



# Next-generation Compound Libraries: from Virtual to High-throughput Screening

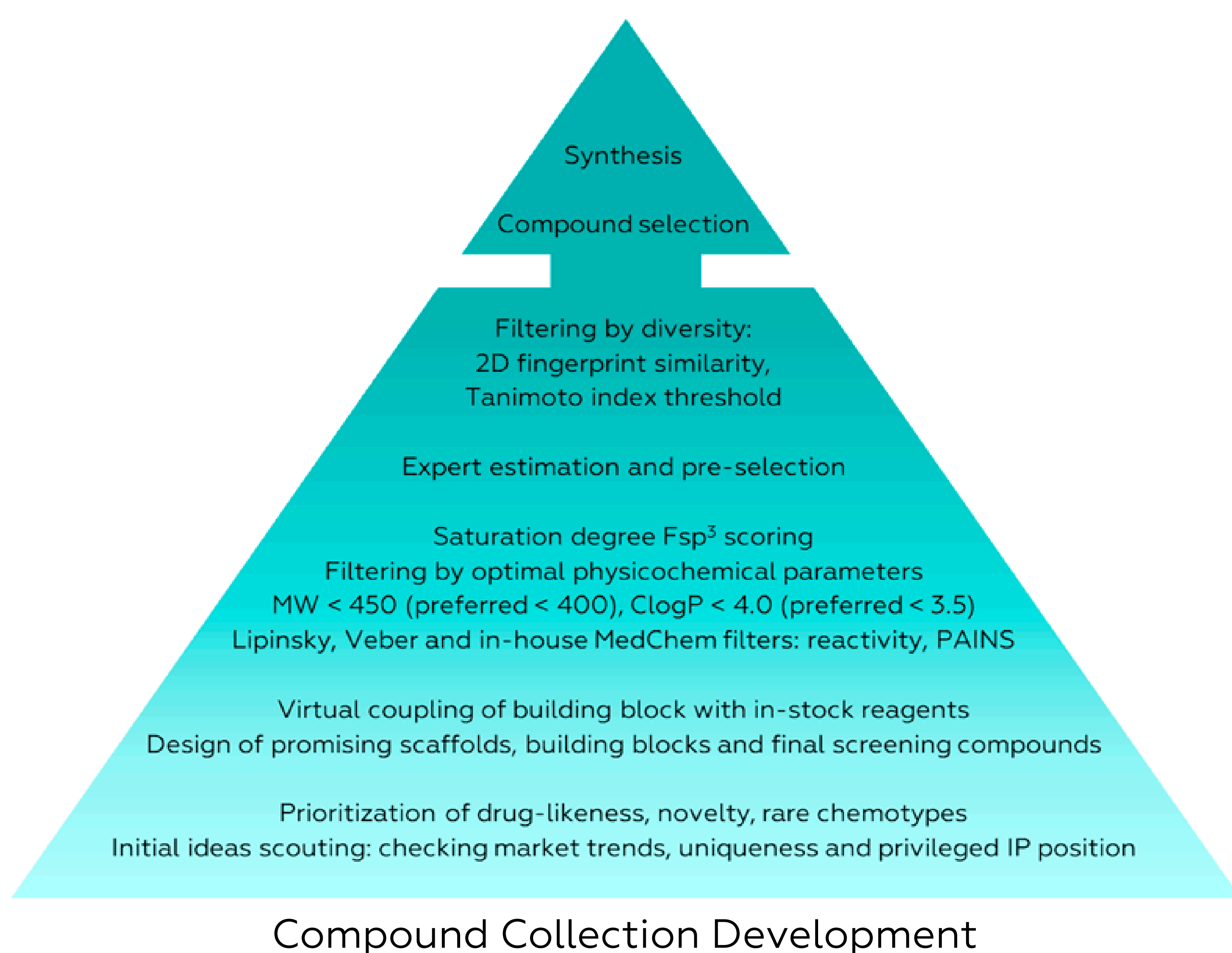
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## Proprietary Screening Compound Collection

- 575,000 stock compounds synthesized on site
- Novel structures with privileged IP position
- Structural diversity and chemotypes rarity
- Optimal physicochemical properties
- In-house structural and MedChem filtering
- > 90 % purity confirmed by LCMS or 400MHz NMR
- Customizable formatting: solids or DMSO solution



