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**Rosa davurica** Pall., **Rosa rugosa** Thumb., and **Rosa acicularis** Lindl. Originating from Far Eastern Russia: Screening of 146 Chemical Constituents in Three Species of the Genus Rosa

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Abstract: **Rosa rugosa** Thumb., **Rosa davurica** Pall., and **Rosa acicularis** Lindl. contain a large number of target analytes which are bioactive compounds. High performance liquid chromatography (HPLC), in combination with the ion trap (tandem mass spectrometry), was used to identify target analytes in MeOH extracts of **R. rugosa**, **R. davurica**, and **R. acicularis**, originating from the Russian Far East, Trans-Baikal Region, and Western Siberia. The results of initial studies revealed the presence of 146 compounds, of which 115 were identified for the first time in the genus **Rosa** (family *Rosaceae*). The newly identified metabolites belonged to 18 classes, including 14 phenolic acids and their conjugates, 18 flavones, 7 flavonols, 2 flavan-3-ols, 2 flavanones, 3 stilbenes, 2 coumarins, 2 lignans, 9 anthocyanins, 3 tannins, 8 terpenoids, 3 sceletium alkaloids, 4 fatty acids, 2 sterols, 2 carotenoids, 3 oxylipins, 3 amino acids, 5 carboxylic acids, etc. The proven richness of the bioactive components of targeted extracts of **R. rugosa**, **R. davurica**, and **R. acicularis** invites extensive biotechnological and pharmaceutical research, which can make a significant contribution both in the field of functional and enriched nutrition, and in the field of cosmetology and pharmacy.

Keywords: **Rosa rugosa**; **Rosa davurica**; **Rosa acicularis**; ion trap; tandem mass spectrometry; polyphenolic compounds

1. Introduction

Plants have been used as medicines since the existence of human civilization [1,2]. More than 35 thousand varieties of plants from different parts of the world are actively used for medical purposes, since they contain numerous phytocomponents that can potentially treat many diseases, including infectious ones [3]. Numerous medical systems of treatment, such as Ayurveda, Unani, homeopathy, naturopathy, Siddha, and others, rely on plants as effective remedies for various life-threatening diseases [4,5]. Due to the presence of secondary metabolites in plants, they have significant potential as antimicrobial agents. The diversity of these natural products offers an endless number of possibilities for the discovery of new drugs for the treatment of various diseases [6–8].
In recent years, traditional medicine based on oral herbal preparations has attracted the attention of both consumers and healthcare professionals. However, the use of these medicinal products requires improved knowledge of their composition and stability over time in order to support or validate these therapies in humans. Liquid preparations from medicinal plants, such as tinctures and extracts from plant buds, are typical products that are widely used but still poorly understood. Plant bud extracts are defined as extracts obtained exclusively from fresh buds, shoots, young leaves, and/or roots, which are macerated and extracted with hydro–glycerol and water–alcohol mixtures [9]. Kidney extracts represent a new category of herbal products well known and widely used in gemmotherapy, as well as in homeopathy and herbal medicine [10].

The genus *Rosa* (family *Rosaceae*) is represented on the territory of the Trans-Baikal region, Far East (Russian Federation), and Western Siberia by 3 species—*Rosa rugosa* Thumb., *Rosa davurica* Pall., and *Rosa acicularis* Lindl. (Figures 1 and 2). Fresh fruits and leaves contain up to 900 mg% ascorbic acid per dry pulp weight. Fresh petals contain 0.25–0.38% essential oil. Its neutral volatile fraction contains 86.3% phenylethyl alcohol, some linalool, citronellol, geraniol, nerol, etc. Eugenol was found in the phenolic fraction, phenylacetic, benzoic, and other acids in the acid fraction. *R. rugosa* is a medicinal plant widely used in traditional and folk medicine. Extracts of *R. rugosa* have been valued for Asian culinary, cosmetic, and aromatherapy purposes, and used in herbal medicines for diabetes mellitus and osteoarthritis [11]. The medicinal effects seem to be involved in the presence of many phytochemicals in *R. rugosa* extracts, for example flavonoids, phenylpropanoid, tannins, fatty acids, and terpenoids [12].

