

REPUBLIC OF AZERBAIJAN

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ABSTRACT

of the dissertation submitted for the degree of Doctor of
Science in Biology

**PHYTOCHEMICAL RESEARCH AND RESOURCE
POTENTIAL OF SOME SPECIES OF THE *ASTERACEAE*
GISEKE. AND *APIACEAE* LINDL. FAMILIES IN THE
FLORA OF AZERBAIJAN**

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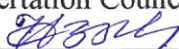
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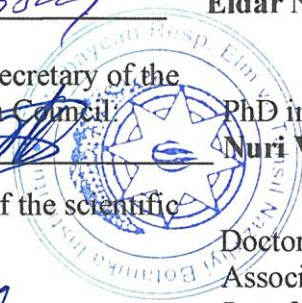
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INTRODUCTION

The relevance of the topic and the degree of development.

Since ancient times, plants have been widely used in the treatment of various diseases. Despite the widespread use of numerous synthetic drugs in medical practice, the use of plant extracts, herbal preparations, as well as various groups of biologically active substances obtained from plants, still remains relevant^{1, 2}. The species composition of the Azerbaijani flora is very rich, represented by approximately 4500 plant species^{3,4}. It is known that plant species belonging to the *Asteraceae* family contain a number of biologically active substances⁵. These compounds include flavonoids, sesquiterpene lactones, and steroid compounds. The main advantage in plants belonging to the *Apiaceae* family is the presence of coumarin-derived compounds⁶.

The use of these biologically active substances of great importance in medicine, pharmacy, and the food industry⁷. The chemical study of plants from the *Asteraceae* and *Apiaceae* families in the Azerbaijani flora is still ongoing. Therefore, the individual extraction of substances from plants belonging to this

¹ Eskandani, M. Galbanic acid inhibits HIF-1 α expression via EGFR/HIF-1 α pathway in cancer cells / M. Eskandani, J. Abdolalizadeh, H. Hamishehkar [et al.] // *Fitoterapia*, – 2015. v. 101, – p. 1–11.

² Sytar, O. COVID-19 Prophylaxis Efforts Based on Natural Antiviral Plant Extracts and their Compounds/ O.Sytar, M. Brestic, S. Ibadullayeva [and et al.]// *Molecules*, - 2021. V. 26, Is. 3, p. 727.

³ Əsgərov, A. Azərbaycanın bitki aləmi /A. Əsgərov. –Bakı:TEAS Press, –2016. – 443 s.

⁴ İbadullayeva, S., Huseynova, İ. An Overview of the Plant Diversity of Azerbaijan [Chapter]: Biodiversity, Conservation and Sustainability in Asia / Editors - Munir Öztürk, Volkan Altay, Recep Efe. Springer, -2021, Volume 1, -p. 431-478.

⁵ Cahangirova, İ.R. *Ambrosia artemisiifolia* L. və *Telekia speciosa* (Schreb.) Baumg. (*Asteraceae*) növlərinin bioloji fəal maddələrinin öyrənilməsi: /biologiya üzrə fəlsəfə doktoru dis.../–Bakı, 2010. – 174.

⁶ Серкеров, С.В. Терпеноиды и фенолпроизводные растений семейств *Asteraceae* и *Apiaceae*. Баку: CBS Production, –2005. – 312 с.

⁷ Tosun, F., Biltekin, S.N., Karadağ, A.E. Biological activities of the Natural coumarins from *Apiaceae* Plants / F.Tosun, S.N. Biltekin, A.E. Biltekin [et al.] // *Rec. Nat. Prod.*, –2023. v. 17, N5, –p. 867-877.

family, their identification, and the study of their structural formulas and pharmacological activities are among the current issues. Our prominent scientist, S. Sarkarov, once known in the field of chemistry of natural compounds, devoted his research to investigating the chemical composition of plants from these families⁸. He studied the chemical composition of both the aboveground and underground organs of some species belonging to the *Asteraceae* and *Apiaceae* families, isolated several compounds that were new to science, and studied them using modern spectroscopic methods. Among the compounds belonging to this group and studied are sesquiterpene lactones, terpenoid esters, alcohols, coumarin and furocoumarin derivatives, steroid compounds, flavonoids, aliphatic sugar alcohols, etc. The chemical composition of species belonging to the genus *Ferula* L. of the *Apiaceae* family is rich in terpenoid coumarins, lactones, esters and other compounds^{9,10}. The terpenoid coumarins found in plants belonging to this genus have several isomers. Isolation of new isomers from plants and their study by spectroscopic methods means the discovery of structures of new substances for science^{11,12}. Natural coumarin compounds are constantly in the focus of researchers' attention due to their diverse biological activities¹³.

⁸ Серкеров, С.В., Алескерова, А.Н. Инфракрасные спектры и строение сесквитерпеновых лактонов и кумаринов / С.В. Серкеров, А.Н. Алескерова, – Баку: CBS Production, –2006. – 223 с.

⁹ Jiang, M. Quality evaluation of four *Ferula* plants and identification of their key volatiles based on non-targeted metabolomics / M. Jiang, M. Peng, Y. Li [et al.] // Front. Plant Sci., –2024. v.14, e1297449.

¹⁰ Yaqoob, U., Nawchoo, I.A. Distribution and taxonomy of *Ferula* L.: A review. // Res. Rev. J. Bot., – 2016, 5(3), – p. 15–23.

¹¹ Heydərov, İ.Q. *Ferula calcarea* M. Pimen, *Prangos biebersteinii* Karjag. və *Angelica purpurascens* (Ave-Lall.) Gilli (*Apiaceae*) növlərinin kimyəvi tədqiqi./ biologiya üzrə fəlsəfə doktoru dis. /– Bakı, 2018. – 131 s.

¹² Назаров, М.Н., Джамшедов, Дж.Н., Борониев, Н.С. Литературная справка род *Ferula* L. // Наука и инновация, –2018. т. 2, – с.176–181.

¹³ Wang, J.-L. Sesquiterpene coumarins from *Ferula sinkiangensis* and their anti-pancreatic cancer effects / J.-L. Wang, C.-Y. Sang, J. Wang [et al.] // *Phytochemistry* – 2023, v. 214, e 113824.

The chemical composition and biological activities of most plants in the Azerbaijani flora, especially species belonging to the genus *Ferula* L., have been poorly studied. Therefore, the individual extraction of substances from these plants, their identification, and in cases where new substances are obtained, the study of their structural formulas and pharmacological activities is one of the current issues. Thus, most researchers have noted in their works the antimicrobial, antiviral, antiestrogenic, opioid, antioxidant, antimalignant, photosensitizing, anti-leishmanial, anthelmintic, wound healing, antiulcer, anti-neuroinflammatory, and other properties of coumarin derivatives^{14,15,16,17,18,19,20}.

Object and subject of research. The objects of the research have been selected as *Ferula persica* Wild., *Ferula caucasica* Korovin. (syn. *F. caspica* M. Bieb.) belonging to the family *Apiaceae* Lindl. and *Artemisia campestris* subsp. *marschalliana* (Spreng.), Elenevsky & Radygina, *Achilleae nobilis* L. from the family

¹⁴ Bashir, S. A. New antileishmanial sesquiterpene coumarins from *Ferula narthex* Boiss / S. Bashir, M. Alam, A. Adhikari [et al.] // *Phytochemistry Lett.*, – 2014. v. 9, – p. 46–50.

¹⁵ Verma, S. Valuating the role of dithiolane rich fraction of *Ferula asafoetida* (*Apiaceae*) for its antiproliferative and apoptotic properties: in vitro studies / S. Verma, P. Khambhala, S. Joshi [et al.] // *Exp Oncol.*, – 2019, 41(2), – p. 90-94.

¹⁶ Hashemi, Z. Green synthesis of silver nanoparticles using *Ferula persica* extract (Fp-NPs): Characterization, antibacterial, antileishmanial, and in vitro anticancer activities / Z. Hashemi, M. Mohammadyan, M. Fakhar [et al.] // *Materialstoday communication*, – 2021. v. 27, e 102264.

¹⁷ Hasanpour, M. Efficacy of Covexir (*Ferula foetida* Oleo-Gum) Treatment in symptomatic improvement of patients with mild to moderate COVID-19: A randomized, double-blind, placebo-controlled trial // M. Hasanpour, H. Safari, A.H. Mohammadpour [et al.] // *Phytother. Res.* – 2022. v. 36, – p. 4504–4515.

¹⁸ Nasri, S. Phytochemical study of methanolic extract of *Ferula persica* Willd. Inflorescence and its antinociceptive effect in male mice / S. Nasri, M. Gh. Nohooji, G.R. Amin [et al.] // *J. Med. Plants*, – 2018. 17 (68), – p. 136-144.

¹⁹ Sistani, P. Structural and kinetic Insights into HIV-1 reverse transcriptase inhibition by farnesiferol C / P. Sistani, G. Dehghan, L. Sadeghi [et al.] // *Int. J. Biol. Macromol.*, – 2021. v.174, – p. 309–318.

²⁰ Wang, L. Research on the development of chemical components, pharmacological activities and toxicity of resina *Ferulae* / L. Wang, R. Sun, M. Xu [et al.] // *World Tradit. Chin. Med.*, – 2020. v. 15, – p. 3887–3894.

Asteraceae Giseke., which are widespread in the flora of Azerbaijan. The subject of the study is the phytochemical study of these species.

Aim and objective of research: The aim of the research has been to study the chemical composition of terpenoid compounds in the species *Ferula persica* Wild., *Ferula caucasica* Korovin., *Artemisia campestris* supsb. *marschalliana* (Spreng.) Elenevsky & Radygina, *Achillea nobilis* L., theoretical quantum chemical calculations of isolated compounds, in silico studies, determination of the distribution areas of the studied species, raw material reserves, accumulation dynamics and storage period of biologically active substances, identification of macro and micromorphological diagnostic signs, and study of the microbiological, antioxidant and parasitological properties of the identified substances. To achieve all this, the following tasks are planned to be carried out:

➤ Acquisition of individual substances from *Ferula persica*, *Ferula caucasica*, *Artemisia campestris* supsb. *marschalliana* species by means of extraction and column chromatography;

➤ Identification of individual substances using (1D) and (2D) dimensional NMR spectroscopic analysis methods;

➤ Study of the individual substances by X-ray structural analysis;

➤ Theoretical quantum chemical calculations of sesquiterpene coumarins and lactones identified from the species *Ferula persica* and prediction of in silico studies using a computer program;

➤ Extraction and study of essential oils from *Ferula persica*, *Ferula caucasica* and *Achillea nobilis* species;

➤ Study of macro-microelement composition of roots and fruits of *Ferula persica* and *Ferula caucasica*;

➤ Investigation of the distribution areas and raw material reserves of the studied species;

➤ Determination of the optimal accumulation dynamics and storage time of biologically active substances in the roots and fruits of *Ferula persica* and *Ferula caucasica* species;

➤ Determination of macro and micromorphological diagnostic features of the roots and fruits of *Ferula persica*, *Ferula caucasica* species;

➤ Study of microbiological, antioxidant, and parasitological activities of identified substances;

Research methods. The following research methods have been used during the implementation of the dissertation:

In the study of substances, chemical-acetylation and spectroscopic (IR-Infrared spectroscopy; UV-Ultraviolet spectrophotometry; GC-MS-gas-chromatography-mass spectrometry; 1D-dimensional PMR-¹H NMR, ¹³C NMR, ¹³C DEPT 135, ¹³C DEPT 90, ¹³C DEPT 90, ¹³C DEPT 45 and 2D-dimensional COSY, HSQC, HMQC, HMBC spectroscopy; X-ray structural analysis methods have been used. The melting point of individual substances has been determined using a Stuart SMP10 device, and the optical rotation angle has been measured using a Rudolph Research Analytical digital polarimeter (model Autopol I, USA) (λ 589 nm) at 20°C.

For *in silico* prediction of biological activity and toxicity of substances, computer modeling programs Pass Online, ProTox-3.0, SwissTargetPrediction, Swiss ADME and Admet Lab 3.0 have been used.

Microscopic studies have been performed using a BIOLAM-C microscope, MBC-1 binoculars and a L74WIDE Samsung camera. Microbiological studies used *Methicillin – sensitive Staphylococcus aureus* – MSSA, code: ATCC 700699; *Methicillin-resistant Staphylococcus aureus* MRSA, code: ATCC 29213; *Bacillus subtilis*, code: MIK; *Esherichia coli*, ATTCC 25922; *Pseudomonas*, *Klebsiella* sp. 505562; *Candida albicans* ATCC 2091) microbial and fungal strains. Parasitological studies used ticks of the genus *Rhipicephalus* and *Trichocephalus* eggs found in sheep stool samples. Japanese-made JEM-1400 electron microscopes with an acceleration voltage of 80-120 kV have been used to examine stained and unstained ultra-cut microbiological preparations. The recording and acquisition of morphometric parameters of the structural elements of the raw material has been carried out using a side-mounted digital camera (Veleta and iTEM software, Japan, Germany). A Leica EM UC7 ultramicrotome has been used to obtain ultrathin sections.

The main provisions put forward for defense.

1. The fact that *Ferula persica*, *Ferula caucasica* species and

Artemisia campestris subsp. *marschalliana* subspecies are rich in sesquiterpene lactones and coumarins in their chemical composition and that these substances have biological activity provides the basis for the development and preparation of new medicines containing this group of compounds and for their use as a raw material source for the production of these substances in the future. In particular, the species *Ferula persica* and *Ferula caucasica* are included in the “Red Book” of the Republic of Azerbaijan (2023), indicating the need for their introduction and increasing.

2. Diagnostic features discovered during morphological and anatomical studies of *Ferula persica* and *Ferula caucasica* can be used in the systematic identification of the species.

3. The sulfur-containing organic compounds and sesquiterpene coumarins in the essential oils obtained from the roots and fruits of the species *Ferula persica* and *Ferula caucasica* allow these species to be grouped in terms of their chemical chemotaxonomic position.

Scientific novelty of the research. For the first time, the chemical composition of two species of the genera *Achillea* L. and *Artemisia* L. of the family *Asteraceae*, as well as two species of the the genus *Ferula* L. of *Apiaceae* family, has been studied using phytochemical, chromatographic, and modern spectroscopy methods. 36 components have been obtained from the essential oil of the aerial part of *Achillea nobilis*, two substances and one monoacetyl derivative from the aerial part of *Artemisia campestris* subsp. *marschalliana*.

Fifteen substances have been isolated and studied from the lipophilic fraction of the roots of *Ferula persica*, 10 individual substances from other fractions, and three individual substances from its fruits. Three substances have been isolated and identified from the roots of the species *Ferula caucasica*. The substances have been studied using GC–MS, (1D) and (2D) dimensional NMR spectroscopic and X-ray structural analysis methods. The identified substances have been determined to belong to sulfur-containing organic compounds, sesquiterpene coumarins, and lactones. Santonin, artemisinin, monoacetylartemisinin have been identified from the aboveground parts of *Artemisia campestris* subsp.

marschalliana; mogoltavidin, badrakemin, badkhysidin, badkhysin, badkhysin, feselol from the roots of *Ferula persica*; conferon, conferol, badrakemin from the fruits of this species; hydrate compounds of conferon, conferol, samarkandin have been identified from the roots of *Ferula caucasica* and are new for these species. For the first time, quantum chemical calculations of osthol, conferol, badrakemin, badkhysidin and badkhysin compounds obtained from *Ferula persica* roots have been performed. For the first time, X-ray structural analysis of badrakemin and badkhysidin compounds has been performed.

