Discover. Synthesize. Analyze. Customize.

Maybridge HitCreator
the ultimate diversity library!

Diversity-based screening continues to be a vital tool for drug discovery. Efficiency and productivity can be improved by using screening libraries that offer maximum diversity whilst retaining drug-like properties. Faced with a bewildering array of commercially available screening libraries, each with their own differing characteristics, it can be difficult for drug discovery scientists to pick the ideal screening library for their specific requirements.

Our unique new offering takes away the need to choose between different libraries by providing exceptional coverage of drug-like chemical space with a single library. Building on more than 50 years of expertise in designing industry-leading screening libraries, the pre-plated Maybridge™ HitCreator consists of 14,000 screening compounds, derived from a rigorous analysis of more than 500,000 commercially available screening compounds. These compounds have been selected using a clustering algorithm, based on standard Daylight fingerprints and Tanimoto similarity. Each Maybridge HitCreator is conveniently supplied as dry films in Thermo Scientific™ Matrix 96 shallow-well plates or 384-well microplates.

Key features and benefits:

- **High diversity** – applied Daylight fingerprints and Tanimoto similarity calculations based on the Tanimoto coefficient of 0.65 to produce an exceptionally diverse commercial library providing the best opportunity to find hits
- **High hit probability** – all the compounds are drug-like, conforming to "Lipinski's Rule of Five" and additional filters, such as PSA ≤ 140Å^2
- **Reliability** – the compounds contained within the library have been screened to remove any inappropriate chemical structures, avoiding "false hits"
- **Convenience** – all 14,000 compounds are available off the shelf, as 1 micromole in 96-well plates or 0.25 micromole in 384-well plates

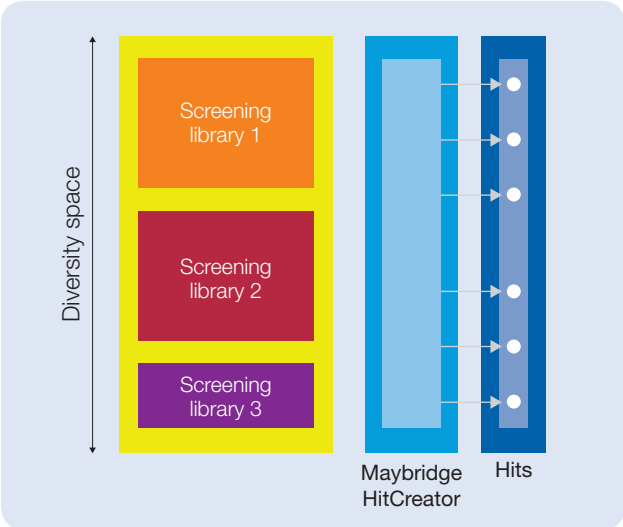


Figure 1. Importance of diversity in finding hits

The figure above illustrates how a highly diverse screening library will provide a greater hit probability than larger, but less diverse libraries.

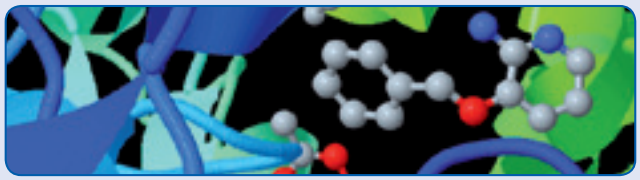
MAYBRIDGE

Accelerate your fragment screening program with the 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™ Ro3 library is a proven industry-leading library due to its diversity, pharmacophoric content and novelty.

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



Discover our entire range at www.maybridge.com.

To place an order, contact your local distributor.

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