



## 1. Physicochemical Property

Property	Value	Comment
Molecular Weight	316.2	Contain hydrogen atoms. Optimal:100~600
Volume	344.632	Van der Waals volume
Density	0.918	Density = MW / Volume
nHA	3	Number of hydrogen bond acceptors. Optimal:0~12
nHD	2	Number of hydrogen bond donors. Optimal:0~7
nRot	2	Number of rotatable bonds. Optimal:0~11
nRing	3	Number of rings. Optimal:0~6
MaxRing	14	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	17	Number of rigid bonds. Optimal:0~30
Flexibility	0.118	Flexibility = nRot / nRig
Stereo Centers	2	Optimal: ≤ 2
TPSA	57.53	Topological Polar Surface Area. Optimal:0~140
logS	-3.684	Log of the aqueous solubility. Optimal: -4~0.5 log mol/L
logP	4.091	Log of the octanol/water partition coefficient. Optimal: 0~3
logD	3.406	logP at physiological pH 7.4. Optimal: 1~3

## 2. Medicinal Chemistry

Property	Value	Decision	Comment
QED	0.627	●	■ A measure of drug-likeness based on the concept of desirability; ■ Attractive: > 0.67; unattractive: 0.49~0.67; too complex: < 0.34
SAscore	3.894	●	■ 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	0.65	●	■ The number of sp <sup>3</sup> hybridized carbons / total carbon count, correlating with melting point and solubility. ■ Fsp <sup>3</sup> ≥ 0.42 is considered a suitable value.
MCE-18	76.667	●	■ MCE-18 stands for medicinal chemistry evolution. ■ MCE-18 ≥ 45 is considered a suitable value.

NPscore	2.242	-	<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>■ <math>MW \leq 500</math>; <math>\log P \leq 5</math>; <math>Hacc \leq 10</math>; <math>Hdon \leq 5</math></p> <p>■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.</p>
Pfizer Rule	Rejected	●	<p><math>\log P &gt; 3</math>; <math>TPSA &lt; 75</math></p> <p>Compounds with a high log P (&gt;3) and low TPSA (&lt;75) are likely to be toxic.</p>
GSK Rule	Rejected	●	<p>■ <math>MW \leq 400</math>; <math>\log P \leq 4</math></p> <p>■ Compounds satisfying the GSK rule may have a more favorable ADMET profile</p>
Golden Triangle	Accepted	●	<p>■ <math>200 \leq MW \leq 500</math>; <math>-2 \leq \log D \leq 5</math></p> <p>■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile.</p>
PAINS	1 alerts	-	Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound.
ALARM NMR	2 alerts	-	Thiol reactive compounds.
BMS	1 alerts	-	Undesirable, reactive compounds.
Chelator Rule	1 alerts	-	Chelating compounds.

### 3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-4.748	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	1.8e-05	●	<p>■ low permeability: <math>&lt; 2 \times 10^{-6}</math> cm/s</p> <p>■ medium permeability: <math>2-20 \times 10^{-6}</math> cm/s</p> <p>■ high passive permeability: <math>&gt; 20 \times 10^{-6}</math> cm/s</p>
Pgp-inhibitor	0.83	●	<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	0.012	●	<p>■ Human Intestinal Absorption</p> <p>■ Category 1: HIA+ (HIA &lt; 30%); Category 0: HIA- (HIA &lt; 30%); The output value is the probability of being HIA+</p>
F <sub>20%</sub>	0.995	●	<p>■ 20% Bioavailability</p> <p>■ Category 1: F<sub>20%</sub> + (bioavailability &lt; 20%); Category 0: F<sub>20%</sub> - (bioavailability ≥ 20%); The output value is the probability of being F<sub>20%</sub> +</p>

$F_{30\%}$	0.988	●	<ul style="list-style-type: none"> <li>■ 30% Bioavailability</li> <li>■ Category 1: <math>F_{30\%} +</math> (bioavailability &lt; 30%); Category 0: <math>F_{30\%} -</math> (bioavailability <math>\geq</math> 30%); 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	95.13%	●	<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	5.237	●	<ul style="list-style-type: none"> <li>■ Volume Distribution</li> <li>■ Optimal: 0.04-20L/kg</li> </ul>
BBB Penetration	0.266	●	<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	1.850%	●	<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	0.1	<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	0.796	<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	0.135	<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	0.701	<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	0.147	<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	0.885	<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	0.864	<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	0.552	<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	0.518	<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	0.331	<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	3.164	●	<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>	0.287	-	<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	0.008	●	<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	0.051	●	<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	0.037	●	<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	0.319	●	<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	0.254	●	<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	0.814	●	<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	0.954	●	<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	0.086	●	<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	0.015	●	<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	0.921	●	<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	0.933	●	<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	2.104	<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>	4.748	<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	5.377	<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	6.178	<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	0.183	●	<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	0.234	●	<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	0.613	●	<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	0.932	●	<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	0.825	●	<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	0.732	●	<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	0.983	●	<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	0.896	●	<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	0.714	●	<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	0.948	●	<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	0.973	●	<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	0.983	●	<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	7 alerts	<ul style="list-style-type: none"> <li>■ 155 substructures</li> <li>■ skin irritation</li> </ul>
Aquatic Toxicity Rule	0 alerts	<ul style="list-style-type: none"> <li>■ 99 substructures</li> <li>■ toxicity to liquid(water)</li> </ul>
NonBiodegradable Rule	1 alerts	<ul style="list-style-type: none"> <li>■ 19 substructures</li> <li>■ non-biodegradable</li> </ul>
SureChEMBL Rule	2 alerts	<ul style="list-style-type: none"> <li>■ 164 substructures</li> <li>■ MedChem unfriendly status</li> </ul>