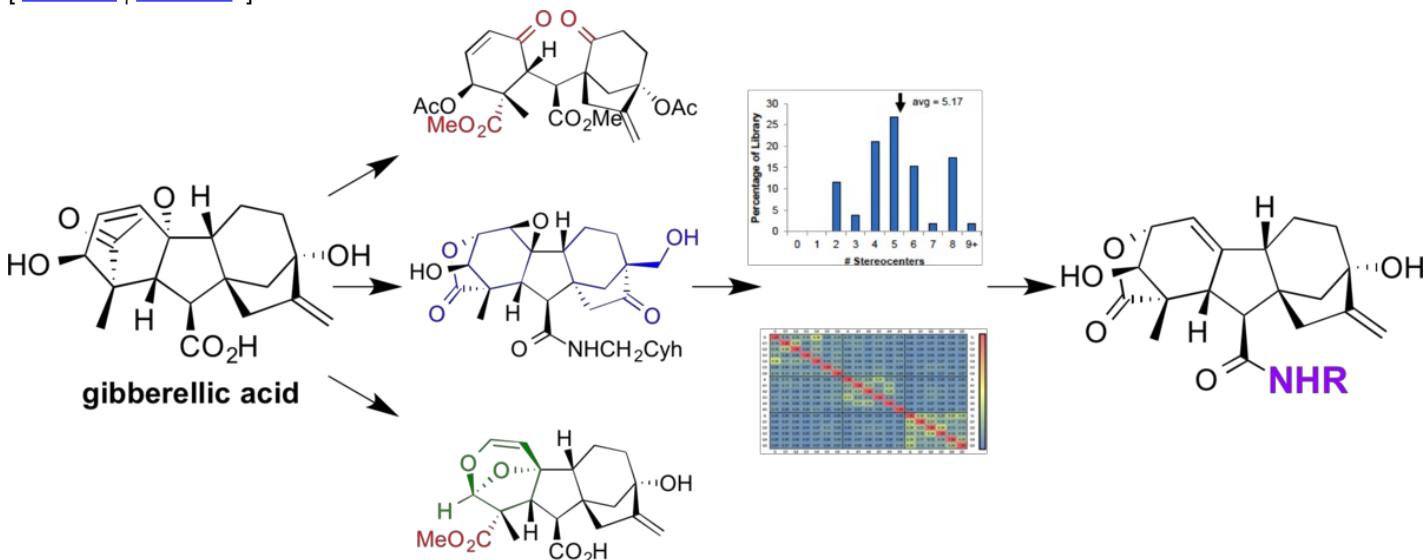
[ Abstract | PubMed | PMC ]



37. Diversifying complexity.

Sharma, I.; Tan, D. S.\* *Nat. Chem.* 2013, 5, 157–158.

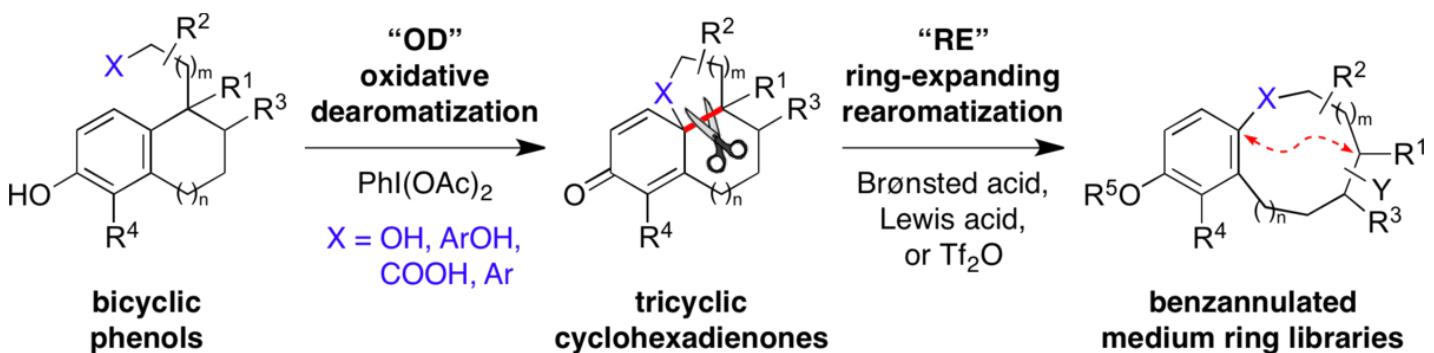
[ Abstract | PubMed ]



36. Biomimetic diversity-oriented synthesis of benzannulated medium rings via ring expansion.

Bauer, R. A.; Wenderski, T. A.; Tan, D. S.\* *Nat. Chem. Biol.* 2013, 9, 21–29.

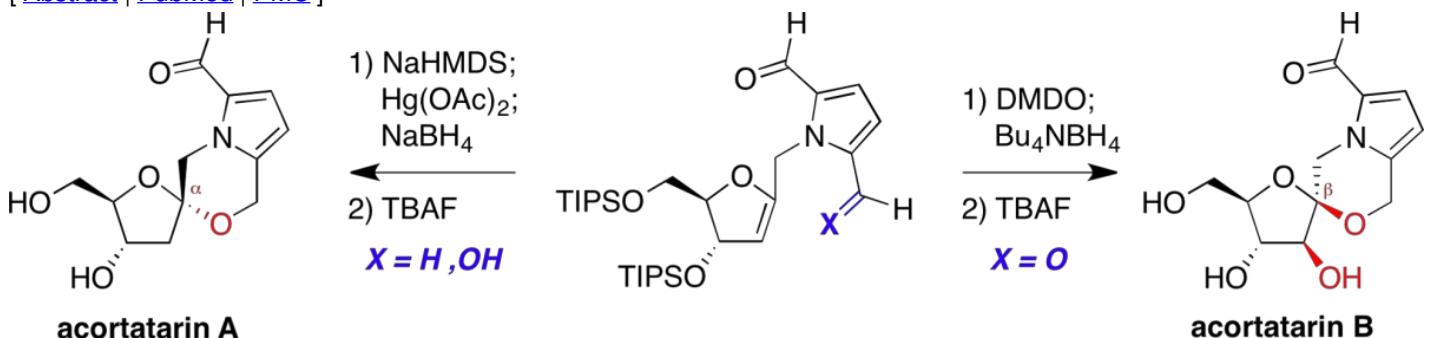
[ Abstract | PubMed | PMC ]



35. Stereoselective synthesis of acortatarins A and B.

Wurst, J. M.; Verano, A. L.; Tan, D. S.\* *Org. Lett.* 2012, 14, 4442–4445.

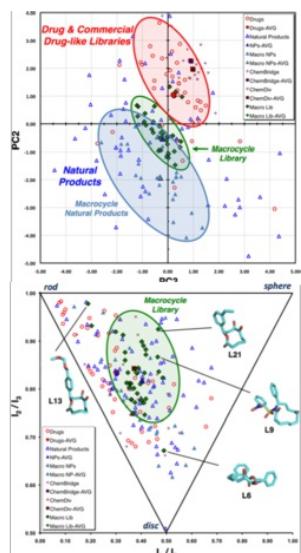
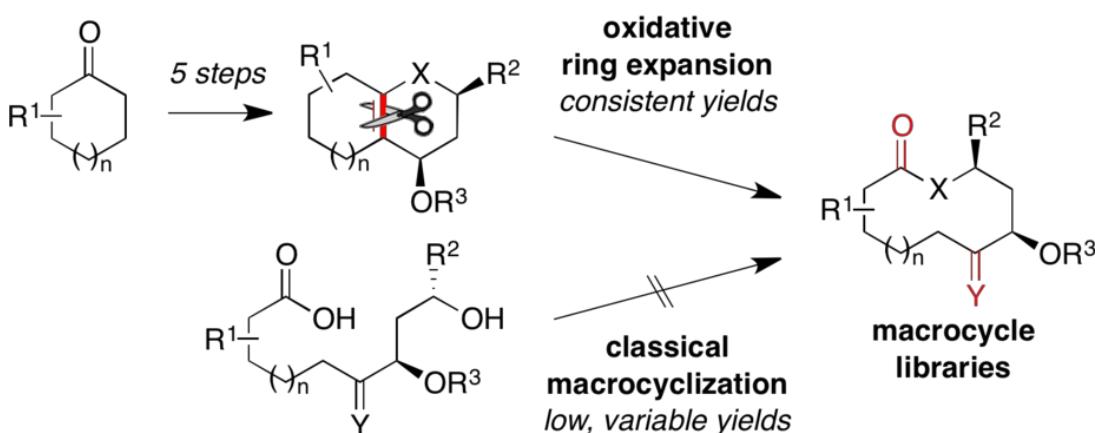
[ Abstract | PubMed | PMC ]



34. A diversity-oriented synthesis approach to macrocycles via oxidative ring expansion.

Kopp, F.; Stratton, C. F.; Akella, L. B.; Tan, D. S.\* *Nat. Chem. Biol.* 2012, 8, 358–365.

[ Abstract | PubMed | PMC ]

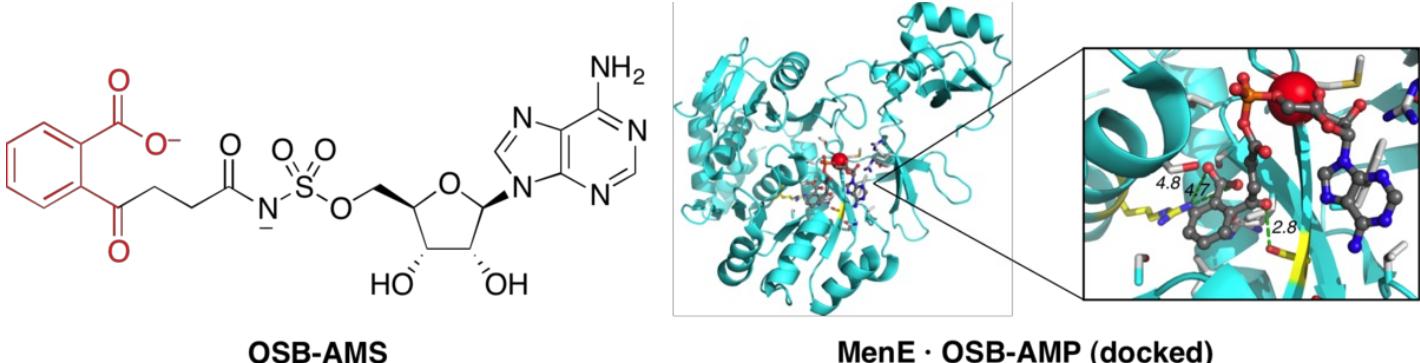


(Highlighted in SciBX)

33. Stable analogues of OSB-AMP: Potent inhibitors of MenE, the *o*-succinylbenzoate-CoA synthetase from bacterial menaquinone biosynthesis.

