

Poster Session II

Carissa spinarum L.: a study using ethnomedicine-guided systems pharmacology in identifying a mechanism of action of a medicinal plant

C Smyth*, J Liu, S Yuan, I Obaidi, H Sheridan

> Author Affiliations

> Further Information

Congress Abstract

Full Text

References

Figures

> References

The literature of Pokot ethnomedicine (Kenya) shows that several species used by the Pokot are widely used throughout Kenya [1]. One of these species, *Carissa spinarum* L. (CS) (Apocynaceae), was selected for further ethnomedical [2] and phytochemical investigation. The use of the inhaled root in chest congestion led to the analysis of steam distillate of CS root, finding a major metabolite, 2'-hydroxyacetophenone (2-HAP), with little known bioactivity [3]. This study aims to investigate the mechanism of action (MOA) of 2-HAP relative to traditional usage of root volatile using systems pharmacology (SP). General SP analysis found 2-HAP to be a druggable molecule with predicted overlaps with ethnomedical use of volatilised root in respiratory, central nervous system and inflammatory conditions. As a folk treatment of respiratory disease, further research is required to elucidate its MOAs and explore its therapeutic potential for treating lung inflammatory disorders. Literature and SP studies revealed core targets for molecular docking analysis. Good results for PTGS2, IL18, NOS3, ACE2, PTGS1, CCNA2 and ALB were confirmed by molecular computational analyses indicating a potential MOA of 2-HAP in pulmonary inflammatory and immune responses. This study confirmed the therapeutic effect of CS, a tree widely used in African and Asian countries to treat different diseases. The potential mechanisms of 2-HAP were revealed by network pharmacology and molecular computational analyses. Our results offer a different perspective using modern pharmacological mechanisms which may assist in the global fight against the COVID-19 pandemic. Further cell and animal models are necessary to verify the relevant pathways and targets.

