1. Physicochemical Property

Property	Value	Comment
Molecular Weight	504.32	Contain hydrogen atoms. Optimal:100~600
Volume	499.387	Van der Waals volume
Density	1.01	Density = MW / Volume
nHA	12.0	Number of hydrogen bond acceptors. Optimal:0~12
nHD	4.0	Number of hydrogen bond donors. Optimal:0~7
nRot	12.0	Number of rotatable bonds. Optimal:0~11
nRing	4.0	Number of rings. Optimal:0~6
MaxRing	10.0	Number of atoms in the biggest ring. Optimal:0~18
nHet	12.0	Number of heteroatoms. Optimal:1~15
fChar	0.0	Formal charge. Optimal:-4 ~4
nRig	23.0	Number of rigid bonds. Optimal:0~30
Flexibility	0.522	Flexibility = nRot /nRig
Stereo Centers	0.0	Stereo Centers. Optimal: ≤ 2
TPSA	145.44	Topological Polar Surface Area. Optimal:0~140
logS	-4.056	The logarithm of aqueous solubility value.
logP	2.18	The logarithm of the n-octanol/water distribution coefficients at pH=7.4.
logD	2.353	The logarithm of the n-octanol/water distribution coefficient.
pka (Acid)	8.627	Acid-base dissociation constant (pKa) value represents the strength of a drug molecule's acidity or basicity.
pka (Base)	5.844	Acid-base dissociation constant (pKa) value represents the strength of a drug molecule's acidity or basicity.
Melting point	158.703	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	364.067	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

QED	0.308	🔴	■ 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	🟢	■ 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	🟢	■ 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	0.75	🟢	■ The number of sp3 hybridized carbons / total carbon count, correlating with melting point and solubility. ■ Fsp^3 ≥0.42 is considered a suitable value.
MCE-18	54.476	🟢	■ MCE-18 stands for medicinal chemistry evolution. ■ MCE-18≥45 is considered a suitable value.
NPscore	-0.518	-	■ 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	1.0	🔴	■ 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	🟢	■ logP > 3; TPSA < 75 ■ Compounds with a high log P (>3) and low TPSA (<75) are likely to be toxic.
GSK Rule	1.0	🔴	■ MW ≤ 400; logP ≤ 4 ■ Compounds satisfying the GSK rule may have a more favorable ADMET profile
Golden Triangle	1.0	🔴	■ 200 ≤ MW ≤ 500; -2 ≤ logD ≤ 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	0 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	0.489	-	■ 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	0.001	●	■ 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	0.994	●	■ 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	0.464	●	■ 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	0.02	●	■ 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	0.992	●	■ 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	-5.327	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	-4.825	●	■ low permeability: < 2 × 10-6 cm/s ■ medium permeability: 2-20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
PAMPA	0.02	●	■ 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	0.371	●	■ Category 1: Inhibitor; ■ Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	0.22	●	■ Category 1: substrate; ■ Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.001	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); ■ Category 0: HIA-(HIA >= 30%); ■ The output value is the probability of being HIA+

$F_{20\%}$	0.0	●	■ 20% Bioavailability ■ Category 1: F 20% + (bioavailability < 20%); ■ Category 0: F 20% - (bioavailability ≥ 20%); ■ The output value is the probability of being F 20% +
$F_{30\%}$	0.0	●	■ 30% Bioavailability ■ Category 1: F 30% + (bioavailability < 30%); ■ Category 0: F 30% - (bioavailability ≥ 30%); ■ The output value is the probability of being F 30% +
$F_{50\%}$	0.002	●	■ 50% Bioavailability ■ Category 1: F 50% + (bioavailability < 50%); ■ Category 0: F 50% - (bioavailability ≥ 50%); ■ The output value is the probability of being F 50% +

