



1. Physicochemical Property

Property	Value	Comment
Molecular Weight	418.2	Contain hydrogen atoms. Optimal:100~600
Volume	433.427	Van der Waals volume
Density	0.965	Density = MW / Volume
nHA	7.0	Number of hydrogen bond acceptors. Optimal:0~12
nHD	1.0	Number of hydrogen bond donors. Optimal:0~7
nRot	7.0	Number of rotatable bonds. Optimal:0~11
nRing	1.0	Number of rings. Optimal:0~6
MaxRing	9.0	Number of atoms in the biggest ring. Optimal:0~18
nHet	7.0	Number of heteroatoms. Optimal:1~15
fChar	0.0	Formal charge. Optimal:-4 ~4
nRig	22.0	Number of rigid bonds. Optimal:0~30
Flexibility	0.318	Flexibility = nRot / nRig
Stereo Centers	0.0	Stereo Centers. Optimal: ≤ 2
TPSA	84.25	Topological Polar Surface Area. Optimal:0~140
logS	-4.968	The logarithm of aqueous solubility value.
logP	4.222	The logarithm of the n-octanol/water distribution coefficients at pH=7.4.
logD	3.718	The logarithm of the n-octanol/water distribution coefficient.
pka (Acid)	10.297	Acid-base dissociation constant (pKa) value represents the strength of a drug molecule's acidity or basicity.
pka (Base)	6.342	Acid-base dissociation constant (pKa) value represents the strength of a drug molecule's acidity or basicity.
Melting point	132.535	The predicted melting point of a compound is expressed in degrees Celsius (°C). Melting points below 25°C are classified as liquids, while melting points above 25°C are classified as solids.
Boiling point	321.359	The predicted melting point of a compound is expressed in degrees Celsius (°C). A normal boiling point below 25°C is categorized as a gas.

2. Medicinal Chemistry

Property	Value	Decision	Comment
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QED	0.5	●	<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
GASA	0.0	●	<ul style="list-style-type: none"> ■ ES: Easy to synthesize; HS: Hard to synthesize; ■ The output value represents the probability of being difficult to synthesize, ranging from 0 to 1.
Synth	2.0	●	<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	0.292	●	<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	24.0	●	<ul style="list-style-type: none"> ■ MCE-18 stands for medicinal chemistry evolution. ■ MCE-18 ≥ 45 is considered a suitable value.
NPscore	-1.362	-	<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	0.0	●	<ul style="list-style-type: none"> ■ MW ≤ 500; logP ≤ 5; Hacc ≤ 10; Hdon ≤ 5 ■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.
Pfizer Rule	0.0	●	<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	1.0	●	<ul style="list-style-type: none"> ■ MW ≤ 400; logP ≤ 4 ■ Compounds satisfying the GSK rule may have a more favorable ADMET profile
Golden Triangle	0.0	●	<ul style="list-style-type: none"> ■ 200 \leq MW \leq 500; -2 \leq logD \leq 5 ■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile.
PAINS	0 alerts	-	frequent hitters, Alpha-screen artifacts and reactive compound 480 substructures (J Med Chem 201053:2719-40)
ALARM NMR	2 alerts	-	Thiol reactive compounds.
BMS	0 alerts	-	undesirable, reactive compounds 176 substructures (J Chem Inf Model 200646:1060-8)
Chelator Rule	0 alerts	-	Chelating compounds.
Colloidal aggregators	0.121	-	<ul style="list-style-type: none"> ■ Category 0: non-colloidal aggregators; ■ Category 1: colloidal aggregators. ■ The output value is the probability of being colloidal aggregators, within the range of 0 to 1.

