

Covalent Fragments





Many drugs people have been using for a really long time are actually covalent binders. Examples of covalent modifiers include cancer and arthritis treatments and as antibacterial and antiviral agents.

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

Although reversibly binding ligands are commonly pursued, covalent fragments provide an alternative route to small-molecule probes. Compounds with covalent warhead that comply with Rule of 3 enable the access of protein regions that are difficult to target with "classical" ligands.



Compounds for our **Covalent Fragments** library were picked from Chemspace Selected Screening set. All compounds comply with Ro3 and contain possible covalent binder.

Library size:

11 038 in-stock compounds

25 665 make-on-demand compounds

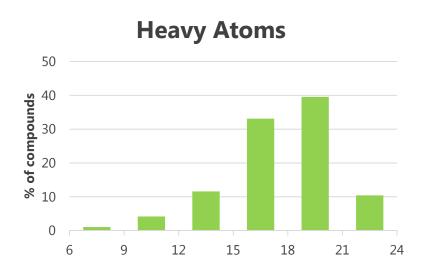
You can order full set or selected subset based on your criteria; all compounds are supplied as powders, solutions, or dry films. Please contact us at sales@chem-space.com for more information.

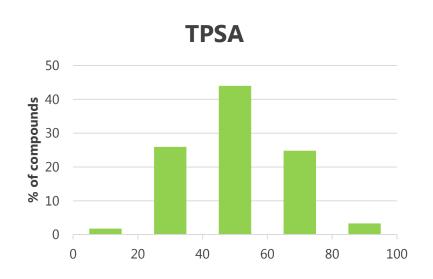
Covalent warheads include:

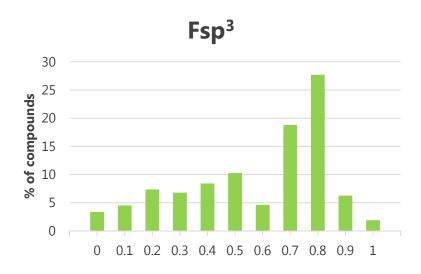
alkyl thiols and halides, oxirane and oxetane rings, sulfonyl halides, Michael acceptors, carbamates, terminal alkynes and methylene-active compounds.

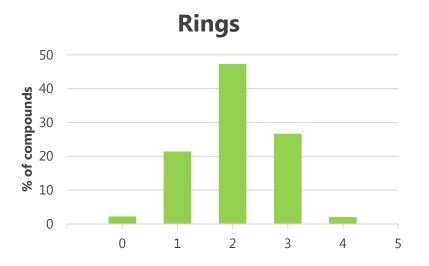


PhyChem properties











Chemspace Compound sets

Discover our **Fragment Libraries**:

- **General** Fragments
- **3D-Shaped** Fragments
- Acid and Amine Fragments
- **Covalent** Fragments

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

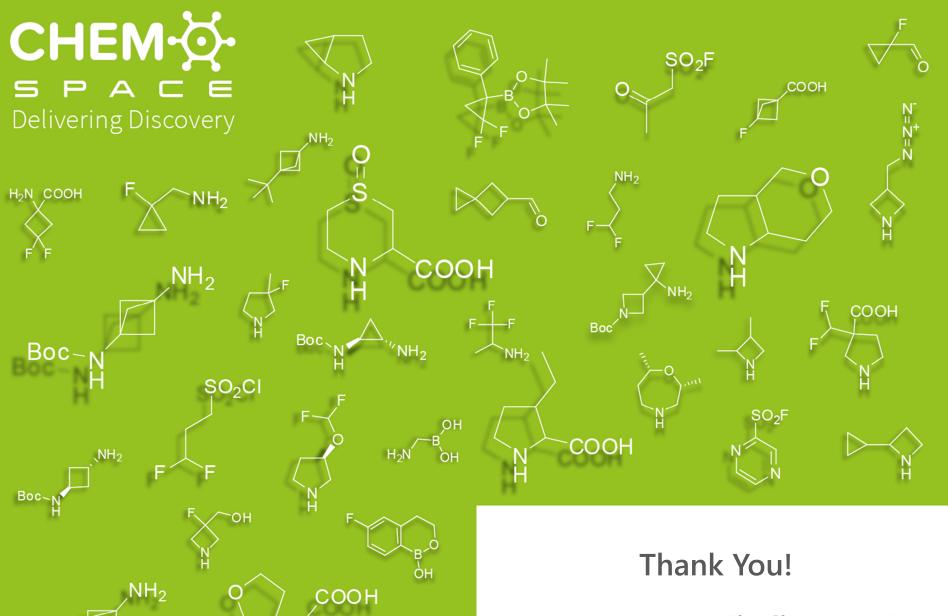


Chemspace Compound sets

Discover our **Screening compounds**:

- ChEMBL analogs
- CNS-Focused library
- Covalent Modifiers
- Drug Impurities
- Drug Repurposing
- Framework-Derived set

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



The Chemspace Team

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