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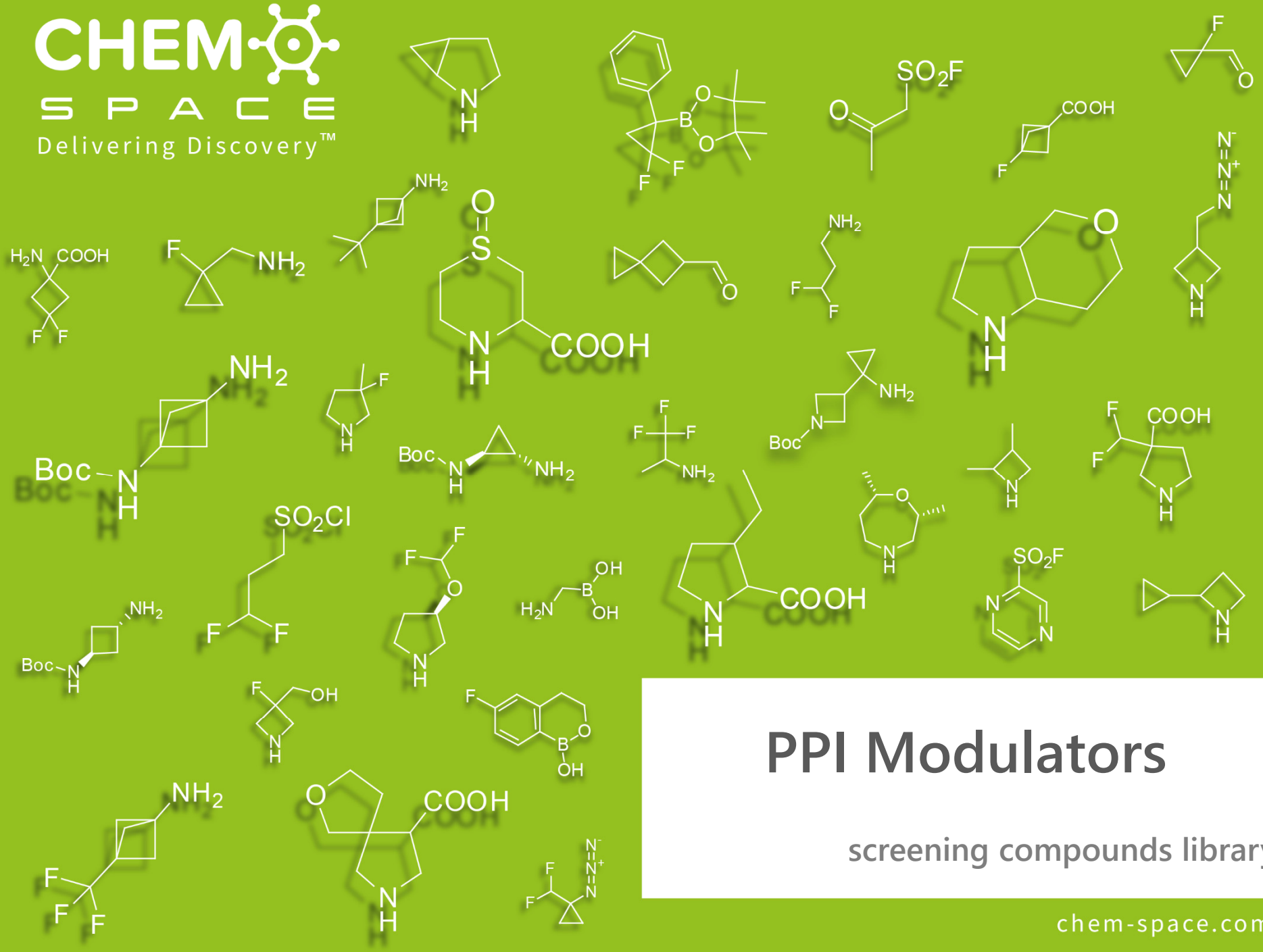

PPI Modulators

screening compounds library

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Description

Targeting Protein-Protein Interactions is a promising strategy since PPIs are involved in numerous cell processes – and, therefore, various diseases may be associated with them.

As promising as difficult the PPI studying and targeting is. Regarding this, we aimed to create the PPI modulators library of large, but not “greasy” molecules that accord with the “Rule of 4” for iPPI and, moreover, included compounds possess functional groups that interact with important Arg, Trp, Tyr residues.

