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Supplementary Material



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 ($4-5 \times 10^4 \text{ M}^{-1}$). 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.

Article History

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SUPPLEMENTARY TABLE AND FIGURE

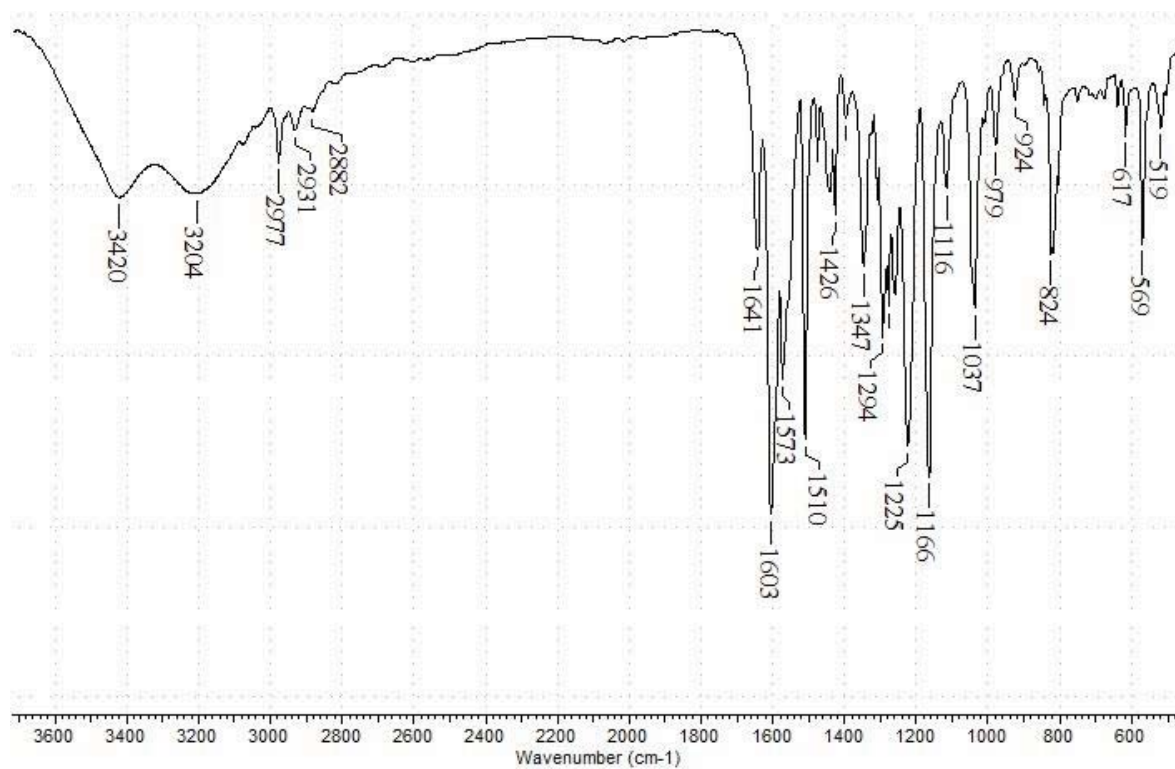
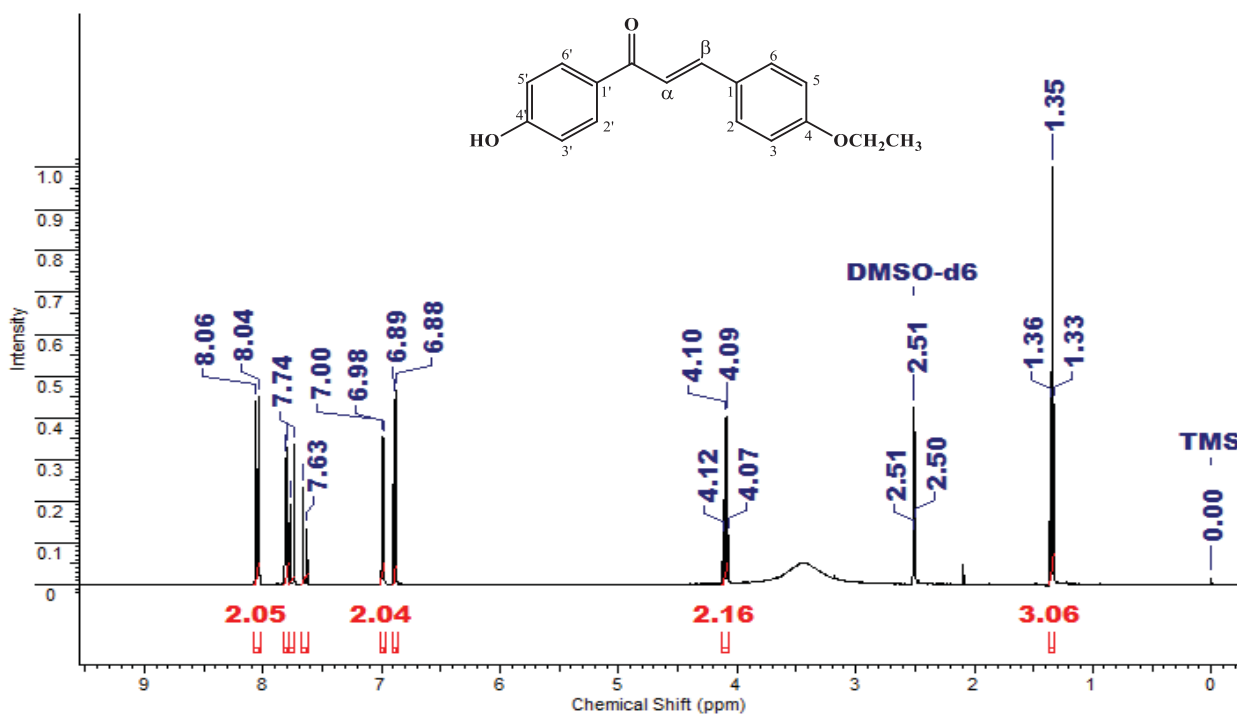


