Network pharmacology predicts potential mechanisms of 18β-glycyrrhetinic acid against triple-negative breast cancer

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Introduction：

Triple-negative breast cancer(TNBC) is the prominent malignant subtype of breast cancer, and targeted therapeutic agents acting on it still need to be investigated for addition. It is well known that natural products with a variety of pharmacological activities can be developed as potential antitumor agents. Among them, pentacyclic triterpenoid 18β-glycyrrhetinic acid(GA) is widely recognized to have a wide range of pharmacological effects such as anti-inflammatory, antibacterial, antitumor and antivirus. We showed the potential targets and mechanisms of GA against TNBC through network pharmacology and molecular docking.

Methods：

In this paper, R was used to analyze the differences of TNBC samples and interact with the predicted target of GA to obtain common genes. Through the protein interaction study and enrichment analysis of the common genes, the possible related pathways and targets of GA against TNBC were obtained, and the molecular docking study of the core targets was carried out.

Results：

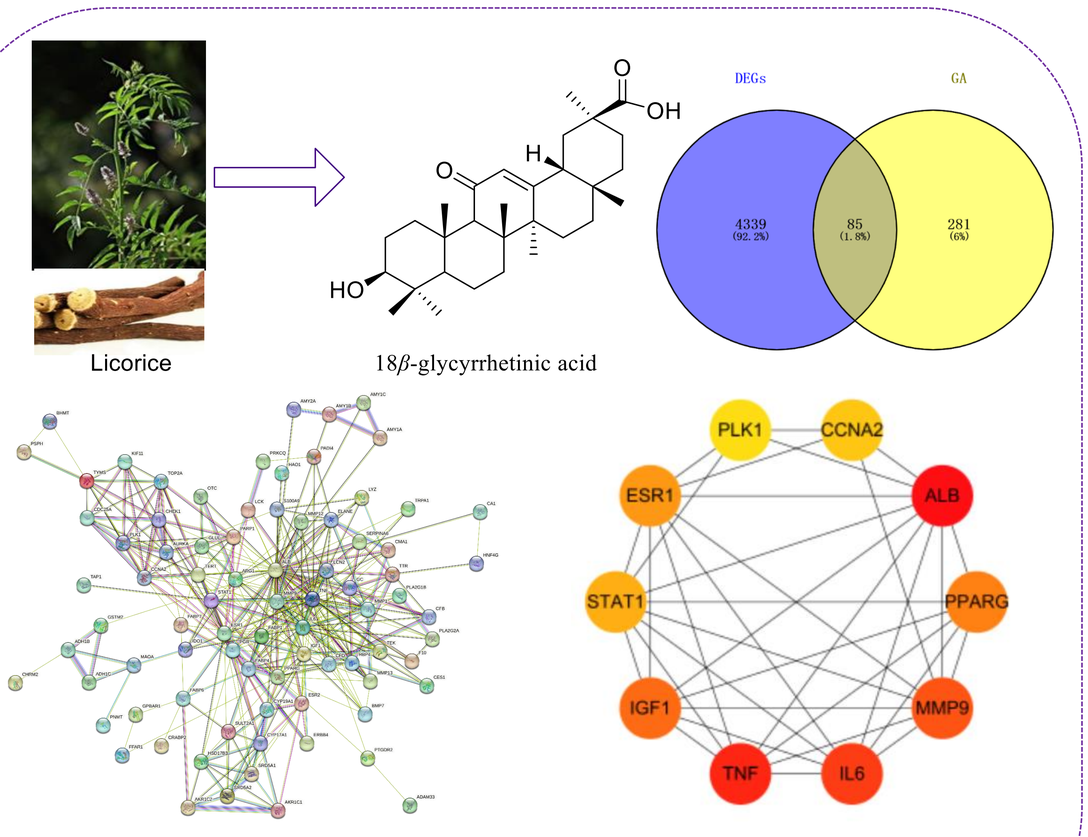

Fig.1 Common gene screening and protein-protein interaction topology analysis core target screening

