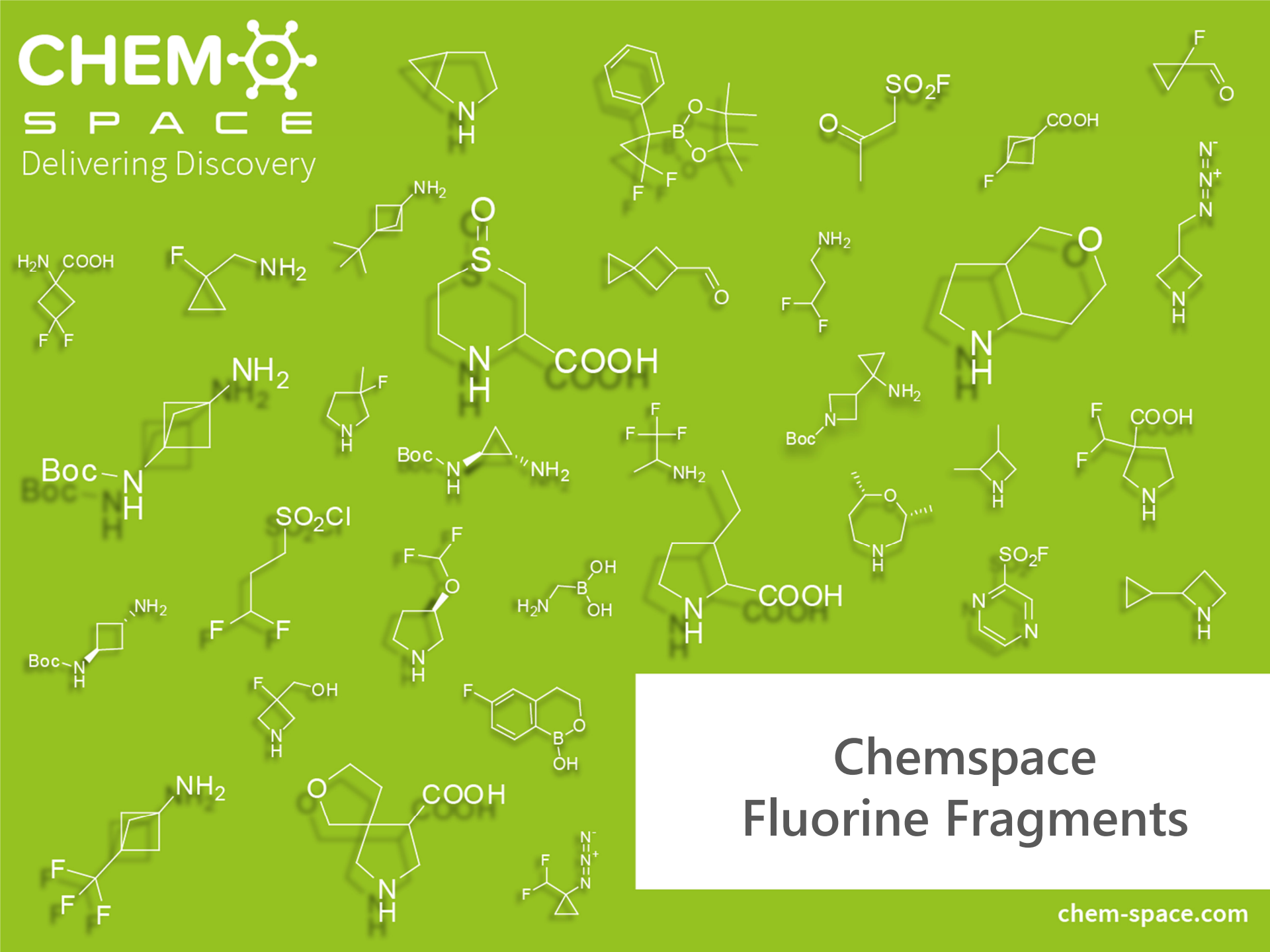
CHEM SPACE

Delivering Discovery



Chemspace Fluorine Fragments

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Description

Presence of Fluorine atom has been noticed to improve overall ADMET properties, which includes improving metabolic stability and increasing of bioavailability through increasing lipophilicity, decreasing basic and increasing acidic character of the compound. Fluorinated compounds have different uses: from modulators of the blood pressure and anaesthetics to labeling for the PET screens.

But in the Fragment-based drug discovery projects, the major use of fluorinated compounds is ^{19}F NMR-assisted screening. Fluorine atom shows strong and distinct signal in the NMR spectra. This, and also its sensitivity to local environment changes, allowed usage of the “fragment cocktails” in the NMR studies.

