



# Article Study of the Chemical Composition of *Rosa beggeriana* Schrenk's Fruits and Leaves

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**Abstract:** *Rosa* species are widely used in folk medicine in different countries of Asia and Europe, but not all species are studied in-depth. For instance, *Rosa beggeriana* Schrenk, a plant which grows in Central Asia, Iran, and some parts of China, is little described in articles. Column and thin-layer chromatography methods were used to isolate biologically active substances. From a study of fruits and leaves of *Rosa beggeriana* Schrenk, a large number of compounds were identified, seven of which were isolated:  $3\beta$ ,23-dihydroxyurs-12-ene (1),  $\beta$ -sitosterol (2), betulin (3), (+)-catechin (4), lupeol (5), ethyl linoleate (6), and ethyl linolenoate (7). Their structures were elucidated by <sup>1</sup>H, DEPT and <sup>13</sup>C NMR spectroscopy, mass spectrometry, and GC-MS (gas chromatography–mass spectrometry). The study also identified the structures of organic compounds, including volatile esters and acids. Consequently, comprehensive data were acquired concerning the chemical constitution of said botanical specimen.

**Keywords:** *Rosa beggeriana* Schrenk; 3β,23-dihydroxyurs-12-ene; β-sitosterol; betulin; (+)-catechin; lupeol; ethyl linoleate; ethyl linolenoate

# 1. Introduction

The genus *Rosa* holds big commercial significance and is renowned in the domain of folk medicine. Numerous wild species within this genus have played a pivotal role in the development of valuable and economically viable cultivars of ornamental roses [1]. Despite the relative under-examination of certain rose species, several of them possess significant potential due to the presence of rosehip fruits. Commercially traded rosehip fruit is derived from several different species. They are long-lived woody perennials found mainly on forest margins and in disturbed habitats, such as roadsides and open fields. The genus *Rosa* (Rosaceae) has around 150–200 species [1–3]. Roses have also been cultivated since ancient times as medicinal plants in many countries across Europe and Asia. Rosehips contain many pharmacologically active compounds, such as organic acids, vitamin C and E, flavonoids, carotenoids, and tannins. Therapeutic properties and benefits of rosehips are their nourishing, mild laxative, mild diuretic, mild astringent, diuretic, ophthalmic and tonic effects [1,4–6]. *Rosa* extracts derived from these plants are also widely used in cosmetics, promising antioxidant and moisturizing effects [1,5–8]. All parts of this wild rose have been used in Asian folk medicine [4,5,9–11].

The intrinsic value of rosehip fruit has been acknowledged for centuries; however, efforts have only recently been made to domesticate and cultivate wild roses specifically for their fruit and to advance agronomic techniques in this regard. This shift in focus can be attributed to an enhanced comprehension of the pivotal role that dietary fruits play in



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**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). enhancing human health and mitigating disease risks [12]. The Rosaceae family is one of the most employed as a consolidated source of phytoproducts with functional properties [13]. Within this family, the genus *Rosa* provides various species, and their essential oils possess a wide range of applications as flavor, fragrance, and additive in cosmetic and toiletries [14]. In addition to their aromatic composition, many Rosa species from all over the word have been evaluated for their food-related biological properties and multiple functional uses have been suggested [15–19]. For example, teas made from the fruits of *Rosa canina* have mild laxative and diuretic tendencies [12]. Rosehips have a longstanding history of utilization in folk medicine spanning centuries, primarily for the prevention and treatment of various ailments such as the common cold, influenza-like infections, fever, infectious diseases, vitamin C deficiency, general exhaustion, gastritis and gastric ulcers prevention, diarrhea, gallstones and gallbladder discomforts, urinary tract diseases and discomforts, as well as for their potential anti-inflammatory, anti-obesity, anticancer, and diabetes management properties. Furthermore, rosehips have been employed to address inadequate peripheral circulation concerns [5,6,15–18,20,21]. Mixed with small amount of vinegar, rosehips were used as an antidote for the treatment of iron toxicity [20,22]. For nutritional purposes, fruits are used for the production of different products like tea, marmalade, jam, stewed fruit, wine, and juices [23]. Ground in a hand mill and cooked with milk, they could be used as children's snack and baby food as reported by the latter authors. The functional properties of some Rosa species are attributable to a wide range of bioactive ingredients, such as minerals, flavonoids, tannins, anthocyanin, organic acids, phenolic compounds fatty acids, volatile oils, ascorbic acid, phenols, and sugar. Through the examination of a species within the same taxonomic family as the subject of investigation, co-occurring within the identical geographical region, it becomes feasible to assess the potential anticancer properties of compounds derived from Begger's rosehip [5,24–28].

*Rosa beggeriana* Schrenk is an indigenous species predominantly distributed in Central Asia (Kazakhstan, Kyrgyzstan), China (Xinjiang Uygur Autonomous Region), and Iran [29–33]. It has been identified as an essential resource for hybridization purposes, particularly in the development of cold-resistant germplasm, when combined with contemporary rose varieties [29]. Begger's rosehip contains a large number of compounds with antioxidant activity, including activity against cancer cells. Rosehip hips have a high concentration of the carotenoid lycopene, which is considered a compound with a powerful antioxidant effect and is used as a therapeutic and prophylactic agent for various diseases, including cancer. Begger's rosehip extracts display cytotoxicity and antiproliferative properties against human liver and breast cancer cells, which might be associated with the presence of polyphenols in it [34].

According to the studies mentioned earlier, we can tell that Begger's rosehips have not been studied sufficiently even though other species are very well known in the folk medicine of different countries.

# 2. Results

#### 2.1. Identification of the Isolated Compounds from Leaves of Rosa beggeriana Schrenk

Utilizing column chromatography, a total of seven distinct substances were successfully isolated from both the fruits and leaves of the wild rose species known as Begger (Rosa sp.). The isolated substances encompassed a diverse range of chemical classes, including triterpenoids, catechins, and fatty acid esters. Remarkably,  $3\beta$ ,23-dihydroxyurs-12-ene had not been previously reported in this particular plant species. Additionally, no NMR characterization data were available for this newly isolated substance [35–37]. Apart from this novel isolate, the triterpenoids, catechins, and a mixture of fatty acid esters were also successfully identified and isolated from the aforementioned plant material.

## 2.2. GC-MS Data

GC-MS analysis was used to obtain data on the fatty acid composition of the leaves (Table 1) and fruits (Table 2) of *Rosa beggeriana* Schrenk.