The essential oil and macro- and microelement composition of the roots and fruits of the species *Ferula persica* and *Ferula caucasica* have been studied for the first time. The distribution areas of these species and the determination of their raw material reserves have been investigated. Macro and micromorphological characteristics of the studied species have been determined. The antibacterial, antifungal, antioxidant, and parasitological activities of substances obtained from these species have been evaluated.

Theoretical and practical significance of the research.

Sesquiterpene coumarins - badrakemin and conferol isolated from the species *Ferula persica* and *Ferula caucasica* can be applied in clinical practice due to their cytotoxic effect on HCT116 (human colorectal carcinoma cell line) in colon culture, Colo205 and (UO31 and A498) kidney cancer cell lines and the sesquiterpene lactone - badkhysidin and badkhysin obtained from the roots of *Ferula persica* for their wound-healing, anti-burn, regenerative, and even nootropic effects. Mogoltavidin, a bicyclic sesquiterpenoid coumarin with aphrodisiac properties, extracted from the roots of the *Ferula persica* species, may be used as a biological food supplement in the future. The structure of the anthelmintic alpha santonin obtained from the species *Artemisia campestris* supsb. *marschalliana*, the antimicrobial, antifungal, antioxidant and parasitological effects of essential oils obtained from the root and fruits of *Ferula persica* and *Ferula caucasica*, as well as the aerial parts of the *Achillea nobilis* plant have been studied, which in turn will contribute to the preparation of new medicines based on these raw materials in the future. Studying the

phytochemical and biological aspects of these species may have practical application importance in laboratory classes held in departments of biological, chemical, and pharmaceutical-oriented universities. Also, substances identified from the studied plants can be used in the preparation of future famcopeia articles.

Approbation and implementation. The results of the dissertation have been presented at the following local and international conferences and symposia: International conference on “Actual problems of contemporary natural and economic sciences” (Ganja-2018); International conference on “Actual problems of contemporary natural and economic sciences” (Ganja-2019); III Medical Drugs for Human. Modern Issues of Pharmacotherapy and Prescription of Medicine (Ukraine-2019); V Medical Drugs for Human. Modern Issues of Pharmacotherapy and Prescription of Medicine (Ukraine -2021); Actual Problems of the Chemistry of Natural Compounds, International scientific conference (Tashkent-2023); Actual Problems of the Chemistry of Natural Compounds, International scientific and technical conference (Tashkent-2024); International scientific and practical congress on the topic “Actual problems of medicine” dedicated to the 100th anniversary of the birth of the National Leader Heydar Aliyev (Baku-2023); 11th scientific and practical conference of residents and graduate students dedicated to the 100th anniversary of the birth of the National Leader of the Azerbaijani People Heydar Aliyev ATUREK-11 (Baku-2023); Materials of the 5th International Scientific Congress on “Modern Problems of Pharmacy” (Baku-2021); Program and materials of the conference of the student scientific society of the Faculty of Pharmacy dedicated to the 95th anniversary of the Azerbaijan Medical University (Baku-2025); Collection of abstracts of the Medical Festival dedicated to the 102nd anniversary of the National Leader Heydar Aliyev and the 95th anniversary of the Azerbaijan Medical University, ATUREK-13, (Baku-2025) and at the scientific seminar of the Institute of Botany, MSERA.

The 23 scientific works, including 13 articles and 10 theses, have been published on the results of the dissertation work. Ten (10) of the articles have been published in foreign and three in local

journals. Eight of the articles have been published in foreign journals indexed in Web of Science and Scopus International databases.

Organizations where the dissertation work has been performed.

The main experimental part of the scientific research has been implemented in the Ethnobotany and Plant Resources Departments of the Institute of Botany of the Ministry of Science and Education of the Republic of Azerbaijan, the others have been carried out in the Nuclear Magnetic Resonance of the Institute of Petrochemical Processes, the Central Analytical Laboratories of the Geology and Geophysics Scientific Research Institute, as well as in the laboratories of the departments of Pharmacognosy, Pharmaceutical Chemistry, Medical Microbiology and Immunology, Cytology, Embryology and Histology of the Azerbaijan Medical University. The research has been also carried out in the analytical phytochemical laboratories of the V.L. Komarova Institute of Botany in St. Petersburg, Russia, and the N.D. Zelinsky Institute of Organic Chemistry in Moscow. I express my gratitude to all the organizations mentioned above.

The total volume of the dissertation in characters, with the volume of its structural sections indicated separately. The volume of dissertation is 406 pages (375 452 characters): introduction (17405 characters), Chapter I (45518 characters), Chapter II (64499 characters), Chapter III (139995 characters), Chapter IV (16641 characters), Chapter V (32877 characters), Chapter VI (33369 characters), Chapter VII (6557 characters), Conclusion (12890 characters), Results (4830 characters), Recommendations (871 characters), list of used literature with 228 titles and appendices. The dissertation is illustrated with 65 tables, 157 figures, and 3 schemes.

CHAPTER I. LITERATURE REVIEW

This chapter of the dissertation examines literature materials and provides information about the species included in the genera *Ferula* L., *Artemisia* L. and *Achillea* L., their chemical composition, and prospects for use in medicine. Since the research deals with the identification of sesquiterpene coumarins and lactones, an extensive

literature review has been conducted on this group of coumarins, and a classification of coumarins and lactones has been provided by dividing them into groups.

CHAPTER II

RESEARCH OBJECTS AND METHODS

2.1. Research objects

The species *Ferula persica* Wild., *Ferula caucasica* Korovin., belonging to the family *Apiaceae* Lindl., and *Achillea nobilis* L., *Artemisia campestris* subsp. *marschaliana* (Spreng.) Elenovsky & Radygina from the family *Asteraceae* Giseke. have been collected as the object of the research. The roots and fruits of *F. persica* Wild. raw material were collected from the Jangi area of Gobustan on 21.07.2021, at the stage of full seed ripening. The second species of the *Ferula* genus is *F. caucasica*. The roots of the plant were collected on 01.05.2024, when the flowers were blooming, and the fruits were collected on 27.07.2024, when the seeds were fully ripe, in Gizagi and Godughgiran, Arabgadim village, Gobustan district. The above-ground part of *Artemisia campestris* subsp. *marschaliana* was collected on 28.07.2018 during the budding stage from the vicinity of the River Araz, which runs along the border of Imishli and Beylagan districts of the Republic of Azerbaijan. *Achilleae nobilis* L. - Noble yarrow was collected in the flowering phase on 18.06.2020 from the vicinity of the village Malham, Shamakhi district of the Republic of Azerbaijan. These paragraphs provide information about the botanical characteristics of the species and their distribution in the flora of Azerbaijan²¹.

2.2. Research methods

In the experimental part of the dissertation, extraction methods have been used to obtain the total amount of extractive substances from plant raw materials, column methods to separate the substances from the total amount of extractive substances into fractions, and thin layer chromatography (TLC) methods to check the individuality of the collected

²¹ Флора Азербайджана: [в VIII томах]. – Баку: Флора Азербайджана, – т. VI; т. VIII. – 1955; -1961. 479–483 с.; – 270-318 с.

fractions. Chemical (acetylation), physical chemical ultraviolet (–UV), infrared (–IR), nuclear magnetic resonance (–NMR), and X-ray structural analysis methods have been used to study the individual substances obtained²².

Theoretical quantum calculations of the studied compounds have been performed using the DFT method, and the 6-31G(d,p) basis set B3LYP theory has been used in geometric optimization. The ORCA-4.2.1 computational package has been used for the calculations²³.

For *in silico* prediction of biological activity and toxicity of substances, computer modeling programs Pass Online, ProTox-3.0, SwissTargetPrediction, Swiss ADME and Admet Lab 3.0 have been used²⁴.

The determination of the ranges and reserves of the studied species has been carried out on the basis of field routes and expeditions. Macroscopic and microscopic methods have been also used to determine the macro-micromorphological properties of plant raw materials^{25,26}. Antioxidant, microbiological, and histological methods have been used to study some of the biological activities of plant-derived substances²⁷.

2.2.1. Methodology for studying plant resources

The model sampling method has been used to determine raw

²² Kərimli, E.H. *Fraxinus* L. cinsinə aid bəzi növlərin farmakoqnostik tədqiqi: /əczaçılıq üzrə fəlsəfə doktoru dis. /– Bakı, 2016. – 178 s.

²³ Abbasov, V.M. Green synthesis and DFT calculations of 4'-(2-phenyl-1H-phenanthro[9,10-d]imidazol-1-yl)-[1,1'-biphenyl]-4-amine / V.M. Abbasov, A.M. Mammadov, R.E. Azizov [və b.] // Processes of Petrochemistry and Oil Refining, – 2025. v. 26, N1, –p. 97-106.

²⁴ Xiong, G. ADMETlab 2.0: an integrated online platform for accurate and comprehensive predictions of ADMET properties / G. Xiong, Z. Wu, Y. Jiakai [et al.] // Nucleic Acids Res. –2021, 49(W1), W5–W14.

²⁵ Практикум по ботанике. / Ю.Б. Керимов, Н.А. Исламова, Д.С. Халилов [и др] – Баку: nəşr, – 1999. – 238 с.

²⁶ Khamraeva, D.T. Comparative anatomical study of underground and aboveground organs in *Ferula tadshikorum* Pimenov under natural and introduced environments / D.T. Khamraeva, D.N. Tukhtaeva, Khojimatov O.K. [et al.] // Acta Biologica Sibirica, –2024. v. 10, – p. 9–29.

²⁷ Beladjal, H. HPLC-DAD analysis and antioxidant potential of *Ferula assa foetida* resin ethanol /H. Beladjal, Dj. Bouhadi, H. Belkhodja [et al.] //Extract Trop J. Nat. Prod. Res., –2024, 8(4) – p. 6906-6910.

material reserves²⁸. To determine the yield of raw materials in test plots, the number and size of test plots are first determined depending on the number of mature plants. The number of test plots should be such that the results obtained in statistical processing are within ± 10 -15% of the average mathematical calculation.

2.2.2. Acquisition of coumarin derivatives and their determination by chemical methods

The extraction process of individual coumarins is best performed using petroleum ether (hexane) as an organic solvent. This is because fewer other ballast substances pass into the obtained hexane or petroleum ether extract, making it easier to later obtain their crystals. All chemical methods (saponification, chemical decomposition, hydrolysis, oxidation, acetylation, hydrogenation, dehydrogenation, dehydration, etc.) applied in the study of other natural compounds are used to determine the structural structures of coumarin derivatives.

2.2.3. Methods for spectroscopic study of coumarins

Infrared spectroscopy. The study of information obtained from the detection of infrared (IR-) spectra is of great importance in determining the structural formulas of natural coumarin derivatives.

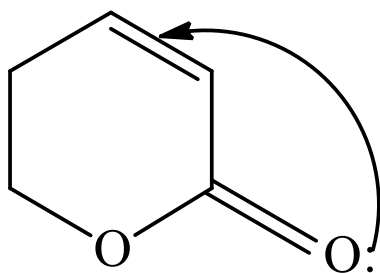
The wavelength in the IR spectrum covers the range between 4000-650 cm^{-1} , with the unit of measurement used in IR spectroscopy being “ cm^{-1} ”. The absorption band of coumarins is in the 1750-1700 cm^{-1} region of the IR spectrum as a result of the neutralization of the one electron pair of the oxygen atom of the carbonyl group ($>\text{C}=\text{O}$) in α -pyron cycle by the conjugated one double bond^{29,30}.

The exact value of the carbonyl group depends on the location of the functional groups in the benzene ring and other factors.

²⁸ Ресурсоведение лекарственных растений (Учебно-методическое пособие для вузов)/ Составитель: Негробов В.В., - Воронеж: - 2015. -с 57.

²⁹ Наканиси, К. Инфракрасные спектры и строение органических соединений. – Москва: изд. Мир, –1965. – 207 с.

³⁰ Хасанов, Т.Х. Саидходжаев, А.И. Никонов, Г.К. Структура и конфигурация новых кумаринов корней *Ferula mogoltavica* //Химия природных соединений, –1974. №1, –с. 10-14.

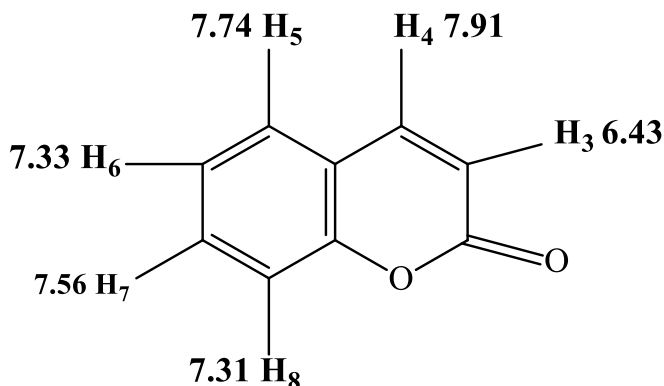


α -piron

In addition, coumarin derivatives give intense absorption bands in the 1620-1470 cm^{-1} region associated with the double bonds of the aromatic system.

The chemical shifts of the signals in the NMR spectra of mono- and disubstituted coumarins vary depending on the position of the protons of the coumarin system in the structural formula.

The chemical shifts (δ , ppm relative to tetramethylsilane (SiH_4)) and spin-spin coupling constants (J , Hz) of the substituted coumarin protons are shown below³¹.



³¹ Xing, Y. Sesquiterpene coumarins from *Ferula sinkiangensis* act as neuroinflammation inhibitors / Y. Xing, N. Li, D. Zhou [et al.] // *Planta Med.*, – 2016. v. 83, p. 135–142.

$\delta_{H-3}=6.43$ $\delta_{H-5}=7.74$ $\delta_{H-7}=7.56$
 $\delta_{H-4}=7.91$ $\delta_{H-6}=7.33$ $\delta_{H-8}=7.31$
J=9,8 Hs J=8.5 Hs

The sequence of chemical shifts in the NMR spectrum of substituted coumarin in increasing order: $\delta_{H-4} > \delta_{H-5} > \delta_{H-7} > \delta_{H-6} > \delta_{H-8} > \delta_{H-3}$

2.2.4. Acquisition of sesquiterpene lactones and determination by chemical methods

Sesquiterpene lactones, as in the case of coumarins, are usually obtained using organic solvents. Petroleum ether, hexane, benzene, chloroform, carbon-4-chloride, ethyl acetate, ethanol, methanol, etc. are used as organic solvents. Thin-layer, HPLC, GC-MS, and other methods are used to obtain sesquiterpene lactones individually. Column chromatography is more widely used for the individual extraction of sesquiterpene lactones. Aluminum oxide, silica gel powder, etc. are used as sorbents.

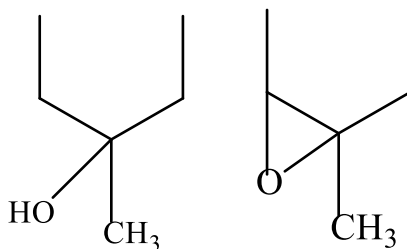
2.2.5. Methods for spectroscopic study of sesquiterpene lactones

Ultraviolet (-UV) spectroscopy. Most sesquiterpene lactones (eudesmanolides, guaianolides, germacranolides, etc.) contain endo- and exocyclic methylene double bonds conjugated to the carbonyl of the γ -lactone ring. In the UV spectrum, this chromophore gives maximum absorption in the 197-225 nm range at an intensity of 8000-14000.

