

## 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	0	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	0.0	Flexibility = nRot /nRig
Stereo Centers	0	Optimal: ≤ 2
TPSA	0.0	Topological Polar Surface Area. Optimal:0~140
logS	-2.905	Log of the aqueous solubility. Optimal: -4~0.5 log mol/L
logP	3.115	Log of the octanol/water partition coefficient. Optimal: 0~3
logD	3.08	logP at physiological pH 7.4. Optimal: 1~3

## 2. Medicinal Chemistry

Property	Value	Decision	Comment
QED	0.476	●	<ul style="list-style-type: none"> <li>■ A measure of drug-likeness based on the concept of desirability;</li> <li>■ Attractive: &gt; 0.67; unattractive: 0.49~0.67; too complex: &lt; 0.34</li> </ul>
SAscore	1.034	●	<ul style="list-style-type: none"> <li>■ Synthetic accessibility score is designed to estimate ease of synthesis of drug-like molecules.</li> <li>■ SAscore ≥ 6, difficult to synthesize; SAscore &lt;6, easy to synthesize</li> </ul>
Fsp3	0.25	●	<ul style="list-style-type: none"> <li>■ The number of sp<sup>3</sup> hybridized carbons / total carbon count, correlating with melting point and solubility.</li> <li>■ Fsp<sup>3</sup> ≥ 0.42 is considered a suitable value.</li> </ul>
MCE-18	5.0	●	<ul style="list-style-type: none"> <li>■ MCE-18 stands for medicinal chemistry evolution.</li> <li>■ MCE-18≥45 is considered a suitable value.</li> </ul>

NPscore	-0.694	-	<ul style="list-style-type: none"> <li>■ Natural product-likeness score.</li> <li>■ 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.</li> </ul>
Lipinski Rule	Accepted	●	<ul style="list-style-type: none"> <li>■ MW <math>\leq</math> 500; logP <math>\leq</math> 5; Hacc <math>\leq</math> 10; Hdon <math>\leq</math> 5</li> <li>■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.</li> </ul>
Pfizer Rule	Rejected	●	<ul style="list-style-type: none"> <li>logP <math>&gt;</math> 3; TPSA <math>&lt;</math> 75</li> <li>Compounds with a high log P (<math>&gt;3</math>) and low TPSA (<math>&lt;75</math>) are likely to be toxic.</li> </ul>
GSK Rule	Accepted	●	<ul style="list-style-type: none"> <li>■ MW <math>\leq</math> 400; logP <math>\leq</math> 4</li> <li>■ Compounds satisfying the GSK rule may have a more favorable ADMET profile</li> </ul>
Golden Triangle	Rejected	●	<ul style="list-style-type: none"> <li>■ 200 <math>\leq</math> MW <math>\leq</math> 50; -2 <math>\leq</math> logD <math>\leq</math> 5</li> <li>■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile.</li> </ul>
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	-4.245	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	2.8e-05	●	<ul style="list-style-type: none"> <li>■ low permeability: <math>&lt; 2 \times 10^{-6}</math> cm/s</li> <li>■ medium permeability: <math>2-20 \times 10^{-6}</math> cm/s</li> <li>■ high passive permeability: <math>&gt; 20 \times 10^{-6}</math> cm/s</li> </ul>
Pgp-inhibitor	0.001	●	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being Pgp-inhibitor</li> </ul>
Pgp-substrate	0.04	●	<ul style="list-style-type: none"> <li>■ Category 1: substrate; Category 0: Non-substrate;</li> <li>■ The output value is the probability of being Pgp-substrate</li> </ul>
HIA	0.003	●	<ul style="list-style-type: none"> <li>■ Human Intestinal Absorption</li> <li>■ Category 1: HIA+( HIA <math>&lt;</math> 30%); Category 0: HIA-( HIA <math>&lt;</math> 30%); The output value is the probability of being HIA+</li> </ul>
F <sub>20%</sub>	0.103	●	<ul style="list-style-type: none"> <li>■ 20% Bioavailability</li> <li>■ Category 1: F<sub>20%</sub>+ (bioavailability <math>&lt;</math> 20%); Category 0: F<sub>20%</sub>- (bioavailability <math>\geq</math> 20%); The output value is the probability of being F<sub>20%</sub>+</li> </ul>

