

## Identification and configuration study of the sesquiterpene coumarin mogoltavidin from the roots of *Ferula persica*

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**Abstract:** The genus *Ferula* L. (Apiaceae) has 130 species, widespread in the Caucasus, Central Asia, Siberia, China (Xinjiang), Afghanistan, Iran and North Africa. There are eight species of this genus in the Republic of Azerbaijan. The main part of the chemical substances of the plants of genus *Ferula* species are sesquiterpene coumarins, lactones, alcohol esters and essential oils. For the first time, a crystalline substance with the composition  $C_{24}H_{32}O_5$  with a melting point of 157-159°C was isolated from an ethanol extract of *Ferula persica* roots collected in the phase of full ripening of seeds using column chromatography. Based on spectral (UV)-ultraviolet, (IR)-infrared, (NMR)-nuclear magnetic resonance PMR and  $^{13}C$  NMR, DEPT and two-dimensional experimental methods COSY, HSQC, HMBC and physical indicators (polarometry, melting point) data, it has been proven that this substance has a structure identical to mogoltavidin. To determine the configuration of a substance in the PMR spectrum, were used which is a classical method the chemical shift and the value of the spin-spin interaction constant. The purpose of the current study was to identify the coumarin content of *F. persica* roots. Obtained results in the future can be assessed for identifying chemotaxonomic position of the species within the genus.

**Keywords:** chemical shift, sesquiterpen lactone, spin-spin interaction constant, Woodward-Fieser rules, UV, IR, NMR configuration

### INTRODUCTION

*Ferula persica* Willd. is a perennial herb belonging to the family Apiaceae (Umbelliferae), widely distributed in Central Asia, Iran, China, Afghanistan, Siberia and North Africa. The family is represented by 10 species in the Caucasus and eight species in Azerbaijan [Karyagin, 1955]. As it is known, *F. persica* is rich in biologically

active compounds such as essential oils [Kerimli et al., 2024; Javidnia et al., 2005], alkylated coumarin, complex esters, sterol [Kerimov et al., 1992], sulfur-containing compounds [Iranshahi et al.,], sesquiterpene coumarins [Kerimli et al., 2023], sesquiterpene coumarin glycosides [Iranshahia et al. 2008], sesquiterpene germacrene [Iranshahi et al., 2003] and eudesmanolide lactones [Karimli et al. 2023], phenol compounds [Stetskov et al. 1980; Nasri et al. 2018], etc. *F. persica* species is widely used in traditional medicine due to the richness of biologically active substances in its extract. Extracts and isolated compounds obtained from this species are used in cytotoxic, antibacterial, antifungal, leishmaniasis diseases, cancer chemoprevention [Sattar et al., 2017; Hashemi et al., 2021]. The dried juice of the plant is taken in the form of tincture, emulsion, pill, which is used in medicine as an antispasmodic in asthma, in diseases of the nervous system of various origins, homeopathy and folk medicine [Zemlinsky, 1958]. Osthol coumarin obtained from this species increases blood pressure, stimulates the respiratory system, has an antibacterial and is poisonous to fish [Kuznetsova, 1967].

This genus in Azerbaijan is distributed in Dzhangi of Gobustan district, Dzheyrankechmaz, Arabgadim, Maraza; Beshbarmag of Siyazan district, Pirekeshkul, Nardaran settlement, Gyuzdek of Absheron district, Daridagh of (Julfa, Nakhchivan AR) of Azerbaijan [Flora of Azerbaijan, 1955; Karimli et al., 2023]. The purpose of the current study was to identify the coumarin content of *F. persica* roots. Obtained results can be assessed for identifying chemotaxonomic position of the species within the genus.

### MATERIAL AND METHODS

**The research object.** The roots of *Ferula persica* were collected from the Jangi area (40°30'03.04" N 49°15'33.11" E; 356 m) of Gobustan settlement in the vicinity of Baku city. The specimens were collected during fruiting period on July 21, 2021.

**Isolation of substances.** The substances were isolated by the total extraction method (ethanol), and glass column chromatography was used to obtain the substances

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individually. Silufol-254 and silica gel 60 GF254 (Merck) thin-layer (20 x 5) adsorbent, benzene-ethylacetate (9:1) ratio solvent system were taken for the identification of the individuality of the substance. Melting temperature in Stuart SMP10 apparatus was 157-159°C. Iodine vapors and “Camag 254, 365 nm UV lamp” were used to detect spots on the plates. The optical rotation angle was measured with a Rudolph Research Analytical digital polarimeter (model Autopol I, USA) ( $\lambda$  589 nm) at 20°C. UV-spectra were recorded on “Varian Cary 50 Scan”, IR-spectra on a “Bruker ALPHA IR-Fourier” spectrophotometer.

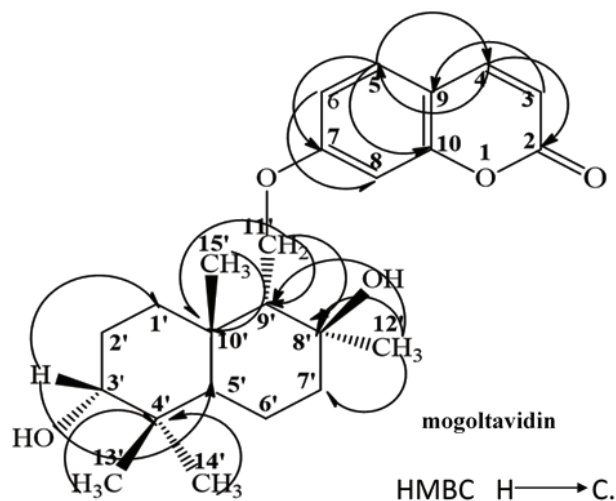
NMR  $^1\text{H}$  and  $^{13}\text{C}$  spectra (1D and 2D dimensions) were performed on a “Bruker Fourier-300” spectrometer at 300 MHz for  $^1\text{H}$  and  $^{13}\text{C}$  isotope taken in  $\text{CDCl}_3$  solvent at 75 MHz. Internal standard TMS-O, chemical shifts are given on the  $\delta$  scale. Chemical shifts s – singlet, d – doublet, d.d.– doublet, doublet, m – multiplet.