L-2-1—Hexane fraction           40.944         Octadeca-9,12,15-trienoic acid         95.8         5.38           L-2-11—n-hexane/ethyl acetate fraction (6/4)         28.259         Methyl dodecanoate         98.0         0.95           32.897         Methyl tetradecanoate         97.5         2.61         37.087         Methyl hexadecanoate         98.6         14.45           39.021         Methyl neptadecanoate         95.0         0.47         40.244         Methyl octadeca-9,12-dienoate         99.2         13.16           40.335         Methyl octadeca-9,12-fi-trienoate         99.3         32.94         40.387         Methyl trans-9-octadecenoate         91.9         5.86           40.483         Methyl octadecanoate         98.6         6.37         44.340         Methyl icosanoate         95.3         1.45           41.340         Methyl icosanoate         95.3         1.45         1.92         1.45           55.902         Methyl tetracosanoate         90.3         1.67         1.45           CH-21dichloromethane/ethyl acetate fraction (6/4)         1.45         1.45           37.078         Methyl hexadecanoate         90.3         3.67           40.225         Methyl hexadecanoate         96.3         3.76	RT	Compound Name	Match Factor	Area, %
40.944       Octadeca-9,12,15-trienoic acid       95.8       5.38         L-2-11—n-hexane/ethyl acetate fraction (6/4)       28.259       Methyl dodecanoate       98.0       0.95         32.897       Methyl tetradecanoate       97.5       2.61         37.087       Methyl hexadecanoate       98.6       14.45         39.021       Methyl neptadecanoate       95.0       0.47         40.244       Methyl octadeca-9,12,15-trienoate       99.3       32.94         40,335       Methyl octadeca-9,12,15-trienoate       99.3       32.94         40,387       Methyl octadeca-9,12,15-trienoate       99.3       32.94         40,387       Methyl octadeca-9,12,15-trienoate       99.3       32.94         40,387       Methyl octadecanoate       91.9       5.86         40.483       Methyl octadecanoate       96.5       3.06         40.878       Methyl docosanoate       95.1       2.16         51.111       Methyl tetracosanoate       90.3       1.67         CH-21—dichloromethane/ethyl acetate fraction (7/3)       37.078       Methyl hexadecanoate       90.4       5.04         CH-39—dichloromethane/ethyl acetate fraction (6/4)       1.45       32.897       Methyl hexadecanoate       96.3       3.76		L-2-1—Hexane fraction		
L-2-11—n-hexane /ethyl acetate fraction (6/4)28.259Methyl dodecanoate98.00.9532.897Methyl tetradecanoate97.52.6137.087Methyl hexadecanoate98.614.4539.021Methyl heptadecanoate95.00.4740.244Methyl octadeca-9,12-dienoate99.213.1640.335Methyl octadeca-9,12,15-trienoate99.332.9440,387Methyl octadeca-9,12,15-trienoate99.332.9440,387Methyl octadeca-9,12,15-trienoate96.53.0640.878Methyl octadecanoate96.53.0640.878Methyl icosanoate96.21.9247.540Methyl docosanoate95.31.4555.902Methyl Hexacosanoate90.31.67CH-21—dichloromethane/ethyl acetate fraction (7/3)7.078Methyl hexadecanoate90.437.078Methyl tetradecanoate96.34.8337.078Methyl tetradecanoate93.12.0040.225Methyl tetradecanoate93.12.0040.225Methyl octadeca-9,12,15-trienoate97.69.7528.259Methyl octadeca-9,12,15-trienoate96.33.7640.297Methyl octadeca-9,12,15-trienoate96.30.5835.5216,10,14-Trimethyl-g-methyl-lexadec-1-ene92.90.3336.125(2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl22.30.5336.125(2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl93.22.10	40.944	Octadeca-9,12,15-trienoic acid	95.8	5.38
28.259       Methyl dodecanoate       98.0       0.95         32.897       Methyl tetradecanoate       97.5       2.61         37.087       Methyl hexadecanoate       98.6       14.45         39.021       Methyl heptadecanoate       95.0       0.47         40.244       Methyl octadeca-9,12,15-trienoate       99.2       13.16         40.335       Methyl octadeca-9,12,15-trienoate       99.3       32.94         40,387       Methyl trans-9-octadecenoate       91.9       5.86         40.483       Methyl octadecanoate       96.5       3.06         40.878       Methyl octadecanoate       96.2       1.92         47.540       Methyl docosanoate       95.3       1.45         55.902       Methyl Hexacosanoate       90.3       1.67         CH-21—dichloromethane/ethyl acetate fraction (7/3)       31.67         CH-39—dichloromethane/ethyl acetate fraction (6/4)       1.45         14.411       2-Ethylhexan-1-ol       96.4       1.85         32.897       Methyl hexadecanoate       93.1       2.00         40.225       Methyl hexadecanoate       96.3       3.76         40.297       Methyl hexadecanoate       96.3       3.76         40.297		L-2-11—n-hexane/ethyl acetate fraction	(6/4)	
32.897Methyl tetradecanoate97.52.6137.087Methyl hexadecanoate98.614.4539.021Methyl heptadecanoate95.00.4740.244Methyl octadeca-9,12-dienoate99.213.1640.335Methyl octadeca-9,12,15-trienoate99.332.9440,387Methyl trans-9-octadecenoate91.95.8640.483Methyl (gZ)-9-octadecenoate96.53.0640.878Methyl octadecanoate96.53.0640.878Methyl icosanoate95.12.1651.111Methyl docosanoate95.31.4555.902Methyl Hexacosanoate90.31.67CH-21dichloromethane/ethyl acetate fraction (7/3)37.078Methyl hexadecanoate90.453.997Methyl hexadecanoate96.34.8337.078Methyl tetradecanoate93.12.0040.225Methyl hexadecanoate93.12.0040.225Methyl octadeca-9,12,15-trienoate96.60.5835.5216,10,14-Trimethylpentadecan-2-one96.30.5835.6497,11,15-Tietramethylhexadec-1-ene92.90.3336.125 $(2E,7R,11R)-3,7,11,15-Tetramethylhexadec-1-ene92.90.5336.5023,7.11,15-Tetramethyl-2-hexadecen-1-ol93.22.10$	28.259	Methyl dodecanoate	98.0	0.95