Fig. (1S). IR-FT spectrum of compound 1A.

Fig. (2S). ^1H NMR (500 MHz, DMSO-d_6) spectrum of compound 1A.

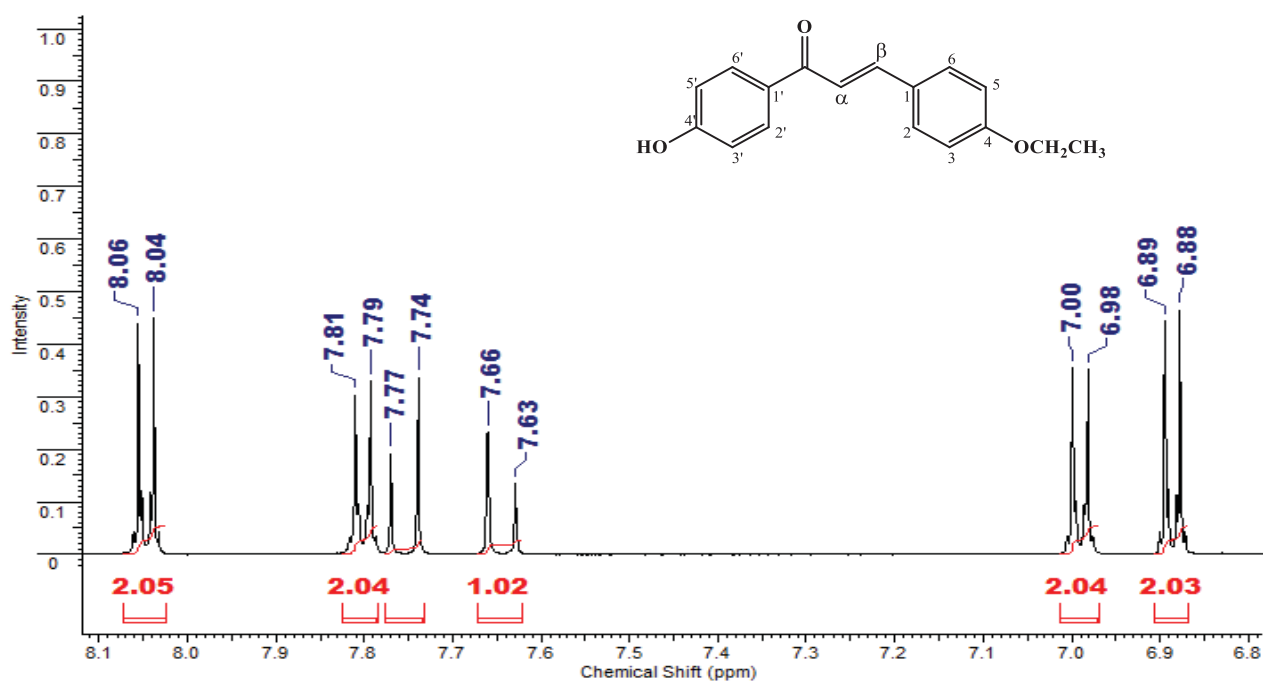


Fig. (3S). Expanded ^1H NMR (500 MHz, DMSO-d_6) spectrum from 6,7 ppm to 8,2 ppm of compound 1A.

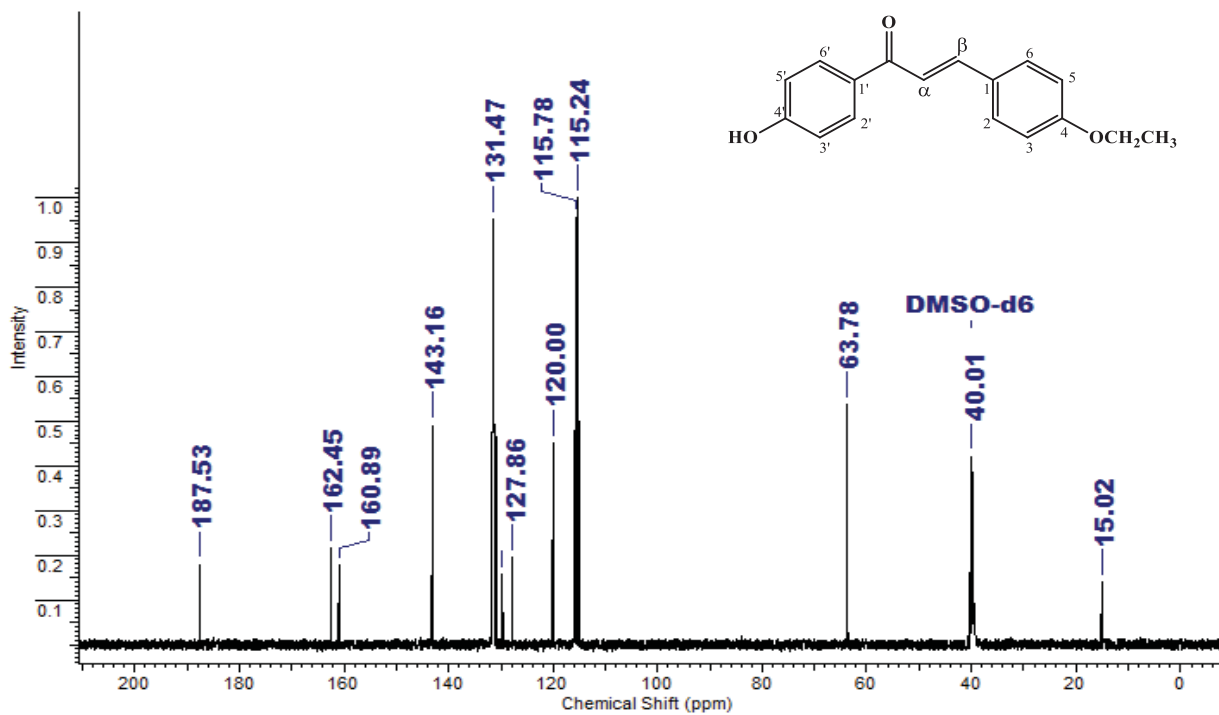


Fig. (4S). ^{13}C NMR spectrum (126 MHz, DMSO-d_6) of compound 1A.

