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# *Computer-Aided Screening of anti-TNF Traditional Chinese Medicine*

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***Keywords:*** Computer Assisted Screening; Small Molecule Inhibitors; TNF; Traditional Chinese Medicine

***Abstract:*** Tumor Necrosis Factor (TNF, also known as Tumor Necrosis Factor, TNF-Alpha), is an important inflammatory factor that plays an important role in autoimmune diseases. Its monoclonal antibodies have been widely used in rheumatic immune diseases, but they require injection and are expensive, and may produce corresponding antibodies, leading to a decrease in efficacy. Developing oral formulations with anti TNF effects can compensate for the shortcomings of monoclonal antibodies, which has significant significance. This study used computer-aided methods to screen small molecule compounds with anti-TNF effects from the active ingredient datebases of traditional Chinese medicine, and identified traditional Chinese medicine with anti-TNF effects. 100 compounds with the strongest binding force to TNF were selected from databases such as TCM, TCMD, and ZINC, respectively. The ADMET lab2.0 online database was used to predict the oral absorption and toxicity of selected small molecule compounds. Compounds with an oral absorption ≥ 20% and no carcinogenic, teratogenic, mutagenic, or cardiac toxicity were retained. TCM retained 19 compounds, TCMD retained 13 compounds, and ZINC retained 25 compounds. Using AutoDock Vina 1.1.2 software, 13 compounds screened from TCMD were molecularly docked with TNF, resulting in the removal of Vitamin K2 and Saussureamine A, due to their low binding energy. Finally, 11 small molecule compounds with potential anti-TNF effects were obtained, and these compounds were searched through the TCMD database to obtain their sources of traditional Chinese medicine or medicinal plants. Sophoranochrome from the Sophora subprostrata, Neoarctin B from the Arctium lappa, 5-Hydroxy-7-methoxy-3', 4'-diacetoxy-6-(6,6-dimethyl-2-oxo-cyclohexylmethyl) flavone from the Helminthostachys zeylanica and 8-Geranyloxy psoralen from the Pleurospermum rivulorum are likely to have significant anti-TNF effects. Therefore, these traditional Chinese medicines are worthy of further in vitro experimental research.

## 1. Introduction

Tumor necrosis factor (TNF, also known as Tumor Necrosis Factor, TNF-Alpha), is an important inflammatory factor that plays an important role in autoimmune diseases. Its monoclonal antibodies, such as Adalimumab, are widely used in rheumatic immune diseases, and its sales rank among the

top 5 of all monoclonal antibody drugs. However, it requires injection and is expensive, and may produce corresponding antibodies, leading to a decrease in efficacy. [1] Developing oral formulations with anti-TNF effects can compensate for the shortcomings of monoclonal antibodies, which is of great significance. Since 1992, small molecule inhibitors of TNF (1) have been reported, which has been more than 30 years, and researchers have been trying various methods to screen or synthesize TNF small molecule inhibitors[2]. Due to various reasons, such as the side effects of compounds, the therapeutic effects, and the most importantly, the long research and development cycle and high investment of Western drugs, there are still no available oral TNF small molecule inhibitors on the market so far. Therefore, screening small molecule compounds with anti-TNF effects from the active ingredient datebases of traditional Chinese medicine and identifying traditional Chinese medicine with anti-TNF effects have practical significance. Because traditional Chinese medicine has a long history of use and its safety has been verified, it can avoid the problems of long research and development cycle and large investment in Western medicine [3].

## 2. Materials and Methods

### 2.1 Virtual screening of TNF small molecule inhibitor

Adopting the Vina solution from Yin Fu Cloud Computing Platform (https://cloud.yinfotek.com/), we completed virtual screening work. We obtained the crystal structure (2) or NMR structure (PDB ID: 7JRA, resolution: 2.1 Å) of the TNF protein from the RCSB Protein Data Bank (http://www.rcsb.org/). We then used databases containing traditional Chinese medicine or natural drug compounds, including TCM (35,308 small molecules), TCMD (23,025 small molecules), and ZINC (127,695 small molecules), for virtual screening. The binding pocket was defined based on the crystal ligand, and semi-flexible docking was performed using the AutoDock Vina program (3). Finally, we visualized and analyzed the binding patterns of the first 1,000 docking results and sorted them in order of binding energy. The top 100 compounds with the highest binding energy from each database were selected for further screening [4].

