

Screening Compound Libraries

- HTS Compound Collection
- Targeted and Focused Libraries
- Diversity and Pre-plated Screening Sets
- Fragment Libraries for FBDD
- Custom Compound Libraries Design
- Tangible Screening Compounds

MedChem CRO Services

- Custom Synthesis
- Off-the-shelf Building Blocks
- Fine Organic Chemicals
- Scaffold Hopping
- Route Scouting, Scale-up
- Process Optimization

Computational Chemistry Services

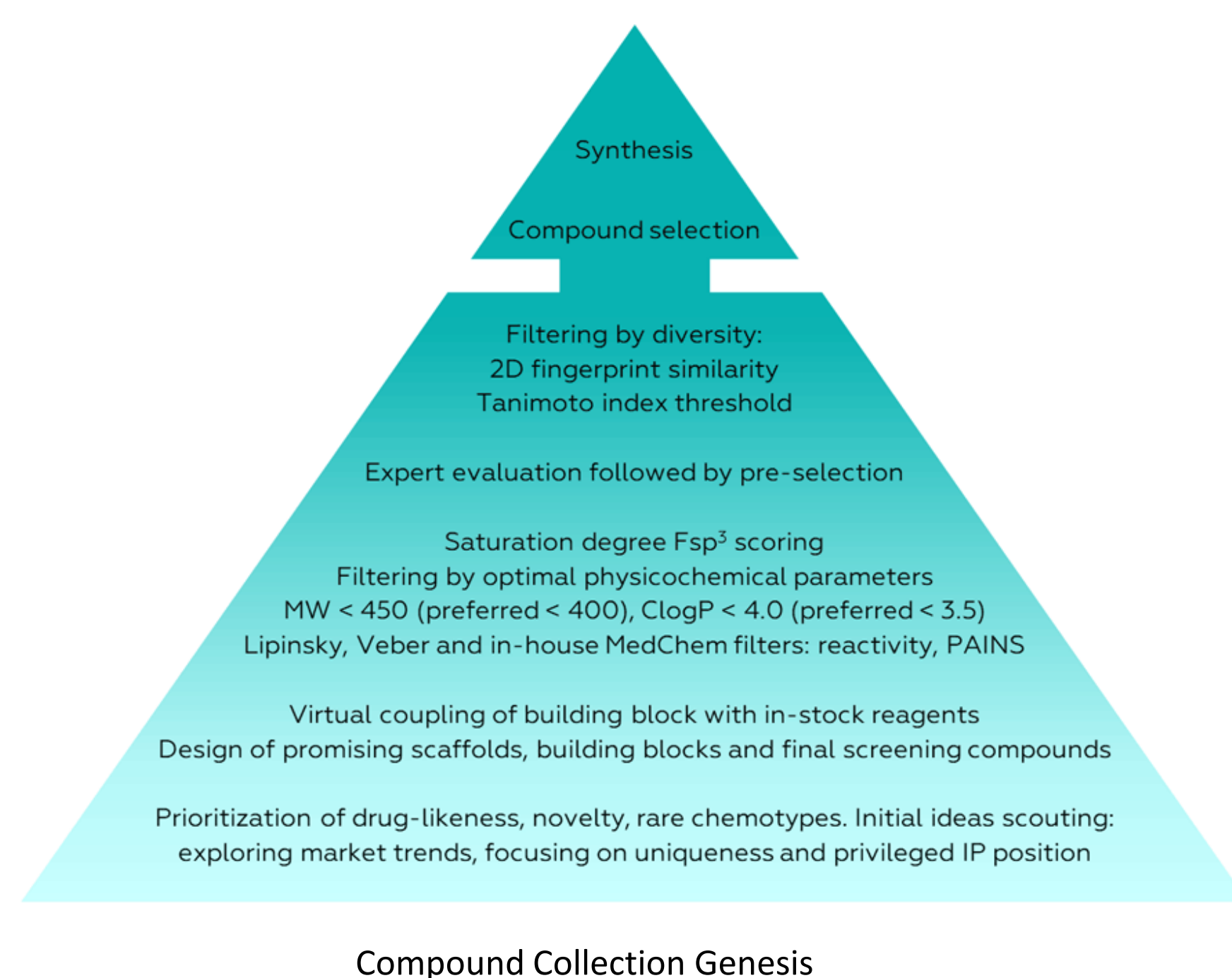
- Physicochemical Properties Calculations
- ADMET Prediction, QSAR, Diversity
- Computer-Aided Molecular Design: Virtual Screening, Machine Learning
- Molecular Dynamics Simulation
- Structural Bioinformatics

In Vitro ADMET Tests

- Solubility, LogP, LogD
- Permeability Evaluation (Caco-2, MDCK)
- Plasma Protein Binding
- Volume of Distribution
- Brain and Lung Tissue Binding
- Proteinase, Thrombin Inhibition Assays

