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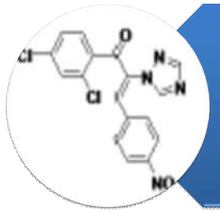
IDENTIFICATION OF NITROTRIAZONE BY NUCLEAR MAGNETIC RESONANCE 1H, 13C

Drumea Maria, Catedra de Chimie farmaceutică și toxicologică, USMF „Nicolae Testemițanu”
Macaev Fliur, Laboratorul Sinteză organică, Institutul de chimie MEC
Valica Vladimir, Catedra de Chimie farmaceutică și toxicologică, USMF „Nicolae Testemițanu”

Introduction

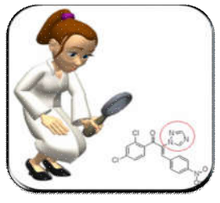


Nuclear magnetic resonance (NMR) is a high-performance instrumental analytical method that allows elucidation and confirmation of the steric structure of organic compounds. NMR is based on measuring the absorption of electromagnetic radiation by the method: ^{1}H NMR, ^{13}C NMR.

Keywords

Nitrotriazone, ^{1}H NMR, ^{13}C NMR, DMSO (*Dimethylsulfoxide*).

Purpose



- Identification and confirmation of the steric structure of Nitrotriazone by the method of nuclear magnetic resonance with the ^{1}H proton and ^{13}C carbon technique.

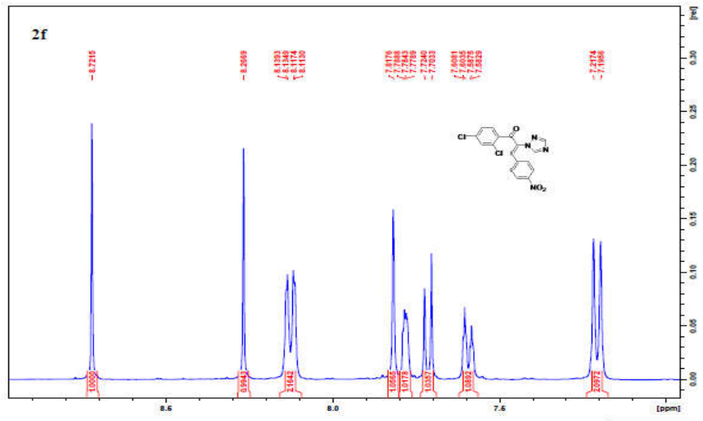
Material and methods

^{1}H and ^{13}C NMR spectra were recorded for 2% d6-DMSO solutions using a “Bruker-Avance III” (400.13 and 100.61 MHz). The chemical changes δ were expressed in ppm, referring to the center of the signal, using the solvent peaks as reference: d6-DMSO 2.50 ppm.

The assumption and confirmation of the molecular skeleton is carried out with the help of the NMR spectra that gather the resonance signals resulting from the interaction of the nuclear spin of the analyzed atom in a magnetic field with an electromagnetic radiation with long wavelength (hertzian waves) and low energy.

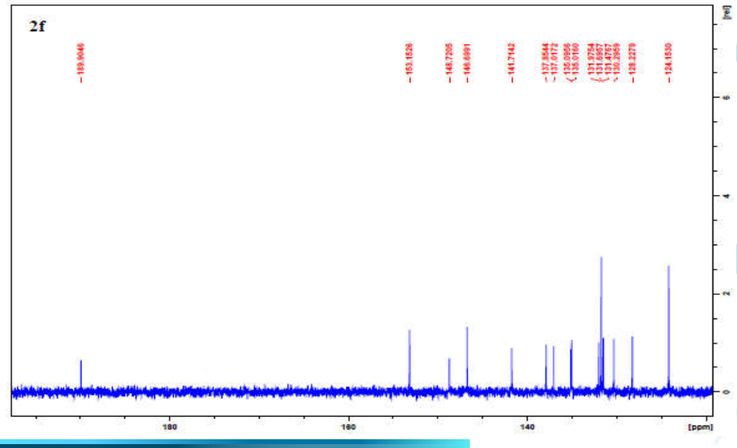
Results

1H RMN (DMSO-d6, 400 MHz): 8,72 (1H, s), 8,27 (1H, s), 8,13 (1H, d, d, J = 8,9, 1,9, Hz), 7,82 (1H, s), 7,78 (1H, td, J = 3,9, 1,6 Hz), 7,71 (2H, d, J = 8,3Hz), 7,59 (1H, dt, J = 8,3, 1,9 Hz), 7,21 (2H, d, J = 8,9 Hz) . RMN 13C (DMSO-d6, 100 MHz): 189,9, 153,2, 148,7, 146,7, 141,7, 137,9, 137,0, 135,1, 135,0, 132,0, 131,7, 131,5, 130,3, 128,2, 124,2. Anal. Calculated for C17H10Cl2N4O3, C 52,52, H 2,64%. Finder C 52,46, H 2,59%.



In the ^{1}H NMR spectrum of Nitrotriazon the chemical shifts have values in the range of 8.7-7.1 ppm. The signals at 8.72 and 8.27 ppm belong to the protons of the 1,2,4-triazole group. The bands at 8.13; 7.78; 7.71; 7.59 and 7.21 ppm are decomposed into peaks called doublets.

The doublet at 8.13 and 7.21 ppm is attributed to four protons in the p-nitrophenyl substituent. Vinyl strips and aromatic ring are in the region of 7.82-7.59 ppm. In the ^{13}C NMR spectrum, signals at 189.9 ppm belong to the C = O group; 153.2 and 146.7 ppm are attributed to the triazole ring. The peak at 148.7 ppm belongs to the carbon in the nitro group in the aromatic ring.



Conclusions

The ^{1}H proton and ^{13}C carbon spectra of Nitrotriazone were investigated, highlighting absorption bands, which distinguish Nitrotriazone from other substances and allow their use to identify and confirm the steric structure.