

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 accepted¹ 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.

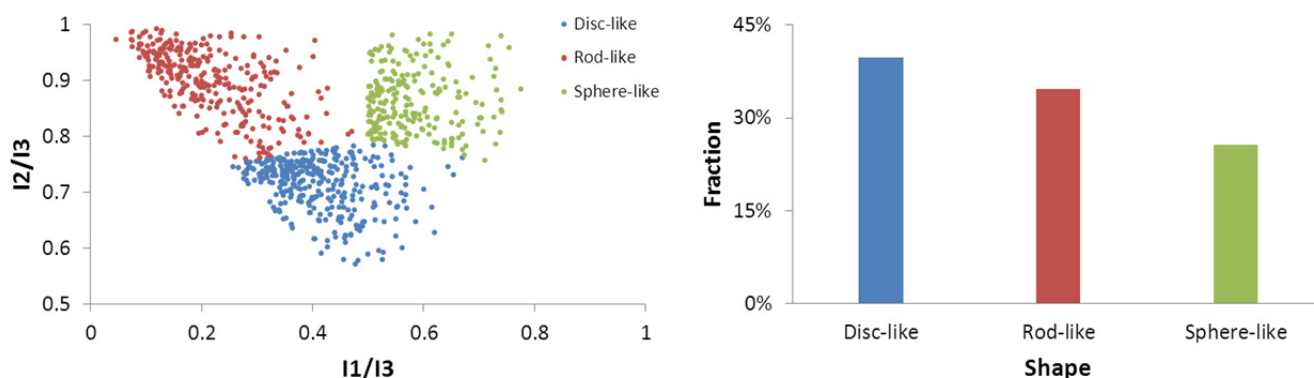
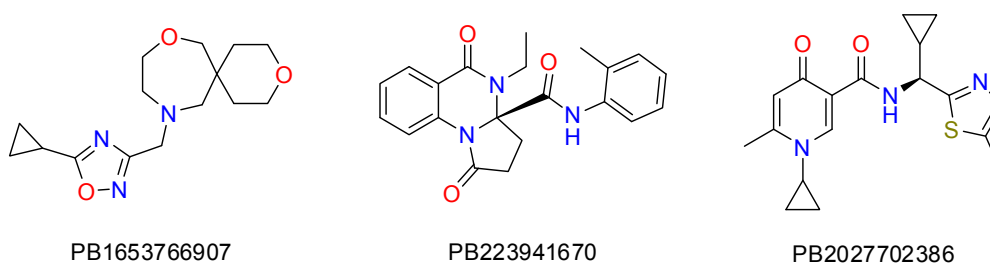


Figure 1. PMI analysis of UORSY mixed shapes compounds.



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 ¹H NMR; analytical data is provided.

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

¹W. H. B. Sauer, M. K. Schwarz, *J. Chem. Inf. Comput. Sci.* **2003**, *43*, 987–1003.

²P. 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.

³F. Lovering, J. Bikker, C. Humblet, *J. Med. Chem.* **2009**, *52*, 6752–6756.

⁴N. C. Firth, N. Brown, J. Blagg, *J. Chem. Inf. Model.* **2012**, *52*, 2516–2525.