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32.897	Methyl tetradecanoate	97.5	2.61
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37.087	Methyl hexadecanoate	98.6	14.45
40.244Methyl octadeca-9,12-dienoate99.213.1640.335Methyl octadeca-9,12,15-trienoate99.332.9440,387Methyl trans-9-octadecenoate91.95.8640.483Methyl (9Z)-9-octadecenoate96.53.0640.878Methyl octadecanoate98.66.3744.340Methyl icosanoate96.21.9247.540Methyl docosanoate95.12.1651.111Methyl tetracosanoate90.31.6755.902Methyl hexacosanoate90.31.67CH-21dichloromethane/ethyl acetate fraction (7/3)37.078Methyl hexadecanoate90.45.04CH-39dichloromethane/ethyl acetate fraction (6/4)14.4112-Ethylhexan-1-ol96.41.8532.897Methyl hexadecanoate93.12.0040.225Methyl octadeca-9,12,15-trienoate96.33.7640.297Methyl octadeca-9,12,15-trienoate96.60.5835.5216,10,14-Trimethylpentadecan-2-one96.30.5835.6497,11,15-Trimethyl-3-methylidenehexadec-1-ene92.90.3336.125 $(2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl92.30.53acetate36.5023,7,11,15-Tetramethyl-2-hexadecen-1-ol93.22.10$	39.021	Methyl heptadecanoate	95.0	0.47
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40.244	Methyl octadeca-9,12-dienoate	99.2	13.16
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40.335	Methyl octadeca-9,12,15-trienoate	99.3	32.94
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40,387	Methyl trans-9-octadecenoate	91.9	5.86
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40.483	Methyl (9Z)-9-octadecenoate	96.5	3.06
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40.878	Methyl octadecanoate	98.6	6.37
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	44.340	Methyl icosanoate	96.2	1.92
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	47.540	Methyl docosanoate	95.1	2.16
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	51.111	Methyl tetracosanoate	95.3	1.45
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	55.902	Methyl Hexacosanoate	90.3	1.67
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		CH-21—dichloromethane/ethyl acetate fract	ion (7/3)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	37.078	Methyl hexadecanoate	90.4	5.04
14.4112-Ethylhexan-1-ol96.41.8532.897Methyl tetradecanoate96.34.8337.078Methyl hexadecanoate93.12.0040.225Methyl octadeca-9,12-dienoate96.33.7640.297Methyl octadeca-9,12,15-trienoate97.69.7528.259Methyl dodecanoate96.60.5835.5216,10,14-Trimethylpentadecan-2-one96.30.5835.6497,11,15-Trimethyl-3-methylidenehexadec-1-ene92.90.3336.125(2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate92.30.5336.5023.7,11,15-Tetramethyl-2-hexadecen-1-ol93.22.10		CH-39—dichloromethane/ethyl acetate fract	ion (6/4)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14.411	2-Ethylhexan-1-ol	96.4	1.85
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32.897	Methyl tetradecanoate	96.3	4.83
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37.078	Methyl hexadecanoate	93.1	2.00
40.297       Methyl octadeca-9,12,15-trienoate       97.6       9.75         28.259       Methyl dodecanoate       96.6       0.58         35.521       6,10,14-Trimethylpentadecan-2-one       96.3       0.58         35.649       7,11,15-Trimethyl-3-methylidenehexadec-1-ene       92.9       0.33         36.125       (2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate       92.3       0.53         36.502       3.7,11,15-Tetramethyl-2-hexadecen-1-ol       93.2       2.10	40.225	Methyl octadeca-9,12-dienoate	96.3	3.76
28.259     Methyl dodecanoate     96.6     0.58       35.521     6,10,14-Trimethylpentadecan-2-one     96.3     0.58       35.649     7,11,15-Trimethyl-3-methylidenehexadec-1-ene     92.9     0.33       36.125     (2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate     92.3     0.53       36.502     3.7,11,15-Tetramethyl-2-hexadecen-1-ol     93.2     2.10	40.297	Methyl octadeca-9,12,15-trienoate	97.6	9.75
35.521       6,10,14-Trimethylpentadecan-2-one       96.3       0.58         35.649       7,11,15-Trimethyl-3-methylidenehexadec-1-ene       92.9       0.33         36.125       (2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate       92.3       0.53         36.502       3.7,11,15-Tetramethyl-2-hexadecen-1-ol       93.2       2.10	28.259	Methyl dodecanoate	96.6	0.58
35.649       7,11,15-Trimethyl-3-methylidenehexadec-1-ene       92.9       0.33         36.125       (2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate       92.3       0.53         36.502       3.7,11,15-Tetramethyl-2-hexadecen-1-ol       93.2       2.10	35.521	6,10,14-Trimethylpentadecan-2-one	96.3	0.58
36.125       (2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate       92.3       0.53         36.502       3.7,11,15-Tetramethyl-2-hexadecen-1-ol       93.2       2.10	35.649	7,11,15-Trimethyl-3-methylidenehexadec-1-ene	92.9	0.33
36.502 3.7.11.15-Tetramethyl-2-hexadecen-1-ol 93.2 2.10	36.125	36.125 (2E,7R,11R)-3,7,11,15-Tetramethylhexadec-2-en-1-yl acetate		0.53
=	36.502	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	93.2	2.10
37.078 Methyl hexadecanoate 98.4 12.43	37.078	Methyl hexadecanoate	98.4	12.43
40.302 Methyl octadeca-9.12.15-trienoate 99.2 4.85	40.302	Methyl octadeca-9,12,15-trienoate	99.2	4.85
40.874 Methyl octadecanoate 96.8 13.58	40.874	Methyl octadecanoate	96.8	13.58
41.440 Ethyl (9Z,12Z)-octadeca-9,12-dienoate 94.6 14.49	41.440	Ethyl (9Z,12Z)-octadeca-9,12-dienoate	94.6	14.49
44.340 Methyl icosanoate 90.1 10.66	44.340	Methyl icosanoate	90.1	10.66
L-2-27—ethyl acetate/methanol fraction $(8/2)$		L-2-27—ethyl acetate/methanol fraction	(8/2)	
37.697 Hexadecanoic acid 94.1 6.28	37.697	Hexadecanoic acid	94.1	6.28
40.926 Octadeca-9,12,15-trienoic acid 93.1 7.28	40.926	Octadeca-9,12,15-trienoic acid	93.1	7.28