![Figure 1](image1.png)

(A) *Rosa rugosa* (Far Eastern Russia); (B) *Rosa davurica* (Trans-Baikal region).

![Figure 2](image2.png)

*Figure 1. (A) Rosa rugosa (Far Eastern Russia); (B) Rosa davurica (Trans-Baikal region).*
Several studies have reported that some compounds from rose hip extracts exhibit anti-inflammatory activity in vitro. The anti-inflammatory property of the crude hydroalcoholic extract of rose hip has been proven in vivo, suggesting its potential role as one of the main therapies for the treatment of diseases associated with inflammation [13]. In Turkish folk medicine, a decoction of fresh rose hips is prepared and used to treat various stomach disorders [14]. Trans-Tiliroside (Tribuloside) has been found to be one of the main active components of aqueous acetone extracts from fruits and seeds that inhibit weight gain and lower plasma triglyceride levels in mice [15]. Additionally, clinical studies have demonstrated the positive effect of rose hip powder in the treatment of osteoarthritis [16]. Rose hip powder enhances in vitro anti-inflammatory and chondroprotective properties in leukocytes and primary chondrocytes of human peripheral blood [17]. Unfortunately, to date, there are few data providing information on the biological action of extracts of buds and leaves, and it should be noted that these preparations have never been used for preclinical and clinical trials.

The present investigation was designed to carry out a phytochemical study involving detailed metabolomic and comparative analysis of fruits and flowers of *Rosa rugosa* Thumb., *Rosa davurica* Pall., and *Rosa acicularis* Lindl. originating from the Trans-Baikal region, Western Siberia, and Russian Far East.

## 2. Results

Approximately 300 mass spectra were assessed for each analytical replicate and MS operating condition in this comprehensive approach for a complete screening of phytochemicals (Figure 3).

![Figure 3. Representative chemical profiles of the *R. rugosa* (Primorye, Russia) total ion chromatogram from the MeOH extract.](image-url)

This procedure allowed a detailed evaluation of the rose MeOH extract fraction and the tentative identification of up to 146 phytochemicals (Table A1 (Appendix A)). The most represented classes of polyphenolic compounds were flavonoids (flavonols, flavones, flavan-3-ols, flavanones) with a total of 68 polyphenols identified for the first time. Some polyphenols were identified for the first time in the genus *Rosa* (family *Rosaceae*).

These are the flavones: Chrysosierol, Hispidulin, 5,7-Dimethoxyluteolin, Cirsimartin, Cirsiliol, Tricin, Jaceosidin, Nevadensin, Syringetin, Isovitexin, Genistein C-glucoside malonylated, Chrysin 6-C-glucoside-6′′-O-deoxyhexoside; flavanols: Dihydrokaempferol, Rhamnetin II, Kaempferol-3-O-α-L-rhamnoside, Taxifolin-O-pentoside, Taxifolin-3-O-hexoside, Isorhamnetin triacetyle hexoside; flavan-3-ols: Epiafzelechin and Galloatechin; flavanone: Naringenin, Fustin; phenolic acids: Caffeic acid, Citric acid, Hydroxy methoxy dimethylbenzoic acid, Hydroxyferulic acid, Ellagic acid, p-Coumaroylquinic acid, Ginkgoic acid, Salvianolic acid D, Salvianolic acid B; stilbenes: Pinosylvin, Resveratrol, 3-Hydroxyresveratrol;
lignans: Pinoresinol, Arctigenin, coumarins: 3,4,5-Trimethoxycoumarin, Fraxin; anthocyanins: Cyanidin 3-O-glucoside, Delphinidin O-pentoside, Pelargonidin 3-O-(6-O-malonyl-β-d-glucoside), Cyanidin 3-(6′-Succinyl-Glucoside), Delphinidin malonyl hexoside, Cyanidin 3-O-dioxyl-glucoside, Delphinidin 3,5-dihexoside, etc.