Lu, X.; Zhou, R.; Sharma, I.; Li, X.; Kumar, G.; Swaminathan, S.; Tonge, P. J.\*; Tan, D. S.\* *ChemBioChem* 2012, 13, 129–

[ Abstract | PubMed | PMC ]



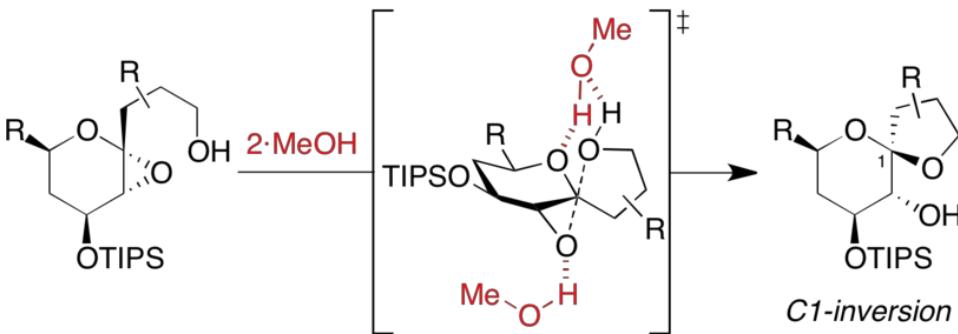
OSB-AMS

MenE · OSB-AMP (docked)

32. Hydrogen-bonding catalysis and inhibition by simple solvents in the stereoselective kinetic epoxide-opening spirocyclization of glycal epoxides to form spiroketals.

Wurst, J. M.; Liu, G.; Tan, D. S.\* *J. Am. Chem. Soc.* 2011, 133, 7916–7925.

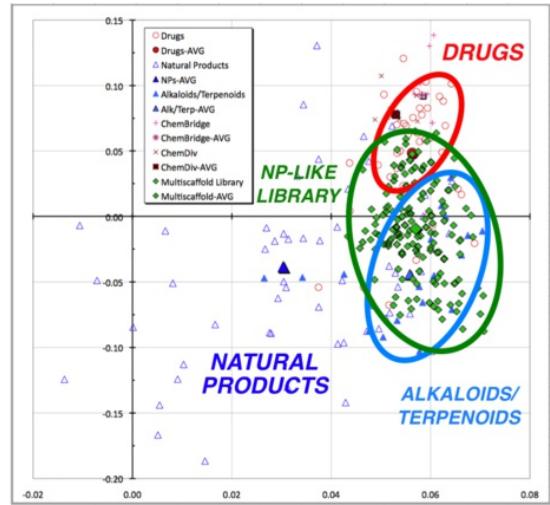
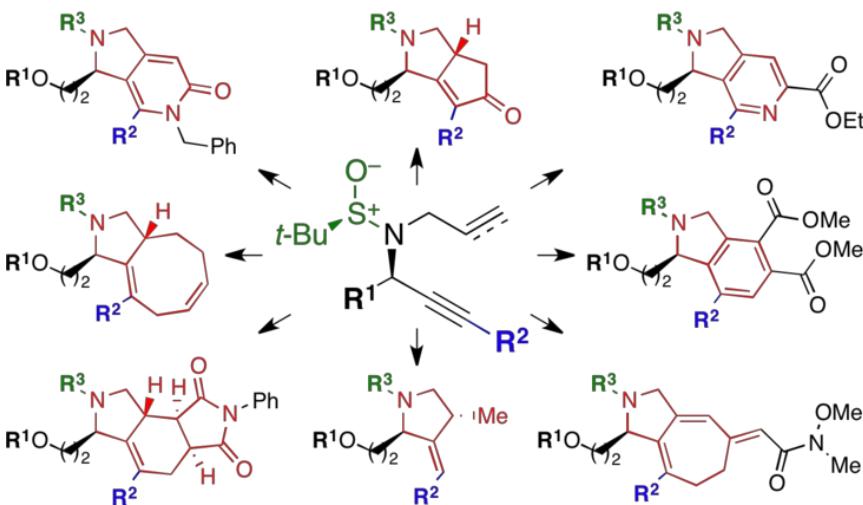
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31. Solid-phase synthesis and chemical space analysis of a 190-membered alkaloid/terpenoid-like library.

Moura-Letts, G.; DiBlasi, C. M.; Bauer, R. A.; Tan, D. S.\* *Proc. Natl. Acad. Sci. USA* 2011, 108, 6745–6750.

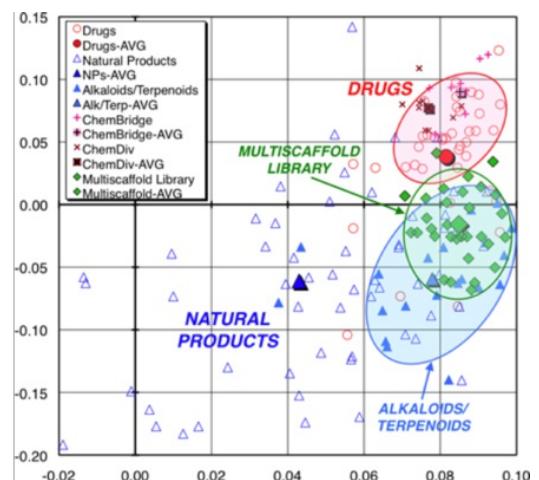
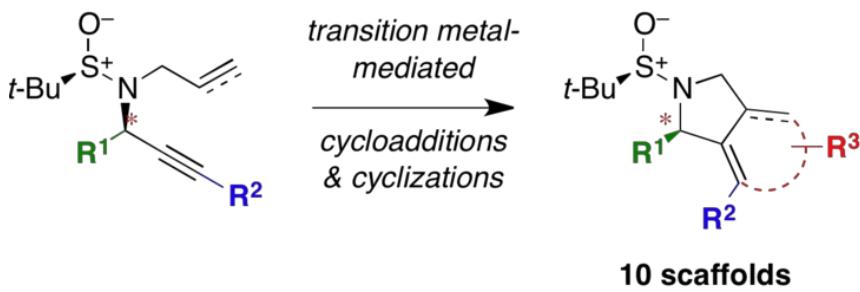
[ Abstract | PubMed | PMC ]



30. The *tert*-butylsulfinamide lynchpin in transition-metal-mediated multisccaffold library synthesis.

Bauer, R. A.; DiBlasi, C. M.; Tan, D. S.\* *Org. Lett.* 2010, 12, 2084–2087.

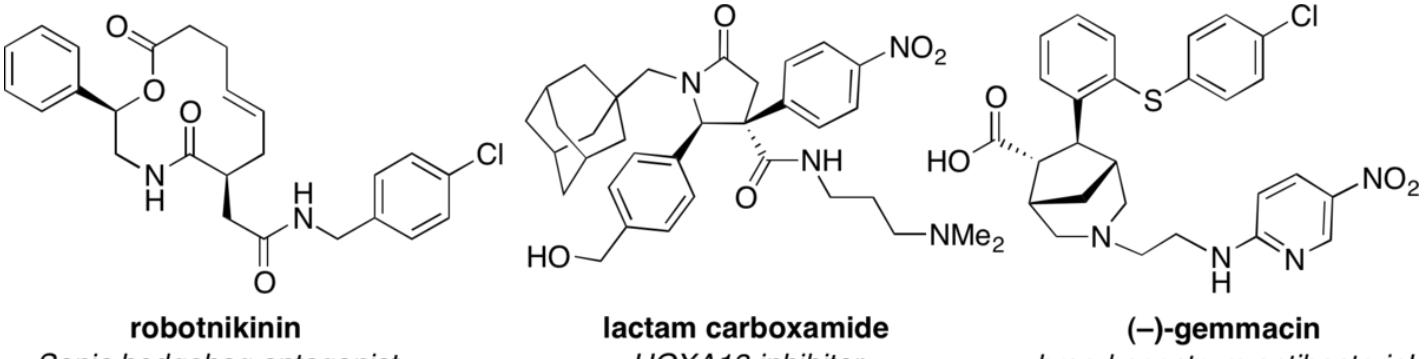
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29. Expanding the range of 'druggable' targets with natural product-based libraries: An academic perspective.

Bauer, R. A.; Wurst, J. M.; Tan, D. S.\* *Curr. Opin. Chem. Biol.* 2010, 14, 308–314.

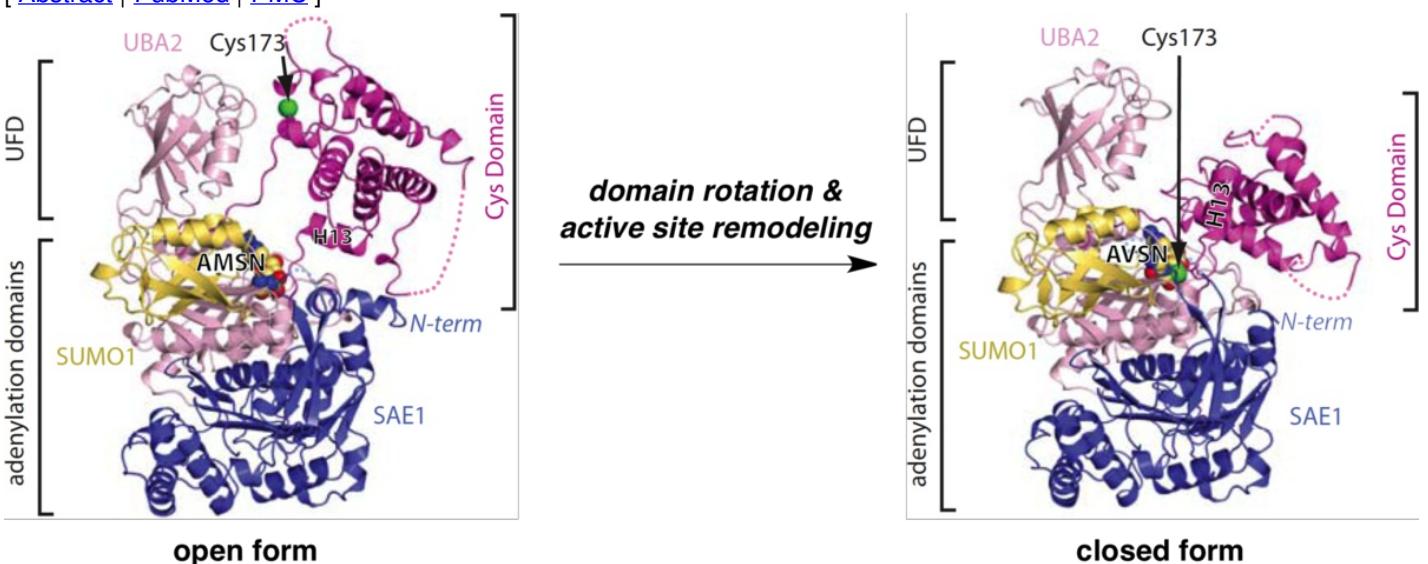
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28. Active site remodelling accompanies thioester bond formation in the SUMO E1.

