Antioxidant properties of 5 herbal plants based of pharmacophore modeling

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ABSTRACT

Malaysian medicinal plants are known to exert therapeutic effects. We have evaluated some species namely *Moringa oleifera, Clinacanthus nutans, Rhodomyrtus tomentosa, Arctium lappa* and *Sonneratia alba* for their antioxidant properties assisted by using pharmacophore modeling approach. We displayed five major compounds from each plant namely: 3-caffeoylquinic, benzylglucosinolate, kaempferol, leucodelphinidin and quercetin (*Moringa oleifera*), adenosine, arctigenin, arctiin, kaempferol, and solasonine (*Arctium lappa*), 2-cis-entadamine A, phaeophytin, clinamides B, isovetaxin, and vitexin (*Clinancathus nutans*), 5-hydroxymethylfurfural, alphitolic acid, betulin, mtheyl gallate, oleanolic acid (*Sonneratia alba*) and lupeol, rhodomyrtosone A, rhodomyrtosone B, rhodomyrtosone C and rhodomyrtosone D (*Rhodomyrtus tomentosa*).

Keywords: Pharmacophore Modeling, antioxidant properties, *Moringa oleifera, Clinacanthus nutans, Rhodomyrtus tomentosa, Arctium lappa, Sonneratia alba,* ligand-based pharmacophore.

1. INTRODUCTION

Antioxidant refers to compound which is able to scavenge, cease formation or counteracting the damaging action of oxidants on cells [1]. They act as reducing agent, hydrogen donor, singlet oxygen quencher and metal chelator. Naturally, our body produces free radicals in small amount for particular functions such as modulation of inflammation, killing pathogens, detoxifying toxins and producing signaling molecules [2,3]. Even though the generation of these free radicals is kept in check by defense and repairs system, the uncontrolled generation of free radical species particularly of oxygen species and decreased in antioxidant protection within cells cause oxidative stress to healthy body cells [4]. Excess free radicals participate in various chemical reactions subsequently produce more reactive species of oxygen, nitrogen and sulphur which is linked to many chronic diseases like cancers, cardiovascular diseases, neurological disorder, auto-immune deficiency diseases and degenerative disorders associated with aging [5].

Considering the extensive damages arise from oxidative stress on human health, it is uncommon that antioxidant is one of the interest compound in the study of plant medicinal value as it provides protection against various oxidative stress-related diseases. In plants, polyphenols such as flavonoids, phenolic acids, stilbenes, coumarins, lignin and lignins are the interest compounds that possess free radical scavenging activity [6]. In this study antioxidant properties are identified based on pharmacophore modeling; the focus is on five plants from South Asia namely *Moringa oleifera, Clinacanthus nutans, Rhodomyrtus tomentosa, Arctium lappa* and *Sonneratia alba*.

These plants have been well known for centuries as alternative medicine to cure various diseases. Among the prominent uses of *C. nutans* are as cure for various types of cancers and skin inflamation, *M. olifera* and *R. tomentosa* as anti-diabetic [7,8]. Meanwhile, *A. lappa* has been studied for is anti-inflammatory which can prevent or treat gout attack and *S. alba* as anti-diabetic [9]. The five major compounds found in each plant are as follow respectively: 3-caffeoylquinic, benzylglucosinolate, kaempferol, leucodelphinidin and quercetin (*M .oleifera*), adenosine, arctigenin, arctiin, kaempferol, and solasonine (*A. lappa*), 2-cis-entadamine, phaeophytin, clinamides B, isovetaxin, and vitexin (*C. nutans*), 5-hydroxymethylfurfural, alphitolic acid, betulin, methyl gallate, oleanolic acid (*S. alba*) and lupeol, rhodomyrtosone A, rhodomyrtosone B, rhodomyrtosone C and rhodomyrtosone D (*R. tomentosa*).

Pharmacophore modeling method simulates the search of potential and promising drugs candidates by virtual screening. Pharmacophore modelling provides useful structural and chemical information for future development of more potent molecules [10]. Ligand-based pharmacophore model plays a major role in searching drugs and treatment of certain diseases. Pharmacophore modelling has been applied in combination with other molecular modelling technique [11].