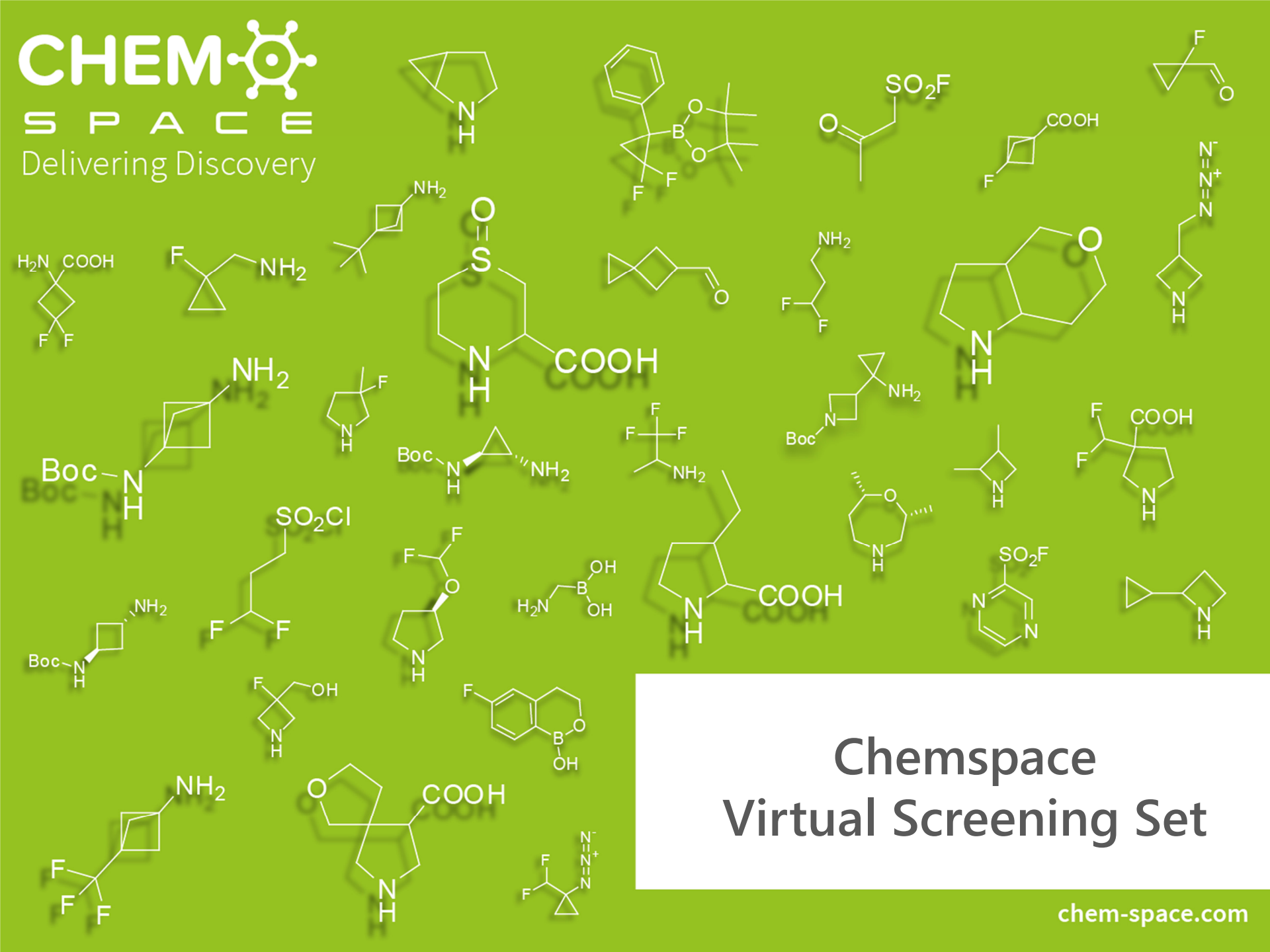
CHEM SPACE

Delivering Discovery



Chemspace Virtual Screening Set

chem-space.com

Description

Virtual screening (VS) has been a tool to identify primary hits, to study structure-activity relationship, and to tweak the structures using scaffold hopping, – to name a few. VS enables screening of large compound collections without actually having them on the shelf.

High quality of compounds for virtual screening is as important as for the 'wet lab' experiments. Therefore, we created a Chemspace **Virtual Screening set** by selecting blending compounds with favorable physicochemical profiles and high QED with known bioactives from ChEMBL and their analogs.