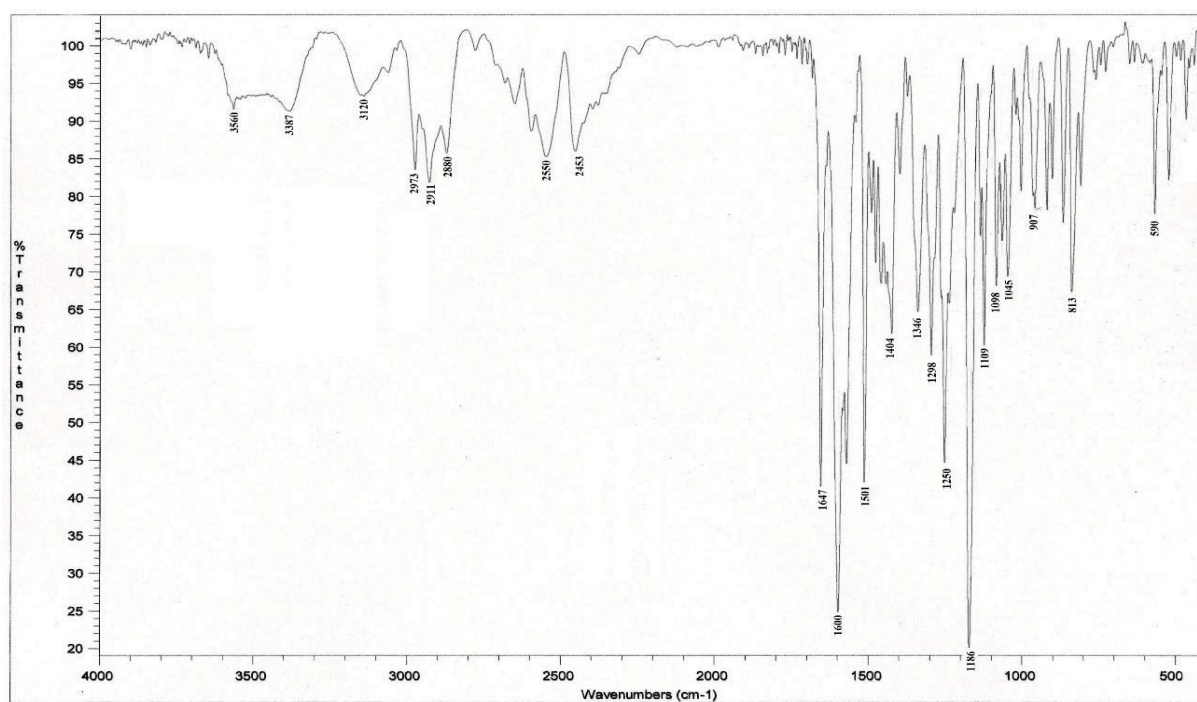
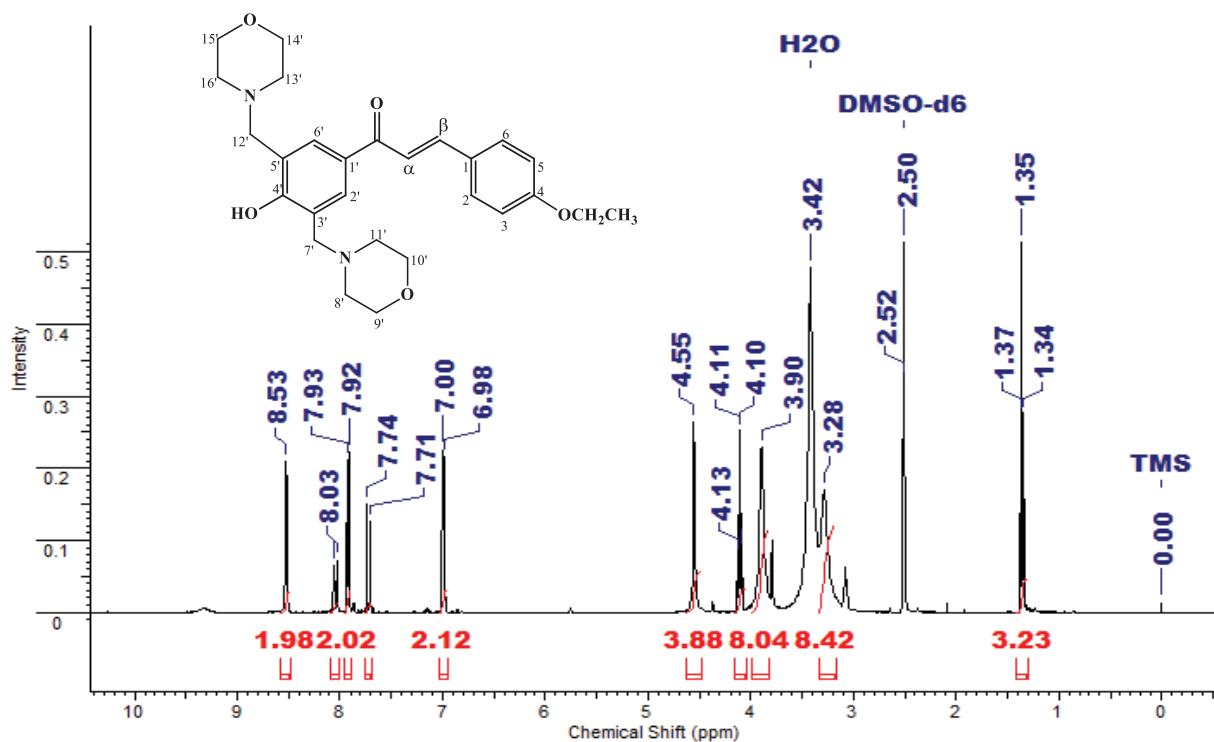