3. Discussion

A total of 146 compounds were identified in extracts of Rosa rugosa Thumb., Rosa davurica Pall., and Rosa acicularis Lindl. based on their accurate MS, fragment ions, and by searching online databases and the reported literature. A total of 115 compounds were identified for the first time in the genus Rosa (family Rosaceae). The newly identified metabolites belonged to 18 classes, including 14 phenolic acids and their conjugates, 18 flavones, 7 flavonols, 2 flavan-3-ols, 2 flavanones, 3 stilbenes, 2 coumarins, 2 lignans, 9 anthocyanins, 3 tannins, 8 terpenoids, 3 sceletium alkaloids, 4 fatty acids, 2 steroids, 2 carotenoids, 3 oxylipins, 3 amino acids, 5 carboxylic acids, etc. Metabolomic screening of polyphenols from extracts of R. rugosa, R. davurica, and R. acicularis included flavones, flavonols, flavan-3-ols, flavanones, anthocyanins, condensed tannins, phenolic acids, lignans, stilbenes, and coumarins.

3.1. Dimethoxyflavones

The flavones 5,7-Dimethoxyluteolin (compound 5), Cirsimaritin (compound 6), Chrysoseric methyl ether (compound 7), Cirsiliol (compound 8), Tricin (compound 9), Jaceosidin (compound 10), and Syringetin (compound 13) (Table A1 (Appendix A)) have been already characterized as components of Syzygium aromaticum [18], Ocimum [19], Rosmarinus officinalis [20], Bougainvillea [21], Triticum aestivum [22]; millet grains [23]; Sasa veitchii; Phyllostachys nigra [24], etc. Thus, the flavone Jaceosidin was found in extracts of R. davurica. The flavone 5,7-Dimethoxyluteolin was found in extracts of R. rugosa and R. davurica. The CID-spectrum (collision induced dissociation spectrum) in negative ion modes of Tricin from extracts of R. davurica is shown in Figure 4.

![Figure 4. CID-spectrum of Tricin from extracts of R. davurica, m/z 329.19.](image_url)

The [M – H]– ion produced three fragment ions at m/z 313, m/z 259, and m/z 229 (Figure 4). The fragment ion with m/z 313 produced two daughter ions at m/z 298 and m/z 271. The fragment ion with m/z 298 yielded two daughter ions at m/z 271 and m/z 227. It was identified in the bibliography in extracts of Triticum aestivum [22]; millet grains [23]; Sasa veitchii; Phyllostachys nigra [24].

3.2. Trimethoxyflavones

The flavones Nevadensin (compound 12) and Pentahydroxy trimethoxy flavone (compound 15) (Table A1 (Appendix A)) have been already characterized as components of Ocimum [19], F. glaucescens; C. edulis [25], Mentha [26], etc. Thus, the flavone Nevadensin was
found in extracts of R. acicularis. The CID-spectrum in positive ion modes of Nevadensin from extracts of R. acicularis is shown in Figure 5.

The [M + H]+ ion produced two fragment ions at m/z 330 and m/z 212 (Figure 5). The fragment ion with m/z 330 yielded one daughter ion at m/z 314. The fragment ion with m/z 314 yielded five daughter ions at m/z 312, m/z 286, m/z 259, m/z 182, and m/z 133. It was identified in the bibliography in extracts of Ocimum [19] and Mentha [26].

3.3. Trihydroxyflavones

The flavones Apigenin (compound 2), Chrysoeriol (compound 3), Isovitexin (compound 16), and flavonol Isokaempferide (compound 22) have been already characterized as components of Mentha [26], Hedyotis diffusa [27], Andean blueberry [28], Stevia rebaudiana [29], Rosa rugosa [30], Propolis [31], Rhus coriaria [32], Mexican lupine species [33], etc. Thus, the flavonol Isokaempferide was found in extracts of R. davurica. The CID-spectrum in positive ion modes of Isokaempferide from extracts of R. davurica is shown in Figure 6.

