

## 1. Physicochemical Property

Property	Value	Comment
Molecular Weight	118.08	Contain hydrogen atoms. Optimal:100~600
Volume	130.841	Van der Waals volume
Density	0.902	Density = MW / Volume
nHA	0	Number of hydrogen bond acceptors. Optimal:0~12
nHD	0	Number of hydrogen bond donors. Optimal:0~7
nRot	2	Number of rotatable bonds. Optimal:0~11
nRing	0	Number of rings. Optimal:0~6
MaxRing	0	Number of atoms in the biggest ring. Optimal:0~18
nHet	1	Number of heteroatoms. Optimal:1~15
fChar	0	Formal charge. Optimal:-4 ~4
nRig	0	Number of rigid bonds. Optimal:0~30
Flexibility	inf	Flexibility = nRot / nRig
Stereo Centers	0	Optimal: $\leq 2$
TPSA	0.0	Topological Polar Surface Area. Optimal:0~140
logS	-2.764	Log of the aqueous solubility. Optimal: -4~0.5 log mol/L
logP	3.069	Log of the octanol/water partition coefficient. Optimal: 0~3
logD	3.326	logP at physiological pH 7.4. Optimal: 1~3

## 2. Medicinal Chemistry

Property	Value	Decision	Comment
QED	0.529	●	<ul style="list-style-type: none"> <li>■ A measure of drug-likeness based on the concept of desirability;</li> <li>■ Attractive: <math>&gt; 0.67</math>; unattractive: <math>0.49 \sim 0.67</math>; too complex: <math>&lt; 0.34</math></li> </ul>
SAscore	3.026	●	<ul style="list-style-type: none"> <li>■ Synthetic accessibility score is designed to estimate ease of synthesis of drug-like molecules.</li> <li>■ SAscore <math>\geq 6</math>, difficult to synthesize; SAscore <math>&lt; 6</math>, easy to synthesize</li> </ul>
Fsp3	1.0	●	<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> <math>\geq 0.42</math> is considered a suitable value.</li> </ul>
MCE-18	0.0	●	<ul style="list-style-type: none"> <li>■ MCE-18 stands for medicinal chemistry evolution.</li> <li>■ MCE-18 <math>\geq 45</math> is considered a suitable value.</li> </ul>

NPscore	0.23	-	<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	Accepted	●	<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	Rejected	●	<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	0 alerts	-	Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound.
ALARM NMR	1 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	-4.226	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	3.3e-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	0.0	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being Pgp-inhibitor</p>
Pgp-substrate	0.0	●	<p>■ Category 1: substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being Pgp-substrate</p>
HIA	0.028	●	<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>	0.005	●	<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>

$F_{30\%}$	0.002	●	■ 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	97.74%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	2.849	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.249	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	5.251%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5~20%; High: > 20%

## 5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.624	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.863	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.155	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.901	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.067	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C9 substrate	0.855	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2D6 inhibitor	0.007	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2D6 substrate	0.74	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP3A4 inhibitor	0.017	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP3A4 substrate	0.207	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.

## 6. Excretion

Property	Value	Decision	Comment
CL	9.805	●	<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>	0.647	-	<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	0.779	●	<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	0.231	●	<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	0.006	●	<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	0.063	●	<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	0.027	●	<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	0.291	●	<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	0.191	●	<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	0.965	●	<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	0.987	●	<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	0.099	●	<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	1.99	<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>	3.042	<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	3.437	<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	4.951	<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	0.003	●	<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	0.002	●	<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	0.005	●	<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	0.081	●	<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	0.006	●	<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	0.019	●	<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	0.003	●	<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	0.02	●	<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	0.007	●	<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	0.007	●	<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	1 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	0 alerts	<ul style="list-style-type: none"> <li>■ 19 substructures</li> <li>■ non-biodegradable</li> </ul>
SureChEMBL Rule	1 alerts	<ul style="list-style-type: none"> <li>■ 164 substructures</li> <li>■ MedChem unfriendly status</li> </ul>