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Study of β-cyclodextrin inclusion complexes with volatile molecules geraniol and α-terpineol enantiomers in solid state and in solution

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ABSTRACT

Geraniol and α-terpineol are insoluble in water volatile compounds. α-Terpineol is a potentially important agent for medical applications. Formation of molecular complexes with β-cyclodextrin would lead to the increase of water solubility and bioavailability. β-Cyclodextrin forms 2:2 inclusion complexes with both enantiomers of α-terpineol and their precursor geraniol. Solid state complexes are thoroughly characterized by single X-ray crystallography and their stability over vast range of temperatures is proven by TG analysis. Intermolecular host–guest, host–host and guest–guest interactions give good insight into the nature of formed inclusion complexes. Stability constants of the complexes in solution are determined by HPLC.

1. Introduction

Geraniol [3,7-dimethylocta-trans-2,6-dien-1-ol] and both (+)- and (−)-α-terpineol [2-(4-methyl-1-cyclohex-3-enyl)propan-2-ol] belong to the class of terpenoids (Figure 1). Geraniol is an acyclic alcohol, which, under acidic conditions, may be converted into a cyclic α-terpineol [1]. α-Terpineols' precursor geraniol is a monoterpenoid. It is a basic component of rose oil, palmarosa oil, and citronella oil (Java type). It also occurs in small quantities in geranium, lemon, and many other essential oils. Geraniol exhibits acaricidal properties (studied against storage food mite) [2], antimicrobial activity, which is due to its solubility in the phospholipid biolayer of cell membranes [3], it is also known for its antitumor activity against leukemia, hepatoma and melanoma cancers [4,5]. Due to its specific scent, it is also widely used in as a fragrance. Moreover, it can also be used as plant-based mosquito repellent [6]. Terpineol is a naturally occurring monoterpene alcohol that has been isolated from a variety of sources such as cajuput oil, pine oil and petitgrain oil. α-Terpineol exhibits strong antifungal properties as shown by Zhou et al. [7]. Both enantiomers of α-terpineol, as well as geraniol are volatile and insoluble in water compounds. Their poor water solubility requires formulation involving solubilizing agents, one of the possibilities being molecular encapsulation with cyclodextrins to form inclusion compounds. β-Cyclodextrin (Figure 1) is a nontoxic macrocyclic carbohydrate compound toroid-like shaped, consisting of 7 glucopyranose units linked by 1,4-glycosidic bonds. Cyclodextrins have been used for analysis, separation including separation of enantiomers, chiral recognition as well as for physicochemical studies of inclusion phenomena of terpenoids like anethol, borneol, bornyl acetate, camphene, camphor, carvone, cineole, citral, citronellal, citronellene, eugenol, fenchone, geraniol, α-ionone, isomenthol, isomenthone, isopinocampheol, limonene, linalool, menthol, menthone, myrcene, neomenthol, nerol, α-phellandrene, perillaldehyde, pinenes, pulegone, terpinen-4-ol, terpineols, terpinolene, tricyclic diterpenoid acids, etc. by a number of researchers [8–29]. β-Cyclodextrin may also be used to encapsulate active pharmaceutical ingredients (API) and thus it can be used in the process of drug design. Nevertheless, due to the crystallization problems, there are only a few examples of crystalline complexes of cyclodextrins with APIs [30–32].

The possibility of formation of inclusion compounds by geraniol and α-teerpineol with β-cyclodextrin was first suggested by Araujo et al. [33] and Mazzobre et al. [34]. To gain insight in the

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