The [M + H]+ ion produced five fragment ions at m/z 300, m/z 274, m/z 256, m/z 212, and m/z 184 (Figure 6). The fragment ion with m/z 300 yielded three daughter ions at m/z 285, m/z 241, and m/z 200. The fragment ion with m/z 285 yielded one daughter ion at m/z 239. It was identified in the bibliography in extracts of Rosa rugosa [30] and Propolis [31].
3.4. Tetrahydroxyflavones

The flavonols Kaempferol (compound 20), Dihydrokaempferol (compound 21), Kaempferol-3-α-L-rhamnside (compound 30), Kaempferol diacetyl hexoside (compound 34), Kaempferol 3-O-rutinoside (compound 35), and Kaempferol 3-O-deoxyhexosylhexoside (compound 36) have been already characterized as components of F. glaucescens [25], *Andean blueberry* [28], *Rhus coriaria* (Sumac) [32], *Lonicerajaponica* [34], *Potato leaves* [35], *Rapeseed petals* [36], *Camellia kucha* [38]. Thus, the flavonol Kaempferol was found in extracts of *R. rugosa*, *R. davurica*, and *R. acicularis*. The CID-spectrum in positive ion modes of *F. glaucescens* is shown in Figure 7.

![Figure 7](image_url)

*Figure 7. CID-spectrum of Kaempferol from extracts of R. acicularis, m/z 287.*

The [M + H]+ ion produced six fragment ions at m/z 269, m/z 242, m/z 213, m/z 175, m/z 157, and m/z 139 (Figure 7). The fragment ion with m/z 175 yielded two daughter ions at m/z 157 and m/z 139. It was identified in the bibliography in extracts of *Andean blueberry* [28], *Rhus coriaria* (Sumac) [32], *Lonicerajaponica* [34], and *Potato leaves* [35].

3.5. Pentahydroxyflavones

The flavonols Quercetin (compound 23), Morin (compound 24), Rhamnetin I (compound 25), Rhamnetin II (compound 26), Isorhamnetin (compound 27), Avicularin (compound 31), Taxifolin-O-pentoside (compound 32), Taxifolin-3-O-hexoside (compound 33), and Isorhamnetin trimethyl hexoside (compound 37) have been already characterized as components of *Bougainvillea* [21], *Rosa rugosa* [30], *Propolis* [31], *Rhus coriaria* [32], and *Potato leaves* [35]. Thus, the flavonol Taxifolin-O-pentoside was found in extracts of *R. davurica*. The CID-spectrum in negative ion modes of Taxifolin-O-pentoside from extracts of *R. davurica* is shown in Figure 8.

![Figure 8](image_url)

*Figure 8. CID-spectrum of Taxifolin-O-pentoside from extracts of R. davurica, m/z 285.03.*
The [M − H]$^-$ ion produced three fragment ions at m/z 387, m/z 300, and m/z 177 (Figure 8). The fragment ion with m/z 300 yielded two daughter ions at m/z 284 and m/z 177. The fragment ion with m/z 284 yielded two daughter ions at m/z 240 and m/z 175. It was identified in the bibliography in extracts of millet grains [23] and A. cordifolia [25].

3.5. Pentahydroxyflavones

The flavonols Quercetin (compound 23), Rutin (compound 24), Myricetin (compound 25), and Quercetin 3-O-β-D-glucoside (compound 26) have been already characterized as components of millet grains [23], G. linguiforme [25], Camellia kucha [35], strawberry, cherimoya [39], Rosa rugosa [40], Myrtle [41], Radix polygoni multiflori [42], Licania ridigna [43], and Rhodiola rosea [44]. The flavan-3-ol Gallocatechin (compound 41) was found in extract of R. rugosa and R. davurica. The CID-spectrum in negative ion modes of Gallocatechin from R. rugosa is shown in Figure 9.