Screening Compounds Synthesized In-house

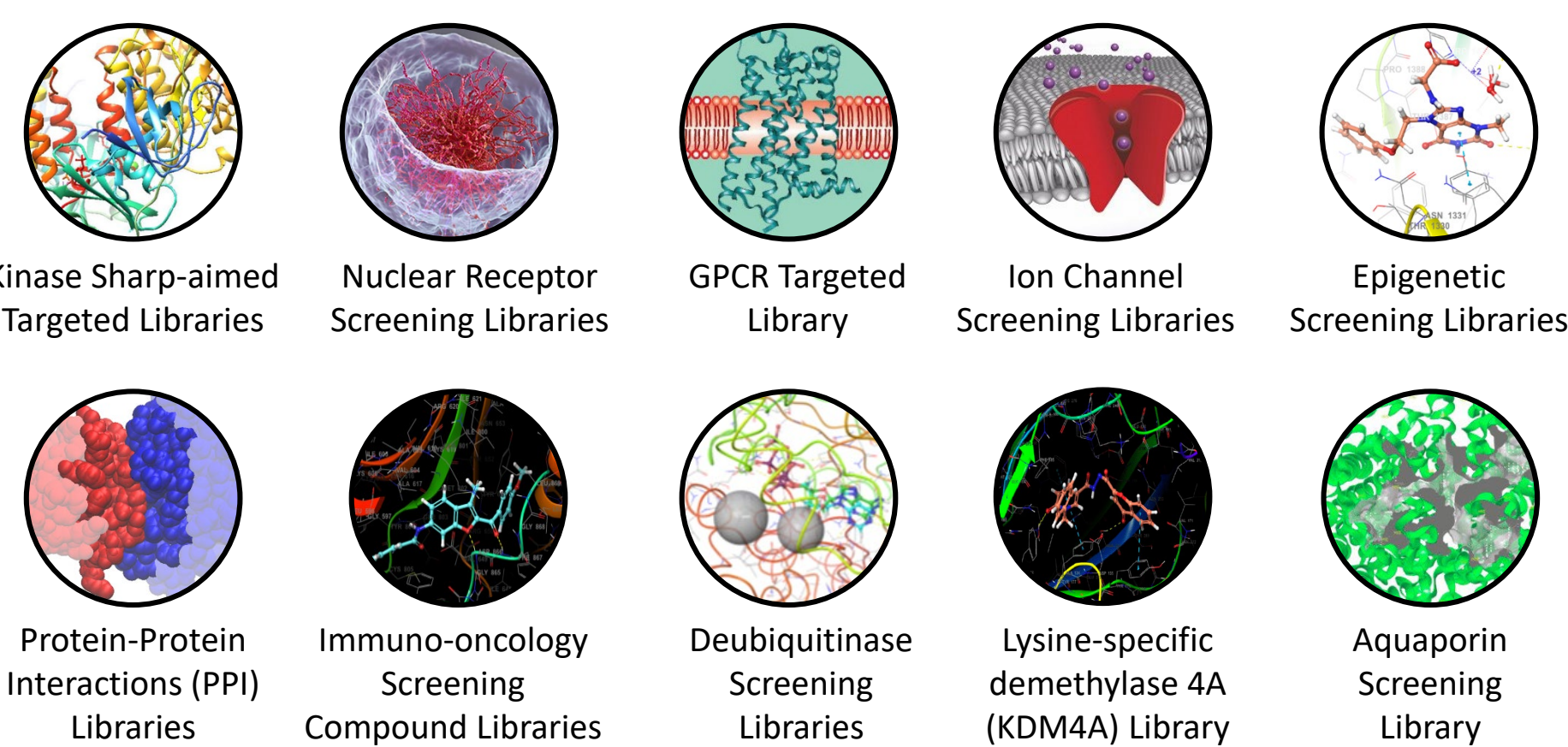
- 510,000 compounds in-stock
- 1,300 original scaffolds
- 2,500,000 tangible molecules
- > 90 % purity confirmed by LCMS or 400MHz NMR
- Prompt delivery worldwide
- Formatting: solids or DMSO solution
- Customized bar-coding and labeling