Infrared (-IR) spectroscopy. In the IR spectra of all sesquiterpene lactones, regardless of the group to which the lactone belongs (guayan, pseudoguayan, eudesman, eleman, germacrane, etc.), the absorption band in the range of 1750-1800 cm^{-1} characterizes the carbonyl of the γ -lactone cycle.

NMR spectroscopy of sesquiterpene lactones. The chemical shift intervals of different representatives of sesquiterpene lactones are different. The signals with high intensity in the PMR spectrum are signals of methyl groups. The chemical shift of the double methyl group signals (doublets, $\text{CH}_3\text{-CH}<$, 5-7 Hz) and the singlet signals of

the triple methyl group are detected in the range of 0.6-1.4 ppm. Singlet signals that appear in the region of three proton units (1.3-1.6 ppm.) indicate the presence of heteroatoms (e.g., oxygen, i.e., epoxy, hydroxy) groups attached to the carbon atom in the heminal position of the methyl group.



The chemical shift of the signals of the vinyl methyl group ($\text{CH}_3\text{-C=}$) is in the range of 1.5-2.5 ppm. In this chemical shift region (1.8-2.2 ppm), signals from the ester group are also detected. If the signals of the vinyl methyl group are conjugated to the carbonyl group inside the cycle, its chemical shift undergoes a weaker paramagnetic (2.4 ppm., etc.) chemical shift than the vinyl methyl signals of the ester group attached outside the cycle.

X-ray structural analysis. X-rays have been discovered by Wilhelm Röntgen (1895) and have been called X-rays. On the scale of electromagnetic waves, it lies in the wavelength range between gamma radiation and ultraviolet radiation. Many chemical compounds, such as terpenoids, coumarins, and alkaloids, occur in crystalline or soft powder form. The X-ray structural analysis method is used to analyze these compounds³².

2.3. Devices, materials, reagents and sorbents used during the studies

Ethyl alcohol and acetone have been used to obtain the total extractive substances from plant raw materials ($\geq 99\%$ Merck KGaA, EMD Millipore Corporation), sorbent in column chromatography (II

³² Кузнецова, Г.А. Качественный рентгенофазовый анализ Методические указания/ Г.А. Кузнецова, – Иркутск: – 2005. – 28 с.

degree of activity, filled with neutral Al₂O₃ powder) and thin-layer plates (NTX) “Silufol-UV 254, silica gel 60 GF254 (Merck)” to check the individuality of the substances. The Stuart SMP10 device has been used to determine the melting temperature of individual substances, the “Varian Cary 50 Scan” spectrophotometer to record UV (ultraviolet spectra), and the “Bruker ALPHA IR-Fourier” device to record IR (infrared spectra). The optical rotation angle has been measured using a Rudolph Research Analytical digital polarimeter (model Autopol I, USA) (λ 589 nm) at 20°C.

In the study of the identified individual substances, nuclear magnetic resonance (1D) and (2D) NMR spectra have been recorded on a Bruker 300 and 500 spectrometer, at resonance frequencies of 300 and 500 MHz for ¹H, and at frequencies of 75 and 125 MHz for ¹³C. Deuterated dimethylsulfoxide and deuterium chloroform CDCl₃ have been used as solvents. Tetramethylsilane (TMS) has been used as an internal standard. The chemical shift has been field calibrated for deuterium chloroform solvent (¹H δ 7.27; ¹³C δ 77.0 ppm) and for dimethyl sulfoxide (¹H δ 2.5; ¹³C δ 39.52 ppm.).

X-ray structural analysis has been used to determine the crystal structure and isomerism of the studied compounds. The studied crystal has been immersed in cryo-oil and attached to a nylon loop, intensity data have been collected at 150 (2) K on a “Smart Apex II diffractometer” (Germany) using Mo K α radiation (λ =0.71073 Å). Diffraction experiments have been performed on a Bruker APEX II CCD diffractometer.

A BIOLAM-C microscope, MBC-1 binoculars, and an L74WIDE Samsung camera have been used in microscopic studies. Microbiological studies used (*Methicillin-sensitive Staphylococcus aureus* – MSSA, code: ATCC 700699; *Methicillin-resistant Staphylococcus aureus* MRSA, code: ATCC 29213; *Bacillus subtilis*, code: MIK, *Esherichia coli*, ATCC 25922; *Pseudomonas*, *Klebsiella* sp. 505562; *Candida albicans* ATCC 2091) microbial and fungal strains.

Japanese-made “JEM-1400” electron microscopes with an acceleration voltage of 80-120 kV have been used to examine stained and unstained ultra-sectioned microbiological preparations.

EXPERIMENTAL PART

CHAPTER III. PHYTOCHEMICAL STUDY OF THE SPECIES *FERULA PERSICA* WILD., *FERULA CAUCASICA* KOROVIN., *ARTEMISIA CAMPESTRIS* SUPSB. *MARSCHALIANA* (SPRENG.) ELENEVSKY & RADYGINA AND *ACHILLEA NOBILIS* L. DISTRIBUTED IN THE FLORA OF AZERBAIJAN

3.1. Study of the bioorganic chemical composition of the roots of *Ferula persica* Wild.

In the phytochemical study of the species *F. persica* and *F. caucasica* distributed in the flora of Azerbaijan, (1D) and 2D) NMR, GC-MS, X-ray structural analysis methods have been used.

3.1.1. Obtaining and studying the lipophilic fractions of sulfur-containing organic compounds

A thick yellow-greenish liquid mass with an oily, sharp odor has been obtained from fractions 5-15 of the hexane elution of the total extractive substances by column chromatography. The obtained lipophilic fraction has been analyzed by gas chromatography-mass spectrometry (GC-MS). The main predominated components as a result of the analysis are as follows: 1) Disulfide, bis(1-methylpropyl), 2) Thiophene, 2,3,4-trimethyl-, 3) 1,2-dithiolane, 4) 3,5-diethyl-1,2,4-trithiolane have been identified.

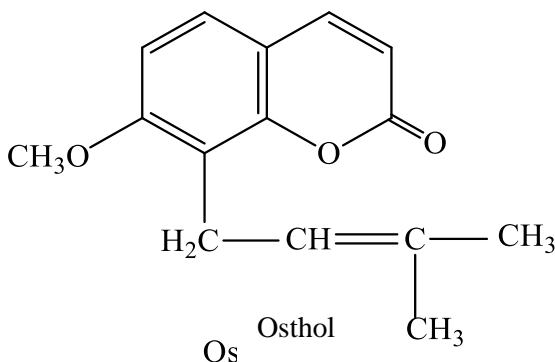
3.1.2. Identification of substance Fp-1 (Osthol)

A whitish-yellow crystalline substance has been obtained from fractions 22-30 of the glass column chromatography of the total extractive substances with ethanol residue, eluted with a mixture of hexane+benzene (7:3). By recrystallization (from aqueous ethanol), a substance with an elemental composition of $C_{15}H_{16}O_3$ and m.t. 84-85°C has been obtained individually.

$$[\alpha_{20}^D] = -13,3^\circ \text{ (c 0,60, } CHCl_3\text{)}.$$

In the UV spectrum λ_{max} , nm (EtOH) 212, 249, 258, 322 wavelength and in the IR spectrum (ν_{max} cm^{-1}) 3487 (OH group), 2922, 2855 (valent vibrational C-H bond CH_2 , CH_3), 1722, 1708 (CO- δ -lactone) 1608, 1555, 1507 $-C=C-$ in the aromatic nucleus), the absorption bands indicate that the compound is a sesquiterpenoid

derivative of coumarin. ^1H NMR spectrum (300 MHz, CDCl_3 , ppm, J/Hs): 1.67 (3H, s, H-5'), 1.84 (3H, s, H-4'), 3.55 (2H, d, J=7.2, H-1'), 3.92 (3H, s, $\text{CH}_3\text{O}-6'$), 5.25 (1H, t, J=7.3, H-2'), 6.25 (1H, d, J=9.6, H-3), 6.85 (1H, d, J=8.7, H-6), 7.31 (1H, d, J=8.7, H-5), 7.63 (1H, d, J=8.7, H-5). J=9.6, H-4). ^{13}C NMR spectrum (75MHz, CDCl_3 , δ , ppm): 161.43 (C=O, C-2), 112.97 (C-3), 143.80 (C-4), 126.23 (C-5), 107.35 (C-6), 160.21 (C-7), 117.93 (C-8), 112.97 (C-9), 132.66 (C-10), 21.92 (C-1'), 121.12 (C-2'), 152.80 (C-3'), 17.94 (C-4'), 25.81 (C-5'), 56.05 (CH_3O , C-6').



3.1.2.1. X-ray structural analysis of substance Fp-1 (Osthol)

The main crystallographic parameters and characteristics of the X-ray diffraction experiment. The crystal system is triclinic, the crystal size is 0.283x0.293x0.052 mm, the crystal bond accuracy C-C=0.0016 Å, the crystal lattice a=7.43628 (16), b=9.34450 (19), c=10.7464 (3), α =65.406 (2), β =74.647 (2), γ =70.3107 (19), temperature T=100K, h=1.54184. Based on the spectral data, the studied substance has been identified as osthol (7-methoxy-8-isopentenylcoumarin)³³ (Figure 1).

³³ Farozi, A., Shah A.Sh., Banday J.A. Structural and optical studies of 7-methoxy-8-(3-methylbut-2-enyl)-2-chromenone (osthol), a plant based coumarin // Optik, – 2016 v.127, – p. 2802-2805.

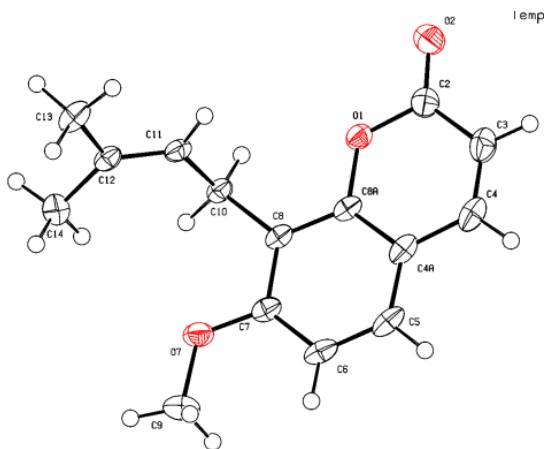


Figure 1. Spatial structure of substance Fp-1 (Osthol).

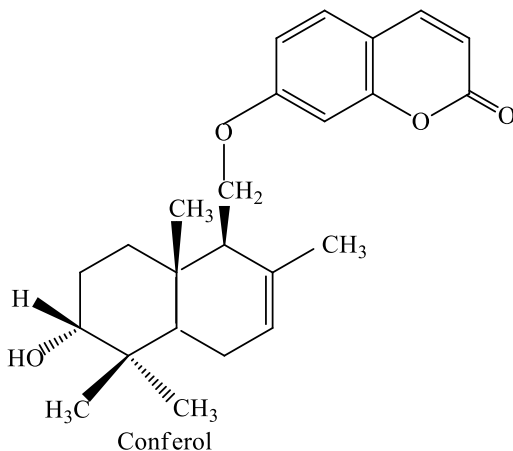
3.1.3. Identification of substance Fp-2 (Conferol)

A whitish-yellow mixed crystalline substance has been obtained from fractions 32-38 of the 1st glass column chromatography of the total extractive substances with ethanol residue, eluted with hexane+benzene. A white crystalline compound with elemental composition $C_{24}H_{30}O_4$ and m.t. 137-138°C has been obtained from fractions 20-25 of the secondary glass column chromatographed with the hexane. Crystallization (with aqueous ethanol) has been performed.

$$[\alpha]_{20}^D = -7,27^\circ \text{ (c 0,55, CHCl}_3\text{)}.$$

In the UV spectrum λ_{\max} , nm (EtOH): 212, 242, 258, 324 wavelength and in the IR spectrum ν_{\max} (cm^{-1}): 3487 (OH group), 2922, 2855 (valent vibrational C–H bond CH_2 , CH_3), 1722, 1708 (CO- δ -lactone) 1608, 1555, 1507 ($-\text{C}=\text{C}-$) in the aromatic nucleus), the absorption bands indicate that the compound is a sesquiterpenoid derivative of coumarin. ^1H NMR spectrum (300 MHz, CDCl_3 , ppm, J/Hz): 0.93 (3H, s, H-15'), 0.94 (3H, s, H-14'), 0.98 (3H, s, H-13'), 1.54 (1H, br. s, 3'-OH), 1.69 (2H, m, m, H-2'), 1.70 (3H, s, H-12'), 1.73 (1H, m, H-5'), 1.75 (2H, m, H-1'), 1.97 (2H, m, H-6'), 2.34 (1H, br.s, H-9'), 3.49 (1H, br. s, H-3), 5.56 (1H, m, H-7'), 4.03(1H, dd, J=9.6, 6.0, H-11'a), 4.18 (1H, dd, J=9.75, 3.45, H-11'b), 6.25 (1H, d, J=9.6, H-3), 6.82 (1H, s, H-8), 6.85 (1H, d, J=2.4, H-6), 7.36 (1H, d,

J=8.7, H-5), 7.64 (1H, d, J=9.3, H-4). ^{13}C NMR spectrum (75MHz, CDCl_3 , δ , ppm): 161.20 (C=O, C-2), 112.97 (C-3), 143.44 (C-4), 128.69 (C-5), 113.18 (C-6), 161.27 (C-7), 101.35 (C-8), 155.94 (C-9), 112.45 (C-10), 31.80 (C-1'), 25.15 (C-2'), 75.78 (C-3'), 37.20 (C-4'), 43.38 (C-5'), 23.21 (C-6'), 123.21 (C-7'), 132.51 (C-8'), 53.52 (C-9'), 35.64 (C-10'), 67.08 (CH_2O , C-11'), 22.36 (C-12'), 28.09 (C-13'), 21.74 (C-14'), 14.81 (C-15')³⁴.



3.1.3.1. X-ray structural and supramolecular Hirshfeld surface analysis of substance Fp-2 (Conferol)

Compound Fp-2 (Figure 2) consists of two trans-fused cyclohexane rings (C10–C14/C19 and C14–C19) connected to a chromen-2-one fragment via an oxymethylene bridge. Cyclohexane rings adopt C10–C14/C19 and C14–C19 semi-chair and chair conformations.

The parameters of the compound³⁵ are $QT = 0.5458 (15) \text{ \AA}$, $\theta = 49.18 (17)^\circ$ and $\varphi = 273.3 (2)^\circ$, and $QT = 0.5405 (15) \text{ \AA}$, $\theta = 9.33$

³⁴Вандышев, В.В. Конферол-новый кумарин из корней *Ferula conocaula* и *F. moschata* /В.В. Вандышев, Ю.Е. Скляр, М.Е. Перельсон [и др.] //Химия природных соединений, –1972. №5, –с. 670-671.

³⁵Cremer D., Pople, J.A. A general definition of ring puckering coordinates // *J. Am. Chem. Soc.*, –1975. v. 97, –p. 1354–1358.

(16)° and $\phi = 188.4$ (10)°, respectively, with an equatorial hydroxyl at C16 and an olefinic bond at C11–C12³⁶.