## Design and Synthesis of Compound Libraries

- R&D projects, original chemistry, custom-tailored collections
- Hit-to-lead, SAR studies, process optimization and scale-up
- Scaffold-hopping, bioisosteric replacements, conformational restrictions, peptidomimetics
- Optimization of ADMET, potency and selectivity

### Structure-Based Design

- Flexible docking
- Homology modelling
- Pharmacophore refinement

### Shape & Chemotype Expansion

- 3D shape profiling
- Chemotype clustering
- Drug-like filtering

➔ *Broadest coverage of novel scaffolds*

## LifeCheMyriads: Virtual Compound Hyperspace

*Chemistry and HTS of tomorrow*

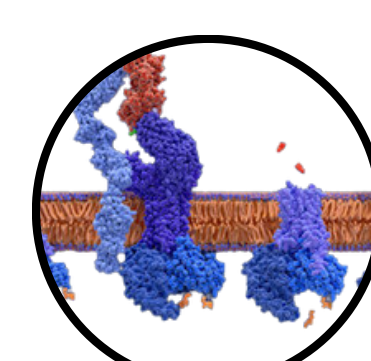
- Most dynamic proprietary hyperspace of over **50 billions** synthesizable and Med Chem-relevant compounds
- Created in collaboration with ➤ **Alipheron**
- Real-time ultra-fast AI-accelerated search
- Cheminformatics support, CRO services, prompt delivery

## Targeted and Focused Screening Libraries

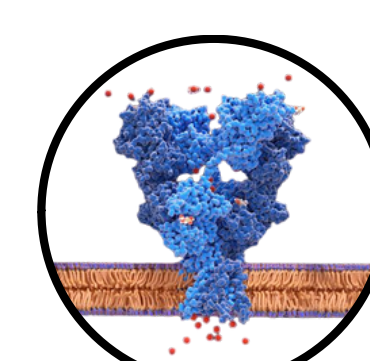
- More than 120 specialized screening libraries
- Rapidly growing portfolio of pre-plated assay-ready sets

### Receptor-based Targeted Libraries

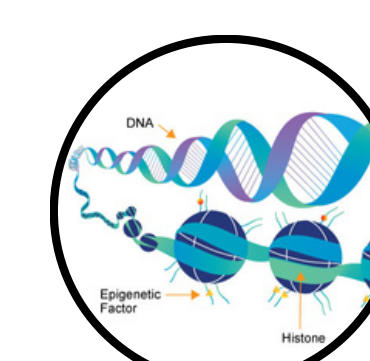
- Flexible docking to X-ray target structures
- High-throughput virtual screening, homology modeling



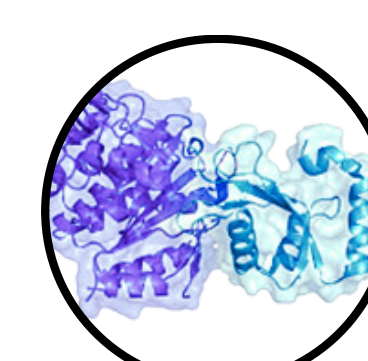
GPCR Targeted Library



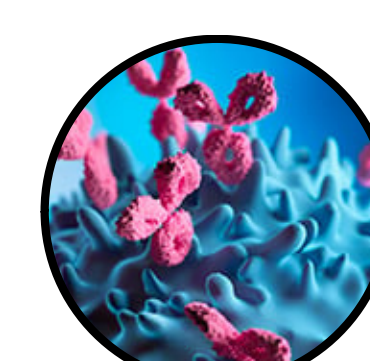
Ion Channel Libraries



Epigenetic Libraries



Protein-Protein Interactions (PPI) Libraries



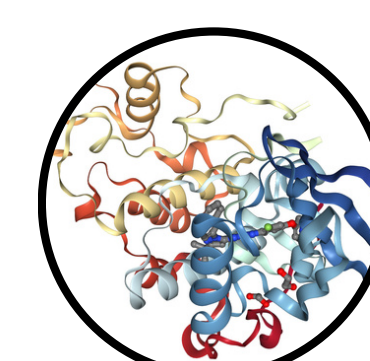
Immuno-oncology Libraries

### Ligand-based Focused Libraries

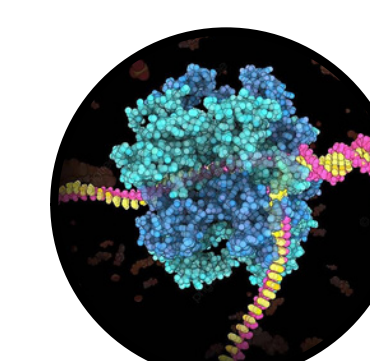
- 2D fingerprint similarity search
- Decision tree method, structure-activity relationships