## RESULTS

**Obtaining the sum of extractives.** Two kg of dried, crushed roots extracted with ethanol alcohol ( $\geq 99\%$  Merck KGaA, EMD Millipore Corporation). Extraction process performed 3 times, each time for 1 day. The obtained extract is filtered, expelled through a rotary evaporator on a water bath (90°C). The amount of the obtained brown residue was 146 g. The yield for raw materials is 7.3%. The resin of 60 g was dissolved in a small amount of ethyl alcohol and chromatographed on a glass column (h=1m, d=3.5 cm) filled with neutral  $\text{Al}_2\text{O}_3$  with II activity according to Brockman. The ratio of resin and sorbent was in the ratio of 1:10. Chromatographic column was eluted with hexane (20 fractions), hexane+benzene (51 fractions, 9:1, 8:2, 7:3, 6:4, 1:1, 1:2, 1:3, 1:4 ratios), benzene (44 fractions), benzene+ethyl acetate (15 fractions 4:1, 3:2, 1:1) and ethyl acetate, ethyl acetate+alcohol (8 fractions 9:1, 8:2, 7:3).

The sesquiterpene coumarin compound was obtained individually as a result of the separation of the sum of extractive substances by chromatographic method. Identified compounds were determined by comparing spectral (UV, IR, NMR spectra) and physical constants (melting temperature, spin angle) described in the literature [Kerimli et al. 2023]. The studied compound is a bicyclic coumarin and consists of five asymmetric centers where the chiral carbon atoms belong to C3', C8', C9', C10', accepts R- or S-configuration. 3R, 8'S, 9'S, 10'R.

The element composition of the 55-70 th fraction eluted with benzene of the chromatography column is



**Figure 1.** Structure of mogoltavidin obtained from the roots of *Ferula persica*.

$\text{C}_{24}\text{H}_{32}\text{O}_5$  m.p. 157-159°C white crystalline substance was obtained (crystallization with benzene).  $\lambda_{\text{max}}$  (EtOH) wavelengths of 202, 260, 325 nm in the UV-spectrum indicate that the studied compound is an irezan-type terpenoid coumarin, a derivative of umbelliferone (Fig. 2).

According to the Woodward-Fieser rules, the maximum absorption wavelength of a molecule can be calculated. Thus, due to the conjugated double bond in the pyrone ring here, the molecule acquires the characteristic of a cyclic enone. The maximum absorption wavelength of the molecule can be calculated using the summation rule for cyclic enones. If cyclic enones are 6-membered, then the main maximum absorption wavelength of the molecule is assumed to be 215 nm. Each additional conjugated double bond increases by 30 nm, and alkyl groups (ring thickness) by 10, 12, and 18 nm, depending on the condition considering that a radical is attached to the 9th position of the molecule. This radical causes an increase of 18 nm. The maximum absorption wavelength of this molecule was calculated as follows according to L.Fiser, M. Fiser [1964].

$$\lambda_{\text{max}} = 215 + 18 (\text{Radical}) + 30 + 30 + 30 = 323 \text{ nm } \nu_{\text{max}} (\text{cm}^{-1})$$

$\nu_{\text{max}}$  of asymmetric and symmetric valence oscillations in the IR spectrum ( $\text{cm}^{-1}$ ) 2922, 2855 ( $\text{CH}_2$ ,  $\text{CH}_3$  with C-H bond), 3630-3350 (OH group), 1721 ( $\text{CO}-\delta$ -lactone), 1688, 1620, 1612, 1554, 1505 (double bonds of the aromatic core) absorption bands were clarified and compared with S.Serkerov et al. [2006] and L. Bellamy et al. [1963] (Fig. 3).

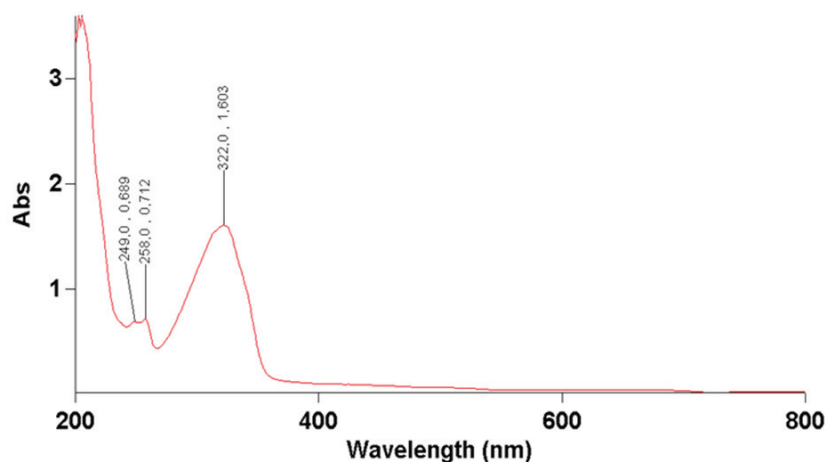


Figure 2. UV spectrum of mogoltavidin.