Targeted and Focused Screening Libraries

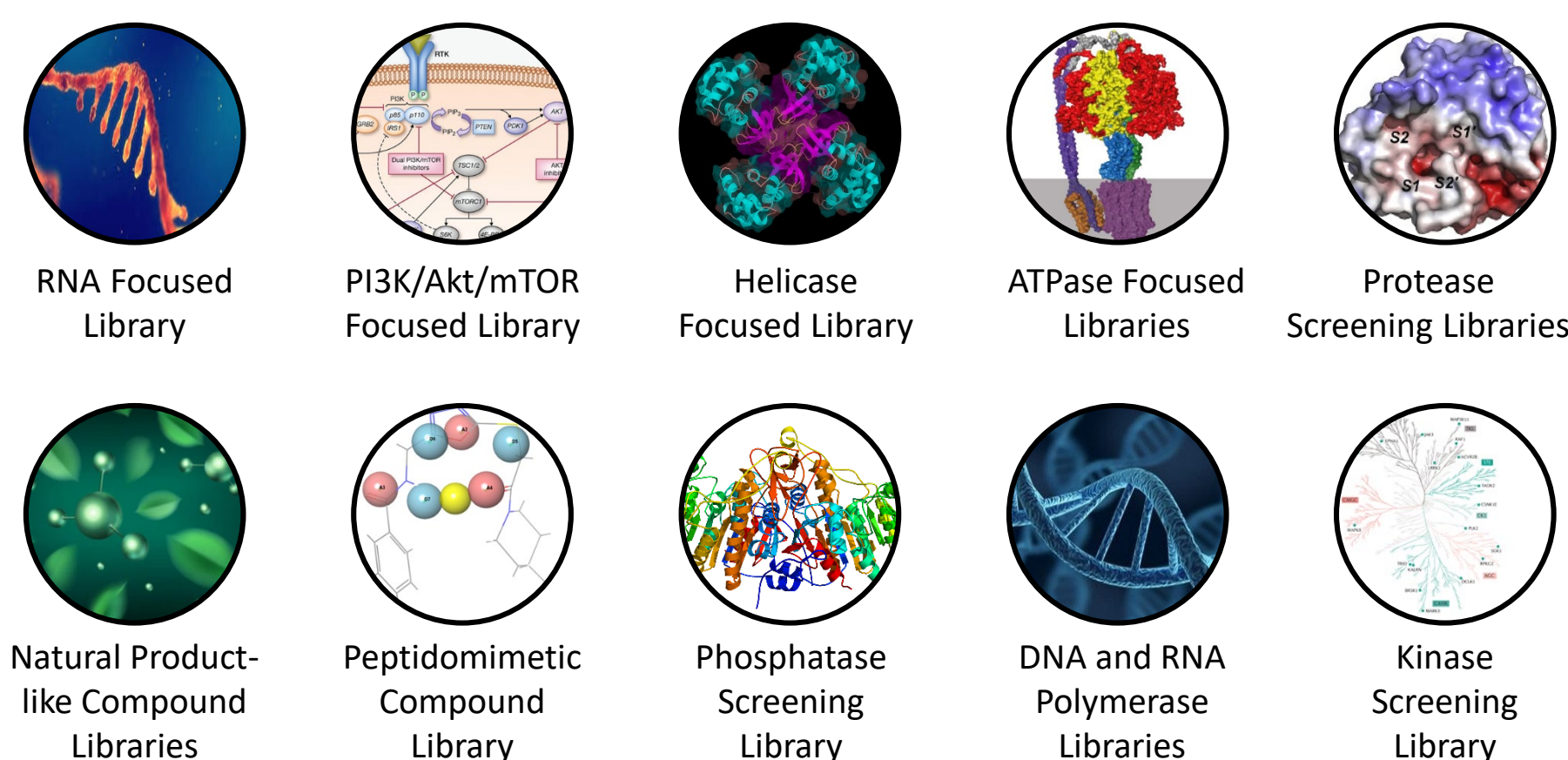
Receptor-based Targeted Libraries

- Flexible docking to X-ray target structures
- High-throughput virtual screening, homology modeling



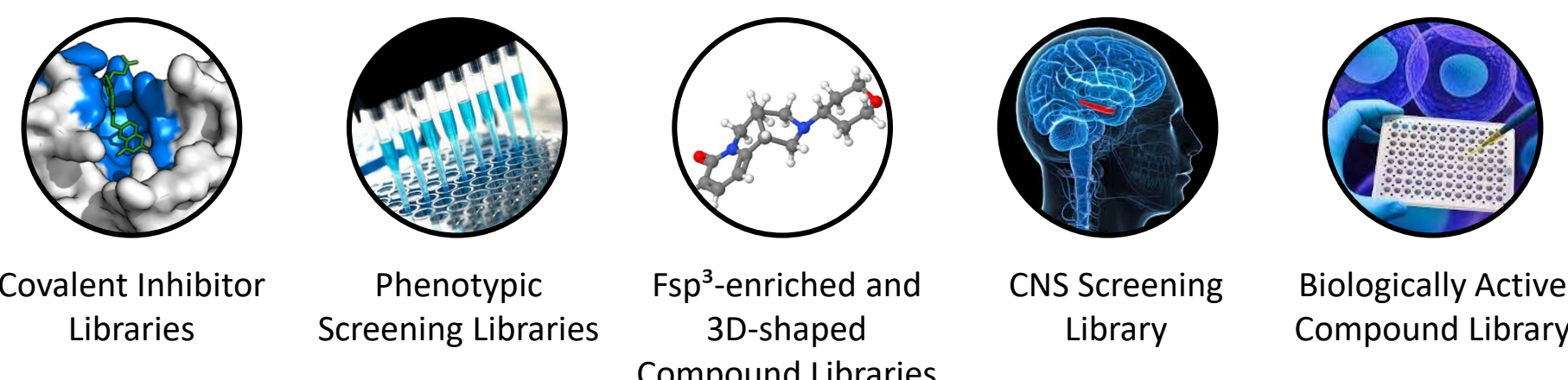
Ligand-based Focused Libraries

- 2D fingerprint similarity search
- Decision tree method, structure-activity relationships



