

What types of chemical libraries are used?

Type of library	Analogy	Examples
Comprehensive	Search in the dark	<u>ZINC15</u> : ~1 billion compounds in vendor catalogs. ~11 million in stock.
Combinatorial	Search in the dark	<u>Enamine REAL</u> : 13 billion “readily accessible” molecules.
Diverse	Efficient search in the dark	<u>Diverse REAL drug-like</u> : 15 million. <u>NCI Diversity Set VI</u> : 1548 free.
“Focused” or “Targeted” for lead identification	Search with a flashlight	Filtered for a structural motif or pharmacophore
“Focused” or “Targeted” for lead optimization	Focusing the spotlights	Riboflavin analogues

Molecular weight is an important factor

Class	Weight	Why do virtual screening?
Fragments	< 300 Da	to join together into leads
Lead-like	300-375 Da	low potency compounds that can be optimized
Drug-like	<500 Da	potential to be highly potent and suitable for preclinical testing