In the proton magnetic resonance (PMR) spectrum, one-proton signals belonging to the coumarin core are  $\delta_{\text{H}}$  6.26-7.64 ppm. detected in the interval. The 5-protonated signals correspond to the 7-substituted coumarin. In the diamagnetic field, singlet signals (0.85, 0.95, 0.98, 1.23 ppm.), each with an area equal to 3 proton units were detected: The singlet clarification of the signals characterizing the methyl groups that appear in the spectrum indicates that the methyl groups are connected to 4-substituted carbon atoms, that is, they are triple methyl groups. Of these, 0.85, 0.95, 0.98 ppm.

belong to 3 methyl groups signals corresponding to the C-10 and C-4 carbon atoms, 1.23 ppm. the singlet signal belongs to the triple hydroxyl group ( $\text{C}_8\text{-CH}_3$ ) located in the geminal position. The location of the hydroxyl group at the C-3 position was determined based on the HMBC NMR spectrum. Expanded singlet 3.43 ppm. signal ( $^1\text{H}$ ) refers to the proton of the gem hydroxyl group (H-C-OH). Total intensity fields equal to 2 proton units, centered (4.15 and 4.41 ppm.) 4.41 ( $J_{\text{gem}} = 9.9$ ,  $J_{\text{vic.}} = 4.5$  Hz) and 4.15 ( $J_{\text{gem}} = 9.9$  Hz,  $J_{\text{vic.}} = 5.7$  Hz) conditions  $\text{ArOCH}_2\text{-}$  group (Fig. 4).

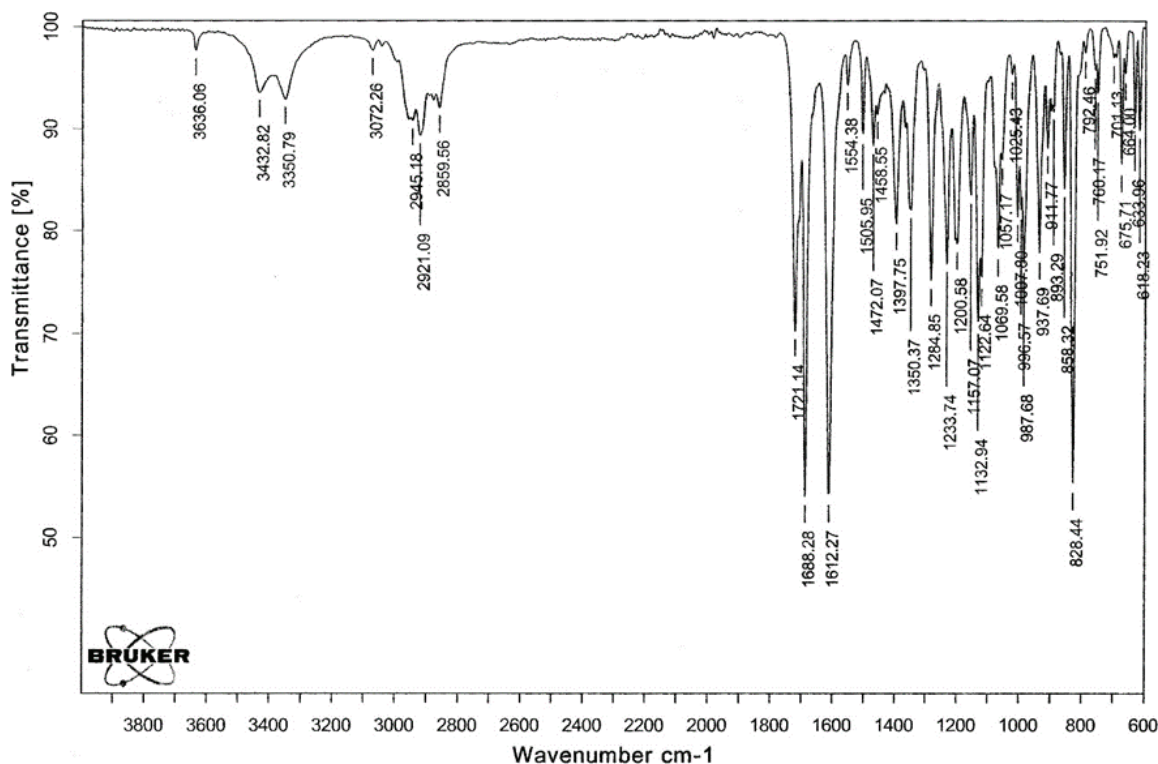


Figure 3. IR spectrum of mogoltavidin.

A  $^{13}\text{C}$  NMR spectrum was recorded to determine the number of carbon atoms in the molecule of the compound. In the  $^{13}\text{C}$  NMR spectrum 24 singlet signals characterizing the 24 carbon atoms in the molecule were detected (Fig.5).

