

FASEB Journal logo

HomeCurrent IssueEarly OnlineArchiveAbout

Pharmacology and Experimental Therapeutics

Gas chromatography-mass spectrometry identification of anticancer phytochemicals in *Aframomum danielli* (LB579)

Solomon Rotimi, Tolulope Bisi-Adeniyi, Isaacson Adelani, Oluwatobi Adegbite

Published Online:1 Apr 2014Abstract Number:LB579

Abstract

Aframomum danielli is one of the African spices used in folklore medicine for the management of several diseases. This study identified the phytochemical components present in the n-hexane seed extract of the *A. danielli* by gas chromatography-mass spectrometry (GC-MS) analysis and also evaluated the anti-cancer potential of the identified phytochemicals by performing molecular docking against human Vascular Endothelial Growth Factor (VEGF) using Molegro Virtual Docker. The GC-MS analysis identified the presence of phytochemical components caryophyllene (RT: 18.479), humulene (RT: 19.189), 2-butanone (RT: 22.976), benzenesulfonamide (RT: 31.651) and 2-pyridine acetic acid (RT: 32.446). 2-Butanone was the strongest binding ligand (-65.744 kcal/mol) while caryophyllene was the weakest binding ligand (-56.311 kcal/mol). These compounds showed relative strong docking to VEGF with docking energies comparable to an anticancer drug, bevacizumab (-77.883 kcal/mol). This *in silico* molecular docking study has shown that these phytochemical components could be responsible for anti-cancer properties of *A. danielli*.

Vol. 28, No. 1_supplement

April 2014

Metrics

Publication History

Published online 1 April 2014

FASEB

9650 Rockville Pike

Bethesda, MD 20814

301-634-7000

Information

For Authors

Meeting Abstracts

FASEB Publication Services

Terms & Conditions

© 2018 by the Federation of American Societies for Experimental Biology