

Study on the Mechanism of Jiedu Sanjie Formula in the Treatment of Gastric Cancer Based on Network Pharmacology and Molecular Docking

Yixin Fu ^{1,2}, Longjian Zhou ¹, Jing'er Huang ^{1,2}, Ruihua Xiong ^{1,3}, Yanli Fu ^{1,3,*}

- ¹ Department of Oncology, Shenzhen (Futian) Hospital of Guangzhou University of Chinese Medicine, 518000 Shenzhen, Guangdong, China
- ² The Sixth Clinical Medical School, Guangzhou University of Chinese Medicine, 518000 Shenzhen, Guangdong, China
- ³ Shenzhen Cancer Center of Traditional Chinese Medicine, 518000 Shenzhen, Guangdong, China

DOI: <https://doi.org/10.62767/jecacm702.1579>



Supplementary Materials

Table S1 The specific grid center coordinates for each ligand-target pair

xyz	3O96	3D0E	akt3	8YP4	6OCO	1H9O
Quercetin	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	9.619 2.157 13.576	-0.161 -0.183 21.854
Kaempferol	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	9.619 2.157 13.576	-0.161 -0.183 21.854
Luteolin	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	9.619 2.157 13.576	9.619 2.157 13.576
Beta-sitosterol	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	9.619 2.157 13.576	9.619 2.157 13.576	9.619 2.157 13.576
Nobiletin	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	20.89 9.664 17.567	9.619 2.157 13.576
β-ecdysone	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	20.89 9.664 17.567	9.619 2.157 13.576
Stigmasterol	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	20.89 9.664 17.567	9.619 2.157 13.576
Cinobufagin	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	20.89 9.664 17.567	9.619 2.157 13.576
Morin	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	20.89 9.664 17.567	9.619 2.157 13.576
Cinobufotalin	6.29 -7.942 17.261	23.898 -62.712 -3.816	-3.076 4.113 5.9	-0.161 -0.183 21.854	20.89 9.664 17.567	9.619 2.157 13.576