Olsen, S. K.; Capili, A. D.; Lu, X.; Tan, D. S.\*; Lima, C. D.\* *Nature* 2010, 463, 906–912.

[[Abstract](#) | [PubMed](#) | [PMC](#)]

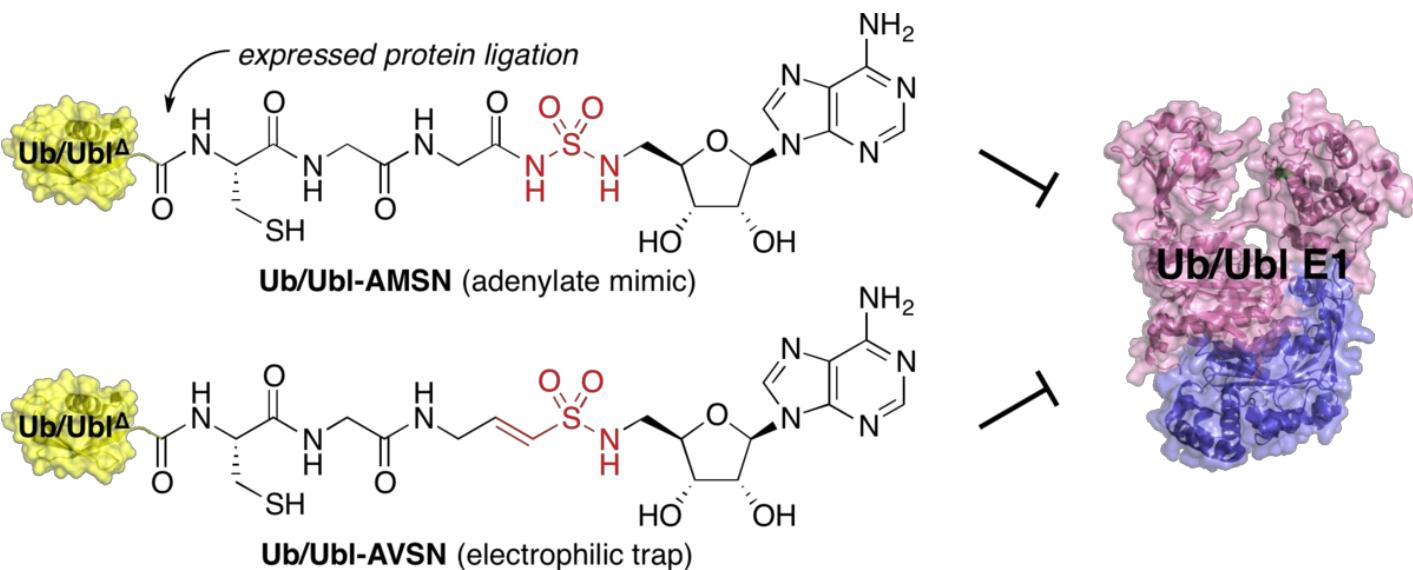


(Highlighted in [Nature](#), [Chem. Eng. News](#), [Nat. Rev. Mol. Cell Biol.](#), [Nat. Chem. Biol.](#), [Structure](#), [ACS Chem. Biol.](#), and [Faculty of 1000 Biology](#) )

27. Designed semisynthetic protein inhibitors of Ub/Ubl E1 activating enzymes.

Lu, X.; Olsen, S. K.; Capili, A. D.; Cisar, J. S.; Lima, C. D.\*; Tan, D. S.\* *J. Am. Chem. Soc.* 2010, 132, 1748–1749.

[[Abstract](#) | [PubMed](#) | [PMC](#)]

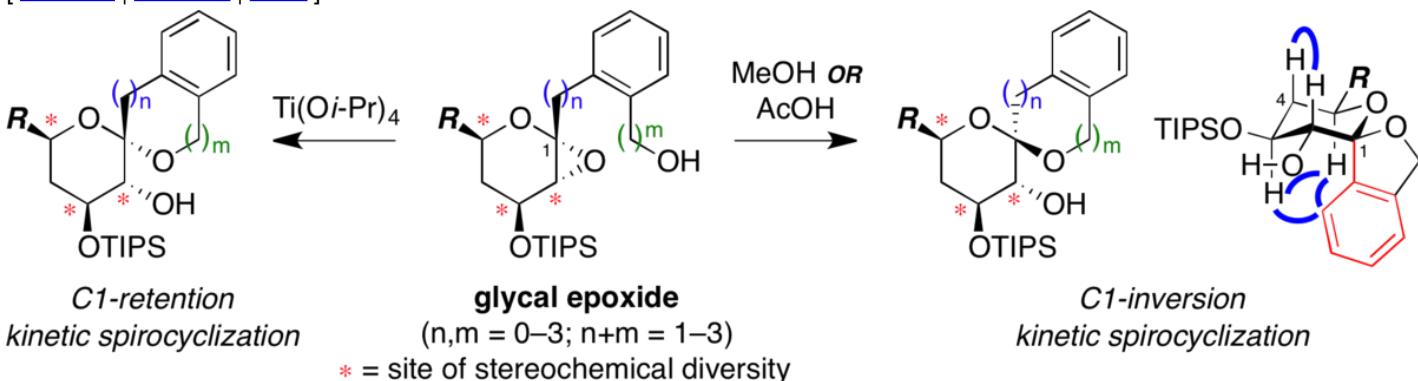


(Highlighted in [Chem. Eng. News](#), [Nat. Rev. Mol. Cell Biol.](#), [ACS Chem. Biol.](#), and [Faculty of 1000 Biology](#) )

26. Stereoselective synthesis of benzannulated spiroketals: Influence of the aromatic ring on reactivity and conformation.

Liu, G.; Wurst, J. M.; Tan, D. S.\* *Org. Lett.* 2009, 11, 3670–3673.

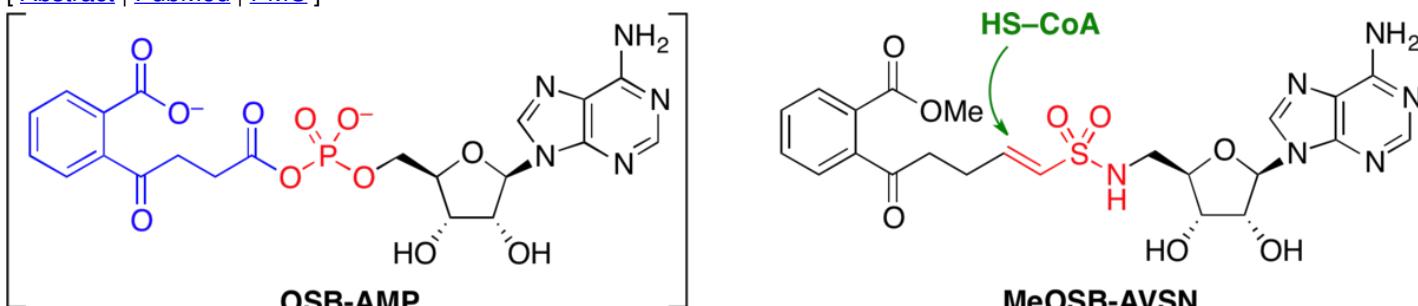
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



25. Mechanism-based inhibitors of MenE, an acyl-CoA synthetase involved in bacterial menaquinone biosynthesis.

Lu, X.; Zhang, H.; Tonge, P. J.\*; Tan, D. S.\* *Bioorg. Med. Chem. Lett.* 2008, 18, 5963–5966.

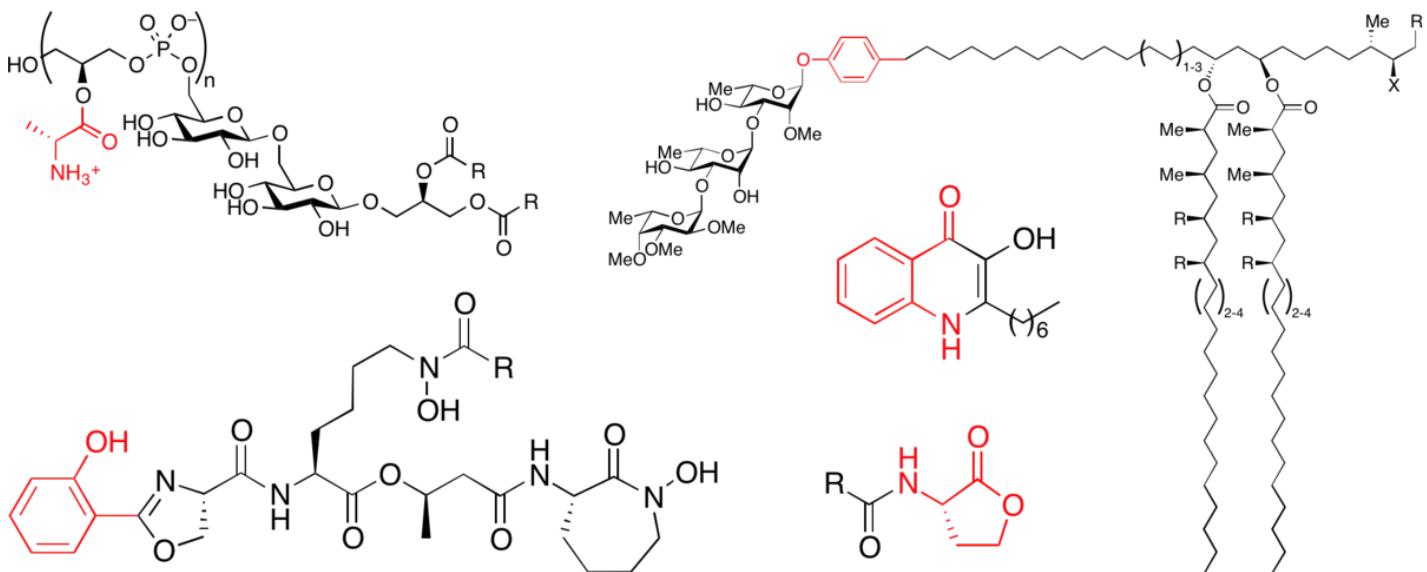
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



24. Small molecule inhibition of microbial natural product biosynthesis – An emerging antibiotic strategy.

Cisar, J. S.; Tan, D. S.\* *Chem. Soc. Rev.* 2008, 37, 1320–1329.

