OTAVA chemicals

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

RNA

RIBONUCLEIC ACID

TARGETED LIBRARY

OTAVACHEMICALS.COM

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OTAVA offers you RNA Targeted Library which is a special screening library that contains compounds with predicted RNA interaction activity based on different types of tertiary structures. The compounds have been selected with Bayesian models using a set of known RNA binding small molecules targeted hairpins, internal loops, bulges, stems and miRNA. Thus, the compounds from OTAVA's RNA Targeted Library match physical and structural parameters of typical RNA binders and contain important molecular fragments, required for interaction with RNA. The library consists of **2,730 compounds***.

All compouds 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.

Target's actuality:

The recent substantial progress in RNA biology underscores the importance of RNA in normal and aberrant cellular functions. Rather, it is now recognized that RNA is essential for transcriptional regulation, translational regulation, protein function, and catalysis, responsibilities that have classically been reserved for proteins.

It also highlights the potential of targeting RNA for treatment of a multitude of diseases including bacterial/viral infection and cancer.

Specificity to secondary structures :

RNAs can form well-defined secondary structures, such as double helices, hairpins, bulges, internal loop, stems, which offer structural basis for designing therapeutic agents. These structural features have been taken into account in the design of RNA Targeted Library, which contains compounds with predicted RNA interaction activity based on different types of secondary structures.

Design speciality:

The compounds have been selected with Bayesian models using most active template compounds from literature data*. We collected a training set of miRNA targeted compounds taken from PubChem database.

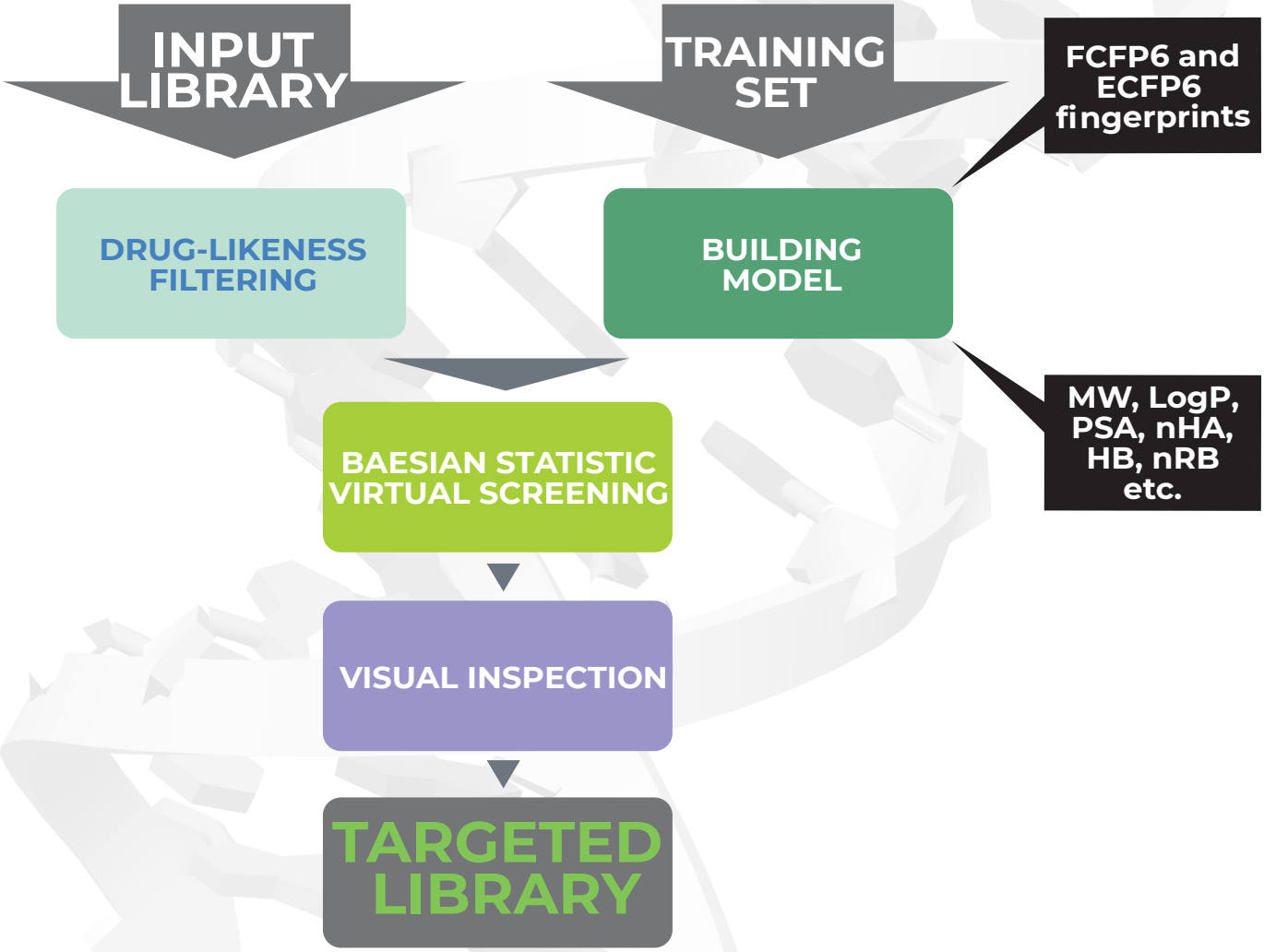
Two models were developed for each training sets. The first one was based on FCFP6 fingerprints, the second one - on ECFP6. Molecular descriptors, such as LogP, molecular weight, number of hydrogen donors and acceptors, number of rotatable bonds, number of rings and molecular polar surface area were involved in the construction of the models for more accuracy.

