Indices of Reactivity of Biomarkers of Naphthalan oil

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Abstract

The compounds contained in the Naphthalan oil have a quad cyclopentanopergyphenanthrene system. In nature, this ring system is found both in animals and in plant organisms. Compounds containing such a ring system are of great importance for the body. The structure and position of the side groups and atoms adjacent to the main cycle, the position of the double bonds in the molecule, the spatial configuration, etc., have a definite influence on the biological activity of these compounds.

Calculated methods for the parameters of the geometry, electronic structure, and stereochemistry of the compounds under study have established that they have an oxygen function at C_3 and *trans*-articulation of the B/C and C/D rings. Some of them include phenolic ring A, while others contain α,β-unsaturated ketone system in ring A. Cholestans correspond to cholesterol in the orientation of the side chain and angular methyl groups, as well as *trans*-articulation of the rings. The compounds studied were found to be *trans*- or 14α-17α-compounds, or *cis*- or 14β-17β-compounds.

In biomarker structures, rings B and C form a rigid system of two chair-shaped rings with simultaneous *trans*- articulation of rings A and B. Ring A can take the form of a bath, but the instability of the form of the cyclohexane bath does not increase much in this case (as in the case of the steroid interactions between methyl and hydroxyl groups located at C_{10} and C_3, respectively). But even in cholestans, the interaction between the 3β-hydrogen atom and the angular methyl group prevents the transformation of cycle A into a bath form and, in the absence of special structural features, it can be assumed that ring A exists in the form of a chair.

Using quantum chemical methods, we calculated the transition states of the interaction of the studied substances contained in Naphthalan oil. Calculated activation energy for each stage of transformation. The results of finding the transient states are confirmed by the presence of one imaginary frequency, as well as by the successful completion of the procedure for reconstructing the reaction coordinates using the IRC method.

Also proposed regions of origin, formation and progress of oil in the territory of the globe. All the names of the Naphthalan oil are indicated by various peoples who were the pioneers of the extraction and use of this product.