Chemspace RNA-Targeted Library

O. Gavrylenko, O. Savych, B. Rogovoy, Y. Moroz

Overview

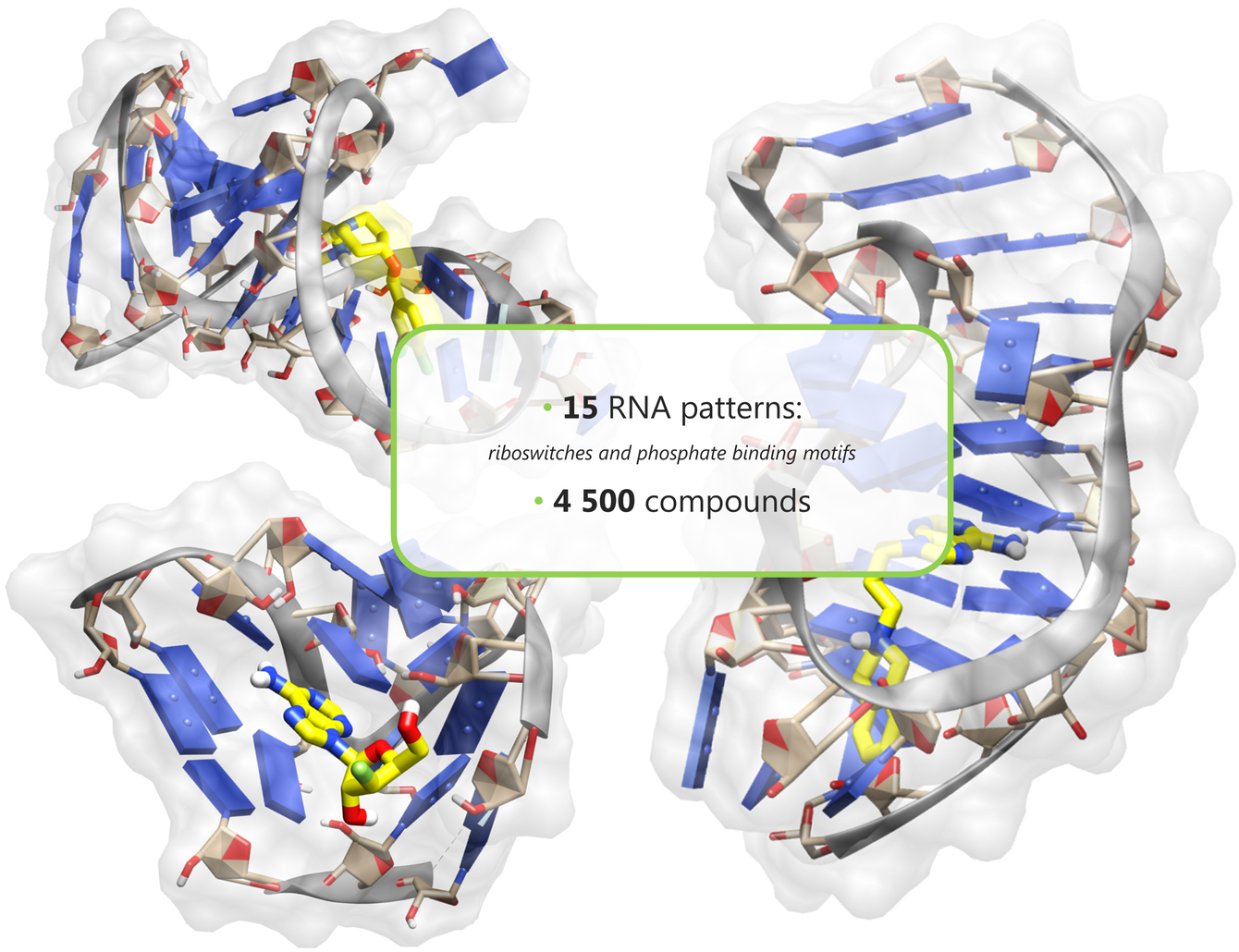
4 515 in-stock compounds

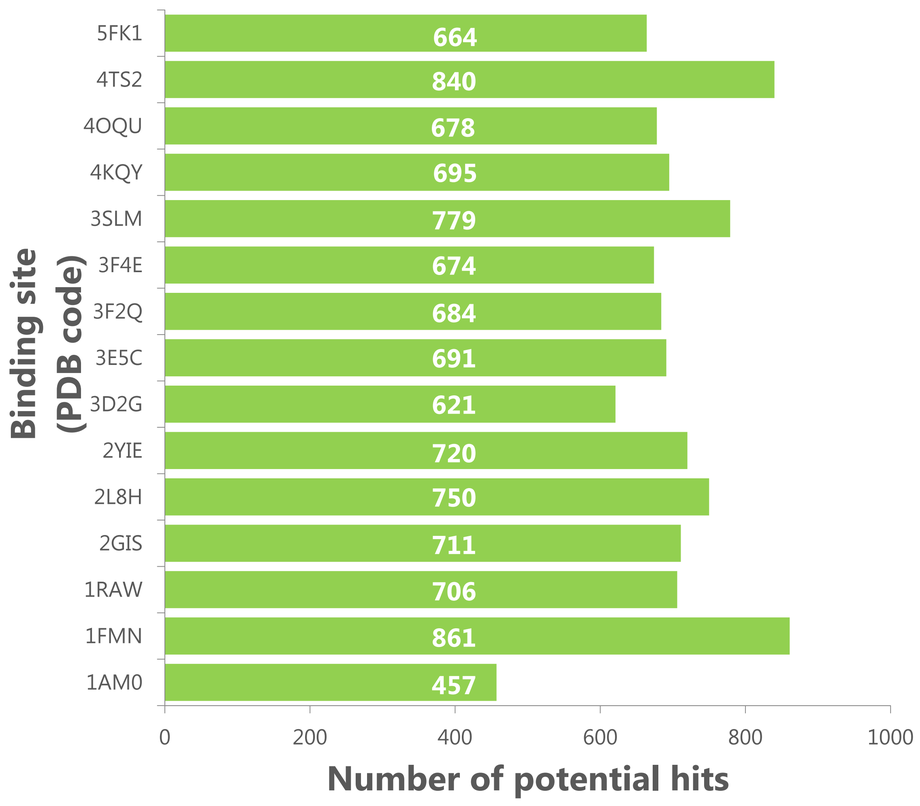
RNAs participate in more cell mechanisms than it has been thought before. Aside from transferring information from the DNA, this type of biomolecules appears to affect numerous cell processes: very small part of the transcripts actually codes proteins.

