

Axxam Compound Collection

Next-Generation Small Molecule Collections for Hit-Finding by HTS

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INTRODUCTION:

These innovative libraries have been assembled by incorporating compounds with structural and molecular properties suitable for hit discovery and hit-to-lead programs, avoiding unwanted reactive chemical groups, frequent hitters, toxicophores, aggregators and other undesirables. The goal was to ensure that the resulting screening hits be readily tractable starting points for further optimization.

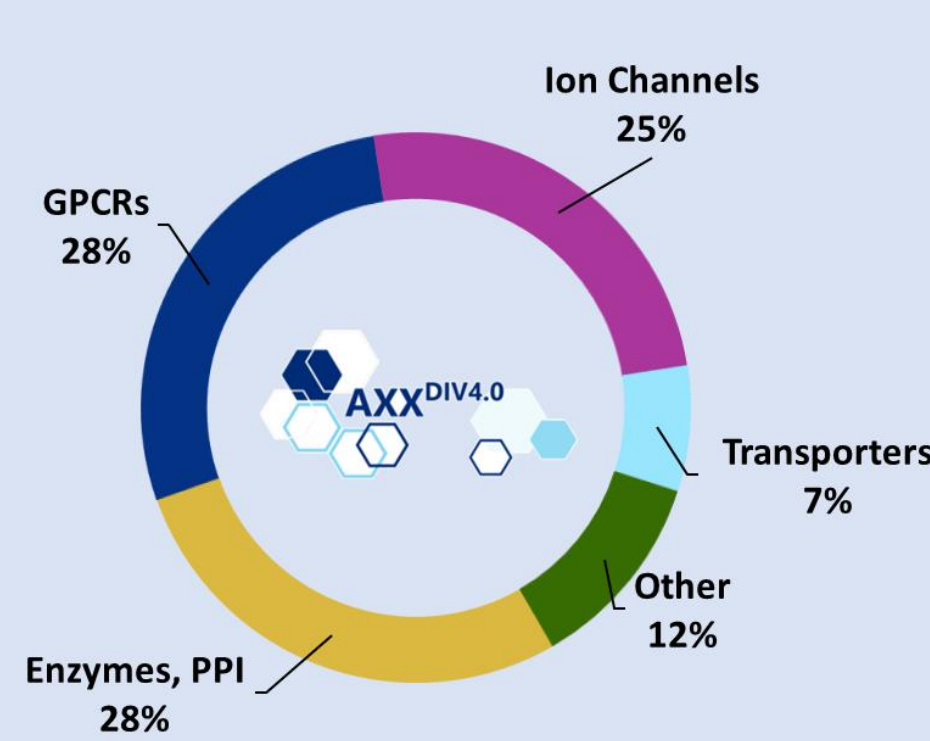


The **AXX^{DIV4.0}** library consists of ~325.000 lead-like small molecules. The selection process has been performed over time on structurally diverse screening compounds with the aim of covering a broad chemical space characterized by optimal physicochemical properties. The collection consists of four independent screening sets, accessible separately or in combination according to project's needs:

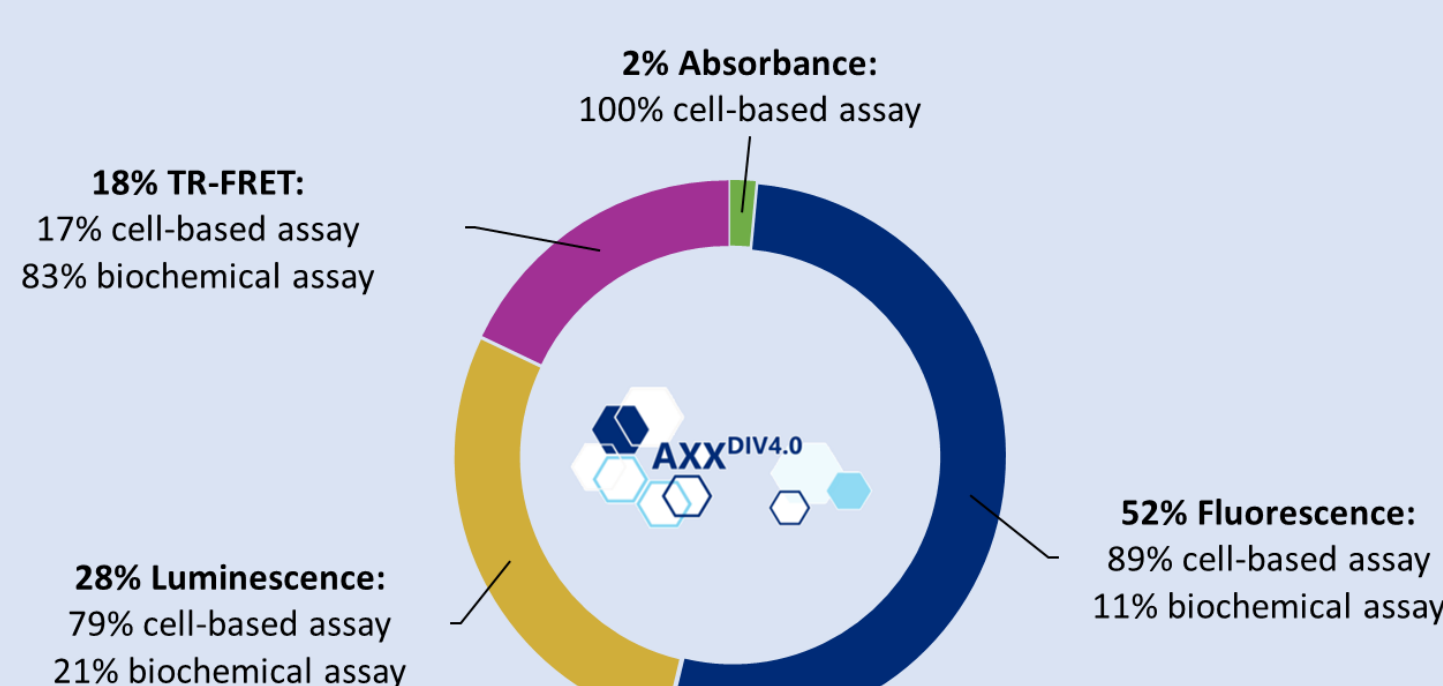
- Discovery**
 - ~179K lead-like molecules
 - ~15 analogues for each chemotype
 - Provides SAR information
- Explorer^{PLUS}**
 - ~98K lead-like singletons
 - High coverage of diversity
 - Ideal for novel peripheral and central targets
- CNS**
 - ~35K lead-like singletons
 - Optimized MPO scores
 - Specifically biased for CNS and intracellular targets
- Probe**
 - ~12K decorated fragment-like compounds
 - Low molecular weight
 - Ideal starting point for structure-enabled programs

PERFORMANCE IN HTS:

Type of Target Classes Screened



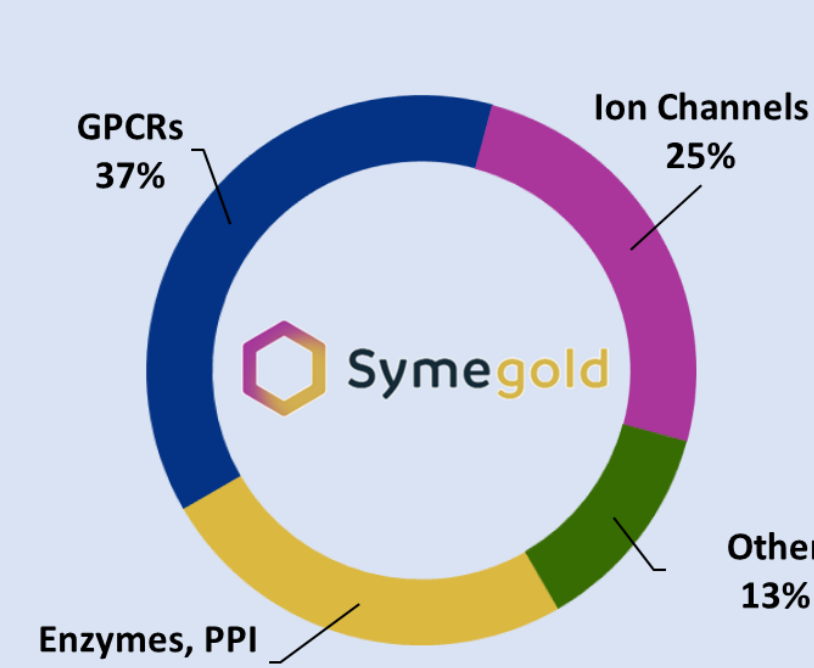
Type of Readouts Screened*



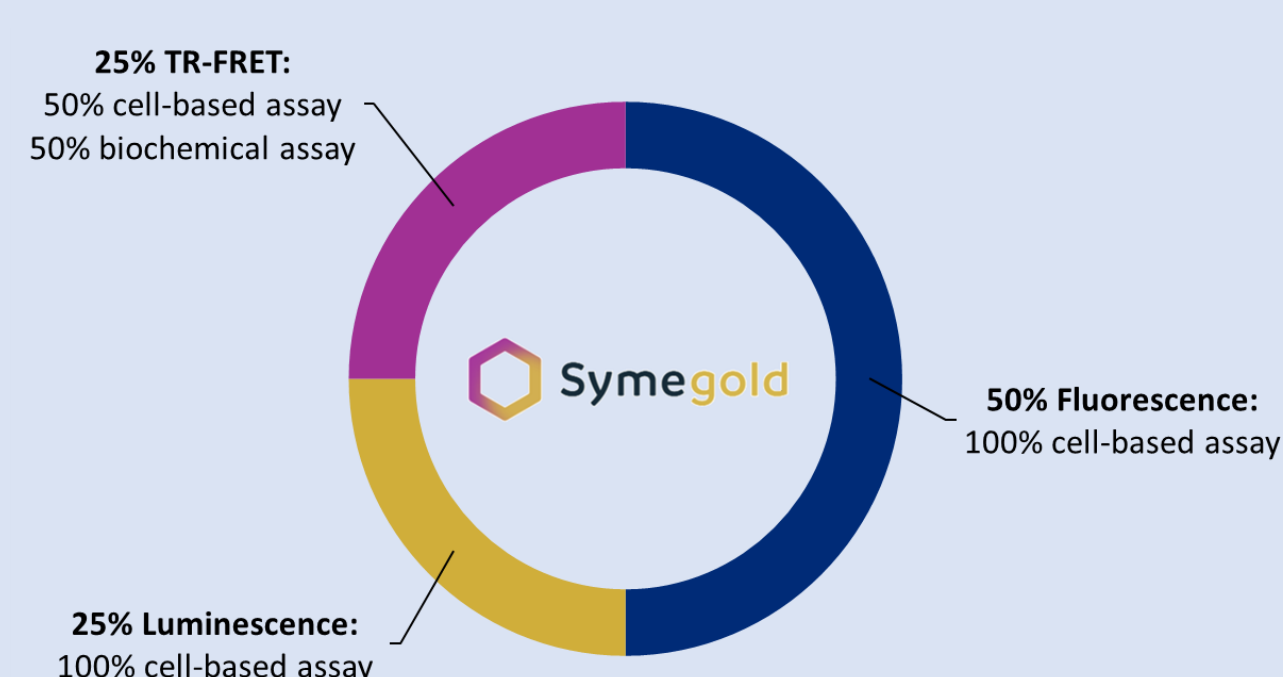
The **Symegold** library is composed of ~75.000 lead-like compounds synthesized at Symeres, as part of the European Lead Factory. The design criteria for preparing this novel and unique compound collection were based on diverse lead-like properties and structural novelty, using Symeres proprietary, rigid, sp³-rich scaffolds synthesized in house via innovative chemistry.

