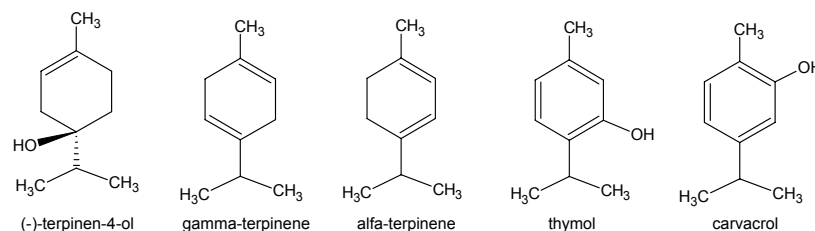


## Conformational and Vibrational Analysis of Selected Monoterpenoids by Using Density Functional Theory

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Monoterpenes are built from two isoprenoid units and represent the most abundant group of terpenoids. Here, we present systematic studies on conformational and vibrational analysis of monocyclic monoterpenoids (Fig. 1).



**Fig. 1:** Structures of the selected monoterpenoids

Until now, studies of the above-mentioned monoterpenes have been focused on identification, quantitative and qualitative analysis of these substances in chemical composition of the plant essential oils. This analysis has been carried out by using GC-MS, [1-3],  $^1\text{H}$  and  $^{13}\text{C}$  NMR, [2, 4], NIR-FT-Raman, and ATR/FT-IR spectroscopies [2, 5, 6,]. Moreover, inhibitory effects and pharmacological properties (e.g. antibacterial, anti-inflammatory, and anti-cancer action) of these substances have been studied.

To this point, there have been very few papers about molecular structures of the selected monoterpenoids. Crystallographic data concern only metal complexes of thymol [4] and carvacrol [7]. To the best of our knowledge, there is no information about the molecular structures of liquid terpinolene, p-cymene,  $\alpha$ -terpinene, and solid state of terpinen-4-ol.

Firstly, the DFT/B3LYP method with a 6-31G(d,p) basis set was used to determine conformational population for each of the terpenoid in respect of dihedral angles of the exocyclic groups. Then, the rotamers of the lowest energy were selected for the further calculations of frequencies of normal modes, and their IR and Raman intensities. The presence/absence of the studied molecular structures was confirmed by comparison of the theoretical vibrational spectra with FT-IR and FT-Raman spectra. Finally, an assignment of the normal vibrations of the molecules presented here was carried out on the basis of potential energy distribution (PED) of normal modes.

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