

Compounds that possess moieties able to react with biological molecules in the cell have been overlooked in drug discovery research projects for a long time. Character of the investigation did not allow to suppose direct binding between the target and the agent.

Covalent modifiers have a scaffold capable of accommodating a reaction moiety, otherwise known as the warhead, which improves the binding affinity and selectivity by forming a covalent interaction with a protein reactive residue.

Now molecules with covalent warheads attract researchers' attention as possible antiviral, antibacterial and anticancer agents.





We have selected a library from the Chemspace **Selected Screening** set: each compound contains possible covalent binder. Warheads include alkyl thiols, oxetane rings, sulfonyl halides, Michael acceptors, etc.

Library size: 71 396 in-stock compounds 243 273 make-on-demand compounds Please discover our <u>Covalent Fragments</u> – set of small molecules with covalent warheads.

You can order full set or selected subset based on your criteria; all compounds are supplied as powders, solutions, or dry films. Please contact us at <u>sales@chem-space.com</u> for more information.

#### 

# **PhyChem properties**

Heavy Atoms





Fsp<sup>3</sup>



**Rotatable Bonds** 





# **Chemspace Compound sets**

### Discover our Fragment Libraries:

- <u>General</u> Fragments
- <u>3D-Shaped</u> Fragments
- Acid and Amine Fragments
- Covalent Fragments

- **<u>Fluorine</u>** and <u>Heavy</u> Fragments
- <u>Selected</u> Fragments
- <u>Singleton</u> Fragments
- <u>Saturated</u> and <u>Spiro</u> Fragments

All libraries' names are clickable links. Visit www.chem-space.com/flyers to find more Chemspace presentations!



# **Chemspace Compound sets**

#### Discover our **Screening compounds**:

- <u>ChEMBL analogs</u>
- **<u>CNS-Focused</u>** library
- <u>Covalent Modifiers</u>
- Drug Impurities
- Drug Repurposing
- Framework-Derived set

- High QED compounds
- **<u>Phenotypic Screening</u>** set
- PPI Modulators
- <u>Pre-Plated</u> compounds
- **<u>RNA-Targeted</u>** library
- Virtual Screening set

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