

1. Physicochemical Property

Property	Value	Comment
Molecular Weight	354.35	Contain hydrogen atoms. Optimal:100~600
Volume	421.308	Van der Waals volume
Density	0.841	Density = MW / Volume
nHA	2	Number of hydrogen bond acceptors. Optimal:0~12
nHD	1	Number of hydrogen bond donors. Optimal:0~7
nRot	21	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	2	Number of heteroatoms. Optimal:1~15
fChar	0	Formal charge. Optimal:-4 ~4
nRig	1	Number of rigid bonds. Optimal:0~30
Flexibility	21.0	Flexibility = nRot /nRig
Stereo Centers	0	Optimal: ≤ 2
TPSA	37.3	Topological Polar Surface Area. Optimal:0~140
logS	-6.662	Log of the aqueous solubility. Optimal: -4~0.5 log mol/L
logP	9.589	Log of the octanol/water partition coefficient. Optimal: 0~3
logD	3.804	logP at physiological pH 7.4. Optimal: 1~3

2. Medicinal Chemistry

Property	Value	Decision	Comment
QED	0.21	•	■ A measure of drug-likeness based on the concept of desirability; ■ Attractive: > 0.67; unattractive: 0.49~0.67; too complex: < 0.34
SAscore	1.665	•	 ■ 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	0.957	•	 ■ 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	0.0	•	■ MCE-18 stands for medicinal chemistry evolution.■ MCE-18≥45 is considered a suitable value.

NPscore 0.277 - ■ 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 Accepted ■ 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. □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. Pfizer Rule Rejected □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. GSK Rule Rejected □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. GSK Rule Rejected □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. GSK Rule Rejected □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. GSK Rule Rejected □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. GSK Rule Rejected □ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable, one is acceptable. GSK Rule Rejected □ If two properties are out of range, a poor acceptable.				
Lipinski Rule Accepted ■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable. Pfizer Rule Rejected logP > 3; TPSA < 75 Compounds with a high log P (>3) and low TPSA (<75) are likely to be toxic.	NPscore	0.277	-	■ This score is typically in the range from –5 to 5. The higher the score is, the higher the probability is
Pfizer Rule Rejected Compounds with a high log P (>3) and low TPSA (<75) are likely to be toxic. GSK Rule Rejected ■ MW ≤ 400; logP ≤ 4 Compounds satisfying the GSK rule may have a more favorable ADMET profile Golden Triangle ■ 200 ≤ MW ≤ 50; -2 ≤ logD ≤ 5 Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile. PAINS 0 alerts - Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound. ALARM NMR 0 alerts BMS 1 alerts Chelator 0 alerts Chelating compounds		Accepted	•	■ If two properties are out of range, a poor absorption or permeability is possible, one is
GSK Rule Rejected ■ Compounds satisfying the GSK rule may have a more favorable ADMET profile Golden Triangle Accepted ■ 200 ≤ MW ≤ 50; -2 ≤ logD ≤ 5 ■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile. PAINS 0 alerts - Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound. ALARM NMR 0 alerts - BMS 1 alerts - Undesirable, reactive compounds. Chelator 0 alerts	Pfizer Rule	Rejected	•	Compounds with a high log P (>3) and low TPSA
Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile. PAINS	GSK Rule	Rejected	•	■ Compounds satisfying the GSK rule may have a
ALARM NMR 0 alerts - Thiol reactive compounds. BMS 1 alerts - Undesirable, reactive compounds. Chelator 0 alerts - Chelating compounds		Accepted	•	■ Compounds satisfying the Golden Triangle rule
NMR 0 alerts - Thiol reactive compounds. BMS 1 alerts - Undesirable, reactive compounds. Chelator 0 alerts - Chelating compounds	PAINS	0 alerts	-	Pan Assay Interference Compounds, frequent hitters, Alpha-screen artifacts and reactive compound.
Chelator Chelating compounds	, . <u></u> ,	0 alerts	-	Thiol reactive compounds.
() alerts - Chelating compounds	BMS	1 alerts	-	Undesirable, reactive compounds.
		0 alerts		Chelating compounds.

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-5.165	•	Optimal: higher than -5.15 Log unit
MDCK Permeability	1.2e-05	•	 ■ low permeability: < 2 x 10⁻⁶ cm/s ■ medium permeability: 2-20 x 10⁻⁶ cm/s ■ high passive permeability: > 20 x 10⁻⁶ cm/s
Pgp-inhibitor	0.0		■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	0.0	•	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.005	•	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
F _{20%}	0.292	•	■ 20% Bioavailability ■ Category 1: F _{20%} + (bioavailability < 20%); Category 0: F _{20%} - (bioavailability ≥ 20%); The output value is the probability of being F _{20%} +

F _{30%}	0.998	•	■ 30% Bioavailability ■ Category 1: $F_{30\%}$ + (bioavailability < 30%); Category 0: $F_{30\%}$ - (bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$ +
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4. Distribution