![Figure 9. CID-spectrum of Gallocatechin from R. rugosa, m/z 305.10.](image)

The [M − H]$^-$ ion produced one fragment ion at m/z 273 (Figure 9). The fragment ion with m/z 273 yielded two daughter ions at m/z 269 and m/z 217. The fragment ion with m/z 245 yielded four daughter ions at m/z 243, m/z 217, m/z 173, and m/z 145. It was identified in the bibliography in extracts from G. linguiforme [25], Licania ridigna [43], and Rhodiola rosea [44].

3.6. Flavan-3-ols

The flavan-3-ols Epiafzelechin (compound 38), Catechin (compound 39), (epi)Catechin (compound 40), and Gallocatechin (compound 41) have been characterized as components of millet grains [23], G. linguiforme [25], Camellia kucha [35], strawberry, cherimoya [39], Rosa rugosa [40], Myrtle [41], Radix polygoni multiflori [42], Licania ridigna [43], and Rhodiola rosea [44]. The flavan-3-ol Gallocatechin (compound 41) was found in extract of R. rugosa and R. davurica. The CID-spectrum in negative ion modes of Gallocatechin from R. rugosa is shown in Figure 9.

![Figure 10. CID-spectrum of (S)-Flavogallonic acid from extracts of R. davurica, m/z 471.11.](image)

3.7. Condensed Tannin

Prodelphinidin A-type (compound 83) and (S)-Flavogallonic acid (compound 84) have been already characterized as components of Vitis vinifera [45], Terminalia arjuna [46], and R. rugosa [47]. CID-spectrum in positive ion modes of (S)-Flavogallonic acid from R. davurica is shown in Figure 10. The [M + H]$^+$ ion produced four fragment ions at m/z 453, m/z 407, m/z 321, m/z 247, and m/z 205 (Figure 10). The fragment ion with m/z 407 yielded three daughter ions at m/z 389, m/z 307, and m/z 205. This compound was identified in the bibliography in extracts from Terminalia arjuna [46] and R. rugosa [47].
The polyphenol composition distribution table of varieties *Rosa rugosa* Thumb., *Rosa davurica* Pall., and *Rosa acicularis* Lindl. is shown below [Table 1]. The comparison table shows the presence of some polyphenols in three types of the genus *Rosa* (kaempferol, ellagic acid). Some polyphenols are present in only one variety of the genus *Rosa*.

**Table 1.** The flavonoid composition distribution of varieties *R. rugosa* Thumb., *R. davurica* Pall., and *R. acicularis* Lindl. Blue square—presence in extracts of *R. rugosa*; red square—in extracts of *R. davurica*; green square—in extracts of *R. acicularis*.