PERFORMANCE IN HTS:

Type of Target Classes Screened



Type of Readouts Screened*



*Among the main readout group "Fluorescence", several different sub-types are included (Calcium Dyes, MP-Dyes, Thallium-Dyes, AlphaLisa, enzymatic coupled cascades and others).

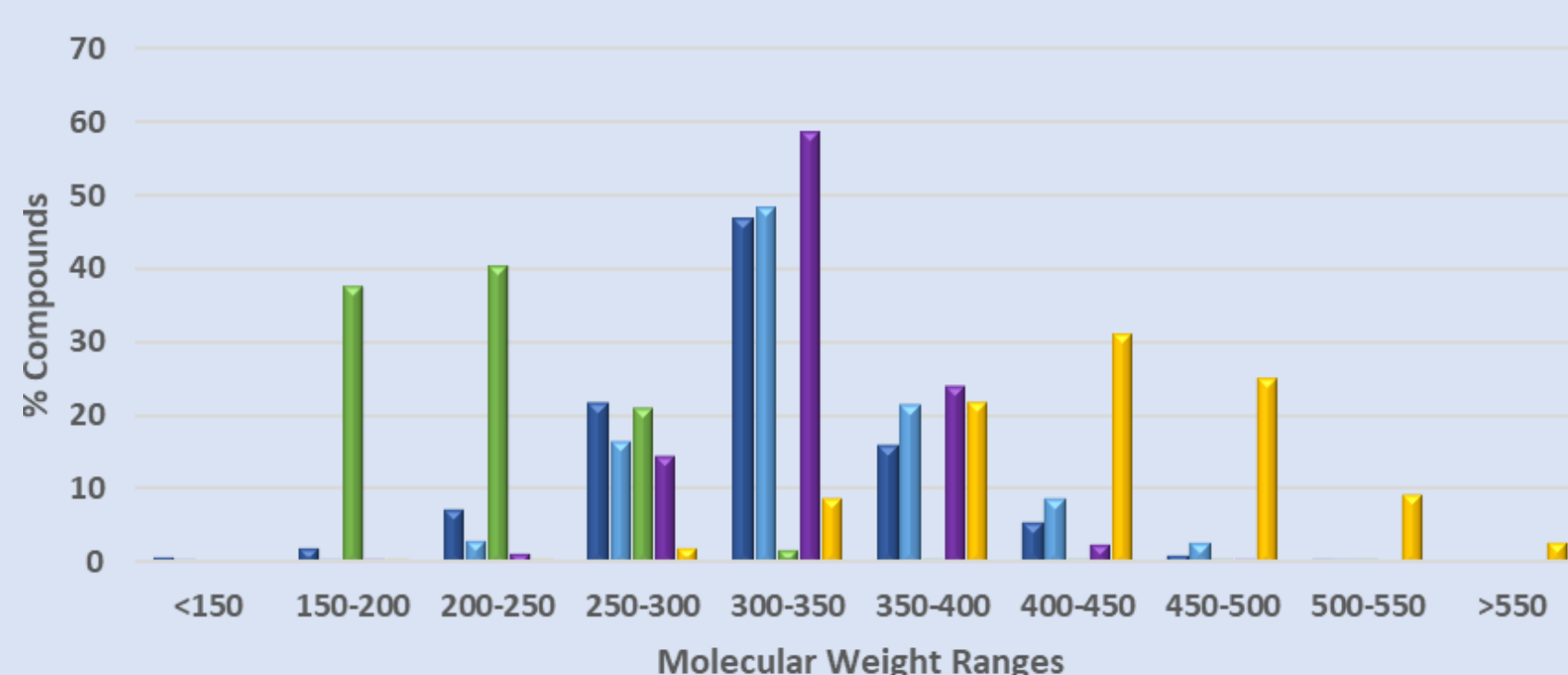
*Among the main readout group "Luminescence", several different sub-types are included (Calcium sensitive Photoproteins, different types of Luciferases, enzymatic coupled cascades and others)

