

Labels Explanation:

In **Herba- compound-target information.csv**:

Herb Name: represents the name of the Chinese herbal medicine;

Mol ID: represents the compound number of the compound in the Chinese herbal medicine in the tcmsp database;

Molecule Name: represents the compound name in TCMSP;

Targets: represents the possible target of the compound;

Gene symbol: represents the target Point corresponding gene.

It's the same in a table called **All compounds and their sources.xlsx**.

MW stands for molecular mass;

OB: oral bioavailability;

DL: Drug Likeness;

FASA-: Fraction of all atoms with negative partial charge Water accessible surface area;

Caco-2: component transport rate in monolayer Caco-2 cells (nm/s);

BBB: blood-brain barrier;

HL: Drug half-life;

AlogP: partition coefficient between octanol and water.

The first row in each table is the Chinese pinyin of the Chinese medicine and the corresponding English name.