FLuc inhibitors	0.394	●	<ul style="list-style-type: none"> ■ Category 0: non-fLuc inhibitors; ■ Category 1: fLuc inhibitors. ■ The output value is the probability of being fLuc inhibitors, within the range of 0 to 1.
Blue fluorescence	0.471	●	<ul style="list-style-type: none"> ■ Category 0: non-blue fluorescence; ■ Category 1: blue fluorescence. ■ The output value is the probability of being blue fluorescence, within the range of 0 to 1.
Green fluorescence	0.675	●	<ul style="list-style-type: none"> ■ Category 0: non-green fluorescence; ■ Category 1: green fluorescence. ■ The output value is the probability of being green fluorescence, within the range of 0 to 1.
Reactive compounds	0.002	●	<ul style="list-style-type: none"> ■ Category 0: non-reactive compound; ■ Category 1: reactive compound. ■ The output value is the probability of being reactive compound, within the range of 0 to 1.
Promiscuous compounds	0.02	●	<ul style="list-style-type: none"> ■ Category 0: non-promiscuous compound; ■ Category 1: promiscuous compound. ■ The output value is the probability of being promiscuous compound, within the range of 0 to 1.

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-4.682	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	-4.576	●	<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
PAMPA	0.003	●	<ul style="list-style-type: none"> ■ The experimental data for Peff was logarithmically transformed (logPeff). ■ Molecules with log Peff values below 2.0 were classified as low-permeability (Category 0), while those with log Peff values exceeding 2.5 were classified as high-permeability (Category 1).
Pgp-inhibitor	0.977	●	<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	0.014	●	<ul style="list-style-type: none"> ■ Category 1: substrate; ■ Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.0	●	<ul style="list-style-type: none"> ■ Human Intestinal Absorption ■ Category 1: HIA+ (HIA $< 30\%$); ■ Category 0: HIA- (HIA $\geq 30\%$); ■ The output value is the probability of being HIA+

$F_{20\%}$	0.003	●	<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 $F_{20\%} +$
$F_{30\%}$	0.019	●	<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 $F_{30\%} +$
$F_{50\%}$	0.37	●	<ul style="list-style-type: none"> ■ 50% Bioavailability ■ Category 1: $F_{50\%} +$ (bioavailability < 50%); ■ Category 0: $F_{50\%} -$ (bioavailability \geq 50%); ■ The output value is the probability of being $F_{50\%} +$

4. Distribution

Property	Value	Decision	Comment
PPB	97.202	●	<ul style="list-style-type: none"> ■ Plasma Protein Binding Optimal: < 90%. ■ Drugs with high protein-bound may have a low therapeutic index.
VDss	-0.043	●	<ul style="list-style-type: none"> ■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB	0.417	●	<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	2.145	●	<ul style="list-style-type: none"> ■ The fraction unbound in plasms ■ Low: <5%; Middle: 5~20%; High: > 20%
OATP1B1 inhibitor	0.997	●	<ul style="list-style-type: none"> ■ Category 0: Non-inhibitor; Category 1: inhibitor. ■ The output value is the probability of being inhibitor, within the range of 0 to 1.
OATP1B3 inhibitor	0.975	●	<ul style="list-style-type: none"> ■ Category 0: Non-inhibitor; Category 1: inhibitor. ■ The output value is the probability of being inhibitor, within the range of 0 to 1.
BCRP inhibitor	0.001	●	<ul style="list-style-type: none"> ■ Category 0: Non-inhibitor; Category 1: inhibitor. ■ The output value is the probability of being inhibitor, within the range of 0 to 1.
MRP1 inhibitor	0.991	●	<ul style="list-style-type: none"> ■ Category 0: Non-inhibitor; Category 1: inhibitor. ■ The output value is the probability of being inhibitor, within the range of 0 to 1.

