



## 1. Physicochemical Property

Property	Value	Comment
Molecular Weight	480.17	Contain hydrogen atoms. Optimal:100~600
Volume	483.215	Van der Waals volume
Density	0.994	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	8.0	Number of rotatable bonds. Optimal:0~11
nRing	1.0	Number of rings. Optimal:0~6
MaxRing	13.0	Number of atoms in the biggest ring. Optimal:0~18
nHet	8.0	Number of heteroatoms. Optimal:1~15
fChar	0.0	Formal charge. Optimal:-4 ~4
nRig	32.0	Number of rigid bonds. Optimal:0~30
Flexibility	0.25	Flexibility = nRot / nRig
Stereo Centers	0.0	Stereo Centers. Optimal: ≤ 2
TPSA	81.39	Topological Polar Surface Area. Optimal:0~140
logS	-5.571	The logarithm of aqueous solubility value.
logP	4.519	The logarithm of the n-octanol/water distribution coefficients at pH=7.4.
logD	4.267	The logarithm of the n-octanol/water distribution coefficient.
pka (Acid)	10.422	Acid-base dissociation constant (pKa) value represents the strength of a drug molecule's acidity or basicity.
pka (Base)	3.805	Acid-base dissociation constant (pKa) value represents the strength of a drug molecule's acidity or basicity.
Melting point	151.653	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	395.679	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	0.244	●	<ul style="list-style-type: none"> <li>■ A measure of drug-likeness based on the concept of desirability;</li> <li>■ Attractive: &gt; 0.67;</li> <li>■ unattractive: 0.49~0.67;</li> <li>■ too complex: &lt; 0.34</li> </ul>
GASA	0.0	●	<ul style="list-style-type: none"> <li>■ ES: Easy to synthesize; HS: Hard to synthesize;</li> <li>■ The output value represents the probability of being difficult to synthesize, ranging from 0 to 1.</li> </ul>
Synth	2.0	●	<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 &lt;6, easy to synthesize</li> </ul>
Fsp3	0.185	●	<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	29.0	●	<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	-1.488	-	<ul style="list-style-type: none"> <li>■ Natural product-likeness score.</li> <li>■ This score is typically in the range from -5 to 5.</li> <li>■ The higher the score is, the higher the probability is that the molecule is a NP.</li> </ul>
Lipinski Rule	0.0	●	<ul style="list-style-type: none"> <li>■ MW <math>\leq 500</math>; logP <math>\leq 5</math>; Hacc <math>\leq 10</math>; Hdon <math>\leq 5</math></li> <li>■ If two properties are out of range, a poor absorption or permeability is possible, one is acceptable.</li> </ul>
Pfizer Rule	0.0	●	<ul style="list-style-type: none"> <li>■ logP &gt; 3; TPSA &lt; 75</li> <li>■ Compounds with a high log P (&gt;3) and low TPSA (&lt;75) are likely to be toxic.</li> </ul>
GSK Rule	1.0	●	<ul style="list-style-type: none"> <li>■ MW <math>\leq 400</math>; logP <math>\leq 4</math></li> <li>■ Compounds satisfying the GSK rule may have a more favorable ADMET profile</li> </ul>
Golden Triangle	0.0	●	<ul style="list-style-type: none"> <li>■ 200 <math>\leq</math> MW <math>\leq</math> 500; -2 <math>\leq</math> logD <math>\leq</math> 5</li> <li>■ Compounds satisfying the Golden Triangle rule may have a more favorable ADMET profile.</li> </ul>
PAINS	0 alerts	-	frequent hitters, Alpha-screen artifacts and reactive compound 480 substructures (J Med Chem 201053:2719-40)
ALARM NMR	1 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	0.972	-	<ul style="list-style-type: none"> <li>■ Category 0: non-colloidal aggregators;</li> <li>■ Category 1: colloidal aggregators.</li> <li>■ The output value is the probability of being colloidal aggregators, within the range of 0 to 1.</li> </ul>

FLuc inhibitors	0.017	●	<ul style="list-style-type: none"> <li>■ Category 0: non-fLuc inhibitors;</li> <li>■ Category 1: fLuc inhibitors.</li> <li>■ The output value is the probability of being fLuc inhibitors, within the range of 0 to 1.</li> </ul>
Blue fluorescence	0.544	●	<ul style="list-style-type: none"> <li>■ Category 0: non-blue fluorescence;</li> <li>■ Category 1: blue fluorescence.</li> <li>■ The output value is the probability of being blue fluorescence, within the range of 0 to 1.</li> </ul>
Green fluorescence	0.839	●	<ul style="list-style-type: none"> <li>■ Category 0: non-green fluorescence;</li> <li>■ Category 1: green fluorescence.</li> <li>■ The output value is the probability of being green fluorescence, within the range of 0 to 1.</li> </ul>
Reactive compounds	0.03	●	<ul style="list-style-type: none"> <li>■ Category 0: non-reactive compound;</li> <li>■ Category 1: reactive compound.</li> <li>■ The output value is the probability of being reactive compound, within the range of 0 to 1.</li> </ul>
Promiscuous compounds	0.026	●	<ul style="list-style-type: none"> <li>■ Category 0: non-promiscuous compound;</li> <li>■ Category 1: promiscuous compound.</li> <li>■ The output value is the probability of being promiscuous compound, within the range of 0 to 1.</li> </ul>

