

Structure based drug discovery vocabulary card

Five words that carry the whole pipeline, and the sentences that keep them honest.

Word	Definition	What it is not
Target	The biological molecule, almost always a protein, that a drug acts on	Not the disease and not the pathway
Ligand	Any molecule that binds the target, here the candidate drug	Not necessarily an inhibitor
Binding pocket	A three dimensional cavity formed by the fold where a ligand fits	Not any gap on the surface
Pose	One position and orientation of the ligand with its rotatable bonds set	Not a structure determined by experiment
Docking score	A predicted value for a pose from an approximate scoring function	Not a measured affinity and not a potency

Drug likeness at a glance

Property	Usual oral range	Why it matters
Molecular weight	under about 500 Da	Heavier molecules are absorbed less easily
LogP	under about 5	Too low will not cross a membrane, too high will not dissolve
Hydrogen bond donors and acceptors	5 and 10	Strong water binding resists membrane crossing
Rotatable bonds and polar surface area	10 and 140 square Angstroms	Veber criteria for oral bioavailability
Breaking the rules	Lenacapavir about 968 Da	Chooses an injectable route rather than signalling failure

Based on the ERAS Africa Molecular Docking using Python course, 2026, and the study "Target Protein Pocket Volume and Antiretroviral Drug Physicochemical Properties" (Hailekiros, 2026) with its reproduction guide. Tool documentation from RDKit, AutoDock Vina, Meeko, RCSB PDB, PubChem and ProteinsPlus. Free to copy and adapt with attribution.