5. Metabolism

Property	Value	Decision	Comment
CYP1A2 inhibitor	0.969	●	<ul style="list-style-type: none"> ■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

CYP1A2 substrate	1.0	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2C19 inhibitor	0.963	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2C19 substrate	0.99	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2C9 inhibitor	0.794	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2C9 substrate	0.944	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2D6 inhibitor	0.437	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2D6 substrate	0.997	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP3A4 inhibitor	0.882	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP3A4 substrate	0.689	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2B6 inhibitor	0.048	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2B6 substrate	0.004	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2C8 inhibitor	0.793	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
HLM Stability	0.721	●	<p>■ human liver microsomal (HLM) stability</p> <p>■ Category 0: stable+ (HLM > 30 min); Category 1: unstable- (HLM ≤ 30 min). The output value is the probability of human liver microsomal instability, where a value closer to 1 indicates a higher likelihood of instability. The range is between 0 and 1.</p>













6. Excretion

Property	Value	Decision	Comment
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CL _{plasma}	5.611	●	<p>■ The unit of predicted CL_{plasma} penetration is ml/min/kg. >15 ml/min/kg: high clearance; 5-15 ml/min/kg: moderate clearance; < 5 ml/min/kg: low clearance.</p>
T _{1/2}	0.414	●	<p>■ The unit of predicted T_{1/2} is hours.</p> <p>■ ultra-short half-life drugs: 1/2 < 1 hour; short half-life drugs: T_{1/2} between 1-4 hours; intermediate short half-life drugs: T_{1/2} between 4-8 hours; long half-life drugs: T_{1/2} > 8 hours.</p>

7. Toxicity

Property	Value	Decision	Comment
hERG Blockers	0.448	●	<p>■ Molecules with IC₅₀ ≤10μM or ≥50% inhibition at 10 μM were classified as hERG+ (Category 1),</p> <p>■ while molecules with IC₅₀ >10μM or < 50% inhibition at 10μM were classified as hERG - (Category 0).</p> <p>■ The output value is the probability of being hERG+, within the range of 0 to 1.</p>
hERG Blockers (10um)	0.477	●	<p>■ Molecules with IC₅₀ ≤10 μM are classified as hERG+ (Category 1),</p> <p>■ and molecules with IC₅₀ > 10μM are classified as hERG- (Category 0).</p> <p>■ The output value is the probability of being hERG+, within the range of 0 to 1.</p>
DILI	0.993	●	<p>■ Drug Induced Liver Injury.</p> <p>■ Category 1: drugs with a high risk of DILI;</p> <p>■ Category 0: drugs with no risk of DILI.</p> <p>■ The output value is the probability of being toxic.</p>
AMES Mutagenicity	0.579	●	<p>■ AMES Toxicity</p> <p>■ Category 1: Ames positive(+);</p> <p>■ Category 0: Ames negative(-);</p> <p>■ The output value is the probability of being toxic.</p>
Rat Oral Acute Toxicity	0.388	●	<p>■ Rat Oral Acute Toxicity.</p> <p>■ Category 0: low-toxicity, > 500 mg/kg;</p> <p>■ Category 1: high-toxicity; < 500 mg/kg.</p> <p>■ The output value is the probability of being toxic, within the range of 0 to 1.</p>
FDAMDD	0.699	●	<p>■ FDA Maximum (Recommended) Daily Dose.</p> <p>■ Category 1: FDAMDD (+);</p> <p>■ Category 0: FDAMDD (-);</p> <p>The output value is the probability of being positive.</p>
Skin Sensitization	0.432	●	<p>■ Category 1: Sensitizer;</p> <p>■ Category 0: Non-sensitizer.</p> <p>■ The output value is the probability of being toxic, within the range of 0 to 1.</p>
Carcinogenicity	0.786	●	<p>■ Category 1: carcinogens;</p> <p>■ Category 0: non-carcinogens;</p> <p>■ The output value is the probability of being toxic.</p>

