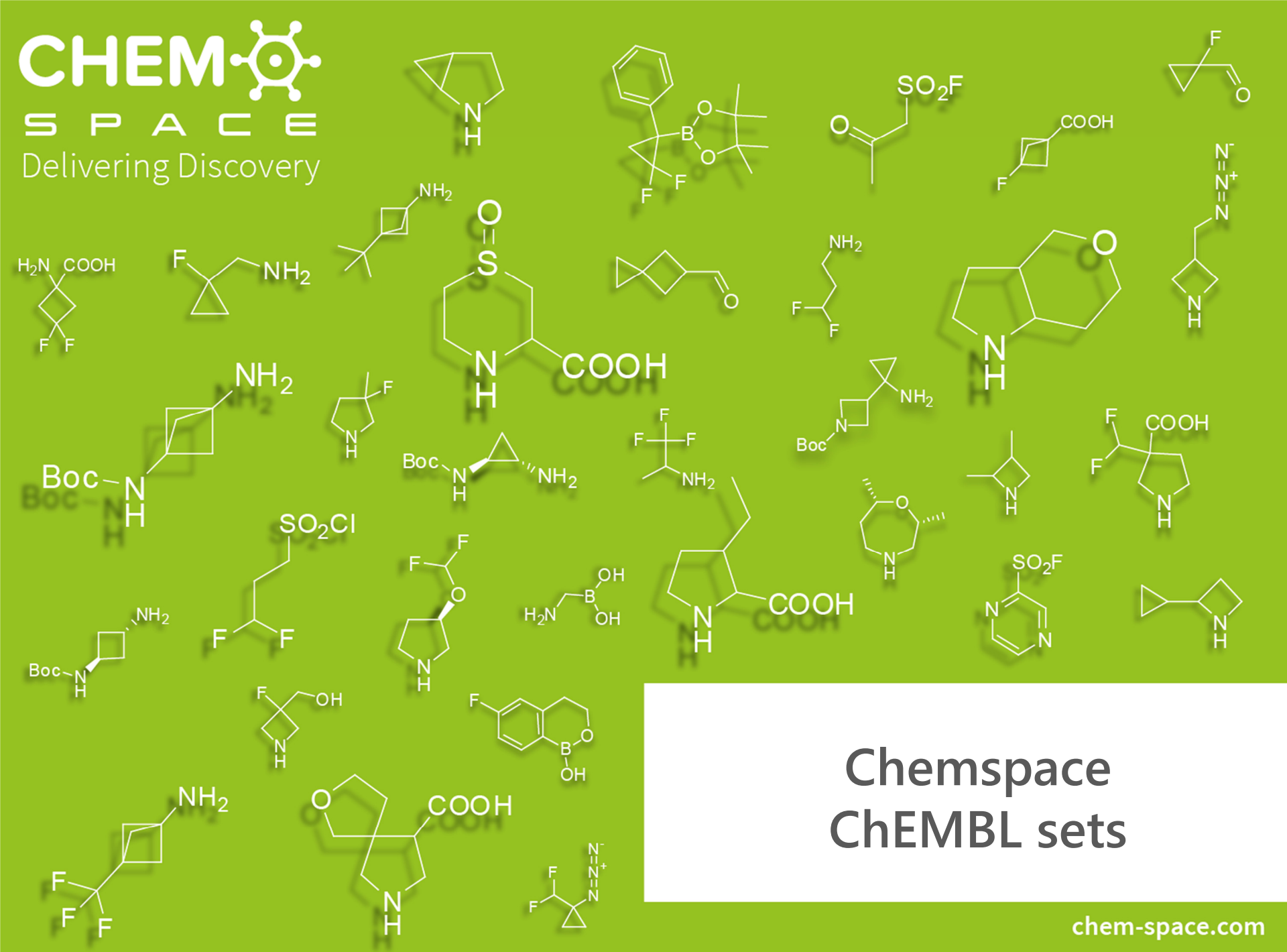
CHEM SPACE

Delivering Discovery



Chemspace ChEMBL sets

chem-space.com

Description

Searching analogs to compounds with the known activity is helpful in hit expansion and repurposing projects. ChEMBL database has become an important reference tool containing an information on potency, binding, ADME/T, and pharmacology of small molecules.

For referencing, we have prepared the library of in-stock compounds that are listed as actives on ChEMBL.

For hit expansion studies, we have selected compounds that are highly similar to ChEMBL actives.

Custom selection is available for the compounds of interest.