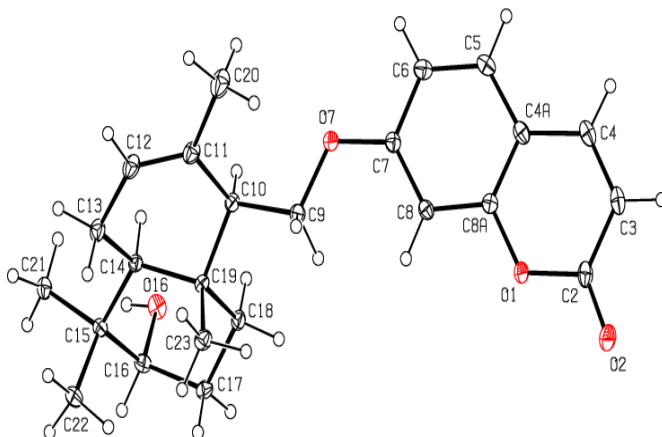


Figure 2. Molecular structure of compound *Fp-2* (Conferol) showing atomic labeling and displacement ellipsoids drawn at the 30% probability level. The small disorder component is omitted for clarity.

Supramolecular properties and Hirshfeld surface analysis. In the crystal, molecules are linked by C–H···O hydrogen bonds along the *c* axis to form layers parallel to the (010) plane, while molecules are linked by O–H···O hydrogen bonds along the *a* axis, forming R22(6) motifs (Figure 3)³⁷.

³⁶ Kerimli, E.H. Crystal structure and hirshfeld surface analysis of 7-((6- hydroxy-2,5,5,8a-tetramethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl) methoxy) -2h-chromen-2-one isolated from *Ferula persica*: A new enantiomorph at 100 K / E.H. Kerimli, S.J. Ibadullayeva, V.N. Khrustalev [et al.] // Химия растительного сырья, – 2024. №4. – с. 232–240.

³⁷ Bernstein, J. Patterns in Hydrogen bonding: functionality and graph set analysis in crystals / J. Bernstein, R.E. Davis, L. Shimoni [et al.] // Angewandte Chemie (Intern. ed. in Engl.), –1995. v. 34, –p. 1555–1573

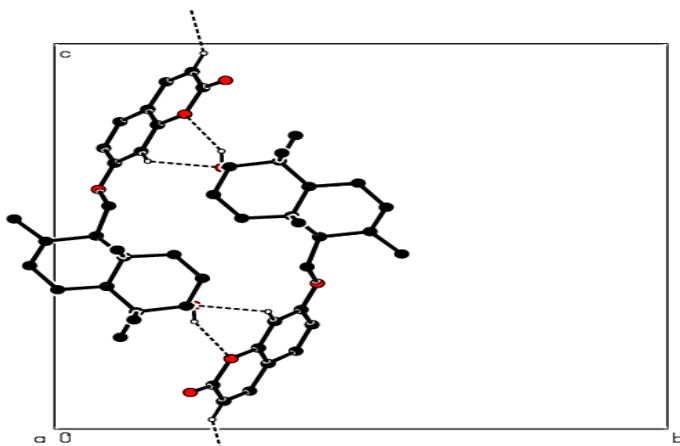


Figure 3. A view of the packing of the compound in question with O-H \cdots O and C-H \cdots O hydrogen bonds along the a-axis. For clarity, H atoms not involved in hydrogen bonding have been omitted.

The Hirshfeld surface is mapped onto the d_{norm} in the range -0.3269 to +1.7684 a.u. It shows intermolecular bonds as red spots indicating O-H \cdots O and C-H \cdots O hydrogen bonds (Figure 4).

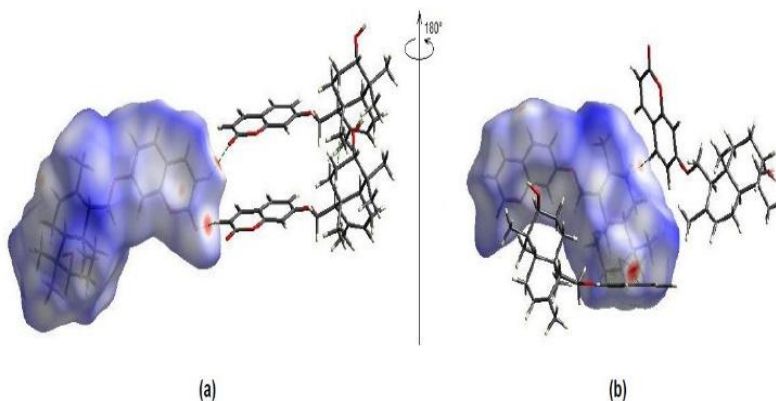


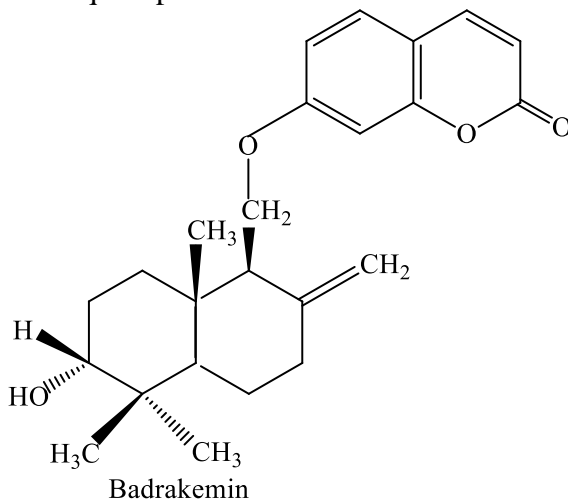
Figure 4. (a) Front and (b) back sides of the three-dimensional Hirshfeld surface of the compound in question, mapped onto d_{norm} with a fixed color scale from -0.3269 to +1.7684 a.u.

3.1.4. Identification of substance Fp-3 (Badrakemin)

A white crystalline compound with elemental composition $C_{24}H_{30}O_4$ and m.t. 198-199°C has been individually obtained from fractions 40-45 of glass column chromatography of the total extractives with residual ethanol eluted with hexane and benzene (1:1). Crystallization has been performed (with 96% ethanol).

$$[\alpha_{20}^D] = -60^\circ (c\ 0,1, CHCl_3).$$

In the UV spectrum λ_{max} , nm (EtOH) 208, 229, 326 wavelengths confirm that the studied compound is of coumarin nature. In the IR spectrum ν_{max} (cm^{-1}) 3609 (OH group), 2934, 2838 (valent vibrational C-H bond CH_2 , CH_3), 1725 (CO- δ -lactone) 1609, 1557, 1509, 1450 (in the aromatic nucleus – C=C–), absorption bands indicate that the compound is a sesquiterpenoid derivative of coumarin.



1H NMR spectrum (300 MHz, $CDCl_3$, ppm, J/Hz): 0.88 (3H, s, H-15'), 0.93 (3H, s, H-13'), 1.00 (3H, s, H-14'), 1.50 (2H, m, H-1'), 1.70 (2H, m, H-2'), 1.72 (1H, m, H-5'), 1.98 (br. s, 3'-OH), 2.14 (2H, m, H-6'), 2.15 (2H, m, H-7'), 2.34 (1H, br. s, H-9'), 3.49 (1H, br. s, H-3'), 4.17 (1H, dd, J=9.6, 7.7, H-11'a), 4.24 (1H, dd, J=9.6, 4.2, H-11'b), 4.54 (1H, s, H-12'), 4.91 (1H, s, H-12'), 6.25 (1H, d, J=9.6, H-3), 6.82 (1H, s, H-8), 6.85 (1H, d, J=2.4, H-6), 7.36 (1H, d, J=8.7, H-5), 7.64 (1H, d, J=9.3, H-4). ^{13}C NMR spectrum (75MHz, $CDCl_3$, δ , ppm):

161.33 (C=O, C-2), 112.91 (C-3), 143.53 (C-4), 128.73 (C-5), 113.22 (C-6), 162.35 (C-7), 101.35 (C-8), 155.90 (C-9), 112.40 (C-10), 31.80 (C-1'), 25.76 (C-2'), 75.74 (C-3'), 37.74 (C-4'), 146.74 (C-8'), 54.70 (C-9'), 38.81 (C-10'), 65.71 (CH₂O, C-11'), 107.59 (C-12'), 22.37 (C-13'), 28.60 (C-14'), 15.29 (C-15').

3.1.4.1. X-ray structural, supramolecular Hirshfeld surface analysis of substance Fp-3 (Badrakemin)

The studied substance Fp-3 C₂₄H₃₀O₄ 7-[(6-hydroxy-5,5,8a-trimethyl-2-methylenedecahydronaphthalen-1-yl)-methoxy]-2H-chromen-2-one (Figure 5) is composed of a chain of carbon atoms from two trans cyclohexane rings (C10–C14/C19 and C14–C19) connected to the chromen-2-one moiety via an oxymethylene bridge. Cyclohexane rings incorporate semi-chair and chair conformations. The folded angle parameters of the C10–C14/C19 carbon atoms are 56 , $Q_T = 0.550 (5) \text{ \AA}^\circ$, $\theta = 14.2 (5)^\circ$ and $\varphi = 292 (2)^\circ$; C14–C19-da $Q_T = 0.546 (5) \text{ \AA}^\circ$, $\theta = 5.1 (5)^\circ$ and $\varphi = 199(5)^\circ$ -degrees. The bond lengths and angles of compound Fp-3 are consistent with those of similar compounds reported in the database query section.

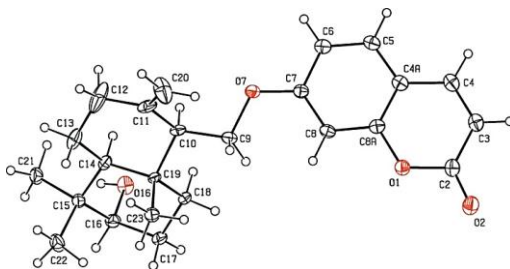


Figure 5. Molecular structure of substance Fp-3 (Badrakemin) showing atomic alignment and displacement ellipsoids drawn at the 30% probability level.

Supramolecular properties and Hirshfeld surface analysis. In the crystal, the molecules are connected by C-H...O and O-H...O hydrogen bonds to form a triperiodic network (Figure 6).

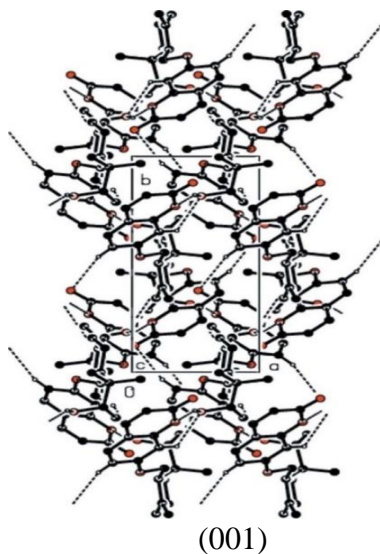


Figure 6. View of the crystal structure of substance Fp-3. O–H·O and C–H·O hydrogen bonds are shown by dashed lines (100) (Fleck parameter).

H atoms that are not involved in hydrogen bonding have been removed for clarity (Figure 7).

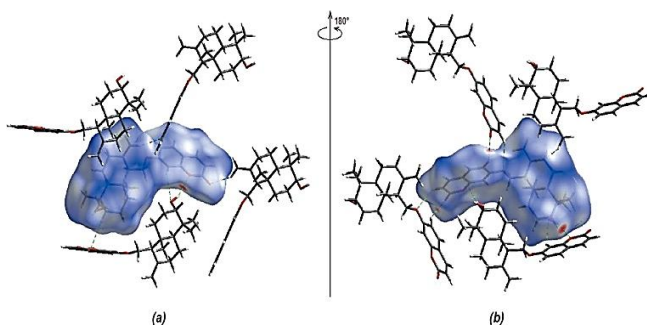


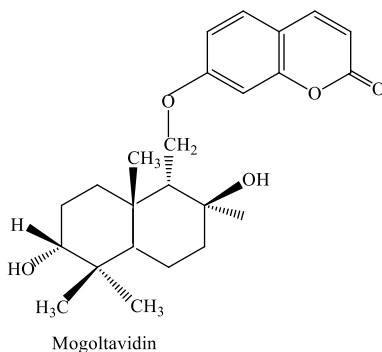
Figure 7. The (a) front and (b) back sides of the three-dimensional Hirshfeld surface of Substance Fp-3 mapped on the $dnorm$ in the fixed color scale from -0.2594 to +1.5213 a.u.

3.1.5. Identification of substance Fp-4 (Mogoltavidin)

A white crystalline substance with elemental composition $C_{24}H_{32}O_5$, and m.t. 157-159°C has been obtained from fractions 55-70 of primary glass column chromatography of the total extractives with residual ethanol, eluting with benzene solvent. Crystallization has been carried out with benzene.

$$[\alpha_{20}^D] = -3,63^\circ \text{ (c 1,1, CHCl}_3\text{)}.$$

In the UV spectrum λ_{\max} , nm (EtOH) wavelengths of 202, 260, 325 nm indicate that the studied compound is a terpenoid coumarin of the irezan type, a derivative of umbelliferone. In the IR spectrum, absorption bands ν_{\max} (cm^{-1}) 2922, 2855 (C-H bonds CH_2 , CH_3), 3630-3350 (OH group), 1721 (CO- δ -lactone), 1688, 1620, 1612, 1554, 1505 (double bonds of the aromatic nucleus) have been revealed. ^1H NMR spectrum (300 MHz, CDCl_3 , ppm, J/Hz): 0.85 (3H, s, H-14'), 0.98 (3H, s, H-13'), 0.95 (3H, s, H-15'), 1.23 (3H, s, H-12'), 1.53 (1H, m, H-5'), 1.58 (2H, m, H-6'), 1.69 (2H, m, H-1'), 1.88 (1H, s, H-9'), 1.90 (2H, m, H-2'), 1.93 (2H, m, H-7'), 2.34 (1H, br. s, 3'-OH), 3.43 (1H, br. s, H-3'), 4.15 (1H, dd, J=9.9, 5.7, H-11'a), 4.41 (1H, dd, J=9.9, 4.5, H-11'b), 6.25 (1H, d, J=9.6, H-3), 6.83 (1H, d, J=2.7, H-8), 6.89 (1H, dd, J=9.0, 2.4, H-6), 7.36 (1H, d, J=9.3, H-5), 7.64 (1H, d, J=9.3, H-4). ^{13}C NMR spectrum (75MHz, CDCl_3 , δ , ppm): 161.28 (C=O, C-2), 113.06 (C-3), 143.46 (C-4), 128.72 (C-5), 101.59 (C-6), 161.82 (C-7), 113.20 (C-8), 112.57 (C-9), 155.84 (C-10), 32.79 (C-1'), 25.13 (C-2'), 75.61 (C-3'), 37.45 (C-4'), 48.43 (C-5'), 19.97 (C-6'), 44.14 (C-7'), 72.61 (C-8'), 59.33 (C-9'), 37.88 (C-10'), 66.61 ($-\text{CH}_2\text{O}-$, C-11'), 24.65 (C-12'), 28.43 (C-13'), 22.11 (C-14'), 15.99 (C-15').

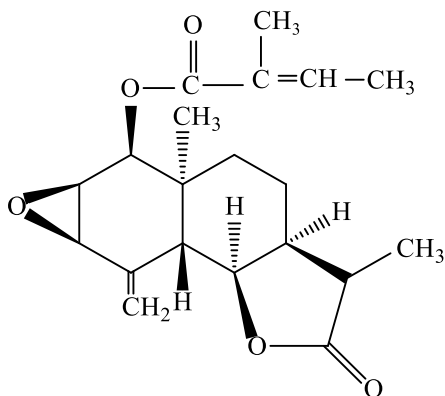


3.1.6. Identification of substance Fp-5 (Badkhysidin)

A yellowish-orange monocrystalline compound with elemental composition $C_{20}H_{26}O_5$, m.t. 111-117°C (1:10 in aqueous ethanol) has been obtained by crystallization from fractions 102-106 of glass column chromatography of the total extractive substances with residual ethanol, eluting with benzene-ethyl acetate (8:2) solvents.

