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PII: S1386-1425(18)30660-7
DOI: doi:10.1016/j.saa.2018.07.007
Reference: SAA 16276
To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date: 13 May 2018
Revised date: 4 July 2018
Accepted date: 5 July 2018

Please cite this article as: Y. Sheeba Sherlin, T. Vijayakumar, J. Binoy, S.D.D. Roy, V.S. Jayakumar , Büchi's model based analysis of local anesthetic action in procaine hydrochloride: Vibrational spectroscopic approach. Saa (2018), doi:10.1016/j.saa.2018.07.007

Büchi's Model based Analysis of Local Anesthetic Action in Procaine Hydrochloride: Vibrational Spectroscopic Approach

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Abstract

The drug action of ester type local anesthetic (LA) procaine hydrochloride (PRC HCl) is activated by blocking Na^+ ion flow when it binds to the ion channel in the ligand gated sodium ion channel protein. Buchi's model, explains binding action of ester type LA drug with receptor in terms of charge transfer, dipole-dipole, hydrogen bonding and van der Waals interactions through lipophilic, ester and hydrophilic moieties. The present work investigates molecular structural and vibrational spectral features of para amino benzoate group, ester part and tertiary amino group respectively belonging to lipophilic, ester and hydrophilic moieties, accountable for the binding of drug to sodium channel. The electron transport mechanism through the ring responsible for structural deviation from benzenoid to quinonoid form and consequent dipolar nature of carbonyl group have been investigated, based on the analysis of XRD, DFT computed molecular structure, 8a ring mode and NBO charges. The characteristic UV absorption peaks and vibrational marker bands of LA drugs have been identified and the charge transfer interaction responsible for lipophilic binding has been investigated. The blocking of Na^+ in the ion channel has been probed using attractive and repulsive energy profile. The molecular polarizability has been computed to substantiate the correlation between the structure activity relationship of LA drug molecule and molecular polarizability. The low toxicity of PRC HCl was evaluated using *in vitro* cytotoxicity study, confirming it as a potential short acting local anesthetic.

Keywords: FT-Raman, DFT, Büchi's model, Quinonoid structure, Local anesthetic spectral bands, Cytotoxicity.

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