 Table 1. GC-MS data for the leaves of Rosa beggeriana Schrenk.

**Table 2.** GC-MS data for the fruits of Rosa beggeriana Schrenk.

RT	Compound Name	Match Factor	Area, %
	B—Ethanol extract		
26.198	Trimethyl 2-hydroxybutane-1,2,3-tricarboxylate	91.7	13.47
39.397	Ethyl hexadecanoate	92.4	5.25
42.430	Ethyl (9E,12E)-octadeca-9,12-dienoate	92.5	6.71
42.506	Ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate	90.0	6.55
39.397	Ethyl hexadecanoate	92.7	4.97
42.430	Ethyl (9E,12E)-octadeca-9,12-dienoate	92.6	6.47
42.506	Ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate	91.6	6.29
42.430	Ethyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate	91.2	3.55
38.068	Methyl hexadecanoate	96.6	4.32
38.959	Ethyl 9-hexadecenoate	92.1	0.83
41.216	Methyl octadeca-9,12-dienoate	99.0	11.16
41.292	Methyl octadeca-9,12,15-trienoate	98.0	8.22
41.364	Methyl (9Z)-9-octadecenoate	93.5	4.57

 Table 2. Cont.

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	RT	Compound Name	Match Factor	Area, %
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41.864	Methyl octadecanoate	90.8	1.53
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.435	Ethyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate	97.9	15.56
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.516	Ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate	98.3	11.37
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.573	Ethyl (E)-octadec-9-enoate	93.2	6.22
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	43.059	Ethyl octadecanoate	93.8	1.50
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.425	Ethyl (9Z,12Z)-octadeca-9,12-dienoate	90.6	4.82
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	42.430	Ethyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate	92.8	3.09
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		14-(5-Ethyl-6-methylheptan-2-yl)-2,15-		
	48.811	dimethyltetracyclo	93.9	30.29
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		[8.7.0.0^{2,7}.0^{11,15}]heptadec-7-en-5-ol		
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	56.445	Nonacosane	92.1	13.69
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		B-M1-16—ethyl acetate/methanol fraction	n (1/1)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37.621	Methyl (Z)-pentadec-8-enoate	96.1	0.85
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38.073	Methyl hexadecanoate	98.5	4.23
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38.968	Ethyl 9-hexadecenoate	97.9	1.81
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	39.402	Ethyl hexadecanoate	98.7	7.97
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41.221	Methyl octadeca-9,12-dienoate	99.2	5.82
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41.297	Methyl octadeca-9,12,15-trienoate	98.8	7.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41.373	Methyl (9Z)-9-octadecenoate	93.0	2.84
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41.873	Methyl octadecanoate	92.2	0.53
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.449	Ethyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate	98.4	27.71
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42.530	Ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate	98.8	28.61
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	43.068	Ethyl octadecanoate	93.2	0.80
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		(2R)-2,7,8-Trimethyl-2-[(4R,8R)-4,8,12-		
ol       B-M2-18—ethyl acetate/methanol fraction (3/7)         32.478       Methyl dodecanoate       96.9       0.61         36.706       Tetradecanoic acid       99.6       3.22         38.321       (9Z)-Hexadec-9-enoic acid       97.9       3.81         38.854       Hexadecanoic acid       98.1       29.50         42.002       (9Z,12Z)-Octadeca-9,12-dienoic acid       97.7       27.43         42.135       (E)-Octadec-9-enoic acid       97.4       23.95         42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       y0.0       6.04       2,7,8,9,11,12,14,15,16,17-decahydro-1H-         cyclopenta[a]phenanthrene       90.0       6.04       2,7,8,9,11,12,14,15,16,17-decahydro-1H-	60.378	trimethyltridecyl]-3,4-dihydro-2H-1-benzopyran-6-	91.4	1.66
$\begin{array}{c c c c c c c c c c } B-M2-18ethyl acetate/methanol fraction (3/7) \\\hline 32.478 & Methyl dodecanoate & 96.9 & 0.61 \\\hline 36.706 & Tetradecanoic acid & 99.6 & 3.22 \\\hline 38.321 & (9Z)-Hexadec-9-enoic acid & 97.9 & 3.81 \\\hline 38.854 & Hexadecanoic acid & 98.1 & 29.50 \\\hline 42.002 & (9Z,12Z)-Octadeca-9,12-dienoic acid & 97.7 & 27.43 \\\hline 42.135 & (E)-Octadec-9-enoic acid & 97.4 & 23.95 \\\hline 42.492 & (E)-Octadec-2-enoic acid & 96.6 & 3.19 \\\hline 26-Aethyl acetate/methanol fraction (2/8) \\\hline 40.549 & Hexadecanoic acid & 95.8 & 8.32 \\\hline 40.549 & Hexadecanoic acid & 98.6 & 29.85 \\\hline 43.535 & (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid & 91.1 & 3.47 \\\hline (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6- \\\hline 62.859 & methylheptan-2-yl]-10,13-dimethyl- \\\hline 2,7,8,9,11,12,14,15,16,17-decahydro-1H- \\\hline cyclopenta[a]phenanthrene \\\hline \end{array}$		ol		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		B-M2-18—ethyl acetate/methanol fractior	n (3/7)	
36.706       Tetradecanoic acid       99.6       3.22         38.321       (9Z)-Hexadec-9-enoic acid       97.9       3.81         38.854       Hexadecanoic acid       98.1       29.50         42.002       (9Z,12Z)-Octadeca-9,12-dienoic acid       97.7       27.43         42.135       (E)-Octadeca-9-enoic acid       97.4       23.95         42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       26.4       29.85         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       cyclopenta[a]phenanthrene       90.0       6.04	32.478	Methyl dodecanoate	96.9	0.61
38.321       (9Z)-Hexadec-9-enoic acid       97.9       3.81         38.854       Hexadecanoic acid       98.1       29.50         42.002       (9Z,12Z)-Octadeca-9,12-dienoic acid       97.7       27.43         42.135       (E)-Octadec-9-enoic acid       97.4       23.95         42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       2       2         40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       cyclopenta[a]phenanthrene       90.0       6.04	36.706	Tetradecanoic acid	99.6	3.22
38.854       Hexadecanoic acid       98.1       29.50         42.002       (9Z,12Z)-Octadeca-9,12-dienoic acid       97.7       27.43         42.135       (E)-Octadec-9-enoic acid       97.4       23.95         42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       2       2         40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       cyclopenta[a]phenanthrene       90.0       6.04	38.321	(9Z)-Hexadec-9-enoic acid	97.9	3.81
42.002       (9Z,12Z)-Octadeca-9,12-dienoic acid       97.7       27.43         42.135       (E)-Octadec-9-enoic acid       97.4       23.95         42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       26.4       26.4       26.4         40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       20.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       cyclopenta[a]phenanthrene       90.0       6.04	38.854	Hexadecanoic acid	98.1	29.50
42.135       (E)-Octadec-9-enoic acid       97.4       23.95         42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       10       10       10         40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         62.859       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04	42.002	(9Z,12Z)-Octadeca-9,12-dienoic acid	97.7	27.43
42.492       (E)-Octadec-2-enoic acid       96.6       3.19         26-A—ethyl acetate/methanol fraction (2/8)       40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       cyclopenta[a]phenanthrene       90.0       6.04	42.135	(E)-Octadec-9-enoic acid	97.4	23.95
26-A—ethyl acetate/methanol fraction (2/8)         40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         2,7,8,9,11,12,14,15,16,17-decahydro-1H-       cyclopenta[a]phenanthrene       91.1       3.47	42.492	(E)-Octadec-2-enoic acid	96.6	3.19
40.549       Hexadecanoic acid       95.8       8.32         40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       90.0       6.04         62.859       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         cyclopenta[a]phenanthrene       90.0       6.04		26-A—ethyl acetate/methanol fraction (	2/8)	
40.549       Hexadecanoic acid       98.6       29.85         43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid       91.1       3.47         (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-       methylheptan-2-yl]-10,13-dimethyl-       90.0       6.04         62.859       2,7,8,9,11,12,14,15,16,17-decahydro-1H-       90.0       6.04         cyclopenta[a]phenanthrene       2,7,8,9,11,12,14,15,16,17-decahydro-1H-       10.1       10.1	40.549	Hexadecanoic acid	95.8	8.32
43.535       (9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid (8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6- methylheptan-2-yl]-10,13-dimethyl- 2,7,8,9,11,12,14,15,16,17-decahydro-1H- cyclopenta[a]phenanthrene       91.1       3.47	40.549	Hexadecanoic acid	98.6	29.85
(8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6- methylheptan-2-yl]-10,13-dimethyl- 2,7,8,9,11,12,14,15,16,17-decahydro-1H- cyclopenta[a]phenanthrene	43.535	(9Z,12Z,15Z)-Octadeca-9,12,15-trienoic acid 91.1 3.		3.47
62.859 methylheptan-2-yl]-10,13-dimethyl- 2,7,8,9,11,12,14,15,16,17-decahydro-1H- cyclopenta[a]phenanthrene		(8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-Ethyl-6-		
02.009 2,7,8,9,11,12,14,15,16,17-decahydro-1H- cyclopenta[a]phenanthrene	() PEO	methylheptan-2-yl]-10,13-dimethyl-	00.0	6.04
cyclopenta[a]phenanthrene	62.839	2,7,8,9,11,12,14,15,16,17-decahydro-1H-	90.0	6.04
		cyclopenta[a]phenanthrene		

When comparing the two tables, a richer composition of the fatty acids in fruits can be observed (Tables 1 and 2).

## 2.3. NMR Data

2.3.1. Identification of the Isolated Compounds from Leaves of Rosa beggeriana Schrenk

From the ethanol extract (45 g) of *Rosa beggeriana* Schrenk (553 g), 3β,23-dihydroxyurs-12-ene (**1**) [35–37] (21 mg) was isolated. The chemical structures are shown in Figure 1.

NMR data for Compound **1** were not found in literature. Hence, the analysis of the NMR spectra (Figures S1–S4) and the comparison of the spectroscopic data (Table 3) with those compounds that have a similar structure and described in the literature [35–37] allowed the identification of the compound **1**. The mass spectra also allowed us to identify compound **1**. Also, the melting point for compound **1** was 226–229 °C.



Figure 1. Chemical structure of 3β,23-dihydroxyurs-12-ene (1).

