UNIVERSITY OF LAGOS
FACULTY OF PHARMACY
3RD SCIENTIFIC CONFERENCE

INVESTIGATION OF SECONDARY METABOLITES PRESENT IN ALKALOIDAL EXTRACTS OF *HUNTERIA UMBELLATA* LEAVES USING COMPUTATIONAL MOLECULAR NETWORKING TOOL

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Background

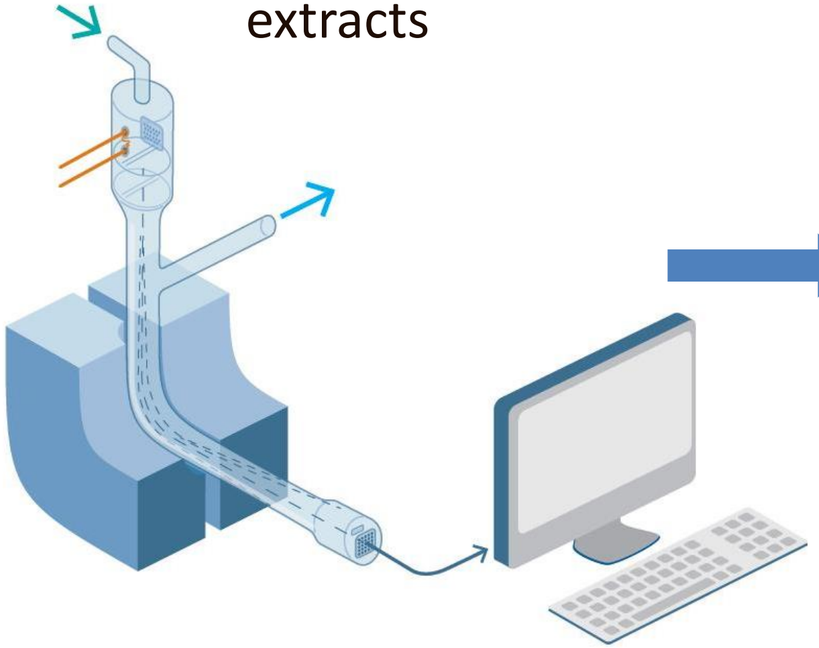
- *Hunteria umbellata* K. Schum, a tropical rainforest tree found in western and central Africa.
- African traditional herbalists use various portions of the plant for a wide variety of medicinal purposes.
- The aim of this study was to investigate the secondary metabolites present in the leave extract of the plant using metabolomics tools and a computational molecular networking platform.

