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

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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 bind lingand (-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.

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