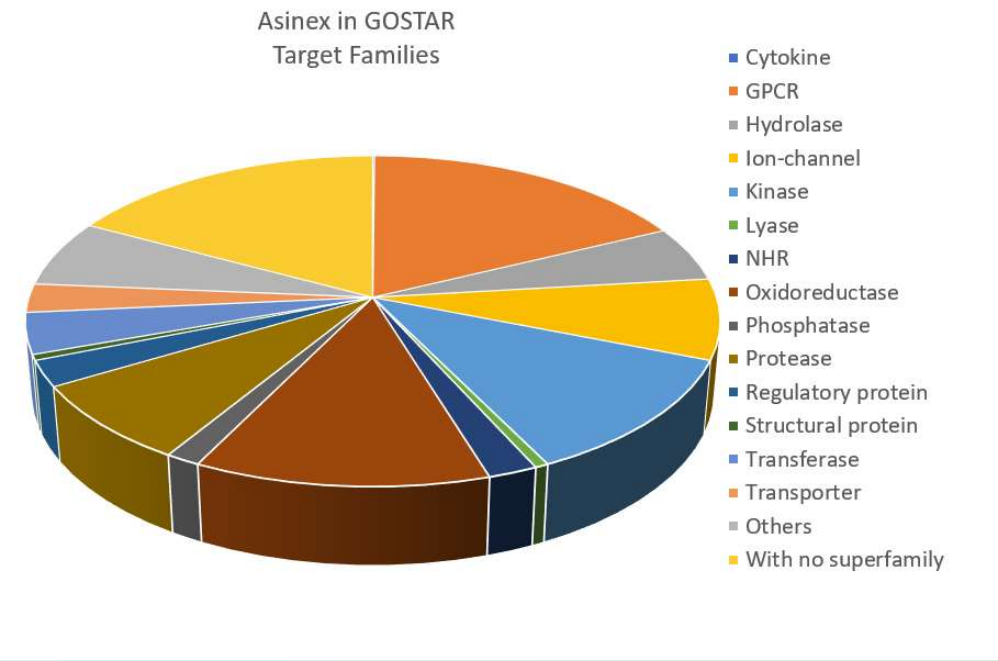
Asinex in GOSTAR
Biologically Annotated Library for Phenotypic or Target-directed Screening

Biologically annotated chemical libraries have long been recognized as a valuable source of small molecules to drive drug discovery efforts [1-2]. Such libraries are often used to probe complex biological pathways in phenotypic assays providing essential clues for target deconvolution and hit prioritization. In some target-directed screens this type of library can also deliver interesting starting points for further chemical optimization leading to novel candidates with improved pharmacological properties [3]. Compared to large HTS-oriented compound collections application of a smaller biologically annotated library in a multiple assay setting can reduce screening costs without compromising efficiency.

Creation of a credible, biologically annotated library requires both extensive data mining in reliable SAR knowledge databases and selection of compounds maximizing chemical and biological diversity. At Asinex, we have opted to use the Global Online Structure Activity Relationship Database (GOSTAR) as an integrated source of data capturing chemical, biological, pharmacological, and therapeutic parameters https://www.gostardb.com/gostar/. The structural overlap between the Asinex (500K+) and GOSTAR (8M+) databases has revealed **17910** unique molecules with associated biological activity. Application of additional structural filters (PAINS, Eli Lilly [4-5]) has resulted in a set of **11923** compounds; diversity-oriented selection supported by computational and medicinal chemistry expertise has further refined this set resulting in **1878** molecules available for computational or *in vitro* evaluation. Biological diversity is represented by multiple target families (Figure 1) where each molecule is associated with a GOSTAR record via a unique structure code identifier (see SDF/SMILES files).

Figure 1



The library of **1878** annotated compounds is complemented by an extended library of **41K+ analogs** that are readily available.

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Literature:

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2. Moffat, J., Vincent, F., Lee, J. et al. Nat Rev Drug Discov 16, 531–543 (2017). https://doi.org/10.1038/nrd.2017.111
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4. Baell, J. B.; Holloway, G. J. Med. Chem. 2010, 53 (7), 2719– 2740, DOI: 10.1021/jm901137j
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