### 2.2 Prediction of toxicity and oral absorption

Using ADMET lab2.0 online database (https://admetmesh.scbdd.com/service/evaluation/cal) predict the oral absorption and toxicity of the selected small molecule compounds, retain compounds with an oral absorption of ≥20% and compounds without carcinogenicity, teratogenicity, mutagenicity, and cardiac toxicity [5].

### 2.3 Molecular docking

The 2D/3D structure of small molecule compounds was obtained from Pubchem in the sdf format and minimized in the ChemBioDraw 3D module. The crystal structure of TNF is based on data from Uniprot database (https://www.uniprot.org/). The TNF structure was modified by AutodockTools 1.5.6(dehydration and hydrogenation) and exported to pdbqt format. After defining the grid on the active site of TNF protein, the docking program was executed by AutoDock-Vina 1.1.2, and the output score was displayed as kcal/mol. PyMOL 2.3.0 and BIOVIA Discovery Studio 2016 were applied to result processing and visualization[6].

## 3. Results

### 3.1 Results of virtual screening from small molecule compound databases

Using the method of 2.1, 100 compounds with the strongest binding force to TNF were selected from databases containing traditional Chinese medicine or natural drug compounds, such as TCM (35308 small molecules), TCMD (23025 small molecules), and ZINC (127695 small molecules), as shown in Table 1.

Table 1: Results of virtual screening of small molecule compound database

| TCM | | TCMD | | ZINC | |
|---|---|---|---|---|---|
| ZINC85543530 | ZINC85597228 | 11107 | 16802 | ZINC04221534 | ZINC12892869 |
| ZINC85543552 | ZINC85597296 | 20053 | 16951 | ZINC03839510 | ZINC85874644 |
| ZINC85593944 | ZINC95912875 | 7687 | 22250 | ZINC15708831 | 20096 |
| ZINC14649947 | ZINC05854709 | 11111 | 23021 | ZINC68601297 | ZINC01792699 |
| ZINC85592933 | ZINC14649954 | 18878 | 6471 | ZINC05415673 | ZINC02092851 |
| ZINC85593903 | ZINC42876749 | 18918 | 7691 | ZINC20503379 | ZINC03844746 |
| ZINC85593946 | ZINC59586817 | 11096 | 8484 | ZINC08296596 | ZINC04024417 |
| ZINC85593863 | ZINC85504524 | 1110 | 8485 | ZINC08296608 | ZINC04701203 |
| ZINC95910777 | ZINC85504702 | 16333 | 906 | ZINC08296706 | ZINC08296533 |
| ZINC13461720 | ZINC85543536 | 17572 | 10039 | ZINC08297093 | ZINC08296611 |
| ZINC14711739 | ZINC85569460 | 5880 | 10352 | ZINC20503374 | ZINC08296681 |
| ZINC85492157 | ZINC85597289 | 6911 | 10368 | ZINC08296860 | ZINC08296864 |
| ZINC85597273 | ZINC85631215 | 1456 | 11093 | ZINC08297105 | ZINC08297869 |
| ZINC13460794 | ZINC85632420 | 14564 | 14601 | ZINC08297129 | ZINC08952261 |
| ZINC85569238 | ZINC95913422 | 18066 | 14707 | ZINC12899148 | ZINC09041421 |
| ZINC85592897 | ZINC03791929 | 19103 | 16394 | ZINC01814811 | ZINC09485757 |
| ZINC85594065 | ZINC13385406 | 21170 | 16966 | ZINC02095133 | ZINC12902247 |
| ZINC85631217 | ZINC14711733 | 21937 | 22313 | ZINC02126276 | ZINC13406683 |
| ZINC70455591 | ZINC15148357 | 10032 | 2363 | ZINC08296519 | ZINC19782239 |
| ZINC85543585 | ZINC22013607 | 11190 | 2489 | ZINC08296677 | ZINC20503402 |
| ZINC85543593 | ZINC29490879 | 12566 | 3067 | ZINC08297088 | ZINC20503522 |
| ZINC85569058 | ZINC33831896 | 18067 | 3392 | ZINC79188145 | ZINC20503535 |
| ZINC85569481 | ZINC38143855 | 21658 | 435 | ZINC08296522 | ZINC20759442 |
| ZINC85570766 | ZINC59728659 | 21675 | 5550 | ZINC08297143 | ZINC68568930 |
| ZINC85592931 | ZINC85490449 | 3294 | 5566 | ZINC08297156 | ZINC79188936 |
| ZINC85593905 | ZINC85510692 | 6077 | 677 | ZINC12898623 | ZINC00619547 |
| ZINC95911417 | ZINC85543541 | 6183 | 8636 | ZINC20503371 | ZINC02107526 |
| ZINC04097753 | ZINC85543591 | 1019 | 8824 | ZINC08296515 | ZINC02112535 |
| ZINC14618800 | ZINC85569126 | 14539 | 15870 | ZINC08297123 | ZINC02125574 |
| ZINC59586930 | ZINC85569217 | 161 | 15871 | ZINC13403248 | ZINC02126683 |
| ZINC85488005 | ZINC85569450 | 16178 | 17378 | ZINC03847085 | ZINC02434789 |
| ZINC85504706 | ZINC85592935 | 16965 | 18508 | ZINC05415069 | ZINC20565258 |
| ZINC85570702 | ZINC85593931 | 19036 | 18871 | ZINC08296903 | ZINC03839491 |
| ZINC85592913 | ZINC85593934 | 20340 | 18916 | ZINC68562976 | ZINC03839539 |
| ZINC85632702 | ZINC85597267 | 3223 | 18921 | ZINC68569328 | ZINC03841779 |
| ZINC85645188 | ZINC85646381 | 5899 | 20769 | ZINC68569437 | ZINC03841895 |