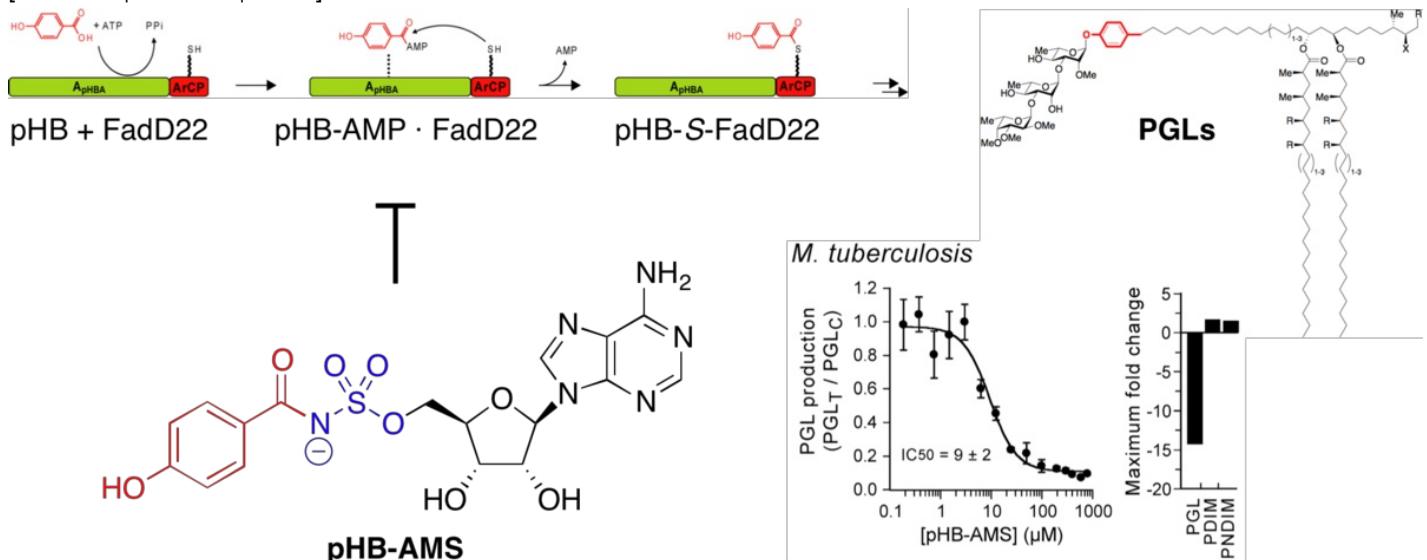
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



23. Mycobacterial phenolic glycolipid virulence factor biosynthesis: Mechanism and small-molecule inhibition of polyketide chain initiation.

Ferreras, J. A.; Stirrett, K. L.; Lu, X.; Ryu, J.-S.; Soll, C. E.; Tan, D. S.; Quadri, L. E. N.\* *Chem. Biol.* 2008, 15, 51–61.

[ [Abstract](#) | [PubMed](#) | [PMC](#) ]

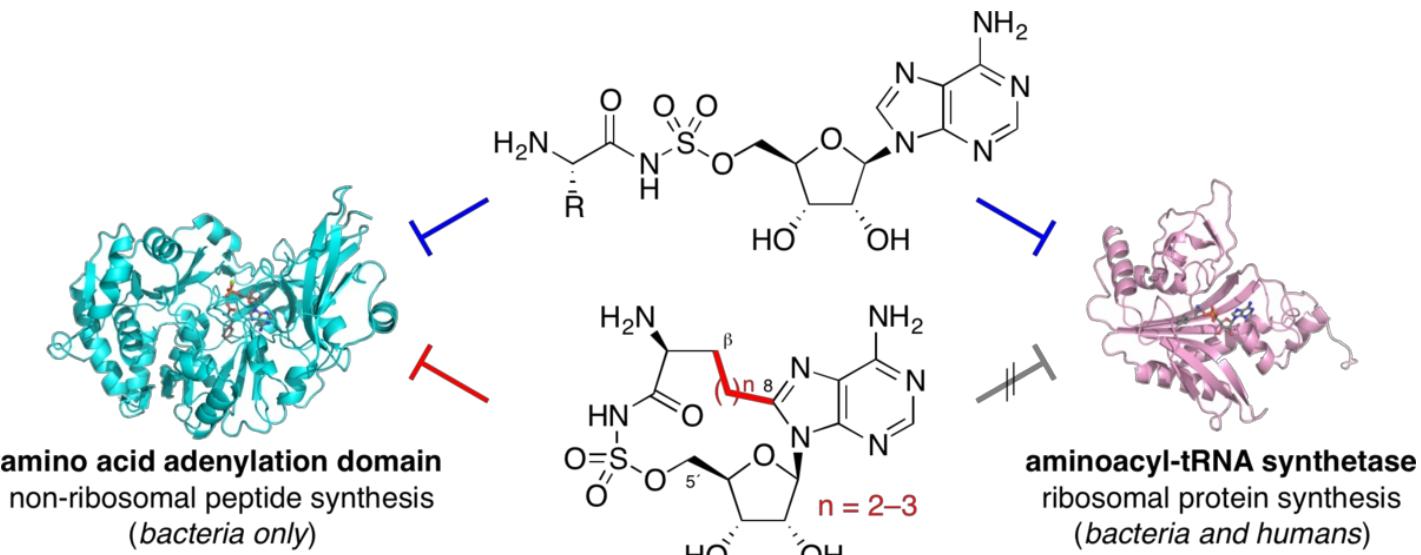


(Highlighted in [Chem. Biol.](#).)

22. Exploiting ligand conformation in selective inhibition of non-ribosomal peptide synthetase amino acid adenylation with designed macrocyclic small molecules.

Cisar, J. S.; Ferreras, J. A.; Soni, R. K.; Quadri, L. E. N.\*; Tan, D. S.\* *J. Am. Chem. Soc.* 2007, 129, 7752–7753.

[ [Abstract](#) | [PubMed](#) | [PMC](#) ]

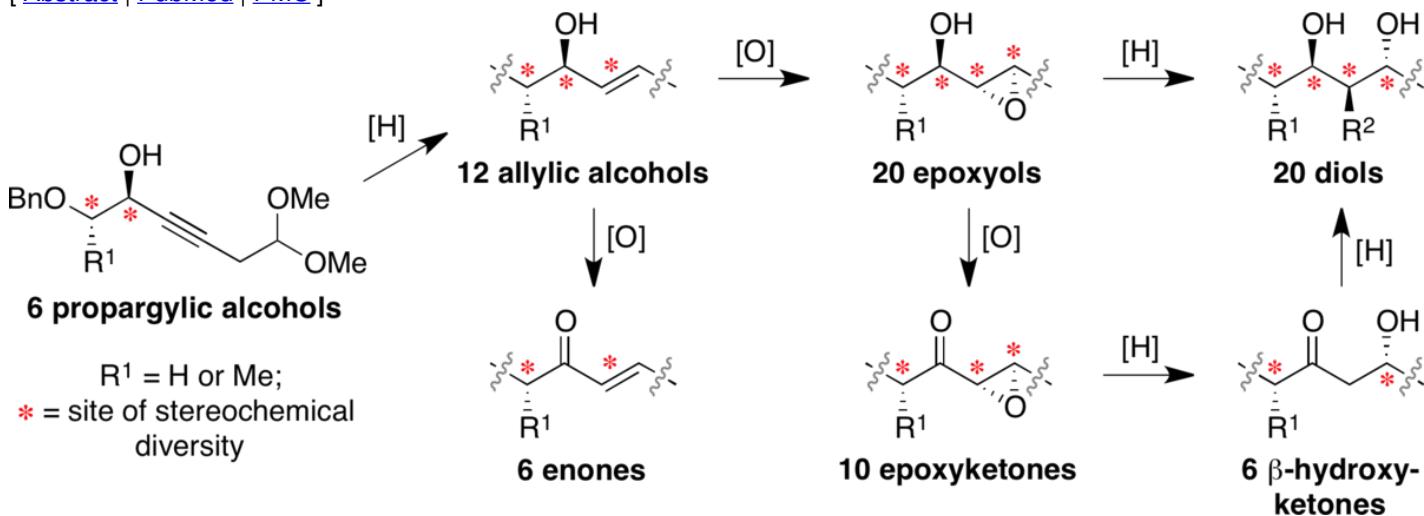


(Highlighted in [Faculty of 1000 Biology](#))

21. A unified synthetic approach to polyketides having both skeletal and stereochemical diversity.

Shang, S.; Iwadare, H.; Macks, D. E.; Ambrosini, L. M.; Tan, D. S.\* *Org. Lett.* 2007, 9, 1895–1898.

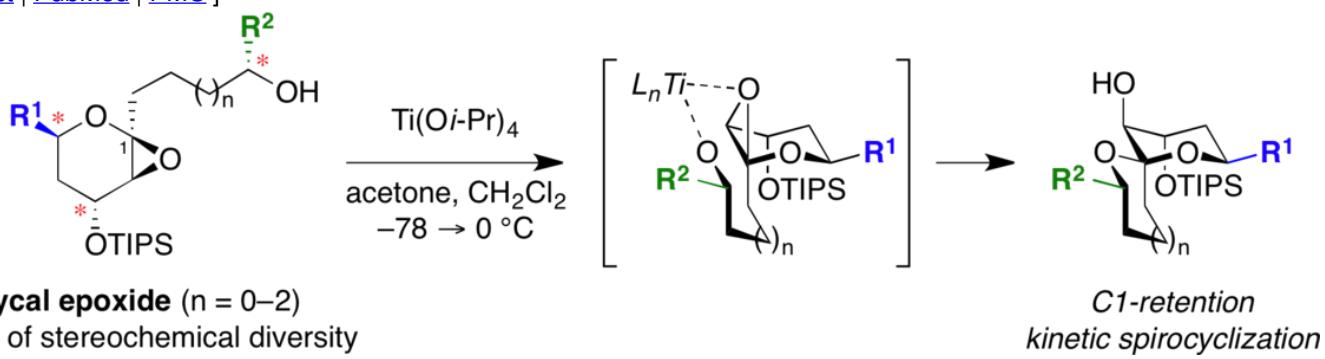
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



20. Stereocontrolled synthesis of spiroketals via  $Ti(O-iPr)_4$ -mediated kinetic spirocyclization of glycal epoxides with retention of configuration.

Moilanen, S. B.; Potuzak, J. S.; Tan, D. S.\* *J. Am. Chem. Soc.* 2006, 128, 1792–1793.

