Abstract

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## In vitro study of the effects of dihydropyrano coumarins isolated from Ferulago macrocarpa on DNA by spectroscopic and molecular modeling methods

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Background and objectives: Coumarins have potential anticancer effects. Ferulago macrocarpa (Fenzl) Boiss, is a perennial herb which has shown to have several dihydropyranocoumarins like grandivittin (GRA) and dihydrofuranocoumarins such as prantschimgin (PRA). Previously the antibacterial, cytotoxic and antioxidant effect of GRA and PRA have been reported. Understanding that how GRA and PRA bind to ct- DNA, can show the mechanism of antibacterial, cytotoxic effects. Methods: F. macrocarpa fruits were collected and dried. Acetone extract of the plant was prepared and defatted. Several coumarins were purified using normal column and high performance liquid chromatographic methods. The structures were determined with NMR analysis. The electrochemical behavior of GRA and PRA was studied by cyclic voltammetry, fluorescence, UV-Vis, FT-IR spectroscopy and molecular modeling methods. Results: The cathodic peaks I and II may corresponded to the reduction of the alkene groups at the electrode surface, respectively. The peak III may be resulted from the opening and oxidation of the furan ring moiety. The complex stability constant, binding site size, diffusion coefficients of free and bounded of GRA-DNA and PRA-DNA complex were obtained by CV, DP and UV-Vis at 25 °C. Conclusion: The binding of GRA and PRA with ct-DNA caused significance changes in electrochemical and spectral characteristics of GRA and PRA and confirming that the interaction mode of GRA and PRA with ct-DNA is major groove with binding site size of 1.

**Keywords:** DNA binding, *Ferulago macrocarpa* (Fenzl) Boiss, grandivittin, major groove, prantschimgin

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