At the final stage, OTAVAchemicals Drug-like Green Collection was screened against these models and top-scored compounds were selected.

The compounds from the RNA Targeted Library match physical and structural parameters of typical RNA targeted compounds and contain important molecular fragments, required for RNA binding.

*Jason R. Thomas and Paul J. Hergenrother, Targeting RNA with Small Molecules, Chemical Reviews, Vol. 108, No. 4, 2008, pp. 1171 -1224.

Virtual screening flowchart:



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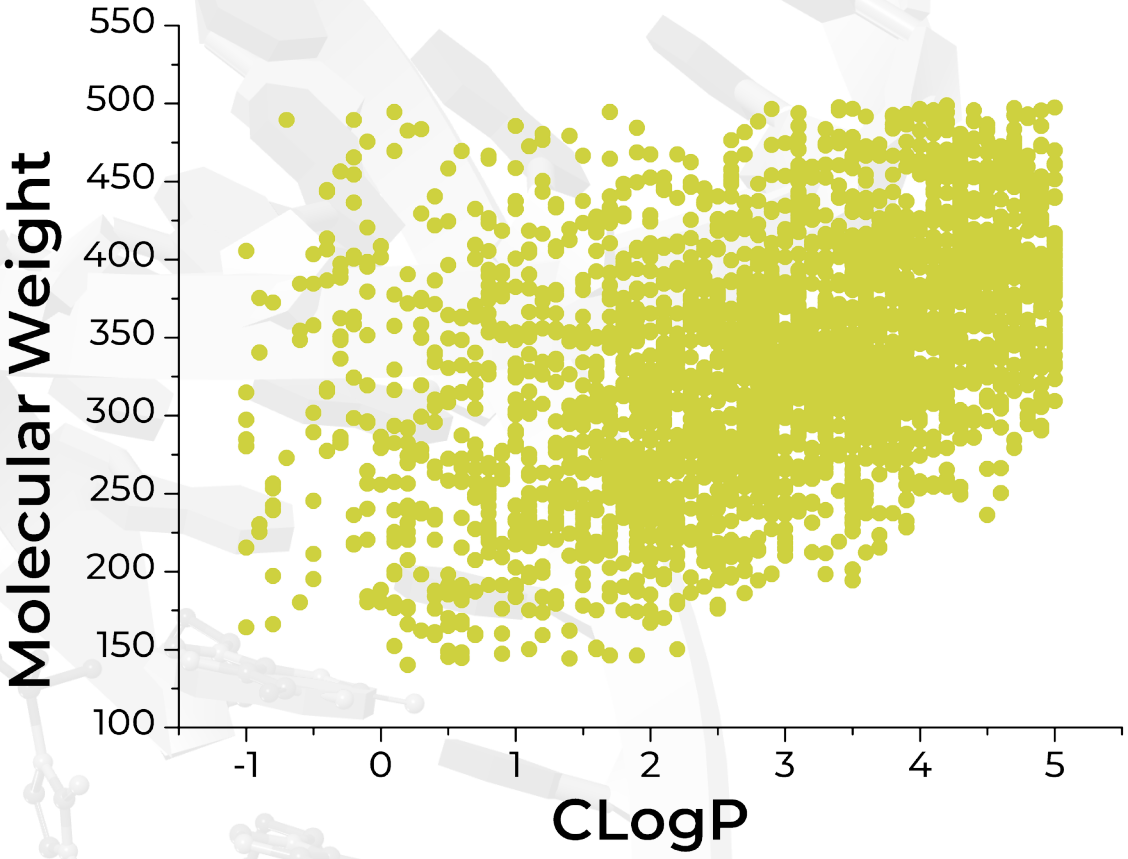
Distribution of physicochemical properties of compounds in the library:

100% Drug-like

58% Lead-like



The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	140.1	498.9	336.8
Number of Hydrogen Bond Donors	0	5	1,4
Number of Hydrogen Bond Aceptors	0	10	3.7
Number of Rotatable Bonds	0	11	4.2
CLogP	-1	5	2.9
Number of Rings	0	6	3.3
Polar Surface Area	6.5	195.1	78.6

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Custom synthesis

Molecular modeling

Amyloids detection

Contract research

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