### 3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-5.031	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	-4.527	●	<ul style="list-style-type: none"> <li>■ low permeability: <math>&lt; 2 \times 10^{-6}</math> cm/s</li> <li>■ medium permeability: <math>2-20 \times 10^{-6}</math> cm/s</li> <li>■ high passive permeability: <math>&gt; 20 \times 10^{-6}</math> cm/s</li> </ul>
PAMPA	0.005	●	<ul style="list-style-type: none"> <li>■ The experimental data for Peff was logarithmically transformed (logPeff).</li> <li>■ 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).</li> </ul>
Pgp-inhibitor	1.0	●	<ul style="list-style-type: none"> <li>■ Category 1: Inhibitor;</li> <li>■ Category 0: Non-inhibitor;</li> <li>■ The output value is the probability of being Pgp-inhibitor</li> </ul>
Pgp-substrate	0.0	●	<ul style="list-style-type: none"> <li>■ Category 1: substrate;</li> <li>■ Category 0: Non-substrate;</li> <li>■ The output value is the probability of being Pgp-substrate</li> </ul>
HIA	0.025	●	<ul style="list-style-type: none"> <li>■ Human Intestinal Absorption</li> <li>■ Category 1: HIA+ (HIA <math>&lt; 30\%</math>);</li> <li>■ Category 0: HIA- (HIA <math>\geq 30\%</math>);</li> <li>■ The output value is the probability of being HIA+</li> </ul>

$F_{20\%}$	0.098	●	<ul style="list-style-type: none"> <li>■ 20% Bioavailability</li> <li>■ Category 1: <math>F_{20\%} +</math> (bioavailability &lt; 20%);</li> <li>■ Category 0: <math>F_{20\%} -</math> (bioavailability <math>\geq</math> 20%);</li> <li>■ The output value is the probability of being <math>F_{20\%} +</math></li> </ul>
$F_{30\%}$	0.969	●	<ul style="list-style-type: none"> <li>■ 30% Bioavailability</li> <li>■ Category 1: <math>F_{30\%} +</math> (bioavailability &lt; 30%);</li> <li>■ Category 0: <math>F_{30\%} -</math> (bioavailability <math>\geq</math> 30%);</li> <li>■ The output value is the probability of being <math>F_{30\%} +</math></li> </ul>
$F_{50\%}$	0.56	●	<ul style="list-style-type: none"> <li>■ 50% Bioavailability</li> <li>■ Category 1: <math>F_{50\%} +</math> (bioavailability &lt; 50%);</li> <li>■ Category 0: <math>F_{50\%} -</math> (bioavailability <math>\geq</math> 50%);</li> <li>■ The output value is the probability of being <math>F_{50\%} +</math></li> </ul>

#### 4. Distribution

Property	Value	Decision	Comment
PPB	98.64	●	<ul style="list-style-type: none"> <li>■ Plasma Protein Binding</li> <li>Optimal: &lt; 90%.</li> <li>■ Drugs with high protein-bound may have a low therapeutic index.</li> </ul>
VDss	0.153	●	<ul style="list-style-type: none"> <li>■ Volume Distribution</li> <li>■ Optimal: 0.04-20L/kg</li> </ul>
BBB	0.889	●	<ul style="list-style-type: none"> <li>■ Blood-Brain Barrier Penetration</li> <li>■ Category 1: BBB+; Category 0: BBB-;</li> <li>■ The output value is the probability of being BBB+</li> </ul>
Fu	0.901	●	<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>
OATP1B1 inhibitor	0.893	●	<ul style="list-style-type: none"> <li>■ Category 0: Non-inhibitor; Category 1: inhibitor.</li> <li>■ The output value is the probability of being inhibitor, within the range of 0 to 1.</li> </ul>
OATP1B3 inhibitor	0.127	●	<ul style="list-style-type: none"> <li>■ Category 0: Non-inhibitor; Category 1: inhibitor.</li> <li>■ The output value is the probability of being inhibitor, within the range of 0 to 1.</li> </ul>
BCRP inhibitor	0.005	●	<ul style="list-style-type: none"> <li>■ Category 0: Non-inhibitor; Category 1: inhibitor.</li> <li>■ The output value is the probability of being inhibitor, within the range of 0 to 1.</li> </ul>
MRP1 inhibitor	0.761	●	<ul style="list-style-type: none"> <li>■ Category 0: Non-inhibitor; Category 1: inhibitor.</li> <li>■ The output value is the probability of being inhibitor, within the range of 0 to 1.</li> </ul>

