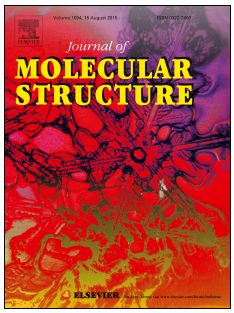
Accepted Manuscript



Synthesis and crystal structure of quinolinium salt: Assignment on nonsteroidal anti-inflammatory activity and DNA cleavage activity

Praveen Singh, Ranjeet Kumar, Ajeet K. Singh, Priyanka Yadav, Ranjana S. Khanna, Manjula Vinayak, Ashish Kumar Tewari

PII: S0022-2860(18)30269-2

DOI: 10.1016/j.molstruc.2018.02.115

Reference: MOLSTR 24937

To appear in: *Journal of Molecular Structure*

Received Date: 21 August 2017

Revised Date: 16 February 2018

Accepted Date: 28 February 2018

Please cite this article as: P. Singh, R. Kumar, A.K. Singh, P. Yadav, R.S. Khanna, M. Vinayak, A.K. Tewari, Synthesis and crystal structure of quinolinium salt: Assignment on nonsteroidal anti-inflammatory activity and DNA cleavage activity, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.02.115.

Synthesis and Crystal Structure of Quinolinium Salt: Assignment on Nonsteroidal Anti-inflammatory Activity and DNA Cleavage Activity

Praveen Singh[a], Ranjeet Kumar[a,c], Ajeet K. Singh[b], Priyanka Yadav[a], Ranjana S Khanna[a], Manjula Vinayak[b], Ashish Kumar Tewari[a*]

[a]Department of Chemistry (Centre of Advanced Studies), Institute of Science, Banaras Hindu University, Varanasi 221005, INDIA.

[b]Department of Zoology (Centre of Advanced Studies), Institute of Science, Banaras Hindu University, Varanasi 221005, India.

[c]Department of Chemistry, C.M.P. Degree college, Allahabad 211002, INDIA.
E*mail:* tashish2002@yahoo.com, ashishtewarichem@gmail.com.

Abstract: To develop new anti-inflammatory and DNA cleavage agent with improved pharmaceutical profile, five quilinium salt based compounds have been synthesized and x-ray characterization of these quinolinium salts have been reported here. These quinolinium salts have potential to show the better anti-inflammatory activity as well as DNA cleavage activity. The anti-inflammatory activities of quinolinium salts **1-5** have been evaluated by complete Freund's adjuvant (CFA) induced rat paw edema method. The DNA cleavage activities of quinolinium salts **1-5** were analyzed by using plasmid pBR322. The crystal structure of quinolium salt **1, 2** and **3** have shown the intermolecular non-covalent interactions such as cation$\cdots\pi$, $\pi\cdots\pi$, C-H$\cdots\pi$, C-H$\cdots$X (X= I and Br) and C-H$\cdots$N interactions.

Keyword: Quinolinium salts, Non-covalent interactions, Anti-inflammatory activity, DNA cleavage activity, Docking studies.

INTRODUCTION: The major biological action of nonsteroidal anti-inflammatory drugs (NSAIDs) is the inhibition of cyclooxygenase (COX) mediated production of pro-inflammatory prostaglandins and thromboxanes.[1] Further, inflammations may implicated in causing cancer therefore nonsteroidal anti-inflammatory drugs (NSAIDS) may be an important target for cancer prevention strategy.[2] At the beginning of the 1990s two COX isoforms were discovered: one (COX-1) constitutively present in many tissues such as stomach, kidney, and