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Description

- Physicochemical criteria (MW ≥ 400, SLogP ≥ 4, HBA≥3, Rings ≥ 3)
- Compounds with toxic and overreactive moieties excluded
- The “hot spot” paradigm (design included functional groups able to interact with Tyr, Trp, Arg residues)[1]
- Ligand-based design (similarity analysis to TIMBAL database)[2]

Library size:

6 416 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 sales@chem-space.com for more information.

[1]Wells, J. A.; McClendon, C. L., Nature 2007, 450, 1001–1009
[2]Higueruelo, A. P.; Jubb, H.; Blundell, T. L., Database (Oxford). 2013, 2013, bat039

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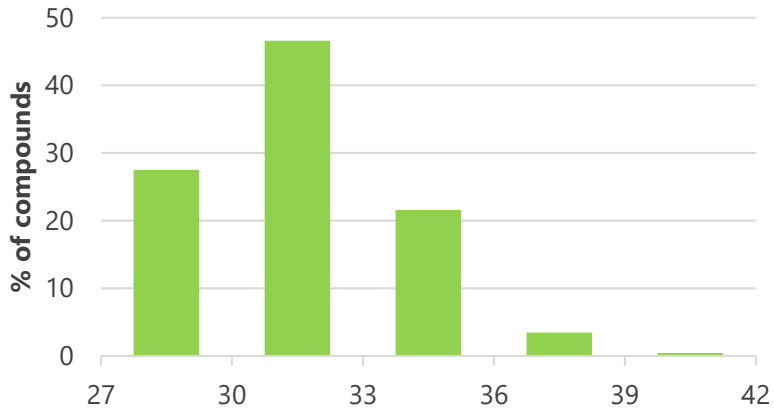
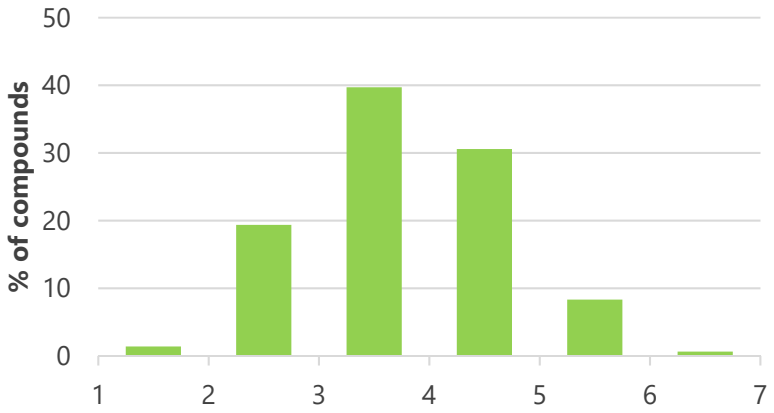
PhysChem properties

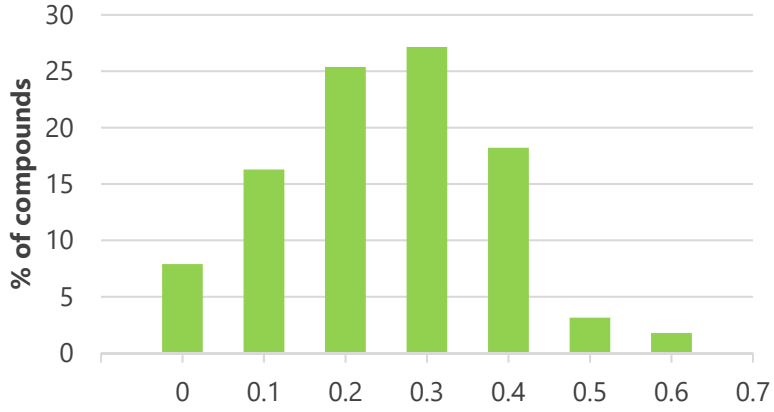
Heavy Atoms count



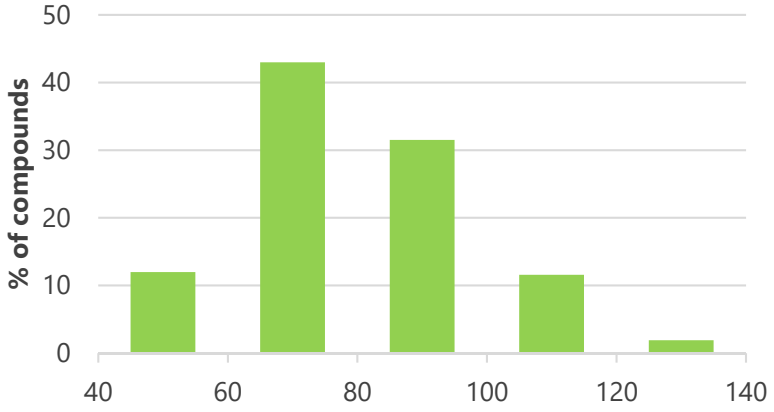
sLogP



Fsp3



TPSA



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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