Picture from www.gbif.org

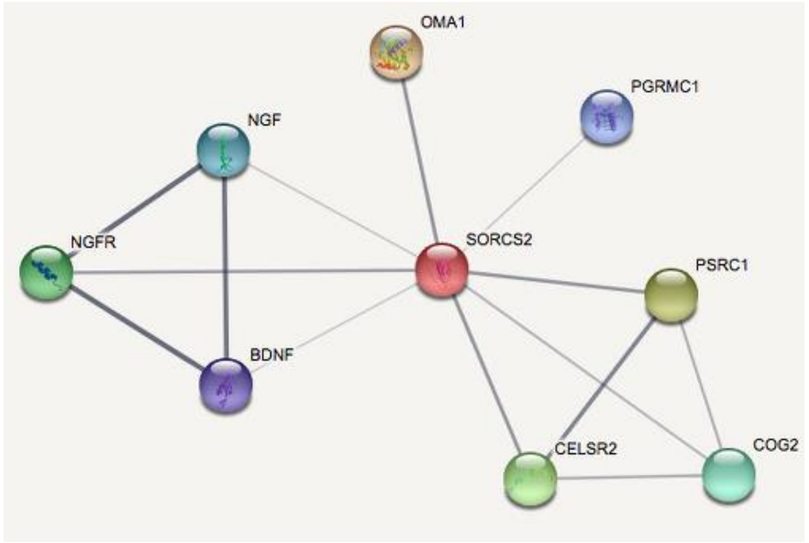
Methodology

Alkaloids extraction using Manske Method

LC-MS/MS Analysis of extracts



Molecular Networking for Compounds Identification



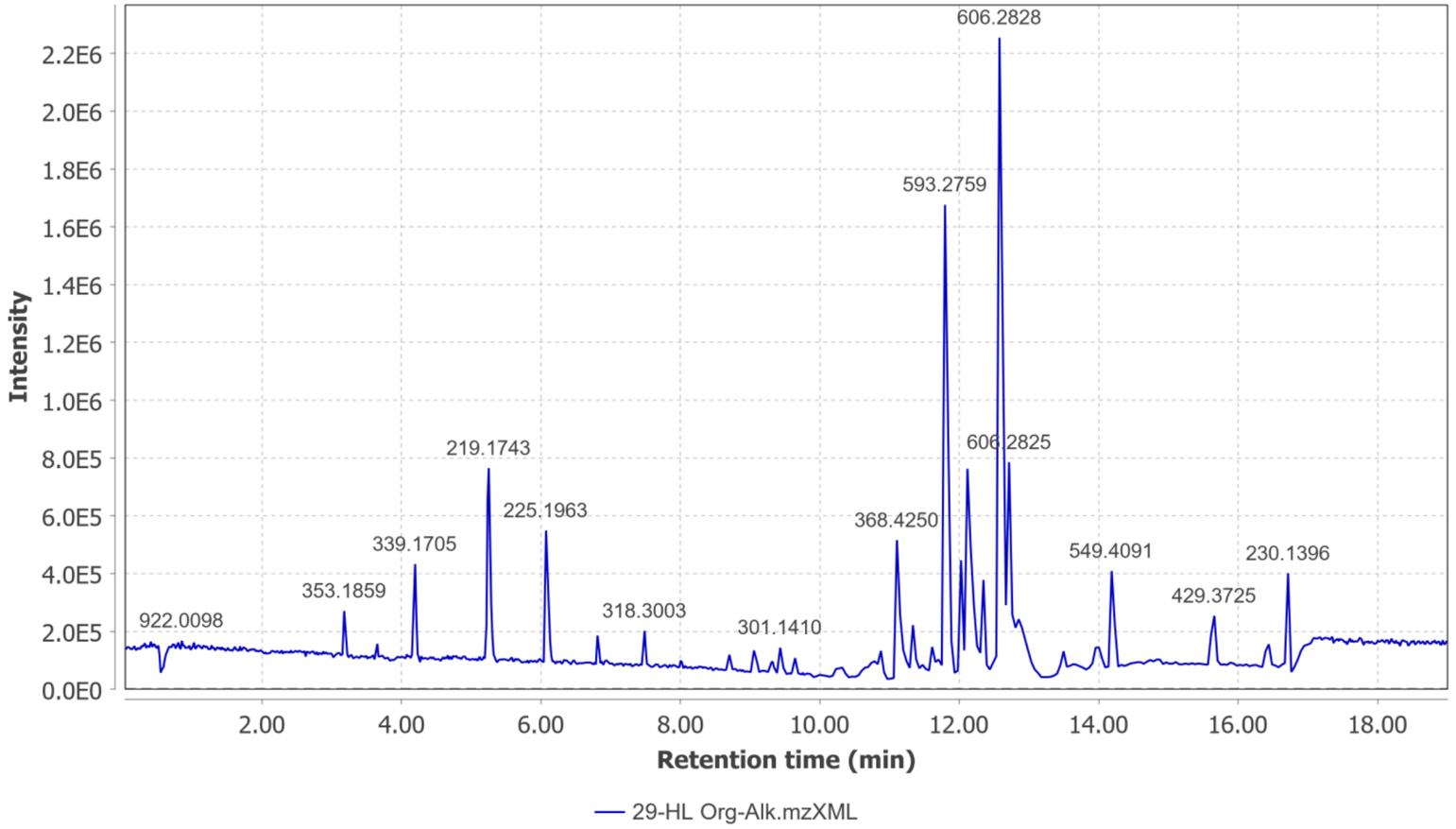
Global Natural Product Social Molecular Networking (GNPS)

Results

- Several alkaloids were isolated as shown in the chromatogram
- 3 unique compounds identified:
  - Picrinine

