



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.

For Chemspace **Singleton Fragments**, we have utilized approaches that allow:

a) to cover wide chemical space: fragment-likeness and diversity selection, and

b) bring novelty (molecules with new Murcko frameworks).





Compounds selection strategy:

- Comply Rule of 3, no PAINS and "toxic" moieties;
- New chemotypes (Tanimoto similarity to the nearest purchasable compound \leq 0.45)
- Highly diverse set (Tanimoto similarity to the nearest compound within the set ≤ 0.5)

Library size: 2 547 in-stock 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

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

– chem-space.com –

delivering discovery -

