

2P2I_{DB} Glossary and Abbreviations

Term	Definition
BASA	Buried Accessible Surface Area (Å ²)
BRD	Bromodomain
Fsp³	Fraction of sp ³ hybridized carbon atoms in a molecule
HBond	Hydrogen Bond
HBond Acceptors	Polar atoms involved in hydrogen bonds (Os and Ns)
HBond Donors	Polar hydrogen donors involved in hydrogen bonds (OHs and NHs)
Kd	Dissociation Constant (Molar units)
Lipinski Rule	Rule of thumb to evaluate drug-likeness or determine if a chemical compound has properties that would make it a likely orally active drug in humans.
LogP	Logarithm of n-octanol/water partition coefficient
MLogP	Moriguchi LogP
MW	Molecular weight (g/mol)
Oprea Rule	Rule of thumb to evaluate lead-likeness of a compound
Orthosteric	Refers to a compound directly targeting the protein-protein interface
PPI	Protein-protein interaction
TPSA	Topological Polar Surface Area (Å ²): sum of tabulated surface contributions of polar fragments
Veber Rule	Rule of thumb to evaluate bioavailability of a compound
