

Systematic review and chemoinformatics analysis of anti-allergic medicinal plants used in Malawi

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Abstract

In Malawi, ethnobotanical surveys have been carried out on the plants used to treat or manage allergies and their symptoms. However, studies focusing on information analysis such as systematic reviews of anti-allergic plants and natural products are not yet published. This review highlighted and analysed data of potential anti-allergic medicinal plants used in Malawi in order to discover potential treatments for allergies through various approaches and improve well-being of people. Literature search strategy was used to collect data of medicinal plants. Chemoinformatics analysis was applied to compile associated natural products and to profile the physicochemical properties (drug-likeness and fingerprint diversity) with references to 60 antihistamine 1 drugs (H1R drugs) and 277 anti-H1 receptor inhibitors. Sixty (60) medicinal plants from 36 families out of 645 reported plant species had information of diseases or symptoms of allergies. The Malawian Natural Products (MNP) data set composed of 1757 unique compounds was compiled for the first time from 39 of 60 medicinal plants and approximately 48.9 % and 45.3 % of the compounds did not violate Lipinski and Veber drug-like rules respectively. Chemical space mapping revealed that compounds from Malawian medicinal plants are structurally diverse and share a small space with antihistamine compounds and drugs. This information is useful in exploring other anti-allergy biological mechanisms for natural products. Similarity screening identified usambarine (CID442121), which is structurally similar to 2,8- Dimethyl-5-(2-pyrazine-2-ylethyl)-gamma-carboline (CHEMBL1783970) and 29 other antihistamine compounds. The results will be used as a baseline for further studies which may eventually lead to the discovery of potential allergy treatments through various approaches. This could improve health and well-being of people which is in line with goal number 3 of Sustainable Development Goals, Africa's Union's Agenda 2063 and National Research Agenda for the Malawi 2063.

Keywords: Allergy, Antihistamine compounds, Chemoinformatics, Medicinal plants, Phytochemicals