



پژوهش‌های شیمیایی ایران

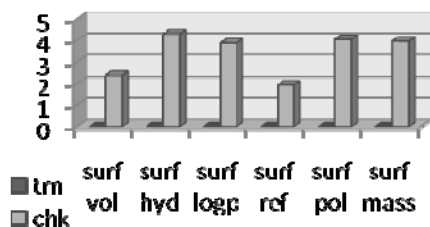


Figure 2. According to obtained results the mass and surface area has most important role on Kraft temperature.

Reference

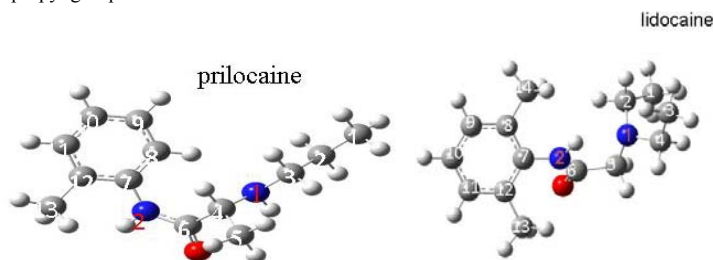
[1] Sateesh Krishna Chand Chandra thesis submitted to the department of chemistry Eastern Michigan University in Partial fulfillment of the requirements for degree of MASTER OF SCIENCE in chemistry.

Structure and conformation of lidocaine and Prilocaine. A DFT study

Mohammad Vakilia, Fatemeh Dolatia*, Sayyed Faramarz Tayyaria, Omid Rajabib, Roshanak Salarib

^aDepartment of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, IRAN, ^bDepartment of Medicinal Chemistry, School of Pharmacy, Mashhad University of Medical Sciences (MUMS), Mashhad 91775-1365, IRAN

Local anesthetics like lidocaine (N-(2,6-dimethylphenyl)-N2,N2-diethylglycinamide) and prilocaine ((RS) N-(2-methylphenyl)N-propylalaninamide) are amide local anesthetic and lidocaine is used topically to relieve itching, burning and pain from skin inflammations, injected as a dental anesthetic or as a local anesthetic for minor surgery. Prilocaine is applied in dentistry and is a sodium channel blocker. Their common forms are salts and insoluble in water which have less toxic effects. Mass spectrometric methods are most commonly used. Unfortunately, these methods are destructive and the sample is no longer available for re-analysis by other laboratories. IR and Raman spectroscopy provide alternatives for non-invasively analyzing drug crystals. Furthermore, these methods are accurate and highly sensitive for lower amounts of these materials [2]. The Raman and IR spectra of the titled compound are obtained and by using quantum chemistry calculations the frequencies are assigned to the normal modes [1]. The aim of this study is investigation on the structure, stable conformer, and vibrational spectroscopy in solid, CCl4 and CH3CN solutions of Prilocaine and lidocaine with using DFT calculations at B3LYP/6-31G** level of theory. 4 different stable conformers were obtained for Lidocaine and Prilocaine. The structures of the most stability of these conformers and atom numbering of the system are shown in Fig 1. The relative stabilities of the lidocaine conformers are in the range of 3.5-4.97 kcal/mol and those for prilocaine are in 3.5-5.1 kcal/mol range, with respect to the most stable conformer. Dihedral angle between Ph ring and N2C6 for prilocaine conformers is about 40-60° and more than those in lidocaine, so there is no resonance between them that it confirmed with calculated N-Ph bond length. The dihedral angles of O=C-CH-N1 in prilocaine and lidocaine are 77.25° and 154.37°, respectively. The difference is due to the presence of two ethyl groups bounded to N1 in Lidocaine while there is only one n-propyl group bounded to N1.



Reference

[1] Andrea C. Schmidt Pharmaceutical Research, Vol. 22, No. 12, December 2005.
 [2] Don Kimberley F. Schrum, Ph.D. Physical Sciences & Mathematics. volume 5 Issue 1, October 2001.

IR and Raman spectrophotometric studies on the effects of pH and temperature on structural stability of human serum albumin (HSA)

a Fatemeh Dolati, b Roshanak Salarib, Mohammad Vakilia, Sayyed Faramarz Tayyari, Omid Rajabib

^aDepartment of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, IRAN

^bDepartment of Medicinal Chemistry, School of Pharmacy, Mashhad University of Medical Sciences (MUMS), Mashhad 91775-1365, IRAN

Human serum albumin is the most abundant protein in human blood plasma. Albumin is a soluble, monomeric protein which comprises about one-half of the blood serum protein. Albumin is essential for maintaining the osmotic pressure needed for proper distribution of body fluids between intravascular compartments and body tissues. It also acts as a plasma carrier by non-specifically binding several hydrophobic steroid hormones and as a transport protein for heme and fatty acids (1). In this paper, we decided to determine the structural kinetic stability of human serum albumin by different factors such as pH and temperature (2). How these factors affected the protein stability, were shown by IR spectrums. In acidic or alkaline environment, the number and type of hydrogen bonds varied due to the