**Table 3.** Spectral data of <sup>1</sup>H NMR and <sup>13</sup>C NMR of  $3\beta$ ,23-dihydroxyurs-12-ene (1) in CDCl<sub>3</sub> and the structures of similar molecules.

No.	<sup>13</sup> C NMR Compound 1	Ref. <sup>13</sup> C NMR (3β,24-Dihydroxyurs- 12-ene) [35]	Ref. <sup>13</sup> C NMR (3β,28-Dihydroxyurs- 12-ene) [36]	<sup>1</sup> H NMR Compound 1	Ref. <sup>1</sup> H NMR (3β,24-Dihydroxyurs- 12-ene) [35]	Ref. <sup>1</sup> H NMR (3β,28-Dihydroxyurs- 12-ene) [36]
1	38.3	38.5	38.78		-	
2	27.3	27.2	26.63		-	
3	79.0	80.9	78.44	3.32, m	3.45 dd, 11.5/4.4 Hz	3.17
4	42.0	42.0	38.60	-	-	_
5	55.2	55.8	55.15		-	
6	18.4	18.6	18.20		-	
7	32.9	33.1	32.72		-	
8	40.0	40.0	39.86	-	-	-
9	47.7	47.7	47.56		-	
10	36.9	36.6	36.75	-	-	-
11	23.4	23.6	23.22		-	
12	124.4	124.2	124.96	5.26, m	5.12 br t, 3.6 Hz	5.1
13	139.5	139.6	138.67	-	_	-
14	42.7	42.7	42.32	-	-	-
15	28.1	28.0	26.24		-	
16	26.6	26.6	23.70		-	
17	33.7	33.7	37.79	-	-	-
18	59.1	59.0	54.07	-	-	-
19	39.6	39.5	39.62		-	
20	39.7	39.6	39.33		-	
21	31.2	31.2	30.80		-	
22	41.5	41.5	35.15		-	
23	63.0	22.4	27.89	3.72, m	1.25	0.80
24	15.6	64.5	16.44	1.33, s	4.23/3.34 d,11.0 Hz	0.93
25	15.7	16.2	15.51	1.06, s	0.90	0.92
26	16.9	16.7	16.44	1.10, s	0.97	0.92
27	23.3	23.3	23.70	1.16, s	1.06	1.09
28	28.8	28.7	69.20	0.89, s	0.79	3.52
29	17.5	17.5	17.23	0.88, s	0.78	0.81
30	21.4	21.4	21.20	0.89, s	0.91	1.00

From the ethanol extract (45 g) of *Rosa beggeriana* Schrenk (553 g), betulin (3) [38,39] (42.5 mg) and (+)-catechin (4) [40–42] (40.0 mg) were isolated. The chemical structures are shown in Figure 2.



Figure 2. Chemical structure of betulin (3) and (+)-catechin (4).

Compound **3** (betulin) was identified by its characteristic <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>)  $\delta$ : 1.57, 1.27 (2H, s, H-1), 1.70 (2H, s, H-2), 3.21 (2H, dd, H-2), 0.96 (1H, s, H-5), 1.38 (2H, s, H-6), 1.57, 1.38 (2H, s, H-7), 1.38 (2H, s, H-11), 1.38 (2H, s, H-12), 1.57, 1.27 (2H, s, H-15), 1.57, 1.27 (2H, s, H-16), 1.92 (1H, m, H-19), 1.57, 1.27 (2H, s, H-21), 1.57, 1.27 (2H, s, H-22), 0.78 (3H, s, H-24), 0.81 (3H, s, H-25), 0.96 (3H, s, H-23), 0.99 (3H, s, H-27), 1.05 (3H, s, H-26), 1.70 (3H, s, H-30), 3.20 (d, H-28a), 3.65 (d, H-28b), 4.58 (dd, H-29a), 4.71 (d, H-29b). <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$ : 38.73 (C-1), 27.41 (C-2), 79.01 (C-3), 38.73 (C-4), 55.32 (C-5), 18.34 (C-6), 34.30 (C-7), 40.84 (C-8), 50.45 (C-9), 37.18 (C-10), 20.95 (C-11), 25.15 (C-12), 37.18 (C-13), 42.84 (C-14), 27.41 (C-15), 29.39 (C-16), 47.99 (C-17,C-19), 48.31 (C-18), 150.94 (C-20), 29.73 (C-21), 33.30 (C-22), 28.01 (C-23), 15.40 (C-24), 16.14 (C-25), 15.99 (C-26), 14.57 (C-27), 63.67 (C-28), 109.36 (C-29), 16.00 (C-30) (Figures S7–S14), all in agreement with values in the literature [39,43]. The melting point of compound **3** was 248–250 °C.

For compound 4 (m.p.175–177 °C, optical rotation [ $\alpha$ ]D +17.2°), a detailed analysis of the NMR data led to the proposed structure, confirmed by the analysis of the spectra and comparison of the NMR resonances (Figures S15–S18) with the literature data summarized in the Table 4 [40].

No.	<sup>13</sup> C NMR	Ref. <sup>13</sup> C NMR	<sup>1</sup> H NMR
2	82.9	83.0	4.59 (d, J = 7.44 Hz)
3	68.9	68.9	4.00 (q, J = 8.2 Hz)
4	28.6	28.6	2.88 (dd, J = 16.12, 5.36 Hz) 2.52 (dd, J = 16.08, 8.08 Hz)
5	157.6	157.7	
6	96.5	96.4	5.89 (d, J = 2.3 Hz)
7	157.9	157.9	
8	95.7	95.6	5.96 (d, J = 2.3 Hz)
9	157.0	157.0	
10	101.0	100.9	
1'	132.3	132.3	
2'	115.4	115.4	6.86 (d, J = 1.96 Hz)
3'	146.3	146.4	
4'	146.3	146.3	
5'	116.3	116.2	6.78 (d, J = 8.16 Hz)
6'	120.2	120.2	6.74 (dd, J = 8.16, 2.0 Hz)

**Table 4.** Spectral data of <sup>1</sup>H NMR and <sup>13</sup>C NMR of (+)-catechin (4) in MeOD and chemical structures of the molecules.

2.3.2. Identification of the Isolated Compounds from Fruits of Rosa beggeriana Schrenk

 $\beta$ -sitosterol (2), lupeol (5), ethyl linoleate (6), and ethyl linolenoate (7) were isolated from the ethanol extract (35 g) of *Rosa beggeriana* Schrenk (400 g). The chemical structures are shown in Figure 3.



Figure 3. Chemical structure of  $\beta$ -sitosterol (2), lupeol (5), ethyl linoleate (6), and ethyl linolenoate (7).

Compound (2) was identified as  $\beta$ -sitosterol (Figures S5 and S6) according to the literature [44,45].

Lupeol (5) (m.p. 215–218°C): (Figures S19–S21) <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$ : 0.77 (3H, s, H-24), 0.80 (3H, s, H-28), 0.84 (3H, s, H-25), 0.96 (3H, s, H-23), 0.98 (3H, s, H-27), 1.04 (3H, s, H-26), 1.69 (3H, s, H-30), 4.58 (1H, s, H-29a), 4.70 (1H, s, H-29b). 3.19 (1H, dd, H-3); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  150.92 (C-20), 109.37 (C-29), 78.99 (C-3), 55.32 (C-5), 50.45 (C-9), 48.31 (C-18), 47.99 (C-19), 43.01 (C-17), 42.84 (C-14), 40.84 (C-8), 40.02 (C-22), 38.87 (C-13), 38.73 (C-4), 38.06 (C-1), 37.18 (C-10), 35.60 (C-16), 34.30 (C-7), 29.86 (C-21), 28.01 (C-23), 27.46 (C-15), 27.40 (C-12), 25.15 (C-2), 20.95 (C-11), 19.33 (C-30), 18.34 (C-6), 18.03 (C-28), 16.14 (C-25), 16.00 (C-26), 15.40 (C-24), 14.57 (C-27) [39,41,46,47]. Optical rotation [ $\alpha$ ]D +27.1°.