In the  $^{13}\text{C}$  DEPT 135 spectrum, a total of 17 signals indicating the number of carbon atoms in hydrogen bonds were clarified (Fig. 6a). The carbon atoms that are not in a bond with hydrogen in the  $^{13}\text{C}$  DEPT 135

spectrum, as a rule, are not clarified, so the signals of the deprotonated carbon atoms in the molecule of the compound as detected are in the  $^{13}\text{C}$  NMR spectrum; 37.45 (C4'); 37.88 (C10'); 72.61 (C8'); 112.57 (C9); 155.84 (C-10); 161.28 (C7); 161.82 (C8) ppm. In the  $^{13}\text{C}$  DEPT 135 spectrum of the substance, 5 signals belonging to protonated olefin atoms of carbon were attributed to the coumarin nucleus, and 4 methyl ( $\text{CH}_3$ ), 5 methylene ( $\text{CH}_2$ ) and 3 methine ( $\text{CH}$ ) groups were attributed to the

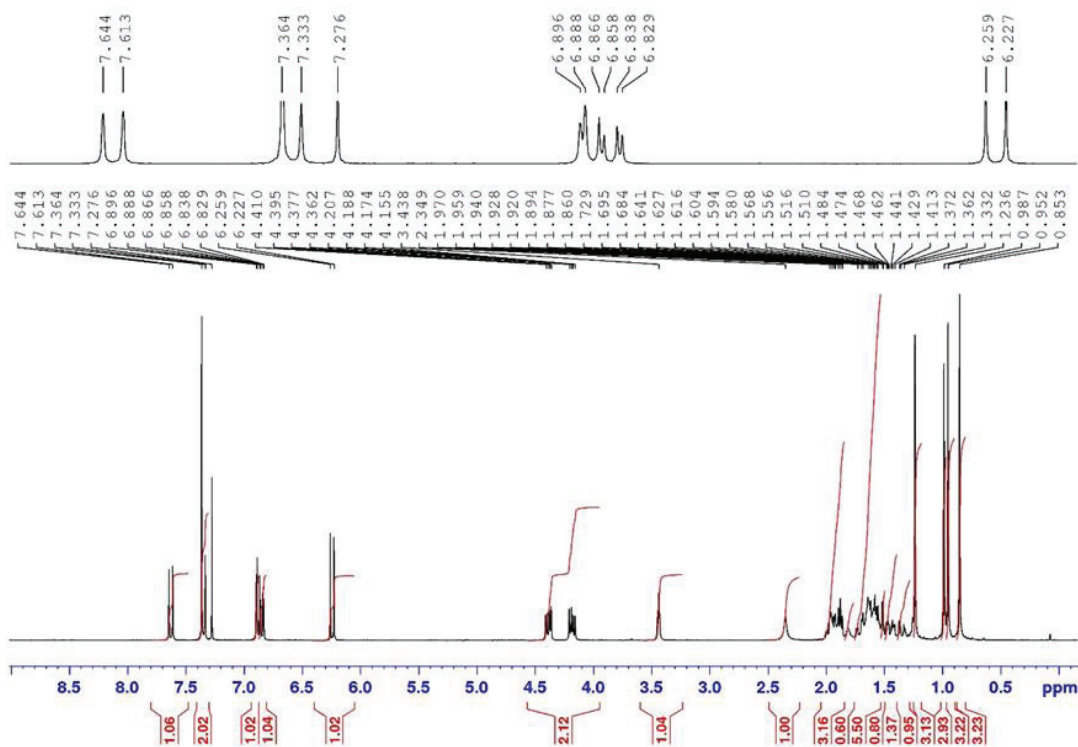


Figure 4. PMR spectrum of mogoltavidin.