$[\alpha_{20}^D] = -8,9^\circ$ (c 0,45, $CHCl_3$).

In the UV spectrum λ_{max} , nm (EtOH) 224, 229 and 232 wavelengths indicate the presence of conjugated double bonds in the studied compound. In the IR spectrum, absorption bands are detected, characterizing the carbonyl of the γ -lactone cycle (1761 cm^{-1}), α , β -unsaturated ester (1704 and 1233 cm^{-1}), and double bond (1644 cm^{-1}). 1H NMR spectrum (300 MHz, $CDCl_3$, ppm, J/Hz): 0.87 (3H, s, H-15), 1.11 (1H, m, H-9), 1.25 (3H, d, $J=6.7$, H-12), 1.60 (2H, m, H-8), 1.93 (3H, t, $J=1.5$, H-5'), 2.10 (3H dt, $J=7.0, 2.0$, H-4'), 2.50 (1H, dt, $J=9.6, 2.0$, H-2), 2.67 (1H, m, H-11), 2.77 (1H, m, H-7), 3.66 (1H, t, $J=2.0$, H-2), 3.66 (1H, t, $J=2.0$, H-3), 4.62 (1H, m, H-1), 4.80 (1H, dd, $J=9.0, 7.5$, H-6), 5.42 (1H, $J=1.8$), 5.59 (1H, $J=2.1$, H-14), 6.10 (1H, m, H-3'). ^{13}C NMR spectrum (75MHz, $CDCl_3$, δ , ppm): 74.43 (C-1), 58.18 (C-2), 52.32 (C-3), 127.24 (C-4), 38.91 (C-5), 77.52 (C-6), 37.41 (C-7), 19.35 (C-8), 31.45 (C-9), 36.28 (C-10), 37.29 (C-11), 179.56 (C=O, C-12), 12.26 (C-13), 118.38 (C-14), 21.87 (C-15), 167.30 (-O-C=O, C-1'), 140.71 (C-2'), 139.41 (C-3'), 15.88 (C-4'), 20.70 (C-5').



Badkhysidin

3.1.6.1. X-ray structural and supramolecular Hirshfeld surface analysis of compound Fp-5 (Badkhysidin)

Crystal structure and Hirshfeld structural analysis of the compound (5a*S*,8a*R*)-3,5a-dimethyl-8-methylidene-2-oxododecahydrooxyreno [2',3':6,7] naphtho [1,2-*b*]furan-6-yl(*Z*)-2-methylbut-2-enoate identified from *Ferula persica* roots. A view of the molecular structure of the Fp-5 compound is shown (in Figure 8). The cyclohexane rings (A: C3A/C4/C5/C5A/ C9A/C9B; B: C5A/C6–C9/C9A) adopt tub and semi-chair conformations, respectively. The bending parameters of rings A and B are $Q_T = 0.7259$ (19) Å, $\theta = 83.29$ (15)°, $\gamma = 51.45$ (15)°, and $Q_T = 0.5337$ (18) Å, $\theta = 52.1$ (2)°, $\gamma = 331.7$ (3)°, respectively³⁸.

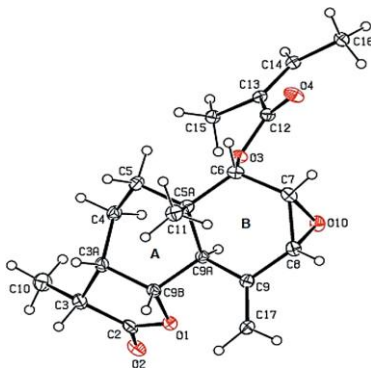


Figure 8. Molecular structure of the compound Fp-5 (Badkhysidin), showing atomic labeling and displacement ellipsoids drawn at the 30% probability level.

“*CrystalExplorer17*” has been³⁹ used to calculate the Hirshfeld surfaces of the molecule of compound Fp-5 (Badkhysidin). The d_{norm}

³⁸ Spackman P.R., Turner M.J., McKinnon J.J. *CrystalExplorer*: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals / P.R. Spackman, M.J. Turner, J.J. McKinnon [et al.] // *J. Appl. Cryst.*, 2021. v. 54, – p. 1006–1011.

³⁹ Karimli, E.G. Crystal structure and Hirshfeld surface analysis of (5a*S*,8a*R*)-3,5a-dimethyl-8-methylidene-2-oxododecahydrooxyreno [20,30:6,7] naphtho[1,2-*b*]furan-6-yl (*Z*)-2-methylbut-2-enoate extracted from *Ferula persica* / E.G. Karimli, V. N. Khrustalev, M.N. Kurasova [et al.] // *Acta crystallographica. Section E*, –2023. v. 79, – p. 474–477.

maps for the molecule have been performed in the range of -0.1633 to +1.3364 a.u. The C—H···O interaction sites are indicated by dense red circles on the d_{norm} surface (in Figure 9).

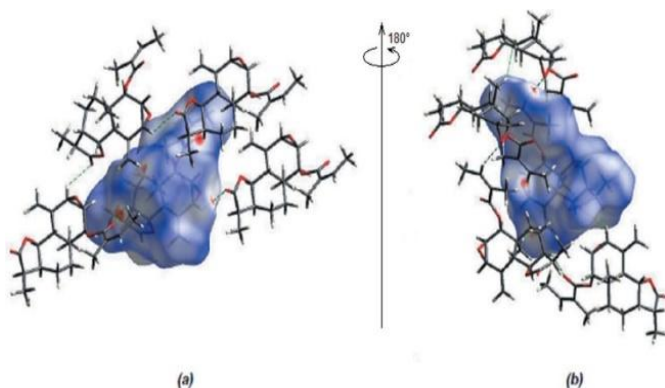


Figure 9. (a) Front and (b) back sides of the three-dimensional Hirshfeld surface of the compound Badkhysidin, mapped onto d_{norm} with a fixed color scale from a,b -0.1633 to +1.3364 a.u.

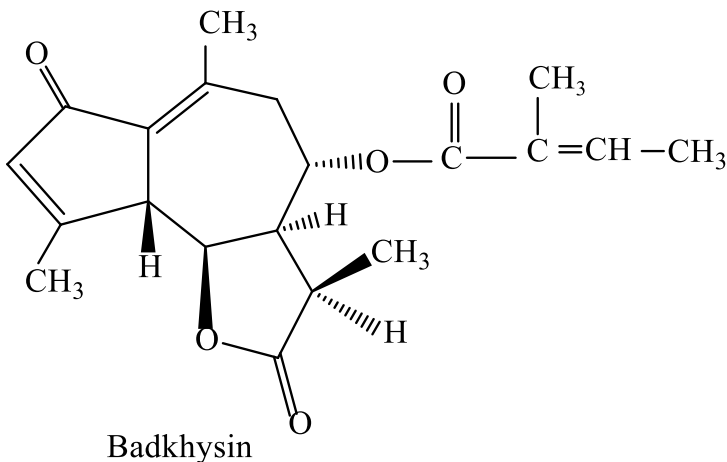
3.1.7. Identification of substance Fp- 6 (Badkhysin)

A yellowish crystalline compound has been obtained from fractions 10-15 of primary glass column chromatography of the total extractives with residual ethanol, eluting with benzene solvent. A colorless crystalline compound with elemental composition $C_{20}H_{24}O_5$, and m.t. 139-140°C (in aqueous ethanol) has been obtained from fractions 30-35 of secondary repeated glass column chromatography of the obtained yellowish crystalline compound, eluting with hexane-benzene (7:3) solvent.

$[\alpha]_{20}^D = +30^\circ$ (c 0,1, $CHCl_3$).

In the UV spectrum (λ_{max} , nm (EtOH): 234, 249, 255 wavelengths indicate the presence of a conjugated double bond in the cycle of the compound. In the IR spectrum ν_{max} (cm^{-1}): related to asymmetric and symmetric valence vibrations) absorption bands related to C-H bonds CH_3 , (2962, 2916), CH_2 (2848); 1765 (CO-group of the lactone cycle), 1706 and 1234 (α and β unsaturated ester group angelic acid), 1681 (CO group conjugated to a five-membered cycle (cyclopentanone)) and 1638, 1615 (double bond) are revealed.

^1H NMR spectrum (300 MHz, CDCl_3 , ppm, J/Hz): 1.35 (3H, d, $J=7.8$, H-13), 1.89 (3H, st, $J=1.5$, H-5'), 2.26 (3H, s, H-14), 2.28 (3H, s, H-15), 2.32 (1H, ddd, $J=18.9, 9.0, 3.6$, H-11), 2.52 (2H, dd, $J=18, 9.3$, H-9), 2.88 (1H, m, H-7), 3.61 (1H, d, $J=10.5$, H-5), 4.46 (1H, dd, $J=10.5, 8.1$, H-6), 5.50 (1H, td, $J=9.9, 3.9$, H-8), 6.18 (1H, m, H-3'), 2.01 (3H, dd, $J=8.7, 1.5$, H-4'), 6.18 (1H, m, H-3). ^{13}C NMR spectrum (75MHz, CDCl_3 , δ , ppm): 166.75 (C-1), 195.26 (C=O, C-2), 135.38 (C-3), 145.59 (C-4), 49.06 (C-5), 80.76 (C-6), 37.21 (C-7), 67.05 (C-8), 43.54 (C-9), 126 (C-10), 45.11 (C-11), 178.03 (C=O lactone carbonyl) C-12), 13.26 (C-13), 19.67 (C-14), 20.21 (C-15), 169 (-COO, C-1), 129 (C-2'), 140 (C-3'), 15.89 (C-4'), 20.48 (C-5').

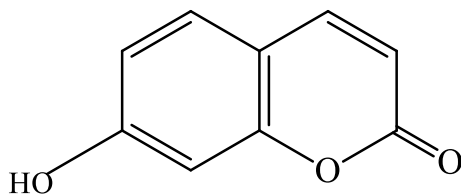


3.1.8. Identification of substance Fp-7 (Umbelliferone)

A dark-yellowish amorphous compound with elemental composition $\text{C}_9\text{H}_6\text{O}_3$, and m.t. $230\text{-}232^\circ\text{C}$ has been obtained by crystallization from the 90-100th fraction (benzene) of the glass column chromatography of the total extractive substances with ethanol residue, eluting with benzene-ethyl acetate (8:2) solvents.

$[\alpha]_{20}^D = -5,9^\circ$ (c 0,40, CHCl_3).

In the UV spectrum (λ_{max} , nm (EtOH): 218, 228, 327, 367 wavelengths indicate that the studied compound is a derivative of 7-oxycoumarin (umbelliferone).



Umbelliferone

In the IR spectrum ν_{\max} (cm^{-1}): absorption bands related to the C=O group of the δ -lactone cycle (1706), double bonds of the aromatic system (1678, 1624, 1603, 1566, 1508) have been revealed. ^1H NMR spectrum (500 MHz, DMSO- d_6 , ppm, J/Hz): 6,27 (1H, d, $J=9,6$, H-3), 7,65 (1H, d, $J=9,6$, H-4), 7,37 (1H, dd, $J_{\text{visinal}}=8,4$, $J_{\text{alil}}=2,3$, H-5), 6,85 (1H, d, $J_{\text{visinal}}=8,4$, H-6), 6,84 (1H, d, $J_{\text{alil}}=2,4$, H-8), 10,59 (1H, br. s., -OH-7). ^{13}C NMR spectrum (150 MHz, DMSO- d_6 , δ , ppm): 160,92 (C-2), 112,54 (C-3), 144,97 (C-4), 129,90 (C-5), 113,57 (C-6), 161,75 (C-7), 102,62 (C-8), 155,95 (C-9), 111,73 (C-10).

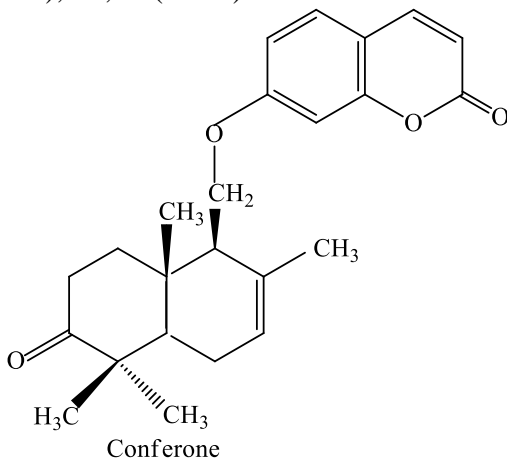
3.1.9. Identification of substance Fp-8 (Conferone)

A yellowish amorphous compound has been obtained from fractions 10-15 of the primary glass column chromatography of the total extractive substances with residual ethanol eluted with benzene solvent. A white amorphous compound with elemental composition $\text{C}_{24}\text{H}_{28}\text{O}_4$, and m.p. 140-142°C has been obtained from crystallization of fractions 5-20 (in aqueous ethanol) of the secondary repeated glass column chromatography of the obtained compound, eluting with hexane-chloroform (8:2) solvent.

Specific rotation angle of the substance $[\alpha_{20}^D] = -20^\circ$ (c 0,1, CHCl_3).

In the UV spectrum λ_{\max} , nm (EtOH): 205, 211, 214, 322 wavelengths indicate that the studied compound is a derivative of 7-oxycoumarin (umbelliferone). In the IR spectrum ν_{\max} (cm^{-1}): absorption bands related to the C=O group of the δ -lactone cycle (1724), the ketone group (1707) and the double bonds of the aromatic system (1610, 1558, 1508) have been revealed. ^1H NMR spectrum (500 MHz, DMSO- d_6 , ppm, J/Hz): 6,27 (1H, d, $J=9,6$, H-3), 7,65

(1H, d, J=9,6, H-4), 7,37 (1H, dd, $J_{\text{visinal}}=8,4$, $J_{\text{allil}}=2,3$, H-5), 6,85 (1H, d, $J_{\text{visinal}}=8,4$, H-6), 6,84 (1H, d, $J_{\text{allil}}=2,4$, H-8), 1,65 (2H, m, H-1'), 2,32 (2H, m, H-2'), 1,70 (1H, m, H-5'), 1,98 (2H, m), 5,62 (1H, m, H-7), 2,30 (1H, gen. s, H-9), 4,15 (1H, dd, $J_{\text{hem.}}=9,80$, $J_{\text{vis.}}=4,7$, H-11'a) 4,05 (1H, dd, $J_{\text{hem.}}=9,80$, $J_{\text{vis.}}=5,2$, H-11' b), 1,80 (3H, s, H-12'), 1,16 (3H, s, H-13'), 1,13 (3H, s, H-14'), 1,19 (3H, s, H-15'). ^{13}C NMR spectrum (150 MHz, DMSO-d₆, δ , ppm): 160,79 (C=O, C-2), 113,47 (C-3), 144,82 (C-4), 129,89 (C-5), 112,91 (C-6), 162,00 (C-7), 101,74 (C-8), 155,91 (C-9), 112,84 (C-10), 37,63 (C-1'), 34,56 (C-2'), 215,50 (C-3'), 47,21 (C-4'), 50,63 (C-5'), 23,83 (C-6'), 123,41 (C-7'), 133,06 (C-8'), 52,29 (C-9'), 35,73 (C-10'), 67,28 (C-11'), 25,49 (C-12'), 21,84 (C-13'), 22,30 (C-14'), 14,34 (C-15').

