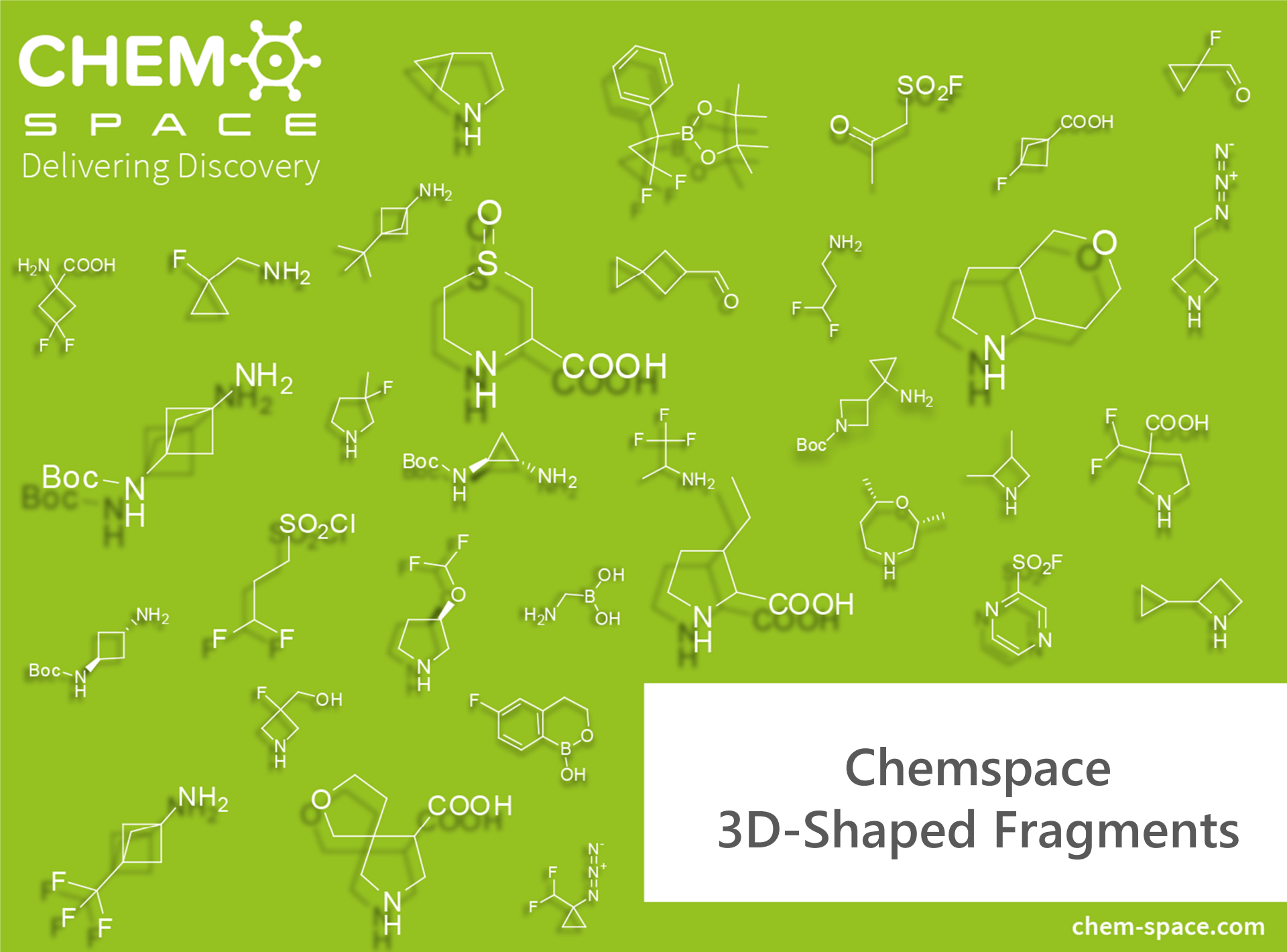
CHEM SPACE

Delivering Discovery



Chemspace
3D-Shaped Fragments

chem-space.com

Description

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.