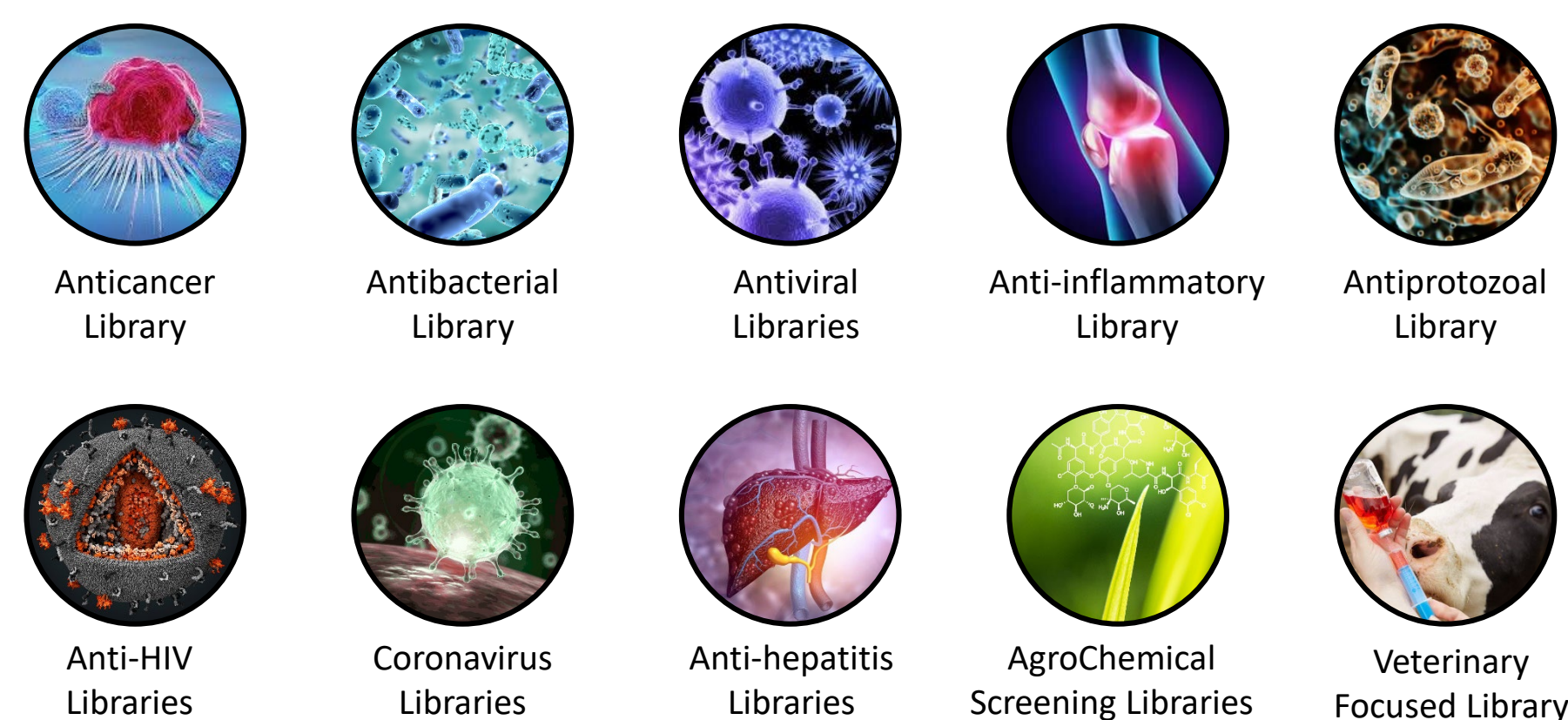
Cheminformatics-based Libraries

- Combination of physicochemical parameters and descriptors, ADMET characteristics
- Selection by relevant chemical moieties



Disease-based Libraries

- Ligand-, receptor- or cheminformatics-based approaches
- Focused on general pharmacological activity rather than particular drug target or drug target family

