# Classifications

Schrödinger classifies screening compounds based on properties calculated on a single, neutralized and desalted representation. Near drug-like compounds are those that fall close, but not quite into the drug-like property space. Drug-like compounds are expected to have properties similar to known marketed drugs. Lead-like compounds typically have a more restrictive set of properties that align with the goals of finding a hit and expanding that hit into a more drug-like compound. Fragments are compounds that are typically very small and are used to probe a target in order to determine the functionalities expressed by compounds that bind to a particular site. All other molecular structures are not given a classification.

Several rubrics are used in a hierarchical funnel to associate a molecular entity to a specific class. Note that even though a molecule may fit into several classifications, in practice, compounds are allowed to match and get assigned to categories further down the funnel in the order: near drug-like, drug-like, lead-like, to fragment. The count of structures in each class is summarized in table below.

**Table 1. Classification criteria.** These properties are discussed below. Note that NCC, NR, and HAC correspond to Num chiral centers, Num rings, and Num heavy atoms as calculated by ligfilter. Structures are assigned to a class by the last successful match on all criteria proceeding from right to left.

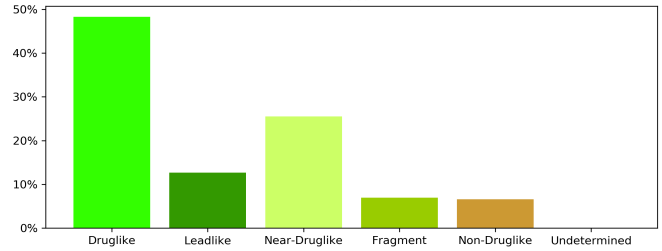
| Near drug-like | Drug-like | Lead-like | Fragment |
|---|---|---|---|
| –1.5 ≤ AlogP ≤ 5.5 | –1 ≤ AlogP ≤ 4 | 0 ≤ AlogP ≤ 3 | AlogP ≤ 3 |
| 150 ≤ MW ≤ 575 | 250 ≤ MW ≤ 500 | 250 ≤ MW ≤ 375 | MW > 110 |
| 30 < PSA < 150 | 50 < PSA < 130 | PSA < 110 | PSA ≤ 110 |
| HBD ≤ 5 | HBD ≤ 5 | HBD ≤ 2 | HBD ≤ 3 |
| HBA ≤ 12 | HBA ≤ 10 | HBA ≤ 5 | HBA ≤ 5 |
| RB ≤ 10 | RB ≤ 10 | RB ≤ 10 | RB ≤ 3 |
| NCC ≤ 3 | NCC ≤ 3 | NCC ≤ 1 | |
| | | | NR ≥ 1 |
| | | | HAC ≤ 18 |

**Table 2. Screening classification**

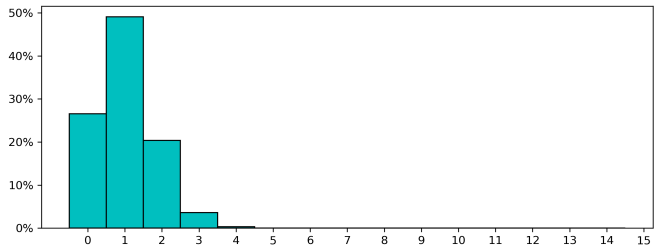
| | Drug-like | Lead-like | Near drug-like | Fragment | Others |
|---|---|---|---|---|---|
| Count | 46,889 | 12,285 | 24,759 | 6,764 | 6,402 |
| Percentage | 48.3% | 12.7% | 25.5% | 7.0% | 6.6% |