| | | | | | |
|---|---|---|---|---|---|
| ZINC14768164 | ZINC86050540 | 7689 | 20776 | ZINC02121309 | ZINC03847585 |
| ZINC44404823 | ZINC00077311 | 8902 | 20983 | ZINC03429535 | ZINC04258814 |
| ZINC85489584 | ZINC08234342 | 10264 | 21167 | ZINC08296659 | ZINC05415064 |
| ZINC85543563 | ZINC14923010 | 15875 | 2364 | ZINC08296891 | ZINC05415130 |
| ZINC85543599 | ZINC32037939 | 19658 | 2494 | ZINC08297108 | ZINC08296662 |
| ZINC85643579 | ZINC59587281 | 21172 | 3161 | ZINC20503516 | ZINC08296820 |
| ZINC95912676 | ZINC59589074 | 3174 | 7097 | ZINC04235733 | ZINC08297080 |
| ZINC33833762 | ZINC70450956 | 8009 | 8647 | ZINC04237519 | ZINC08878685 |
| ZINC70457399 | ZINC70455128 | 12082 | 9123 | ZINC04701202 | ZINC08952083 |
| ZINC85504709 | ZINC70455615 | 13634 | 10151 | ZINC05413613 | ZINC12660323 |
| ZINC85593859 | ZINC85493208 | 13831 | 10182 | ZINC08296861 | ZINC12661719 |
| ZINC85596043 | ZINC85511995 | 13968 | 1139 | ZINC08297147 | ZINC12892129 |
| ZINC85596079 | ZINC85530955 | 15490 | 11739 | ZINC08297159 | ZINC20503389 |
| ZINC85597219 | ZINC85531494 | 16675 | 16176 | ZINC09033168 | ZINC20503491 |

Table 1 summarizes candidate molecule information obtained through virtual screening from different small molecule compound databases (TCM, TCMD, ZINC), and it comprises three main columns. Each column contains the molecule IDs for that database, represented by numbers or alphanumeric combinations. Each main column displays the 100 compounds with the strongest TNF binding affinity selected from each database.

### 3.2 Results after toxicity and oral absorption screening

According to the method in 2.2, the ADMET lab2.0 online database was used to predict the oral absorption and toxicity of the small molecule compounds screened in 3.1. Compounds with an oral absorption of ≥20% and no carcinogenic, teratogenic, mutagenic, and cardiac toxicity were retained, as shown in Table 2. After screening, the TCM database retained 19 compounds, the TCMD database retained 13 compounds, and the ZINC database retained 25 compounds.

