Effects of Force Fields on the Equilibrium State of 5,7-Dihydroxy-4-MethylCoumarin Comparative Study of Molecular and Langevin Dynamic Simulations

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Abstract

We have studied the influence of the two force fields Amber and MM+ in both gas and solution environments. Molecular Dynamic (MD) and Langevin Dynamic (LD) simulations of the 5,7-dihydroxy-4-methylcoumarin were performed with the an efficient program. The geometries, interaction energies, bonds, angles, stretch-bends, electrostatic and the Van der Waals (VDW) interactions were carried out in solution and gas phases. The results show that MD and LD simulations are identical. This comparative study shows that the coumarin acquires the low-energy and has the dipolar characteristic under the MM+ field by using the both methods. This molecule reaches its high stable conformation state in solution environment. So, under MM+ field, the simulation gives best results.

Keywords: AMBER, MM+, molecular dynamics (MD), langevin dynamics (LD), coumarin

1. Introduction

Coumarins are an important class of heterocyclic organic compounds (Borges et al., 2005). They have attracted great interest due to their importance in synthetic organic chemistry, and to their possession of diverse pharmacological properties (Hoult & Payá, 1996). Coumarins consist of a carbon-carbon double bond which is fixed as *trans* conformation as in *trans*-stilbene through a lactone structure. From the molecular structure result a strong fluorescence and photostability in most of coumarin derivatives.

In the late of 1950, Wheelock has shown that substitutions on the coumarin structure shifted the fluorescence band. For example, adding a methyl group to the 4-position of 7-hydroxy- or 7-methoxycoumarin moves the fluorescence spectra. Addition of electron-repelling groups in the 4-, 6-, or 7-position or electron-attracting groups in the 3-position shifts the fluorescence band to longer wavelengths.

As consequence, 4-methylcoumarins have been found to possess choleretic, analgesic, anti-spermatogenic, anti-tubercular and diuretic properties (Goel et al., 2007; Pedersen et al., 2007). Hydroxyl derivatives of 4-methylcoumarin are used as optical brightening, dispersed fluorescent lasers (Shan & Xiao, 2004; Wheelock, 1959). Recently, they are employed as potential bio-antioxidants agents (Borges et al., 2005; Hoult & Payá, 1996; Kumar et al., 2005; Kancheva, 2009).

In our earliest work, we have studied the different properties of some coumarin systems by Molecular dynamics (Mesli & Mahboub, 2010). From these results, we are interested in 5,7-dihydroxy-4-methylcoumarin. For this system, we apply Molecular dynamics (MD) and Langevin dynamics (LD) methods. In this article, we detail the method of simulation using AMBER and MM+ as force fields. We will present here recent results both in water and gas environments and we give geometry optimization, energies and dihedrals angles properties.

In the present work, we describe and characterize the molecular structure of 5,7-dihydroxy-4-methylcoumarin by two methods: MD and LD simulations using two force fields: AMBER and MM+. We discuss the computational chemistry results of the coumarin compound then we compare the two calculations methods and force fields effects.

In section 2, we describe the materials and methods used in this study. In the next section, we have detailed the molecular calculations: i) geometry optimization, and ii) dynamic simulations. In the second part, we discuss the evolution of: i) energies, ii) dihedrals angles, iii) temperatures, and iv) geometry optimization in both vacuum