

## Chemical Compound Libraries at the McMaster High Throughput Screening Lab

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### 1. Bioactives 2 – 11,471

Compounds with confirmed biological activity and targets. These compounds include natural products, FDA approved drugs, and clinical compounds. The collection is structurally diverse and cell permeable and has no overlap with the Bioactives collection that is part of the CCC.

### 2. Gram negative screening set – 73,931 compounds

- a. Custom designed collection with low logD values to target Gram negative bacteria

### 3. Diverse compound collection – 67,934 compounds

- a. Customized collection from Enamine and ChemBridge designed to expand chemical coverage of the McMaster collections

### 4. Canadian Compound Collection (CCC) Library which is approximately 30 000 compounds composed of 6 subsets, each from a different distributor:

- a. Maybridge / from Maybridge (part of Thermo Fisher), Cornwall, UK

16 000 compounds

Average molecular weight: 325 g/mol

This Maybridge custom library is composed of synthetic small molecules from the Maybridge Screening collection. The molecules in this library follow Lipinski's rule of five and have good ADME (absorption, distribution, metabolism and excretion) components.

For more information:

[http://www.maybridge.com/portal/alias\\_Rainbow/lang\\_en/tabID\\_146/DesktopDefault.aspx](http://www.maybridge.com/portal/alias_Rainbow/lang_en/tabID_146/DesktopDefault.aspx)

- b. DIVERSet / from ChemBridge Corp., San Diego, CA, USA

10 000 compounds

Average molecular weight: 325 g/mol

This is a collection of synthetic small molecules with diverse pharmacophores and drug-like compounds.

For more information:

[http://www.chembridge.com/screening\\_libraries/diversity\\_libraries/index.php](http://www.chembridge.com/screening_libraries/diversity_libraries/index.php)

- c. Prestwick Chemical Library / from Prestwick Chemical, Illkirch, France

1120 compounds

Average molecular weight: 372 g/mol

This is a set of small molecules comprised of 100% FDA approved drugs. The compounds in this collection have high chemical and pharmacological diversity and known bioavailability and safety in humans.

For more information:

<http://www.prestwickchemical.fr/index.php?pa=26>

- d. BIOMOL<sup>2865</sup> Natural Products Library / from Enzo Life Sciences, Inc., Farmingdale, NY, USA

502 compounds

Average molecular weight: 401 g/mol

Highly purified natural products of known structure.

For more information:

<http://www.enzolifesciences.com/BML-2865/natural-product-library/>

- e. Lopac<sup>1280</sup> (International Version) / from Sigma-Aldrich Canada Ltd., Oakville, ON, Canada

1280 compounds

Average molecular weight: 337 g/mol

A set of drug-like molecules active in the fields of cell signaling and neuroscience.

For more information:

<http://www.sigmaaldrich.com/catalog/search/ProductDetail/SIGMA/LO3300>

- f. Spectrum Collection / from MicroSource Discovery Systems, Inc., Gaylordsville, CT, USA

2000 compounds

Average molecular weight: 354 g/mol

This collection is comprised of drugs (60%) with defined pharmacological and toxicological profiles, natural products (25%) with unknown biological properties that cover a wide range of chemical classes and structural diversities, and other bioactive components (15%) which include non-drug enzyme inhibitor, receptor blockers, membrane active compounds, and cellular toxins.

For more information:

<http://www.msdiscovery.com/spectrum.html>

5. Maybridge custom made library, 49 907 compounds from Maybridge (part of Thermo Fisher), Cornwall, UK

Average molecular weight: 325 g/mol

This library was made by Maybridge for the McMaster University HTS facility. This library is composed of synthetic small molecules that follow Lipinski's rule of five and have good ADME properties. The library was designed around diversity and good drug/lead-like compounds.

For more information:

[http://www.maybridge.com/portal/alias\\_Rainbow/lang\\_en/tabID\\_146/DesktopDefault.aspx](http://www.maybridge.com/portal/alias_Rainbow/lang_en/tabID_146/DesktopDefault.aspx)

6. ChemBridge custom made library, 96 480 compounds from ChemBridge Corp., San Diego, CA, USA

Average molecular weight: 325 g/mol

This is a collection of synthetic small molecules with diverse pharmacophores and drug-like compounds.

For more information:

[http://www.chembridge.com/screening\\_libraries/diversity\\_libraries/index.php](http://www.chembridge.com/screening_libraries/diversity_libraries/index.php)

7. McMaster collection, 1400 compounds provided by chemists.

This is a collection of novel compounds submitted by chemists to the HTS facility. It aims to form direct links between Canadian chemists and biologists to foster new collaborations.

8. Ontario Institute for Cancer Research (OICR) Collection, 141,861 compounds

Restrictions Apply

Average molecular weight

Chembridge: 320.240 g/mol

ChemDiv: 341.585 g/mol

Asinex: 297.276 g/mol

Enamine:

Overall collection properties (calculated for 141,861 compounds):

Brutto MW =  $344.01 \pm 63.86$  g/mol

Parent MW =  $342.00 \pm 64.19$  g/mol

alogP\_GC =  $2.66 \pm 1.04$

Polar Surface Area =  $79.23 \pm 27.01$

H Bond Donors =  $1.14 \pm 0.83$

H Bond Acceptors =  $4.04 \pm 1.41$

Number of rotatable bonds =  $5.06 \pm 1.87$

9. PKIS (Published Kinase Inhibitor Set ), 363 compounds from GlaxoSmithKline, Durham, NC, USA

The GSK Published Kinase Inhibitor Set. All compounds have been published in the literature.

For more information:

<https://www.ebi.ac.uk/chembl/db/extra/PKIS/>

10. KIS (Kinase Inhibitor Set ), 233 compounds from Hoffmann-La Roche, Nutley, NJ, USA

The Roche Kinase Inhibitor Set.

11. Natural products library, ~10,000 wells

Wright lab collection. Extracts from Actinomycetes collected from around the world.

Requires permission/collaboration with the Wright lab.