Eye Corrosion	0.0		<p>■ Eye Corrosion</p> <p>■ Category 1: corrosives;</p> <p>Category 0: noncorrosives;</p> <p>■ The output value is the probability of being corrosives.</p>
Eye Irritation	0.464		<p>■ Eye Irritation</p> <p>■ Category 1: irritants;</p> <p>Category 0: nonirritants;</p> <p>■ The output value is the probability of being irritants.</p>
Respiratory	0.96		<p>■ Category 1: respiratory toxicants;</p> <p>■ Category 0: non-respiratory toxicants.</p> <p>■ The output value is the probability of being toxic, within the range of 0 to 1.</p>
Human Hep atotoxicity	0.832		<p>■ Human Hepatotoxicity</p> <p>■ Category 1: H-HT positive(+);</p> <p>■ Category 0: H-HT negative(-);</p> <p>■ The output value is the probability of being toxic.</p>
Drug-induce d Nephrotox icity	0.917		<p>■ Category 0: non-nephrotoxic (-);</p> <p>■ Category 1: nephrotoxic (+).</p> <p>■ The output value is the probability of being nephrotoxic (+), within the range of 0 to 1.</p>
Ototoxicity	0.79		<p>■ Category 0: non-ototoxicity (-);</p> <p>■ Category 1: ototoxicity (+).</p> <p>■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.</p>
Hematotoxic ity	0.707		<p>■ Category 0: non-hematotoxicity (-);</p> <p>■ Category 1: hematotoxicity (+).</p> <p>■ The output value is the probability of being hematotoxicity (+), within the range of 0 to 1.</p>
Genotoxicity	0.986		<p>■ Category 0: non-Genotoxicity (-);</p> <p>■ Category 1: Genotoxicity (+).</p> <p>■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.</p>
RPMI-8226 Immunitoxici ty	0.166		<p>■ Category 0: non-cytotoxicity (-);</p> <p>■ Category 1: cytotoxicity (+).</p> <p>■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.</p>
A549 Cytotoxicity	0.201		<p>■ Category 0: non-cytotoxicity (-);</p> <p>■ Category 1: cytotoxicity (+).</p> <p>■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.</p>
Hek293 Cytotoxicity	0.507		<p>■ Category 0: non-cytotoxicity (-);</p> <p>■ Category 1: cytotoxicity (+).</p> <p>■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.</p>
Drug-induce d Neurotox icity	0.869		<p>■ Category 0: non-neurotoxic (-);</p> <p>■ Category 1: neurotoxic (+).</p> <p>■ The output value is the probability of being neurotoxic (+), within the range of 0 to 1.</p>

8. Environmental toxicity

Property	Value	Comment
Bioconcentration Factors	1.241	<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	4.005	<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	4.439	<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	4.587	<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-AhR	0.919	●	<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-AR	0.006	●	<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	0.0	●	<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-Aromatase	0.002	●	<ul style="list-style-type: none"> ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-ER	0.396	●	<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	0.0	●	<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	0.0	●	<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	0.031	●	<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	0.034	●	<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	0.019	●	<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	0.021	●	<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	0.017	●	<ul style="list-style-type: none"> ■ p53, a tumor suppressor protein ■ 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	<ul style="list-style-type: none"> ■ 20 substructures; ■ acute toxicity during oral administration
Genotoxic Carcinogenicity Rule	0	<ul style="list-style-type: none"> ■ 117 substructures; ■ carcinogenicity or mutagenicity
NonGenotoxic Carcinogenicity Rule	0	<ul style="list-style-type: none"> ■ 23 substructures; ■ carcinogenicity through nongenotoxic mechanisms
Skin Sensitization Rule	0	<ul style="list-style-type: none"> ■ 155 substructures; ■ skin irritation
Aquatic Toxicity Rule	0	<ul style="list-style-type: none"> ■ 99 substructures; ■ toxicity to liquid(water)
NonBiodegradable Rule	1 alerts	<ul style="list-style-type: none"> ■ 19 substructures; ■ non-biodegradable
SureChEMBL Rule	0	<ul style="list-style-type: none"> ■ 164 substructures; ■ MedChem unfriendly status
Toxicophores Rule	2 alerts	154 toxic substructures from FAF-Drug4