HIT RATE IN HTS:

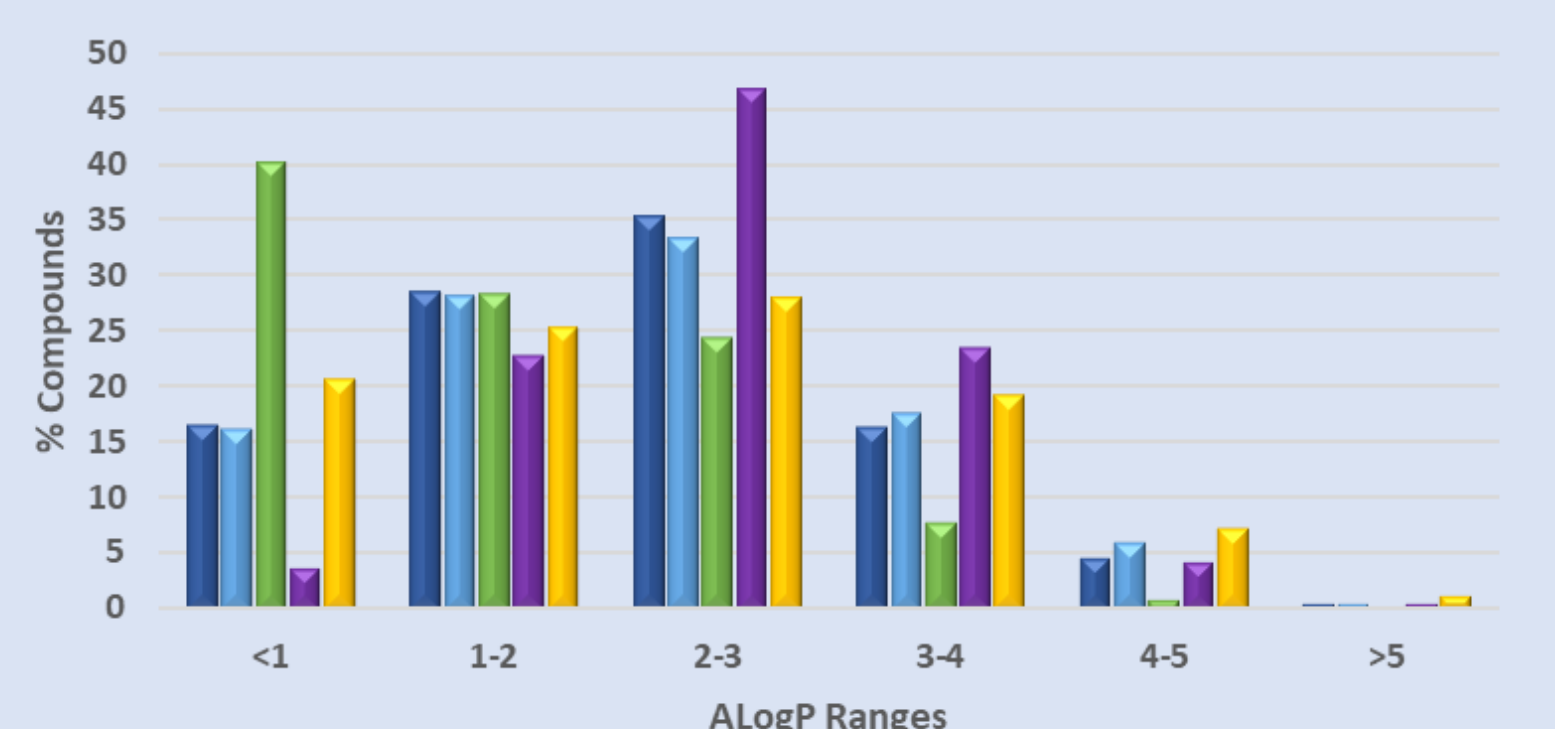
	hit rate%		
	mean	min	max
Discovery set	0.6	0.1	1.4
ExplorerPlus set	1.3	0.1	3.3
Probe set	0.5	0.03	1.8
CNS set	0.9	0.02	6.7
SymeGold library	0.8	0.3	1.6

