OTAVA chemicals

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

DIVERSITY LIBRARIES

OTAVA chemicals

OTAVA offers Diversity Libraries. These sets of diverse drug-like compounds are the best choice for primary screening and can be applied to a wide range of targets.

The library consists of:

- PrimScreen1 – **1,000** compounds;
- PrimScreen2 – **2,000** compounds;
- PrimScreen3 – **3,000** compounds;
- PrimScreen5 – **5,000** compounds;
- PrimScreen10 – **10,000** compounds;
- PrimScreen15 – **15,000** 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 libraries.

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**

*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.

Library overview:

OTAVAchemicals Diversity Libraries **PrimScreen1**, **PrimScreen2**, **PrimScreen3**, **PrimScreen5**, **PrimScreen10** and **PrimScreen15** are prepared by diversity sorting using CheD software. Diversity is a property of dataset and characterizes the similarity (or dissimilarity) of molecules included in it. The goal of Diversity calculation and sorting is to select a maximally diverse subset of a given size from a given large pool of candidate molecules. The diverse data set can be used for screening purposes to reduce expenses for compounds testing or compounds selection.

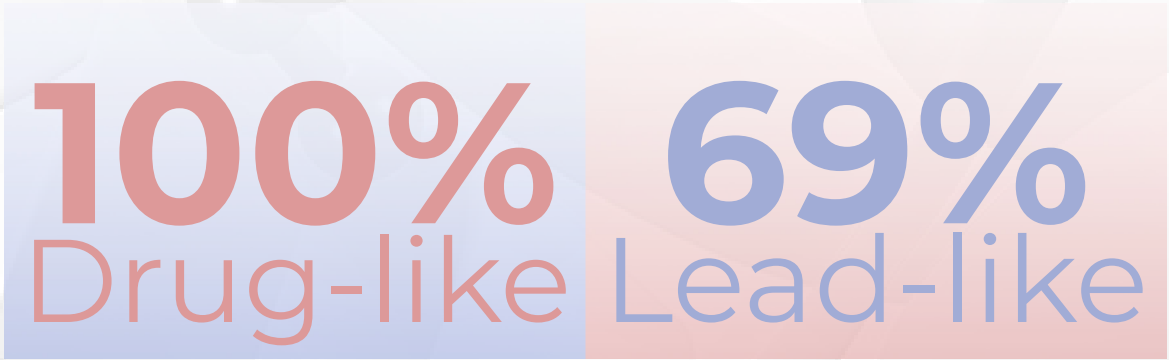
Diversity set	Number of compounds	Min. value of diversity	Number of Scaffolds
PrimScreen1	1,000	0.8922	898
PrimScreen2	2,000	0.8793	1,625
PrimScreen3	3,000	0.8703	2,273
PrimScreen5	5,000	0.8601	3,468
PrimScreen10	10,000	0.8460	5,894
PrimScreen15	15,000	0.8383	7,920

PrimScreen1

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	162.2	499	326.3
Number of Hydrogen Bond Donors	0	5	1.1
Number of Hydrogen Bond Aceptors	0	10	4.1
Number of Rotatable Bonds	0	11	4.1
CLogP	-1	5	2.7
Number of Rings	1	6	2.9
Polar Surface Area	4.9	239.2	79.2

Distribution of physicochemical properties of compounds in the library:

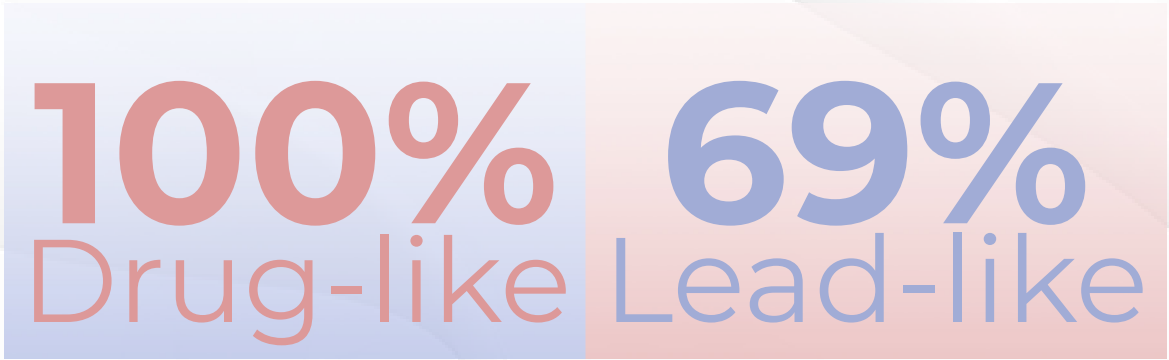


PrimScreen2

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	160.2	499	325.1
Number of Hydrogen Bond Donors	0	5	1.1
Number of Hydrogen Bond Aceptors	0	10	4
Number of Rotatable Bonds	0	11	4.1
CLogP	-1	5	2.8
Number of Rings	1	6	2.9
Polar Surface Area	3.2	239.2	78.6

Distribution of physicochemical properties of compounds in the library:

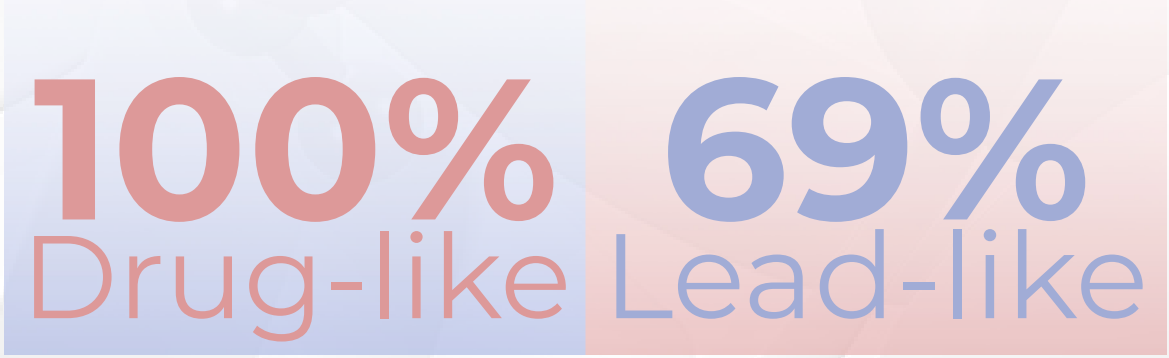


PrimScreen3

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	160.2	499	323.4
Number of Hydrogen Bond Donors	0	5	1.1
Number of Hydrogen Bond Aceptors	0	10	4
Number of Rotatable Bonds	0	11	4.1
CLogP	-1	5	2.8
Number of Rings	1	6	2.9
Polar Surface Area	3.2	239.2	78.2

Distribution of physicochemical properties of compounds in the library:

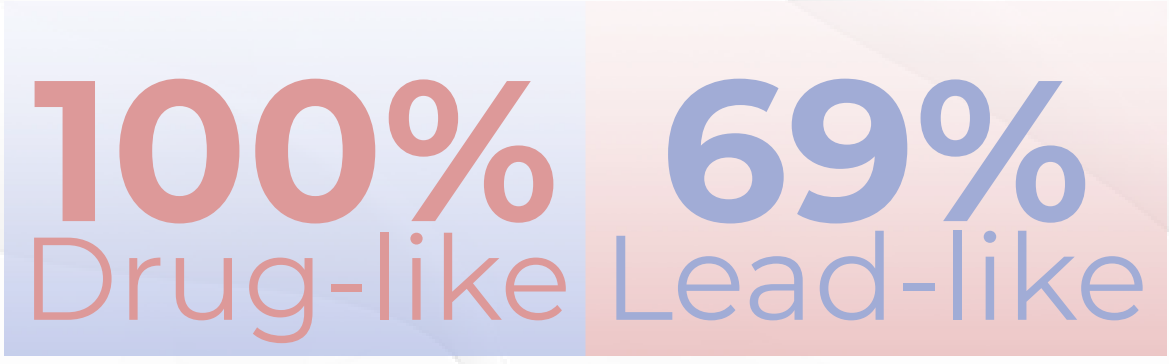


PrimScreen5

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	160.2	500	324.5
Number of Hydrogen Bond Donors	0	5	1.1
Number of Hydrogen Bond Aceptors	0	10	4
Number of Rotatable Bonds	0	11	4.1
CLogP	-1	5	2.8
Number of Rings	1	6	2.9
Polar Surface Area	0	239.2	78.5

