



Hit follow-up usually shifts its physChem parameters 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.

Please discover Chemspace Selected Fragments: compounds added to this set have passed the strict Astex physChem filters and are free of PAINS and supposedly toxic reagents.

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Chemspace **Selected Fragments** set consists of small molecules that are free of PAINS and "toxic" moieties and comply with the following rules:

- $7 \leq$  Heavy atoms count  $\leq 17$
- $130 \leq Molar Weight \leq 230$
- $0 \leq slogP \leq 2$
- TPSA  $\leq 100$

Library size: 10 540 in-stock compounds 38 981 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 <u>sales@chem-space.com</u> for more information.



## **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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