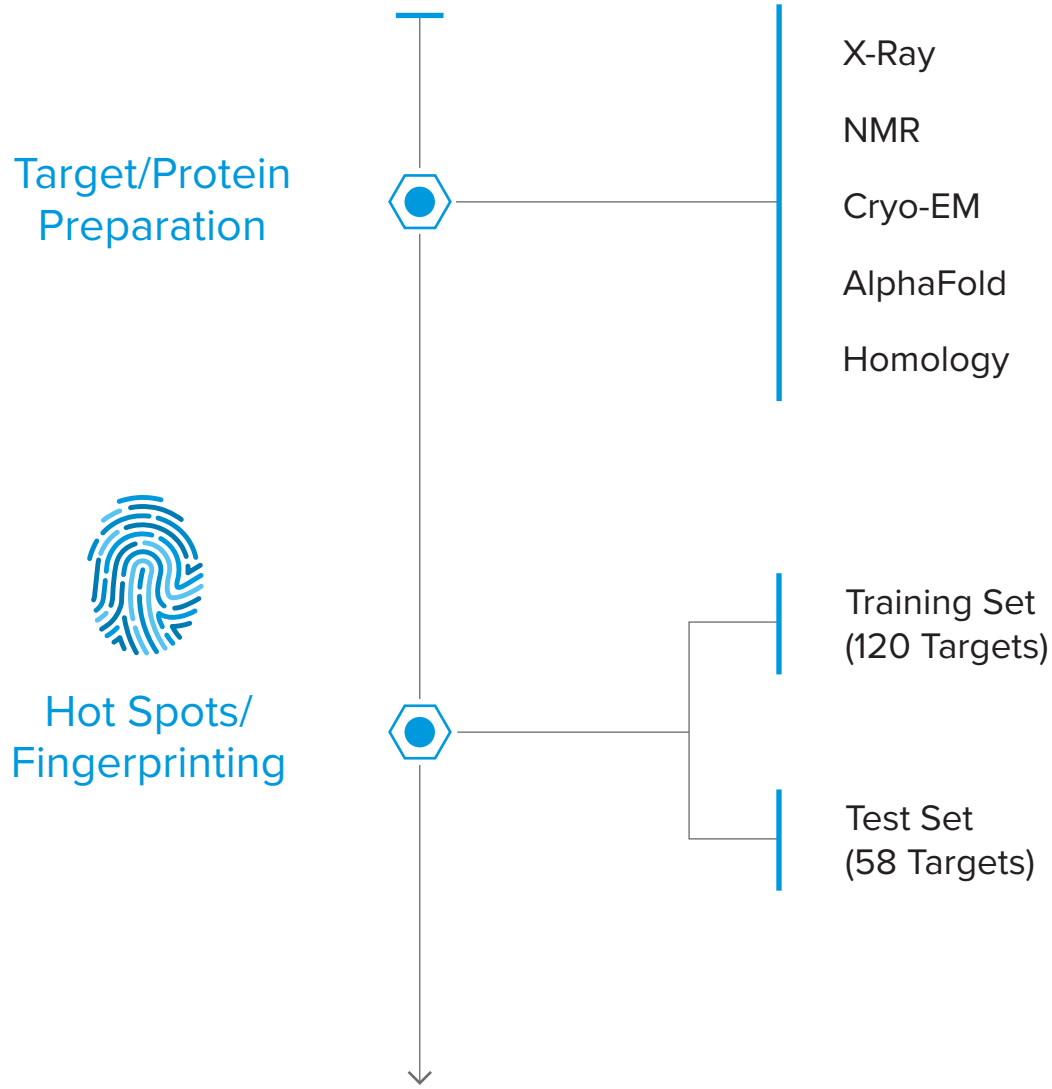