Fig. (5S). IR-FT spectrum of compound 1B.

Fig. (6S). ¹H NMR (500 MHz, DMSO-d₆) spectrum of compound 1B.

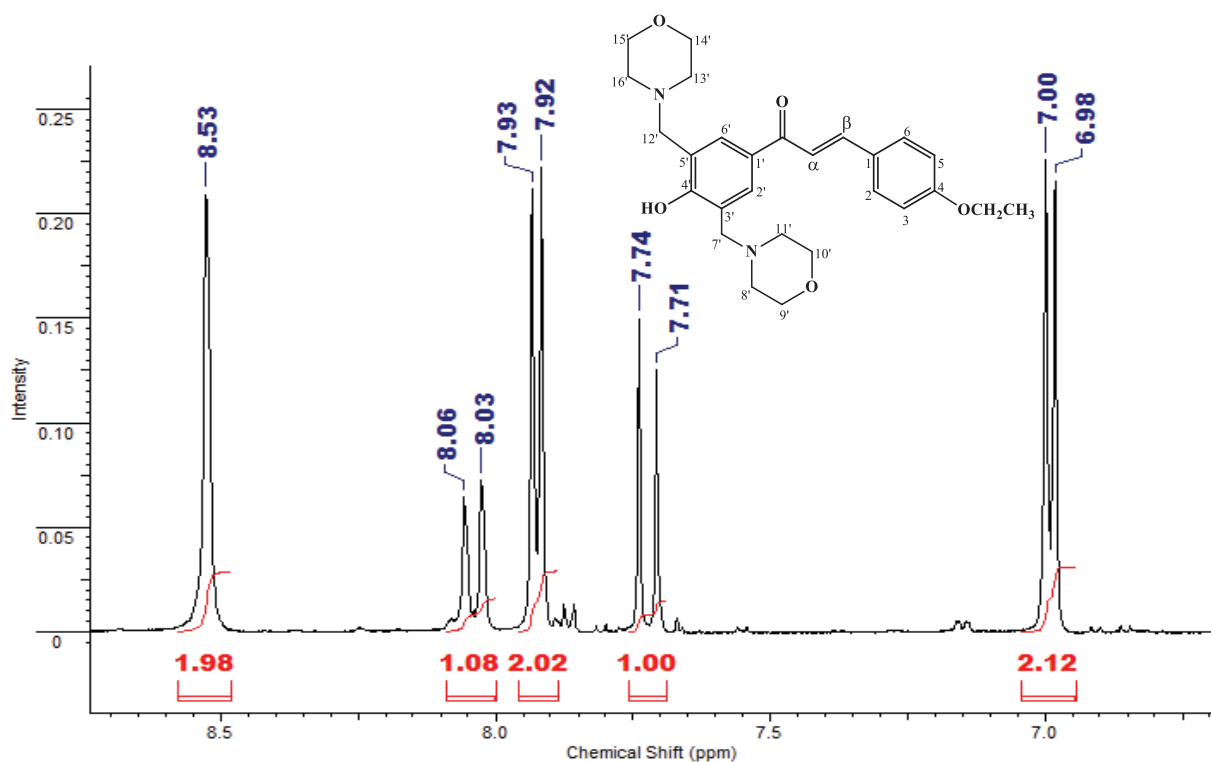


Fig. (7S). Expanded ¹H NMR (500 MHz, DMSO-d₆) spectrum from 6,7 ppm to 8,7 ppm of compound 1B.