#### 5. Metabolism

Property	Value	Decision	Comment
CYP1A2 inhibitor	0.999	●	<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	1.0	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2C19 inhibitor	0.989	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2C19 substrate	0.995	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2C9 inhibitor	0.63	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2C9 substrate	0.004	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2D6 inhibitor	0.993	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2D6 substrate	0.0	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP3A4 inhibitor	0.042	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP3A4 substrate	1.0	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2B6 inhibitor	0.001	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
CYP2B6 substrate	0.284	●	<p>■ Category 1: Substrate; Category 0: Non-substrate;</p> <p>■ The output value is the probability of being substrate.</p>
CYP2C8 inhibitor	1.0	●	<p>■ Category 1: Inhibitor; Category 0: Non-inhibitor;</p> <p>■ The output value is the probability of being inhibitor.</p>
HLM Stability	0.997	●	<p>■ human liver microsomal (HLM) stability</p> <p>■ Category 0: stable+ (HLM &gt; 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 <sub>plasma</sub>	4.901	●	<p>■ The unit of predicted CL<sub>plasma</sub> penetration is ml/min/kg. &gt;15 ml/min/kg: high clearance; 5-15 ml/min/kg: moderate clearance; &lt; 5 ml/min/kg: low clearance.</p>
T <sub>1/2</sub>	0.272	●	<p>■ The unit of predicted T<sub>1/2</sub> is hours.</p> <p>■ ultra-short half-life drugs: 1/2 &lt; 1 hour; short half-life drugs: T<sub>1/2</sub> between 1-4 hours; intermediate short half-life drugs: T<sub>1/2</sub> between 4-8 hours; long half-life drugs: T<sub>1/2</sub> &gt; 8 hours.</p>

## 7. Toxicity

Property	Value	Decision	Comment
hERG Blockers	0.823	●	<p>■ Molecules with IC<sub>50</sub> ≤10μM or ≥50% inhibition at 10 μM were classified as hERG+ (Category 1),</p> <p>■ while molecules with IC<sub>50</sub> &gt;10μM or &lt; 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)	0.928	●	<p>■ Molecules with IC<sub>50</sub> ≤10 μM are classified as hERG+ (Category 1),</p> <p>■ and molecules with IC<sub>50</sub> &gt; 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	0.826	●	<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	0.75	●	<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	0.084	●	<p>■ Rat Oral Acute Toxicity.</p> <p>■ Category 0: low-toxicity, &gt; 500 mg/kg;</p> <p>■ Category 1: high-toxicity; &lt; 500 mg/kg.</p> <p>■ The output value is the probability of being toxic, within the range of 0 to 1.</p>
FDAMDD	0.636	●	<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	0.732	●	<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	0.894	●	<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	0.004	●	<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	0.138	●	<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	0.848	●	<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	0.843	●	<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	0.745	●	<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	0.552	●	<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	0.968	●	<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	0.072	●	<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	0.15	●	<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	0.889	●	<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	0.889	●	<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	1.385	<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>	4.77	<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	6.095	<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	6.168	<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-AhR	0.305	●	<ul style="list-style-type: none"> <li>■ Aryl hydrocarbon receptor</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-AR	0.001	●	<ul style="list-style-type: none"> <li>■ Androgen receptor</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-AR-LBD	0.001	●	<ul style="list-style-type: none"> <li>■ Androgen receptor ligand-binding domain</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-Aromatase	0.595	●	<ul style="list-style-type: none"> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-ER	0.119	●	<ul style="list-style-type: none"> <li>■ Estrogen receptor</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
NR-ER-LBD	0.007	●	<ul style="list-style-type: none"> <li>■ Estrogen receptor ligand-binding domain</li> <li>■ Category 1: actives ;</li> <li>■ 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 ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-ARE	0.277	●	<ul style="list-style-type: none"> <li>■ Antioxidant response element</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>



SR-ATAD5	0.044	●	<ul style="list-style-type: none"> <li>■ ATPase family AAA domain-containing protein 5</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-HSE	0.021	●	<ul style="list-style-type: none"> <li>■ Heat shock factor response element</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-MMP	0.256	●	<ul style="list-style-type: none"> <li>■ Mitochondrial membrane potential</li> <li>■ Category 1: actives ;</li> <li>■ Category 0: inactives;</li> <li>■ The output value is the probability of being active.</li> </ul>
SR-p53	0.068	●	<ul style="list-style-type: none"> <li>■ p53, a tumor suppressor protein</li> <li>■ Category 1: actives ;</li> <li>■ 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	<ul style="list-style-type: none"> <li>■ 20 substructures;</li> <li>■ acute toxicity during oral administration</li> </ul>
Genotoxic Carcinogenicity Rule	3 alerts	<ul style="list-style-type: none"> <li>■ 117 substructures;</li> <li>■ carcinogenicity or mutagenicity</li> </ul>
NonGenotoxic Carcinogenicity Rule	1 alerts	<ul style="list-style-type: none"> <li>■ 23 substructures;</li> <li>■ carcinogenicity through nongenotoxic mechanisms</li> </ul>
Skin Sensitization Rule	0	<ul style="list-style-type: none"> <li>■ 155 substructures;</li> <li>■ skin irritation</li> </ul>
Aquatic Toxicity Rule	0	<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	0	<ul style="list-style-type: none"> <li>■ 164 substructures;</li> <li>■ MedChem unfriendly status</li> </ul>
Toxicophores Rule	3 alerts	154 toxic substructures from FAF-Drug4