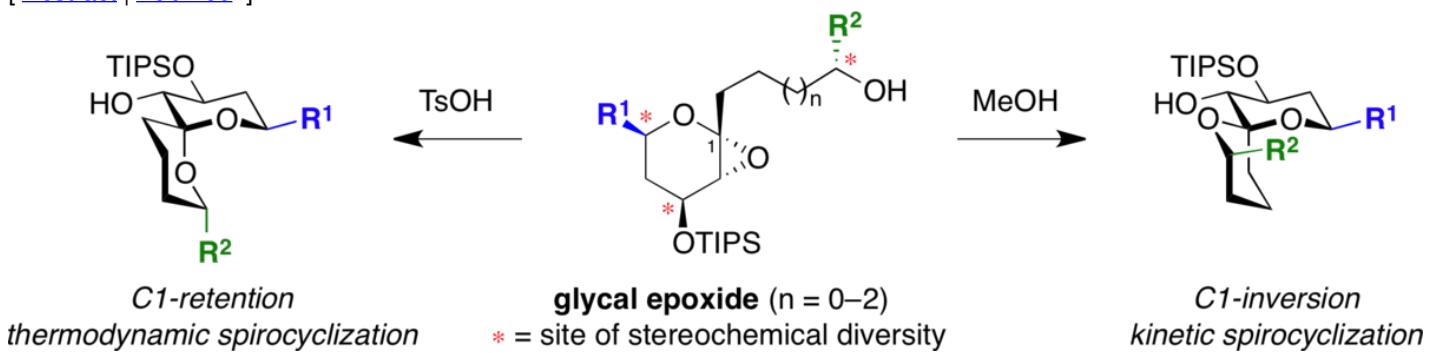
[ [Abstract](#) | [PubMed](#) | [PMC](#) ]



(Highlighted in [Nature](#))

19. Stereocontrolled synthesis of spiroketals via a remarkable methanol-induced kinetic spirocyclization reaction.

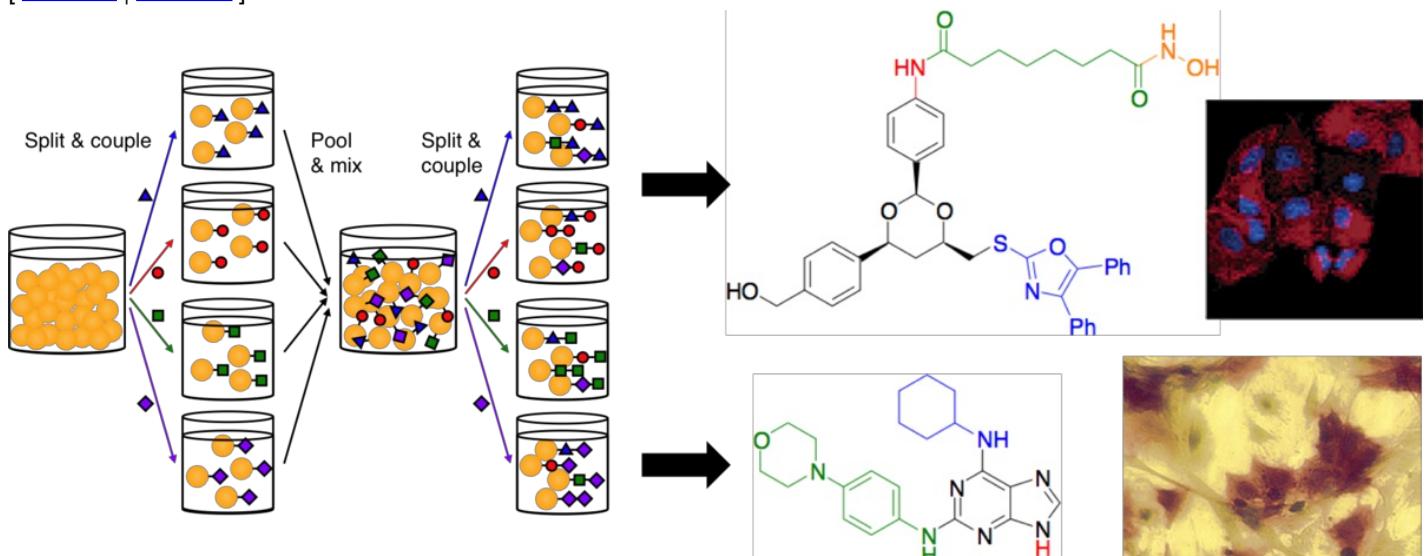
[ Abstract | PubMed ]



18. Diversity-oriented synthesis: Exploring the intersections between chemistry and biology.

Tan, D. S.\* *Nat. Chem. Biol.* 2005, 1, 74–84.

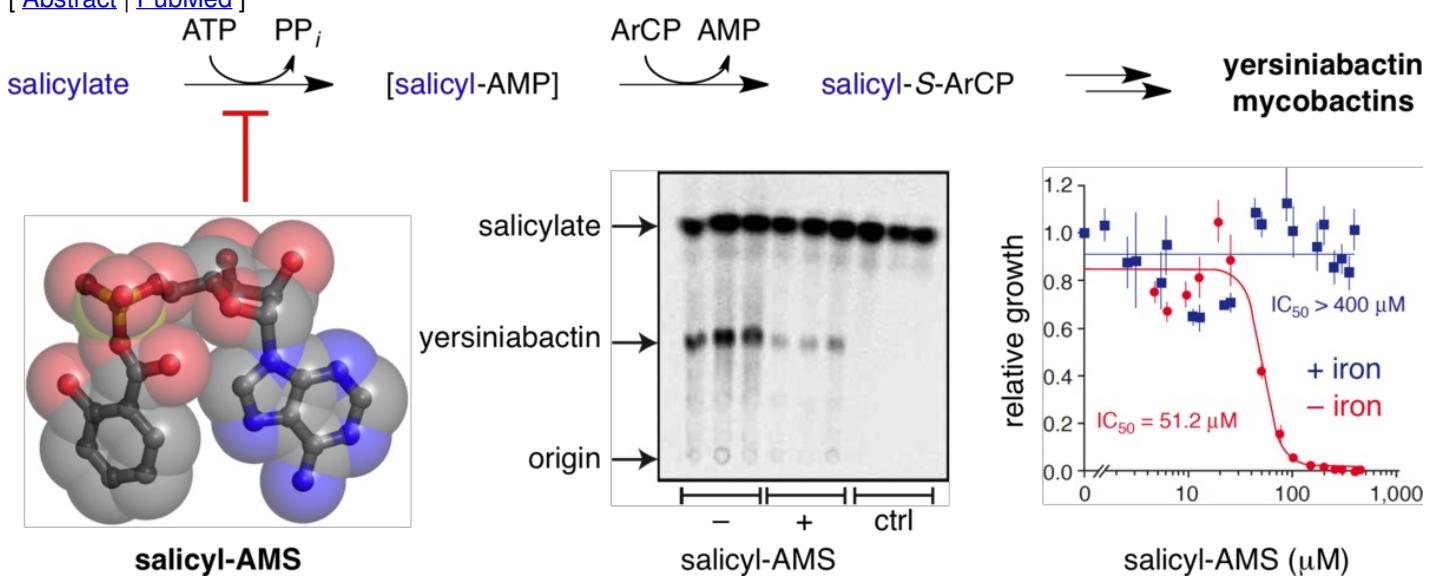
[ Abstract | PubMed ]



17. Small-molecule inhibition of siderophore biosynthesis in *Mycobacterium tuberculosis* and *Yersinia pestis*.

Ferreras, J. A.; Ryu, J.-S.; Di Lello, F.; Tan, D. S.\*; Quadri, L. E. N.\* *Nat. Chem. Biol.* 2005, 1, 29–32.

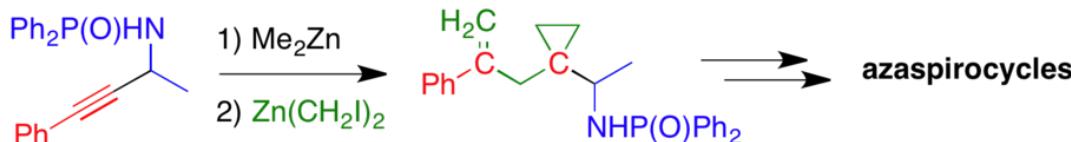
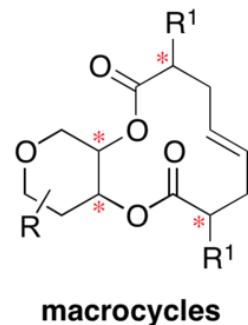
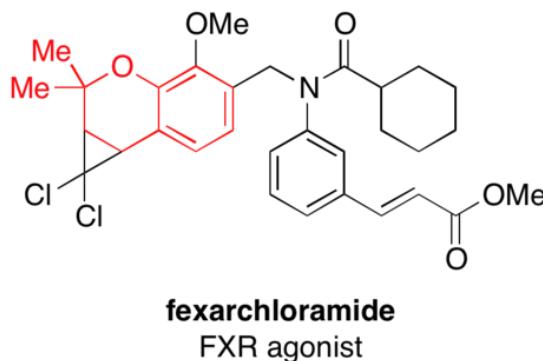
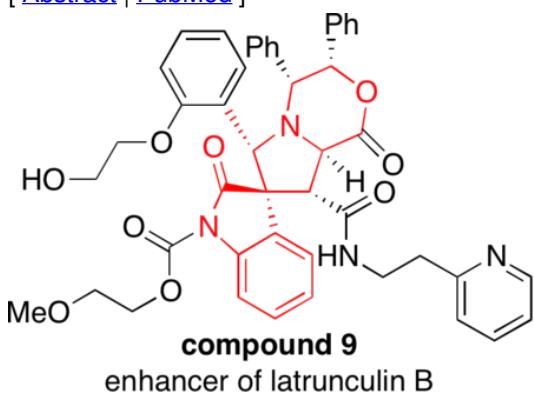
[ Abstract | PubMed ]



(Highlighted in *Nature*, *Nat. Chem. Biol.*, *Chem. Eng. News*, and *Mercosur Económico*)