Fragment libraries mostly consist of *rod*-like and *flat* molecules, with other shapes (*spherical* or *disc*-shaped) being highly diluted. The shape of fragments makes them more conformationally rigid which contributes to the unambiguity of the interaction with the target.

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

We have selected 3D-shaped compounds that have the *disc*- or *sphere*-like shapes. We used Plane of Best Fit (PBF) and Principal Moments of Inertia (PMI; also normalized sum of PMIs - NPR) as descriptors to reflect the shape of the molecule.

Selection

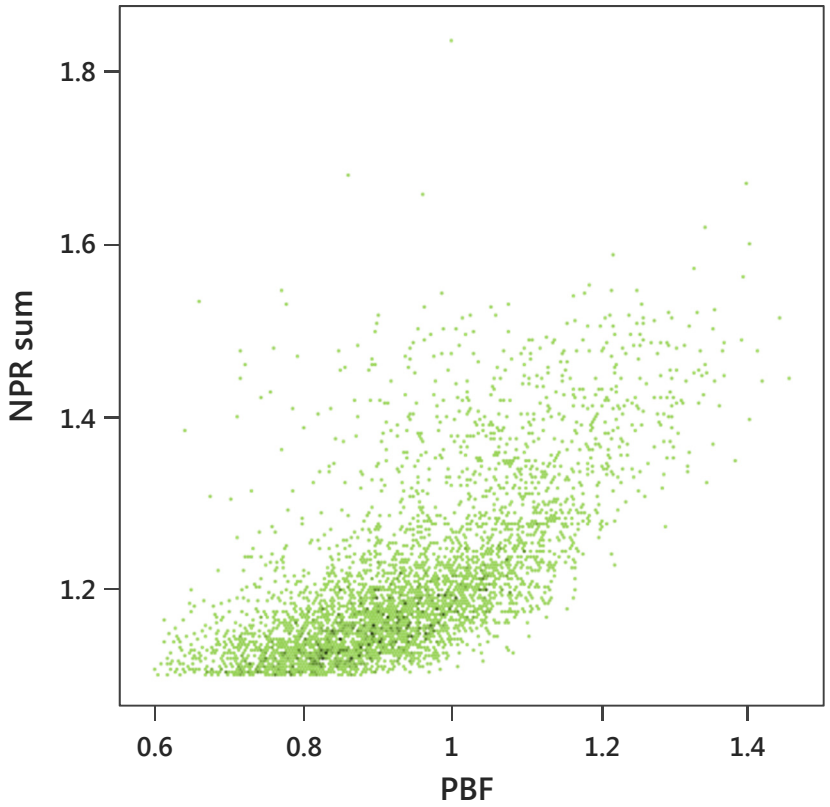
From **Chemspace Selected Screening** collection we picked the compounds with following characteristics:

- PBF ≥ 0.6
- NPRsum ≥ 1.1
- Disc-like and Sphere-like form

Library size:

4 021 in-stock compounds

29 043 make-on-demand compounds

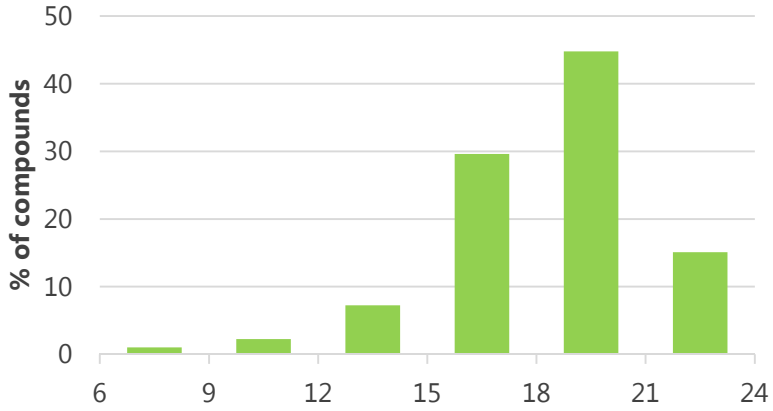


Chemspace 3D fragments distribution in NPRsum-PBF coordinates

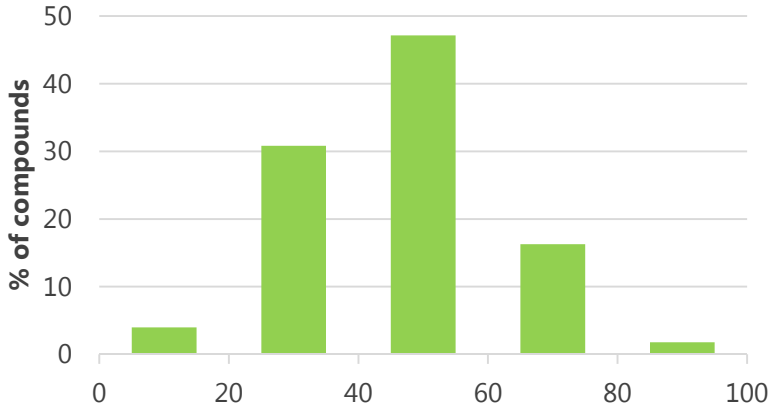
You can order full set or selected subset based on your criteria; all compounds are supplied as powders, solutions, or dry films. Please contact us at sales@chem-space.com for more information.

PhysChem properties

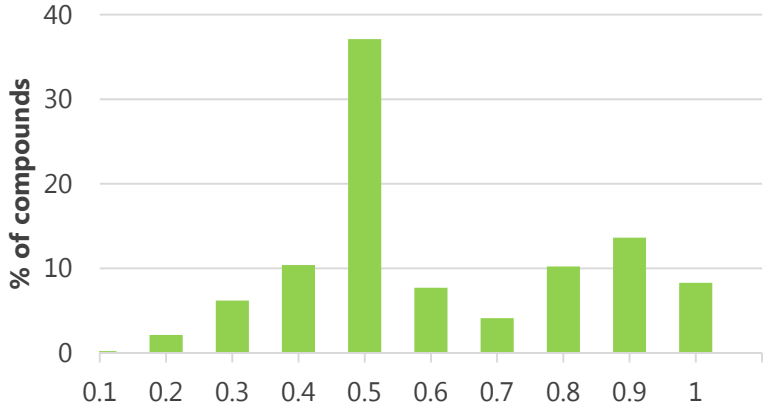
Heavy Atoms



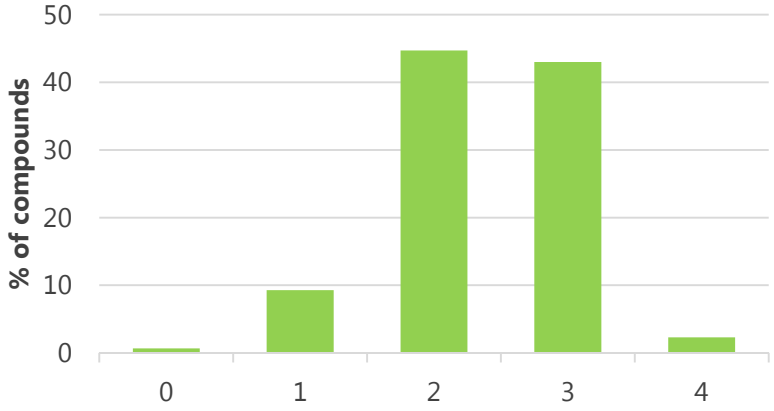
TPSA



Fsp^3



Rings



Chemspace Compound sets

Discover our **Fragment Libraries**:

- **General** Fragments
- **3D-Shaped** Fragments
- **Acid** and **Amine** Fragments
- **Covalent** Fragments
- **Fluorine** and **Heavy** Fragments
- **Selected** Fragments
- **Singleton** Fragments
- **Saturated** and **Spiro** 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**:

- **ChEMBL analogs**
- **CNS-Focused** library
- **Covalent Modifiers**
- **Drug Impurities**
- **Drug Repurposing**
- **Framework-Derived** set
- **High QED** compounds
- **Phenotypic Screening** set
- **PPI Modulators**
- **Pre-Plated** compounds
- **RNA-Targeted** library
- **Virtual Screening** set

