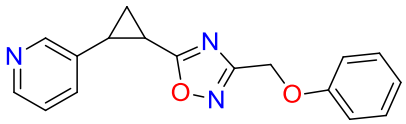
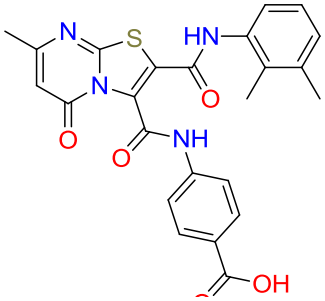
UORSY
unlimited
discovery
opportunities

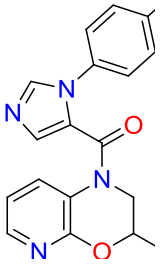
UORSY DYRK1A/B Modulator Library

DYRK family of protein kinases plays crucial role in numerous neurodegenerative diseases (from Alzheimer to Down syndrome). The action of existing kinase modulators is predominantly based on the competitive binding mechanism, for which the knowledge about hinge binding motif is important. Determined hinge binding motif of DYRK1A/B differs them advantageously from the range of other kinases. Considering this, we have summarized the data of modulators' activity and selectivity known from the literature.[1,2,3]

The docking based on hot-spot approach was performed and compounds, which form undesirable hydrogen bonds, were removed to increase selectivity. The resulting set contains 493 compounds and is available in 2D and 3D along with docking scores upon request.







Physicochemical profiles of **UORSY DYRK1A/B modulator library**:
250<MW<540; 2<HbA<8; 0<HbD<3; -0.5<logP<6; RotBonds≤8; TPSA<140.

UORSY DYRK1A/B modulator library is available as powders, dry films or DMSO solutions. 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] Cuny G. et al., *Bioorg. Med. Chem. Lett*. **2012** 22 2015-2019
[2] Anderson K. et al., *Bioorg. Med. Chem. Lett.* **2013** 23 6610-6615
[3] Falke H. et al., *J. Med. Chem*. **2015**, 58, 3131-3143