

Drug Discovery Compound Activity Analysis

Drug discovery relies heavily on analyzing chemical compounds and their interactions with biological targets. Key molecular properties, such as binding affinity, hydrophobicity, and molecular weight, help researchers identify promising drug candidates. This report summarizes important findings from a sample dataset of compounds, highlighting differences between active and inactive molecules and exploring property relationships relevant to drug design.

The dataset was downloaded from - <https://www.kaggle.com/datasets/shahriarkabir/drug-discovery-virtual-screening-dataset>

Compound Activity	Avg. Binding Affinity	Avg. Molecular Weight (g/mol)	Avg. Hydrophobicity	Avg. Rotatable Bonds
Active	7.83	449.7	0.65	5.97
Inactive	5.97	459.2	0.64	5.96

Table 1: Summary of Compound Properties

