Chemspace Fragment Libraries: Fluorine Fragments

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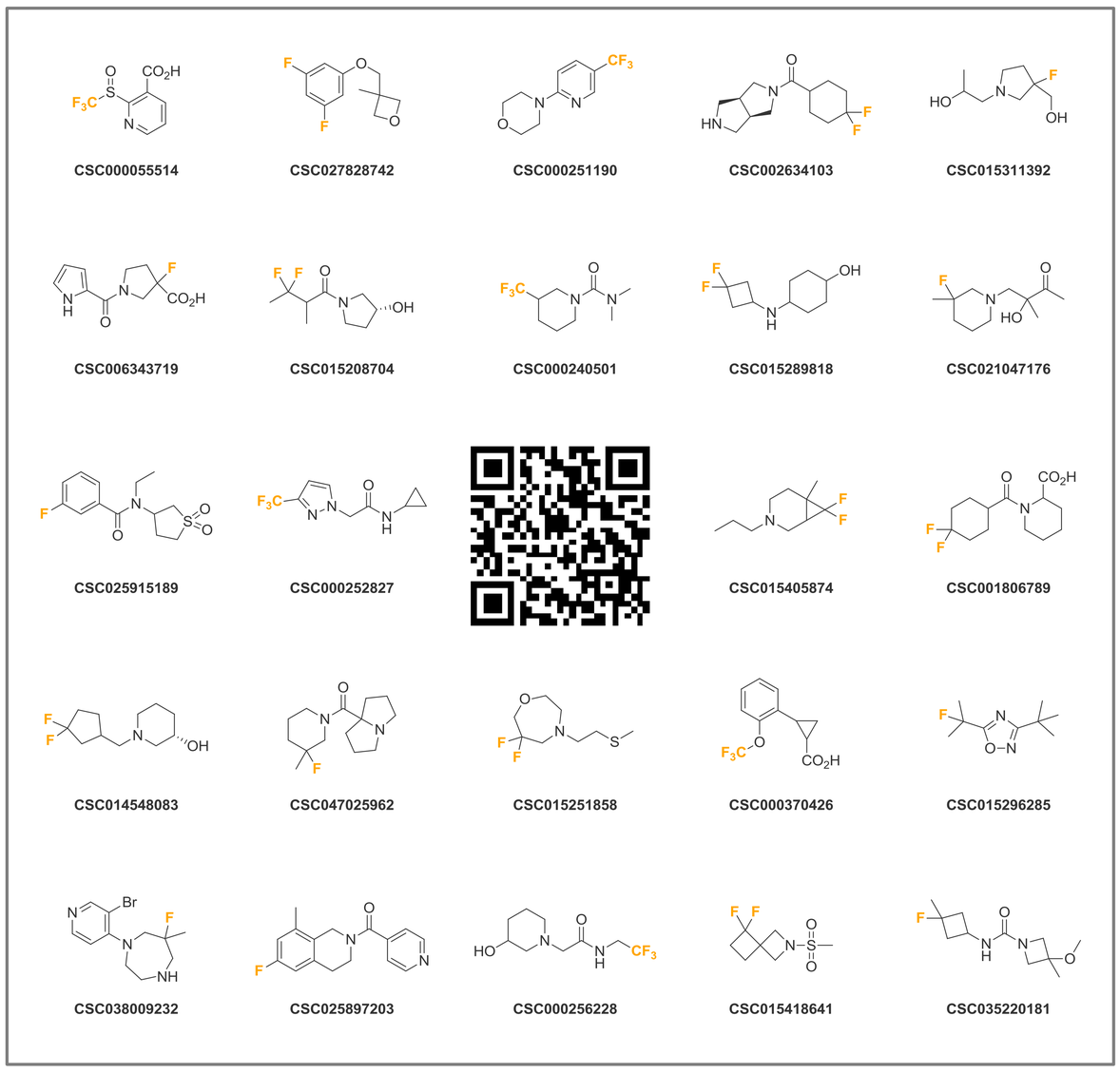


Overview

3 331 in-stock compounds; **24 506** make-on-demand compounds

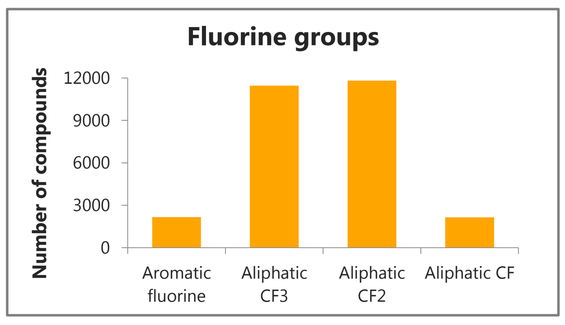
In many instances, presence of fluorine atom in the active molecule improves overall ADMET properties: metabolic stability and bioavailability. Fluorine-substituted groups increase lipophilicity and acidic character of the compounds, and decrease their basicity.

