OTAVA chemicals

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

ALPHA-HELIX PEPTIDOMIMETIC LIBRARY

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OTAVA offers an alpha-Helix Peptidomimetic Library. It is a synthetic compounds which mimic alpha-helixes of proteins. This library provides an excellent basis for drug discovery projects focused on protein-protein interactions.

The library consists of **1,2**32 **compounds***.

All compounds are:

- **in stock**; available amounts: 1 – 50 mg
- **Drug-like only**; 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	207.3	500	387
Number of Hydrogen Bond Donors	0	5	2.3
Number of Hydrogen Bond Aceptors	1	10	4.7
Number of Rotatable Bonds	2	11	7.1
CLogP	-1	5	3.1
Number of Rings	1	6	3.1
Polar Surface Area	26.7	200	97.4

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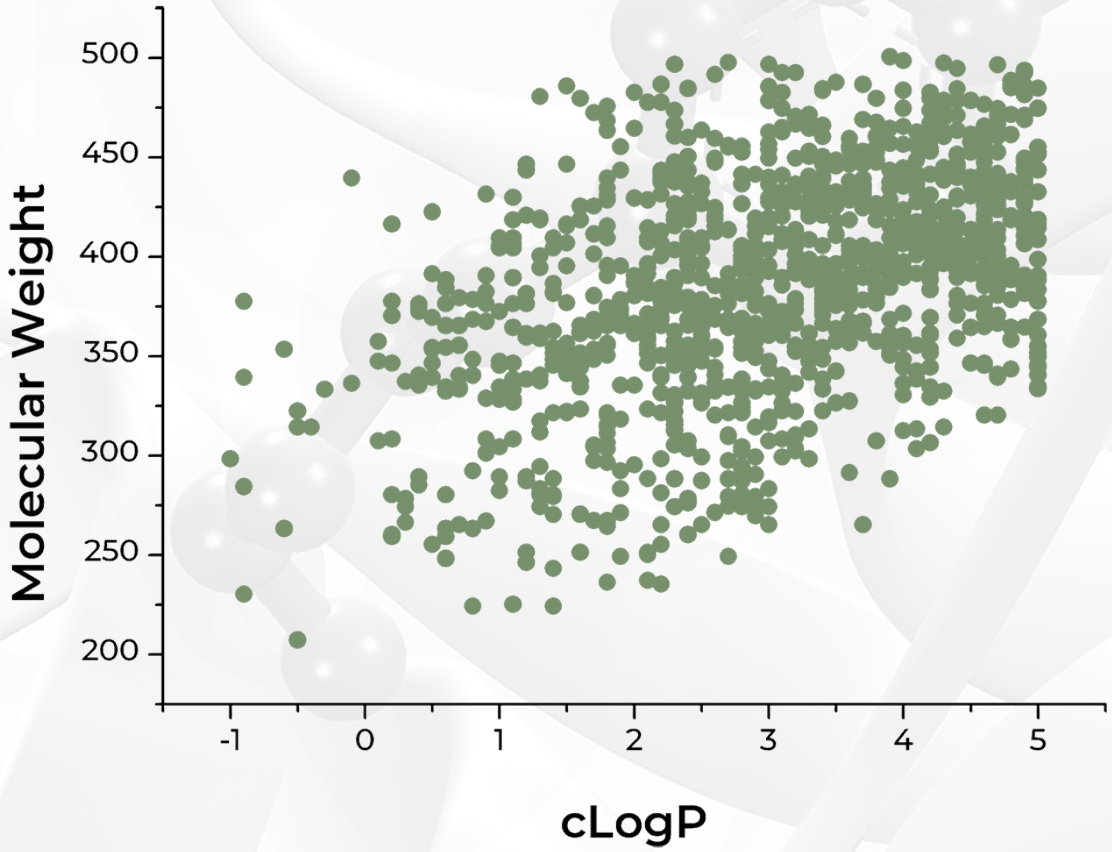
Distribution of physicochemical properties of compounds in the library:

100% Drug-like

41% Lead-like



Design speciality:

The library has been carefully prepared with Bayesian models using active template compounds from ChEMBL database and literature* (Scheme 1). Two models were developed for each training sets. The first one was based on FCFP6 fingerprints, the second one – on ECFP6. Molecular descriptors, such as LogP, molecular weight, number of hydrogen donors and acceptors, number of rotatable bonds, number of rings and molecular polar surface area were involved in the construction of the models for more accuracy.

1,232 **compounds** were selected using this models.

*Maryanna E. Lanning and Steven Fletcher, Multi-Facial, Non-Peptidic a-Helix Mimetics, Biology 2015, 4, 540-555; doi:10.3390/biology4030540.