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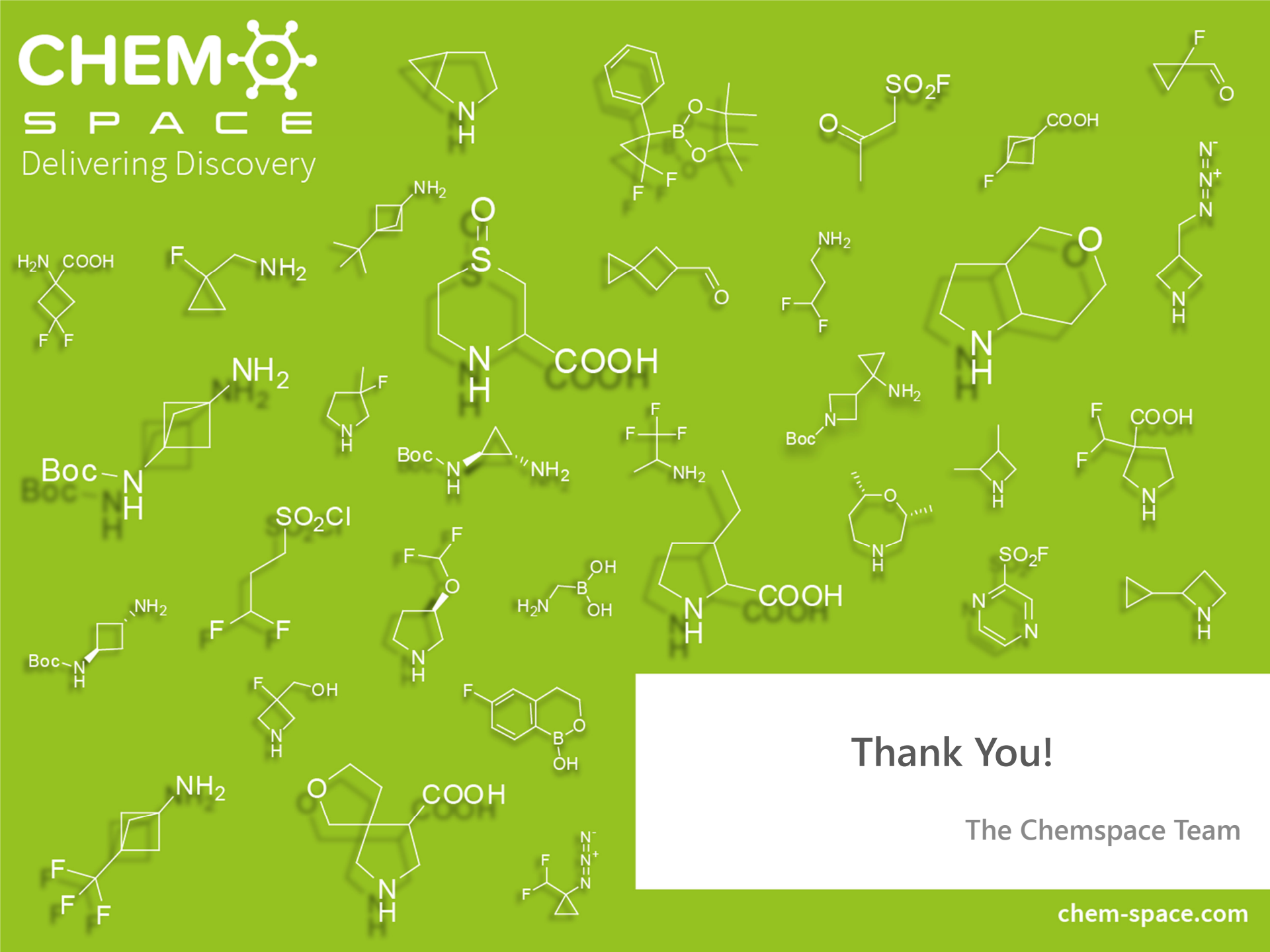

Thank You!

The Chemspace Team

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