16. Advancing chemistry and biology through diversity-oriented synthesis of natural product-like libraries.

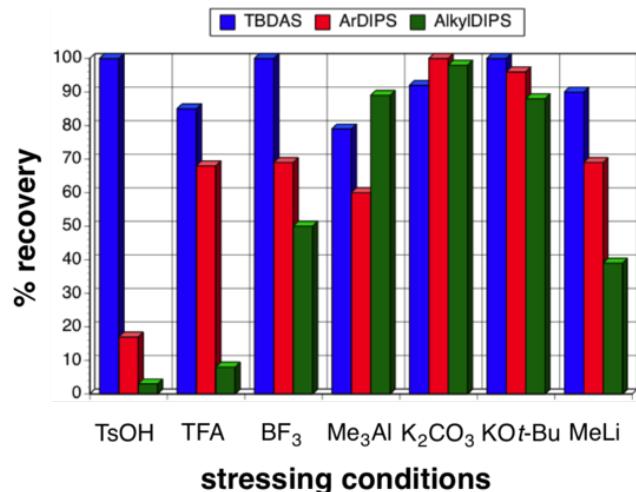
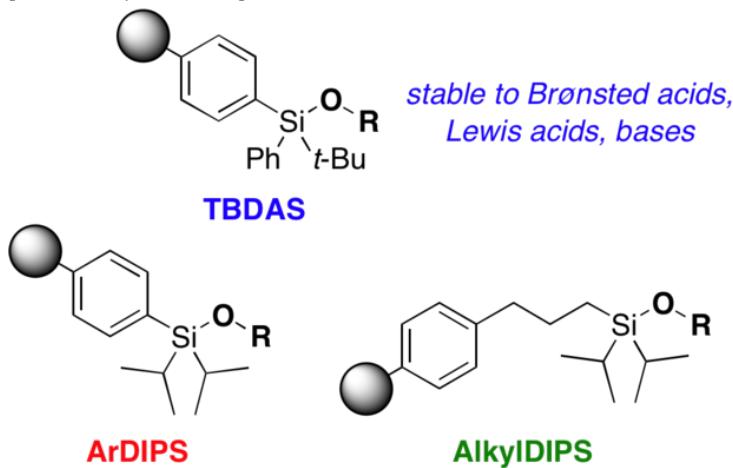
[ Abstract | PubMed ]



15. An acid-stable *tert*-butyldiarylsilyl (TBDAS) linker for solid-phase organic synthesis.

DiBlasi, C. M.; Macks, D. E.; Tan, D. S.\* *Org. Lett.* 2005, 7, 1777–1780.

[ Abstract | PubMed ]

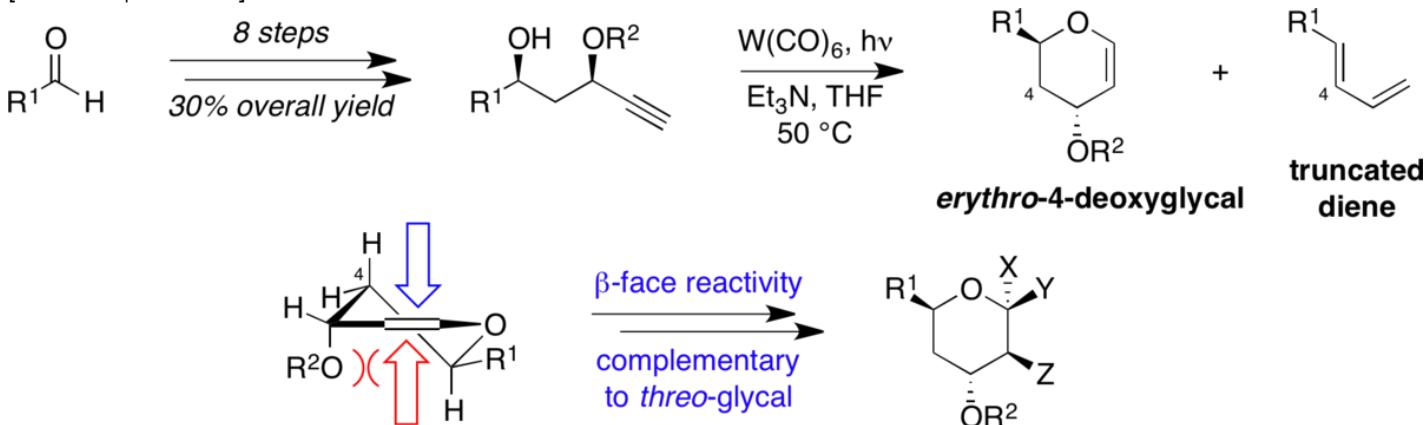


(Highlighted in *Lett. Org. Chem.* [PDF] )

14. Enantioselective synthesis of *erythro*-4-deoxyglycals as scaffolds for target- and diversity-oriented synthesis: New insights into glycal reactivity.

Moilanen, S. B.; Tan, D. S.\* *Org. Biomol. Chem.* 2005, 3, 798–803.

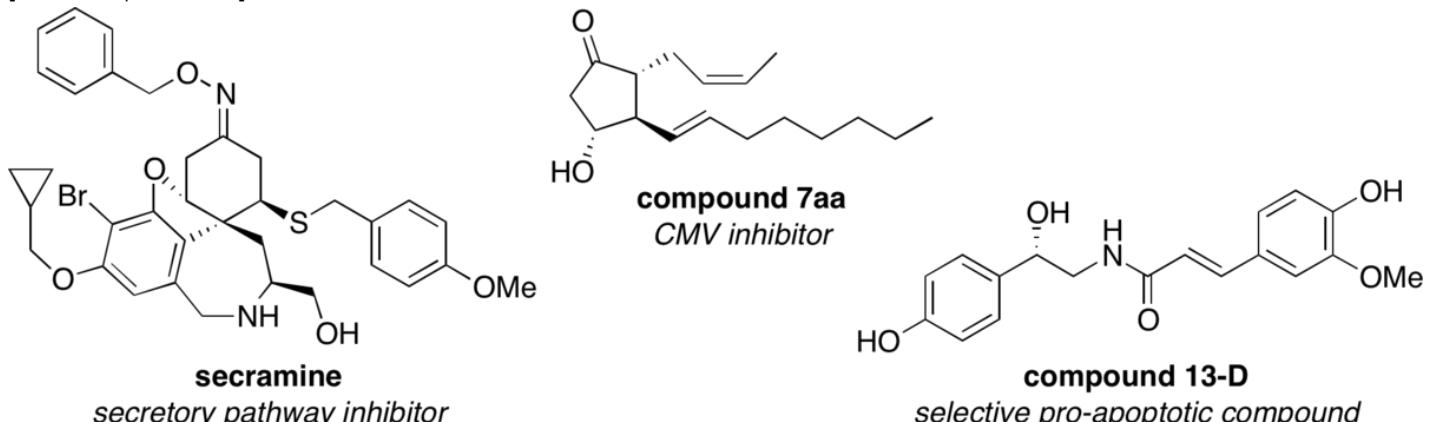
[ Abstract | PubMed ]



13. Current progress in natural product-like libraries for discovery screening.

Tan, D. S.\* *Comb. Chem. High-Throughput Screen.* 2004, 7, 631–643.

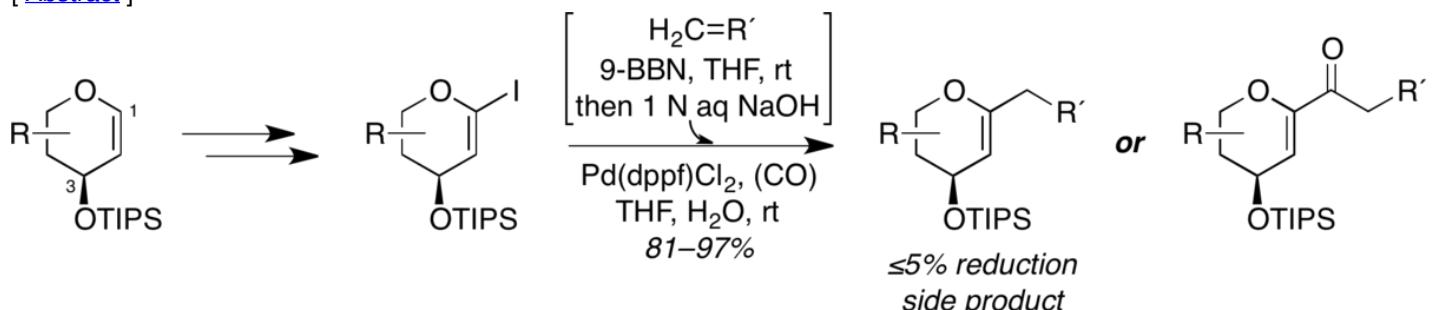
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12. Synthesis of C1-alkyl and C1-acylglycals from glycals using a *B*-alkyl Suzuki–Miyaura cross coupling approach.

Potuzak, J. S.; Tan, D. S.\* *Tetrahedron Lett.* 2004, 45, 1797–1801.

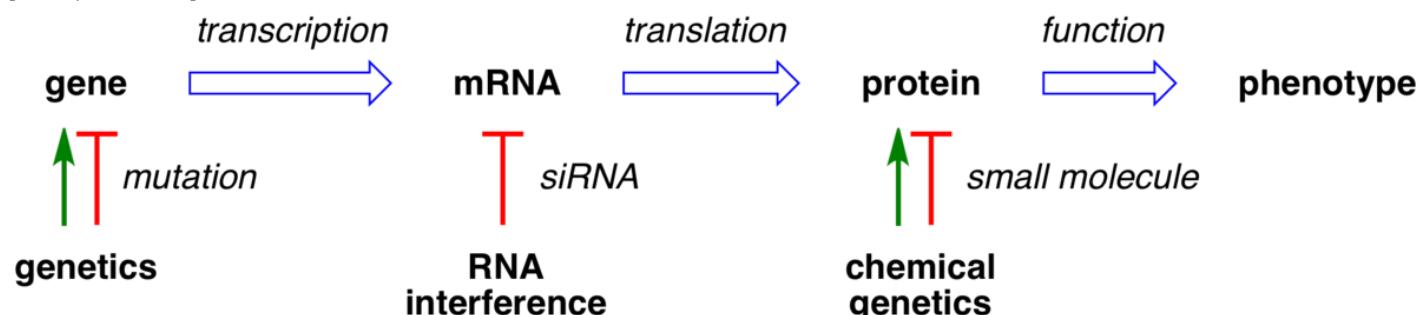
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11. Discovery and applications of small molecule probes for studying biological processes.

Potuzak, J. S.; Moilanen, S. B.; Tan, D. S.\* *Biotechnol. Genet. Eng. Rev.* 2004, 21, 11–78.