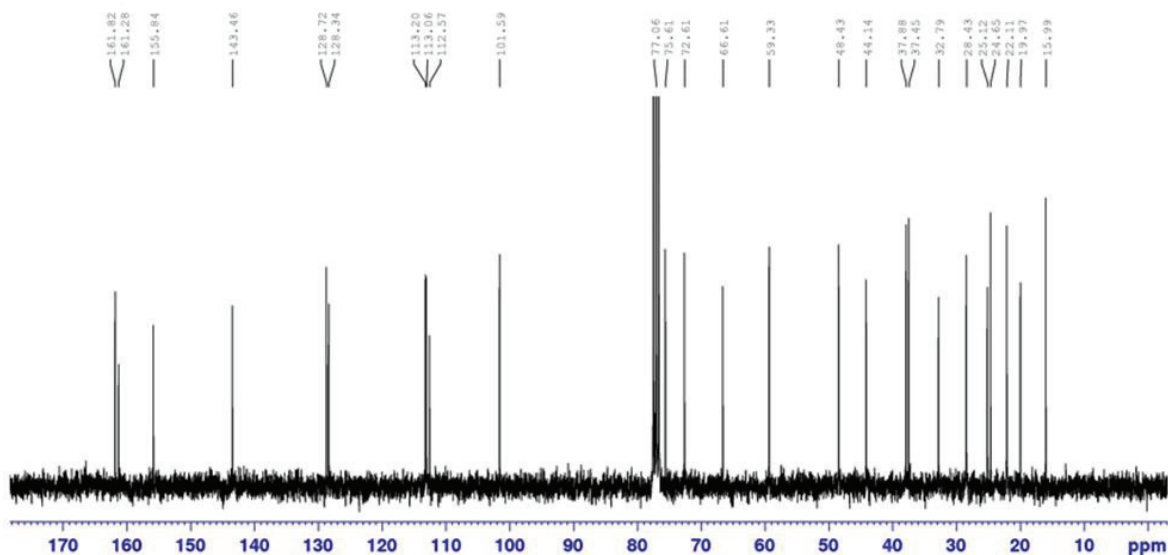
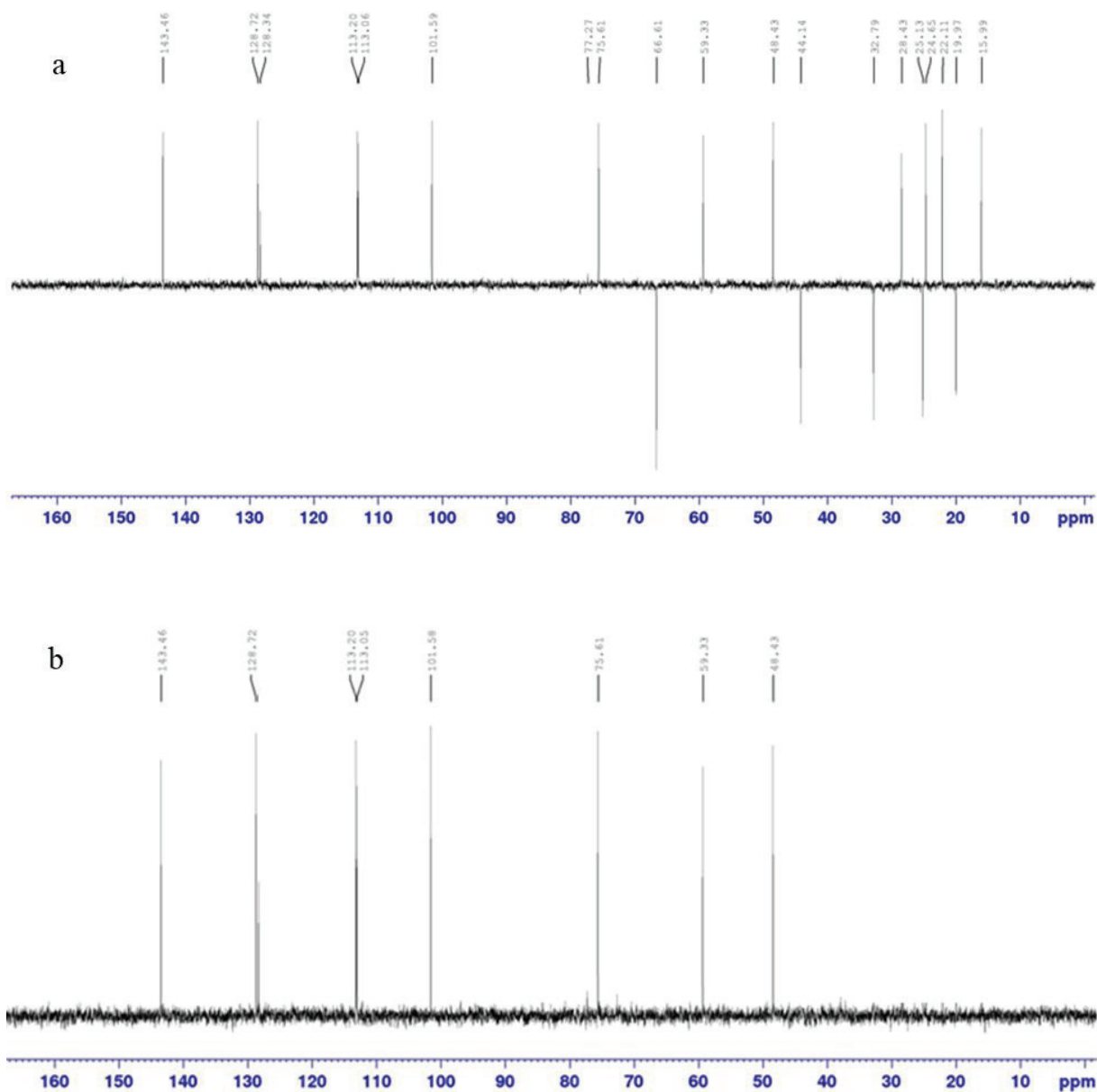


Figure 5.  $^{13}\text{C}$  NMR spectrum of mogoltavidin.



**Figure 6.**  $^{13}\text{C}$  DEPT 135 (a),  $^{13}\text{C}$  DEPT 90 (b) NMR spectrum of mogoltavidin.

terpenoid part. It proves the number of double-bonded and non-double-bonded text groups in the  $^{13}\text{C}$  DEPT. 90 spectrum (Fig. 6b). The molecule of the compound has two hydroxyl groups. Discussing the location of the hydroxyl (-OH) group in the molecule of the studied substance, let us note that one of the (-OH) groups is connected to the carbon atom of C-3 (75.61 ppm.) and the other to C-8' (72.61 ppm.) located in the geminal position. These are confirmed by the Heteronuclear Multiple Bond Correlation (HMBC) spectrum.

In determining the structure of the substance and clarifying the location of each functional group in the molecule, 2D (Fig. 6 a) Heteronuclear Single Quantum

Coherence (HSQC), b) HMBC, c) COSY spectra were used (Fig. 7). The data obtained from the interpretation of both 1D and 2D dimensional spectra are summarized and given in the table.

According to B. Tashkhodzhaev et al. [2015] the investigated compound has eight isomers (Fig. 8).

The IR spectrum of the isomers contains absorption bands in the range at  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) (3300-3500, 1720, 1610-1630, 1400-1550), and the mogoltavidin isomer additionally has a characteristic absorption band in area of  $1688 \text{ cm}^{-1}$  S. Serkerov et al. [2006].

