



The Traditional Chinese Medicine Active Compound Library is a collection of bioactive compounds, bridging ancient medicinal wisdom with modern scientific exploration. This extensive library provides access to a wide array of compounds that influence critical biological pathways, with potential applications in areas such as inflammation, oxidative stress, metabolic regulation, neuroprotection, and more.

Among the well-known compounds are:

- Curcumin, recognized for its potent anti-inflammatory and antioxidant properties. It modulates key pathways like NF- $\kappa$ B and MAPK, contributing to the reduction of inflammation and oxidative damage. It is also potentially active in preventing neurodegenerative diseases like Alzheimer's.

- Resveratrol is a widely researched antioxidant, which regulates pathways such as SIRT1 and AMPK. Its broad therapeutic potential includes aging, cardioprotection, cancer prevention, and metabolic regulation.

- Quercetin, a flavonoid found in many fruits and vegetables, is known for its ability to regulate inflammation by inhibiting enzymes like COX-2 and activating the Nrf2 antioxidant pathway. It has been studied for its protective effects against oxidative stress and potential cancer-preventive properties.

- Theobromine, a compound from cacao, acts as a mild stimulant with cardiovascular benefits. It influences adenosine receptors and serves as a vasodilator, enhancing blood flow, and is of great interest for its potential in mood regulation and heart health.

The **TCM Active Compound Library** integrates solubility, pathway targeting, and biological activity insights, making it an invaluable resource for researchers exploring the pharmacological potential of TCM-derived compounds in modern medicine.

**Related terms:** *chinese medicine, alternative medicine, natural products, inflammation, antioxidants, adenosine receptors, NF- $\kappa$ B, COX-2, MAP kinase*

# Highlights

## Library Composition

Name	Occurrence in the library, times
Others	1166
Antibacterial	188
Oxidoreductases	100
Antiviral	98
Acetylcholine turnover	76
Nitric oxide synthases	48
Antifungal	43
Transient Receptor Potential channels (TRP)	41
Carbonic anhydrases	39
p38 subfamily	35
Nicotinic acetylcholine receptors (nACh)	33
Antiparasitic	31
Voltage-gated calcium channels (Ca <sub>V</sub> )	31

CYP2 family: drug metabolising subset	29
Glycosidases	29
GABA <sub>A</sub> receptors	28
CYP1 family	27
1C. Peroxisome proliferator-activated receptors	21
Type XIII RTKs: Ephrin receptor family	21
3B. Estrogen-related receptors	20
3C. 3-Ketosteroid receptors	19
S1: Chymotrypsin	19
5-Hydroxytryptamine receptors	19
AMPK subfamily	19
Hydrolases	18
Lipoxygenases	18
"Akt (Protein kinase B, PKB) family"	18
3A. Estrogen receptors	16
ABCB subfamily	15
Histone deacetylases (HDACs)	14
Catecholamine turnover	14
Alpha subfamily	14
JNK subfamily	13

Adrenoceptors	13
Ionotropic glutamate receptors	12
"Calcium- and sodium-activated potassium channels (K <sub>Ca</sub> , K <sub>Na</sub> )"	12
"Phosphatidylinositol-4,5-bisphosphate 3-kinase family"	12
P4 P-type ATPases: Phospholipid-transporting ATPases	12
Free fatty acid receptors	12
Class A Orphans	11
Voltage-gated potassium channels (K <sub>v</sub> )	10
Receptor tyrosine phosphatase (RTP) family	8
M2: Angiotensin-converting enzymes (ACE and ACE2)	8
Aryl hydrocarbon receptor	7
Opioid receptors	7
S9: Prolyl oligopeptidase	7
ABCG subfamily	7
Dopamine receptors	7
M28: Aminopeptidase Y	7
Voltage-gated sodium channels (Na <sub>v</sub> )	7
SLC49 family of FLVCR-related heme transporters	7
Succinate receptor	6
Cannabinoid receptors	6

Organic anion transporters (OATs)	6
"CYP11, CYP17, CYP19, CYP20 and CYP21 families"	6
Histamine receptors	6
Type IV RTKs: VEGF (vascular endothelial growth factor) receptor family	6
Glycine receptors	6
Acyltransferases	6
E3 ubiquitin ligase components	5
Adenosine receptors	5
Metabotropic glutamate receptors	5
A1: Pepsin	5
Aurora kinase (Aur) family	5
ABCC subfamily	5
M10: Matrix metalloproteinase	5
Bile acid receptor	5
FRAP subfamily	5
SLC35 family of nucleotide sugar transporters	5
Prostaglandin synthases	5
Dioxygenases	5
UDP glucuronosyltransferases (UGT)	5
Poly ADP-ribose polymerases	5