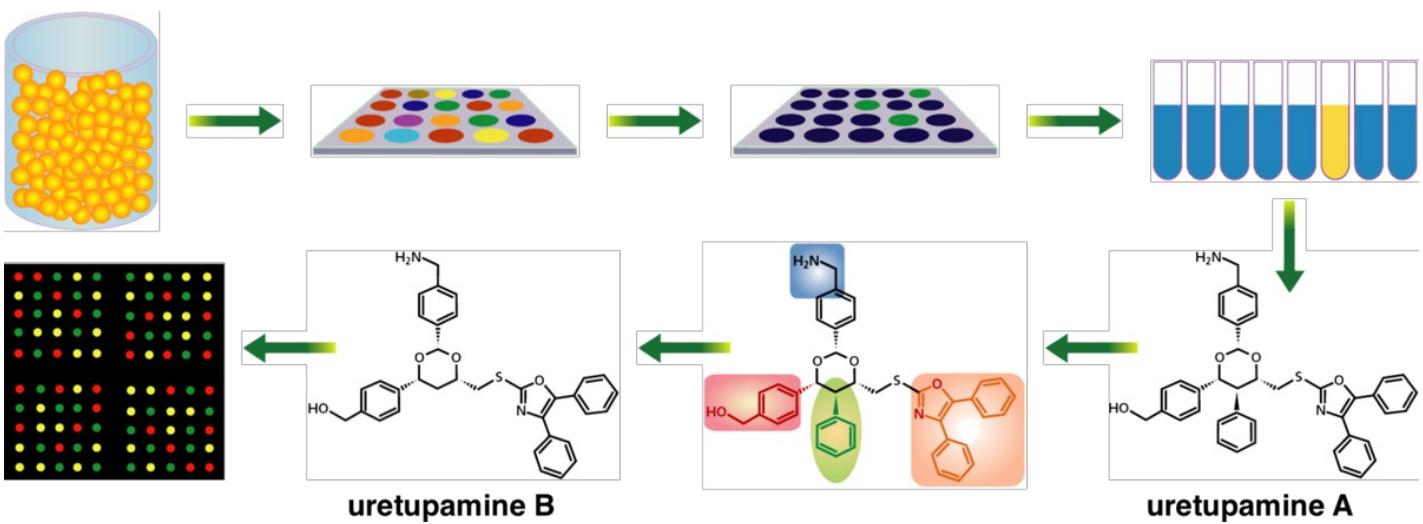
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10. Sweet surrender to chemical genetics.

Tan, D. S.\* *Nat. Biotechnol.* 2002, 20, 561–563.

[ Abstract | PubMed ]

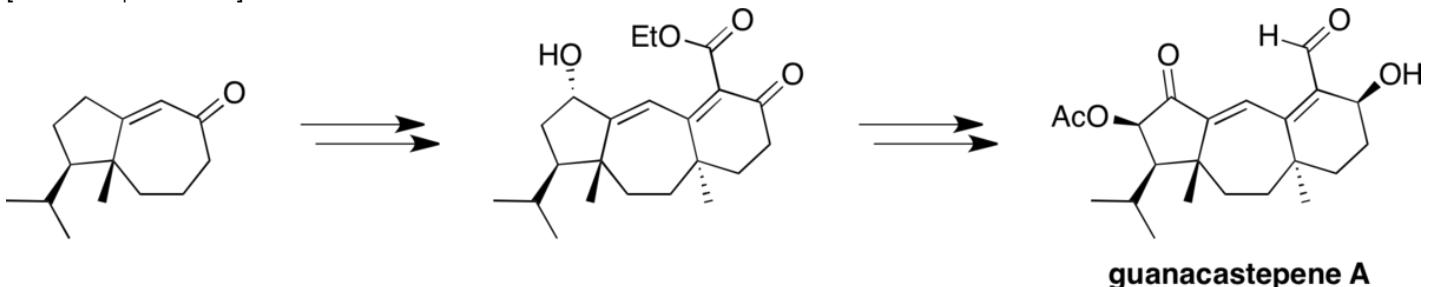


## Postdoctoral Publications

9. Total synthesis of guanacastepene A: A route to enantiomeric control.

Mandal, M.; Yun, H.; Dudley, G. B.; Lin, S.; Tan, D. S.; Danishefsky, S. J.\* *J. Org. Chem.* 2005, **70**, 10619–10637.

[ [Abstract](#) | [PubMed](#) ]

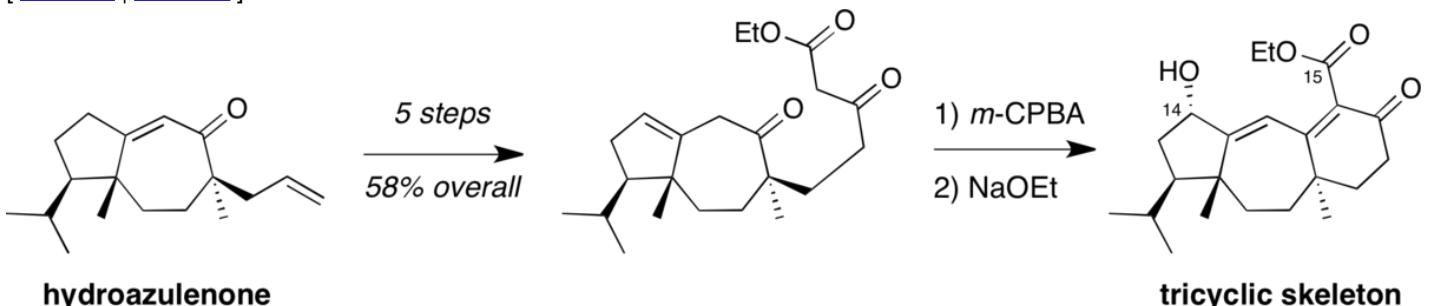


(Featured on the Cover)

8. Synthesis of the functionalized tricyclic skeleton of guanacastepene A: A tandem epoxide-opening  $\beta$ -elimination/Knoevenagel cyclization.

Tan, D. S.; Dudley, G. B.; Danishefsky, S. J.\* *Angew. Chem., Int. Ed.* 2002, **41**, 2185–2188.

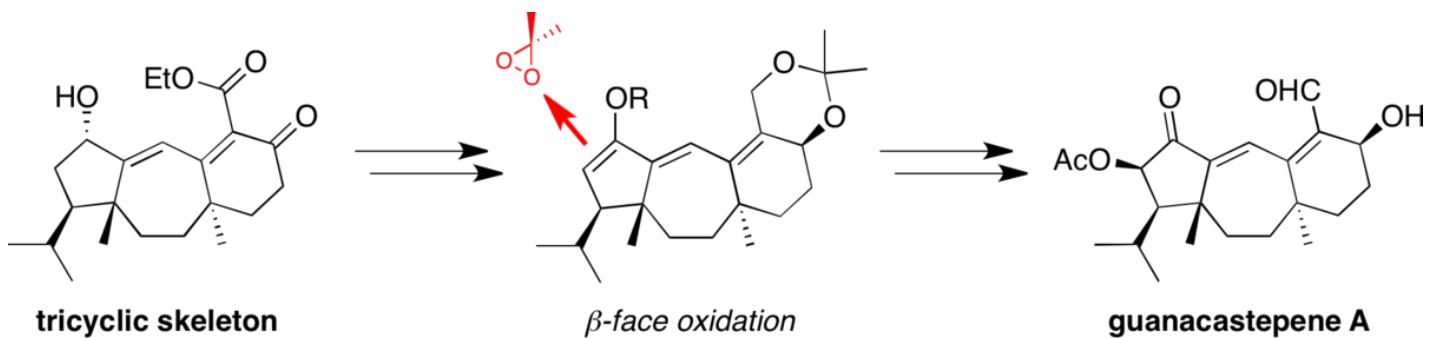
[ [Abstract](#) | [PubMed](#) ]



7. A stereoselective route to guanacastepene A through a surprising epoxidation.

Lin, S.; Dudley, G. B.; Tan, D. S.; Danishefsky, S. J.\* *Angew. Chem., Int. Ed.* 2002, **41**, 2188–2191.

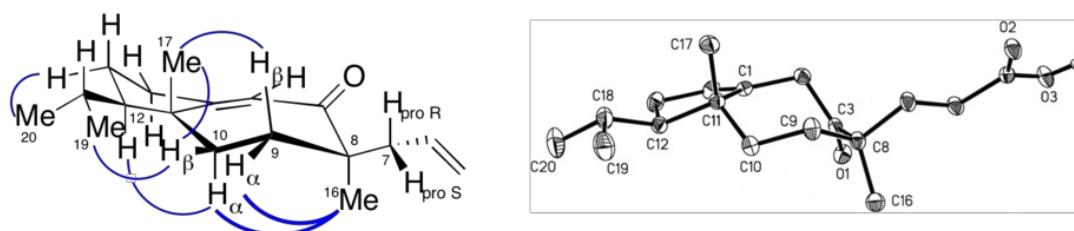
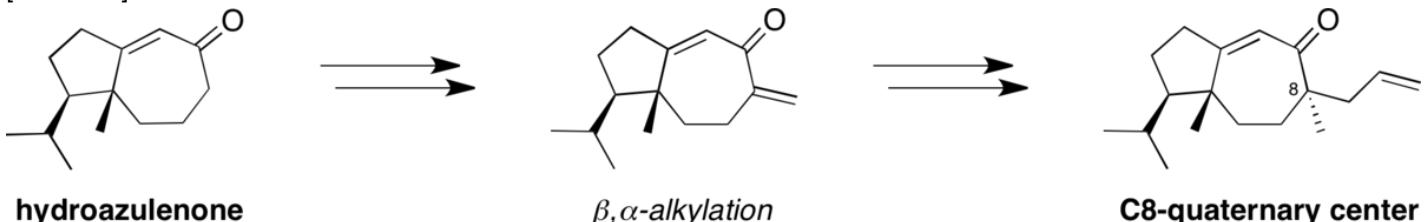
[ [Abstract](#) | [PubMed](#) ]



6. Remarkable stereoselectivity in the alkylation of a hydroazulenone: Progress toward the total synthesis of guanacastepene.

Dudley, G. B.; Tan, D. S.; Kim, G.; Tanski, J. M.; Danishefsky, S. J.\* *Tetrahedron Lett.* 2001, 42, 6789–6791.

[ Abstract ]

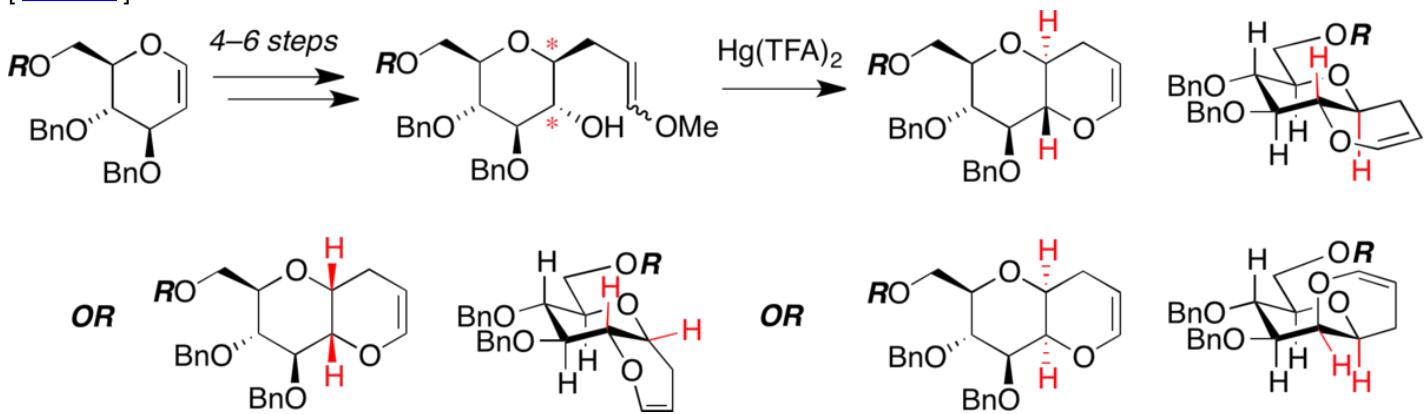


## Graduate Publications

5. A mercury-catalyzed transesterification cyclization leading to fused cyclic polyethers.

Tan, D. S.; Schreiber, S. L.\* *Tetrahedron Lett.* 2000, 41, 9509–9513.

