

1. Physicochemical Property

Property	Value	Comment
Molecular Weight	106.08	Contain hydrogen atoms. Optimal:100~600
Volume	130.459	Van der Waals volume
Density	0.813	Density = MW / Volume
nHA	0	Number of hydrogen bond acceptors. Optimal:0~12
nHD	0	Number of hydrogen bond donors. Optimal:0~7
nRot	1	Number of rotatable bonds. Optimal:0~11
nRing	1	Number of rings. Optimal:0~6
MaxRing	6	Number of atoms in the biggest ring. Optimal:0~18
nHet	0	Number of heteroatoms. Optimal:1~15
fChar	0	Formal charge. Optimal:-4 ~4
nRig	6	Number of rigid bonds. Optimal:0~30
Flexibility	0.167	Flexibility = nRot /nRig
Stereo Centers	0	Optimal: ≤ 2
TPSA	0.0	Topological Polar Surface Area. Optimal:0~140
logS	-2.94	Log of the aqueous solubility. Optimal: -4~0.5 log mol/L
logP	3.059	Log of the octanol/water partition coefficient. Optimal: 0~3
logD	3.094	logP at physiological pH 7.4. Optimal: 1~3

2. Medicinal Chemistry

Property	Value	Decision	Comment
QED	0.515	●	<ul style="list-style-type: none"> ■ A measure of drug-likeness based on the concept of desirability; ■ Attractive: > 0.67; unattractive: 0.49~0.67; too complex: < 0.34
SAscore	1.0	●	<ul style="list-style-type: none"> ■ Synthetic accessibility score is designed to estimate ease of synthesis of drug-like molecules. ■ SAscore ≥ 6, difficult to synthesize; SAscore <6, easy to synthesize
Fsp3	0.25	●	<ul style="list-style-type: none"> ■ The number of sp³ hybridized carbons / total carbon count, correlating with melting point and solubility. ■ Fsp³ ≥ 0.42 is considered a suitable value.
MCE-18	4.0	●	<ul style="list-style-type: none"> ■ MCE-18 stands for medicinal chemistry evolution. ■ MCE-18≥45 is considered a suitable value.

NPscore	-0.773	-	<ul style="list-style-type: none"> ■ Natural product-likeness score. ■ This score is typically in the range from -5 to 5. The higher the score is, the higher the probability is that the molecule is a NP.
Lipinski Rule	Accepted	●	<ul style="list-style-type: none"> ■ MW \leq 500; logP \leq 5; Hacc \leq 10; Hdon \leq 5 ■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.
Pfizer Rule	Rejected	●	<ul style="list-style-type: none"> logP $>$ 3; TPSA $<$ 75 Compounds with a high log P (>3) and low TPSA (<75) are likely to be toxic.
GSK Rule	Accepted	●	<ul style="list-style-type: none"> ■ MW \leq 400; logP \leq 4 ■ Compounds satisfying the GSK rule may have a more favorable ADMET profile
Golden Triangle	Rejected	●	<ul style="list-style-type: none"> ■ 200 \leq MW \leq 50; -2 \leq logD \leq 5 ■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile.
PAINS	0 alerts	-	Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound.
ALARM NMR	0 alerts	-	Thiol reactive compounds.
BMS	0 alerts	-	Undesirable, reactive compounds.
Chelator Rule	0 alerts	-	Chelating compounds.

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-4.114	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	2.6e-05	●	<ul style="list-style-type: none"> ■ low permeability: $< 2 \times 10^{-6}$ cm/s ■ medium permeability: $2-20 \times 10^{-6}$ cm/s ■ high passive permeability: $> 20 \times 10^{-6}$ cm/s
Pgp-inhibitor	0.001	●	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	0.015	●	<ul style="list-style-type: none"> ■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.003	●	<ul style="list-style-type: none"> ■ Human Intestinal Absorption ■ Category 1: HIA+(HIA $<$ 30%); Category 0: HIA-(HIA $<$ 30%); The output value is the probability of being HIA+
F _{20%}	0.921	●	<ul style="list-style-type: none"> ■ 20% Bioavailability ■ Category 1: F_{20%}+ (bioavailability $<$ 20%); Category 0: F_{20%}- (bioavailability \geq 20%); The output value is the probability of being F_{20%}+

$F_{30\%}$	0.134	●	<ul style="list-style-type: none"> ■ 30% Bioavailability ■ Category 1: $F_{30\%}+$ (bioavailability < 30%); Category 0: $F_{30\%}-$ (bioavailability $\geq 30\%$); The output value is the probability of being $F_{30\%}+$
------------	-------	---	---

4. Distribution

Property	Value	Decision	Comment
PPB	90.74%	●	<ul style="list-style-type: none"> ■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	2.411	●	<ul style="list-style-type: none"> ■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.872	●	<ul style="list-style-type: none"> ■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	8.085%	●	<ul style="list-style-type: none"> ■ The fraction unbound in plasms ■ Low: <5%; Middle: 5~20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.968	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.852	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.763	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.406	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.24	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C9 substrate	0.156	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2D6 inhibitor	0.173	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2D6 substrate	0.179	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP3A4 inhibitor	0.023	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP3A4 substrate	0.326	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.

6. Excretion

Property	Value	Decision	Comment
CL	10.388	●	<ul style="list-style-type: none"> ■ Clearance ■ High: >15 mL/min/kg; moderate: 5-15 mL/min/kg; low: <5 mL/min/kg
T _{1/2}	0.717	-	<ul style="list-style-type: none"> ■ Category 1: long half-life ; Category 0: short half-life; ■ long half-life: >3h; short half-life: <3h ■ The output value is the probability of having long half-life.