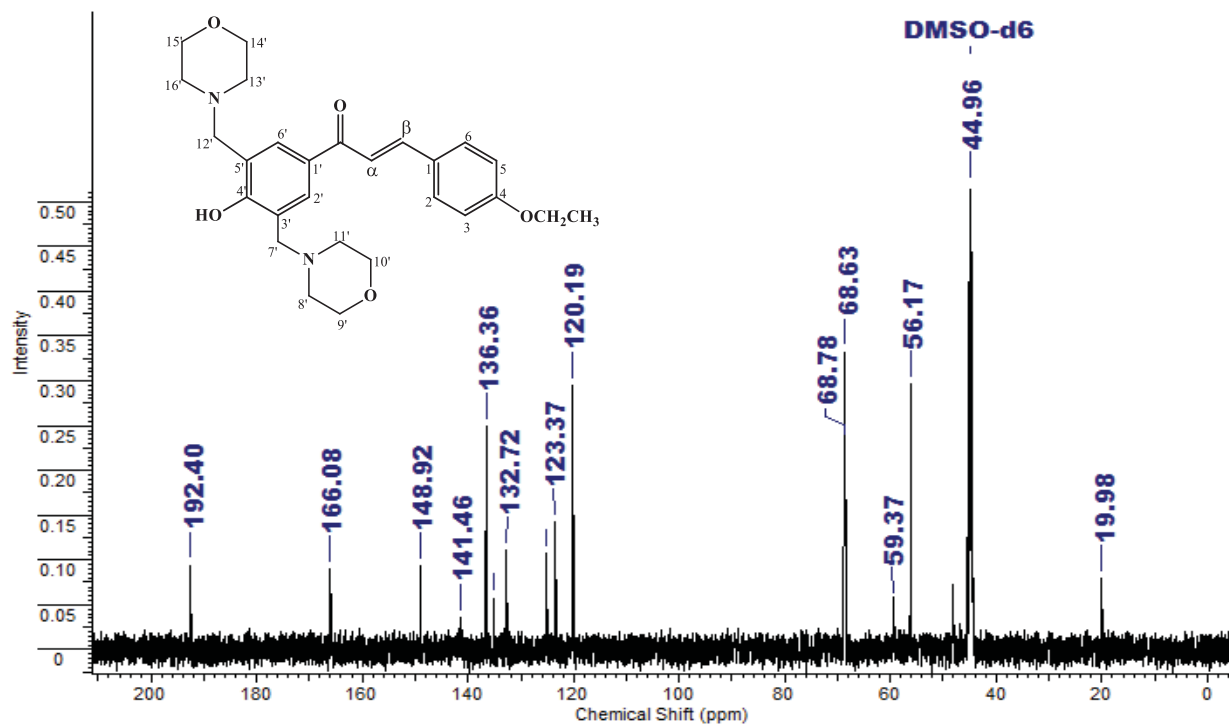
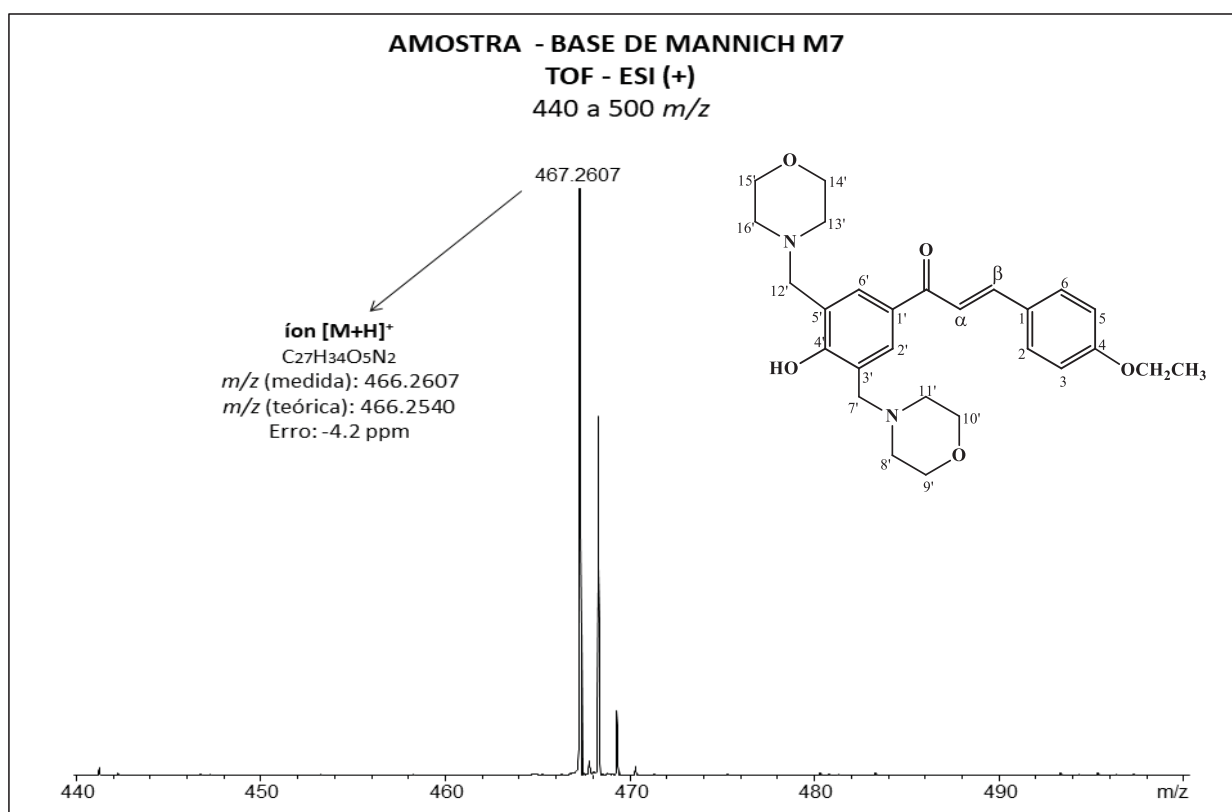


Fig. (8S). ¹³C NMR spectrum (126 MHz, DMSO-d₆) of compound 1B.

**Fig. (9S).** HRMS spectrum of compound **1B**.