Theoretical and Experimental Study of the Reactivity of Naftalan Petroleum Biomarkers

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Abstract

Oil produced on the territory of Naftalan Kasum of the Izmaylovsk region of Azerbaijan is recognized as official medicine and is used as an effective natural source of biologically active substances for both balneology and pharmaceutical chemistry now.

Naftalan petroleum has also become the object of extensive chemical research aimed at identifying the main sources of its therapeutic effects.

Features of the chemical composition of naphthenic hydrocarbons of Naftalan petroleum determine the universality and variety of its therapeutic effect. This action causes more than one type of hydrocarbon (for example, the cyclopentaneperhydrophenantre of the new structure, as was suggested earlier) and the set of petroleum compounds of various naphthenic compounds to which both sterane and triterpane hydrocarbons can be classified as well as hydrocarbons of the bridged type of articulation.

Due to the fact that naphthenic hydrocarbons are the main biological active compounds of therapeutic Nafthalan petroleum it was of interest to study the chemical composition of this group of hydrocarbons using various research methods.

We carried out a component analysis of the white Naftalan oil using a gas chromatograph SHIMADZUGCMS-QP2010 Ultra equipped with a quadrupole mass-selective detector. The IR-spectra of the white Naftalan oil were removed using an IR-Fur'e of the Lumos Microscope. The NMR-spectra were recorded on a Bruker spectrometer at an operating frequency of 300 MHz. The accuracy of the results of the analyzes was confirmed by using the following methods: gas chromatography-mass spectrometry (GCMS, GC & GC-MS, TG-SPI-MS).

Quantum-chemical modeling of the compounds of the interaction of polycyclic naphthenic hydrocarbons with compounds contained in a living body is carried out (the substances under investigation have a quadruple cyclopentanoperhydrophenanthrene system). Using the TS, QST2, and QST3 methods the transient states of the interaction reaction of the investigated substances contained in Naftalan petroleum were calculated. The results of finding the transient states are confirmed by the presence of one imaginary frequency as well as the successful procedure of restoring the coordinate of the reaction by the IRC method.

According to the results of the conducted studies it is established that the metabolism significantly changes under the influence of Naftalan petroleum.