PROPERTIES BY SET:

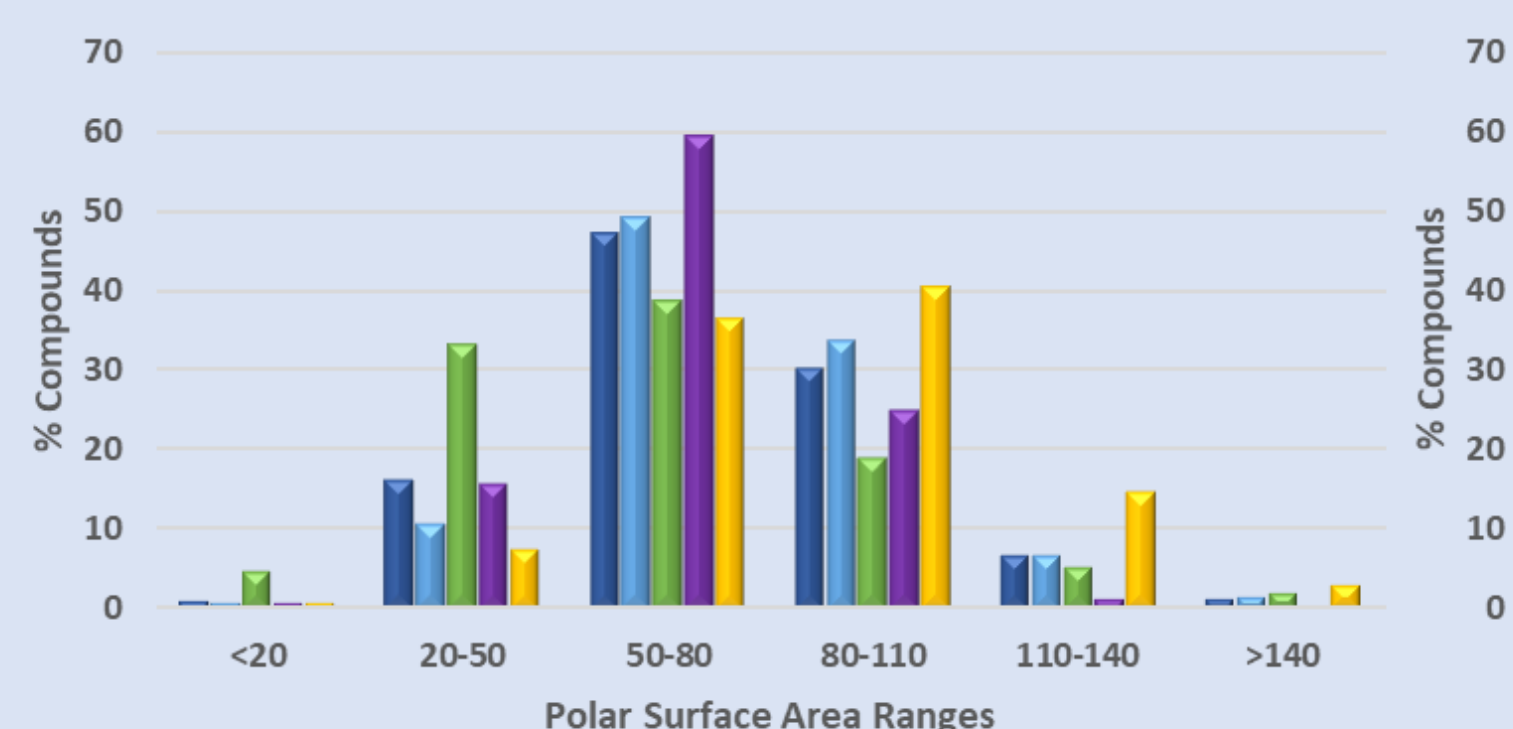
Molecular Weight by Set



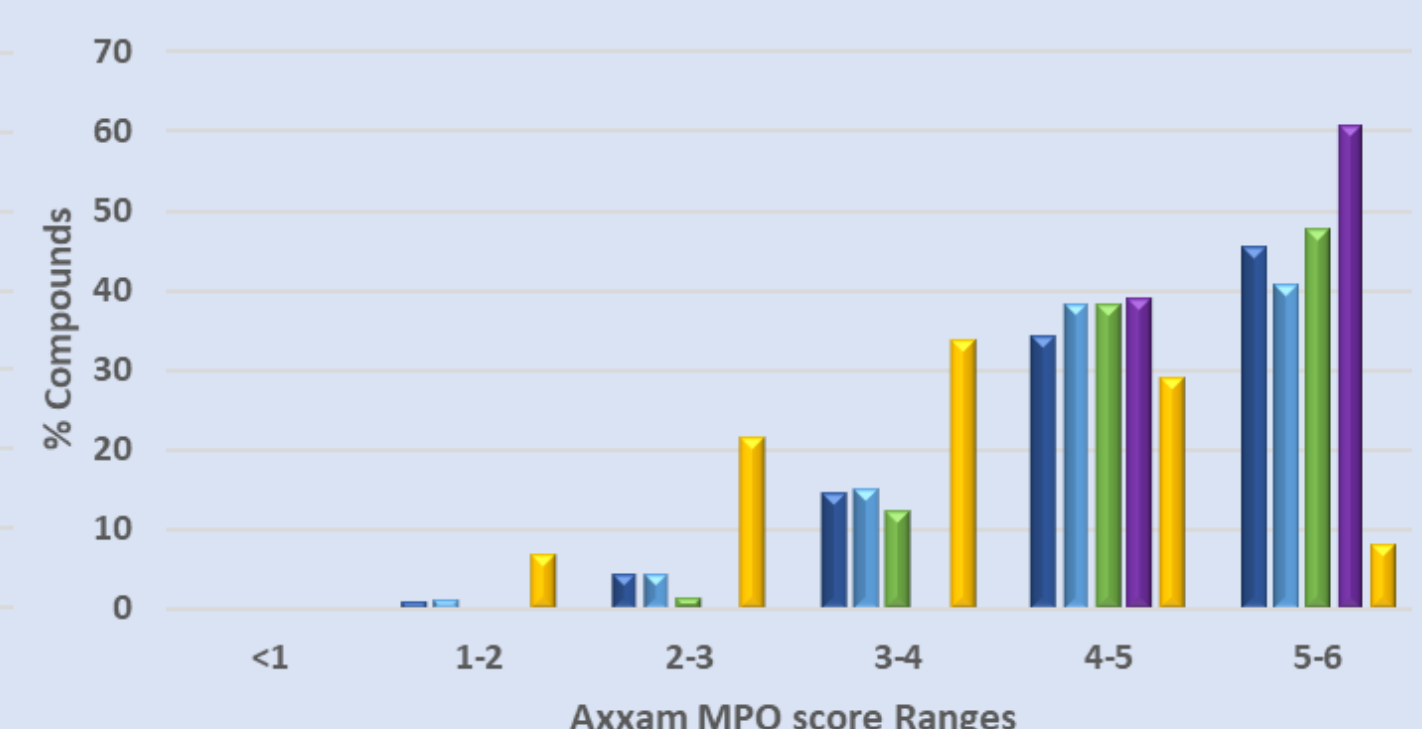
AlogP by Set