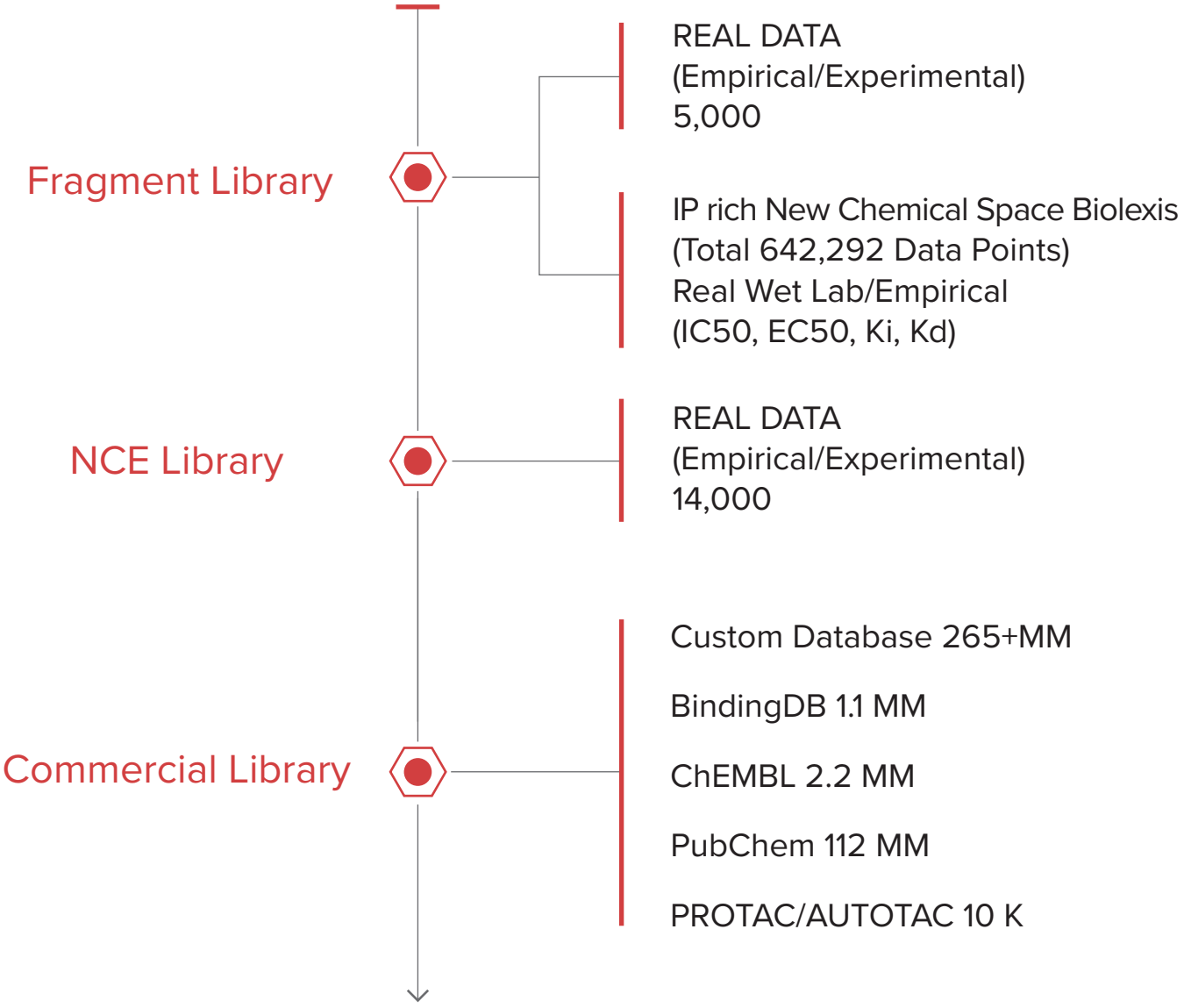
STEP 1
TARGET IDENTIFICATION (TID)