Property	Value	Decision	Comment
PPB	98.93%	•	■ Plasma Protein Binding■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	1.298	•	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.008	•	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	0.713%	•	■ The fraction unbound in plasms■ Low: <5%; Middle: 5~20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.118	■ Category 1: Inhibitor; Category 0: Non-inhibitor;■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.16	■ Category 1: Substrate; Category 0: Non-substrate;■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.229	■ Category 1: Inhibitor; Category 0: Non-inhibitor;■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.056	■ Category 1: Substrate; Category 0: Non-substrate;■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.059	Category 1: Inhibitor; Category 0: Non-inhibitor;The output value is the probability of being inhibitor.
CYP2C9 substrate	0.995	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2D6 inhibitor	0.024	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2D6 substrate	0.028	■ Category 1: Substrate; Category 0: Non-substrate;■ The output value is the probability of being substrate.
CYP3A4 inhibitor	0.067	■ Category 1: Inhibitor; Category 0: Non-inhibitor;■ The output value is the probability of being inhibitor.
CYP3A4 substrate	0.008	■ Category 1: Substrate; Category 0: Non-substrate;■ The output value is the probability of being substrate.

6. Excretion

Property	Value	Decision	Comment
CL	2.715	•	■ Clearance ■ High: >15 mL/min/kg; moderate: 5-15 mL/min/kg; low: <5 mL/min/kg
T _{1/2}	0.24	-	 ■ 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	0.167	•	■ Category 1: active; Category 0: inactive;■ The output value is the probability of being active.	
н-нт	0.017	•	 ■ Human Hepatotoxicity ■ Category 1: H-HT positive(+); Category 0: H-HT negative(-); ■ The output value is the probability of being toxic. 	
DILI	0.057	•	 ■ 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	0.005	•	■ Category 1: Ames positive(+); Category 0: Ames negative(-);■ The output value is the probability of being toxic.	
Rat Oral Acute Toxicity	0.014	•	 ■ Category 0: low-toxicity; Category 1: high-toxicity; ■ The output value is the probability of being highly toxic. 	
FDAMDD	0.013		 ■ Maximum Recommended Daily Dose ■ Category 1: FDAMDD (+); Category 0: FDAMDD (-) ■ The output value is the probability of being positive. 	
Skin Sensiti zation	0.953	•	■ Category 1: Sensitizer; Category 0: Non-sensitizer; ■ The output value is the probability of being sensitizer.	
Carcinogen city	0.033	•	■ Category 1: carcinogens; Category 0: non-carcinogens;■ The output value is the probability of being toxic.	
Eye Corrosion	0.972	•	■ Category 1: corrosives ; Category 0: noncorrosives ■ The output value is the probability of being corrosives.	
Eye Irritation	0.928	•	■ Category 1: irritants; Category 0: nonirritants ■ The output value is the probability of being irritants.	

Respiratory Toxicity	0.862	•	■ 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	1.58	 ■ Bioconcentration factors are used for considering secondary poisoning potential and assessing risks to human health via the food chain. ■ The unit is -log10[(mg/L)/(1000*MW)] 	
IGC ₅₀	5.858	 ■ Tetrahymena pyriformis 50 percent growth inhibition concentration ■ The unit is -log10[(mg/L)/(1000*MW)] 	
LC ₅₀ FM	4.319	■ 96-hour fathead minnow 50 percent lethal concentration ■ The unit is -log10[(mg/L)/(1000*MW)]	
LC ₅₀ DM	5.3	■ 48-hour daphnia magna 50 percent lethal concentration ■ The unit is -log10[(mg/L)/(1000*MW)]	

9. Tox21 pathway

Property	Value	Decision	Comment
NR-AR	0.137	•	 ■ Androgen receptor ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
NR-AR-LBD	0.002	•	 ■ Androgen receptor ligand-binding domain ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
NR-AhR	0.012	•	 Aryl hydrocarbon receptor Category 1: actives; Category 0: inactives; The output value is the probability of being active.
NR-Aromatase	0.108	•	■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
NR-ER	0.359	•	 ■ Estrogen receptor ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
NR-ER-LBD	0.008	•	 ■ Estrogen receptor ligand-binding domain ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
NR-PPAR- gamma	0.972	•	 ■ Peroxisome proliferator-activated receptor gamma ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
SR-ARE	0.341	•	 ■ Antioxidant response element ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
SR-ATAD5	0.002	•	■ ATPase family AAA domain-containing protein 5 ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.

SR-HSE	0.538	•	 ■ Heat shock factor response element ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
SR-MMP	0.151	•	 ■ Mitochondrial membrane potential ■ Category 1: actives; Category 0: inactives; ■ The output value is the probability of being active.
SR-p53	0.027	•	■ 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	■ 20 substructures■ acute toxicity during oral administration
Genotoxic Carcinogenicity Rule	0 alerts	■ 117 substructures ■ carcinogenicity or mutagenicity
NonGenotoxic Carcinogenicity Rule	0 alerts	■ 23 substructures ■ carcinogenicity through nongenotoxic mechanisms
Skin Sensitization Rule	0 alerts	■ 155 substructures ■ skin irritation
Aquatic Toxicity Rule	0 alerts	■ 99 substructures ■ toxicity to liquid(water)
NonBiodegradable Rule	0 alerts	■ 19 substructures ■ non-biodegradable
SureChEMBL Rule	0 alerts	■ 164 substructures■ MedChem unfriendly status