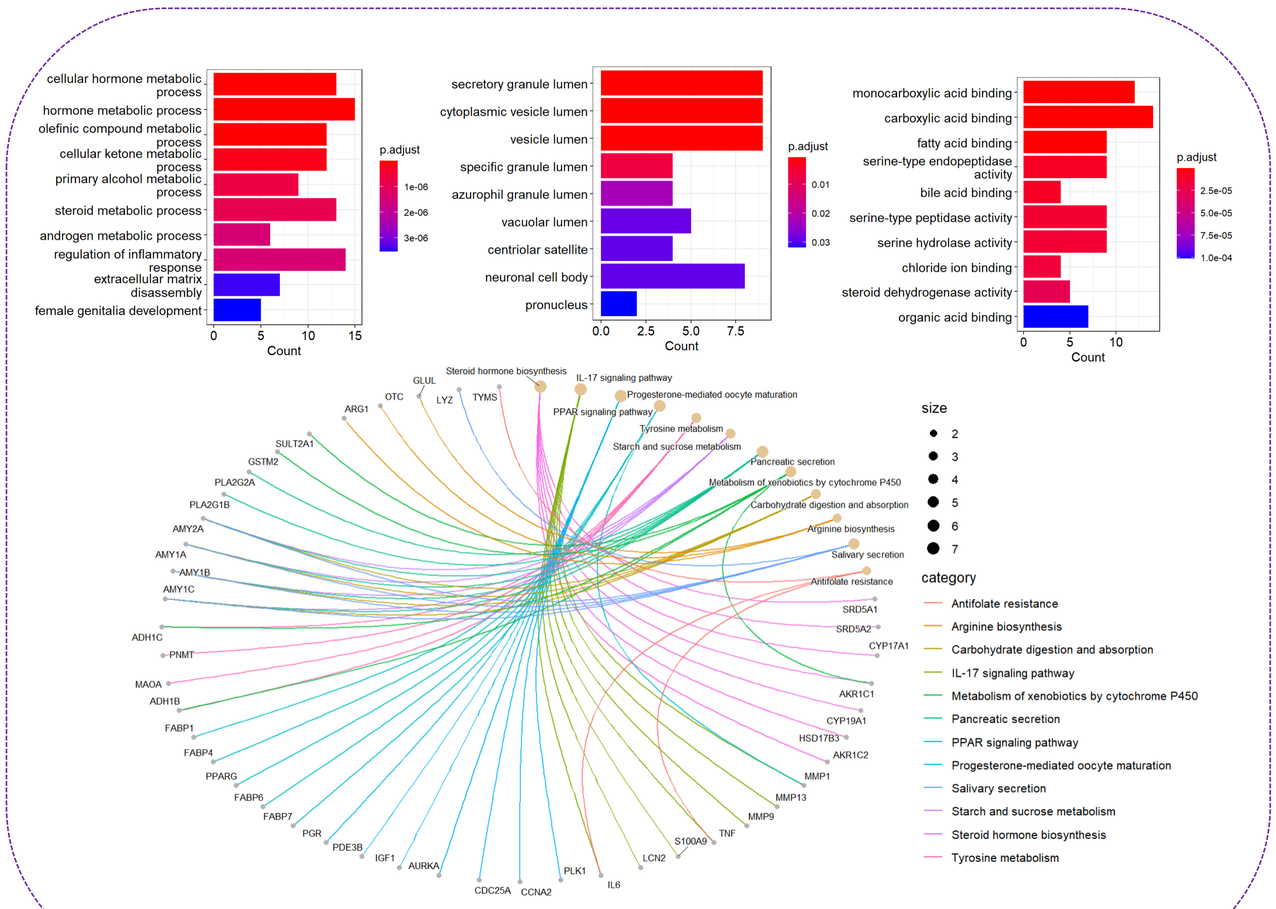

Fig.2 GO and KEGG enrichment analysis

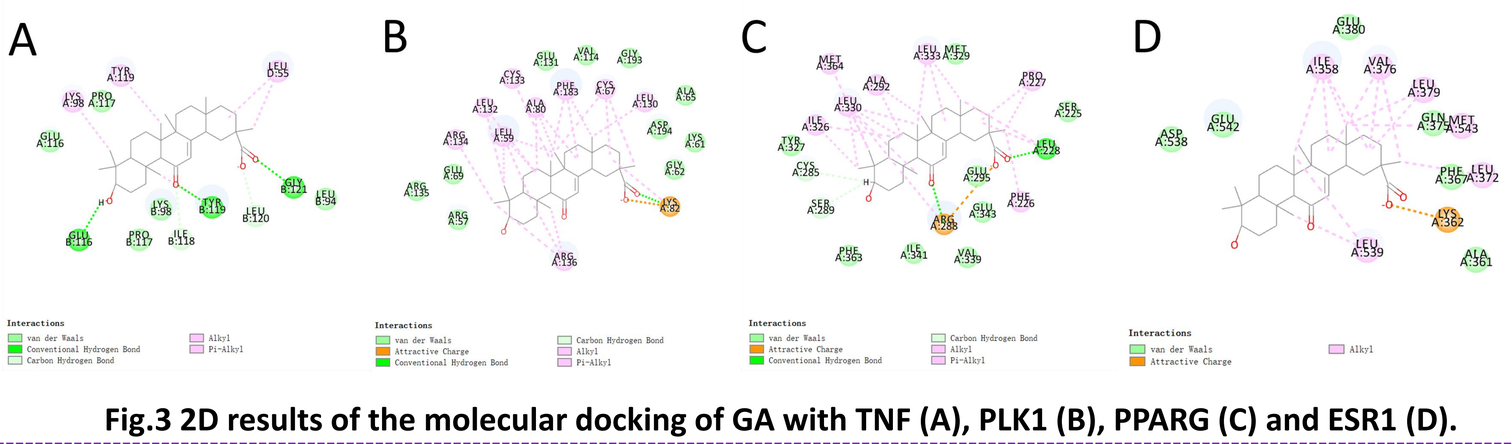

Fig.3 2D results of the molecular docking of GA with TNF (A), PLK1 (B), PPARG (C) and ESR1 (D).

Conclusion:

Through the enrichment analysis of common genes, the possible related pathways of GA inhibiting triple-negative breast cancer are IL-17 signaling pathway, PPAR signaling pathway, arginine biosynthesis, tyrosine metabolism, cytochrome P450 metabolism of exogenous substances and other pathways. Moreover, through the molecular docking study of the core targets, it was found that GA anti-triple negative breast cancer may focus on the 4 targets of TNF, PLK1, PPARG and ESR1 .

References:

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2. Zhang Y., et al. *Antrodia cinnamomea exerts an anti-hepatoma effect by targeting PI3K/AKT-mediated cell cycle progression in vitro and in vivo*. Acta Pharm Sin B. 2022;**12**(2):890-906.