SLC7 family	5
GSK subfamily	5
H <sup>+</sup> /K <sup>+</sup> -ATPases	5
Glycine transporter subfamily	4
Hydroxycarboxylic acid receptors	4
GABA transporter subfamily	4
Organic cation transporters (OCT)	4
Alanine/serine/cysteine transporter subfamily	4
"Phosphodiesterases, 3',5'-cyclic nucleotide (PDEs)"	4
Fatty acid-binding proteins	4
Type I RTKs: ErbB (epidermal growth factor) receptor family	4
Calcium-sensing receptor	4
Arginase	4
Janus kinase (JakA) family	4
Adenosine turnover	4
Fak family	4
Protein kinase A (PKA) family	4
DNA topoisomerases	3
Class Frizzled GPCRs	3
Taste 1 receptors	3

2-Acylglycerol ester turnover	3
SLCO family of organic anion transporting polypeptides	3
Tubulins	3
Heat shock proteins	3
Ryanodine receptors (RyR)	3
CYP3 family	3
Class C Orphans	3
C2: Calpain	3
"CYP39, CYP46 and CYP51 families"	3
C1: Papain	3
11. Vitamin D receptor-like receptors	3
Basic leucine zipper domain TFs	3
Histone acetyltransferases (HATs)	3
CFTR	3
CIC family	3
Lanosterol biosynthesis pathway	3
Type II RTKs: Insulin receptor family	3
Integrins	3
Two-pore domain potassium channels ( $K_{2P}$ )	2
1-phosphatidylinositol 4-kinase family	2

"Type III RTKs: PDGFR, CSFR, Kit, FLT3 receptor family"	2
NOD-like receptor family	2
Melatonin receptors	2
Atypical SLC22B subfamily	2
Polo-like kinase (PLK) family	2
Decarboxylases	2
Toll-like receptor family	2
PIM family	2
Bromodomain kinase (BRDK) family	2
Nucleotide turnover	2
Histone demethylases	2
Monoamine transporter subfamily	2
SLC3 family	2
Tec family	2
Trace amine receptor	2
M1: Aminopeptidase N	2
Platelet-activating factor receptor	2
IRE family	2
"GPR18, GPR55 and GPR119"	2
1H. Liver X receptor-like receptors	2



Blood coagulation components	•	2
Inwardly rectifying potassium channels (K <sub>IR</sub> )	•	2
p70 subfamily	•	2
Lipid phosphate phosphatases	•	2
SGK family	•	1
Adiponectin receptors	•	1
Protein arginine N-methyltransferases	•	1
MAPKAPK subfamily	•	1
Pyrimidine salvage	•	1
Motilin receptor	•	1
SLC29 family	•	1
GABA <sub>B</sub> receptors	•	1
NADPH oxidases	•	1
Eta subfamily	•	1
2B. Retinoid X receptors	•	1
SLC47 family of multidrug and toxin extrusion transporters	•	1
STAT transcription factors	•	1
Type I receptor serine/threonine kinases	•	1
C14: Caspase	•	1
Glucagon receptor family	•	1

M12: Astacin/Adamalysin	-	1
Cyclic GMP-AMP synthase	-	1
Class II transporters	-	1
Csk family	-	1
SLC16 family of monocarboxylate transporters	-	1
Non-enzymatic BRD containing proteins	-	1
Thyroid hormone turnover	-	1
Acetylcholine receptors (muscarinic)	-	1
SLC15 family of peptide transporters	-	1
M14: Carboxypeptidase A	-	1
Haem oxygenase	-	1
Src family	-	1
ATPases	-	1
PDK1 family	-	1
"Sodium iodide symporter, sodium-dependent multivitamin transporter and sodium-coupled monocarboxylate transporters"	-	1
Casein kinase 1 (CK1) family	-	1
Orphan or poorly characterized SLC22 family members	-	1
Adenylyl cyclases (ACs)	-	1
Leukotriene receptors	-	1
Glutaminases	-	1

C44: Phosphoribosyl pyrophosphate amidotransferase	•	1
B-cell lymphoma 2 (Bcl-2) protein family	•	1
<i>N</i>-Acylethanolamine turnover	•	1
Cholecystokinin receptors	•	1
Phospholipase A <sub>2</sub>	•	1
GABA turnover	•	1
Purine-nucleoside phosphorylase	•	1
SLC10 family of sodium-bile acid co-transporters	•	1
Chemokine receptors	•	1
Type X RTKs: HGF (hepatocyte growth factor) receptor family	•	1
Angiotensin receptors	•	1
1A. Thyroid hormone receptors	•	1
CYP4 family	•	1
RSK subfamily	•	1
Glutathione transferases	•	1
NKF2 family	•	1
P2X receptors	•	1
Isocitrate dehydrogenases	•	1
PDHK family	•	1
SLC18 family of vesicular amine transporters	•	1

Vasopressin and oxytocin receptors	•	1
Interferon receptor family	•	1
Glutamate transporter subfamily	•	1
Inhibitors of apoptosis (IAP) protein family	•	1
Histone methyltransferases (HMTs)	•	1
Other pattern recognition receptors	•	1
Interleukin-1 receptor-associated kinase (IRAK) family	•	1