Based on comparisons of spectroscopy, melting point, and polarimetry, compound 2 is an umbelliferone

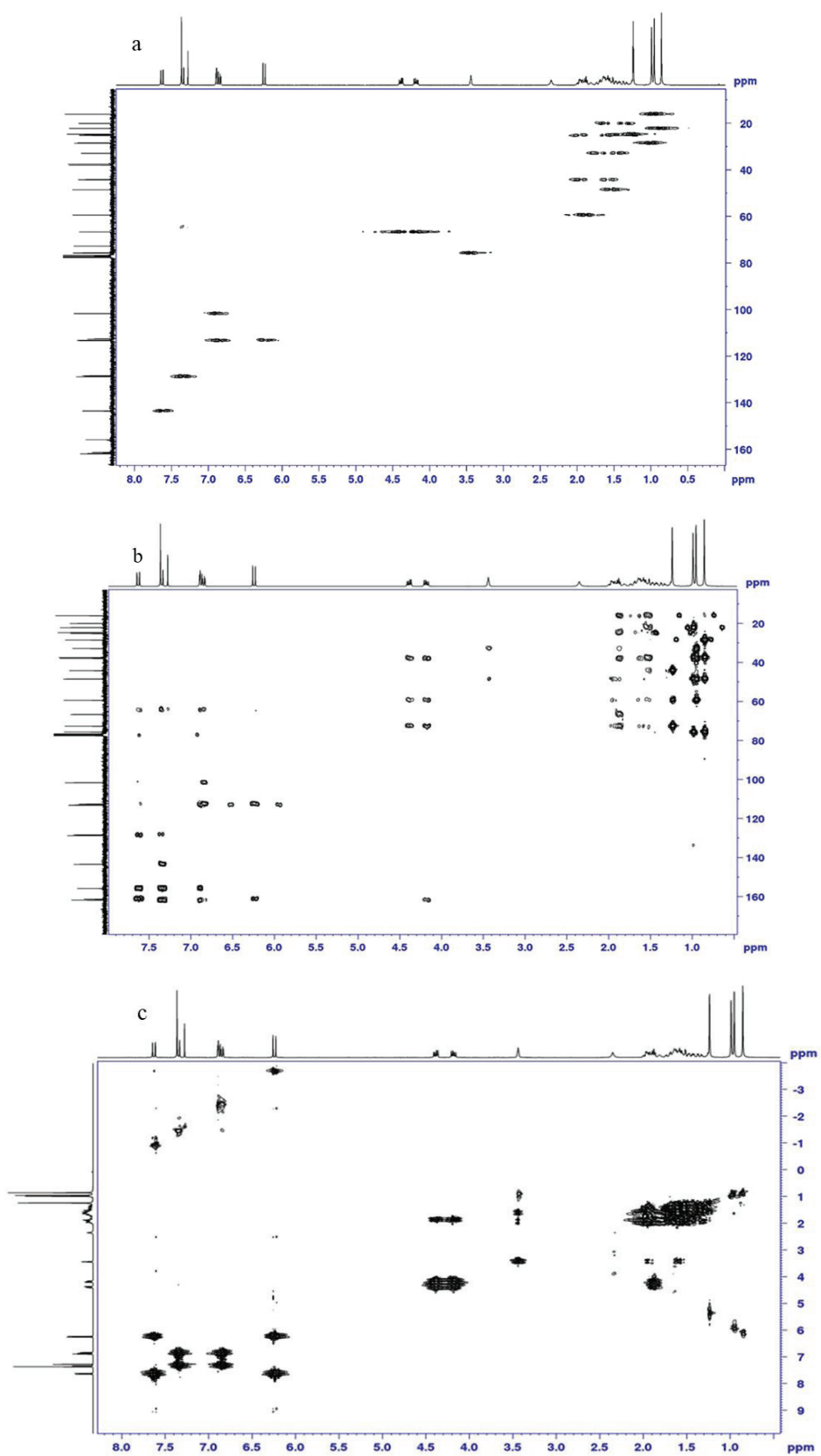
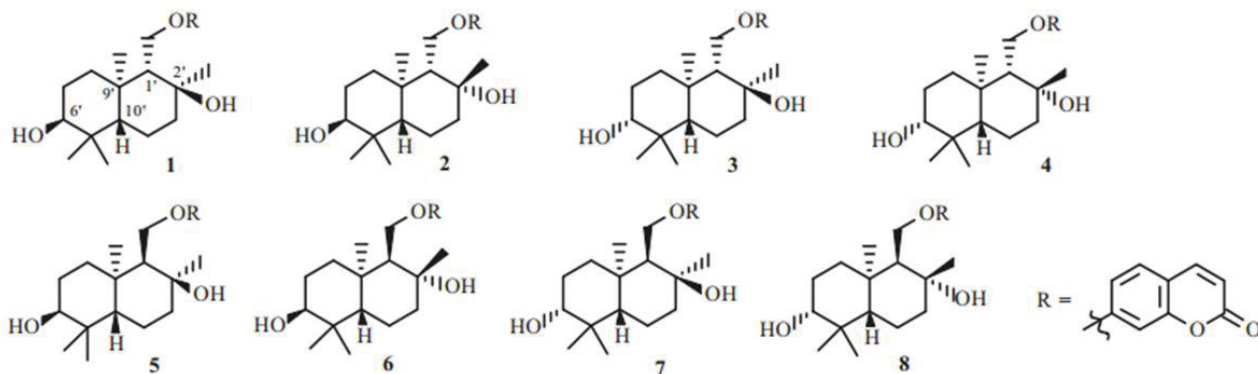


Figure 7. HSQC (a), HMBC (b), COSY (c). NMR spectrum of mogoltavidin.

