UORSY
unlimited
discovery
opportunities

UORSY Mixed Shapes Library

Shape of small molecule compounds has been postulated as an important factor for efficient binding to a biological target. Principal moments of inertia (PMI) is one of the widely accepted[1] approaches to characterize shape diversifying compounds as disc-like, rod-like, and sphere-like. According to PMI analysis, most commercially available collections are enriched with rods or discs but not spheres.[2] 3D shaped molecules, however, are commonly found among natural products and a number of publications showing advantages of 3D structures over planar ones has been released.[3,4]

We offer a mixed shapes library with enriched fraction of sphere-like molecules that allows for equal testing all possible shapes (Figure 1). To ensure high quality of the library, we applied PAINs filtering and "overused" substances removal that yielded a set of 867 lead-like compounds.

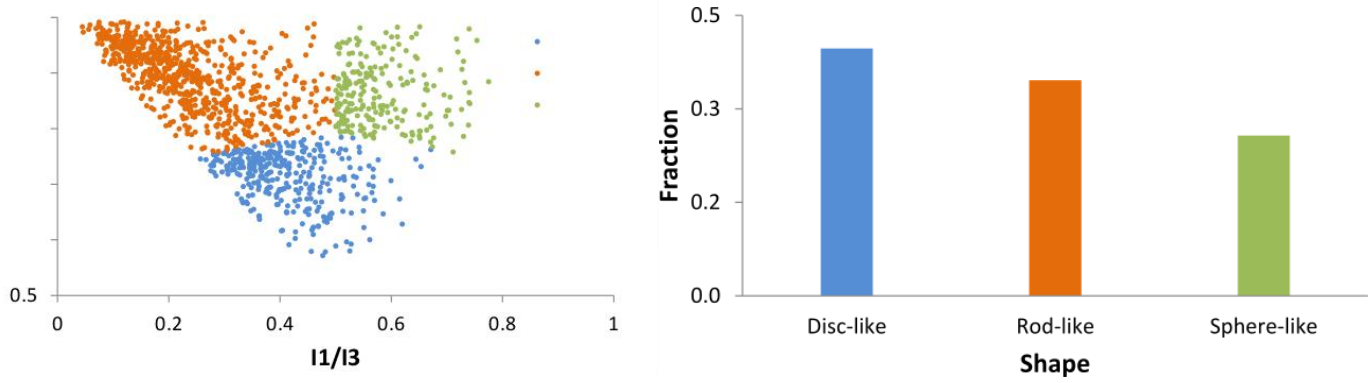
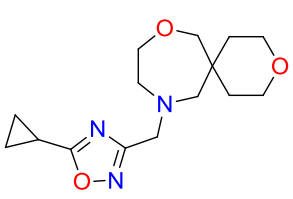


Figure 1. PMI analysis of UORSY **mixed shapes compounds**.



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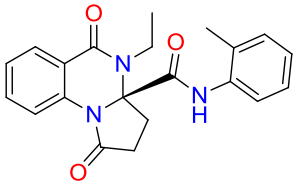

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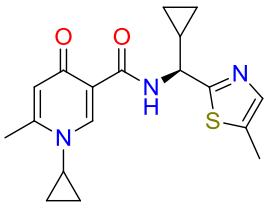

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UORSY mixed shapes compounds are available in stock and could be delivered within 2 weeks in any customer-preferred format: as powders, dry films or DMSO solutions formatted in vials, 96 or 384-well plates. All compounds have a minimum purity of 90%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

For more information, please contact us at **screenlibs@uorsy.com**

[1]W. H. B. Sauer, M. K. Schwarz, *J. Chem. Inf. Comput. Sci.* **2003**, *43*, 987–1003.
[2]P. A. Clemons, J. A. Wilson, V. Dančík, S. Muller, H. A. Carrinski, B. K. Wagner, A. N. Koehler, S. L. Schreiber, *PNAS* **2011**, *108*, 6817–6822.
[3]F. Lovering, J. Bikker, C. Humblet, *J. Med. Chem.* **2009**, *52*, 6752–6756.
[4]N. C. Firth, N. Brown, J. Blagg, *J. Chem. Inf. Model.* **2012**, *52*, 2516–2525.