4. Distribution

Property	Value	Decision	Comment
PPB	92.354	●	■ Plasma Protein Binding Optimal: < 90%. ■ Drugs with high protein-bound may have a low therapeutic index.
VDss	0.078	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB	0.003	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; ■ The output value is the probability of being BBB+
Fu	7.817	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5~20%; High: > 20%
OATP1B1 inhibitor	0.401	●	■ 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	0.888	●	■ 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	0.979	●	■ 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	0.772	●	■ 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	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

CYP1A2 substrate	0.93	🔴	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.0	🟢	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	1.0	🔴	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.0	🟢	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C9 substrate	0.002	🟢	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2D6 inhibitor	0.001	🟢	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2D6 substrate	0.978	🔴	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP3A4 inhibitor	1.0	🔴	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP3A4 substrate	0.006	🟢	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2B6 inhibitor	0.0	🟢	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2B6 substrate	0.0	🟢	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C8 inhibitor	0.0	🟢	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
HLM Stability	1.0	🔴	■ human liver microsomal (HLM) stability ■ 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.

6. Excretion

Property	Value	Decision	Comment

CL_{plasma}	5.997	🟡	■ The unit of predicted CLplasma penetration is ml/min/kg. >15 ml/min/kg: high clearance; 5-15 ml/min/kg: moderate clearance; < 5 ml/min/kg: low clearance.
$T_{1/2}$	1.291	🟡	■ The unit of predicted T1/2 is hours. ■ ultra-short half-life drugs: 1/2 < 1 hour; short half-life drugs: T1/2 between 1-4 hours; intermediate short half-life drugs: T1/2 between 4-8 hours; long half-life drugs: T1/2 > 8 hours.

7. Toxicity

Property	Value	Decision	Comment
hERG Blockers	0.347	🟠	■ Molecules with IC50 ≤10μM or ≥50% inhibition at 10 μM were classified as hERG+ (Category 1), ■ while molecules with IC50 >10μM or < 50% inhibition at 10μM were classified as hERG - (Category 0). ■ The output value is the probability of being hERG+, within the range of 0 to 1.
hERG Blockers (10um)	0.164	🟢	■ Molecules with IC50 ≤10 μM are classified as hERG+ (Category 1), ■ and molecules with IC50 > 10μM are classified as hERG- (Category 0). ■ The output value is the probability of being hERG+, within the range of 0 to 1.
DILI	0.922	🔴	■ 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 Mutagenicity	0.475	🟠	■ AMES Toxicity ■ Category 1: Ames positive(+); ■ Category 0: Ames negative(-); ■ The output value is the probability of being toxic.
Rat Oral Acute Toxicity	0.013	🟢	■ Rat Oral Acute Toxicity. ■ Category 0: low-toxicity, > 500 mg/kg; ■ Category 1: high-toxicity; < 500 mg/kg. ■ The output value is the probability of being toxic, within the range of 0 to 1.
FDAMDD	0.184	🟢	■ FDA Maximum (Recommended) Daily Dose. ■ Category 1: FDAMDD (+); ■ Category 0: FDAMDD (-); The output value is the probability of being positive.
Skin Sensitization	0.997	🔴	■ Category 1: Sensitizer; ■ Category 0: Non-sensitizer. ■ The output value is the probability of being toxic, within the range of 0 to 1.
Carcinogenicity	0.498	🟠	■ Category 1: carcinogens; ■ Category 0: non-carcinogens; ■ The output value is the probability of being toxic.