Table 2: Results after toxicity and oral absorption screening

| TCM | TCMD | ZINC |
|---|---|---|
| ZINC13461720 | 11107 | ZINC08296706 |
| ZINC85597273 | 5880 | ZINC08297093 |
| ZINC85592931 | 1456 | ZINC08296860 |
| ZINC85504706 | 14539 | ZINC08297129 |
| ZINC85543563 | 19036 | ZINC12899148 |
| ZINC85543599 | 5899 | ZINC08296519 |
| ZINC85504709 | 13831 | ZINC08296677 |
| ZINC85597296 | 22250 | ZINC08297088 |
| ZINC59586817 | 10368 | ZINC08296515 |
| ZINC85504702 | 16394 | ZINC08296903 |
| ZINC85597289 | 435 | ZINC08296659 |
| ZINC13385406 | 18921 | ZINC08296891 |
| ZINC15148357 | 20983 | ZINC08297108 |
| ZINC29490879 | | ZINC08296861 |
| ZINC38143855 | | ZINC08297147 |
| ZINC59728659 | | ZINC08296533 |
| ZINC85510692 | | ZINC08296681 |

| | | |
|---|---|---|
| ZINC85592935 | | ZINC08296864 |
| ZINC59587281 | | ZINC12902247 |
| | | ZINC02107526 |
| | | ZINC02112535 |
| | | ZINC02125574 |
| | | ZINC03839539 |
| | | ZINC08296662 |
| | | ZINC08296820 |

Table 2 uses the ADMET Lab 2.0 online database to predict the oral absorption rates and toxicity of the small-molecule compounds screened in Table 1. Compounds with oral absorption ≥20% and no carcinogenic, teratogenic, mutagenic, or cardiotoxic effects were retained. After screening, 19 compounds were retained from the TCM database, 13 from the TCMD database, and 25 from the ZINC database. TCM, TCMD, and ZINC are different small molecule compound databases; the numbers or alphanumeric combinations in each represent the molecule numbers for that database.

### 3.3 Results of molecular docking

Due to copyright, TCM is unable to search for the source of traditional Chinese medicine based on molecular coding. The small molecule compounds screened by ZINC cannot match the corresponding traditional Chinese medicine through commonly used traditional Chinese medicine datebases. Therefore, the small molecule compounds screened by TCMD are used for molecular docking and ultimately screened for traditional Chinese medicine with anti-tNF effects. Using the method of 2.3, the 13 compounds screened from TCMD were molecularly docked with TNF using AutoDock Vina 1.1.2 software, and the binding energy was calculated, as shown in Table 3. Among them, the binding energy of Vitamin K2, Saussureamine A with TNF is greater than -7, and considering the poor binding force, further search and validation experiments for traditional Chinese medicine from TCMD are not considered. The binding energies of 6,6',10,10',12,12'-Hexachloroisoprotetin A, Diospyrosooleanolide with TNF are the highest, with -9.4kcal/mol and -9kcal/mol respectively, which molecular docking diagram is shown in Figure 1.

Table 3. Autodock Vina Rating Results

| Protein | Molecular name | TCMD ID | PubChem ID | Affinity(kcal/mol) |
|---|---|---|---|---|
| TNF (PDB ID:7JRA) | Sophoranochromene | 11107 | 5321396 | -8.8 |
| | Neoarctin B | 5880 | 3083466 | -7.2 |
| | Isochandalone | 1456 | 15907834 | -8.5 |
| | Bisindolylpyrrole | 14539 | 2399 | -8 |
| | Dorsmanin Fa | 19036 | 162908642 | -8.3 |
| | Neo-beta-carotene U | 5899 | 162933483 | -7.4 |
| | Vitamin K2 | 13831 | 5283547 | -5.9 |
| | 6,6',10,10',12,12'-Hexachloroisoperrottetin A | 22250 | 637302 | -9.4 |
| | Saussureamine A | 10368 | 10427798 | -6.9 |
| | (23E)-Coumaroylhederafenin | 16394 | 73812741 | -8 |
| | 5-Hydroxy-7-methoxy-3',4'-diacetoxy-6-(6, 6-dimethyl-2-oxo-cyclohexylmethyl)flavone | 435 | 162960516 | -7.6 |
| | Diospyrosooleanolide | 18921 | 163002369 | -9 |
| | 8-Geranyloxy psoralen | 20983 | 5317564 | -7.5 |

In Table 3, the AutoDock-Vina 1.1.2 software was used to perform molecular docking between 13 compounds screened from TCMD and TNF, and the binding energy was calculated. The target protein is TNF, the PDB ID is the code of this protein domain database, the small molecule name is the compound from TCMD that has been screened for toxicity and oral absorption, the TCMD ID and PubChem ID are the codes of this database, and the binding energy is the energy after TNF docks with the small molecule compound, in kcal/mol.