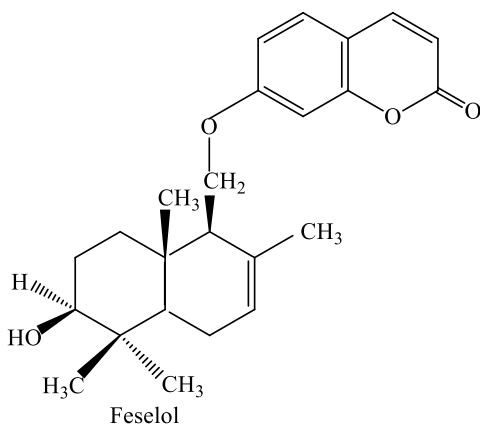


3.1.10. Identification of substance Fp-9 (Feselol)

A yellowish resinous compound has been obtained from fractions 52-55 of the primary glass column chromatography of the resin sum with ethanol residue eluting with benzene solvent. A needle-shaped white crystalline compound with elemental composition $\text{C}_{24}\text{H}_{30}\text{O}_4$, and m.p. 78-80°C has been obtained from fractions 21-30 (chloroform-hexane 2:8) of the secondary repeated glass column chromatography of the yellowish resin, eluting with hexane-benzene (8:2) solvent.

In the UV spectrum λ_{max} , nm (EtOH): 205, 211, 242, 230, 320

wavelength, in the IR spectrum ν_{\max} (cm^{-1}): The detection of absorption bands characteristic of the hydroxyl group (3628 cm^{-1}), the C=O group of the δ -lactone cycle (1724 cm^{-1}), and the double bond of the aromatic system ($1610, 1509 \text{ cm}^{-1}$) indicates that the compound is a coumarin derivative. ^1H NMR spectrum (500 MHz, DMSO- d_6 , ppm, J/Hz): 6,23 (1H, d, $J=9,5$, H-3), 7,65 (1H, d, $J=9,5$, H-4), 7,38 (1H, d, $J_{\text{visinal}}=8,4$, H-5), 6,85 (1H, dd, $J_{\text{visinal}}=8,4$, $J_{\text{alill}}=2,3$, H-6), 6,84 (1H, d, $J_{\text{alill}}=2,2$, H-8), 1,70 dd (2H, $J_1=15,3$, $J_2=4,0$, H-1'), 1,46 (2H, m, H-2'), 3,46 (1H, br. d. $J=11$, H-3'), 1,70 (1H, dd, $J_1=11,5$, $J_2=5$, H-5'), 1,98 (2H, br. m, H-6'), 5,62 (1H, br. s, H-7'), 2,30 (1H, br. s, H-9'), 4,21 (1H, dd, $J_{\text{hem}}=9,6$, $J_{\text{vis}}=3,0$, H-11'a), 4,10 (1H, dd, $J_{\text{hem}}=9,6$, $J_{\text{vis}}=5,5$, H-11'b), 1,75 (3H, s, H-12'), 1,03 (3H, s, H-13'), 0,95 (3H, s, H-14'), 0,94 (3H, s, H-15'). ^{13}C NMR spectrum (150 MHz, DMSO- d_6 , δ , ppm): 160,81 (C=O, C-2), 113,49 (C-3), 144,83 (C-4), 129,88 (C-5), 113,44 (C-6), 162,12 (C-7), 101,70 (C-8), 155,92 (C-9), 112,86 (C-10), 37,84 (C-1'), 27,61 (C-2'), 79,63 (C-3'), 39,94 (C-4'), 49,33 (C-5'), 23,39 (C-6'), 123,86 (C-7'), 132,87 (C-8'), 53,76 (C-9'), 35,79 (C-10'), 67,47 (C-11'), 22,69 (C-12'), 1,03 (C-13'), 0,95 (C-14'), 0,94 (3H, s, H-15').



3.1.11. Identification of substance Fp-10 (Badkhyisinin)

A yellowish resinous compound has been obtained from fractions 52-55 of the primary glass column chromatography of the total extractives with residual ethanol, eluting with benzene solvent.

3.2. Study of the bioorganic chemical composition of the fruits of the species *Ferula persica* Wild.

Three substances have been obtained from the fruits of the species *F. persica* through extraction and chromatographic methods.

3.2.1. Acquisition and study of bicyclic terpenoid coumarins Fp(M)-1 conferon, Fp(M)-2 conferol and Fp(M)-3 badrakemin

Three substances have been isolated from the fruits of *F. persica* by extractive and chromatographic methods. The compounds studied by UV, IR, 1D and 2D NMR spectroscopic methods have been identified as Fp(M)-1 conferon, Fp(M)-2 conferol and Fp(M)-3 badrakemin.

3.3. Acquisition and study of essential oil from the roots and fruits of *Ferula persica* Wild.

From the analysis of the essential oil obtained from the roots of *F. persica* by gas chromatography-mass spectrometry, 12 components have been identified. The main components of the essential oil of the roots are (Z)-1-Propenyl sec-butyl disulfide 41.0%, (E)-1-Propenyl sec-butyl disulfide 51.9%, Di-sec-butyl disulfide 2.2%, Bis-di-sec-butyl trisulfide 2%; in the essential oil of the fruits, (Z)-1-Propenyl sec-butyl disulfide 35.9%, (E)-1-Propenyl sec-butyl disulfide 38.4%, Di-sec-butyl disulfide 2.9% are organic sulfur compounds.

3.4. Study of the inorganic macro- and microelements composition of the roots and fruits of the species *Ferula persica* Wild.

The 23 elements have been identified in the roots and fruits of *F. persica* raw material, of which 12 are macroelements and 11 are microelements. In the composition of *F. persica* raw material, macroelements are more abundant in the roots (3.59% K, 2.99% Ca), and in the fruits (5.43% K, 2.09% S, 1.27% Ca), and microelements are more abundant in the roots (0.0276% Sr, 0.0211% Zn), and in the fruits (0.0895% Zn, 0.0314% Cu).

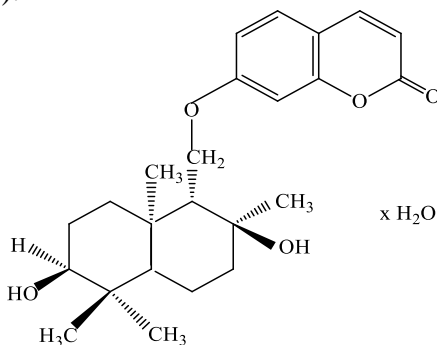
3.5. Study of the bioorganic chemical composition of the roots of the species *Ferula caucasica* Korovin.

Three substances have been identified from the roots of species

F. caucasica through extraction and chromatographic methods.

3.5.1. Acquisition and study of bicyclic terpenoid coumarins with Fc-1 conferon, Fc-2 conferol and Fc-3 samarcandin hydrate

Three substances: conferon, conferol, and samarcandin hydrate have been identified from the roots of *F. caucasica*. Fc-1 Conferon and Fc-2 Conferol are bicyclic terpenoid coumarins also obtained from the species *Ferula persica*. The spectroscopic results of these substances are given in subsections 3.1.3. and 3.1.9. Spectroscopic characteristics of Fc-3 samarcandin hydrate: UV spectrum (λ_{\max} , nm (EtOH): 212, 217, 219, 326. IR spectrum (ν_{\max} , cm^{-1}): 3431 (OH group), 2918, 2849 (valent vibrational C-H bond CH_2 , CH_3), 1703 (CO- δ -lactone) 1617, 1552, 1511, 1509 ($-\text{C}=\text{C}-$ in the aromatic nucleus), absorption bands indicate that the compound is coumarin. ^1H NMR spectrum (500 MHz, (CDCl_3 δ , ppm., J/Hz): 7.60 (1H, d, $J=9.0$, H-4), 7.3 (1H, d, $J=8.4$, H-5), 6.85 (1H, dd, $J=8.4$, $J=2.3$, H-6), 6.80 (1H, d, $J=2.4$, H-8), 6.18 (1H, d, $J=9.0$, H-3), 4.10 (1H, dd, $J=10.0$, 3.6, H-11'b), 4.10 (1H, dd, $J=10.0$, 6.5, H-11'a), 1.80 (2H, m, H-2'), 1.22 (2H, m, H-6'), 1.06 (3H, s, H-12'), 1.35 (1H, m, H-5'), 0.93 (3H, s, H-15'), 0.85 (3H, s, H-14'). 0.71 (3H, s, H-13'). Interpretation of the ^{13}C NMR spectrum of the compound: ^{13}C NMR (125 Hz, (CDCl_3 δ , ppm): 161.20 (C=O, C-2), 112.52 (C-3), 143.40 (C-4), 128.67 (C-5), 113.00 (C-6), 161.85 (C-7), 101.63 (C-8), 155.79 (C-9), 112.95 (C-10), 32.79 (C-1'), 25.14 (C-2'), 72.50 (C-3'), 37.42 (C-4'), 48.44 (C-5'), 19.97 (C-6'), 44.15 (C-7'), 72.52 (C-8'), 59.39 (C-9'), 37.89 (C-10'), 66.59 (C-11'), 22.09 (C-12'), 24.80 (C-13'), 15.63 (C-14'), 15.95 (C-15').



Samarcandin hydrate

X-ray structural analysis has been performed to determine the exact structure of the studied single-crystal compound (Figure 10).

Crystal lattice parameters: $a=10.79037(7)$, $b=13.02033(8)$, $c=15.27905$, $\alpha=90$, $\beta=90$, $\gamma=90$, temperature 100K, $M_r=402.30$, chemical formula $C_{24}H_{32}O_5$, $Z=4$, radiation type Cu Ka, $F_{000}=868$, $F_{000}'=870.65$; reflected numbers 4696,4687; h, k, l_{max} 13,16,19; $T_{min}=0.858, 0.870$; $3/2-x, 2-y, 1/2+z = 2_675$ Check. All H atoms bound to C atoms are geometrically positioned with C-H = 0.95 (aromatics), 0.99 (methylene), 0.98 Å (methyl) and 1.00 Å (methyne), with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for all other atoms.

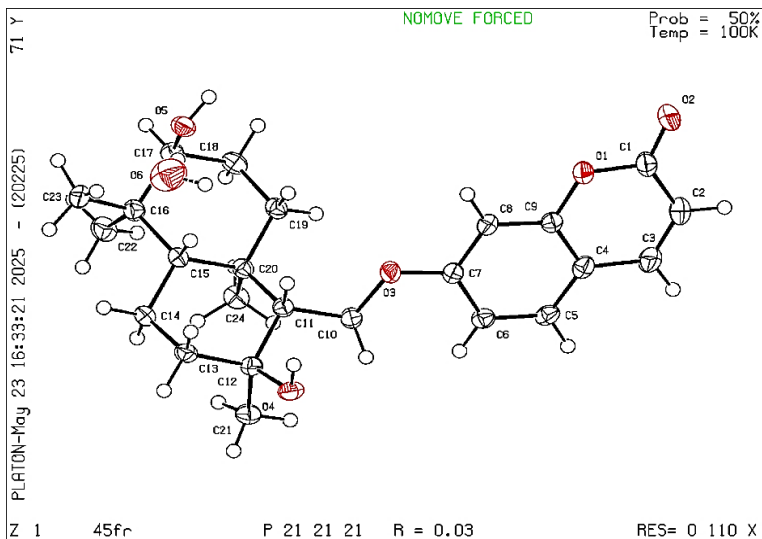


Figure 10. Molecular structure of the samarcandin hydrate, showing atomic labeling and displacement ellipsoids drawn at the 30% probability level.

3.6. Acquisition and study of essential oil from the roots and fruits of *Ferula caucasica* Korovin.

The 13 components have been identified from the analysis of the essential oil of *Ferula caucasica* roots by gas chromatography-mass spectrometry. The main components in the essential oil of the

roots are (Z)-1-Propenyl sec-butyl disulfide 45.9%, (E)-1-Propenyl sec-butyl disulfide 46.0%, Bis-di-sec-butyl trisulfide 2.5%; Di-sec-butyl disulfide 1.7%, in the essential oil of the fruits (Z)-1-Propenyl sec-butyl disulfide 51.2%, (E)-1-Propenyl sec-butyl disulfide 38.1%, Di-sec-butyl disulfide 1.3% are sulfur-containing organic compounds. Selina 3,7(11)-diene is predominant among sesquiterpenes of the selinane type in the fruits.

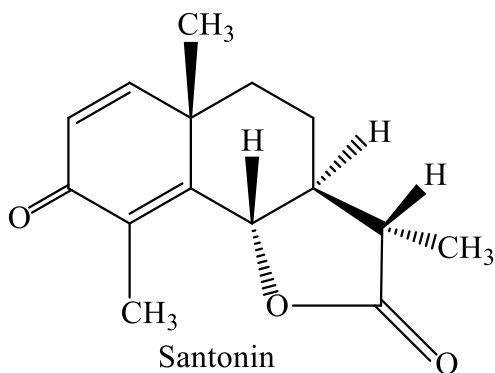
3.7. Study of the inorganic macro- and micronutrient composition of the roots and fruits of *Ferula caucasica* Korovin.

As a result of the analysis, 25 elements have been identified in the roots and fruits of the raw material, of which 12 are macroelements and 13 microelements. As shown in the table, the composition of the *F. caucasica* raw material contains 0.57% K, 0.60% Ca in the roots, 1.06% K, 0.50% Ca in the fruits, and 0.0035% Sr, 0.0017% Cr, 0.0016% Zn in the roots, and 0.0031% Zn, 0.0026% Cr, 0.0021% Zn in the fruits, which are more prevalent in percentage terms than other components.

3.8. Study of the chemical composition of the above-ground part of *Artemisia campestris* supsb. *marschalliana* (Spreng.) Elenevsky & Radygina

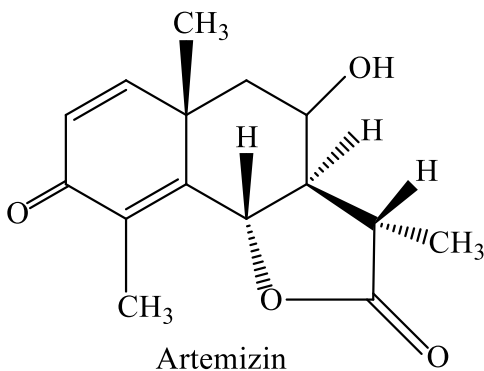
3.8.1. Identification of substance Am-1 (Santonin).

Interpretation results of Santonin: In the UV spectrum (λ_{\max} , nm (EtOH): 238 nm. In the IR spectrum (ν_{\max} , cm^{-1}): carbonyl of the γ -lactone cycle (1783), cyclohexenone (1658), conjugated double bond (1630) have been detected. ^1H NMR spectrum (300 MHz, CDCl_3 , ppm, J/Hz): 6.70 (1H d, J=9.9, H-1), 6.24 (1H d, J=9.9, H-2), 4.77 (1H, d, J=11, H-6), 1.5; 2.0 (1H, m, H-7), 1.4-1.9 (1H, m, H-8), 2.4 (dk, J₁=11.5; J₂=J₃=7, H-11), 1.25 (3H, d, J=6.00, H-13), 1.31 (3H, c, H-14), 2.11 (3H, c, H-15). ^{13}C NMR spectrum (75MHz, CDCl_3 , δ , ppm): 125.84 (C-1), 154.97 (C-2), 177.63 (C-3), 128.65 (C-4), 151.07 (C-5), 41.37 (C-6), 53.53 (C-7), 23.04 (C-9), 37.83 (C-10), 40.98 (C-10), 81.39 (C-11), 186.32 (C-12), 10.90 (C-13), 12.49 (C-14), 25.13 (C-15).