Sensitivity of this method allowed screening numerous compounds at the same time without them interfering with each other. Beyond this, with ^{19}F NMR spectroscopy, structure-activity relationships can be investigated in H2L optimization.

Selection

Chemspace **Fluorine Fragments** library consists of compounds that

- Comply with Ro3
- Possess single-type fluorine group – enabled usage of the "fragment cocktails" in NMR studies

Library size:

4 942 in-stock compounds

70 574 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.

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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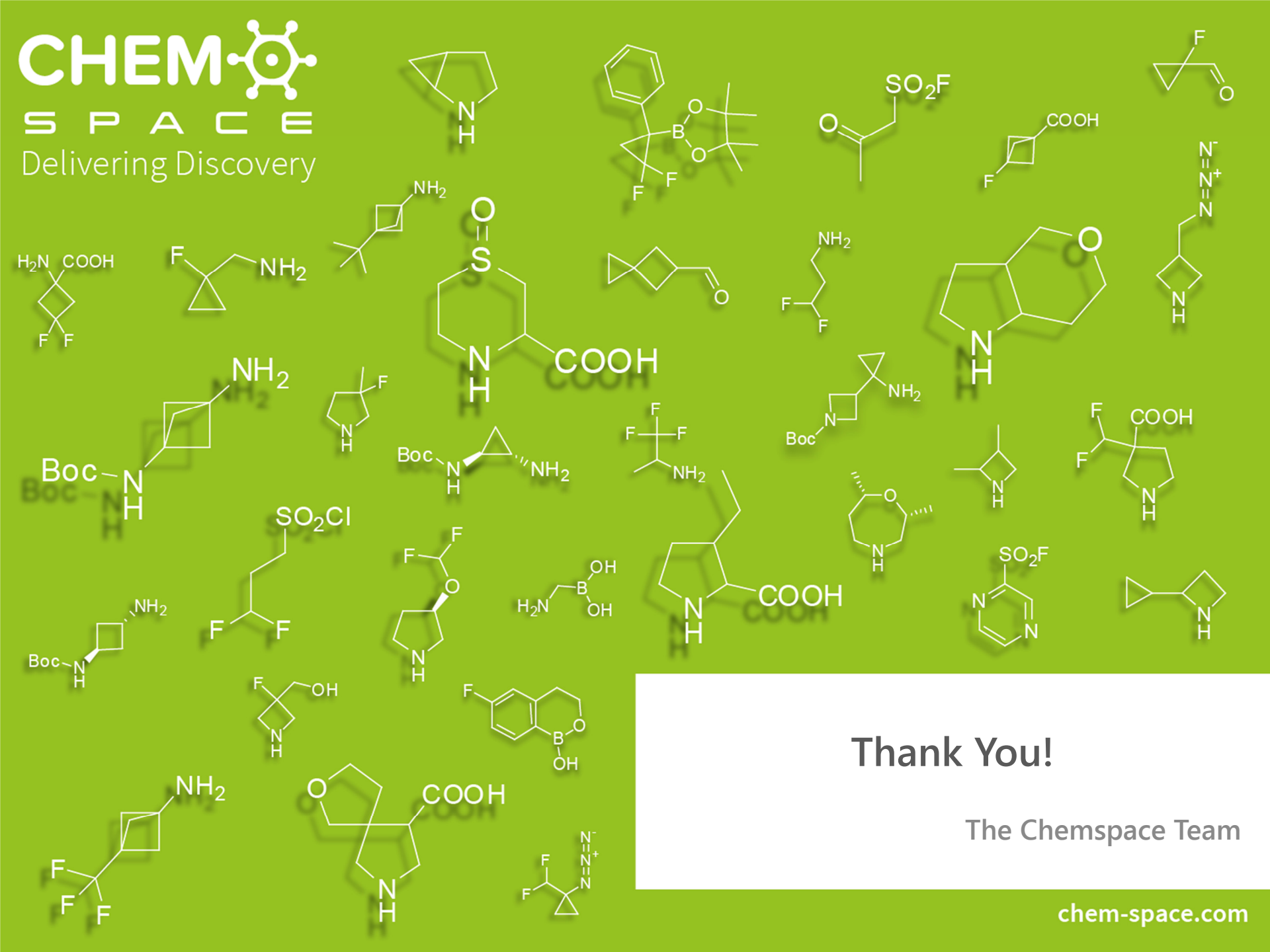

Thank You!

The Chemspace Team

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