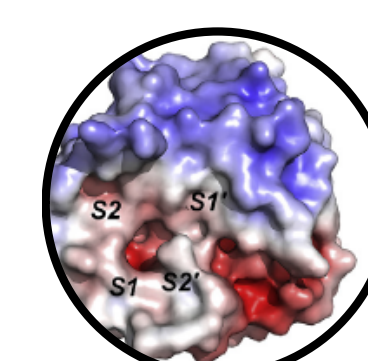
RNA Focused Library



Kinase-focused Libraries



Helicase - focused Library



Protease Libraries



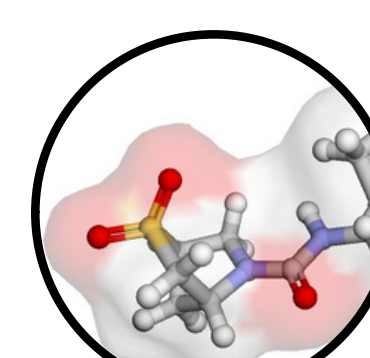
Natural Product-like Compounds

### Cheminformatics-based Libraries

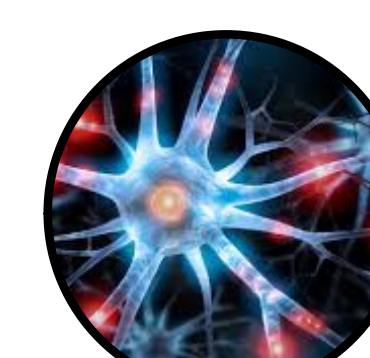
- Integration of physicochemical parameters and descriptors
- Selection by relevant chemical moieties



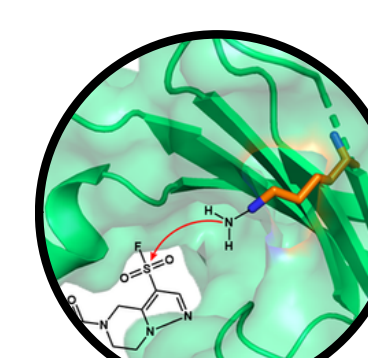
Bioactive Library



Fsp<sup>3</sup>-enriched, 3D-shaped Libraries



CNS-focused Library



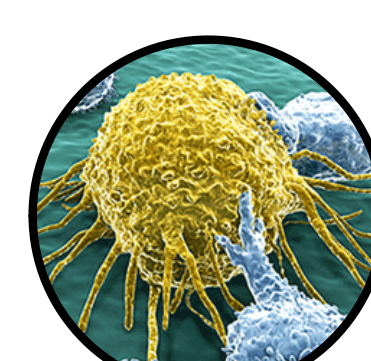
Covalent Inhibitor Libraries



Phenotypic Libraries

### Disease-focused Libraries

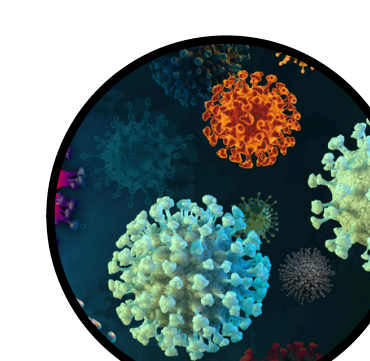
- Ligand-, receptor- or cheminformatics-based approaches
- Focused on general pharmacological activity rather than particular target



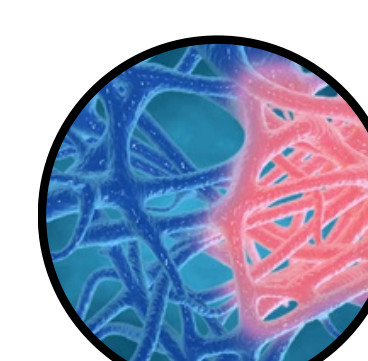
Anticancer Library



Antibacterial Library



Antiviral Libraries



Anti-inflammatory Library



Antiprotozoal Library

### Pre-plated Sets in Screening-ready Formats

- Convenient access to the best-selling screening libraries
- 96- or 384-well plates, 5–100  $\mu$ L per well
- 10 mM DMSO solutions for screening compounds
- 100–200 mM fragment solutions
- Non-overlapping subsets
- Automation-compatible