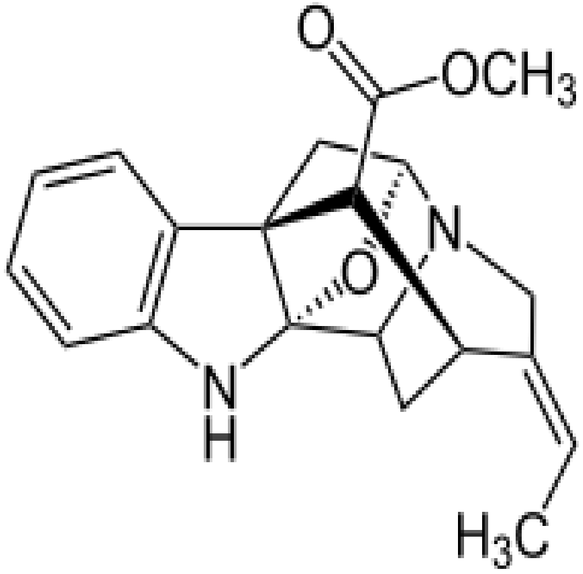
    IUPAC: Methyl 14-ethylidene-18-oxa-2,12-diazahexacyclo[9.6.1.19,15.01,9.03,8.012,17]nonadeca-3,5,7-triene-19-carboxylate
  - (3beta,5xi,9xi,13alpha,17alpha,18xi)-3-Hydroxy-13,28-epoxyurs-11-en-28-one
  - Pheophorbide A

    IUPAC: (3S,4S)-9-Ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoic acid

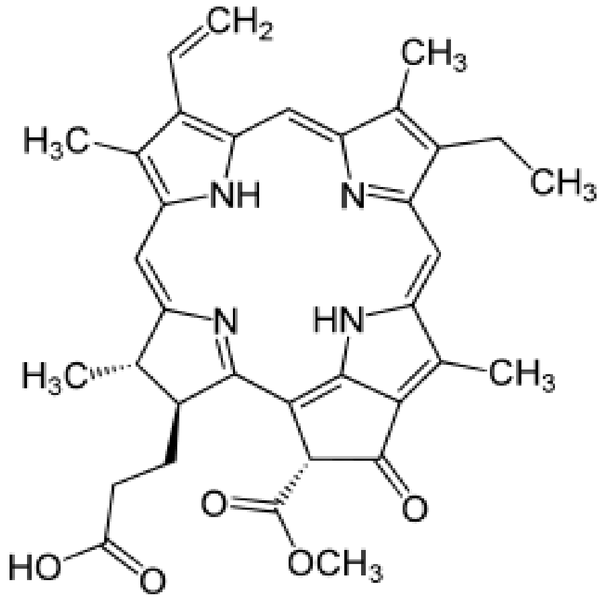


Chromatogram showing the spectrum peaks of the isolated compounds in the alkaloidal extract

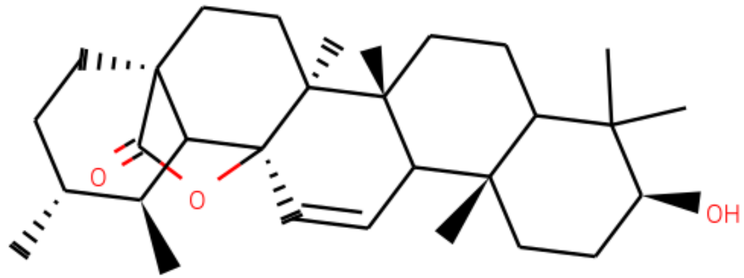
Results



Picrinine



Pheophorbide A



(3beta,5xi,9xi,13alpha,17alpha,18xi)-3-Hydroxy-13,28-epoxyurs-11-en-28-one

Conclusion

Hunteria umbellata demonstrates significant pharmacological potential, highlighted by the rich presence of secondary metabolites in its leaves. Several identified compounds have been associated with therapeutic activities in pharmacological studies. The discovery of both known and novel compounds emphasizes the need for further research in drug development and natural product chemistry.

References

1.Fox Ramos, A.E., Pavesi, C., Litaudon, M., Dumontet, V., Poupon, E., Champy, P., Genta-Jouve, G. and Beniddir, M.A., 2019. CANPA: computer-assisted natural products anticipation. Analytical chemistry, 91(17), pp.11247-11252.

2.Stafford, G. I., Jäger, A. K., & Van Staden, J., 2009. African psychoactive plants. African Natural Plant Products: New Discoveries and Challenges in Chemistry and Quality, 323, 346.

3.Wang, M., Carver, J.J., Phelan, V.V., Sanchez, L.M., Garg, N., Peng, Y., Nguyen, D.D., Watrous, J., Kapono, C.A., Luzzatto-Knaan, T. and Porto, C., 2016. Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. Nature biotechnology, 34(8), pp.828-837.