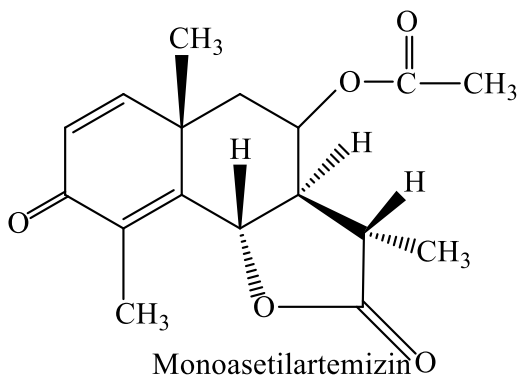
3.8.2. Identification of substance Am-2 (Artemisinin).

Results of artemisinin interpretation: UV spectrum (λ_{\max} , nm (EtOH): 245 nm. In the UV spectrum (ν_{\max} , cm^{-1}): Characteristic absorption bands at 3492 (OH-group), 1772 (C=O γ -lactone cycle), 1664 (C=O of hexenone cycle) and 1634 (conjugated double bond) are detected.



3.8.2.1. Identification of the acetyl derivative of Am-2 (monoacetylartemisinin)

Interpretation of monoacetylartemisinin: In the IR spectrum (ν_{\max} , cm^{-1}): 1780 (carbonyl of the C=O γ -lactone cycle), 1727, 1260 (acetyl group), 1651 (C=O cyclohexenone) and 1632 (conjugated double bond) characteristic absorption bands are detected.



3.9. Identification of essential oil from the aerial part of *Achillea nobilis* L.

As a result of gas-chromatographic mass spectrometric analysis, 35 components have been identified in the composition of *A. nobilis* essential oil. This constitutes 89.916% of the total oil. The main predominant components of the essential oil are the following: artemisinin ketone (23.706%), α -thujone (22.400%), β -thujone (2.933%), 2-bornanone (6.367%), lavandulol (2.975%), terpinen-4-ol (1.715%), limonen-6-ol pivalate (1.188%), cubenol (3.317%), β -eudesmol (2.702%), methylquinoate (2.108%).

CHAPTER IV. STUDY OF THEORETICAL CALCULATIONS OF IDENTIFIED INDIVIDUAL SUBSTANCES AT THE QUANTUM CHEMICAL LEVEL, IN SILICO PREDICTION OF THEIR BIOLOGICAL ACTIVITIES AND TOXICITIES USING COMPUTER PROGRAMS

4.1. Quantum chemical calculation of osthol, badrakemin, conferol, mogoltavidin, badkhyzidin, badkhyisin substances

Chemical hardness of osthol, badrakemin, conferol, mogoltavidin, badxizidine, badxizine compounds studied for the first time, E_{HOMO} , E_{LUMO} orbitals, chemical softness (expresses the ability to attract electron flow), electronegativity, chemical potential, electrophilicity index, ionization potential, electron affinity (E_{ea})

have been defined (as the amount of energy released when an electron is bound to a neutral atom or molecule).

4.2. In silico prediction of biological activities and toxicities of osthol, badrakemin, conferol, mogoltavidin, badkhisidin, badkhisin substances using computer programs

According to predictions, 1) osthol substance has antispasmodic (78.0%) and anti-inflammatory (71.0%) activity in the urinary tract. LD50 is 2905 mg/kg. FDAMDD is 0.568 mmol/kg-bw/day. $Cl_{\text{plasma}} = 8.867$, $T_{1/2} = 0.721$. 2) Badrakemin: LD50 is 3200 mg/kg. $Cl_{\text{plasma}} = 10.062$, $T_{1/2} = 0.827$. 3) Konferol LD50: 3200 mg/kg, FDAMDD (FDA *Maximum recommended Daily Dose*) 0.711 mmol/kg-bw/day. Mogoltavidin: The substance has antineoplastic (76.0%) and hypolipemic (71.6%) activities. LD50 is 3200 mg/kg, FDAMDD is 0.818 mmol/kg-bw/day. $Cl_{\text{plasma}} = 10.488$, $T_{1/2} = 1.269$. 5) The LD50 of badxizin is 7 mg/kg. FDAMDD shows 0.365 mmol/kg-bw/day. $Cl_{\text{plasma}} = 11.509$, $T_{1/2} = 1.342$. 6) The substance badxizin has high cytostatic (93.3%) and antineoplastic (88.4%) activities. The LD50 is 452 mg/kg. FDAMDD shows 0.659 mmol/kg-bw/day. $Cl_{\text{plasma}} = 5.922$, $T_{1/2} = 1.457$.

CHAPTER V. RESERVE SCIENCE AND STUDY OF MORPHOLOGICAL-ANATOMICAL FEATURES OF THE SPECIES *FERULA PERSICA* WILD., *FERULA CAUCASICA* KOROVIN., *ARTEMISIA CAMPESTRIS* SUBSP. *MARSCHALIANA* (SPRENG.) ELENEVSKY & RADYGINA AND *ACHILLEA NOBILIS* L.

5.1. Distribution areas of the species *Ferula persica* Wild.

As a result of route reconnaissance studies, new distribution areas of *F. persica* have been identified. Geographic coordinates of the plant's distribution area have been recorded.

The areas where *F. persica* is distributed are Pirakashkul, Jangi, Maraza, and Jeyrankechmez villages of Gobustan district, Boyanat mountain area, Beshbarmag of Siyazan district, and Khanabad areas of Yevlakh district.

The average density of the mass distribution area of *F. persica* species in Gobustan has been determined. The density of the

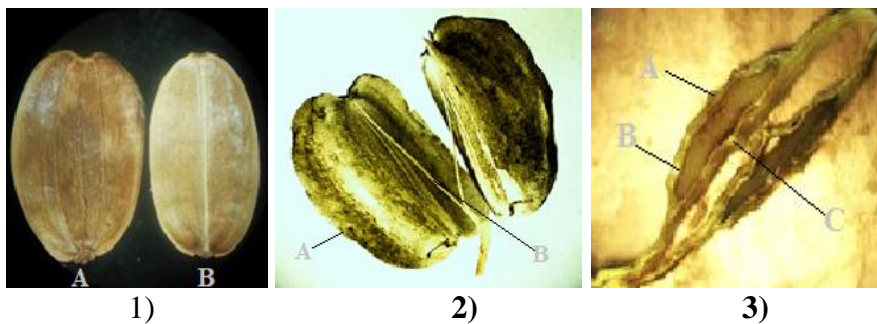
distribution area of this species in Jangi village of Gobustan is $122.4 \pm 14.6 \text{ m}^2$. It covers an area of $24 \pm 3.96 \text{ m}^2$ in Jeyrankechmaz village.

5.2. Determination of the optimal accumulation dynamics and storage time of biologically active substances in the roots and fruits of the species *F. persica* Wild.

The optimal accumulation dynamics of coumarins and essential oils in the roots and fruits of *F. persica* species have been determined. It has been found that the lowest amount of coumarins in the roots has been in the phase of full flowering (5%), and the highest amount in the phase of full ripening of the fruit (7.3%). Coumarins in the fruits have been collected more in the phase of full ripening of the fruit (9,53%). The maximum amount of essential oil is 0.78% in the roots and 0.72% in the fruits during the full ripening phase of the fruit. Also, changes in the total amount of coumarins and the amount of essential oils have been observed when storing the roots and fruits of the plant. This allows the raw material to be stored for 2 years.

5.3. Study of the morphological and anatomical characteristics of the roots and fruits of *Ferula persica* Wild.

Macroscopic and microscopic studies of the roots and fruits of *F. persica* raw material have been conducted. Four essential oil locations in the form of secretory canals are observed on the ventral side of the mericarp. Essential oil canals, conducting clusters and endosperm have been observed in the cross section of the fruit (Figure 11).



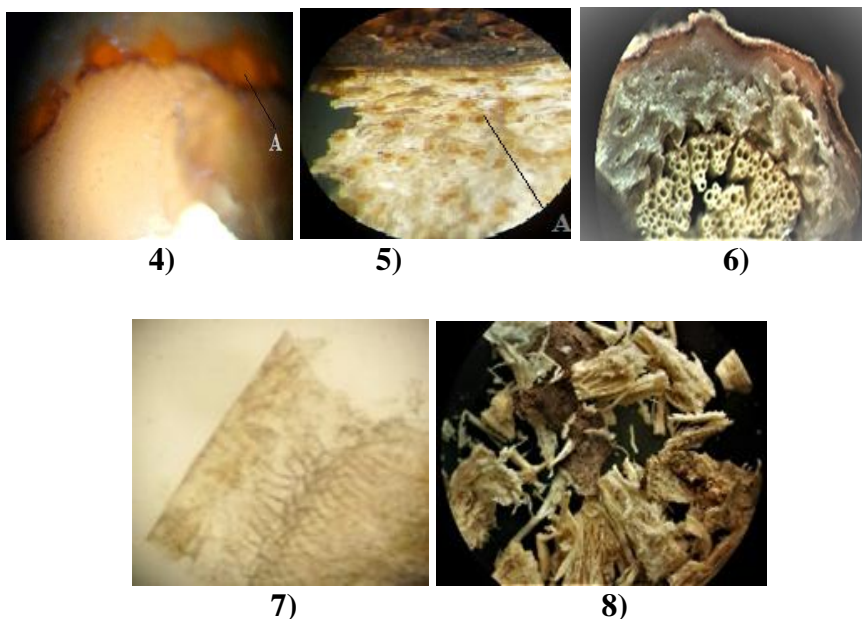


Figure 11. Macroscopic and microscopic characteristics of *F. persica* fruits and roots: 1) Fruit: A– primary three ribs dorsoventrally, B– ventrally. 2) two-mericarp fruit: A– mericarpia, B– divided into two commissural. 3) cross-section of fruit: A–conducting tubules, B– excretory tubules, C– intersection of mericarp commissural tubules. 4) excretory tubules of cross-section of mericarpia, A– essential oil tubules; 5) longitudinal section of root: A– schizogenous cells filled with essential oil and resin. 6) cross-section of root. 7) epidermis of mericarp margin. 8) shredded root.

5.4. Distribution areas of *Ferula caucasica* Korovin.

The distribution areas of the species *F. caucasica* have been identified in the areas of Godughgiran and Gizagi, Shikhlar village, Otmanbozdagh mud volcanoes, and the Gobustan State Historical and Artistic Reserve of the Gobustan district of the Republic of Azerbaijan. The designated areas are shown on the geographical administrative map of the Republic of Azerbaijan. The altitudes above sea level, geographical coordinates, and route distances of the designated areas have been noted.

The density of the distribution area of *F. caucasica* species in Arabgadim village of Gobustan district has been determined. The

density of the distribution area of the species around Godughgiran area of Arabgadim village is $204.75 \pm 20.5 \text{ m}^2$; in Yatag area – $40.54 \pm 7.8 \text{ m}^2$; in the Mid volcano area – $32.15 \pm 3.3 \text{ m}^2$; in Gizagi area – $200 \pm 12.5 \text{ m}^2$.

5.5. Determination of the optimal accumulation dynamics and storage time of biologically active substances in root fruits of the species *Ferula caucasica*

The sum of coumarins and optimal dynamics of accumulation of essential oil in the roots and fruits of *F. caucasica* have been determined, similar to those in *F. persica*. In the roots, the lowest amount of coumarins has been observed during full flowering (7.5%), while the highest amount has been recorded at the full fruit ripening stage (8.2%). In the fruits, coumarins have been accumulated at higher levels during full fruit ripening (8.7%). The amount of essential oils in both roots and fruits also reached its maximum at the full fruit ripening stage (0.77%). In roots: (0.77%), and in fruits: (0.60%). Also, the storage period of the raw material is 2 years.

5.6. Study of morphological and anatomical characteristics of the roots and fruits of the species *Ferula caucasica* Korovin.

Macroscopic and microscopic studies of the roots and fruits of *F. caucasica* have been carried out. In microscopic section, the shape of the mericarps is elliptical and flat. The primary ribs are clearly visible (one in the middle and two lateral) and are marginal. The primary ribs are located on the conducting tubercles, through which the excretory ducts pass..

5.7. Determination of the distribution areas and raw material reserves of *Achillea nobilis* L.

The distribution areas and raw material reserves of the *Achillea nobilis* species have been determined. The biological reserve of the raw material spread (dried in the open air) on a 4 ha area around the village Bayramli in Tovuz district is 62.4 ± 4 (kg), the exploitable quantity is 54.4 ± 3.49 (kg); the biological reserve of the raw material spread in the 3 ha area around the village Chek in Guba district is 53.4 ± 6.6 (kg), the exploitable quantity is 47.4 ± 5.86 (kg); the biological reserve of the raw material spread in the 3 ha area around the village Malham in Shamakhi district is 36.4 ± 5.96 kg, the

exploitable quantity is 24.48 ± 4 kg; the biological reserve of the raw material spread in the 1 ha area around the village Shikhlar in Gobustan district is 12.8 ± 2.26 kg, the exploitable quantity is 8.28 ± 1.46 kg.

5.8. Determination of the distribution areas and raw material reserves of *Artemisia campestris subsp. marschaliana* (Spreng.) Elenevsky & Radygina

The distribution areas and raw material reserves of *A. campestris subsp. marschaliana* have been determined. The biological reserve of raw materials dried in the open air spread on a 2 ha area around the village Otuzikilar in Imishli district is 41.2 ± 4.8 kg, the exploitable amount is 31.6 ± 3.68 kg; the biological reserve of raw materials spread on a 2 ha area around the village Garalar in Imishli district is 32.8 ± 4.4 kg, the exploitable amount is 24 ± 3.21 kg; the biological reserve of raw materials spread on a 1.5 ha area around the Yenikend HPP in Samukh district is 26.1 ± 2.4 kg, the exploitable amount is 21.3 ± 1.95 kg; the biological reserve of raw materials on a 4 ha area around the village Yukhari Tahirjal in Gusar district is 39.2 ± 5.6 kg, the exploitable amount is 28 ± 4 kg.

CHAPTER VI. STUDY OF THE BIOLOGICAL ACTIVITY OF OBTAINED SUBSTANCES

6.1. Antimicrobial and antifungal activities of the extract, essential oil and individual substances obtained from the roots and fruits of *Ferula persica* Wild.

The essential oil extracted from the root of *Ferula persica* has been very effective against the fungi *Pensillum spp.* (30 mm), *Aspergillus flavus* (24 mm). The absolute ethanolic alcoholic extract of the plant's root has been sufficiently effective against the fungi *Aspergillus flavus* (19 mm) and *Candida albicans* (18 mm). The individual substances had little or no activity against fungi. The essential oil of *Ferula persica* root has been effective against *Bacillus anthracoides* (25 mm), and the individual substances such as badkhyisin have been effective against Methicillin-sensitive *Staphylococcus aureus* MSSA (16 mm).

6.2. Antioxidant activities of substances extracted from the roots and fruits of *Ferula persica* Wild.

The antioxidant effects of essential oil extracted from the roots and fruits of *F. persica*, as well as the individually isolated coumarins osthol, badrakemin, conferol, mogoltavidin, and the sesquiterpene lactones eudesmanolide-type badkhysin and guaianolide badkhysin, have been studied. The results obtained have been poor.

