Pharmacophore Modelling Analysis of Burdock Root Extract and Vanillin Derivatives as Anti-Inflammatory Remedy

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ABSTRACT Pharmacophore modelling is an important aspect towards modern medicinal chemistry in drug discoveries and computer aided drug design to ease the understanding between the receptor-ligand interactions. Burdock (*Arctium lappa*), a well-known Traditional Chinese Medicine used in various natural therapeutics was chosen due to its anti-inflammatory characteristics of its constituent (arctiin and arctigenin) which meant to inhibit the metabolism of xanthine oxidoreductase. In this study, virtual screening comparison of burdock root constituent and vanillin derivatives were done *via* structure-based and ligand-based pharmacophore modelling towards the inhibition of xanthine oxidoreductase using Ligand Scout 4.1 software. From pharmacophore modelling analysis burdock root constituents (arctiin and actigenin) are the best anti-inflammatory compared to vanillin derivatives and clinical applied remedy.

KEYWORDS: Structure Based Drug Design, Ligand Based Drug Design, Gout, Burdock Root and Vanillin Derivatives.

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INTRODUCTION

Pharmacophore is defined as 3D arrangement of chemical groups common to active molecules and essential for their biological activities. Pharmacophore modelling is an important tool in drug discovery and in modern medicinal chemistry which was introduced by Ehrlich in 1909 to ease the understanding between the receptor-ligand interactions (Yang, 2010). Structure-based pharmacophore modelling is a strategy in the presences of a target macromolecule to observe the interaction of proposed drug with the active site. Ligand-based drug pharmacophore modelling is a strategy to discover potential drug by generating a pharmacophore model using drug that are being used to treat a diseases or infection without the involvement of a macromolecule.

Gout has become more ordinary among elderly people at a point of their lives due to the longer life expectation and change in diet. Gout is an inflammatory joint disease caused by tiny grit-like crystal in the joint due to high level of uric acid in blood which leads to swelling and pain (gout attack) (Kenny, 2014). Xanthine oxidase is the major enzyme in production of uric acid and also reported to produce superoxide radical and hydrogen peroxide which leads to oxidative stress, inflammation, cancer, aging and many more (Cos *et al.*, 1998). The following chemical reactions are catalysed by xanthine oxidase towards formation of uric acid (Birkett *et al.*, 1997).

$$\text{Hypoxanthine} + H_2O + O_2 \longleftrightarrow \text{Xanthine} + H_2O_2$$
$$\text{Xanthine} + H_2O + O_2 \longleftrightarrow \text{Uric Acid} + H_2O_2$$

Inhibition of this enzyme leads to the reduction of uric acid and prevent gout attacks (Pacher *et al.*, 2006). Allopurinol, febuxostat and other xanthine oxidase inhibitors are consumed, however side effects are tangible and cannot ingest along with other medication such as medication for heart attacks and etc.