

SPARC BioCentre
 Peter Gilgan Centre for Research and Learning (PGCRL)
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Compound Libraries:

Class	Library (# of compounds)	Description
Drug-like collections	Chembridge DIVERSet (50'000)	<ul style="list-style-type: none"> Extensive pharmacophore coverage ideal for initial screening programs that require high diversity and quality drug-like compounds
	Maybridge HitFinder (14'400)	<ul style="list-style-type: none"> Compounds in this library fit Lipinski's guidelines for "drug-likeness", and all have purity >90%. Compounds have undergone a filtration step to remove reactive species leading to fewer false positive hits
	GlycoNet – Chembridge (24'000) Enamine (45'000)	<ul style="list-style-type: none"> The GlycoNet Chembridge library has no structural overlap with the Chembridge DIVERSet collection and is a great tool for initial screening projects The GlycoNet Enamine collection aims to encompass a large variety of chemotypes with a diverse sample of structural features
	Cyclenium's proprietary QUEST Library™ (8'500)	<ul style="list-style-type: none"> Requires signing a Materials Transfer and Research agreement between the researcher and Cyclenium Pharma Inc. Library of macrocyclic molecules designed for blood-brain barrier penetration, ideal for protein-protein interaction disruption, unique scaffolds existing outside patents and exploring unique macrocyclic chemical space
Clinically approved, Bioactive, and Natural Products	ApexBio FDA approved Drug Library (1'496)	<ul style="list-style-type: none"> All the compounds in this library are FDA approved drugs. This collection was acquired in 2019 to update our older Prestwick Collection. This library would be useful for clinicians interested in repurposing drugs
	Prestwick Collection (1'280)	<ul style="list-style-type: none"> All the compounds in this library are FDA approved drugs, safe for use in humans. The drugs were selected to explore a broad chemical and pharmacological space to accelerate lead discovery This library would be useful for clinicians interested in repurposing drugs

Class	Library (# of compounds)	Description
Clinically approved, Bioactive, and Natural Products (cont'd)	LOPAC (1'280)	<ul style="list-style-type: none"> • A Sigma library of small molecule modulators, marketed drugs, failed development candidates, and “gold standards” that have well-characterized activities • 50% of the compound collection interacts with G protein-coupled receptors, the rest of the library interacts with a broad range of cell signaling and neuroscience targets
	ApexBio Epigenetics Library (281)	<ul style="list-style-type: none"> • A valuable tool for chemical genomics, epigenetic target identification in pharmacogenomics, and other biological applications • Inhibitors of epigenetic enzymes including Histone Deacetylase (HDACs), SIRTs, Lysine demethylases, Histone Acetyltransferases (HATs), DNA Methyltransferase (Dnmts), and SIRTs activators among others
	ApexBio Ion Channel Library (199)	<ul style="list-style-type: none"> • Library compounds target ion channels, such as: Calcium, Potassium, and Sodium channels; GABA receptor; and, Proton Pumps among others. • Structurally diverse, medicinally active, and cell permeable.
	Microsource Spectrum Collection (2'320) Contains compounds from 3 collections: 1. Pharmakon 2. Discover 3. Natural Product	<ol style="list-style-type: none"> 1. Pharmakon is a combination of compounds (1'600) that have reached clinical evaluation; many of them are still in the market. The library contains information regarding each compounds' biological profile, generic and market names, literature references, and toxicology 2. Discover is comprised of compounds that have shown biological potential in peer-reviewed publications, but never led to development as drugs for human diseases 3. Natural Product is a portion of the library is derived from commercial sources with >95% purity (full description of the chemical classes contained in this library can be found below)¹ <ul style="list-style-type: none"> • This library would be useful for clinicians interested in repurposing drugs

¹ ~ 75% of the library is composed of: 16% alkaloids, 12% flavonoids, 12% sterols/triterpenes, 10% diterpenes/sesquiterpenes, 10% benzophenones/chalcones/stilbenes, 9% limonoids/quassinoids, 6% chromones/coumarins.

The rest of the library is made up of quinones/quinonemethides, benzofurans/benzopyrans, rotenoids/xanthanones, carbohydrates, and benzotropolones/depsides/depsidones, in descending order

Class	Library (# of compounds)	Description
Ontario Institute of Cancer Research (OICR) Libraries	OICR Kinase Inhibitor Library (640)	<ul style="list-style-type: none"> • Kinase inhibitors targeting protein kinases and lipid kinases • Library is made up of public structures whose target kinases are known
	OICR Tool Kit (560)	<ul style="list-style-type: none"> • Mechanism of Action library: known biological targets. • Many inhibitors in this collection have reached clinical phase development or exist as marketed therapeutics. • Collection includes: PARP inhibitors, STAT3 inhibitors, and anti-cancer or chemotherapeutic compounds
	Prestwick Phytochemical Library (320)	<ul style="list-style-type: none"> • Natural product collection, mostly derived from plants, rich in chemotype diversity, thus ideal for follow-up chemistry
	Peptidomimetic Library (3'000)	<ul style="list-style-type: none"> • Collection from OICRs ChemDivs' Non-peptide Peptidomimetics library • Contains α-helix and β/γ-turn mimetics
	Microsource Natural Products Library (800)	<ul style="list-style-type: none"> • 88% overlap between this collection and the larger Microsource Spectrum collection
	Tocris Library (1'185)	<ul style="list-style-type: none"> • Biologically active compound collection • Some overlap with other SPARC library collections (see % Compound Overlap between Libraries table for more information)

% Compound Overlap between Libraries:

OICR Collections Other SPARC Collections	Tocris Library (% Overlap)	Microsource Natural Products Library (% Overlap)
Prestwick Collection	9%	0%
LOPAC	27%	0%
Microsource Spectrum Collection	12%	88%