# Database Property Distribution

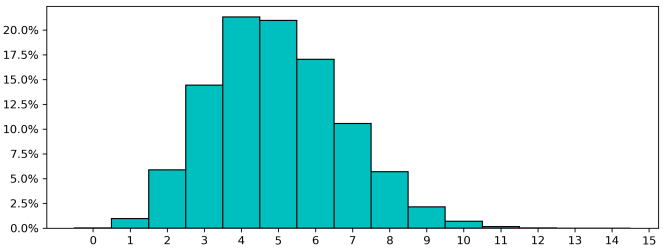
Class



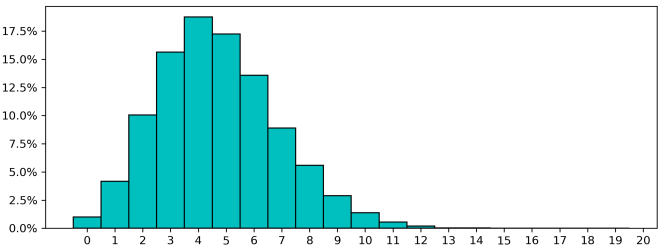

HBD



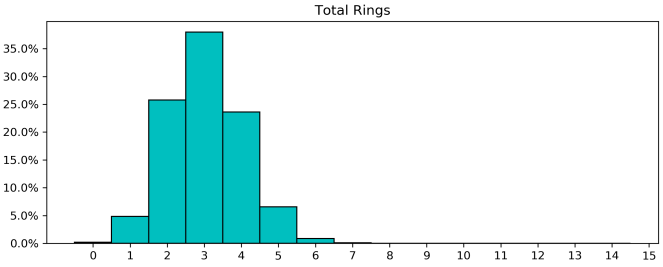

HBA



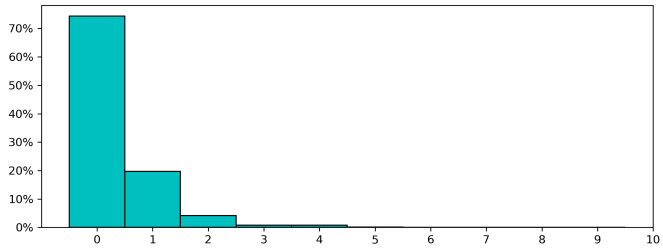

RB



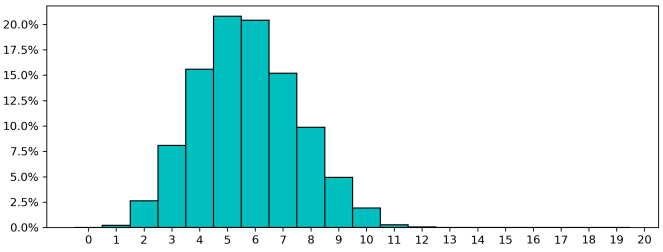

Total Rings



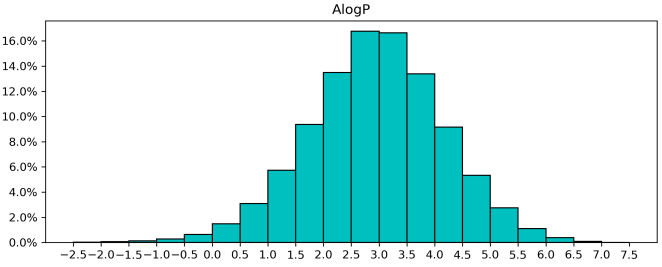

Stereo Centers



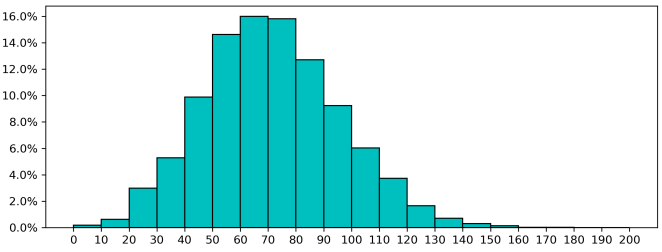

N+O



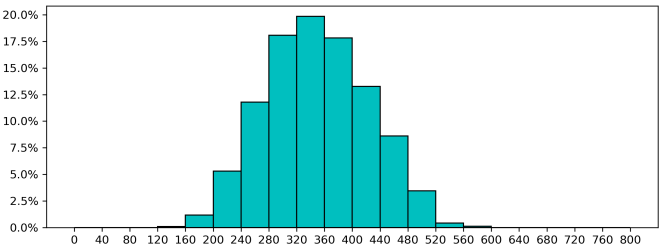

AlogP



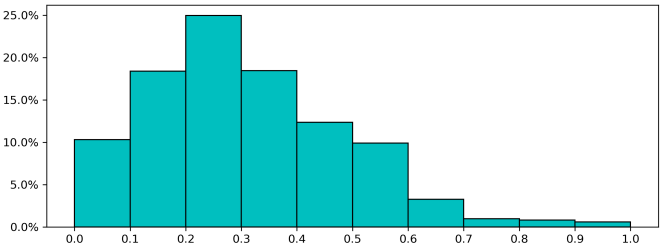

PSA




MW




Frac. CSP3



# Property Description

A brief description of each property is provided below.

**HBD:**
Number of hydrogen bond donors

**HBA:**
Number of hydrogen bond acceptors

**RB:**
Number of rotatable bonds

**Total Rings:**
Number of rings

**Stereo Centers:**
Number of stereogenic centers

**N+O:**
Sum of nitrogen and oxygen atoms

**AlogP:**
Logarithm of the atomistic partition coefficient

**PSA:**
Fragment-based topological polar surface area

**MW:**
Molecular weight

**Frac. CSP3:**
Frequency of sp3-hybridized carbon atoms with respect to total carbon atom count