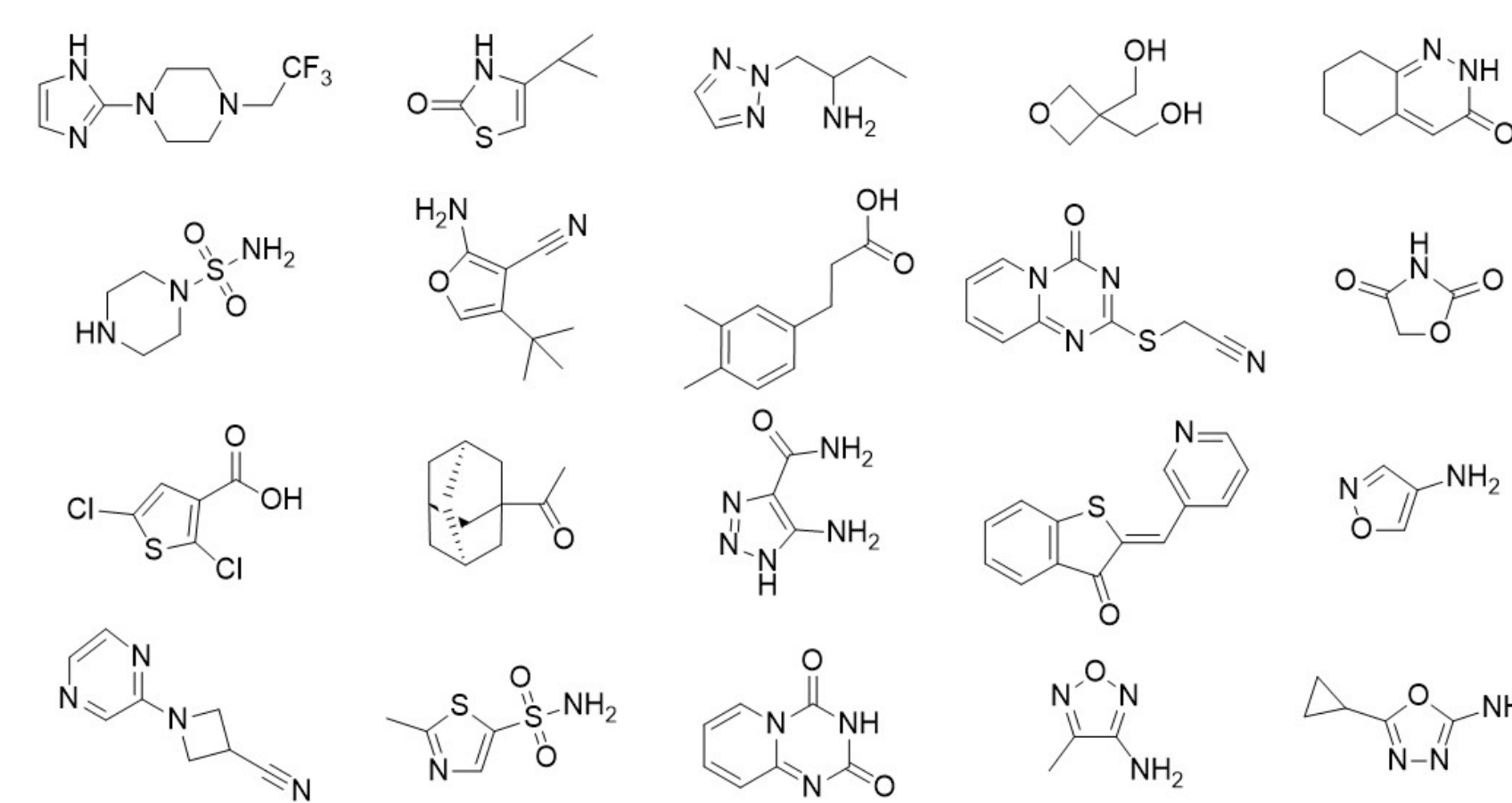


Fragment Libraries for FBDD

- 55,000 in-stock fragment-like compounds
- MW ≤ 300 and ClogP ≤ 3.0
- Available for immediate delivery
- Small diversity sets available

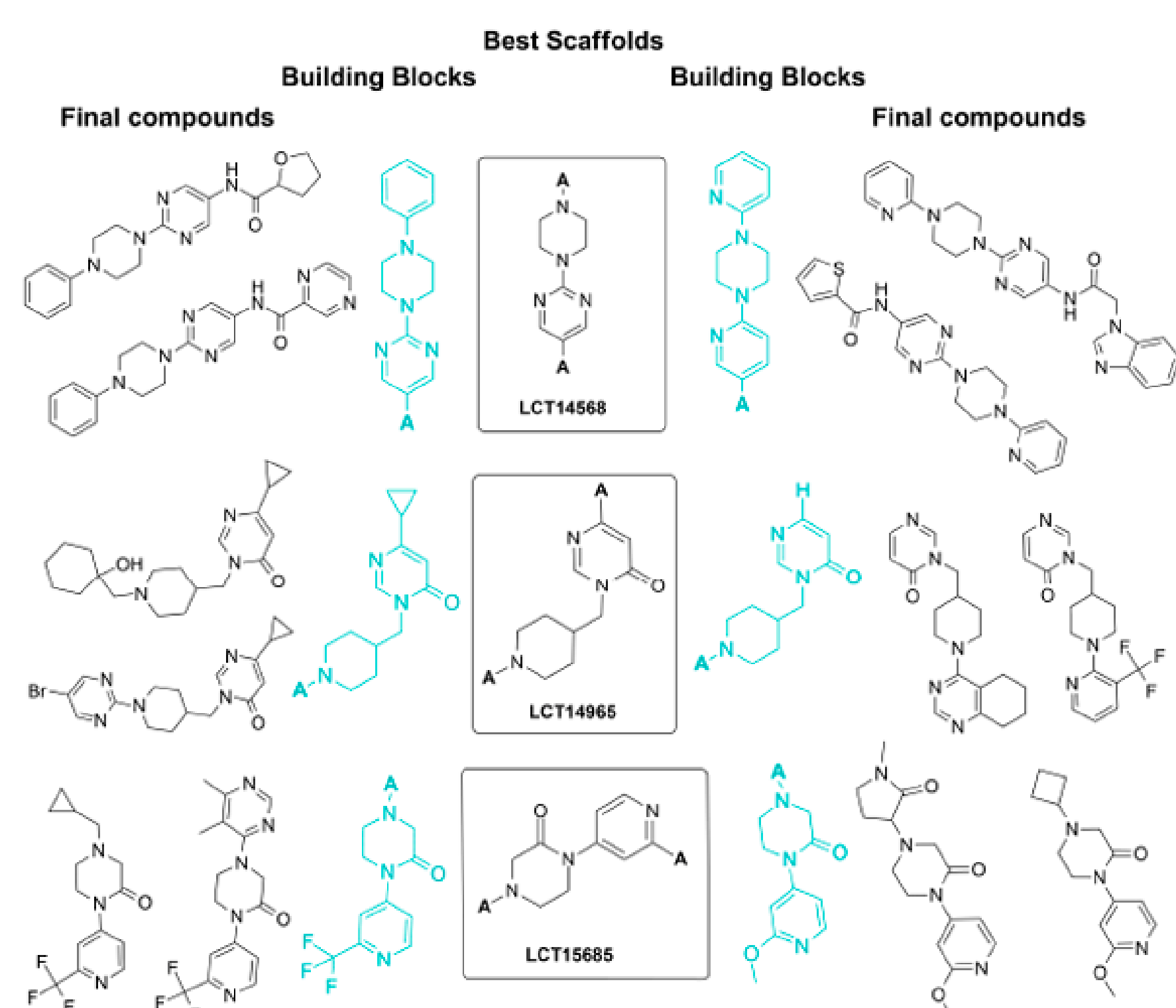
Specialized fragment screening subsets, including:

- Fluorine Fragment Library (6,800)
- Fluorine Fragment Cocktails (1,300 in 130 cocktails)
- Bromine Fragment Library (2,300)
- Fragment Library Experimental Solubility (22,500)
- Fsp³-enriched Fragment Library (19,900)
- Low MW Fragment Library (7,200)
- PPI Fragment Library (7,100)
- Natural Product-like Fragment Library (3,800)
- Covalent Fragment Library (6,200 compounds) and many more...



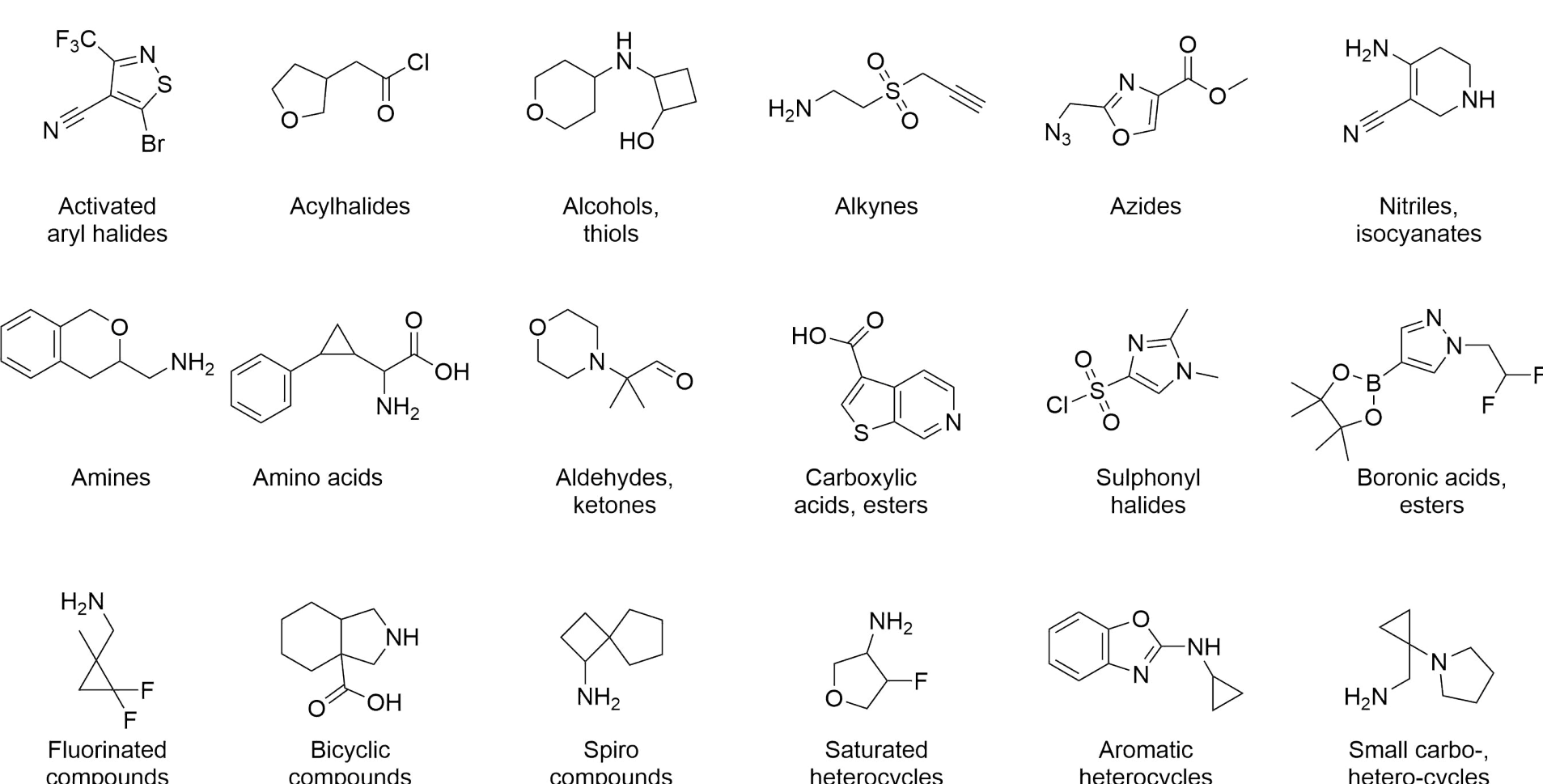
Exclusive Molecular Scaffolds

- Maximum structural diversity and rare chemotypes
- Aimed at lead-orientated libraries
- Novel structures with privileged IP position
- 2-3 variation points per scaffold
- Optimal physicochemical properties
- In-house structural and MedChem filters