Selection

Chemspace **Virtual Screening set**:

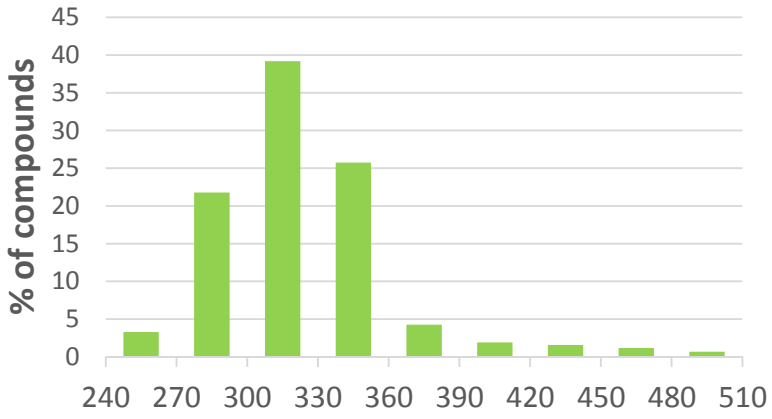
1) **High-QED** – compounds with Quantitative Estimation of Druglikeness of ≥0.9;
2) **ChEMBL actives** – full analogs to active compounds from ChEMBL;
3) **ChEMBL analogs** – compounds that have high similarity to actives from ChEMBL.

Library size:
5 053 840 make-on-demand compounds

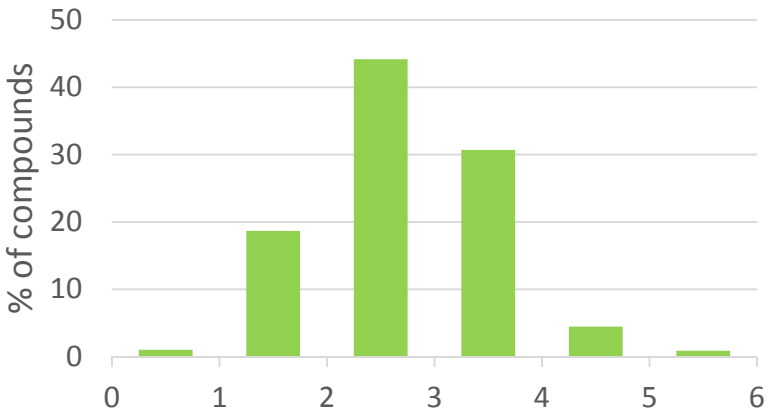
You can order full set or selected subset based on your criteria;
all compounds are supplied as powders, solutions, or dry films.
Please contact us at sales@chem-space.com for more information.

