Quercetin-induced apoptosis in HepG2 cells and identification of quercetin derivatives as potent inhibitors for Caspase-3 through computational methods

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Abstract

Quercetin is a bioflavonoid which possesses immune-enhancing activity, anti-inflammatory, antioxidant properties and considered effective against various cancers. In the present study, quercetin has been extracted from *Ocimum basilicum* and was used to evaluate its anticancer activity against human liver cancer cell lines (HepG2) by assessing cell viability (MTT) and variations in nuclear morphology (AO/EtBr dual staining) during apoptosis. Since Caspase-3 enables the activation of cascade which is responsible for apoptosis, their effects were also investigated using computational approaches like molecular docking, molecular dynamics, covalent docking, ADME prediction, DFT approaches, and pharmacophore modeling besides identifying the binding affinity, stability, drug likeliness properties of top-ranked compounds. Amount of quercetin extracted from *O. basilicum* leaves was found to be 0.82 mg with the retention time of