Our team rapidly identifies and validates druggable targets of interest based on powerful AI/ML training models combined with decades of experience in early drug discovery and disease-causing target gene expression.



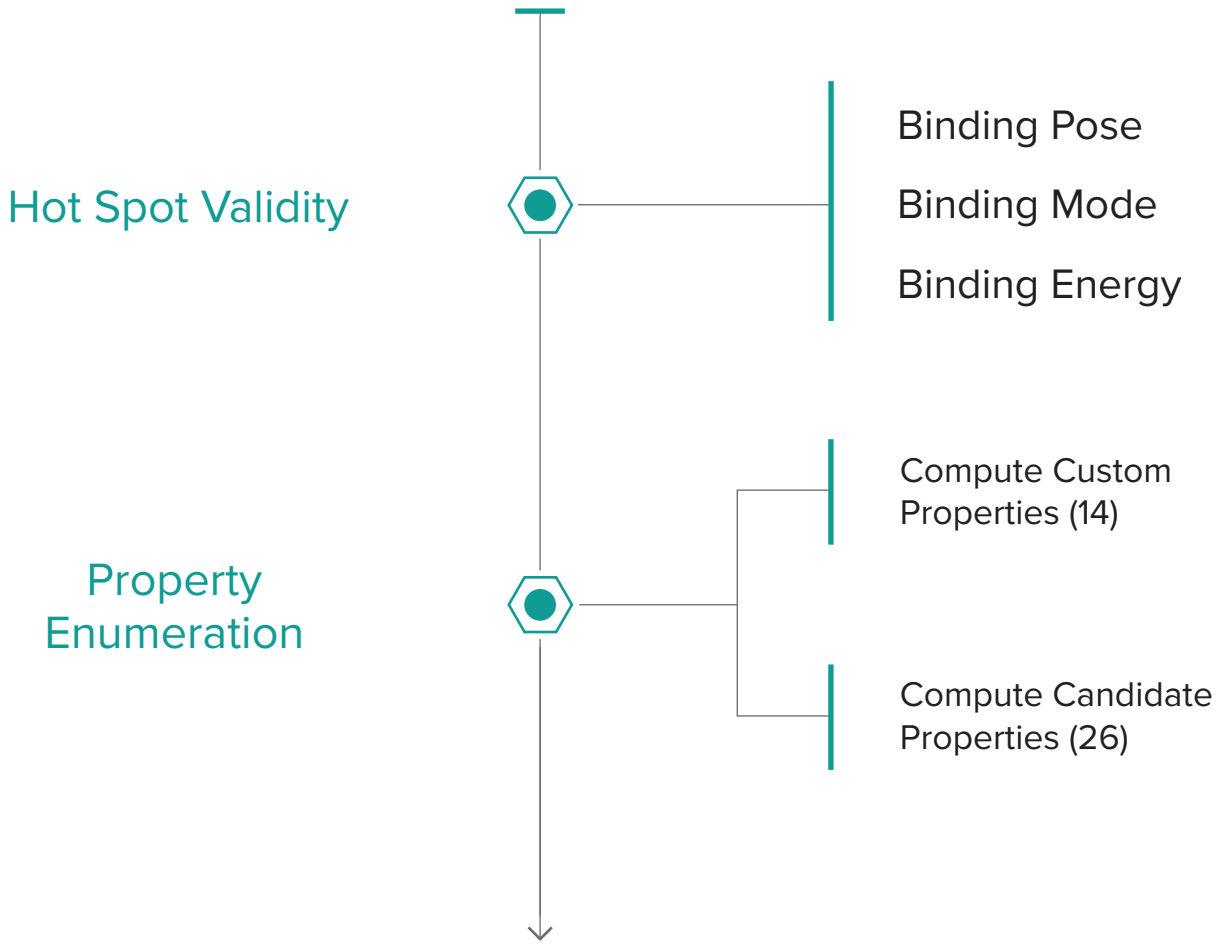
STEP 2
MOLECULERN™ 2HITS (F2H)

Using our proprietary set of over half a million real, wet lab/empirical data points, we analyze a spectrum of protein/small molecule interactions to determine high-quality hits against the protein targets of interest – all with unprecedented speed, exceptional accuracy, and IP-rich qualities.



