

COMPOUND LIBRARIES

diversity libraries

ChemDiv SMART library (10,000 compounds)

A 10K subset of SMART ChemDiv library that (1) is pruned for known frequent hitters (PAINS and alike), (2) is balanced in terms of diversity of chemical scaffolds, (3) functional groups are equally represented, (4) has several representative analogs for each of the scaffolds in the library.

Enamine Discovery Diversity Set c. 2022

10,240 lead-like compounds

Chembridge DIVERSet (50,000 compounds)

Structurally diverse small molecule library with broad 3D pharmacophore coverage for hit identification

ChemDiv PPI library (10,000 compounds)

A curated 10K subset of the ChemDiv protein-protein interaction library.

targeted libraries

TargetMol Bioactive Compound Library (5370)

1,257 FDA-approved drugs, 729 internationally approved drugs, 920 pre-clinical or clinical compounds, and ~2,400 annotated compounds targeting various pathways and disease states.

Endocrinology-Hormones Library (297)

Adrenergic Library (117)

Serotonin Library (134)

Epigenetics Inhibitor Library (380)

Chromatin Modification Compound Library (192)

Histone Modification Compound Library (152)

DNA Damage & Repair Compound Library (475)

Immunology Inflammation Compound Library (876)

Cytokines inhibitor Library (182)

Cell cycle related Compound Library (130)

Apoptosis Compound Library (191)

Autophagy Library (623)

Angiogenesis Related Compound Library (378)

Bioactive Plus Compound Library (200)

CNS-Penetrant Compound Library (90)

Coagulation/anticoagulation Compound Library (153)



Anti-cancer Approved Drug Library (313)

Anti-cancer Clinical Compound Library (560)

Anti-Metabolism Disease Compound Library (816)

Anti-Cardiovascular Disease Compound Library (515)

Anti-obesity Compound Library (85)

Anti-aging Library (833)

Anti-diabetic Library (179)

Antiviral Compound Library (1,040) (c.2024)

Anti-infection Compound library (605)

Antibiotics Library (250)

Antifungal Compound Library (66)

Kinase Inhibitor library (900) (*TargetMol*)

Kinase Inhibitor Library (2,700) (*MCE*)

Ion Channel Inhibitor Library (362)

Potassium Channel Blockers Library (60)

Sodium Channel Blockers Library (62)

Calcium Antagonists Library (48)

Protease Inhibitor Library (162)

GPCR Compound Library (730)

Nuclear-receptor Inhibitors Library (239)

TGF- β Smad Compound Library (45)

Wnt & Hedgehog & Notch Compound Library (74)

PI3K/Akt/mTOR Inhibitor Library (190)

JAK STAT Compound Library (145)

NF- κ B Signaling Compound Library (173)