

### UORSY Saturated Fragments Library

Structural motifs with high content of  $sp^3$ -hybridized carbon atoms are widespread in clinically evaluated compounds.<sup>1</sup> Indeed, increasing mean  $F_{sp^3}$  of screening collections, called “escape from flatland,”<sup>2</sup> has been a way to positively influence ADMET profiles. Following the notion, we created a library of saturated fragments. The library contains 1356 compounds that comply with “Rule of Three” and has favorable physicochemical profiles (Figure 1, left). Similarity analysis revealed high dissimilarity to the commercially available fragment sets (Figure 1, right).

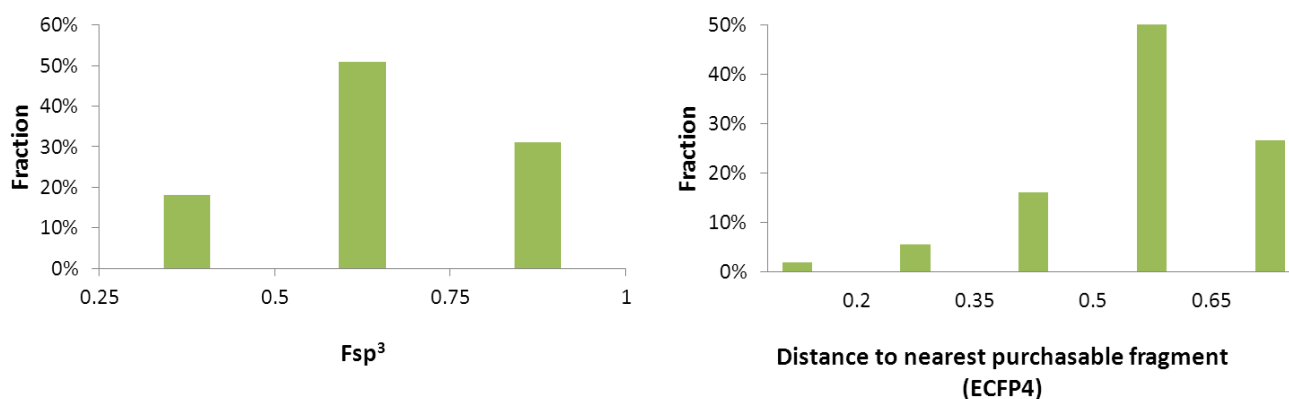
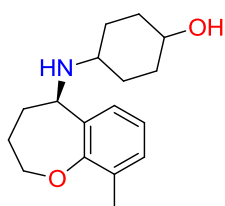
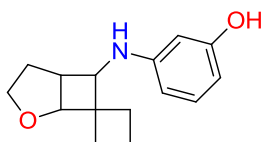


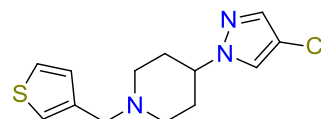
Figure 1. Distribution of  $F_{sp^3}$  (left) and similarity analysis (right) of **C saturated fragments**.



PB1436915828



PB1799337364



PB1631773746

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

$100 < MW < 300$ ;  $HbA \leq 3$ ;  $HbD \leq 3$ ;  $\log P \leq 3$ ;  $RotBonds \leq 3$ ;  $ChiralCenters \leq 4$ .

**UORSY saturated 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  $^1H$  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 Discovery Today*, **2013**, *18*, 1221–1227

<sup>2</sup>Lovering et al, *J. Med. Chem.* **2009**, *52*, 6752–6756