OMICS International
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Clin Pharmacol Biopharm 2015, 4:4
http://dx.doi.org/10.4172/2167-065X.C1.014

Pharma Middle East

November 02-04, 2015 Dubai, UAE

Anatomical investigation of aerial vegetative organs of *Piper amalago* L. (Jaborandi-manso) for the quality control

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Piper amalago L. is popularly known in Brazil by the terms Jaborandi-manso, Jaborandi-falso and Jaborandi-nhandi which is a shrub that measures 2-7 m in length and is found in a region that stretches from Central America to Rio Grande do Sul in the south of Brazil. Pharmacological studies have demonstrated anti-inflammatory, antimicrobial, cicatrizing, and antileishmanial properties. Additionally, it has been suggested that it has antioxidant properties since it contains vitexin and lupeol which have been isolated through phytochemical analysis.The objective of this study was to analyze its leaf and stem by optical and scanning electron microtechniques so that information could be obtained to identify the species. The leaf and stem morpho-anatomy of *Piper amalago* were similar to other Piper species. The features observed should be evaluated as a representative of the entire species, even though several structures can be highlighted as distinguishable among the species of the genus. The main characteristics include a hypostomatic leaf, a sub-epidermal layer on the surfaces, sac-like glandular trichomes, conical non-glandular trichomes, dorsi-ventral mesophyll, a plano-convex midrib with a single collateral vascular bundle, short petiole with irregularly shaped and adaxially grooved. At the caulinar level that was analyzed,the shape is circular and there are collateral vascular bundles arranged in two rings (the outer one in the vascular cylinder and the inner one in the pith). In the perimedular region, a sinuous sclerenchymatic sheath is apparent. These morphological and anatomical features observed for *Piper amalago* enable this taxon to be identified and differentiated from other species of this plant grouping.

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Design, docking, synthesis and *in vitro* binding studies of few benzamide derivatives with glucokinase enzyme

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Glucokinase (GK) enzyme is involved in glucose utilization in liver and has also been implemented in Glucose-dependant release of insulin in the pancreatic β-cell. Activation of glucokinase enzyme therefore, has emerged as a strategy to increase glucose utilization. The world-wide endeavours to design compounds (GKA: Glucokinase activators) that would activate the glucokinase enzyme so as to develop suitable drugs to treat Type 2 diabetes, has culminated in library of numerous compounds; benzamide derivatives have been at mainstay amongst them. The ligand-protein interaction involves ARG63 as the anchoring residue, and many more residues as TYR210, TYR215, etc. which are submerged in a cleft between two domains. Albeit, binding of the ligands with amidine backbone of ARG63 and the hydrogen-bond interactions of the free amino group on ligands with TYR215 is believed to be involved in activation of the enzyme, the free amino group had been noticed to elicit mutagenic effects. Present work describes the design, docking of benzamide derivatives that bind with ARG63, much the way similar to the standard GKA, RO-28-1675, and interact with other set of amino acid residues in much similar way, however, without the presence of free amino group. Molecular modeling studies involved, Molecular Design Suite (VLife MDS 3.5), simulated protein 1V4S, virtual structures of standard and newly designed benzamide derivatives. The structures were docked in the catalytic site of 1V4S to obtain respective docking score (in KJ/mol) and the amino acid residue involved in each interaction. Based on the study, few molecules were selected for synthesis and other molecules were outright rejected. The criteria for such selection, scheme of reactions to synthesize selected molecules, results of their *in vitro* binding with glucokinase enzyme are presented. The obtained results do not promise to yield better GKA than the standard compound. However, the molecules could further be subjected to rational changes in structure and re-subject to *in silico* studies so as to yield molecules to activate GK.

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