Docking Prediction for Six Phenoic Compounds Inhibiting TNF-α and NF-κB Pathway

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ABSTRACT

In this article, we select 6 frequently used polyphenols with strong efficacy from anti-inflammatory herbal medicines: curcumin、EGCG (epigallocatechin -3- gal -late) 、sinapyl alcohol、syringin, triptolide and luteolin to perform docking study. First part addresses on extracellular links to TNF-α. We dock TNF – α with curcumin、 EGCG、 sinapyl alcohol、 syringing、triptolide and luteolin by Autodock 4， respectly. We discover that triptolide and curcumin have stronger effect and better stability on inhibiting TNF-α in these six polyphenols. There are three combinectives of compounds on inhibiting TNF-α: (1). Curcumin、EGCG 、 sinapyl alcohol and luteolin. (2). Curcumin、 sinapyl alcohol 、 syringin and luteolin. (3). EGCG、 syringing、triptolide and luteolin. In the second part, we discuss luteolin inhibits NF-κB pathway in intracellular.We use luteolin as ligand， NF-κB pathway in intracellular as macromolecular to perform docking prediction with Autodock 4. We discoverd that luteolin can strongly inhibit TRAF2 and TNFR1; dock with RIP1 to block the signal passing of RIP1; strongly dock with C-terminal of IKKβ to inhibit IKKβ、 IKKα and IKKγ from forming trimer. In other words， luteolin can be an inhibitor for TNF-α on extracellular and NF-κB pathway in intracellular.

Keywords : Curcumin、EGCG、syringin、sinapyl alcohol、Triptolide、Luteolin、NF-κB pathway

Table of Contents

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