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Chromoto-Mass Methods for Detecting Simple Esters in Chromatography-Mass Spectrometry Method

Kholmirzaev Mekhroj Murodillayevich ¹, Khaydarov Gayrat Shoyimovich ², Saitkulov Foziljon Ergashevich ³, Kholiqova Kamola O'tkir qizi ⁴, Umarova Aziza Ikrom qizi ⁵

^{1, 2} Uzbekistan-Finland Pedagogical Institute, Faculty of Natural and Physical Culture, Department of Natural Sciences

³ Tashkent State Agrarian University

^{4, 5} Student Tashkent State Agrarian University

Abstract: This paper shows a detailed study of the features of the structural organization of compounds that determine the chemical composition of the organic substance cuminium, on the example of its ethanol extract, using chromatography-mass spectrometry, expanding the set of individual compounds, in addition to those known in the scientific literature, to calculate the composition of the extract of esters.

Keywords: Detailed study of the structural organization of compounds, ethanol extract, chromatography-mass spectrometry, individual compounds, mannan, hydrolyzed to mannose, as well as dextrins, starch, protein substances, pentosans, methylpentosans, sugars, esters simple and complex, mineral salts.

Introduction

A detailed study of the features of the structural organization of compounds that determine the chemical composition of the organic substance cuminium, on the example of its ethanol extract, using chromatography-mass spectrometry, expanding the set of individual compounds, in addition to those known in the scientific literature, calculate the structural and group composition of the extract, in order to determine the quantitative ratio of various groups of components, to obtain their mass-spectra and structural formulas; to make an assumption about the direction of the pharmacological action of cuminium preparations, taking into account the peculiarities of the structure of compounds of its organic matter.

Medicinal raw materials were cuminium seeds collected by cuminium. In dried form, they are called salep. The chemical composition of cuminium is determined by the content of mucus, the basis of which is determined by the high-molecular polysaccharide mannan, hydrolyzed to mannose, as well as dextrins, starch, protein substances, bitterness, pentosans, methylpentosans, sugars, esters simple and complex, mineral salts and others [1-10].

Cumin is used as a seasoning in cooking. Sometimes it is used instead of pepper. Cumin is suitable for any dish. This is another advantage of it compared to other seasonings. It is also used in medicine to improve the condition of diabetes, in the treatment of anemia and pathologies of the nervous system. regulates carbohydrate, water-salt metabolism, the functional state of the male sex glands [1-10].

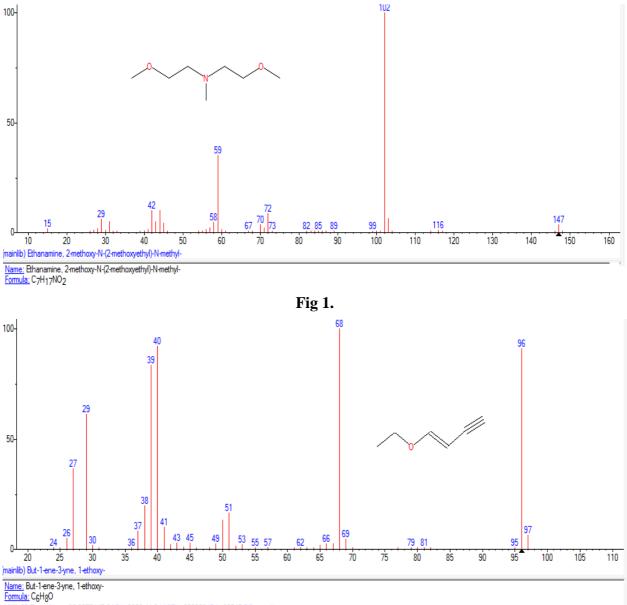


Methods and Results

The object of the study was an ethanol extract of cuminium obtained by exhaustive extraction of raw materials with ethanol with a mass of 95% in a Scraper apparatus. The extract was released from ethanol in a vacuum rotary evaporator model RE-52 AA Rotary Evaporator, the residue was weighed and its chemical composition was studied by chromatography-mass spectrometry.

The registration of analytical signals was carried out with the following parameters of the mass spectrometer: the temperature of the transition line and the ion source is 250 and 280°C, respectively, electronic ionization (EI), the range of recorded masses is from 50 to 500 Da.

The composition of esters is dominated by simple esters of the type: *But-1-ene-3-yne-1-ethoxy*, *Cyclohexane*, *ethoxy*, *2*,7-*Octadiene*, *1-butoxy*.



MW: 96 Exact Mass: 96.0575147 CAS#: 2806-41-9 NIST#: 250268 ID#: 30545 DB: mainlib

Fig 2.



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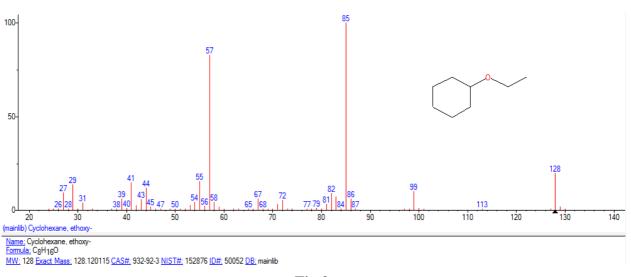


Fig 3.

It is shown (Fig. 1-3) that cumin contains esters in the spectrum.

The given list of compounds, the features of their structural organization, the presence of various functional groups in them allows us to conclude about the rather complex chemical composition of the organic matter of the spotted hawthorn, and, consequently, about the specificity of its pharmacological action.

Conclusion

Cumin's found in the extract are responsible for antispasmodic, anticoagulant, photosensitizing, antitumor effects, especially in combination with steroid compounds, aldehydes and ketones. Nitrogen- and sulfur-containing compounds have a highly selective pharmacological effect, significant amounts of which, different in structure, are found in cumin extract.

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