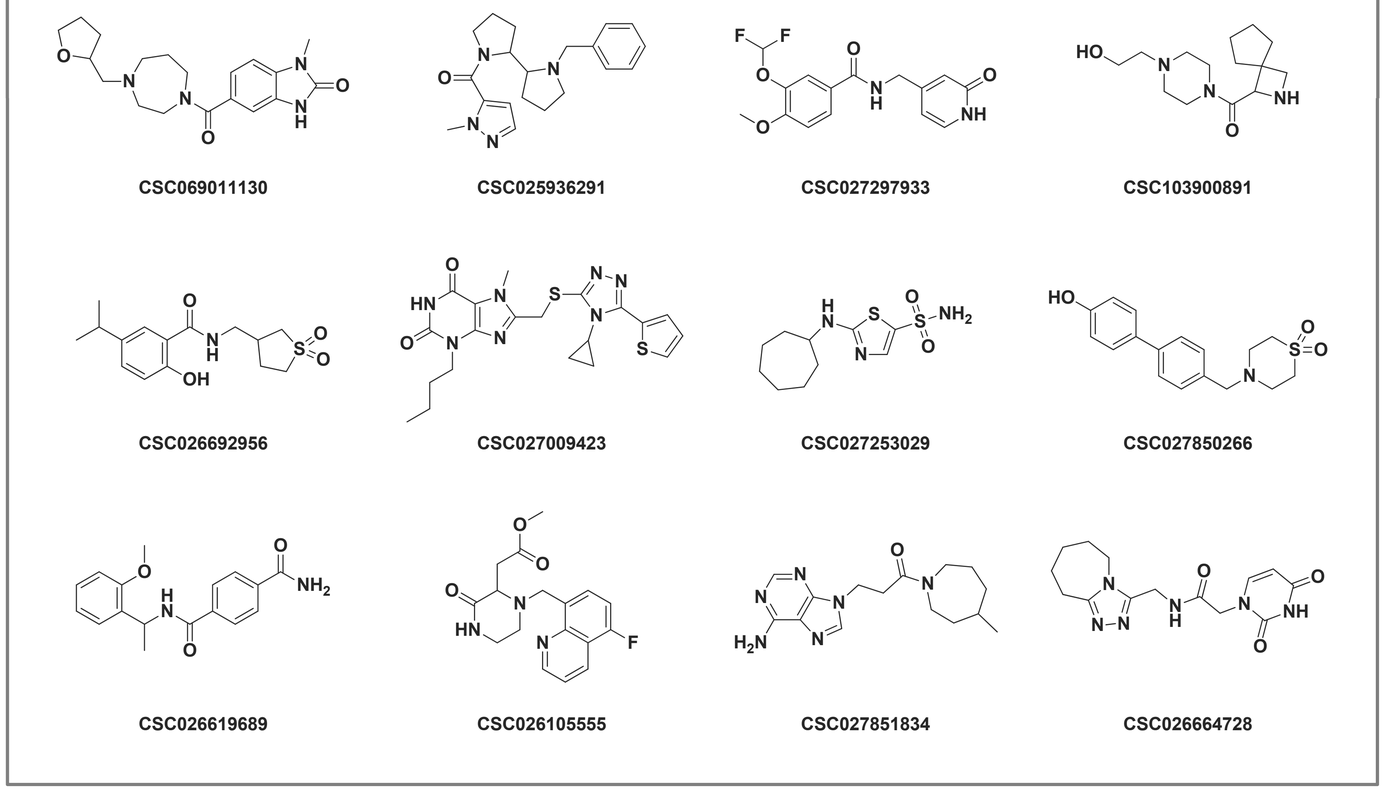
Targeting RNA with small molecules was suggested after discovering "druggability" of the nucleic acids similar to that of proteins. The targeting could be aimed at cell processes in humans or blocking RNA functions in bacteria or viruses.

For **Chemspace RNA-targeted library**, we focused on 15 binding motifs in different RNAs associated with bacterial and viral infections. We have selected the compounds from our Screening Compound Collection utilizing both ligand- and target-based approaches.

Compounds similar to the known RNA binders have been scored using molecular docking, and only those with high predicted activity were picked. The annotations to the target and docking score are available.







Discover other Chemspace Screening Compounds libraries

High QED Compounds

Among the other metrics, **Quantitative Estimate of Druglikeness** (QED) is an integrative score to evaluate compounds' favorability to become a hit. It is a method to quantify the drug-likeness considering the main molecular properties together.

A compound could have high QED score and not necessarily fall into Lipinski boundaries, and many approved drugs are a clear example to that.

See more:

Macrocyclic Compounds

Macrocyclic compounds possess features that push them out of the traditional Druglikeness space. At the same time, these features allow them to act in the cases small molecules seem to not being able to.

Chemspace Macrocycles are custom-designed scaffolds of non-peptidic nature, that could be further modified as well as totally assembled macrocyclic molecules.

See more:

Phenotypic Screening Set

Phenotypic screening (PS) is one of the two major approaches at early stage drug discovery projects, apart from the target-based screens.

Target identification in PS is a complex problem but the outcome could be very attractive: a number of new, first-in-class drugs have been discovered through phenotypic screens.

See more:

Pre-Plated Compounds

Our **Hit Discovery Set** of **72 000** compounds in our pre-plated Hit Discovery Set that includes thematic subsets:

57 280	Drug-Like set
960	Fragments set
4 480	Lead-Like set
4 800	Representative set
4 480	Unique set

See more:

Availability

- In-stock and Make-on-demand sets are available
- Ordering options: full or cherry-picked set
- Purity, 90%+ (LC-MS)
- Various formatting: solids, DMSO solutions (96-, 384-well plates)

Contacts

Yurii Moroz, PhD
yurii.moroz@chem-space.com
7 Deer Park Drive, Suite M-5
Monmouth Junction, NJ 08852