

Pharmacy Section

Application of the NMR Spectroscopy in the Structural Analysis of Clonidine

Alexandru Lisnic, Vasile Palii

Academic adviser: Tamara Cotelea, M.D., Alic Barba, M.D.

State Medical and Pharmaceutical University "Nicolae Testemitanu", Chisinau, Republic of Moldova

NMR spectroscopy is one of the most powerful techniques available for studying the structure of molecules. It involves the absorption of radio waves by the nuclei of some combined atoms (^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P) in a molecule that is located in a magnetic field. Nuclear magnetic resonance spectroscopy is the use of the NMR phenomenon to study physical, chemical, and biological properties of matter. The most important applications are proton NMR and carbon-13 NMR spectroscopy. In principle, NMR is applicable to any nucleus possessing spin. This property of nuclei to have a spin, was used to establish the structure of clonidine using ^1H and ^{13}C spectrum. Clonidine-N-(2,6-dichlorophenyl)-4,5-dihydro-1H-imidazol-2-amine- treats high blood pressure by stimulating α_2 receptors in the brain, which decreases cardiac output and peripheral vascular resistance, lowering blood pressure. It has specificity towards the presynaptic α_2 receptors in the vasomotor center in the brainstem. This binding decreases presynaptic calcium levels, and inhibits the release of norepinephrine (NE). The net effect is a decrease in sympathetic tone. Was determined : • the number of carbon atoms using ^{13}C spectrum(DMSO), and their shift's, ppm : 158.5(C7), 134.5(C8), 129.7(C9), 131.5(C10), 129.7(C11), 130.5(C12). • the number of hydrogen atoms using ^1H spectrum(DMSO), and their shift's, ppm : 7.58(H9), 7.46(H10), 7.58(H11), 10.72(H6), 8.51(H1), 43.2(2H4d, 2H5d). The obtained spectrum gave us the possibility to establish the spatial structure of the analyzed sample. The impact of NMR spectroscopy on the natural sciences has been substantial. It can, among other things, be used to study mixtures of analytes, to understand dynamic effects such as change in temperature and reaction mechanisms, and is an invaluable tool in understanding protein and nucleic acid structure and function. It can be applied to a wide variety of samples, both in the solution and the solid state.

Application of Physical-Chemical Methods in Chemical-Toxicological Analysis of Pyroxicam

Vasile Palii, Alexandru Lisnic

Academic adviser: Tamara Cotelea, M.D.

State Medical and Pharmaceutical University "Nicolae Testemitanu", Chisinau, Republic of Moldova

Pyroxicam (4 hydroxy-2 methyl-N-2 pyridinil-2H-1,2 benzotiazin-3 carboxamide-1,1 dioxide) is used in medicine to treat the rheumatoid polyarthritis, ankylopoetic spondilitis, gout attack, periartthritis, traumatic pains. It concerns to the group of drugs with antiinflammatory features, analgesic. The action mechanism can be explained by the synthesis inhibition of prostaglandines and the inhibition of the synthesis of cyclooxygenase and the migration of leucocytes to the inflammatory focus inhibiting the phagocytosis and releasing of lysosomal hydrolysis. In certain conditions (overdosage, hepatic diseases) pyroxicam possesses toxic features. In this context the study of pyroxicam is a specific interest in biological fluids. As a result we intended to study the factors (the pH