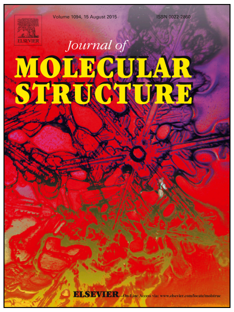

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Synthesis, NMR and computational studies on tautomerism of dichloroacetate of hydroxyanthraquinone

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Abstract: Three dichloroacetate derivatives of hydroxyanthraquinone were synthesized. NMR studies showed that only monoesterified derivative compound 1 had a tautomerization. Since monoetherified derivative of hydroxyanthraquinone did not show tautomerization, a hypothesis that nucleophilicity played an important role in the tautomerization was proposed. The molecular structures of monoesterified derivative compound 1 and diesterified derivative compound 2 were calculated by using DFT method, and the result showed that the electronic density of carbonyl at 9-position of compound 1 was much larger than that of compound 2, which indicated that the hypothesis mentioned above was reasonable.

Keyword: Tautomerism, hydroxyanthraquinone, NMR, computation, nucleophilicity

1. Introduction

Anthraquinone ring is an important privileged structure of anticancer drugs [1]. Anthraquinone ring can intercalate double helix structures of DNA of cancer cells due to its planar structure, which inhibits the duplication of DNA and leads death of cancer cells [2,3]. Anthraquinone ring also can transfer electrons to O_2 (see scheme 1) to generate ROS (reactive oxidative species) which can kill cancer cells selectively [4,5]. The existence of hydroxyl can strengthen the privileged structure of anthraquinone ring because it can stabilize the