Mod Chem Appl 2017, 5:3(Suppl)
DOI: 10.4172/2329-6798-C1-006

5th Global Chemistry Congress

Chemical constituents from the rhizomes of Curcuma zedoaria and assessment of their biological activities The influence of preparation methods on halloysite nanotubes supported Ni catalysts for hydrogenation of benzene

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Phytochemical investigation of C. zedoaria resulted in the isolation of 21 compounds. Isolated compounds includes eighteen sesquiterpenes and three labdane diterpenes. Various chromatographic techniques were used for the detection and isolation of the compounds. Extensive spectroscopic methods including NMR, IR, UV, GC-MS, LC-MS were used for the identification of the isolated compounds. Isolated compounds were subjected to cytotoxicity, anti-oxidant and neuroprotective assays. Curcumenol and dehydrocurdione showed the highest protection (100%) against hydrogen peroxide induced oxidative stress in NG108-15 cells at the concentrations of 4 and 8 μM, respectively. In the oxygen radical antioxidant capacity assay, zerumbone epoxide showed the highest antioxidant activity with a Trolox equivalent (TE) of 35.41 μM per 100 μg of sample. In the MTT based cytotoxicity assay against four cancer cell lines (Ca 41 Ski, MCF-7, PC-3 and HT-29), curcumenone and curcumenol displayed strong antiproliferative activity (IC50 8.3 and 9.3μg/ml, respectively). A quantum chemical study was performed to investigate their relationship with cytotoxic activity and revealed that the dipole moment (μ), molecular volume (V), molecular area (A), polarizability (α) and hydrophobicity (log P) are the most important descriptors that influence the cytotoxic activity of the compounds under investigation. The two most active compounds; curcumenol and curcumenone were investigated for their binding to human serum albumin (HSA). The spectroflurometric analysis, in conjunction with molecular docking study suggested that both curcumenol and curcumenone could bind to binding sites I and II of HSA with intermediate affinity while site I was the preferred binding site for both molecules.

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