The analysis of the NMR spectra (Figures S22–S28) and the comparison of the spectroscopic data with those described in the literature allowed the identification of the mixture of two fatty acids known as ethyl linoleate (6) and ethyl linolenoate (7), and GC-MS helped to verify the accuracy of our assumptions. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$ : 2.30 (2H, t, H-2), 1.63 (2H, t, H-3), 1.35 (14H, s, H-4, 5, 6, 7, 15, 16, 17), 2.07 (4H, m, H-8, 14), 5.41— 5.30 (4H, m, H-9, 10, 12, 13), 2.77 (2H, t, J\_7.0 Hz, H-11), 5.37 (4H, m, H-9, 10, 12, 13), 4.14 (2H, m, –OCH<sub>2</sub>–), 0.90 (3H, t, H-18) 1.26 (3H, m, H-20). <sup>13</sup>C NMR: 174.06 (C-1), 33.76 (C-2) 25.21 (C-3) 26.84(C-4) 29.32 (C-5) 29.45 (C-6) 29.45 (C-7) 27.84 (C-8) 131.36(C-9) 129.49 (C-10) 25.81 (C-11) 129.56(C-12) 129.69 (C-13), 28.81(C-14) 29.45 (C-15) 31.74 (C-16) 22.40 (C-17) 59.97 (–OCH<sub>2</sub>–) 13.24 (C-18) 14.35 (C-20) [48].

## 3. Discussion

#### 3.1. GC-MS Data

The GC-MS analysis uncovered a heterogeneous chemical composition encompassing various classes of volatile compounds, which has been meticulously documented and organized in Tables 1 and 2. Considering the paucity of scholarly investigations on the

phytochemical composition of *R. beggeriana*, the GC-MS data were juxtaposed with data obtained from other species belonging to the *Rosa* genus, as cited in [49–52]. The comparative analysis of compositions, specifically the leaves and fruits, revealed a higher degree of complexity in the composition of the latter. It is noteworthy that this study represents the inaugural examination of the fatty acids' profiles pertaining to this plant species.

Table 1 presents the GC-MS data in the analysis of fractions L-2-1, L-2-11, L-2-27, CH-21, CH-39, and HIJK obtained from leaves of *R. beggeriana*. The richest one was L-2-11— n-hexane/ethyl acetate fraction (6/4).

The composition of leaves was found to include various compounds such as terpenoids, specifically (-)-aristolene, as well as phytosterols like stigmastan-3,5-diene. Additionally, saturated and unsaturated fatty acids, along with their corresponding esters, were identified. The majority of the fatty acids detected exhibited unsaturation, including 9-hexadecenoic acid methyl ester (*Z*)-, 9,12-octadecadienoic acid (*Z*,*Z*)-methyl ester, 9,12,15-octadecatrienoic acid methyl ester (*Z*,*Z*,*Z*)-, methyl linoleate, methyl linolenate, methyl elaidate, 9-octadecenoic acid methyl ester (*E*)-, 9-octadecenoic acid (*Z*)- methyl ester, 9,12,15-octadecatrienoic acid (*Z*,*Z*,*Z*)-, and cis-13-eicosenoic acid methyl ester.

The GC-MS data obtained from the analysis of ethanol extract (B) and various fractions (B-1, B-2, B-3, B-4, B-5, B-DCM, B-M1-16, B-M2-18, 26-A, 26-S8) derived from *R. beggeriana* fruits are presented in Table 2. Among these fractions, the most abundant one was B-4, which corresponded to the chloroform/ethyl acetate fraction with a ratio of 1:1.

The fruits of the plant exhibited a comprehensive array of both saturated and unsaturated fatty acids, along with their respective esters. Moreover, several additional fatty acids were identified, including myristic acid, palmitic acid, palmitoleic acid, ethyl linoleate, (e)-9-octadecenoic acid ethyl ester, ethyl oleate, alpha-linolenic acid, 11-octadecenoic acid (z)-, 11-octadecenoic acid (e)-, oleic acid (z)-, stearic acid, 9,12-octadecadienoic acid (z,z)-, and 2-hydroxy-1-(hydroxymethyl)ethyl ester. The abundance of unsaturated fatty acids in the composition of the fruits holds significant potential for application in the food industry.

In addition, the fruits were found to encompass phytosterols such as beta-sitosterol, gamma-sitosterol, stigmastan-3,5-diene, gamma-tocopherol, and lupeol.

Upon comprehensive analysis of the collective findings presented in Tables 2 and 3, it becomes evident that both the leaves and fruits of *R. beggeriana* exhibited a substantial abundance of saturated and unsaturated acids, terpenoids, and various other substances. These results collectively indicate a highly diverse and rich composition within the examined plant components.

## 3.2. Isolation and Identification of Individual Compounds

Identification of the isolated compounds (1–5) was based on spectroscopic analyses (<sup>1</sup>H, DEPTQ, DEPT135, <sup>13</sup>C NMR) compared with the data published in the literature.

In this study, the presence of  $3\beta$ ,23-dihydroxyurs-12-ene (compound 1—white and crystalline) in the leaves of *R. beggeriana* was established and confirmed using NMR data analysis, coupled with relevant literature sources [35–37]. A structurally similar compound, 3β,24-dihydroxyurs-12-ene, had been previously isolated from *Protium heptaphyllum*. By comparing the <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of the two compounds, it was observed that all peaks were identical, except for those corresponding to C-23 and C-24. For  $3\beta$ ,23dihydroxyurs-12-ene, the chemical shifts for C-23 and C-24 were 63.0 and 15.6 ppm, respectively, whereas for  $3\beta$ ,24-dihydroxyurs-12-ene, these values were reversed [35]. The presence of an oxygen moiety at C-23 in  $3\beta$ ,23-dihydroxyurs-12-ene was deduced based on the chemical shift at 63.0 ppm. The <sup>1</sup>H-NMR spectrum displayed signals corresponding to seven methyl groups: 1.25 (H-24), 0.98 (H-25), 1.02 (H-26), 1.08 (H-27), 0.81 (H-28), 0.80 (H-29), and 0.81 (H-30). The <sup>13</sup>C-NMR spectrum exhibited two peaks at 124.4 (C-12) and 139.5 (C-13), indicating the presence of a double bond in the ring. Overall, the number of observed peaks suggested the presence of 30 carbon atoms in compound 1. Importantly, this study represents the first isolation of  $3\beta$ ,23-dihydroxyurs-12-ene from the *Rosa* genus. Compound 1 was further compared to  $3\beta$ ,28-dihydroxyurs-12-ene, which contained a

-CH<sub>2</sub>OH group at the 28th carbon atom, resulting in a chemical shift of 69.20 ppm. Consistent correlations were observed in the <sup>1</sup>H-NMR spectra, supporting the structural analysis. High-resolution mass spectrometry (HR MS), as depicted in Figure S4, furnishes valuable insights pertaining to the molecular attributes of the compound under investigation. Specifically, it elucidated a molecular weight of 442 m/z, thereby affording a comprehensive breakdown of constituent particles within this compound. For instance, it is reasonable to deduce the presence of two highly mobile hydrogen atoms (m/z 440). Furthermore, the observation of protonation events at 424 [M + H<sub>2</sub>O]<sup>+</sup> and 406 [M + H<sub>2</sub>O]<sup>+</sup> suggests the existence of two hydroxyl (-OH) groups.