PhysChem properties

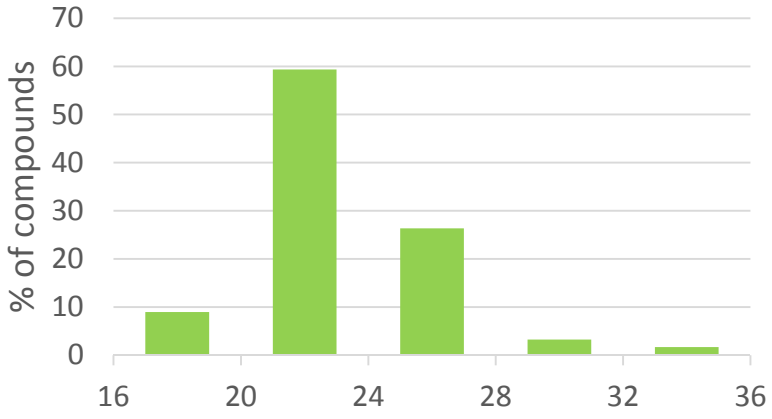
MW



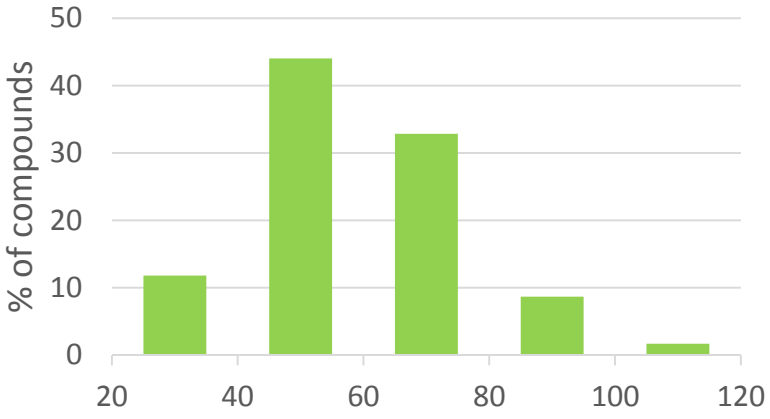
SLogP



Heavy Atoms count



TPSA



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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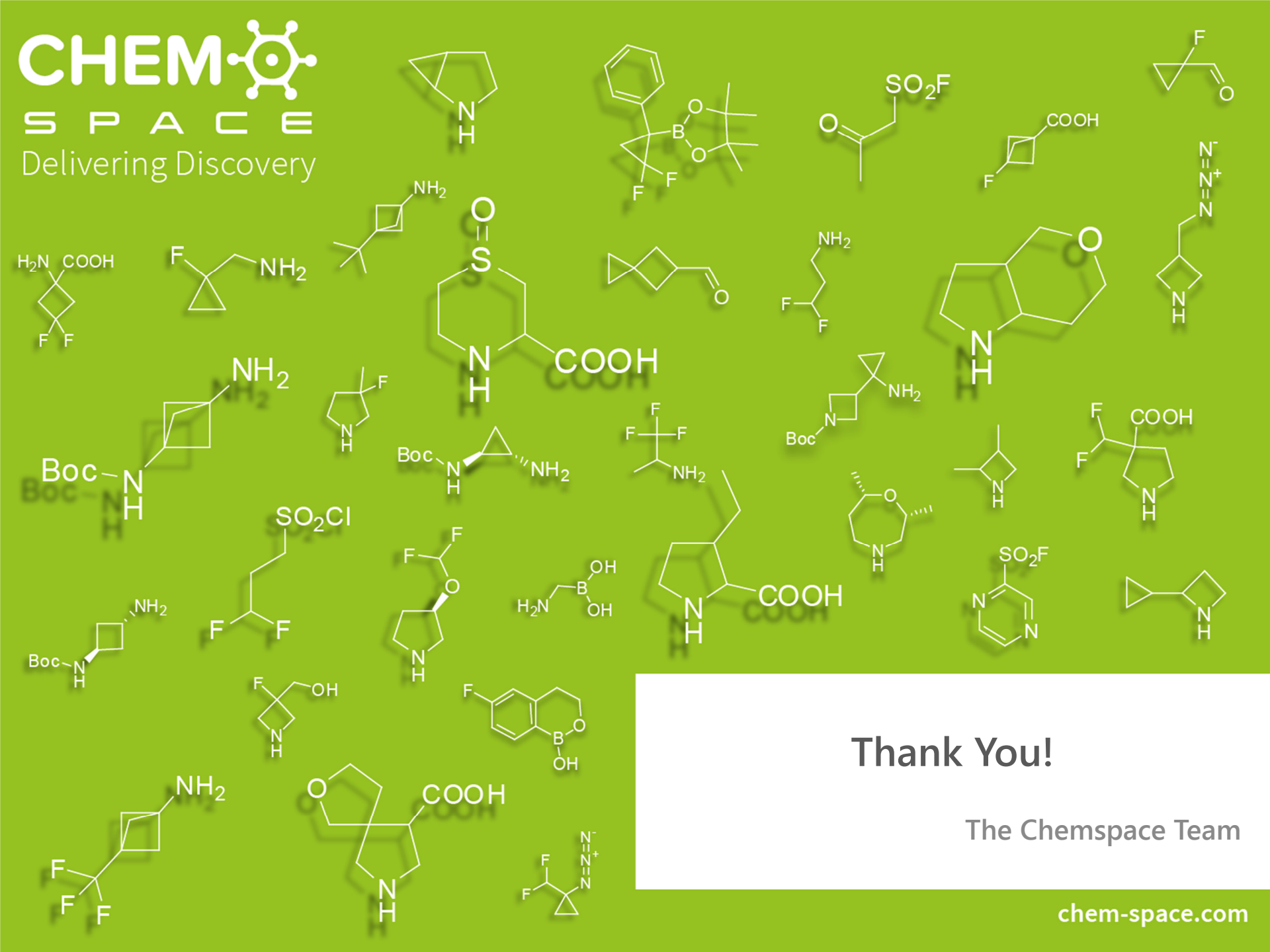

Thank You!

The Chemspace Team

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