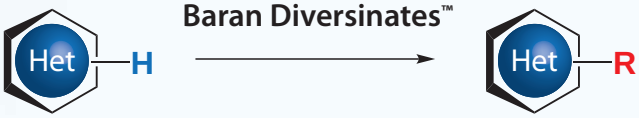
BARAN DIVERSINATES™
LEAD DIVERSIFICATION AND METABOLISM PREDICTION

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.



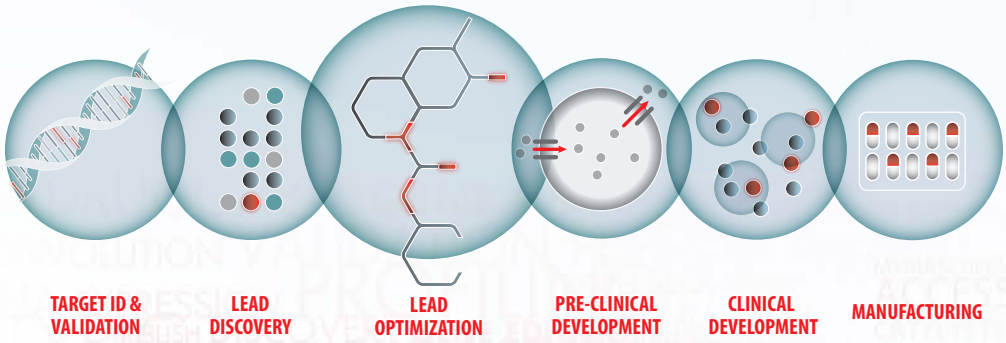
Metabolism Prediction

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.

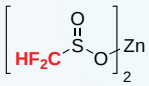
THE SCRIPPS RESEARCH INSTITUTE AND SIGMA-ALDRICH:

Your Innovation Pipeline for Lead Optimization

TRANSLATIONAL WORKFLOW SOLUTIONS



Fluorine Containing



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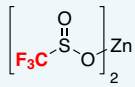
DFMS



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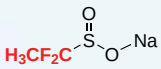

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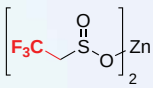
DFES-Na



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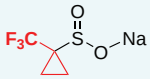

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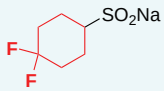

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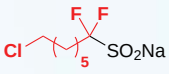

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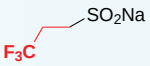
Coming Soon!



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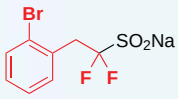

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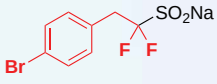

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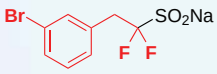

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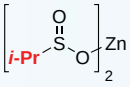
Alkyl Groups



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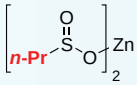

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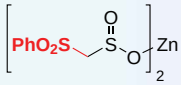

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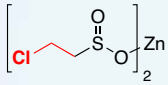

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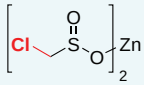

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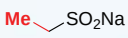

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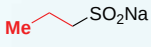

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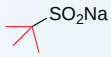

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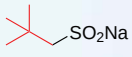

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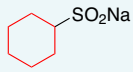
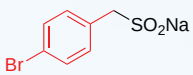


ALD00434

ALD00272
Coming Soon!

Aryl Groups



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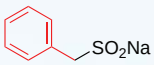

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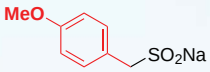

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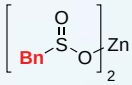

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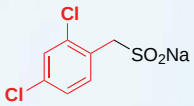

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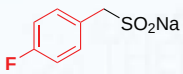

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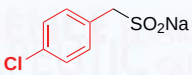

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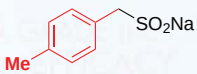

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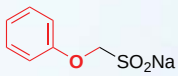

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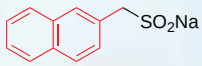

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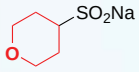
Saturated Heterocycles



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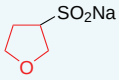

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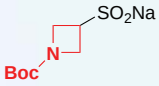

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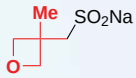

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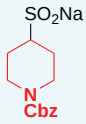

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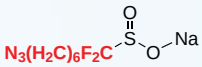
Linkers



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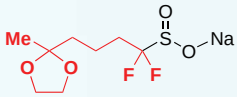

792446
Shabat Sulfinate

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