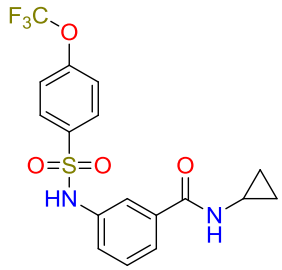
UORSY
unlimited
discovery
opportunities

UORSY PPI Modulators

Modulating protein-protein interactions (PPIs) has been considered as an important goal for drug discovery because of their role in numerous cell disorders.[1] PPIs, however, are both highly promising and highly difficult to study.[2] Much of the success in finding "hidden gems" – small molecule modulators of PPIs, – relies on the quality of the starting library. Understanding this, we created a set of PPIs modulators utilizing the following approaches:

1) physicochemical criteria ("Rule of 4" for inhibitors of PPIs);
2) the "hot spot" paradigm (design included functional groups able to interact with Tyr, Trp, Arg residues);[3]
3) ligand-based design (similarity analysis to TIMBAL database).[4]

Additional filtering to remove PAINS, toxic, and "overused" substances yielded a set of 6482 compounds.



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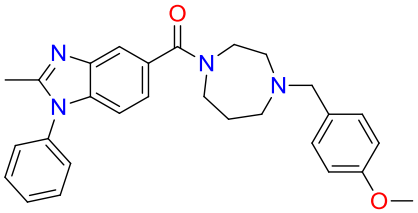

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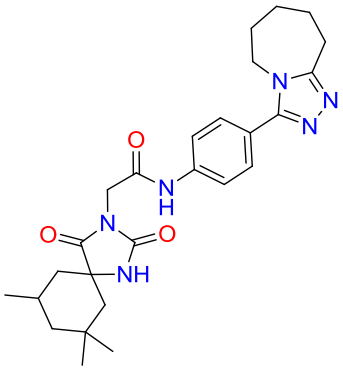

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Physicochemical profiles of **UORSY PPI modulators**:
400<MW<600; 2<HbA<10; 0<HbD<4; 2<logP<6; 1≤RotBonds≤12; TPSA>50.

UORSY PPI modulators 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]Morelli, X.; Hupp, T., *EMBO Rep*. **2012**, 13, 877–879
[2]Surade, S.; Blundell, T. L., *Chemistry and Biology*, **2012**, 19, 42–50
[3]Wells, J. A.; McClendon, C. L., *Nature* **2007**, 450, 1001–1009
[4]Higueruelo, A. P.; Jubb, H.; Blundell, T. L., *Database (Oxford)*. **2013**, 2013, bat039