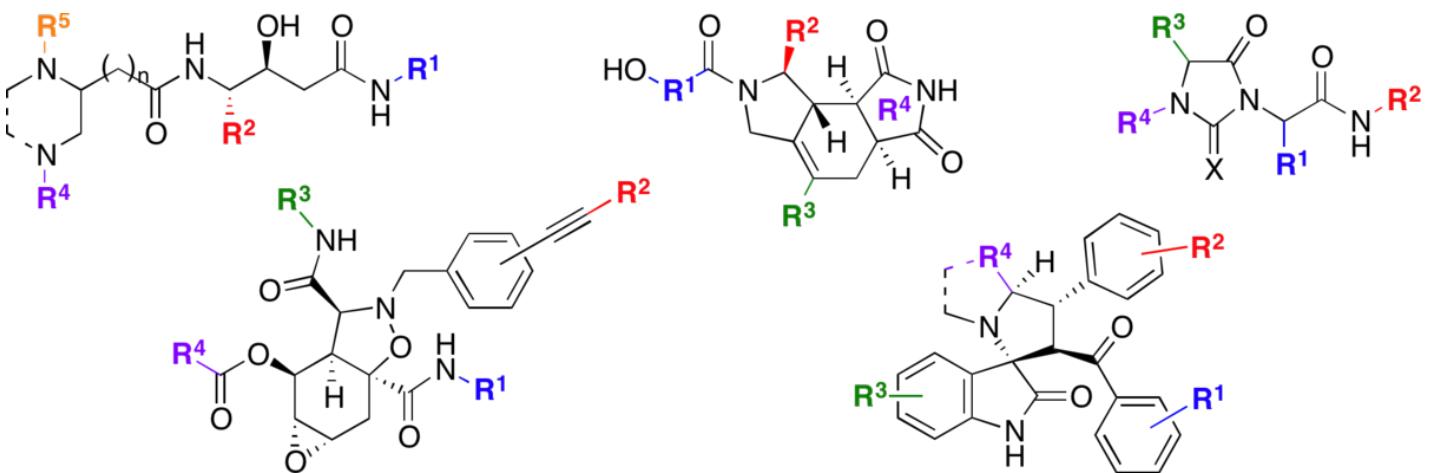
[ Abstract ]



4. Ligand discovery using encoded combinatorial libraries.

Tan, D. S.\*; Burbaum, J. J.\* *Curr. Opin. Drug Discovery Dev.* 2000, 3, 439–453.

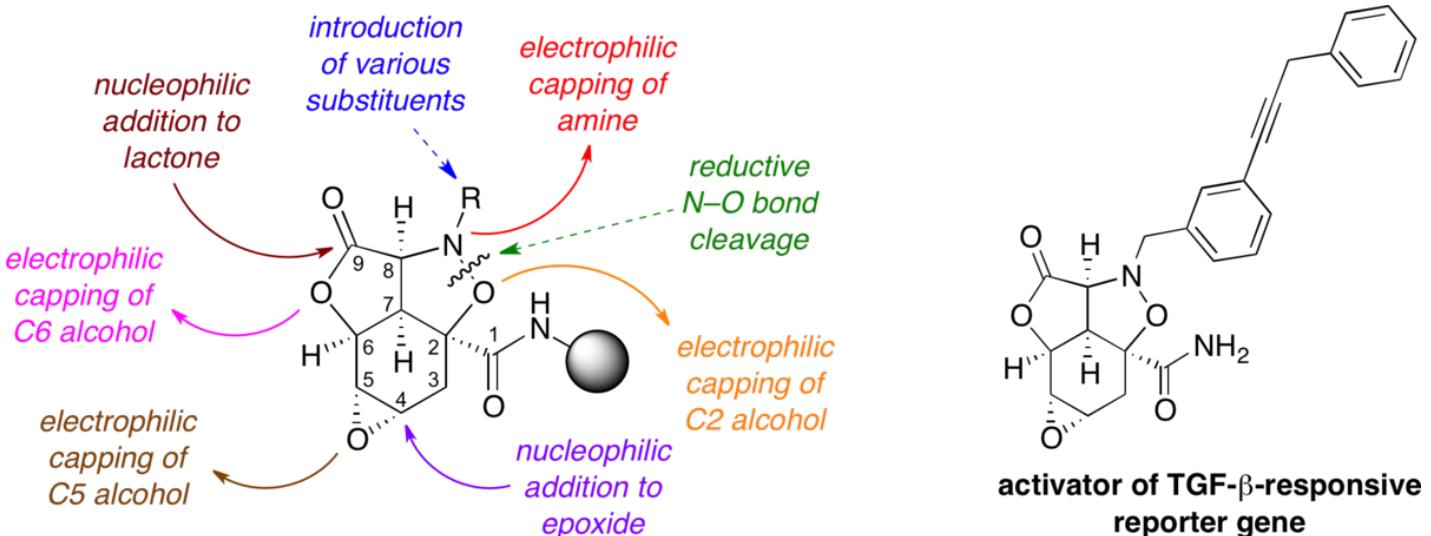
[Abstract]



3. Synthesis and preliminary evaluation of a library of polycyclic small molecules for use in chemical genetic assays.

Tan, D. S.; Foley, M. A.; Stockwell, B. R.; Shair, M. D.; Schreiber, S. L.\* *J. Am. Chem. Soc.* 1999, 121, 9073–9087.

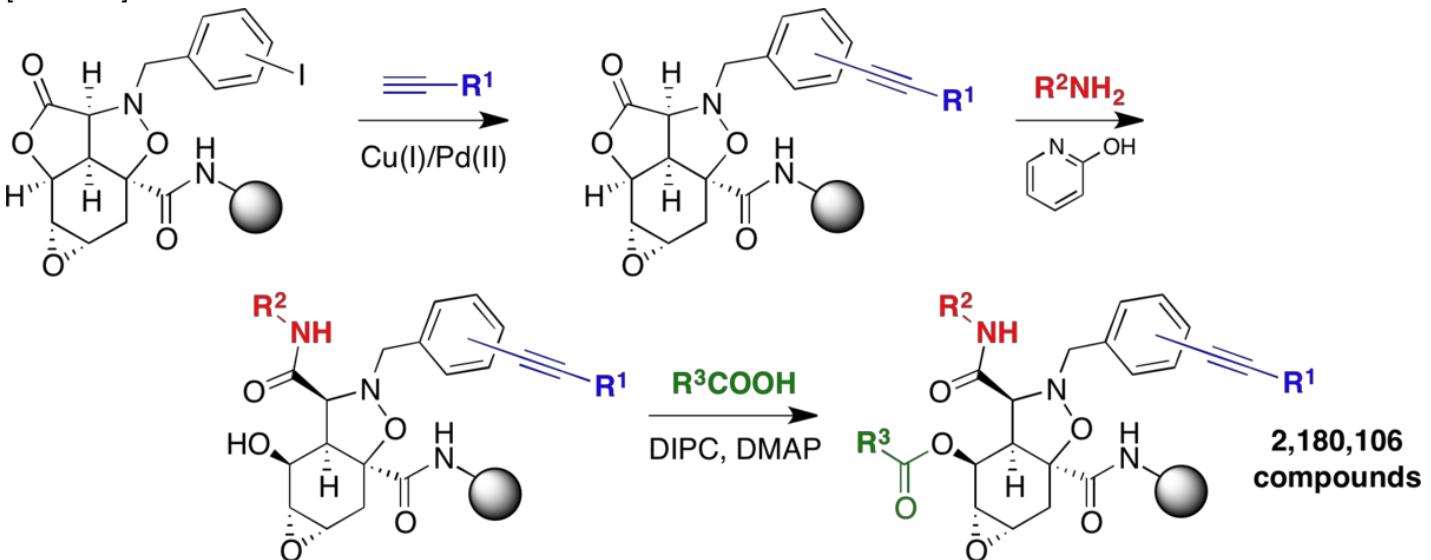
[ Abstract ]



2. Stereoselective synthesis of over two million compounds having structural features both reminiscent of natural products and compatible with miniaturized cell-based assays.

Tan, D. S.; Foley, M. A.; Shair, M. D.; Schreiber, S. L.\* *J. Am. Chem. Soc.* 1998, 120, 8565–8566.

[ Abstract ]



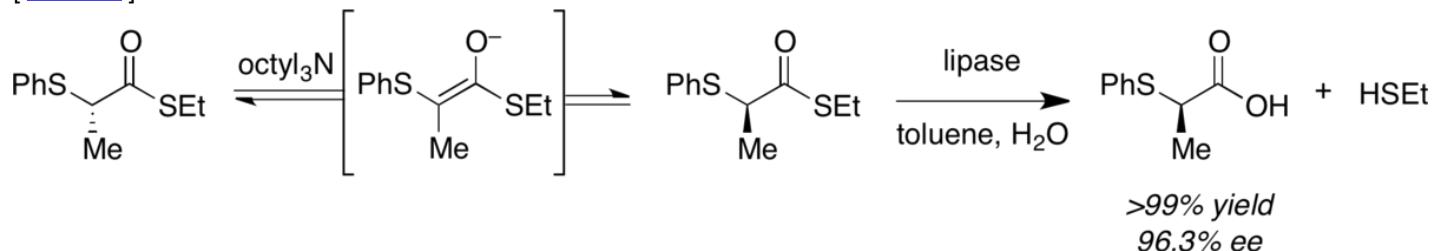
(Highlighted in *Science*, *Chem. Eng. News.*.)

## Undergraduate Publication

- Enzymatic resolution coupled with substrate racemization using a thioester substrate.

Tan, D. S.; Günter, M. M.; Dueckhammer, D. G.\* *J. Am. Chem. Soc.* 1995, 117, 9093–9094.

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