Christopher G Cummings and Andrew D Hamilton, Disrupting protein–protein interactions with non-peptidic, small molecule a-helix mimetics, Current Opinion in Chemical Biology 2010, 14:341–346

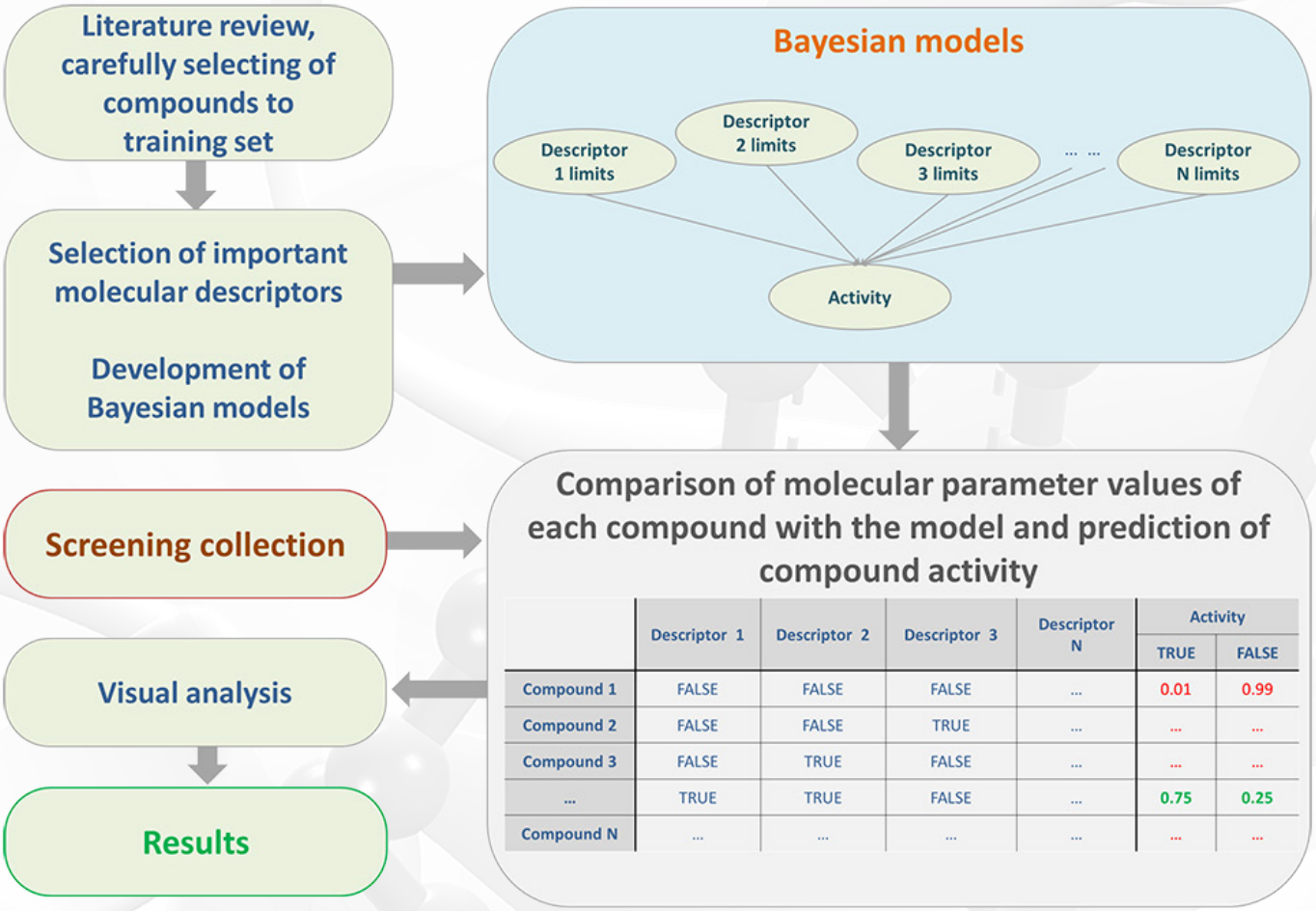
Jessica M. Davis, Lun K. Tsoub and Andrew D. Hamilton, Synthetic non-peptide mimetics of a-helices, Chem. Soc. Rev., 2007, 36, 326–334.

Madura K. P. Jayatunga, Sam Thompson, Andrew D. Hamilton, a-Helix mimetics: Outwards and upwards, Bioorganic & Medicinal Chemistry Letters 24 (2014) 717–724.

Maryanna Lanning & Steven Fletcher, Recapitulating the a-helix: nonpeptidic, low-molecular-weight ligands for the modulation of helix-mediated protein–protein interactions, Future Med. Chem. (2013) 5(18), 2157–2174.

Andrew J. Wilson, Helix mimetics: Recent developments, Progress in Biophysics and Molecular Biology (2015), doi:10.1016/j.pbiomolbio.2015.05.001.

Scheme 1. Application of Bayesian modeling for design of targeted library



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