Antiviral Nucleoside Mimetic Library

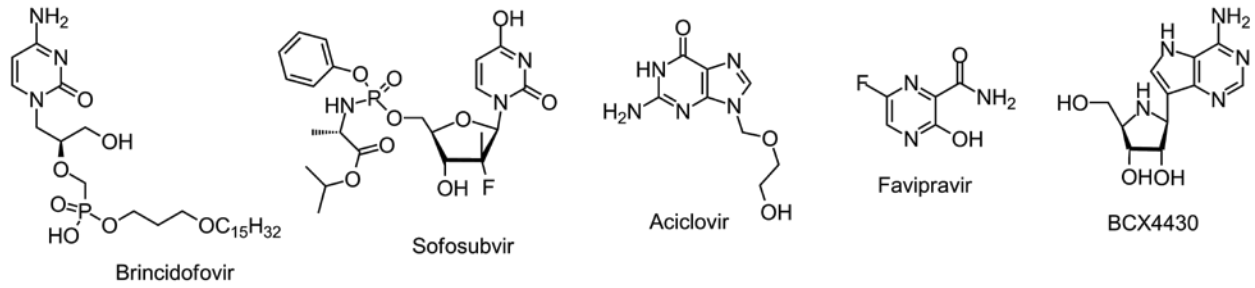
3,700 compounds

In spite of significant success in medicine last decades the development of effective antiviral agents and vaccines continue to be a chalenging task for the modern drug discovery.
Viruses share most of metabolic processes of the host cells thereby making difficult search of selective antiviral agent. However, some enzymes are only present in viruses and these are potential targets for antiviral drugs. For instance, there are several key enzymes which are involved in process with nucleic acids e.g. DNA- and RNA-polymerases as reverse transcriptases which indicates high potential as antiviral targets. Recent FDA approval of RNA-polymerase inhibitor Sofosubvir as anti-HCV drug as well promising results of application such agents as Favipiravir and BCK4430 for Ebola treatment demonstrates that the target inhibition can be effective against different viruses.

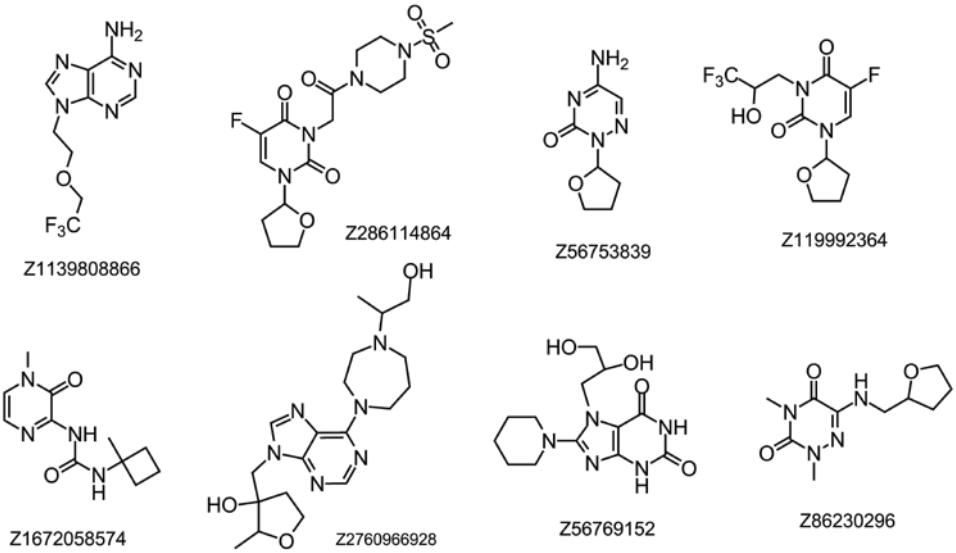
Library Design

Analyzing the structures of known inhibitors we found that most of them are nucleoside mimetics which are not distinguished from the nucleosides by virus enzymes in the active site.
Therefore taking into account pharmacophores and topology of nucleosides and reported nucleoside-like antiviral agents we carefully selected the set of *Nucleoside mimetics* from our screening collection. The compounds from the set contain natural-like moieties and diverse heterocycles as bioisosters of nucleosides. Additionally, special emphasis has been made on compounds that possess several H-bond donors and potentially can form similar interactions with the protein nucleoside-binding sites as a native nucleoside.

Examples of nucleoside mimetics as antiviral agents



Examples of representative compounds from Antiviral Library



Molecular Profile of the library

Selected compounds have attractive drug/lead-like physical chemical and structural properties that are characteristic for nucleosides and their mimetics:
MW 150…400, ClogP -2…4; TPSA < 150, RotBonds <7; HBD 1…5, HBA 1…7.

The library is considered to be a convenient starting point for a wide range of antiviral drug discovery projects.