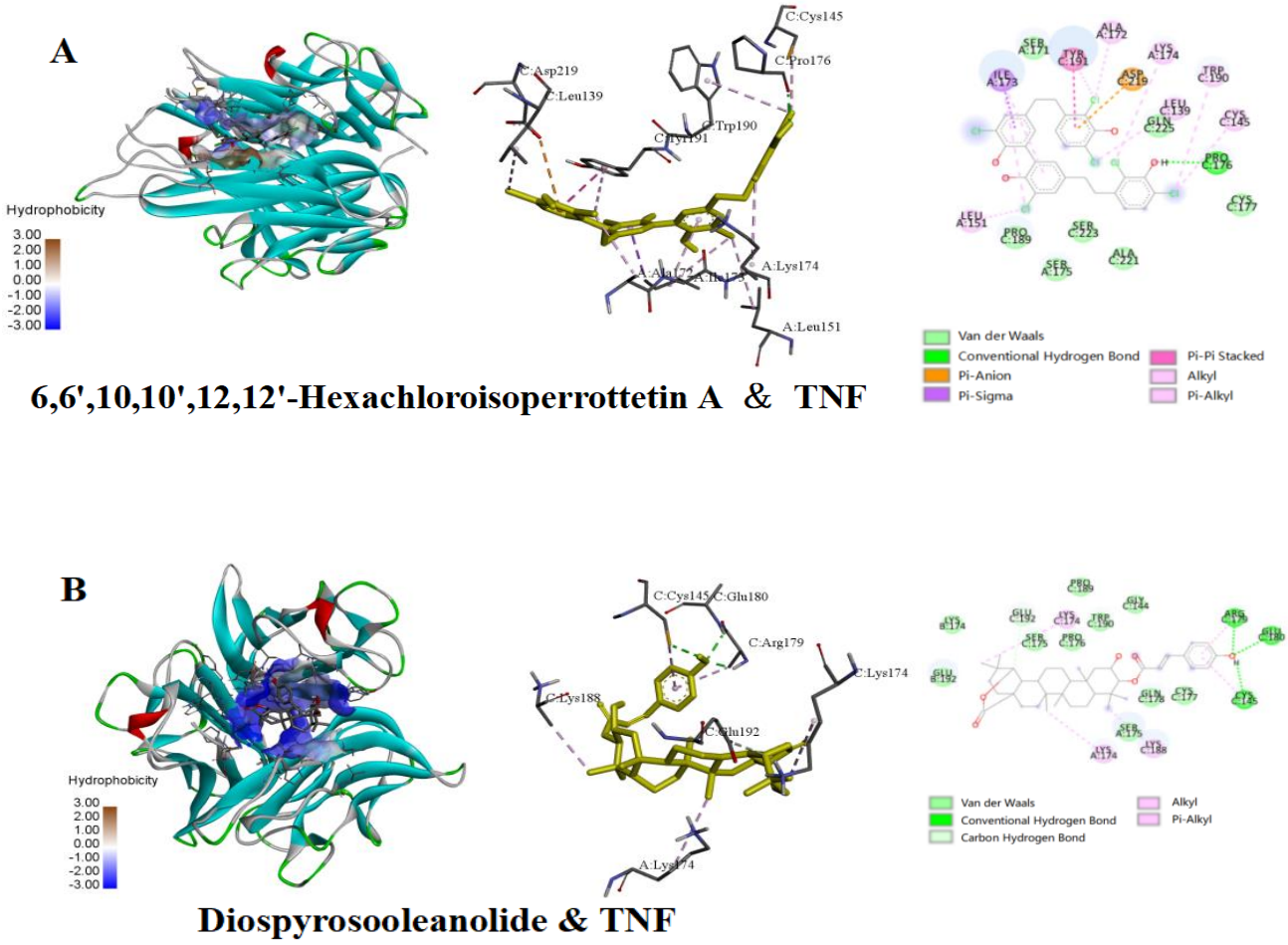


Figure 1. Molecular docking diagram of small molecule compounds with TNF

(A) Molecular docking diagram of 6,6',10,10',12,12'-Hexachloroisoperrottetin A with TNF. The small molecule compound forms a Pi-Pi stacking bond with the residue TYRC: 191 of TNF, a hydrogen bond with PROC: 176, which helps to stabilize the structure. Other residues also form Pi-Alkyl bonds, Alkyl bonds, and van der Waals forces. (B) Molecular docking diagram of Diospyrosooleanolide with TNF. Hydrogen bonds are formed with the residues CYSC: 145, ARGC: 179, GLUC: 180 of TNF, which contribute to structural stability. Other residues also form Alyl bonds, Pi-Amyl bonds, hydrocarbon bonds, and van der Waals forces.

### 3.4 Searching for anti-TNF traditional Chinese medicine from small molecular compounds

After screening through steps 3.1, 3.2, and 3.3, 11 small molecule compounds with potential anti-TNF effects were ultimately obtained. These compounds were searched through the TCMD database to obtain their sources of traditional Chinese medicine or medicinal plants. The results are shown in Table 4. The results showed that Sophoranochrome from the Sophora subprostrata , Neoarctin B from the Arctium lappa, 5-Hydroxy-7-methoxy-3', 4'-diacetoxy-6-(6,

6-dimethyl-2-oxo-cyclohexylmethyl) flavone from the Helminthostachys zeylanica, and 8-Geranyloxy psoralen from the Pleurospermum rivulorum are likely to have significant anti-TNF effects. Therefore, these traditional Chinese medicines are also likely to have anti-TNF effects, worth further research.