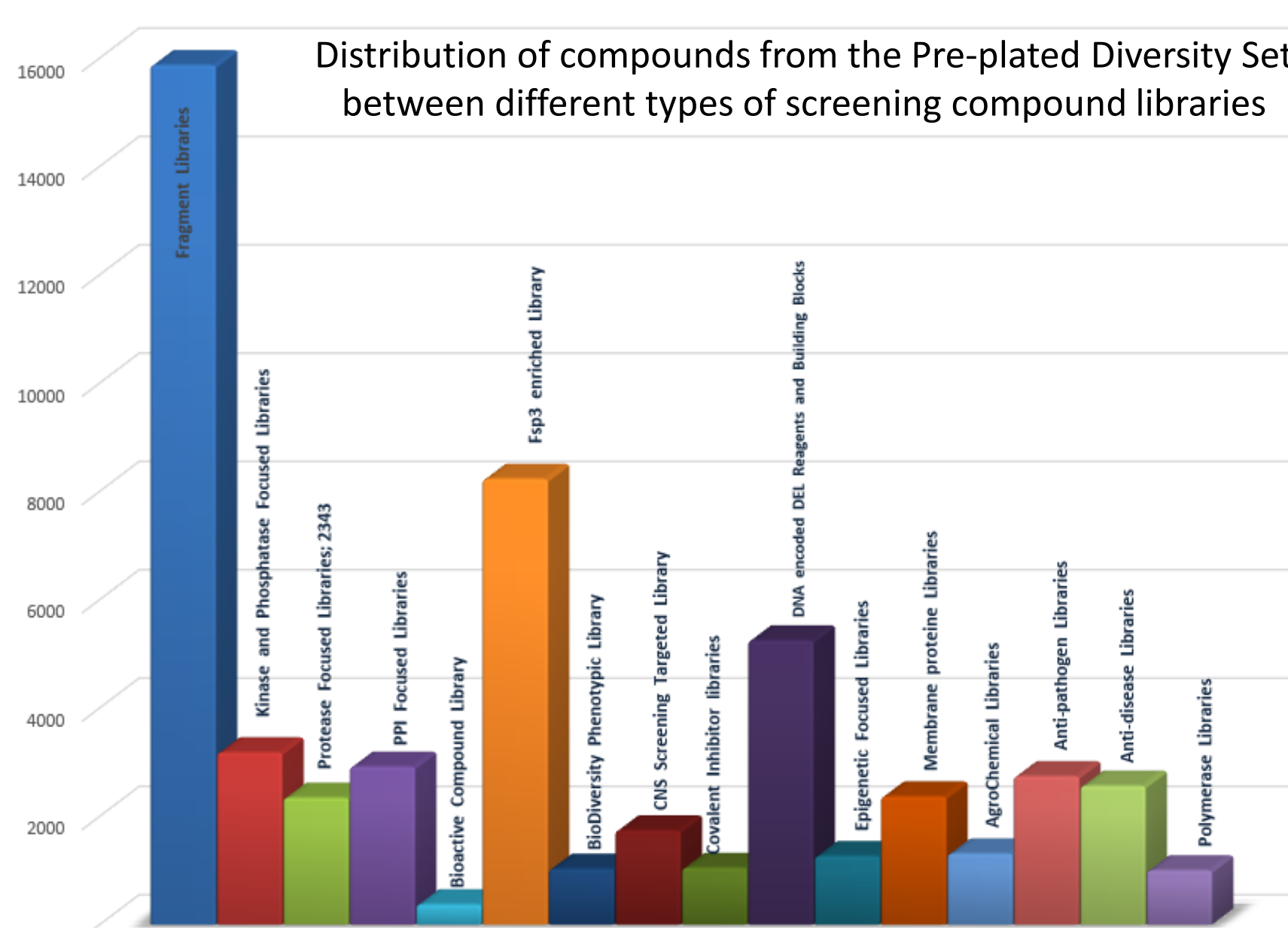
Advanced Building Blocks

- 63,000 original building blocks, including: 13,000 in-stock compounds in multi-gram quantities, 50,000 tangible molecules, synthesized on request
- Re-synthesis and scale-up to 50 kg



