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Small Molecule Libraries

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We are participating in the NIH Molecular Libraries Program (MLP) under our grant entitled "Diversity-Oriented Synthesis of Natural Product-based Libraries for the MLSMR" ([P41 GM076267](#)). Our novel natural product-based libraries are being submitted to the NIH Molecular Libraries Small Molecule Repository (MLSMR), where they are available to the scientific community for high-throughput screening in the NIH Molecular Libraries Probe Production Centers Network (MLPCN). Investigators interested in MLPCN screening under the R21 or R01 mechanisms should see program announcements [PAR-12-058](#) and [PAR-12-059](#). The results of these screens are available to the public via the [PubChem](#) database.

We use diversity-oriented synthesis to produce several different natural product-based libraries for the MLSMR. Some of these libraries are being synthesized in collaboration with members of the [Chemical Biology Platform](#) at the [Broad Institute](#).

A list of our compounds that are currently available for screening in the MLPCN (updated quarterly) can be accessed via the following live search links:

[All Tan Lab Libraries](#)

[SK1 Spiroketal Library \(Aliphatic\)](#)

(48 compounds submitted)

[SK2 Spiroketal Library \(Benzannulated\)](#)

(68 compounds submitted)

[SK3 Spiroketal Library \(Functionalized Benzannulated\)](#)

(30 compounds submitted)

[PK1 Polyketide Fragment Library](#)

(74 compounds submitted)

[AT1 Alkaloid/Terpenoid Library \(Multiscaffold\)](#)

(94 compounds submitted)

[AT2 Alkaloid/Terpenoid Library \(Pyrrolidinopyridines, 2-position full matrix\)](#)

(29 compounds submitted)

[AT3 Alkaloid/Terpenoid Library \(Pyrrolidinopyridines, 2-position sparse matrix\)](#)

(31 compounds submitted)

[AT4 Alkaloid/Terpenoid Library \(Pyrrolidinopyridines, 3-position sparse matrix\)](#)

(62 compounds submitted)

[MC1 Macrocyclic Library \(Macrolides and Macrolactams\)](#)

(18 compounds submitted)

[MR1 Medium Ring Library and CD1 Tricyclic Cyclohexadienone Library](#)

(37 compounds submitted)

Screening results for these libraries are appearing regularly. To access screening data, click on one of the live search links above, then click on the Bioactivity Analysis button on the search results page.

Full experimental details on the synthesis and purification of these compounds have been published previously in the following papers:

Spiroketal Diversity-Oriented Synthesis Libraries

These rigid, stereochemically diverse scaffolds from natural products present sidechains along well-defined three-dimensional vectors.

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.

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

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](#)]

Stereocontrolled synthesis of spiroketals via Ti(*O*-*i*-Pr)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](#))

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

Potuzak, J. S.; Moilanen, S. B.; Tan, D. S.* *J. Am. Chem. Soc.* 2005, *127*, 13796–13797.

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

Polyketide Diversity-Oriented Synthesis Libraries

These structural motifs from natural products exhibit skeletal and conformational diversity.

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](#)]

Alkaloid/Terpenoid Diversity-Oriented Synthesis Libraries

This multiscaffold library is comprised of polycyclic structures related to alkaloid and terpenoid natural products.

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](#)]

The *tert*-butylsulfonamide lynchpin in transition-metal-mediated multiscaffold library synthesis.

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

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

Macrocycle Diversity-Oriented Synthesis Libraries

These scaffolds are comprised of 10- to 12-membered macrolactones and macrolactams.

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](#))

Benzannulated Medium Ring Diversity-Oriented Synthesis Libraries

These scaffolds are comprised of diverse medium rings with aryl ether, aryl lactone, diaryl ether, and biaryl linkages.

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](#)]

TBDAS Linker for Solid Phase Diversity-Oriented Synthesis

This robust linker is stable to a wide range of organic reaction conditions and is cleaved chemoselectively with fluoride reagents. [Click here](#) for more details.

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](#)])

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