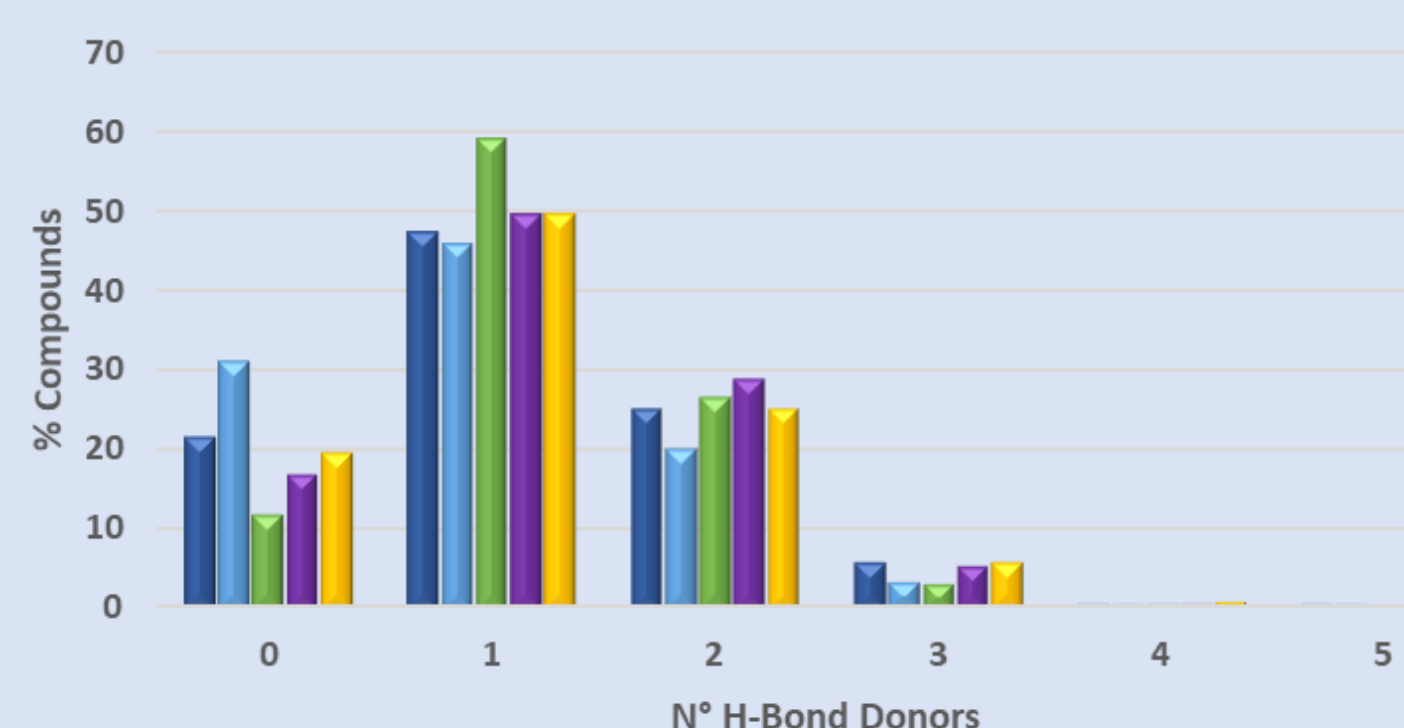
Polar Surface Area by Set



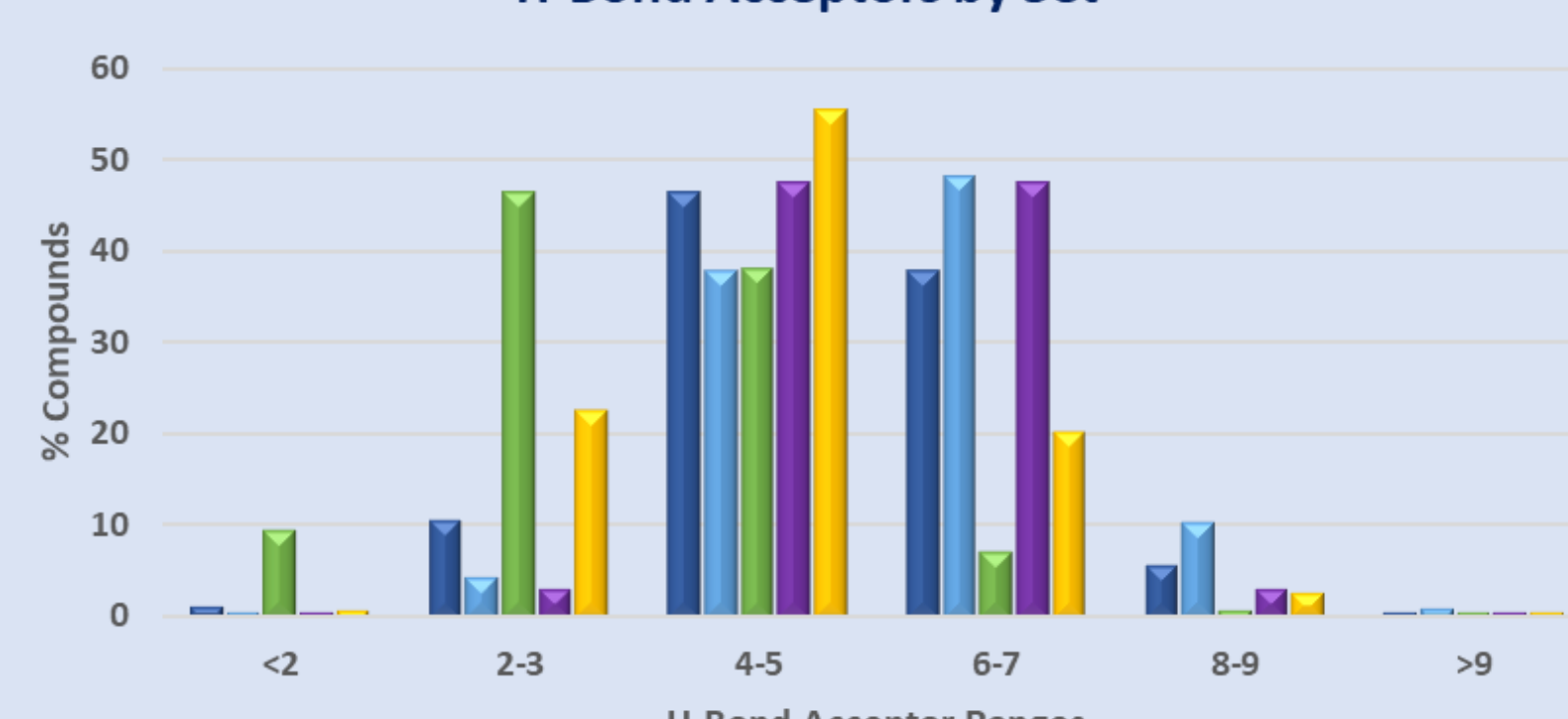
Axxam MPO score by Set



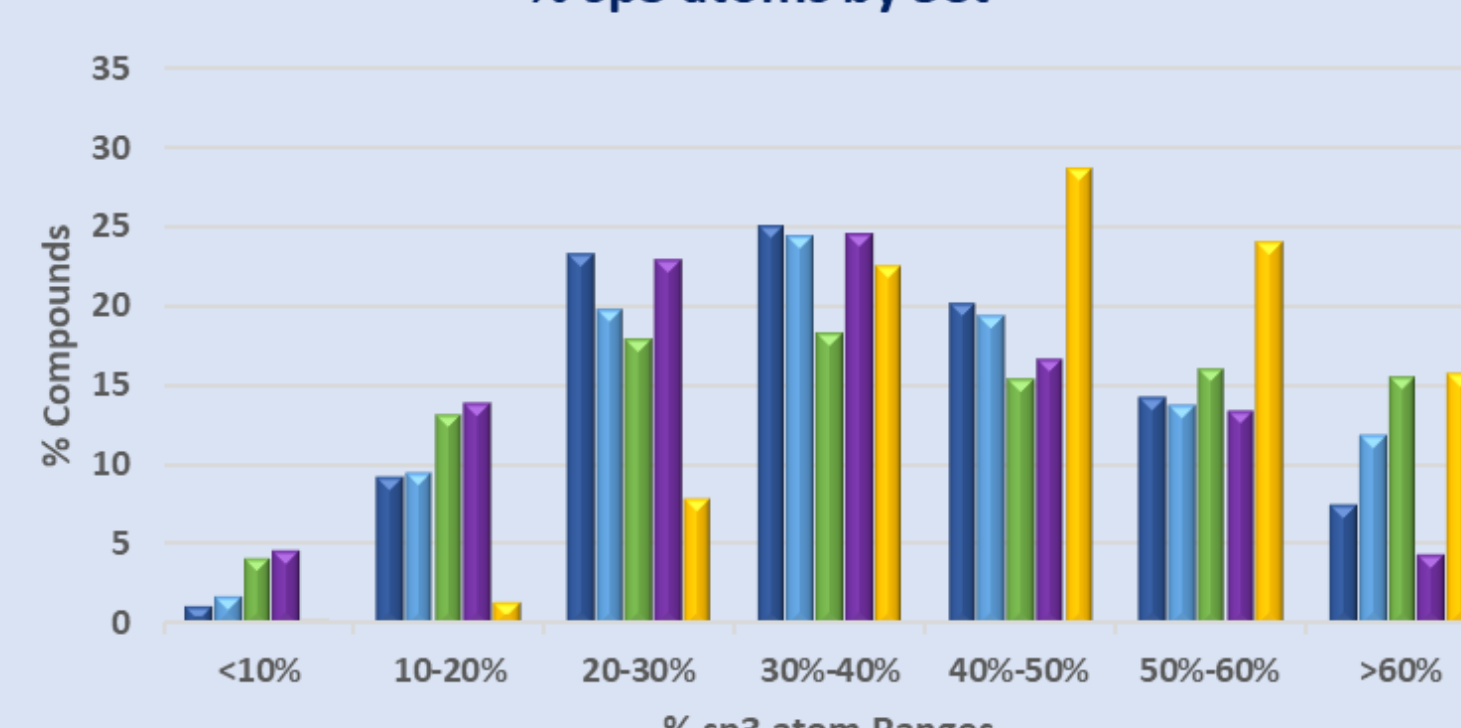
H-Bond Donors by Set



H-Bond Acceptors by Set



% sp³ atoms by Set



■ Discovery set
■ Explorer^{PLUS} set
■ Probe set
■ CNS set
■ SymeGold library