Study on the Interaction of 4'-Hydroxychalcones and their Mannich Derivatives with Calf Thymus DNA by TLC and Spectroscopic Methods, a DNA Cleavage Study

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Abstract:
Background:
Phenolic Mannich bases derived from hydroxychalcones show remarkable cytotoxic potencies towards cancer cell lines. However, the exact mechanism of action is still partially unclear.

Objective:
Interaction of two hydroxychalcones and their Mannich derivatives with calf thymus DNA (ctDNA) has been investigated.

Methods:
Thin-layer chromatography and UV-Vis spectroscopic method were used for studying the interaction. The binding constant has been determined by UV-Vis spectrophotometric titration. The DNA cleavage activity of the compounds was studied by agarose gel electrophoresis.

Results:
Interaction of the compounds with ctDNA exhibited relatively high intrinsic binding constant (4-5×10⁴ M⁻¹). The results indicate existence of weak, non-covalent interactions between the investigated derivatives with ctDNA. Some compounds showed a slight DNA cleavage activity with pBR322.

Conclusion:
The obtained results provide additional knowledge on the previously documented cytotoxicity against tumor cell lines of the hydroxychalcones and their Mannich-derivatives.

Keywords: Chalcones, Hydroxychalcones, Mannich bases, DNA binding, UV-Vis spectroscopy, DNA cleavage.

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SUPPLEMENTARY TABLE AND FIGURE
Fig. (1S). IR-FT spectrum of compound 1A.

Fig. (2S). $^1$H NMR (500 MHz, DMSO-d$_6$) spectrum of compound 1A.
Fig. (3S). Expanded $^1$H NMR (500 MHz, DMSO-d$_6$) spectrum from 6.7 ppm to 8.2 ppm of compound 1A.

Fig. (4S). $^{13}$C NMR spectrum (126 MHz, DMSO-d$_6$) of compound 1A.
Fig. (5S). IR-FT spectrum of compound 1B.

Fig. (6S). $^1$H NMR (500 MHz, DMSO-d$_6$) spectrum of compound 1B.
Fig. (7S). Expanded $^1$H NMR (500 MHz, DMSO-d$_6$) spectrum from 6.7 ppm to 8.7 ppm of compound 1B.

Fig. (8S). $^{13}$C NMR spectrum (126 MHz, DMSO-d$_6$) of compound 1B.
Fig. (9S). HRMS spectrum of compound 1B.