Table 4. Anti-TNF small molecule compounds and sources of TCMD

| Compound name | Source | Smiles structural formula |
|---|---|---|
| Sophoranochromene | Sophora subprostrata | [C@@H]1Oc2c(C(=O)C1)ccc(c2CC=C(C)C)Oc1ccc2c(c1)C=CC(O2)(C)CCC=C(C)C |
| Neoarctin B | Arctium lappa | [C@H]1[C@@H](Cc2cc(ccc2)c2c(cc2c)C[C@H]2[C@H](C=O)OC2)Cc2cc(c(c2)OC)OOC)OC)COC1=O)Cc1cc(c(c(c1)OC)O)OC |
| Isochandalone | Derris scandens | c1c(c(c2c(c1)occ(c2=O)c1ccc2c(c1)C=CC(O2)(C)C)O)CC=C(C)CO |
| Bisindolylpyrrole | Lycogala epidendrum, Arcyria | c1(c[nH]c2c1cccc2)C1=C(c2c[nH]c3c2cccc3)C=ONC1=O |
| Dorsmanin Fa | Dorstenia mannii | c1c(CC=C(C)C)c2c(c3c1C(=O)C[C@H](O3)c1cc(c(cc1)O)O)C[C@H](O2)C(C)(C)OO |
| Neo-beta-carotene U | Spinacia oleracea | C1([C@H])[C@@H](CC=C1)C/C=C/C=C/C=C/C(=C/C=C/C=C/C(=C/C=C/C(./C)=C\C1=C(CCCC1(C)C)C)C/C)C(C)CC |
| 6,6',10,10',12,12'-Hexachloroisoperrottetin A | Jamesoniella colorata | c1(cc(cc(c1O)Cl)CCc1ccc(c(c1Cl)O)Cl)c1cc(cc(c1O)Cl)CCc1c(c(c(cc1)Cl)O)Cl |
| (23E)-Coumaroylhederagenin | Ludwigia octovalvis | C1[C@H]([C@@])[C@H]2[C@](C1)([C@H]1[C@](CC2)([C@]2(C(=CC1)[C@H]1[C@@](CC2)(CCC1(C)C)C(=O)O)C)C)C(C)COC(=O)/C=C/c1ccc(cc1)OO |
| 5-Hydroxy-7-methoxy-3',4'-diacetoxy-6-(6,6-dimethyl-2-oxo-cyclohexylmethyl)flavone | Helminthostachys zeylanica | Oc1c2c=Occoc2cc(c1C[C@H]1C(CCCC1=O)(C)C)OCc1cccc(c1)OC(=O)COC=OC |
| Diospyrosooleanolide | Diospyros angustifolia | c1(ccc(cc1)O)/C=C/C=OO[C@H]1C([C@H]2[C@](C[C@H]1O)[C@H]1[C@](CC2)([C@]2([C@H](CC1)[C@H]1[C@]3(CC2)CCC([C@H]1OC3=O)(C)C)C)CC(C)C |
| 8-Geranyloxy psoralen | Pleurospermum rivulorum | c1c2c(cc3c1ccc3)ccc(=O)o2OC/C=C/CCC=C(C)CC |