$F_{30\%}$	0.124	●	<ul style="list-style-type: none"> <li>■ 30% Bioavailability</li> <li>■ Category 1: <math>F_{30\%}+</math> (bioavailability &lt; 30%);</li> <li>Category 0: <math>F_{30\%}-</math> (bioavailability <math>\geq 30\%</math>); The output value is the probability of being <math>F_{30\%}+</math></li> </ul>
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## 4. Distribution

Property	Value	Decision	Comment
PPB	89.00%	●	<ul style="list-style-type: none"> <li>■ Plasma Protein Binding</li> <li>■ Optimal: &lt; 90%. Drugs with high protein-bound may have a low therapeutic index.</li> </ul>
VD	2.662	●	<ul style="list-style-type: none"> <li>■ Volume Distribution</li> <li>■ Optimal: 0.04-20L/kg</li> </ul>
BBB Penetration	0.844	●	<ul style="list-style-type: none"> <li>■ Blood-Brain Barrier Penetration</li> <li>■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+</li> </ul>
Fu	11.94%	●	<ul style="list-style-type: none"> <li>■ The fraction unbound in plasms</li> <li>■ Low: &lt;5%; Middle: 5~20%; High: &gt; 20%</li> </ul>

## 5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.928	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being inhibitor.</li> </ul>
CYP1A2 substrate	0.934	<ul style="list-style-type: none"> <li>■ Category 1: Substrate; Category 0: Non-substrate;</li> <li>■ The output value is the probability of being substrate.</li> </ul>
CYP2C19 inhibitor	0.761	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being inhibitor.</li> </ul>
CYP2C19 substrate	0.872	<ul style="list-style-type: none"> <li>■ Category 1: Substrate; Category 0: Non-substrate;</li> <li>■ The output value is the probability of being substrate.</li> </ul>
CYP2C9 inhibitor	0.192	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being inhibitor.</li> </ul>
CYP2C9 substrate	0.721	<ul style="list-style-type: none"> <li>■ Category 1: Substrate; Category 0: Non-substrate;</li> <li>■ The output value is the probability of being substrate.</li> </ul>
CYP2D6 inhibitor	0.095	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being inhibitor.</li> </ul>
CYP2D6 substrate	0.907	<ul style="list-style-type: none"> <li>■ Category 1: Substrate; Category 0: Non-substrate;</li> <li>■ The output value is the probability of being substrate.</li> </ul>
CYP3A4 inhibitor	0.079	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being inhibitor.</li> </ul>
CYP3A4 substrate	0.443	<ul style="list-style-type: none"> <li>■ Category 1: Substrate; Category 0: Non-substrate;</li> <li>■ The output value is the probability of being substrate.</li> </ul>

## 6. Excretion

Property	Value	Decision	Comment
CL	10.483	●	<ul style="list-style-type: none"> <li>■ Clearance</li> <li>■ High: &gt;15 mL/min/kg; moderate: 5-15 mL/min/kg; low: &lt;5 mL/min/kg</li> </ul>
T <sub>1/2</sub>	0.619	-	<ul style="list-style-type: none"> <li>■ Category 1: long half-life ; Category 0: short half-life;</li> <li>■ long half-life: &gt;3h; short half-life: &lt;3h</li> <li>■ The output value is the probability of having long half-life.</li> </ul>