6.3. Antimicrobial and antifungal activities of the extract, essential oil and individual substances obtained from the roots and fruits of the species *Ferula caucasica* Korovin.

The strains used to study the antimicrobial effects of substances obtained from the *F. persica* plant have been also experimentally tested on the *F. caucasica* species. The essential oil extracted from the root of *Ferula caucasica* inhibited the growth of *Aspergillus flavus* fungi 32 mm and *Penicillium* spp. fungi 30 mm in the field. The essential oil extracted from the fruit inhibited the growth of *Aspergillus flavus* 18 mm and *Candida albicans* 22 mm in the field. A 99% ethanol extract of the fruit of the plant has been effective against the fungi *Aspergillus flavus* (28 mm) and *Penicillium* spp. (22 mm). The antibacterial and antifungal effects of the individual substances have been weak.

6.4. Antioxidant activities of essential oil and extract from the roots and fruits of *Ferula caucasica* Korovin.

The antioxidant effects of essential oil isolated from *F. caucasica* and individual substances, conferol and samarkand hydrate bicyclic coumarins, have been studied. Based on the results of the study, it can be noted that the IC₅₀ indicator has been high. This indicates that the antioxidant activity of these compounds is weak.

6.5. Antimicrobial activity of essential oil obtained from the aerial part of *Achillea nobilis* L.

The antimicrobial effect of essential oils obtained from the aerial parts of *A. nobilis* has been studied by dilution method. When diluted 1:1 (0.085%) of the essential oil in 1.7% aqueous-alcoholic solution, it showed an effective effect against the test culture starting from the 10th minute of exposure. However, the effect against the yeast *C. albicans* has been weak.

6.6. Effect properties of the essential oil obtained from the aerial part of *A. nobilis* L. against SA bacteria at ultrastructural level

The effect properties of the essential oil obtained from the aerial part of *A. nobilis* against *Staphylococcus aureus* (SA) bacteria have been studied at ultrastructural level. In experimental studies, the following traits subject to ultrastructural changes have been observed in the cells of SA (*Staphylococcus aureus*) ATCC 25923 strains: disruption of the integrity and permeability of the plasmolemma, as well as structural changes in wall elements and cell partitions, mechanical deformation, and cell destruction, each of which is individually evaluated to be due to the bacteriostatic effect of the *A. nobilis* essential oil on MSSA strain. The loss of the overall negatively charged teicholic acid and peptidoglycan due to the action of *A. nobilis* essential oil on MSSA bacteria leads to the destruction of the adherent bacterial cell, surrounded by disintegrated structural wall elements.

6.7. Parasitological activities of essential oils obtained from the roots and fruits of *F. persica* Wild. and *F. caucasica* Korovin.

The parasitological effects of essential oils extracted from the roots of *F. persica* and *F. caucasica* have been studied. The 7.5 and 5% essential oil solutions of both plants in 96% ethyl alcohol had a time-dependent effect on ticks of the genus *Rhipicephalus*, paralyzing them. In the second experiment of parasitological studies, *Trichocephalus* eggs found in sheep feces have been treated with a solution of the essential oil of both plants in 96% ethyl alcohol. The results have been poor.

CHAPTER VII

PRACTICAL SIGNIFICANCE OF THE DISSERTATION

In our research, Osthol, Conferol, Badrakemin, Mogoltavidin, Umbelliferone, Conferone, Feselol, Badkhysidin, Badkhysin, Badkhysin, have been identified from the roots of *Ferula persica*

Three coumarins, conferon, conferol, and badrakemin, have been isolated from the fruits of this species.

Also, bicyclic sesquiterpenoid coumarins belonging to the samarkand group: conferon, conferol, samarkand hydrate have been

identified from the roots of *F. caucasica*, and sulfur-containing organic compounds from the essential oil of their roots and fruits.

Osthol has a number of interesting physiological properties. Osthol increases blood pressure, stimulates breathing, and has antibacterial activity. It is toxic to fish. Osthol inhibits the progression of breast cancer GNG7. It affects many types of tumors by inhibiting tumor cell proliferation⁴⁰. Studies have shown that osthol can also be used in the treatment of ovarian cancer in gynecological diseases.

As indicated in the literature, the cytotoxic activity of compounds such as conferol, badrachem, and mogoltavidin (IC50 - an indicator of the inhibitory effect of a substance on biochemical and biological objects) obtained from other species of the *Ferula* genus has been studied against HCT116 (human colorectal carcinoma cell line), Colo205, and (UO31 and A498) kidney cancer cell lines in colon culture. The inhibitory effect (> IC 50) has been effective⁴¹. It should also be noted that the amount of substances such as conferol, badrakemin, and mogoltavidin obtained from the roots of *Ferula persica* is sufficient in the plant. Thus, 100 g of raw material contains 1 g of isolated substances. Mogoltavidin has been tested in comparison with the sesquiterpene coumarin sildenafil citrate preparation. It has been found that the effect of this substance in stimulating male sexual activity is not inferior to this preparation sildenafil.

The resin extracted from *Ferula persica* roots has also shown therapeutic effects in Alzheimer's disease^{42,43}. The sesquiterpene lactone

⁴⁰ Mei, J. Osthole Inhibits Breast Cancer Progression through Upregulating Tumor Suppressor GNG7 / J. Mei, T. Wang, Sh. Zhao // Hindawi Journal of Oncology, – 2021. v. 2021, – p. 1-12.

⁴¹ Eruçar, F.M. Sesquiterpene coumarin ethers with selective cytotoxic activities from the roots of *Ferula huber-morathii* Peşmen (*Apiaceae*) and Unequivocal Determination of the Absolute Stereochemistry of Samarcandin / F.M. Eruçar, F.K. Kuran, G. Altıparmak Ülbeği // *Pharmaceuticals*, – 2023. v. 16, e792.

⁴² Ghadami, Sh. Oleo-Gum-Resin of *Ferula persica*: Phytochemical Analysis and Enzyme Inhibitory Activity Related to Alzheimer's Disease / Sh. Ghadami, M. Saeedi, R.M. Delnavazi [et al.] // *Journal of Pharmacognosy (RJP)*, – 2024. v.11, N4, – p. 39–48.

⁴³ Mohammadnezhad, P., Valdés A., Cifuentes A. Optimization and Chemical Characterization of Extracts Obtained from *Ferula persica* var. *latisecta* Aerial Parts and Roots and Their Neuroprotective Evaluation / P. Mohammadnezhad, P.A. Valdés, A. Cifuentes // *Nutrients*, – 2024, 16 (23), e 4210.

badkhsin has been isolated from the roots of *Ferula persica*, while this compound has been originally obtained from the species *Ferula oopoda*, which has been studied for its wound-healing, anti-burn, regenerative, and even nootropic effects.

The effect of the sesquiterpenoid coumarins badracemin on U87MG, A549 and PC3 cancer cells and healthy embryonic kidney cell lines HEK293 has been studied. In the studies conducted, it has been determined that the IC₅₀ of badrakemin on U87MG cell lines has been 9.92 μM and 11.85 μM. The cytotoxic effect of these compounds on healthy human embryonic kidney cells has been weak. The cytotoxic activity of the compound has been tested by comparing its inhibitory effect with 5-LOX, collagenase, and elastase⁴⁴.

The essential oil extracted from the roots and fruits of *F. persica* and *F. caucasica* showed effective activity against the fungi *Aspergillus flavus* and *Penicillium spp.*

Alpha santonin, which has anthelmintic effects, has been obtained from the *Artemisia campestris subsp. marschalliana* species.

The antimicrobial, antifungal, antioxidant, and parasitological effects of essential oils extracted from the roots and fruits of *F. persica* and *F. caucasica* species⁴⁵, as well as from the aerial parts of the *Achillea nobilis* plant, have been studied, which will contribute to the development of new medicines from the identified substances in the future⁴⁶.

⁴⁴ Tosun, F., Biltekin, S.N., Karadağ, A.E. Biological activities of the Natural coumarins from Apiaceae Plants / F.Tosun, S.N. Biltekin, A.E. Biltekin [et al.] // Rec. Nat. Prod., –2023. v. 17, N5, –p. 867-877.

⁴⁵ Kerimli, E. H., Kerimov, Yu. B., Shavarda, A.L. Constituent composition and antimicrobial activity of essential oil from roots and fruit of *Ferula caucasica* // Chemistry of Natural Compounds, – 2025, v. 61, N 3, – p. 606-607.

⁴⁶ Керимли, Э.Г. Изучение состава эфирного масла *Achillea nobilis* L. и его антибактериальное влияние на изменение ультраструктуры клеток *Staphylococcus aureus* / Э.Г. Керимли, Э.К. Гасымов, С.В. Серкерев [и др.] //Химия растительного сырья. –2021. №1, – с. 93–104.

RESULTS

1. For the first time, new ranges of *Ferula persica* and *F. caucasica*, rare species of Azerbaijani flora, have been identified. It has been found that the average density of the mass distribution of the *Ferula persica* species in the 20550 m² area of Jangi and Jeyrankechmez areas of Gobustan district is 146,4±18,56 m², and the average density of the mass distribution area of *F. caucasica* species in the areas around Godughiran, Yatag areas, Mid volcano, and Gizagi in the village Arabgadim of Gobustan district- 477,44±44,1 m². Also, raw material reserves of *Achillea nobilis* and *Artemisia campestris* subsp. marschaliana species have been identified. The biological reserve of the above-ground part of the raw material, dried in the open air and spread over 10 ha of the villages of Bayramli in Tovuz district, Chek in Guba district, and Malham in Shamakhi district, is 1165±16.56 kg, and the exploitable amount is 134.48±14.81 kg; the biological reserve of the above-ground part of the raw material, dried in the open air and spread over 9.5 ha of Otuzikilar and Garalar villages of Imishli district, Yenikend HPP of Samukh district and Yuxhari Tahirjal villages of Gusar district, is 139.3±11.66 kg, and the exploitable amount is 104.9±12.76 kg.

2. The optimal accumulation dynamics and storage time of the sum of coumarins and essential oils in the roots and fruits of *Ferula persica* and *F. caucasica* have been determined. The amount of coumarins and essential oil in the roots and fruits of both species has been found to be higher during the fully ripening phase of the fruit. The sum of coumarins in the root of the species *Ferula persica* is 7.3%, and in the fruits 9.53%, the amount of essential oil in the root - 0.78%, and in the fruits - 0.72%; the sum of coumarins in the root of the species *F. caucasica* is 8,2% and in the fruits 8.7%, the amount of essential oil in the root - 0.77%, and in the fruits - 0.60%;

3. For the first time, fifteen substances have identified from the component composition of the lipophilic fraction obtained from column chromatography of *F. persica* roots by gas chromatography-mass spectrometry (GC-MS). From other fractions, 10 individual substances have been identified: 1) Osthol; 2) Conferol; 3) Badrakemin;

4) Mogoltavidin; 5) Badkhysidin; 6) Badkhysin; 7) Umbelliferone; 8) Conferone; 9) Feselol; 10) Badkhysin; and from the fruits, three substances have been identified: Conferone, Conferol, and Badrakemin. Three individual substances: Conferon, Conferol, and Samarcandin hydrate have been identified from the roots of the species *F. caucasica*. Three substances have been isolated from the aerial parts of *Artemisia campestris subsp. marshalliana*: Santonin, Artemisinin, and a derivative of Monoacetylartemisinin.

4. As a result of the analysis of the essential oils obtained from the roots of the species *Ferula persica* and *F. caucasica* by gas chromatography-mass spectrometry the main (Z)-1-Propenyl sec-butyl disulfide, (E)-1-Propenyl sec-butyl disulfide, Di-sec-butyl disulfide, Bis-di-sec-butyl trisulfide and from the essential oil of fruits: (Z)-1-Propenyl sec-butyl disulfide, (E)-1-Propenyl sec-butyl disulfide and Di-sec-butyl disulfide, sulfur-containing organic compounds have been identified. As a result of the analysis of component composition of essential oil of *Achillea nobilis* by gas chromatography-mass spectrometry (GC-MS), the main predominant components have been determined to be artemisinin ketone (23.706%), α -thujone (22.400%), β -thujone (2.933%), 2-bornanone (6.367%), lavandulol (2.975%), terpinen-4-ol (1.715%), limonen-6-ol pivalate (1.188%), cubenol (3.317%), β -eudesmol (2.702%), methylquinolineate (2.108%).

5. Based on the analysis of the elemental composition of the roots and fruits of *Ferula persica*, 23 elements have been identified, of which 12 are macroelements, 11 - microelements. In the roots and fruits of *F. caucasica* raw material, 25 elements have been identified, of which 12 - macroelements and 13 - microelements.

6. As a result of morpho-anatomical studies, four essential oil locations in the form of secretory canals are observed on the ventral side of the mericarp in the longitudinal section of *Ferula persica* fruits. In the transverse section of the fruit, essential oil canals, conducting clusters, and endosperm are visible, in the transverse and longitudinal sections of the root, essential oil canals are observed.

7. During the study of the biological activity of the studied species against fungal and bacterial strains, the essential oil extracted from the root of *Ferula persica* has been found to be very effective against the

fungi *Penicillium* spp. (30 mm), *Aspergillus flavus* (24 mm), *Bacillus anthracoides* (25 mm) bacteria, and the individual components, badkhisinin very effective against *Methicillin-sensitive Staphylococcus aureus* MSSA (16 mm). The essential oil extracted from the roots of *F. caucasica* inhibited the growth of *Aspergillus flavus* fungi as 32 mm and *Penicillium* spp. fungi 30 mm in the field. The essential oil extracted from the fruit inhibited the growth of *Aspergillus flavus* 18 mm and *Candida albicans* 22 mm in the field. The 99% ethanol extract from the plant root and individual compounds had weak antibacterial and antifungal effects. All identified compounds had weak antioxidant activity. The disruption of the integrity of the plasmolemma in bacteria, structural changes in cell partitions, mechanical deformation, and cell destruction due to the action of essential oil obtained from the aboveground part of *Achillea nobilis* has been found to subject to bacteriostatic effects of the MSSA strain.

8. The parasitological effects of essential oils extracted from the roots of *Ferula persica* and *F. caucasica* have been studied. The 7.5 and 5% essential oil solutions of both plants in 96% ethyl alcohol had a time-dependent effect on ticks of the genus *Rhipicephalus*, paralyzing them. The 96% ethyl alcohol solution of the essential oil had a weak effect on *Trichocephalus* eggs.

RECOMMENDATIONS

1. The information provided on the chromatographic extraction of Osthonol, Conferone, Conferol, Badrakemin, Mogoltavidin, Badkhisidin, Badkhyisinin, and Badkhyisin compounds identified from the roots and fruits of *Ferula persica* and *F. caucasica* species, and the interpretation of UV-ultraviolet, IR-infrared, (1D) and (2D)-dimensional NMR spectra used in the study of these substances can be applied in the future for chemotaxonomic grouping of species belonging to these genera.

2. The biological activities determined as a result of studying the antifungal, parasitological and antibacterial effects of the species create conditions for conducting clinical research and developing medicines in this direction.

3. It is recommended to organize the reintroduction of the

species *Ferula persica* and *Ferula caucasica*, assessed as rare species in the “Red Book” of the Republic of Azerbaijan (2023), in new distribution areas and introduction in suitable areas as medicinal plant raw materials.

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