

### UORSY Shaped fragments

Until recently, fragment libraries have been mostly dominated by planar, rod-like compounds. However, adding shape descriptor upon designing fragments will result in broad coverage of chemical space and allow to increase diversity without increasing the complexity.<sup>12</sup> Following this notion, we created a collection of 598 fragment-like molecules with remarkable shape diversity (Figure 1, left). The library complies with “Rule of Three”, has been filtered to remove PAINS and “overused” motifs. Similarity analysis revealed novelty and uniqueness of **UOrSy shaped fragments** compared with commercially available collections (Figure 1, right).

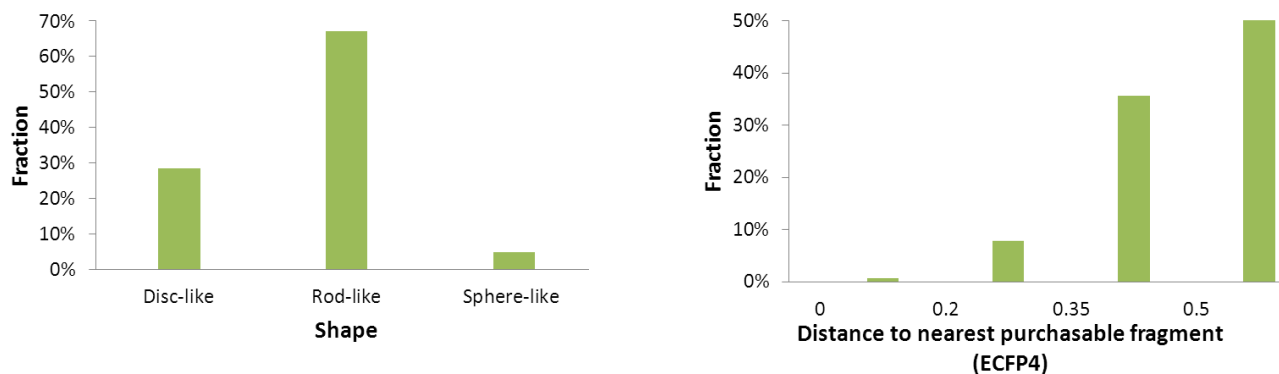
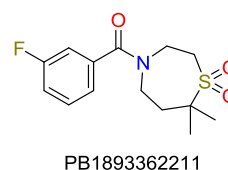
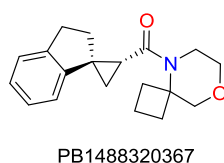
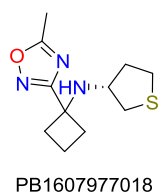


Figure 1. Shape analysis<sup>2</sup> (left) and similarity analysis (right) of **UOrSy shaped fragments**.



#### Physicochemical profiles of **UORSY shaped fragments**:

110<MW<300; HbA≤3; HbD≤3; logP≤3; RotBonds≤3.

**UORSY shaped fragments** are available in stock and could be delivered within 2 weeks in any customer-preferred format: as powders, dry films or DMSO solutions formatted in vials, 96 or 384-well plates. All compounds have a minimum purity of 90% assessed by <sup>1</sup>H NMR; analytical data is provided.

For more information, please contact us at [screenlibs@uorsy.com](mailto:screenlibs@uorsy.com)

<sup>1</sup>Morley *et al.*, Drug Discov Today, 2013, 18, 1221–1227

<sup>2</sup><http://practicalfragments.blogspot.com/2013/08/3d-fragmentsan-analysis.html>