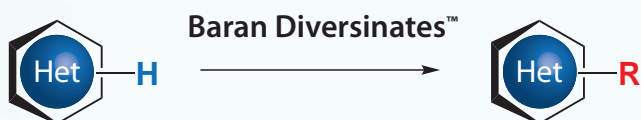


BARAN DIVERSINATES™

LEAD DIVERSIFICATION AND METABOLISM PREDICTION

Lead Diversification

As a ready alternative to the *de novo* synthesis of analogs, the Baran Diversinates™ allow medicinal chemists to modify heterocycle-containing compounds *directly* into a variety of structural analogs in one step. Notably, this technology can also be used to conveniently functionalize heterocyclic C-H bonds with **linkers** containing either an azide or protected ketone, both of which allow for the bioconjugation of small molecules to biomolecules like antibodies or fluorescent tags. The Baran Diversinates™, including the native chemical tagging reagents, can be used in biologically relevant conditions like water and air.

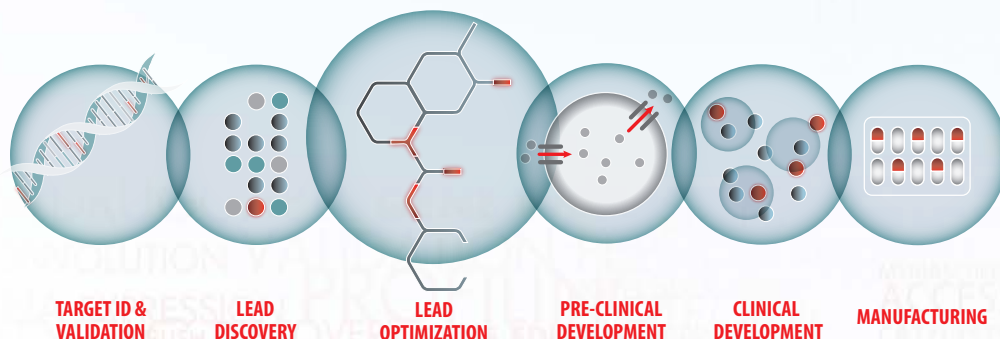


Metabolism Prediction

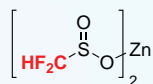
Metabolism of small molecules *via* the aldehyde oxidase enzyme (AO) is difficult to predict, and has derailed several promising drug candidates at a late stage. By providing a ready source of CF_2H radical, DFMS (767840) functionalizes many of the small molecules shown to ultimately be susceptible to the AO metabolic pathway *in vivo*. With this in mind, DFMS has therefore been shown to be a quick and inexpensive chemical litmus test for early prediction of susceptibility to AO metabolism. Beyond prediction, DFMS (and the other Baran Diversinates™) can then be used to chemically block these sites of AO susceptibility, thus generating a set of analogs with lessened metabolic liability.



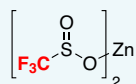
TRANSLATIONAL WORKFLOW SOLUTIONS



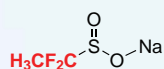
Fluorine Containing



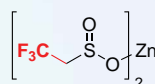
767840
DFMS



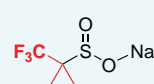
771406
TFMS



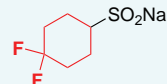
745405
DFES-Na



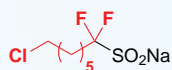
745499
TFES



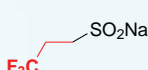
790184
TFCS-Na



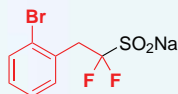
ALD00230
DFHS-Na



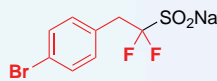
ALD00484
Coming Soon!



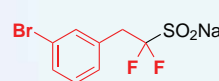
ALD0238
TFPS-Na



ALD00462

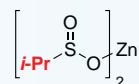


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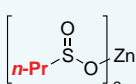


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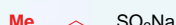
Alkyl Groups



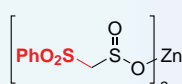
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IPS



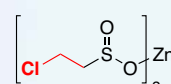
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NPS



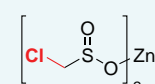
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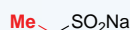
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PSMS



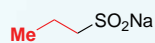
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MCES



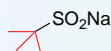
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MCMS



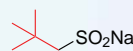
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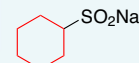
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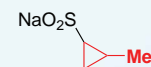
ALD00288
TBS-Na



ALD00290
DMPS-Na

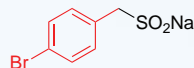


ALD00434

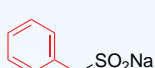


ALD00272
Coming Soon!

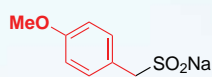
Aryl Groups



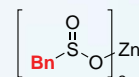
ALD00476
Coming Soon!



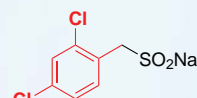
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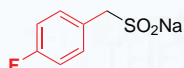
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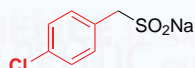
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BNS



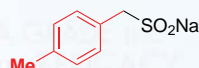
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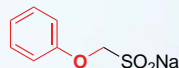
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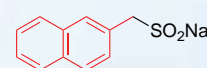
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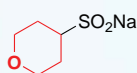


809063
Coming Soon!

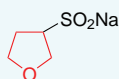


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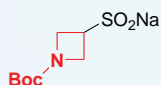
Saturated Heterocycles



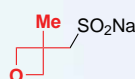
ALD00232
THPS-Na



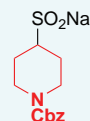
ALD00234
TFHS-Na



ALD00236
AZS-Na

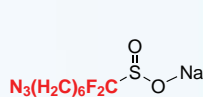


ALD00302

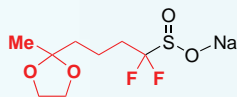


ALD00456

Linkers



746118
DAAS-Na



792446
Shabat Sulfinate

Late Stage Functionalization Toolkit (ALD00444)

The Aldrich LSF Toolkit provides ready access to screening quantities of Baran Diversinates™ capable of installing alkyl, fluorinated alkyl, benzyl, cyclic halogenated and heterocyclic functionalities to a small molecule. The Toolkit also includes Palau'Chlor® (792454) which is able to directly chlorinate a variety of heterocycles, providing easy access to further diversification through this versatile chemical handle.

Share your diversinate needs with us at diversinates@sial.com.

For more information about our commitment to Drug Discovery, visit sigma-aldrich.com/translational

TRANSLATIONAL RESEARCH SOLUTIONS

ALDRICH LATE STAGE FUNCTIONALIZATION TOOLKIT (ALD00444)

Late Stage Functionalization

Late Stage Functionalization (LSF) allows synthetic and medicinal chemists to structurally modify one Lead Compound into a small library of analogs for further screening and eventual optimization. Diversification achieved directly from a compound *already in hand* obviates the need for ground-up syntheses of each analog, a task often hampered by time, cost and the availability of appropriate starting materials.

The Aldrich Late Stage Functionalization Toolkit provides screening quantities of our most popular and effective LSF reagents to date. Armed with this Toolkit, you can generate a diverse library of value-added analogs.

Intelligent Diversification

The components of the kit have:

- High-purity reagents
- On-site quality control (QC) control
- Low-temperature storage
- Low-temperature stability

ALD00232-100mg THPS-Na 152.10 g/mol

ALD00234-100mg TFHS-Na 158.19 g/mol

ALD00236-100mg AZS-Na 172.18 g/mol

ALD00230-100mg THPS-Na 206.19 g/mol

ALD00456-100mg THPS-Na 144.17 g/mol