## 4. Discussion

The research on TNF small molecule inhibitors has a history of more than 30 years, but currently there are no available oral TNF small molecule inhibitors on the market. The main technical bottlenecks currently lie in safety , cost and time needed for research and development (4). And TNF small molecule inhibitors derived from traditional Chinese medicine can effectively avoid this problem. Because traditional Chinese medicine has long-term history in safe use, and the entire cycle from research and development to production and application is not at the same level as Western medicine. This study used the Yin Fu Cloud Computing Platform to search for small molecule compounds that may have anti-TNF effects from databases such as TCM, TCMD, and

ZINC, which aim was to develop oral TNF small molecule inhibitors, screen out traditional Chinese medicine or medicinal plants containing these components, accelerate the development and application of safe and effective TNF small molecule inhibitors.

Previously, many scholars had screened TNF small molecule inhibitors (5-6) from other small molecule compound databases, but these screened small molecules were often not from traditional Chinese medicine or medicinal plants, and the TNF small molecule inhibitors screened from these databases often cannot match the corresponding traditional Chinese medicine or medicinal plants, even the results of the ZINC database screening that is most likely to match the corresponding traditional Chinese medicine or medicinal plants, wat the same situation. Therefore, this study focuses on virtual screening of TNF small molecule inhibitors through TCM and TCMD databases, that is the difference between this study and similar studies in the past.

Hundreds of TNF small molecule inhibitors were preliminarily screened from tens of thousands of small molecule compounds in the database, and further screening was conducted through oral absorption, toxicity, and other conditions. Small molecule compounds derived from traditional Chinese medicine are generally believed to have an oral absorption rate of ≥ 20% in order to achieve effective blood drug concentration and therapeutic effects. Therefore, this study predicted the oral absorption rate of small molecule compounds through software and removed compounds with an oral absorption rate less than 20%. Diseases treated with TNF inhibitors are often chronic immune diseases that require long-term medication, thus requiring lower toxicity than ordinary drugs. Therefore, this study used software to predict the toxicity of small molecule compounds and removed compounds that were cardiotoxic, carcinogenic, teratogenic, and mutagenic. After screening under these two conditions, nearly 80-90% of the initially screened TNF small molecule inhibitors were removed.

Due to copyright restrictions, the small molecule compounds screened from the TCM database cannot obtain their Smiles structure and search for their sources of traditional Chinese medicine or medicinal plants. The small molecule compounds screened from the ZINC database cannot match the corresponding traditional Chinese medicine or medicinal plants when searched in commonly used traditional Chinese medicine databases. Only small molecule compounds screened from the TCMD database can match the corresponding drug sources. After screening with oral absorption rate and toxicity, only 13 small molecule compounds were selected from the TCMD database in this study. After molecular docking of these 13 compounds with TNF using AutoDock-Vina 1.1.2 software, the two compounds with low binding power were removed. Among the remaining 11 compounds, only four compounds come from commonly used traditional Chinese medicine, while the rest come from other medicinal plants or fungi. Respectively, the four compounds were Sophoranochrome from the Sophora subprostrata, Neoarctin B from the Arctium lappa , Hydroxy-7-methoxy-3',4'-diacetoxy-6-(6,6-dimethyl-2-oxo-cyclohexylmeth-yl) flavone from the Helminthostachys zeylanica, and 8-Geranyloxy psoralen from the Pleurospermum rivulorum. Because these screenings are all based on computer-aided technology, further in vitro experiments are needed to verify the anti-TNF effect of the selected compounds, and whether commonly used traditional Chinese medicine containing these compounds also has anti-TNF effects.

## 5. Conclusion

Through computer-aided screening, this study obtained 11 compounds that may have anti-TNF effects and worth further research. Commonly used traditional Chinese medicine such as the Sophora subprostrata, the Arctium lappa , the Helminthostachys zeylanica, the Pleurospermum rivulorum, are also worth further studying for their anti-TNF effects, and are most likely to become oral drugs against TNF.

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