7. Toxicity

Property	Value	Decision	Comment
hERG Blockers	0.054	●	<ul style="list-style-type: none"> ■ Category 1: active; Category 0: inactive; ■ The output value is the probability of being active.
H-HT	0.041	●	<ul style="list-style-type: none"> ■ Human Hepatotoxicity ■ Category 1: H-HT positive(+); Category 0: H-HT negative(-); ■ The output value is the probability of being toxic.
DILI	0.059	●	<ul style="list-style-type: none"> ■ Drug Induced Liver Injury. ■ Category 1: drugs with a high risk of DILI; Category 0: drugs with no risk of DILI. The output value is the probability of being toxic.
AMES Toxicity	0.022	●	<ul style="list-style-type: none"> ■ Category 1: Ames positive(+); Category 0: Ames negative(-); ■ The output value is the probability of being toxic.
Rat Oral Acute Toxicity	0.034	●	<ul style="list-style-type: none"> ■ Category 0: low-toxicity; Category 1: high-toxicity; ■ The output value is the probability of being highly toxic.
FDAMDD	0.026	●	<ul style="list-style-type: none"> ■ Maximum Recommended Daily Dose ■ Category 1: FDAMDD (+); Category 0: FDAMDD (-) ■ The output value is the probability of being positive.
Skin Sensitization	0.551	●	<ul style="list-style-type: none"> ■ Category 1: Sensitizer; Category 0: Non-sensitizer; ■ The output value is the probability of being sensitizer.
Carcinogenicity	0.411	●	<ul style="list-style-type: none"> ■ Category 1: carcinogens; Category 0: non-carcinogens; ■ The output value is the probability of being toxic.
Eye Corrosion	0.98	●	<ul style="list-style-type: none"> ■ Category 1: corrosives ; Category 0: noncorrosives ■ The output value is the probability of being corrosives.
Eye Irritation	0.995	●	<ul style="list-style-type: none"> ■ Category 1: irritants ; Category 0: nonirritants ■ The output value is the probability of being irritants.

Respiratory Toxicity	0.129	●	<ul style="list-style-type: none"> ■ Category 1: respiratory toxicants; Category 0: respiratory nontoxicants ■ The output value is the probability of being toxic.
----------------------	-------	---	--

8. Environmental toxicity

Property	Value	Comment
Bioconcentration Factors	1.662	<ul style="list-style-type: none"> ■ Bioconcentration factors are used for considering secondary poisoning potential and assessing risks to human health via the food chain. ■ The unit is $-\log_{10}[(\text{mg/L})/(1000*\text{MW})]$
IGC ₅₀	3.219	<ul style="list-style-type: none"> ■ Tetrahymena pyriformis 50 percent growth inhibition concentration ■ The unit is $-\log_{10}[(\text{mg/L})/(1000*\text{MW})]$
LC ₅₀ FM	3.788	<ul style="list-style-type: none"> ■ 96-hour fathead minnow 50 percent lethal concentration ■ The unit is $-\log_{10}[(\text{mg/L})/(1000*\text{MW})]$
LC ₅₀ DM	4.077	<ul style="list-style-type: none"> ■ 48-hour daphnia magna 50 percent lethal concentration ■ The unit is $-\log_{10}[(\text{mg/L})/(1000*\text{MW})]$

9. Tox21 pathway

Property	Value	Decision	Comment
NR-AR	0.01	●	<ul style="list-style-type: none"> ■ Androgen receptor ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-AR-LBD	0.004	●	<ul style="list-style-type: none"> ■ Androgen receptor ligand-binding domain ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-AhR	0.005	●	<ul style="list-style-type: none"> ■ Aryl hydrocarbon receptor ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-Aromatase	0.005	●	<ul style="list-style-type: none"> ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-ER	0.194	●	<ul style="list-style-type: none"> ■ Estrogen receptor ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-ER-LBD	0.008	●	<ul style="list-style-type: none"> ■ Estrogen receptor ligand-binding domain ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-PPAR-gamma	0.003	●	<ul style="list-style-type: none"> ■ Peroxisome proliferator-activated receptor gamma ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
SR-ARE	0.016	●	<ul style="list-style-type: none"> ■ Antioxidant response element ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
SR-ATAD5	0.006	●	<ul style="list-style-type: none"> ■ ATPase family AAA domain-containing protein 5 ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.

SR-HSE	0.021	●	<ul style="list-style-type: none"> ■ Heat shock factor response element ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
SR-MMP	0.011	●	<ul style="list-style-type: none"> ■ Mitochondrial membrane potential ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
SR-p53	0.003	●	<ul style="list-style-type: none"> ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.

10. Toxicophore Rules

Property	Value	Comment
Acute Toxicity Rule	0 alerts	<ul style="list-style-type: none"> ■ 20 substructures ■ acute toxicity during oral administration
Genotoxic Carcinogenicity Rule	0 alerts	<ul style="list-style-type: none"> ■ 117 substructures ■ carcinogenicity or mutagenicity
NonGenotoxic Carcinogenicity Rule	0 alerts	<ul style="list-style-type: none"> ■ 23 substructures ■ carcinogenicity through nongenotoxic mechanisms
Skin Sensitization Rule	0 alerts	<ul style="list-style-type: none"> ■ 155 substructures ■ skin irritation
Aquatic Toxicity Rule	1 alerts	<ul style="list-style-type: none"> ■ 99 substructures ■ toxicity to liquid(water)
NonBiodegradable Rule	0 alerts	<ul style="list-style-type: none"> ■ 19 substructures ■ non-biodegradable
SureChEMBL Rule	0 alerts	<ul style="list-style-type: none"> ■ 164 substructures ■ MedChem unfriendly status