In addition, the HR MS data imitate the potential stability of a fragment with an m/z value of 273, indicative of a cleavage point that partitions the molecule into two relatively stable subunits. Moreover, the ensuing particles predominantly originated from the cleavage of the molecule at the central region of its third ring, yielding fragments with m/z values of 133, 189, 203, and 234. These findings contribute to a more intricate understanding of the compound's structural composition and fragmentation pattern. Notably, structurally related compounds (although not identical) [37,43,53,54] have been identified within the *Rosa* family, specifically in the fruits of *R. multiflora* and the roots of *R. taiwanensis*, and have been associated with anti-inflammatory activity. Based on the available data, it is plausible to postulate that  $3\beta$ ,23-dihydroxyurs-12-ene may possess similar activities to those of the structurally related compounds mentioned earlier. However, further investigation and experimental studies are necessary to validate and ascertain its potential biological activities. This compound have potential for use in medicine because there many studies of almost structurally identical compounds that have different types of activities [37,55,56].

Betulin (3) and (+)-catechin (4) have been identified in various Rosa species, present not only in leaves, but also in the roots, stems, with (+)-catechin present in the fruits and flowers [43,57–59]. The identification of compound 3 (betulin—solid and white crystalline) was accomplished through the analysis of its characteristic <sup>1</sup>H NMR (400 MHz; CDCl<sub>3</sub>) and <sup>13</sup>C NMR (CDCl<sub>3</sub>) spectra. The carbon peaks were meticulously examined, revealing the presence of 30 carbon atoms in this compound. Utilizing the DEPT135 method, it was determined that betulin comprises 12 -CH<sub>2</sub> groups, 5 unhydrolyzed carbons (because we can see them in  ${}^{13}$ C NMR spectra but not there), 13 -CH<sub>3</sub> and/or -CH groups, two oxygenated carbons (63.06 and 79.01), and one double bond (109.35). Proton magnetic resonance spectra further confirmed these structural features. Specifically, the <sup>1</sup>H NMR spectra exhibited signals corresponding to six methyl groups: 0.78 (3H, s, H-24), 0.81 (3H, s, H-25), 0.96 (3H, s, H-23), 0.99 (3H, s, H-27), 1.05 (3H, s, H-26), and 1.70 (3H, s, H-30). Additionally, signals of methylene groups were observed at 1.57, 1.27 (2H, s, H-1), 1.70 (2H, s, H-2), 3.21 (2H, dd, H-2), 1.38 (2H, s, H-6), 1.57, 1.38 (2H, s, H-7), 1.38 (2H, s, H-11), 1.38 (2H, s, H-12), 1.57, 1.27 (2H, s, H-15), 1.57, 1.27 (2H, s, H-16), 1.57, 1.27 (2H, s, H-21), 1.57, and 1.27 (2H, s, H-22). Based on the data presented in Figures S10–S14, encompassing 2D nuclear magnetic resonance (NMR) and gas chromatography-mass spectrometry (GC-MS) spectra, it is discernible that compound **3** corresponds to betulin. The GC-MS spectra provides essential information such as the retention time and molecular weight of this compound. Additionally, compound (+)-catechin (4) has been identified through a combination of NMR analysis, which was previously elucidated, and mass spectrometry. The mass spectra of compound 4 exhibited a discernible molecular weight of approximately 290 units. This determination is in accordance with our NMR-based assumption of it being catechin. Notably, the mass spectra also revealed distinct ions with molecular weights of 110, 138, and 55 units. These observations are congruent with the structural features of catechin, particularly with regard to the presence of vulnerable chemical bonds in its structure. Betulin was isolated from the roots of Rosa taiwanensis [43], and catechin was reported in the roots of *R. taiwanensis* [43], rosehips of *Rosa canina* [57,58]. Notably, betulin was reported to have anti-inflammatory and anticancer properties [60]. The structural identification of (+)-catechin (4) was established based on the analyses of the <sup>1</sup>H NMR, DEPT135, and <sup>13</sup>C NMR signals.

The NMR data of  $\beta$ -sitosterol (2) were subjected to a comprehensive comparison with relevant literature data [44,45,61].

Lupeol (5) is a triterpenoid that was found in the fruits of *R. beggeriana* and identified through comparison with NMR data from the literature data [39,46,47]. *R. rugosa* was also reported to have lupeol [62]. Using carbon nuclear magnetic resonance, it was found that the compound had 30 carbon atoms, 10 of which were methylene groups. The presence of a hydroxyl group and a double bond due to the presence of a shift was also established. Also, thanks to proton magnetic resonance, it was possible to establish the structure by calculating the number and area of peaks.

Ethyl linoleate (6) and ethyl linolenoate (7) were isolated together, and structure was elucidated by GC-MS data (Figures S21 and S22) and NMR, which were compared to literature [48].

Regardless of the precise study of several species, like *R. canina*, *R. rugosa*, and others, there are many species in the *Rosa* genus with minimal data. Many species of the *Rosa* family grow in diverse conditions, hence they can have different chemical composition [1,4,5].

## 4. Materials and Methods

## 4.1. Plant Material

The plant was harvested at a 23–25 °C temperature near Ili River and in the Almaty oblast N44°79.3959, E76°29.8245 in September 2021, by a biologist employee of the Botanical Garden in Almaty, Madina Ramazanova. Then, the plant was dried in the drying cabinet at 35 °C for 6 h and 48 h at room temperature, And it was deposited at the herbarium collection at the Institute of Botany and Phytointroduction of the Ministry of Higher Education and Science, Almaty, Kazakhstan (0002540).

#### 4.2. General Experimental Procedures

Solvents used in this work, n-hexane, chloroform, dichloromethane (DCM), ethyl acetate (EtOAc), methanol (MeOH), and ethanol (EtOH), were purchased from Fisher Scientific, Waltham, MA USA. Deuterated solvents (Sigma-Aldrich, Darmstadt, Germany), including methanol (MeOD) and chloroform (CDCl<sub>3</sub>), were used for nuclear magnetic resonance (NMR) spectroscopic analyses. Column chromatography (CC) was performed using silica gel 60 (0.063–0.200 mm; Merck, Darmstadt, Germany) or Sephadex LH-20 (0.25–0.1 mm, GE Healthcare, Cytiva, Sweden). Vacuum liquid chromatography column (VLC) (diameter 15 cm  $\times$  length 30 cm, 300 g) at room temperature was used to isolate substances from five main fractions. Thin-layer chromatography (TLC) analyses were carried out using pre-coated silica G plates w/UV254 (20 cm  $\times$  20 cm, 200  $\mu$ m in thickness; Sorbent Technologies, Norcross, GA, USA). An ultraviolet lamp (UVP, LLC, Spectroline, Westbury, NY, USA) was used for the visualization of spots on thin-layer chromatograms at 254 and/or 365 nm. Spots were visualized by spraying with 2% vanillin–sulfuric acid in ethanol followed by heating at 110 °C on a hot plate. Moreover, <sup>1</sup>H, DEPT135, DEPTQ and <sup>13</sup>C NMR spectra were recorded on a Bruker Avance 400 MHz instrument (Bruker, MA, USA). An LTQ Orbitrap XL mass spectrometer (Agilent Technologies, Santa Clara, CA, USA) was used for high-resolution-electrospray ionization-mass spectrum (HR-ESI-MS). The GC-MS analysis was performed with a Agilent 7890A gas chromatograph (Agilent Technologies, Santa Clara, CA, USA) coupled with an Agilent 5975C single quadrupole mass spectrometer (Agilent Technologies, Santa Clara, CA, USA).