Eye Corrosion	0.0	●	■ Eye Corrosion ■ Category 1: corrosives; Category 0: noncorrosives; ■ The output value is the probability of being corrosives.
Eye Irritation	0.015	●	■ Eye Irritation ■ Category 1: irritants; Category 0: nonirritants; ■ The output value is the probability of being irritants.
Respiratory	0.97	●	■ Category 1: respiratory toxicants; ■ Category 0: non-respiratory toxicants. ■ The output value is the probability of being toxic, within the range of 0 to 1.
Human Hepatotoxicity	0.991	●	■ Human Hepatotoxicity ■ Category 1: H-HT positive(+); ■ Category 0: H-HT negative(-); ■ The output value is the probability of being toxic.
Drug-induced Nephrotoxicity	0.984	●	■ Category 0: non-nephrotoxic (-); ■ Category 1: nephrotoxic (+). ■ The output value is the probability of being nephrotoxic (+), within the range of 0 to 1.
Ototoxicity	0.966	●	■ Category 0: non-ototoxicity (-); ■ Category 1: ototoxicity (+). ■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.
Hematotoxicity	0.959	●	■ Category 0: non-hematotoxicity (-); ■ Category 1: hematotoxicity (+). ■ The output value is the probability of being hematotoxicity (+), within the range of 0 to 1.
Genotoxicity	1.0	●	■ Category 0: non-Genotoxicity (-); ■ Category 1: Genotoxicity (+). ■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.
RPMI-8226 Immunitoxicity	0.294	●	■ Category 0: non-cytotoxicity (-); ■ Category 1: cytotoxicity (+). ■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.
A549 Cytotoxicity	0.104	●	■ Category 0: non-cytotoxicity (-); ■ Category 1: cytotoxicity (+). ■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.
Hek293 Cytotoxicity	0.852	●	■ Category 0: non-cytotoxicity (-); ■ Category 1: cytotoxicity (+). ■ The output value is the probability of being ototoxicity (+), within the range of 0 to 1.
Drug-induced Neurotoxicity	0.973	●	■ Category 0: non-neurotoxic (-); ■ Category 1: neurotoxic (+). ■ The output value is the probability of being neurotoxic (+), within the range of 0 to 1.

8. Environmental toxicity

Property	Value	Comment
Bioconcentration Factors	0.679	■ 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}	3.361	■ Tetrahymena pyriformis 50 percent growth inhibition concentration. ■ The unit is –log10[(mg/L)/(1000*MW)]
$LC_{50}FM$	4.055	■ 96-hour fathead minnow 50 percent lethal concentration. ■ The unit is –log10[(mg/L)/(1000*MW)]
$LC_{50}DM$	4.843	■ 48-hour daphnia magna 50 percent lethal concentration. ■ The unit is –log10[(mg/L)/(1000*MW)]

9. Tox21 pathway

Property	Value	Decision	Comment
NR-AhR	0.0	🟢	■ Aryl hydrocarbon receptor ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-AR	0.499	🟠	■ Androgen receptor ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-AR-LBD	0.0	🟢	■ Androgen receptor ligand-binding domain ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-Aromatase	0.202	🟢	■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-ER	0.004	🟢	■ Estrogen receptor ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-ER-LBD	0.0	🟢	■ Estrogen receptor ligand-binding domain ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
NR-PPAR-gamma	0.006	🟢	■ Peroxisome proliferator-activated receptor gamma ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
SR-ARE	0.913	🔴	■ Antioxidant response element ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.

SR-ATAD5	0.169	●	■ ATPase family AAA domain-containing protein 5 ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
SR-HSE	0.002	●	■ Heat shock factor response element ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
SR-MMP	0.0	●	■ Mitochondrial membrane potential ■ Category 1: actives ; ■ Category 0: inactives; ■ The output value is the probability of being active.
SR-p53	0.014	●	■ 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	■ 20 substructures; ■ acute toxicity during oral administration
Genotoxic Carcinogenicity Rule	1 alerts	■ 117 substructures; ■ carcinogenicity or mutagenicity
NonGenotoxic Carcinogenicity Rule	0	■ 23 substructures; ■ carcinogenicity through nongenotoxic mechanisms
Skin Sensitization Rule	0	■ 155 substructures; ■ skin irritation
Aquatic Toxicity Rule	0	■ 99 substructures; ■ toxicity to liquid(water)
NonBiodegradable Rule	1 alerts	■ 19 substructures; ■ non-biodegradable
SureChEMBL Rule	0	■ 164 substructures; ■ MedChem unfriendly status
FAF-Drugs4 Rule	0	154 toxic substructures from FAF-Drug4