A STUDY OF H-BOND IN A GROUP OF NSAID HYDROXAMIC ACID DERIVATIVES BY FTIR AND NMR SPECTROSCOPY

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INTRODUCTION

The investigation of drug properties, e.g., chemical structure, physical-chemical properties, the possibility of H-bonding and drug molecular geometry, is necessary in pharmacological study, medicinal, drug biotransformation pathways and selection of investigational bases as well as in deciphering physiological and pharmacological processes.

The growing interest is in the characterization of the H-bonding function in a large group of NSAIDs, which are in the focus of intensive research. The H-bonding ability of such compounds is important due to their possible use as drug candidates.

RESULTS AND DISCUSSION

Material and Methods

The investigated compounds were synthesized from NSAID and were isolated by sublimation techniques, and the subsequently reduced of intermediates with H-bonding interactions. The following sections are devoted to the FTIR and NMR spectroscopy techniques.

FTIR spectroscopy

FTIR-ATR spectra were recorded on a Perkin Elmer Spectrum 100 spectrophotometer. The absorbance was measured at 4000–400 cm⁻¹ wave numbers, with a resolution of 2 cm⁻¹.

NMR spectroscopy

The compounds were investigated by 1D-1H and 13C NMR spectroscopy, using HMBC, HSQC, and NOESY methods. The spectra were recorded on a Bruker AMX 400 spectrometer. The chemical shifts are referred to SiMe₃ as an internal standard.

Table 6: 1H and 13C NMR chemical shifts (ppm) of synthesized NSAID hydroxamic acids and their intermediates

Table 7: NOESY interactions in HMBC of synthesized NSAID hydroxamic acids and their intermediates

Table 8: HSQC interactions in HMBC of synthesized NSAID hydroxamic acids and their intermediates

Table 9: MBC interactions in HMBC of synthesized NSAID hydroxamic acids and their intermediates

Table 10: MBC of synthesized NSAID hydroxamic acids and their intermediates

Table 11: MS of synthesized NSAID hydroxamic acids and their intermediates

Table 12: NMR spectra of synthesized NSAID hydroxamic acids and their intermediates

Table 13: Chemical shifts (δ) and H-N coupling constants (J) of synthesized NSAID hydroxamic acids and their intermediates

CONCLUSIONS

The structure of synthesized NSAID hydroxamic acids and their intermediates were determined by means of FTIR (Table 1) and 1H- and 13C NMR spectroscopy (Tables 2 to 7).

The H-bonding was observed in FTIR spectra of all investigated compounds.

Although there is a possibility of H-bonding, detailed study of FTIR spectra and 1H- and 13C NMR spectra of all investigated compounds was done.

The results of this study of structural behavior of NSAID hydroxamic acids and their intermediates are interesting as potential drug candidates.