ChEMBL-PDB Linker

Linking Bioactivity Data with Validated Protein-Ligand Structures

ChEMBL
Bioactivity

IC_{50}, K_i, K_d, EC_{50}

PDB
3D Structures

Protein-Ligand Complexes

Protein Linking
UniProt IDs

Ligand Linking
InChIKey

Pair Validation
Same PDB structure?

Removes 99% false positives

Curated Dataset
98,500 pairs
8,946 compounds
1,297 proteins

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