Selection

We calculated similarity using Morgan fingerprints of radius 2, length 1024. We picked only compounds that have Tanimoto similarity coefficient to ChEMBL active higher than 0.6.

In-stock sets are downloadable from our website:
www.chem-space.com/compounds/chembl-analogs

For Make-on-Demand sets please contact us at **info@chem-space.com**

Library size:

117 445 ChEMBL actives available from Chemspace stock;

(expandable up to 150 000)

2 725 205 analogs to ChEMBL actives on Chemspace available in stock.

(expandable up to 7 200 000)

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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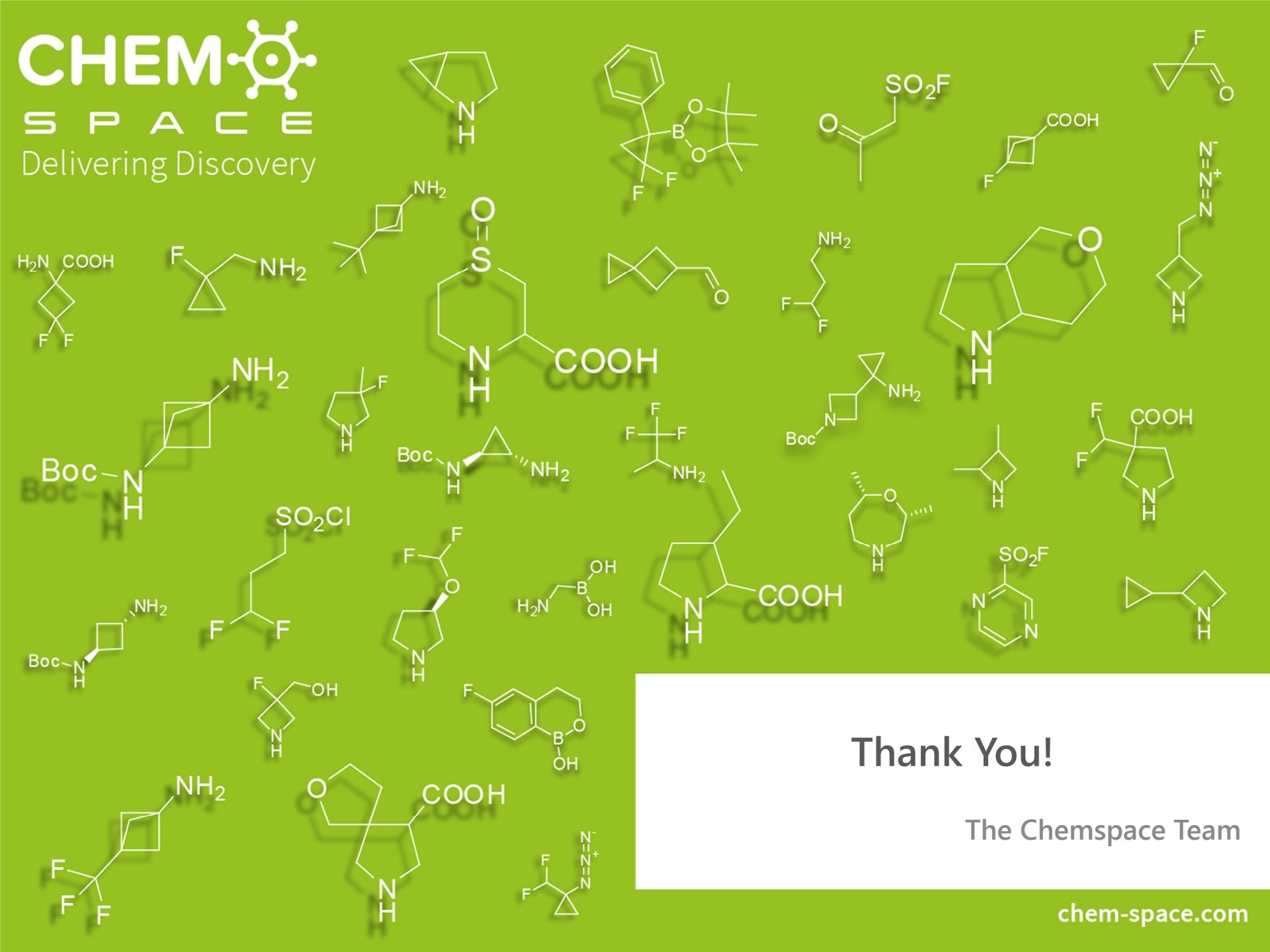

Thank You!

The Chemspace Team

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