OTAVA chemicals

Compounds for HTS
Chemical building blocks
Fragment libraries
Targeted libraries
Drug discovery services

BETA-TURN PEPTIDOMIMETIC LIBRARY

OTAVA chemicals

OTAVA offers a beta-Turn Peptidomimetic Library. It contains synthetic compounds which mimic beta-turns of proteins. This library provides an excellent basis for drug discovery projects focused on protein-protein interactions.

The library consists of 94**8 compounds***.

All compounds are:

- **in stock**; available amounts: 1 – 50 mg
- reactive, pan-assay interference (PAINS), redox-active and aggregator compounds were removed from the library.

QA/QC passed:

- minimal purity of compounds is **90%**;
- by **NMR** and/or **GC/LC/MS**
- **NMR spectra are available** upon request

Frendly packing services:

- **Cherry-picking is available**
- Supplied as dry powder or DMSO solution**
- Packaging in deep-well plates or barcoded vials***
- **Weighing out is free**

*Please note that the library does not contain known inhibitors. The compounds were selected with computational approach and are intended for screening projects

**there is additional fee for preparation of the solution

***4 ml amber glass vials or Deep-well plates: Matrix cat# 4247 (1.4 mL, Blank, Polypropylene, Round Bottom Tubes) w/CapMats. Or plates and vials provided by customer.

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	222.3	537	405.1
Number of Hydrogen Bond Donors	0	7	1.1
Number of Hydrogen Bond Aceptors	2	9	4.9
Number of Rotatable Bonds	0	14	5.4
CLogP	-2	6.6	3.4
Number of Rings	1	7	3.7
Polar Surface Area	16.9	183,4	86.6

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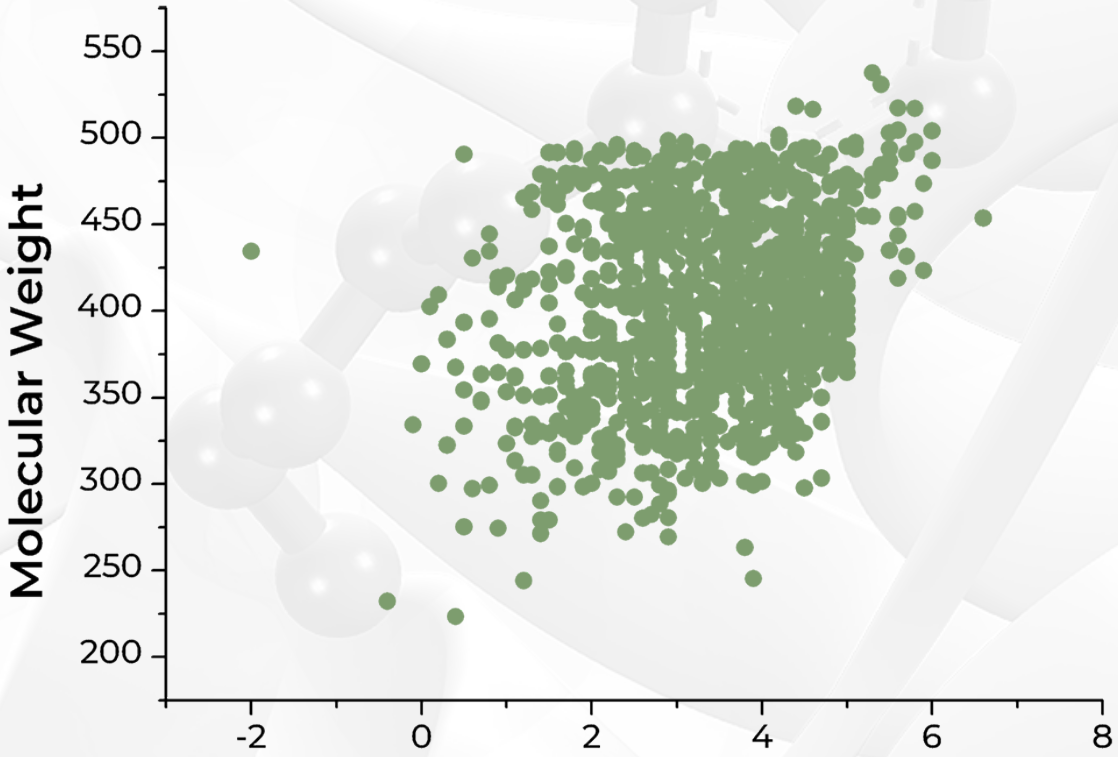
Distribution of physicochemical properties of compounds in the library:

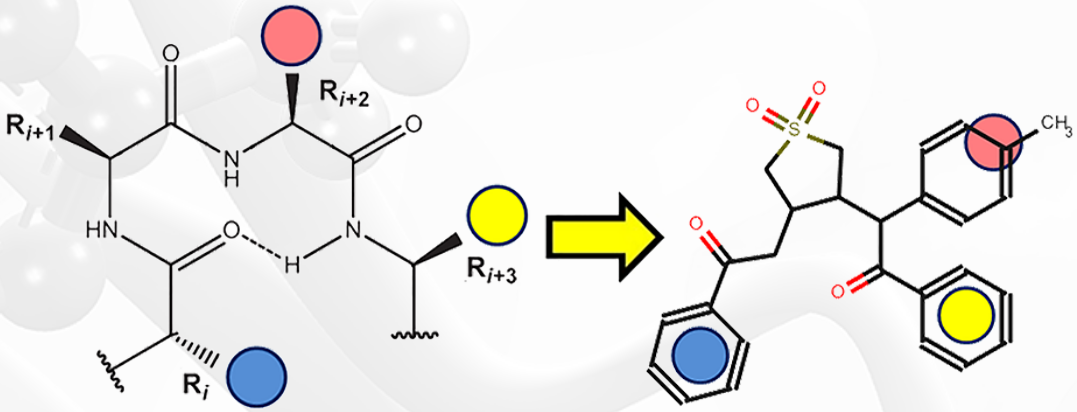
79% Drug-like

30% Lead-like



Design speciality:

The library has been carefully prepared with two selection procedures and diversity clustering. The first selection was made using pharmacophore screening where the pharmacophore model was based on real beta-turn structures*. The second selection was performed using similarity search to already known scaffolds of beta-turn peptidomimetics such as pentameric** and hexameric*** cycle scaffolds, bicyclic scaffolds**** and others.



*Jari J. Koivisto, Esa T. T. Kumpulainen and Ari M. P. Koskine, Conformational ensembles of flexible b-turn mimetics in DMSO-d6. Org. Biomol. Chem. – 2010 – Vol. 8, p. 2103–2116.

**Landon R. Whitby, Yoshio Ando, Vincent Setola, Peter K. Vogt, Bryan L. Roth, and Dale L. Boger, Design, Synthesis, and Validation of a beta-Turn Mimetic Library Targeting Protein-Protein and Peptide-Receptor Interactions. J. Am. Chem. Soc. – 2011 – Vol. 133, p. 10184–10194.

***Ralph F. Hirschmann et al., The beta-D-Glucose Scaffold as a beta-Turn Mimetic. Acc Chem Res. – 2009 – Vol. 42(10), p. 1511–1520.

****Adam Golebiowsk et al., Solid-Supported Synthesis of Putative Peptide beta -Turn Mimetics via Ugi Reaction for Diketopiperazine Formation. J. Comb. Chem. – 2002 – Vol. 4, p. 584–590.

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Custom synthesis

Molecular modeling

Amyloids detection

Contract research

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