## 7. Toxicity

Property	Value	Decision	Comment
hERG Blockers	0.028	●	<ul style="list-style-type: none"> <li>■ Category 1: active; Category 0: inactive;</li> <li>■ The output value is the probability of being active.</li> </ul>
H-HT	0.046	●	<ul style="list-style-type: none"> <li>■ Human Hepatotoxicity</li> <li>■ Category 1: H-HT positive(+); Category 0: H-HT negative(-);</li> <li>■ The output value is the probability of being toxic.</li> </ul>
DILI	0.076	●	<ul style="list-style-type: none"> <li>■ Drug Induced Liver Injury.</li> <li>■ 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.</li> </ul>
AMES Toxicity	0.055	●	<ul style="list-style-type: none"> <li>■ Category 1: Ames positive(+); Category 0: Ames negative(-);</li> <li>■ The output value is the probability of being toxic.</li> </ul>
Rat Oral Acute Toxicity	0.038	●	<ul style="list-style-type: none"> <li>■ Category 0: low-toxicity; Category 1: high-toxicity;</li> <li>■ The output value is the probability of being highly toxic.</li> </ul>
FDAMDD	0.065	●	<ul style="list-style-type: none"> <li>■ Maximum Recommended Daily Dose</li> <li>■ Category 1: FDAMDD (+); Category 0: FDAMDD (-)</li> <li>■ The output value is the probability of being positive.</li> </ul>
Skin Sensitization	0.434	●	<ul style="list-style-type: none"> <li>■ Category 1: Sensitizer; Category 0: Non-sensitizer;</li> <li>■ The output value is the probability of being sensitizer.</li> </ul>
Carcinogenicity	0.702	●	<ul style="list-style-type: none"> <li>■ Category 1: carcinogens; Category 0: non-carcinogens;</li> <li>■ The output value is the probability of being toxic.</li> </ul>
Eye Corrosion	0.983	●	<ul style="list-style-type: none"> <li>■ Category 1: corrosives ; Category 0: noncorrosives</li> <li>■ The output value is the probability of being corrosives.</li> </ul>
Eye Irritation	0.997	●	<ul style="list-style-type: none"> <li>■ Category 1: irritants ; Category 0: nonirritants</li> <li>■ The output value is the probability of being irritants.</li> </ul>

Respiratory Toxicity	0.039	●	<ul style="list-style-type: none"> <li>■ Category 1: respiratory toxicants; Category 0: respiratory nontoxicants</li> <li>■ The output value is the probability of being toxic.</li> </ul>
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## 8. Environmental toxicity

Property	Value	Comment
Bioconcentration Factors	1.629	<ul style="list-style-type: none"> <li>■ Bioconcentration factors are used for considering secondary poisoning potential and assessing risks to human health via the food chain.</li> <li>■ The unit is <math>-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]</math></li> </ul>
IGC <sub>50</sub>	3.176	<ul style="list-style-type: none"> <li>■ Tetrahymena pyriformis 50 percent growth inhibition concentration</li> <li>■ The unit is <math>-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]</math></li> </ul>
LC <sub>50</sub> FM	3.816	<ul style="list-style-type: none"> <li>■ 96-hour fathead minnow 50 percent lethal concentration</li> <li>■ The unit is <math>-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]</math></li> </ul>
LC <sub>50</sub> DM	3.94	<ul style="list-style-type: none"> <li>■ 48-hour daphnia magna 50 percent lethal concentration</li> <li>■ The unit is <math>-\log_{10}[(\text{mg/L})/(1000 \cdot \text{MW})]</math></li> </ul>

## 9. Tox21 pathway

Property	Value	Decision	Comment
NR-AR	0.016	●	<ul style="list-style-type: none"> <li>■ Androgen receptor</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-AR-LBD	0.003	●	<ul style="list-style-type: none"> <li>■ Androgen receptor ligand-binding domain</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-AhR	0.006	●	<ul style="list-style-type: none"> <li>■ Aryl hydrocarbon receptor</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-Aromatase	0.004	●	<ul style="list-style-type: none"> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-ER	0.149	●	<ul style="list-style-type: none"> <li>■ Estrogen receptor</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-ER-LBD	0.011	●	<ul style="list-style-type: none"> <li>■ Estrogen receptor ligand-binding domain</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-PPAR-gamma	0.002	●	<ul style="list-style-type: none"> <li>■ Peroxisome proliferator-activated receptor gamma</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-ARE	0.015	●	<ul style="list-style-type: none"> <li>■ Antioxidant response element</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-ATAD5	0.006	●	<ul style="list-style-type: none"> <li>■ ATPase family AAA domain-containing protein 5</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>

SR-HSE	0.013	●	<ul style="list-style-type: none"> <li>■ Heat shock factor response element</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-MMP	0.006	●	<ul style="list-style-type: none"> <li>■ Mitochondrial membrane potential</li> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-p53	0.003	●	<ul style="list-style-type: none"> <li>■ Category 1: actives ; Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>

## 10. Toxicophore Rules

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