#### 4.3. Extraction and Isolation

## 4.3.1. Extraction and Isolation of Leaves

The air-dried leaves (553.0 g) were macerated with ethanol 95% (1.5 L  $\times$  3 times) at room temperature. The ethanol extracts were combined, and the solvent was distilled under reduced pressure at low temperature to afford a 10.0 g yield.

The ethanol extract was processed using vacuum liquid chromatographic techniques with silica gel in a column (600 g, 0.063–0.200 mm; Merck, Darmstadt, Germany). The

extract was eluted using a gradient system with n-hexane, DCM, ethyl acetate, and ethanol, with growing polarity as a mobile phase starting with 100% n-hexane and ending with 100% methanol, and 5 fractions were obtained. Fractions were grouped depending on their chemical similarity and monitored using thin-layer chromatography and concentrated using a rotary evaporator. The obtained fractions were L-F1 (1.35 g), L-F2 (0.56 g), L-F3 (0.74 g), L-F4 (1.85 g), and L-F5 (2.37 g).

L-F1, L-F2, and L-F3 were concentrated together to fraction L-F1 according to similar spots on TLC. L-F4 and L-F5 was collected to fraction L-F2. Then, each fraction was separated using chromatographic fractionation in a glass column with silica gel 60 (200 g, 0.063–0.200 mm; Merck, Darmstadt, Germany) and Sephadex LH-20 (Lipophilic, 25–100  $\mu$ m, Sigma). The mobile phase was n-hexane and ethyl acetate, and 12 fractions were obtained.

Some fractions that were isolated from fractions L-F1 and L-F2 were studied by GC-MS. To analyze fatty acids by GC-MS, it was prepared by refluxing 20 mg of the isolated fractions with 20 mL CH<sub>3</sub>OH and 2 mL  $H_2SO_4$  for 4 h.

#### 4.3.2. Extraction and Isolation of Fruits

The air-dried fruits (400.0 g) were macerated with ethanol 95% (1.5 L  $\times$ 3 times) at room temperature. The ethanol extracts were combined, and the solvent was distilled under reduced pressure at low temperature to afford a 15.0 g yield.

The ethanol extract was processed using vacuum liquid chromatographic techniques with silica gel premium-grade C18 (40–63  $\mu$ m; 60Å; Sorbtech, Norcross GA, USA) in a column. The extract was eluted using a gradient system with DCM, methanol, and water, with decreasing polarity as a mobile phase starting with 100% water and ending with 100% DCM, and 6 fractions were obtained.

Fractions were grouped depending on their chemical similarity and monitored using thin-layer chromatography and concentrated using a rotary evaporator. The obtained fractions were B-F1 (2.32 g), B-F2 (2.56 g), B-F3 (2.15 g), B-F4 (1.85 g), and B-F5 (1.37 g).

Subsequently, the fractions were separated on Sephadex LH-20 (0.25–0.1 mm, GE Healthcare, Sweden) using methanol as the eluent. As a result, compounds 2, 5, 6, and 7 were obtained.

Some fractions that were isolated from fractions B-F1, B-F2, B-F3, B-F4, and B-F5 were studied by GC-MS. To analyze fatty acids by GC-MS, it was prepared by refluxing 20 mg of the isolated fractions with 20 mL CH<sub>3</sub>OH and 2 mL H<sub>2</sub>SO<sub>4</sub> for 4 h.

## 5. Conclusions

Previously, this type of rosehip (*Rosa beggeriana* Schrenk) had not been studied in terms of chemical composition, hence there are no articles on isolated compounds from this plant. However, there are many research articles about species from the genus *Rosa*, which are very well known in traditional medicine. The fractionation of *Rosa beggeriana* Schrenk leaves and fruits resulted in the isolation and structural elucidation of seven compounds, including phytosterol, triterpenoids, polyphenol, and mixture of fatty acids.  $\beta$ -sitosterol (2), betulin (3), (+)-catechin (4), lupeol (5), ethyl linoleate (6) have already been isolated from the genus *Rosa* but not from *Rosa beggeriana* Schrenk. And compounds like 3 $\beta$ ,23-dihydroxyurs-12-ene (1) and ethyl linolenoate (7) were isolated for the first time for both *Rosa and Rosa beggeriana* Schrenk.

**Supplementary Materials:** The following supporting information can be downloaded at: https: //www.mdpi.com/article/10.3390/plants12183297/s1, Figure S1: <sup>1</sup>H NMR spectrum of 3 $\beta$ ,23-Dihydroxyurs-12-ene (1); Figure S2: DEPT135 NMR spectrum of 3 $\beta$ ,23-Dihydroxyurs-12-ene (1); Figure S3: <sup>13</sup>C NMR spectrum of 3 $\beta$ ,23-Dihydroxyurs-12-ene (1); Figure S4: Mass spectrum of 3 $\beta$ ,23-Dihydroxyurs-12-ene (1); Figure S5: <sup>1</sup>H NMR spectrum of  $\beta$ -sitosterol (2); Figure S6: DEPTQ NMR spectrum of  $\beta$ -sitosterol (2); Figure S7: <sup>1</sup>H NMR spectrum of Betulin (2); Figure S8: DEPT135 NMR spectrum of Betulin (2); Figure S1: HSQC NMR spectrum of Betulin (2); Figure S1: HSQC NMR spectrum of Betulin (2); Figure S1: HSQC NMR spectrum of Betulin (2); Figure S14: GC-MS s of Betulin (2); Figure S15: <sup>1</sup>H NMR spectrum of (+)-Catechin (3); Figure S16: DEPT NMR spectrum (+)-Catechin (3); Figure S17: <sup>13</sup>C NMR spectrum of (+)-Catechin (3); Figure S18: Mass spectrum of (+)-Catechin (3); Figure S19: <sup>1</sup>H NMR spectrum of Lupeol (4); Figure S20: DEPT135 NMR spectrum of Lupeol (4); Figure S21: GC-MS Data of Lupeol (4); Figure S22: <sup>1</sup>H NMR spectrum of Ehyl linoleate (5) and Ethyl linolenoate (6); Figure S23: <sup>1</sup>H NMR spectrum of Ehyl linoleate (5) and Ethyl linolenoate (6); Figure S23: <sup>1</sup>H NMR spectrum of Ehyl linoleate (5) and Ethyl linolenoate (6); Figure S25: <sup>13</sup>C NMR spectrum of Ehyl linoleate (5) and Ethyl linoleate (5); Figure S27: GC-MS Data of Ethyl linolenoate (6); Figure S28: GC-MS Data of Ethyl linoleate (5).

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