Distribution of physicochemical properties of compounds in the library:

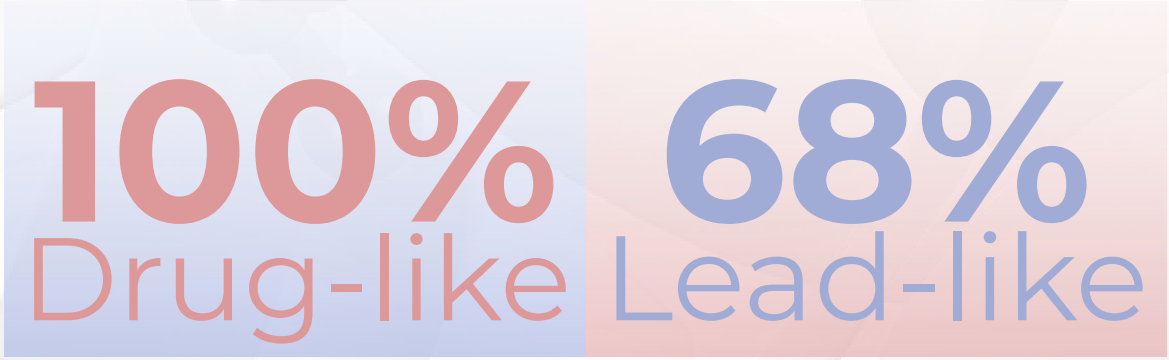


PrimScreen10

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	160.1	500	324.7
Number of Hydrogen Bond Donors	0	5	1.1
Number of Hydrogen Bond Aceptors	0	10	4
Number of Rotatable Bonds	0	11	4.1
CLogP	-1	5	2.8
Number of Rings	1	6	2.9
Polar Surface Area	0	239.2	78.2

Distribution of physicochemical properties of compounds in the library:

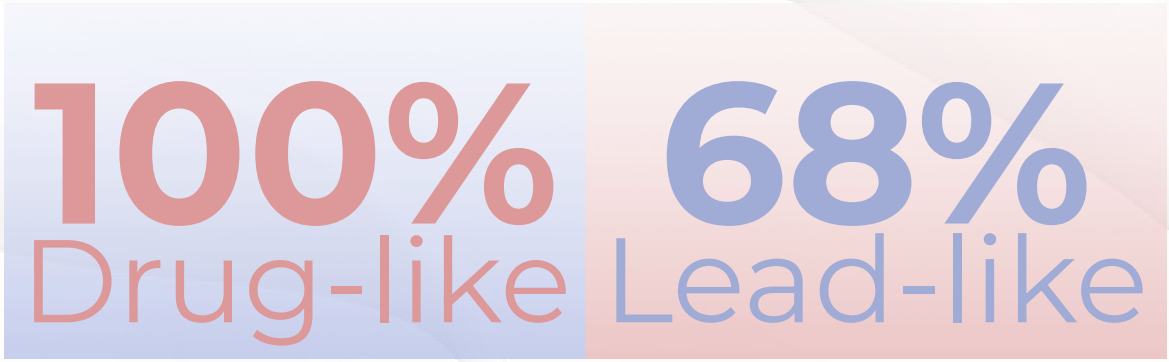


PrimScreen15

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	160.1	500	324.7
Number of Hydrogen Bond Donors	0	5	1.1
Number of Hydrogen Bond Aceptors	0	10	4
Number of Rotatable Bonds	0	11	4.1
CLogP	-1	5	2.8
Number of Rings	1	6	2.9
Polar Surface Area	0	239.2	78.3

Distribution of physicochemical properties of compounds in the library:



OTAVA chemicals

Custom synthesis

Molecular modeling

Amyloids detection

Contract research

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