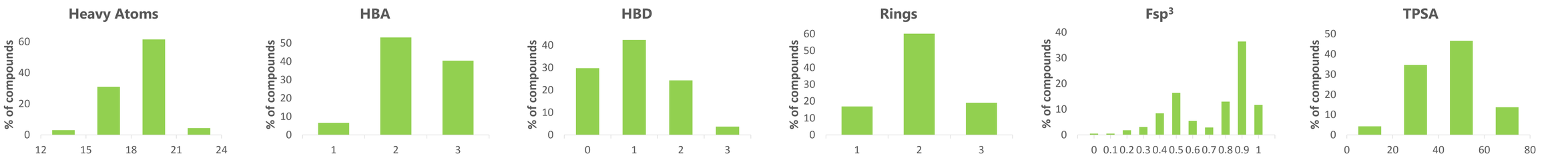
Fluorinated compounds found different uses: from modulators of the blood pressure and anaesthetics to labeling for the PET screens.

But in the Fragment-based drug discovery projects, the major use of fluorinated compounds is ^{19}F NMR-assisted screening. Fluorine atom shows strong and distinct signal in the NMR spectra. This, and also its sensitivity to local environment changes, allowed usage of the "fragment cocktails" in the NMR studies. The method has enabled screening numerous compounds at the same time without interference with each other. Beyond this, with ^{19}F NMR spectroscopy, structure-activity relationships enables additional investigations in H2L optimization.

Selection criteria for the library:

- 'Rule of 3' compliant
- No PAINS, toxic moieties
- Fluorinated group in substructure
- Chlorine atoms count ≤ 2





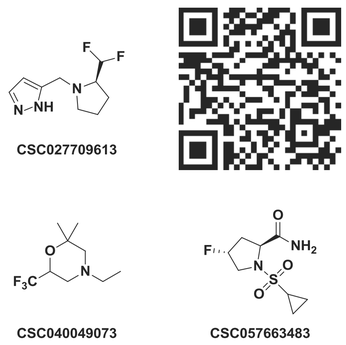
Discover Chemspace fragment libraries:

3D-Shaped Fragments

The shape of the molecule is an important factor in its affinity to the binding site. Thanks to its shape, the molecule could become a specific "key" to the host molecule.

It is also important that rigid 3D-shaped molecules not necessarily have high fsp3: dimensional orientation is more significant than a saturation degree of the molecule.

See more:

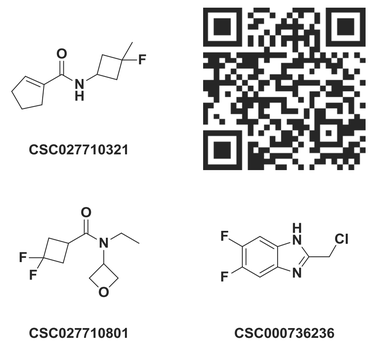


Covalent Fragments

In the early years of drug discovery, compounds able to form covalent bonds with target were consciously omitted as too reactive, promiscuous or toxic.

Now, many drugs people have been using for a really long time are actually covalent binders. Covalent modifiers are used in treatment of arthritis, and have been reported as antibacterial and antiviral agents.

See more:

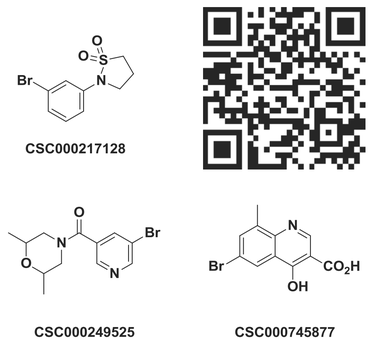


Heavy Fragments

Aside of NMR, X-ray crystallography is a technique that is often used to determine/prove the interaction of the molecule with target protein.

Fragments for this type of screening are brominated small molecules as Bromine atom causes anomalous diffraction of the X-rays and can be clearly detected in the crystal of protein.

See more:

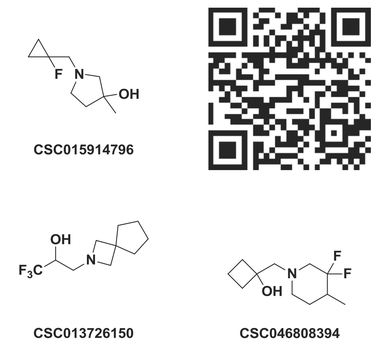


Selected Fragments

Hit optimization usually shifts physicochemical profiles of compounds to less desirable area. Initial library of high quality is a key to enhance the probability of hit obtaining and chance that is would be suitable for follow-up.

Compounds added to this set have passed the strict Astex filters and are free of PAINS and supposedly toxic reagents.

See more:

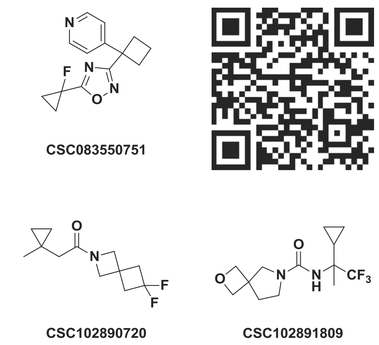


Singleton Fragments

Fragment screening has been an important tool to generate new potent leads.

The screening generates high-quality results (i.e. new starting points) if correct fragment library has been utilized. Chemspace Singleton Fragments *a*) to cover wide chemical space: fragment-likeness and diversity selection, and *b*) bring novelty (molecules with new Murcko frameworks).

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: powders, DMSO solutions (96-, 384-well plates)

Contacts

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