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Opinion Article

Neuro-Protection Drug Target Identification Using Pharmacokinetics and Molecular Docking

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DESCRIPTION

Matrix metallo proteinases and inflammatory cytokines are among the proteins that contribute to the elucidation of the lipopolysaccharide induction and subsequent anti-inflammatory cascades. Computer-aided drug design strategies have been promoted for high throughput screening and interaction pathway analyses corresponding pharmacological targets as a result of the development of systems pharmacology techniques. Additionally, lipopolysaccharide induction, microglial activation, and differential modulation of the neuro-inflammatory protective signal cascade pathways, ranging from the NF-B pathway to the PI3K/Akt pathway, are all ascribed to neuro protection mediated by natural products. In order to envision the safety and efficacy of low molecular weight medicinal molecules for broad spectrum bioactivity, high-throughput virtual screening methods with a specific focus on traditional Chinese medicine and other relevant therapies were used. Through simulated testing for pharmacokinetics and pharmacodynamics, it has recently been demonstrated that the prominent application characteristics of tangeretin are effective against the Zika fever and Corona viruses. However, network pharmacology and docking by themselves were unable to confirm the (Absorption, Distribution, Metabolism and Elimination) ADME characteristics and blood brain permeability of important phenolic compounds. The scenario of tangeretin's chemi informatics and systems biology's neuro protection and anti-inflammatory characteristics necessitates avoiding the difficulties so that commercial applications are made simple. The difficulties for confirming tangeretin's efficacy, safety, drug likelihood, assimilatory patterns, and pursuit of possible gene/protein targets were preceded based on the restrictions to solve them. Thus, the current analysis includes molecular docking with target proteins for non-steroidal anti-inflammatory drugs, pharmacokinetic analysis for drug safety profiles, and comparative mining for potential gene targets for tangeretin.

Scientists all across the world appreciate ADME prediction studies because they help with drug discovery by demonstrating cost-effectiveness and minimizing *in vivo* experiments. Through chemi informatics and molecular research, similar studies evaluating the therapeutic potentials of tangeretin against COVID-19 and the Zika virus were demonstrated. Numerous researches demonstrate the anti-inflammatory properties of tangeretin, although there is no conclusive evidence of its effects on microglial activation, the blood-brain barrier, or neuro protection through lipopolysaccharide induction. Immuno informatics analysis of the proteins and signaling pathways involved in neuro protection led to the hypothesis that immunization against neuro degeneration proteins like TRAF6 and SQSTM1 might have beneficial effects. Citrus tangeretin's specific ADME profiles were demonstrated by research using enzyme kinetics, spectroscopic analysis, and dynamics simulation. These investigations also demonstrated a precise structure-activity relationship and efficient inhibition against pancreatic lipase. An *in silico* analysis of tangeretin for the prevention of hepatocellular carcinoma revealed the participation of Cox-2 enzymes, demonstrating the hepato protective efficacy comparable to the pharmacokinetic findings from the current investigation. 3BV7 (5-Beta-reductase), AKT1, and C1PYA1 are possible targets for tangeretin that are shown in the assessment to have anti-inflammatory capabilities against neurodegenerative disorders. After this level ahead, tangeretin research has a long history of excellence in biomedical applications, including medicinal and nutraceutical potentials. However, the commercialization, patent situation, and large-scale randomized controlled trials will drastically reduce tangeretin's future applications. However, analysis of the relationship between tangeretin and 5-Beta-reductase in the presence of AKT1 points to a similar mechanism for anti-inflammatory neuro protection. Assimilatory levels and bioavailability of the small molecule are positively impacted by additional hepato-protectivity for tangeretin, which also reduces mitochondrial toxicity with matrix metalloproteinases-9.

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