



# Maybridge Fragments

**Open the door to accelerated lead generation by incorporating our extensive, class leading range of Maybridge Fragments into your structure based screening programme.**

The Maybridge Fragment range has been developed to provide not only the quality and structural diversity you have come to expect from Maybridge products, but also the flexibility to meet your needs. The choice of superior off the shelf collections and the ability to "cherry pick" from our carefully selected Fragment lists when creating your own bespoke libraries gives you both convenience and total control of your Fragment screening programmes.

## The Maybridge Ro3 Fragment Library

A premier 'off the shelf' set of 1000 compounds which offer optimal physico-chemical properties. In addition to the ease of ordering an off the shelf product this library benefits from being:

- > Rule of Three (Ro3) compliant<sup>1</sup>
- > Quantifiably diverse through the application of industry standard chemometrics<sup>2</sup>
- > Pharmacophorically rich with the inclusion of many unique Maybridge heterocycles
- > High purity ( $\geq 95\%$ )
- > Aqueous solubility assured (ALogGPS – with outliers confirmed by actual solubility measurement).<sup>3</sup>

## The Maybridge Ro3 500 Fragment Library

An 'off the shelf' offering of 500 compounds selected from the original Maybridge Ro3 set and designed to be a convenient, cost effective entry point to fragment screening.

## The Maybridge Fragment Collection

Over 30,000 Maybridge compounds assembled to provide convenient access to the extensive Maybridge portfolio when building your own bespoke fragment screening libraries or searching for Hit analogues. The Collection has been filtered in terms of purity ( $\geq 90\%$ ), molecular weight ( $\leq 350\text{Da}$ ) and removal of inappropriate functionality to allow you complete freedom to design a library to your own specific needs.<sup>4</sup>

## The Maybridge Bromo-Fragment Collection

A collection of over 1500 bromine containing Maybridge Fragments constructed as an aid to X-ray based fragment screening and to provide a set of Fragments suited to rapid hit evolution.

## The Maybridge Fluoro-Fragment Collection

A set of over 5300 fluorine containing fragments which are a convenient source for <sup>19</sup>F NMR based applications.<sup>5</sup>

## The Maybridge Pre-Fragment Collection

Is an invaluable source of reactive "pre-fragments" which can be used to either synthesise your own bespoke fragments or to evolve your Hits. We currently have available sets of:

- > Sulfonyl chlorides
- > Isocyanates
- > Acid chlorides and pentafluorophenyl esters

In addition we have produced a set of **Self Assembly Fragments** that contain a reactive aldehyde moiety for use in specialised screens which link fragments to generate active ligands *in situ* at the protein target site.<sup>6</sup> Amine containing self assembly partners can be selected from The Maybridge Fragment Collection.

**Maybridge Fragments are available custom weighed to your requirements in milligram ( $\geq 5\text{mg}$ ) or micromolar quantities ( $\geq 25\mu\text{mol}$ ) and have been selected to ensure that they are readily available for re-supply.**

**Download the structures and physicochemical data for each set in the range at [www.maybridge.com](http://www.maybridge.com)**

**Please contact us for a quotation or more information at [maybridge.sales@thermofisher.com](mailto:maybridge.sales@thermofisher.com)**

### References

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2. D. J. Butina, *J. Chem. Inf. Comput. Sci.*, 1999, **39**, 747-750
3. I. Tetko *et al.*, *J. Chem. Inf. Comput. Sci.*, 2002, **42**, 1136-45 ([www.vclab.org](http://www.vclab.org))
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5. C. Dalvit *et al.*, *Drug. Dev. Res.*, 2005, **64**, 105-113
6. I. Huc and J. M. Lehn, *Proc. Natl. Acad. Sci.*, 1994, 2106-2110

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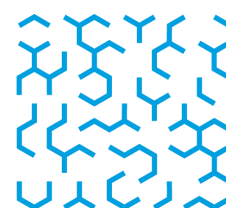
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Compounds for  
Drug Discovery