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Experimental and Theoretical Investigations of Barbaloin in a DMPC Bilayer

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Barbaloin (10-glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone, BBH), is the major anthraquinone glycoside of the Aloe vera. It can be extracted from plants of the family Asphodelaceae such as Aloe vera, Asphodelus and Asphodeline, which are widely used in the food, cosmetic and pharmaceutical industries [1]. Barbaloin has been found to have several pharmacological activities, such as laxative, antimicrobial, anti-inflammatory, antioxidant, antifungal and anticancer activities [2]. Previous studies have shown that barbaloin present strong inhibitory effects on histamine release from human mast cells [3]. This inhibitory effect of barbaloin is much higher than of some anti-inflammatory drugs. Due these effects, more and more scientific workers devote themselves to studying the structural and electronic properties of this molecule and its interactions with the biological environment [4,5]. In a recent work [6], we discussed the absorption spectra of emodin (a small antraquinone) in different solvents and its chemical processes in aqueous solution, such as protonation/deprotonation and tautomerism. These processes changes the molecular properties and its interactions with the environment. In this work, we report a study experimental and theoretical of Barbaloin into solvents and lipid bilayer addressed to examine the partition, location and interaction of this molecule in these environments. As experimental, we present the UV/Visible spectra of these species in solvents of different polarity (range from water to benzene) and in lipid dispersions of DMPC in two pH conditions acid and alkaline. Additionally, we performed molecular dynamics (MD) simulations of Barbaloin in fully hydrated lipid bilayers of DMPC to investigate at atomic detail the molecular mechanism of the interaction of this molecule with lipid membrane and its preferred location and orientation in these environments. In addition, we investigate the partition, orientation and mobility of barbaloin in the bilayer. As main results, we obtained that barbaloin have a strong tendency to insert into the lipid bilayer, collecting near the head groups of DMPC, with the anthracene almost fully oriented parallel to the membrane normal axis and the glucose moieties anchored in the head groups of DMPC. Analysis of various structural properties (area per lipid, electron

density profile and order parameters of the phosphatidylcholine tails) showed that the barbaloin causes a stronger disorder in phosphatidylcholine tails of the lipids.

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