**Table 1.** Mogoltavidin PMR (300 MHz) and  $^{13}\text{C}$  (75 MHz) NMR chemical shifts, spin-spin interaction constants ( $\text{CDCl}_3$ , ppm., J/Hz), HSQC, HMBC, COSY experimental data.

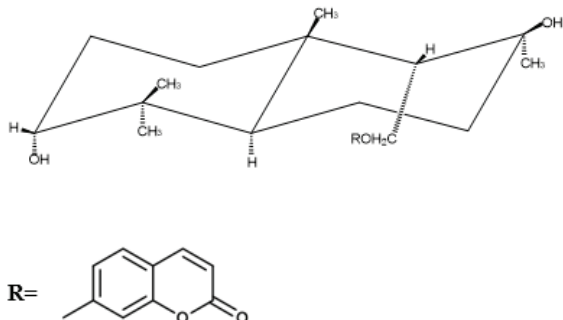
C Atoms	$\delta_{\text{C}}$ (m.h.)	HSQC		$\delta_{\text{C}}$ DEPT	HMBC (H $\rightarrow$ C)	$^1\text{H}$ - $^1\text{H}$ COSY
		$\delta_{\text{H}}$ (m.h.) (J/Hz)				
2	161.82			-C=O		
3	113.06	6.25 (1H, d, J=9.6)		-CH=	C-9	H-4
4	143.46	7.64 (1H, d, J=9.3)		-CH=	C-2, 5, 10	H-3
5	128.72	7.36 (1H, d, J=9.3)		-CH=	C-4, 7, 10,	H-6
6	101.59	6.87 (1H, dd, J=9, $J_{\text{al}}=2.4$ )		-CH=	C- 7, 8	H-5
7	161.28	-		>C=	-	-
8	113.20	6.89 (1H, d, $J_{\text{al}}=2.4$ ).		-CH=	-	-
9	112.57	-		>C=	-	-
10	155.84	-		>C=	-	-
1'	32.79	1.42, 1.69 (2H, m)		-CH <sub>2</sub> -	-	-
2'	25.13	1.9 (2H, m)		-CH <sub>2</sub> -	-	-
3'	75.61	3.43 (1H, br. s)		-CH-	C-1', 5'	-
		2.34 (1H, br. s, -OH)			-	-
4'	37.45	-		-C-	-	-
5'	48.43	1.53 (1H, m)		-CH-	-	-
6'	19.97	1.34 (1dd, $J_1=3$ , $J_2=12$ ), 1.58 (1H, m)		-CH <sub>2</sub> -	-	-
7'	44.14	1.59, 1.93 (1H, m)		-CH <sub>2</sub> -	-	-
8'	72.61	2.34 (1H, br. s, -OH)		-C-	-	-
9'	59.33	1.88 (1H, m)		-CH-	-	-
10'	37.88	-		-C-	-	-
11'a	66.61	4.41 (1H, dd, $J_{\text{gem}}=9.9$ , $J_{\text{vis}}=4.5$ )		-CH <sub>2</sub> O-	C-8', 9', 10'	H-11'b
11'b	66.61	4.15 (1H, dd, $J_{\text{gem}}=9.9$ , $J_{\text{vis}}=5.7$ )				H-11'a
12'	24.65	1.23 (3H, s)		-CH <sub>3</sub>	C-7', 8', 9'	-
13'	28.43	0.98 (3H, s)		-CH <sub>3</sub>	C-4'	-
14'	22.11	0,85 (3H, s)		-CH <sub>3</sub>	C-5'	-
15'	15.99	0,95 (3H, s)		-CH <sub>3</sub>	C-10'	-

**Figure 8.** Eight isomers of the investigated compound:

1: samarcandin m.p. 176-177°C,  $1'R, 2'S, 6'S$  ( $[\alpha]_{\text{D}} +30^\circ$  ( $\text{C}_2\text{H}_5\text{OH}$ ); 2: feshurin m.p. 183-184°C  $1'R, 2'R, 6'S$  [ $\alpha$ ]  $\text{D} -51^\circ$  ( $\text{C}_2\text{H}_5\text{OH}$ ); 3: isosamarcandin m.p. 221°C,  $1'R, 2'S, 6'R$  [ $\alpha$ ]  $\text{D} +27^\circ$  ( $\text{C}_2\text{H}_5\text{OH}$ ); 4: nevskin m.p. 193-194°C,  $1'R, 2'R, 6'R$  [ $\alpha$ ]  $\text{D} -79^\circ$  ( $\text{CHCl}_3$ ); 5: fepaldin m.p. 219-221°C,  $1'S, 2'S, 6'S$  [ $\alpha$ ]  $\text{D} -55^\circ$  ( $\text{CHCl}_3$ ); 6: Deacetylkellerin m.p. 134-136°C,  $1'S, 2'R, 6'S$  [ $\alpha$ ]  $\text{D} +$ ; 7: Episamarcandin  $1'S, 2'S, 6'R$ ; 8: ferucrin 213-215°C,  $1'S, 2'R, 6'R$   $+32^\circ$  ( $\text{C}_2\text{H}_5\text{OH}$ ); mogoltavidin m.p. 159-160°C.

ester and was identified as the sesquiterpenoid coumarin trans-4,4,8,10-tetramethyl-3-,8-dioxydecalin-9-carbinol mogoltavidin. This compound was previously isolated from the roots *Ferula mongolstanica* and *Ferula huber-morathii* [Khasanov et al. 1974; Aydogana et al. 2020].

