

1. Physicochemical Property

Property	Value	Comment
Molecular Weight	340.3	Contain hydrogen atoms. Optimal:100~600
Volume	386.95	Van der Waals volume
Density	0.879	Density = MW / Volume
nHA	3	Number of hydrogen bond acceptors. Optimal:0~12
nHD	0	Number of hydrogen bond donors. Optimal:0~7
nRot	19	Number of rotatable bonds. Optimal:0~11
nRing	1	Number of rings. Optimal:0~6
MaxRing	3	Number of atoms in the biggest ring. Optimal:0~18
nHet	3	Number of heteroatoms. Optimal:1~15
fChar	0	Formal charge. Optimal:-4 ~4
nRig	4	Number of rigid bonds. Optimal:0~30
Flexibility	4.75	Flexibility = nRot / nRig
Stereo Centers	1	Optimal: ≤ 2
TPSA	38.83	Topological Polar Surface Area. Optimal:0~140
logS	-6.284	Log of the aqueous solubility. Optimal: -4~0.5 log mol/L
logP	7.769	Log of the octanol/water partition coefficient. Optimal: 0~3
logD	4.487	logP at physiological pH 7.4. Optimal: 1~3

2. Medicinal Chemistry

Property	Value	Decision	Comment
QED	0.17	●	<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	2.52	●	<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	0.952	●	<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	10.488	●	<ul style="list-style-type: none"> ■ MCE-18 stands for medicinal chemistry evolution. ■ MCE-18 ≥ 45 is considered a suitable value.

NPscore	0.359	-	<p>■ Natural product-likeness score.</p> <p>■ 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.</p>
Lipinski Rule	Accepted	●	<p>■ $MW \leq 500$; $\log P \leq 5$; $Hacc \leq 10$; $Hdon \leq 5$</p> <p>■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.</p>
Pfizer Rule	Rejected	●	<p>$\log P > 3$; $TPSA < 75$</p> <p>Compounds with a high log P (>3) and low TPSA (<75) are likely to be toxic.</p>
GSK Rule	Rejected	●	<p>■ $MW \leq 400$; $\log P \leq 4$</p> <p>■ Compounds satisfying the GSK rule may have a more favorable ADMET profile</p>
Golden Triangle	Accepted	●	<p>■ $200 \leq MW \leq 500$; $-2 \leq \log D \leq 5$</p> <p>■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile.</p>
PAINS	0 alerts	-	Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound.
ALARM NMR	0 alerts	-	Thiol reactive compounds.
BMS	2 alerts	-	Undesirable, reactive compounds.
Chelator Rule	0 alerts	-	Chelating compounds.

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-4.924	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	1.9e-05	●	<p>■ low permeability: $< 2 \times 10^{-6}$ cm/s</p> <p>■ medium permeability: $2-20 \times 10^{-6}$ cm/s</p> <p>■ high passive permeability: $> 20 \times 10^{-6}$ cm/s</p>
Pgp-inhibitor	0.014	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being Pgp-inhibitor</p>
Pgp-substrate	0.001	●	<p>■ Category 1: substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being Pgp-substrate</p>
HIA	0.001	●	<p>■ Human Intestinal Absorption</p> <p>■ Category 1: HIA+ (HIA < 30%); Category 0: HIA- (HIA < 30%); The output value is the probability of being HIA+</p>
F _{20%}	0.85	●	<p>■ 20% Bioavailability</p> <p>■ Category 1: F_{20%} + (bioavailability < 20%); Category 0: F_{20%} - (bioavailability ≥ 20%); The output value is the probability of being F_{20%} +</p>

$F_{30\%}$	0.983	●	<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 $F_{30\%} +$
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4. Distribution

Property	Value	Decision	Comment
PPB	97.62%	●	<ul style="list-style-type: none"> ■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	1.223	●	<ul style="list-style-type: none"> ■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.086	●	<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	1.565%	●	<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	0.193	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.187	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.299	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.058	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.099	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C9 substrate	0.739	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2D6 inhibitor	0.064	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2D6 substrate	0.051	<ul style="list-style-type: none"> ■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP3A4 inhibitor	0.359	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP3A4 substrate	0.063	<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	4.694	●	<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}	0.186	-	<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	0.332	●	<ul style="list-style-type: none"> ■ Category 1: active; Category 0: inactive; ■ The output value is the probability of being active.
H-HT	0.037	●	<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	0.25	●	<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	0.36	●	<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	0.038	●	<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	0.023	●	<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	0.969	●	<ul style="list-style-type: none"> ■ Category 1: Sensitizer; Category 0: Non-sensitizer; ■ The output value is the probability of being sensitizer.
Carcinogenicity	0.172	●	<ul style="list-style-type: none"> ■ Category 1: carcinogens; Category 0: non-carcinogens; ■ The output value is the probability of being toxic.
Eye Corrosion	0.93	●	<ul style="list-style-type: none"> ■ Category 1: corrosives ; Category 0: noncorrosives ■ The output value is the probability of being corrosives.
Eye Irritation	0.974	●	<ul style="list-style-type: none"> ■ Category 1: irritants ; Category 0: nonirritants ■ The output value is the probability of being irritants.

Respiratory Toxicity	0.598	●	<ul style="list-style-type: none"> ■ Category 1: respiratory toxicants; Category 0: respiratory nontoxicants ■ The output value is the probability of being toxic.
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8. Environmental toxicity

Property	Value	Comment
Bioconcentration Factors	1.887	<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 $-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]$
IGC ₅₀	5.737	<ul style="list-style-type: none"> ■ Tetrahymena pyriformis 50 percent growth inhibition concentration ■ The unit is $-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]$
LC ₅₀ FM	4.352	<ul style="list-style-type: none"> ■ 96-hour fathead minnow 50 percent lethal concentration ■ The unit is $-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]$
LC ₅₀ DM	5.528	<ul style="list-style-type: none"> ■ 48-hour daphnia magna 50 percent lethal concentration ■ The unit is $-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]$

9. Tox21 pathway

Property	Value	Decision	Comment
NR-AR	0.071	●	<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	0.003	●	<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	0.02	●	<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	0.637	●	<ul style="list-style-type: none"> ■ Category 1: actives ; Category 0: inactives; ■ The output value is the probability of being active.
NR-ER	0.297	●	<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	0.007	●	<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	0.068	●	<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	0.148	●	<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	0.341	●	<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	0.045	●	<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	0.071	●	<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	5 alerts	<ul style="list-style-type: none"> ■ 117 substructures ■ carcinogenicity or mutagenicity
NonGenotoxic Carcinogenicity Rule	1 alerts	<ul style="list-style-type: none"> ■ 23 substructures ■ carcinogenicity through nongenotoxic mechanisms
Skin Sensitization Rule	1 alerts	<ul style="list-style-type: none"> ■ 155 substructures ■ skin irritation
Aquatic Toxicity Rule	2 alerts	<ul style="list-style-type: none"> ■ 99 substructures ■ toxicity to liquid(water)
NonBiodegradable Rule	2 alerts	<ul style="list-style-type: none"> ■ 19 substructures ■ non-biodegradable
SureChEMBL Rule	2 alerts	<ul style="list-style-type: none"> ■ 164 substructures ■ MedChem unfriendly status