Pre-plated Diversity Set

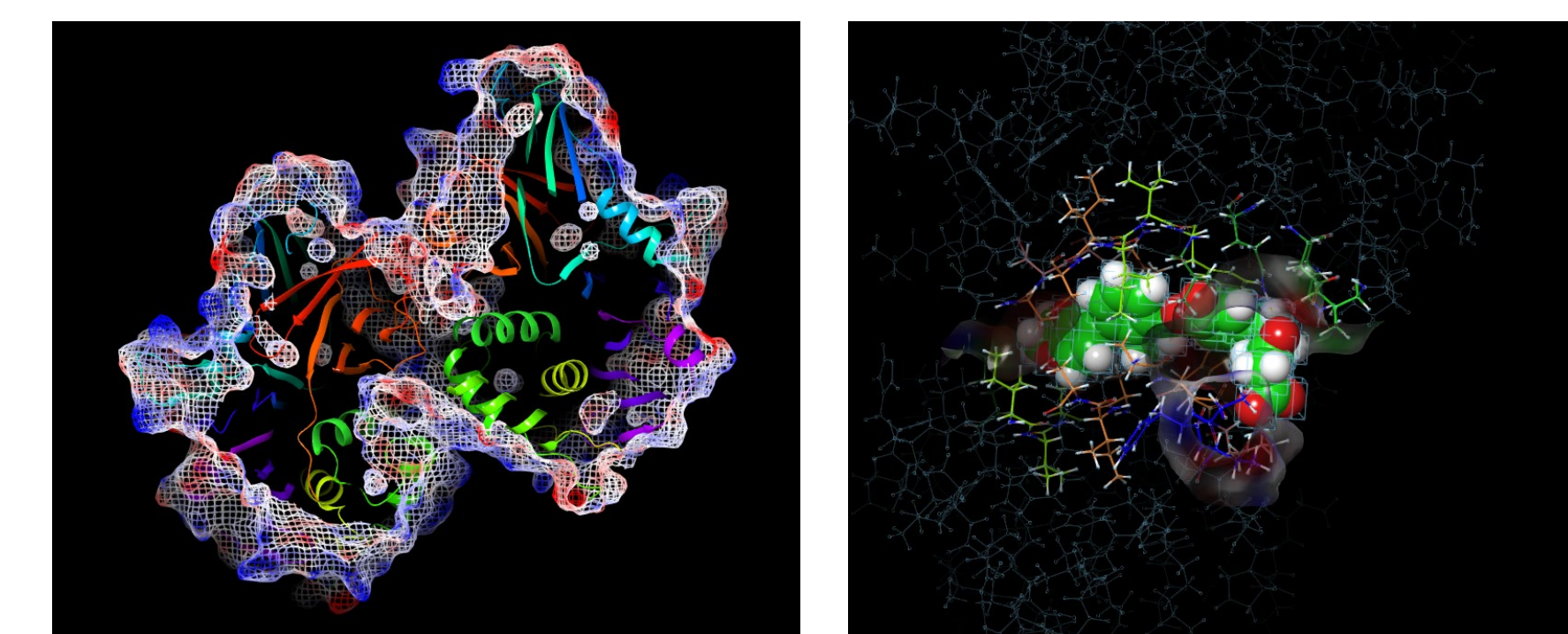
- 100,000 novel screening compounds
- Ideal for phenotypic (cell-based) and target-based HTS
- Non-overlapping subsets of 5K, 10K, 15K, 20K molecules
- Convenient access to the best-selling screening libraries



Life Chemicals Services

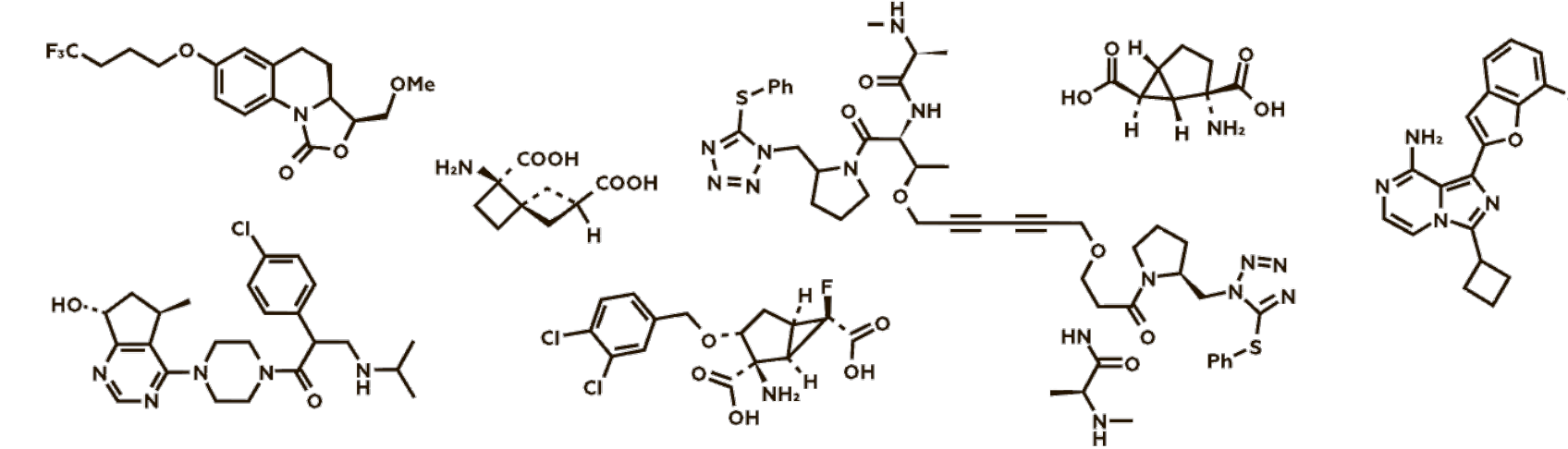
Computational Chemistry

- Computer-aided rational design of small organic molecules against any biological target
- Drug-likeness and lead-likeness prediction
- Receptor-based virtual screening: molecular docking
- Ligand-based virtual screening: shape similarity and pharmacophore search
- Molecular dynamics simulation of macromolecules
- Protein structure modeling, *de novo* or by homology



Custom Synthesis

- Synthesis of individual compounds
- New chemical entities and analogs for H2L development
- Reference compounds and potential impurities
- Scaffold hopping and fragment linking



Synthesis of Compound Libraries

- Based on in-house or customers' scaffolds
- Design and synthesis of custom targeted libraries
- Optimization of ADMET, potency and selectivity