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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

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

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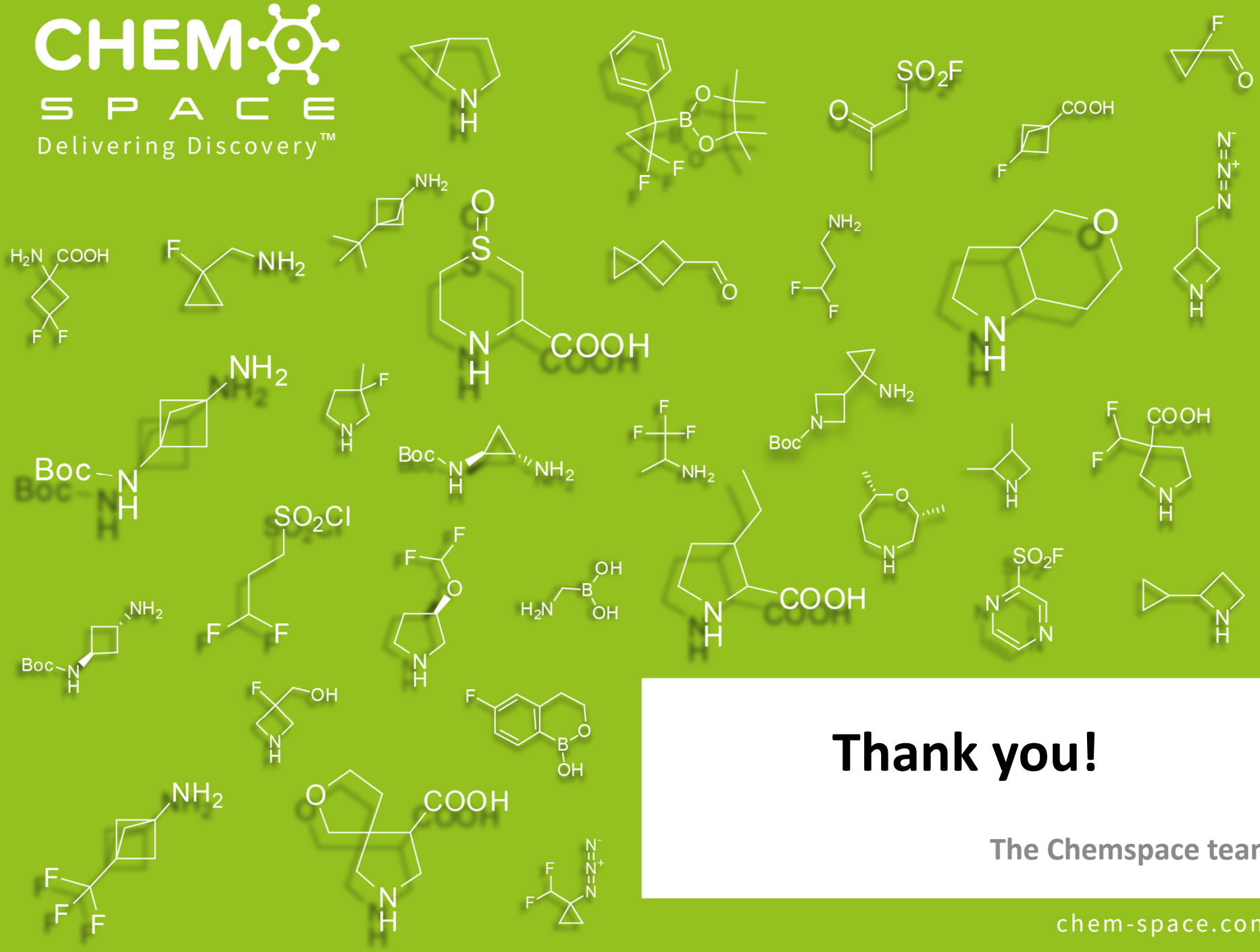

Thank you!

The Chemspace team

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