Subset	Number of compounds	Description
<b>Custom Library</b> (Maybridge, Ltd. Cornwall, UK)	16,000	Synthetic small molecules; Average MW = 325 g/mol
<b>DIVERSet</b> (ChemBridge Corp., San Diego, CA, USA)	9,989	Synthetic small molecules; Average MW = 325 g/mol
Prestwick Chemical Library (Prestwick Chemical, Illkirch, France)	1,120	Off-patent small molecules; >85% FDA approved; Average MW = 325 g/mol
Natural Products Library (BIOMOL International, L.P., Plymouth Meeting, PA, USA)	361	Natural products; Average MW = 350 g/mol
Lopac1280 (International Version) (Sigma-Aldrich Canada Ltd., Oakville, ON, Canada)	885	Pharmacologically active small molecules; Average MW = 350 g/mol
<b>Spectrum Collection</b> (MicroSource Discovery Systems, Inc., Gaylordsville, CT, USA)	1,214	Natural products and bioactives; average MW = 350 g/mol
<b>Dennis Hall Compounds</b> Chem. Dept., University of Alberta	690	Synthesized lactams, lactones and piperidines
Total # compounds	30,259	

## S1 Table. Canadian Compound Collection (CYCC) Library