Maybridge Ro3 Diversity Fragment Library

MAYBRIDGE

... the industry leading library for fragment-based drug screening

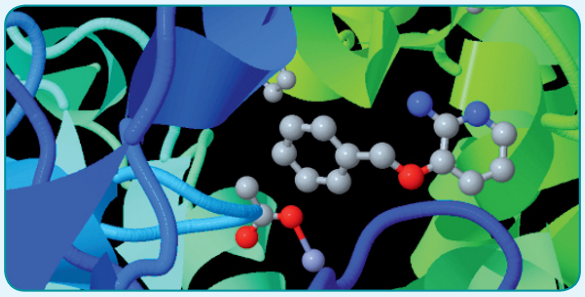
Accelerate your fragment screening program with the expanded Maybridge Ro3 Library

Fragment screening is becoming a method of choice in the quest for rapid identification of new lead molecules in drug discovery due to the higher hit probability and fewer fragments needing to be screened. The Maybridge fragment library is a proven, industry-leading library due to its diversity, pharmacophoric content and novelty.

To further increase the diversity and provide a greater coverage of lead-like chemical space we have redesigned our fragment library. The new library contains 2,500 carefully selected fragments, and it provides the optimal balance between broad coverage of lead-like diversity space and the number of fragments required to be screened.

Key features and benefits:

- Rule of Three (Ro3) compliance delivers superior ADME attributes
- A 30% increase in diversity over the previous library – Tanimoto similarity index of 0.66 based on standard Daylight fingerprinting
- Experimentally measured solubility – guaranteed solubility of fragments in PBS buffer (1mM) ensures robust screening data and minimizes candidate attrition
- Assured quality of >95%, NMR spectrum available for each of the 2,500 compounds
- Chemically "clean" – filtered to remove toxic and reactive groups
- Chemical functionality selected to allow rapid chemical evolution and optimization of fragment hits
- Pharmacaphore rich, but not too complex to allow simpler interpretation of the results
- Fragment hopping is facilitated with the entire Maybridge portfolio, for the full range visit www.maybridge.com



The Maybridge Ro3 Diversity Fragment Library is available in the following formats

Available format	Comments
Entire library with **2,500** compounds	Highly recommended. It provides the highest probability to find a hit.
A **core set** of the entire library with **1,000** compounds	It encompasses the diversity of the entire library. Suitable for rapid and exploratory work.
A **supplement set** of the entire library with **1,500** compounds	For those who have screened the core set. It provides an additional probability to identify more hits.
Customised set	A selection of any number of fragments. Our searchable database allows rapid selection of fragments based on substructure and calculated Ro3 parameters.
Complete convenience	Custom weighed to your requirements in milligram or micromolar quantities.

Leading the way in fragment library design since 2005

2005

The Maybridge Fragment Library

One of the first commercially available fragment libraries.

- 500 compounds cherry-picked from the pharmacophore-rich Maybridge building block portfolio

2007

The Maybridge Ro3 Fragment Library

The first commercially available Ro3-compliant library.

- 1,000 compounds computationally selected to provide:
  - Full "Rule of Three" compliance
  - High structural diversity
  - Pharmacophore-rich fragments containing "linker-friendly" groups for hit evolution

The Maybridge Fragment Collection

- 30,000+ compounds
- Convenient access to the extensive Maybridge portfolio
- Powerful tool for building bespoke fragment screening libraries or searching for hit analogues

2009

The Maybridge Ro3 Fragment Library Solubility Upgrade

The first commercially available fragment library with assured solubility.

- Experimental solubility data acquired for each of the 1,000 Ro3 library compounds
- Each member of the library has been shown to dissolve in:
  - DMSO at 200mM
  - PBS buffer (0.5% DMSO) at 1mM
- The solubility assurance is an additional benefit to the Ro3 and diversity advantages of the original library

2010

The Maybridge Ro3 Diversity Fragment Library

Developed with fragment screening practitioners to provide the most practical and powerful fragment library available.

- 1,500 compounds selected from the Maybridge and Acros Organics portfolios to provide:
  - Improved structural diversity
  - Access to a broader, wider pool of analogues for "fragment hopping"
  - "Linker-friendly" groups allow for rapid hit evolution
  - Full "Rule of Three" compliance
  - Experimental solubility assurance for each compound in the library

2011

Expansion of the Maybridge Ro3 Diversity Fragment Library

As the number of fragments that can be screened during assays increases due to the development of higher throughput biophysical techniques such as surface plasmon resonance, we have added additional fragments.

This has enabled us to:

- Increase the diversity by 30%
- Redesign the library to maximize the diversity across all the subsets
- Offer a greater number of high quality fragments for custom selection

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