To determine the configuration of functional groups in the compound, chemical shifts and spin-spin interaction constants were considered in the PMR spectrum. The fact that the axial orientation of the C-9 ( $-\text{CH}_2\text{OAr}$ ) substituent is in the trans position with respect to the angular methyl group attached to the carbon atom at C10 is due to the determination of the chemical shift of the methyl group in a relatively (0.95 ppm.) weak declination paramagnetic field. The alcohol hydroxyl group in the molecule of the substance is binary and axial ( $3'\alpha\text{-ol}$ ) at C3' in the structure of traditional irezan sesquiterpenoid coumarins. The fact that the configuration of the hydroxyl group in C3' is in the  $\alpha$ -stereoposition is evidenced by the broadened signal of the gem-hydroxyl proton in the NMR spectrum in the form of a triplet (t., 3.43 ppm half-width  $\frac{1}{2} \sum J = 5 \text{ Hz}$ ), the spin-spin coupling constant is 5 Hz, indicating that the hydroxyl group is energetically equatorial and the methine proton is axial (Fig. 9) relevant to the literature by T. Khasanov et al. [1974].



**Figure 9.** Space configuration of mogoltavidin.

### CONCLUSION

For the first time, sesquiterpene coumarins were isolated and studied from the underground part of *Ferula persica* collected in Azerbaijan. From the ethanol extract we obtained elemental composition  $\text{C}_{24}\text{H}_{32}\text{O}_5$  with m.p. 157-159°C white crystalline substance. Based on spectral data established that a substance with an identical structure to mogoltavidin. The conformational isomerism of the substance was determined by classical 1-dimensional PMR spectroscopic method. Also, R and S configurations of asymmetric carbon atoms of the compound were determined.

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### ***Ferula persica* köklərindən izolə edilən sescviterpen kumarin moqoltavidinin identifikasiyası və konfigurasiyasının öyrənilməsi**

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*Ferula* L. (Apiaceae) cinsinin Qafqaz, Orta Asiya, Sibir, Çin (Sincan), Əfqanıstan, İran və Şimali Afrikada geniş yayılmış 130 növü vardır. Azərbaycan Respublikasında bu cinsin səkkiz növünə rast gəlinir. *Ferula* növlərinin tərkibindəki kimyəvi maddələrin əsas hissəsini sescviterpen kumarinlər, laktonlar, mürəkkəb efir spirtləri və efir yağları təşkil edir. Toxumların tam yetişmə mərhələsində toplanmış *Ferula persica* köklərinin etanollu ekstraktından sütunlu xromatoqrafiya üsulundan istifadə etməklə ilk dəfə olaraq C<sub>24</sub>H<sub>32</sub>O<sub>5</sub> tərkibli, ərimə temperaturu 157-159°C olan kristallik maddə alınmışdır. Spektral (UV)-ultrabənövşəyi, (İQ)-infraqırmızı, (NMR)-nüvə maqnit rezonansı PMR və <sup>13</sup>C

NMR, DEPT və iki ölçülü eksperimental üsullar COSY, HSQC, HMBC və fiziki göstəriciləri (polyarometriya, ərimə temperaturu) məlumatları əsasında tədqiq edilən maddənin moqoltavidinlə eyni quruluşa malik olduğu müəyyən edilmişdir. Maddənin konfigurasiyasının təyin edilməsində PMR spektrdəki kimyəvi sürüşmə və spin-spin qarşılıqlı təsir konstantının qiymətindən istifadə edilmişdir. Hazırkı tədqiqatın məqsədi *F. persica* köklərinin kumarin tərkibini müəyyən etməkdir. Bu nəticələrdə gələcəkdə cins daxilində növlərin xemotaksonomik mövqeyini müəyyən etmək üçün qiymətləndirilə bilər.

**Açar sözlər:** kimyəvi sürüşmə, seskiterpen lakton, spin-spin qarşılıqlı təsir konstantı, Vudvord-Fizer qaydası, UV, IR, NMR konfigurasiyası

### Идентификация и исследование конфигурации сесквитерпенового кумарина моголтавидина, выделенного из корней *Ferula persica*

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Род *Ferula* L. (Ariaceae) насчитывает 130 видов, распространенных на Кавказе, в Средней Азии, Сибири, Китае (Синьцзяне), Афганистане, Иране и Северной Африке. В Азербайджанской

Республике встречается восемь видов этого рода. Основную часть химического вещества видов ферулы составляют сесквитерпеновые кумарины, лактоны, сложные эфиры спиртов и эфирные масла. Впервые, из этанолового экстракта корней *Ferula persica*, собранных в фазе полного созревания семян методом колоночной хроматографии, выделено кристаллическое вещество состава  $C_{24}H_{32}O_5$  с температурой плавления 157-159°C. На основании спектральных (УФ)-ультрафиолетовый, (ИК)-инфракрасный, (ЯМР)-ядерный магнитный резонанс ПМР и ЯМР  $^{13}C$ , DEPT и двумерных экспериментальных методов COSY, HSQC, HMBC а также физических показателей (полярометрия, температура плавления) доказано, что это вещество имеет строение идентичное моголтавидину. Для определения конфигурации вещества в ПМР спектре, использовался химический сдвиг и значение константы спин-спинового взаимодействия, который является классическим методом. Целью настоящего исследования было определение содержания кумарина в корнях *F. persica*. Полученные результаты в дальнейшем могут быть оценены для выявления хемотоксонического положения вида внутри рода.

**Ключевые слова:** химический сдвиг, сесквитерпеновый лактон, константа спин-спинового взаимодействия, правила Вудворда-Физера, УФ, ИК, конфигурация ЯМР