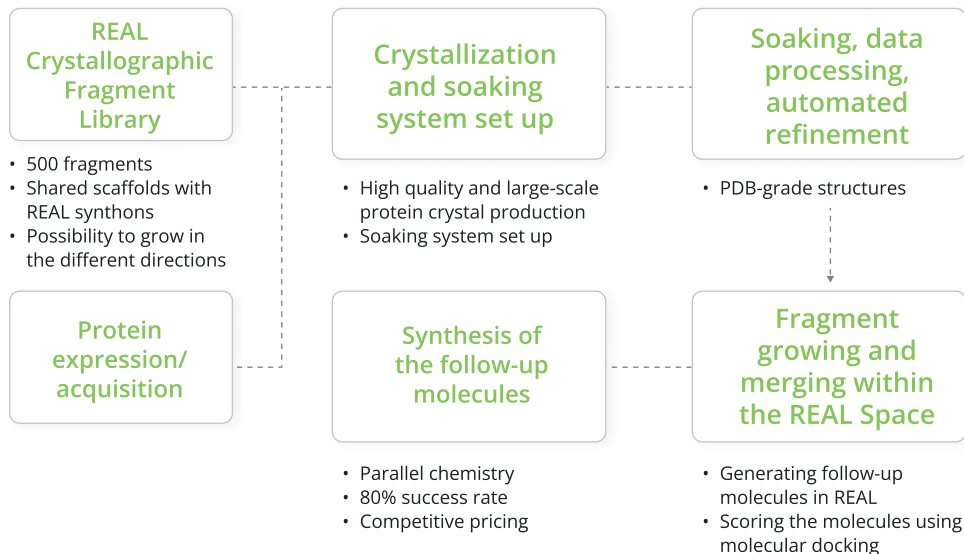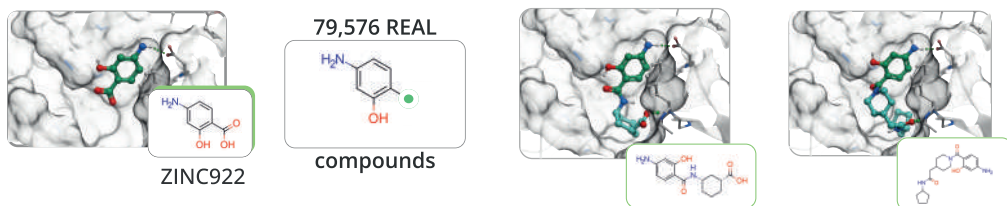# SMART FRAGMENT-BASED DRUG DISCOVERY

Fragment-Based Drug Discovery (FBDD) has proven itself as a reliable method to discover starting points that can be optimized to become clinical candidates. The unique Chemspace REAL Fragment Library built to represent the synthons of the REAL Space insures the easy way to grow the hit fragments withing the REAL Space.

REAL Crystallographic Fragment Library

- 500 fragments
- Shared scaffolds with REAL synthons
- Possibility to grow in the different directions

Crystallization and soaking system set up

- High quality and large-scale protein crystal production
- Soaking system set up

Soaking, data processing, automated refinement

- PDB-grade structures

Protein expression/ acquisition

Synthesis of the follow-up molecules

- Parallel chemistry
- 80% success rate
- Competitive pricing

Fragment growing and merging within the REAL Space

- Generating follow-up molecules in REAL
- Scoring the molecules using molecular docking

HOW TO GROW THE HIT-FRAGMENTS?

A custom subspace is created based on the fragment, which is then docked into the crystal structure using an APF template to select the top-performing compounds.

ZINC922

79,576 REAL compounds

FRAGMENT LINKING

For fragment linking the APF template is constructed from both crystallized fragments.

79,576 REAL compounds   24,050 REAL compounds

chem-space.com
sales@chem-space.com