Phenotypic Screening Library

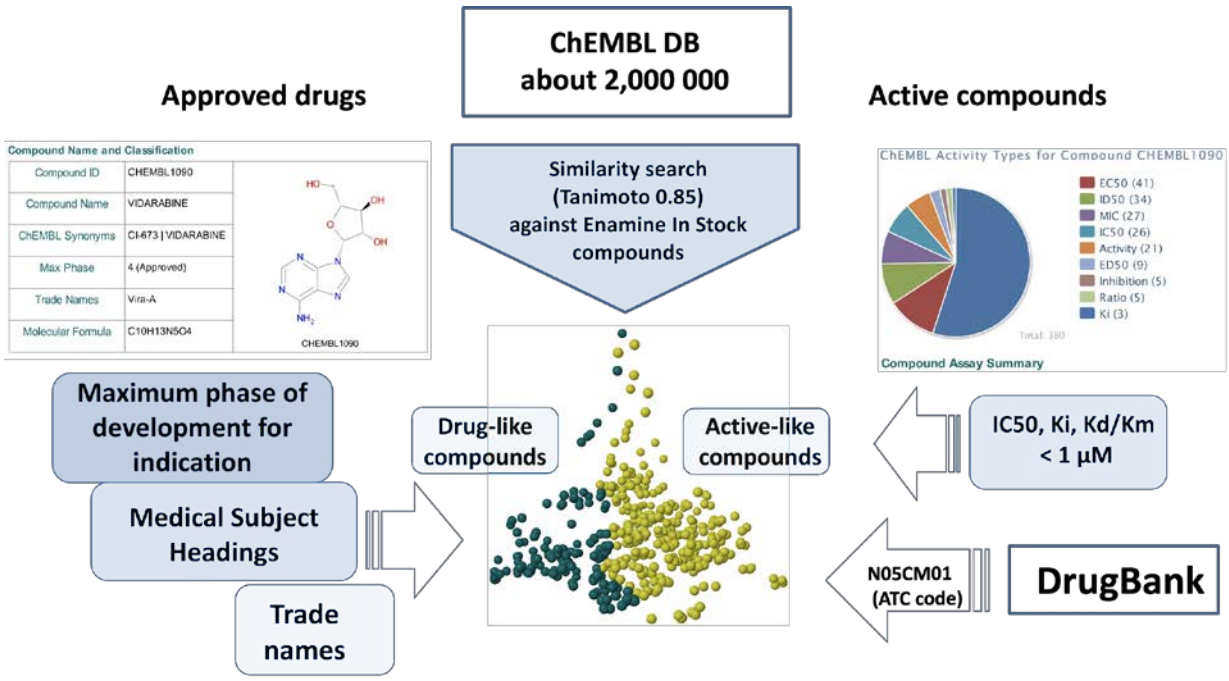
6 370 compounds

Special diversity set created for Phenotypic Screens

A versatile focused library specifically designed to fit both target-based and cell-based screening approaches in search for novel mechanisms of action. This set will be useful in drug repurposing projects, for discovery of the potential targets and investigation of signalling pathways. Phenotypic Screening Library (PSL) from Enamine is composed of the annotated chemical entities and delivered together with all associated cross-linked biological data.

Library Design

To create multipurpose phenotypic library we investigated an optimal balance between diversity of biological activities versus structural diversity of small molecules. The library includes 900+ approved drugs and most similar compounds with identified mechanism of action (T>85%, linear fingerprints). In addition, PSL is enriched with 2000+ of annotated potent inhibitors and their biosimilars, covering a broad diversity of biological targets. Compounds from PSL are cell-permeable and possess pharmacology-compliant physicochemical properties.

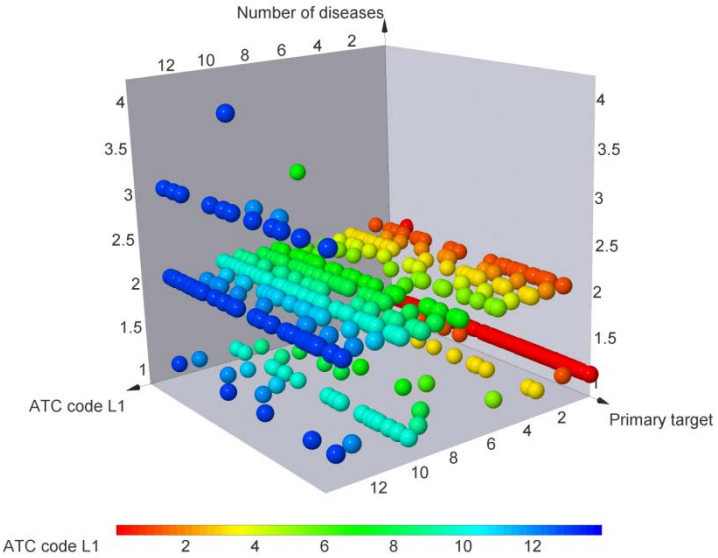


PSL can be divided into smaller focused subsets based on the indicated disease classification (ATC code), target specification or Bayesian fingerprints (applied for Tanimoto similarity search).

Supporting biological data/documentation

- Provides easy access and analyze information from in-fields.
- Covers different aspects: polypharmacology, number of targets and description.
- Numbers and names of associated diseases are indicated for majority of compounds.

Figure below demonstrates chemical space distribution using 2D prop parameters (LogP, fraction of rotatable bonds, donor/acceptor count, etc.), normalized PMI vectors and distribution between classes of the most potent targets, total number of targets per compound and first level of Anatomical Therapeutic Chemical (ATC) Classification.



Our Phenotypic Library can be applied for screening against different protein classes and diseases, affecting adjacent tissues or individual body systems.

Molecular Parameters

Parameter	Range
MW	120 … 450
LogP	-4 – 5.5
TPSA	5 – 210 A^2
RotBonds	0 – 8
Ring count	1 – 5
Isolated benzene rings	≤ 3
Reactive groups and toxicophores were filtered out	
MedChem inspection - no trivial structures and reagents, no amino acids etc.	

All compounds are stored as dry materials and they can be acquired in diverse custom formats. You have also an option to screen the library directly at Enamine. We will be happy to offer you discount on library cost depending on the collaboration scope.