

Theoretical evaluation of some natural polysaccharides as nanocarriers for the terpene alcohols from essential oils

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Abstract. Essential oils have attracted a continuous interest due to their varied biological activity. In order to overcome one of their major drawbacks, the low solubility, various encapsulation methods have been intensively studied. In this paper, nine natural polysaccharides have been investigated as possible nanocarriers for some terpene alcohols. Prior to the molecular docking study, the alcohols have been characterized by means of the global reactivity descriptors like HOMO-LUMO gap, chemical potential and electrophilicity; also, their radical-scavenging ability has been evaluated by means of two thermodynamic parameters, BDE (Bond Dissociation Energy) and IP (Ionization Potential). The results of the molecular docking study showed that best results have been obtained for inulin (among the polysaccharides) and terpineol (among the alcohols).

Keywords: terpenoids; alcohols; polysaccharides; molecular docking.

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