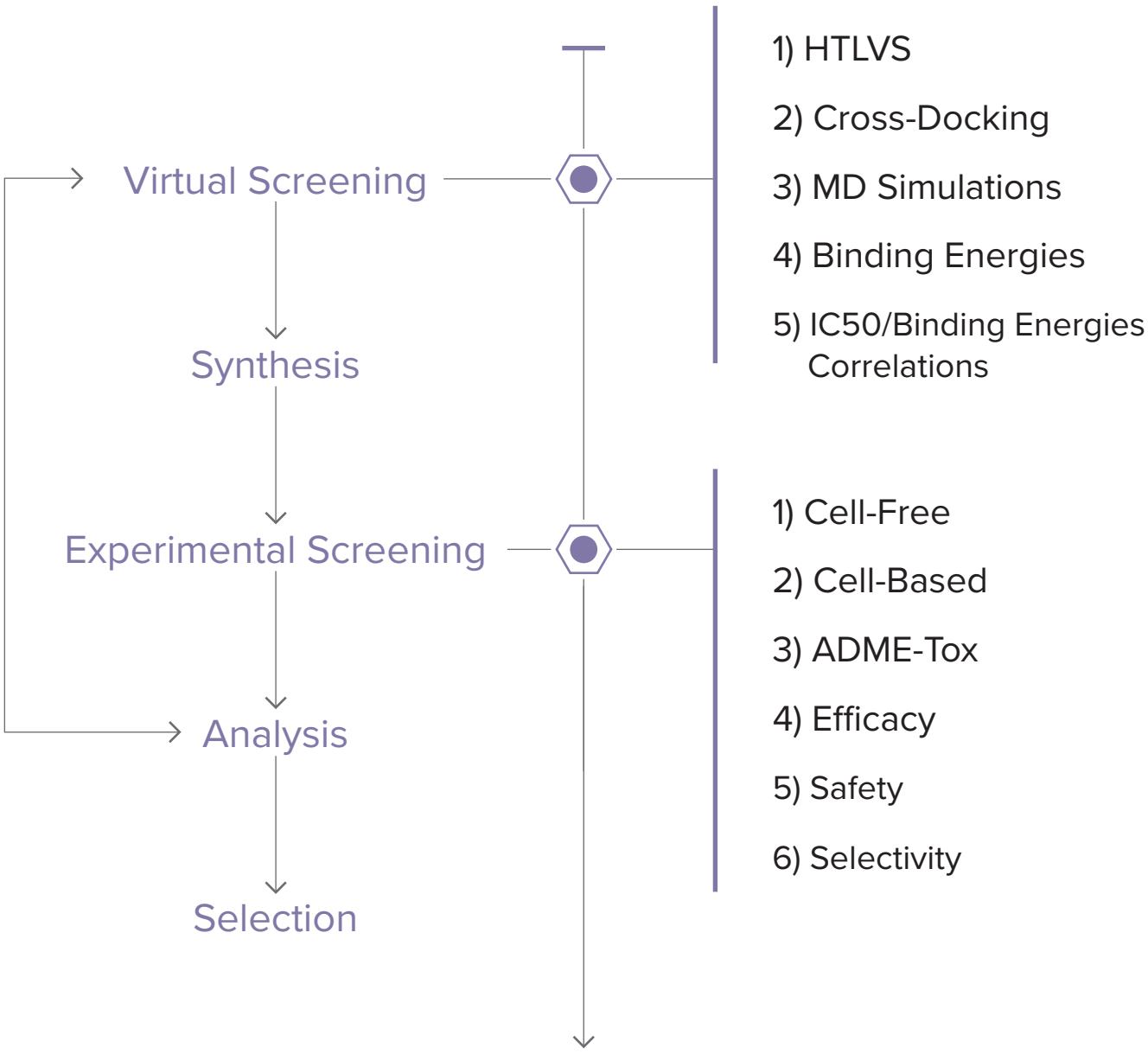
STEP 3
F2H VALIDATION

Our hits validation and selection process utilizes our set of target product profiles and ADME-TOX parameters incorporating our MolecuLern™ Hot Spot residue validation, binding mode, binding energetics, and human feedback loops.



STEP 4
HITS 2LEAD (H2L)

The best hit compounds are further optimized using machine learning / human-in-the-loop structure-based drug discovery methods, ADME-Tox property predictions, and virtual/experimental screening, allowing better drugs with fewer iterations.



STEP 5
LEAD OPTIMIZATION (LO)

Our lead optimization process heavily involves real data, human feedback loops, structure-based activities, and SAR for lead selection and NCEs.

1) Med Chem Tractability
2) Synthesis Feasibility Check
3) Properties
4) Developability Criteria
5) ADME-Tox
6) Safety/Secondary Pharmacology
7) Experimental Feed-Back

STEP 6
CANDIDATE NOMINATION

Our MolecuLern™ process with target binding, cellular efficacy, PK, ADME, pre-tox, biomarkers, and mouse model efficacy studies are the key to our candidate nomination process.

1) ADME-Tox
2) Secondary Pharmacology
3) In-Vivo Efficacy
4) Developability
5) Pre-formulation
6) Route Scout/Scale-up
7) Pre-IND Enabling Studies