| No. | Class of Compounds | Identified Compounds | *R. rugosa* | *R. davurica* | *R. acicularis* |
|-----|-------------------|----------------------|------------|--------------|---------------|
| 1   | Flavone           | Hydroxy-methoxy (iso) flavone * | Blue       | Red          | Green         |
| 2   | Flavone           | Apigenin             |            |              |               |
| 3   | Flavone           | Chrysoeriol [Chryseriol] * | Blue       |              |               |
| 4   | Flavone           | Hispidulin *         | Blue       | Red          | Green         |
| 5   | Flavone           | 5,7-Dimethoxyluteolin * | Blue       | Red          | Green         |
| 6   | Flavone           | Cirsimaritin *       | Blue       | Red          | Green         |
| 7   | Flavone           | Chrysoeriol methyl ether * | Blue       | Red          | Green         |
| 8   | Flavone           | Cirsiliol *          | Blue       | Red          | Green         |
| 9   | Flavone           | Tricin *             | Blue       | Red          | Green         |
| 10  | Flavone           | Jaceosidin *         | Blue       | Red          | Green         |
| 11  | Flavone           | 5,6,4'-Trihydroxy-7,8-dimethoxyflavone * | Blue     | Red          | Green         |
| 12  | Flavone           | Nevadensin *         | Blue       | Red          | Green         |
| 13  | Flavone           | Syringetin *         | Blue       | Red          | Green         |
| 14  | Flavone           | Dihydroxy-tetramethoxy(iso)flavone * | Blue   | Red          | Green         |
| 15  | Flavone           | Pentahydroxy trimethoxy flavone * | Blue   | Red          | Green         |
| 16  | Flavone           | Isovitexin *         | Blue       | Red          | Green         |
| 17  | Flavone           | Genistein C-glucoside malonylated * | Blue  | Red          | Green         |
| 18  | Flavone           | Chrysin 6-C-glucoside-6"-O-deoxyhexoside * | Blue | Red          | Green         |
| 19  | Flavone           | Diosmin *            | Blue       | Red          | Green         |
| 20  | Flavonol          | Kaempferol           | Blue       | Red          | Green         |
| 21  | Flavonol          | Dihydrokaempferol *  | Blue       | Red          | Green         |
| 22  | Flavonol          | Isokaempferide [3-O-Methylkaempferol] | Blue      | Red          | Green         |
| 23  | Flavonol          | Quercetin            | Blue       | Red          | Green         |
| 24  | Flavonol          | Morin                | Blue       | Red          | Green         |
| 25  | Flavonol          | Rhamnetin I         | Blue       | Red          | Green         |
| 26  | Flavonol          | Rhamnetin II *      | Blue       | Red          | Green         |
| 27  | Flavonol          | Isorhamnetin        | Blue       | Red          | Green         |
| 28  | Flavonol          | Myricetin            | Blue       | Red          | Green         |
| 29  | Flavonol          | Mearnsinetin *      | Blue       | Red          | Green         |
| 30  | Flavonol          | Kaempferol-3-O-α-L-rhamnoside * | Blue   |             |               |
| 31  | Flavonol          | Avicularin           | Blue       | Red          | Green         |
| 32  | Flavonol          | Taxifolin-O-pentoside * | Blue       | Red          | Green         |
| 33  | Flavonol          | Taxifolin-3-O-hexoside * | Blue      | Red          | Green         |
| 34  | Flavonol          | Kaempferol diacetyl hexoside | Blue | Red          | Green         |
| 35  | Flavonol          | Kaempferol 3-O-rutinoside | Blue | Red          | Green         |
| 36  | Flavonol          | Kaempferol 3-O-deoxyhexosylhexoside | Blue   | Red          | Green         |
| 37  | Flavonol          | Isorhamnetin triacetyl hexoside * | Blue   | Red          | Green         |
| 38  | Flavan-3-ol       | Epiafzelechin [(epi)Afzelechin] * | Blue     | Red          | Green         |
| 39  | Flavan-3-ol       | Catechin [D-Catechol] | Blue       | Red          | Green         |
| 40  | Flavan-3-ol       | (+)-Epicatechin *    | Blue       | Red          | Green         |
Table 1. Cont.

| No. | Class of Compounds       | Identified Compounds                                                                 | R. rugosa | R. davurica | R. acicularis |
|-----|--------------------------|-------------------------------------------------------------------------------------|-----------|-------------|--------------|
| 41  | Flavan-3-ol              | Gallocatechin [+(-)Gallocatechin] *                                                  |           |             |              |
| 42  | Flavanone                | Naringenin [Naringotel; Naringenine]                                                |           |             |              |
| 43  | Flavanone                | Fustin [2,3-Dihydrofistein] *                                                       |           |             |              |
| 44  | Flavanone                | Eriodictyol [3′,4′,5,7-tetrahydroxy-flavanone]                                       |           |             |              |
| 45  | Flavanone                | Eriodictyol-7-O-glucoside *                                                         |           |             |              |
| 46  | Hydroxycinnamic acid     | Caffeic acid *                                                                      |           |             |              |
| 47  | Phenolic acid            | Quinic acid                                                                         |           |             |              |
| 48  | Phenolic acid            | Citric acid [Anhydrous; Citrate] *                                                  |           |             |              |
| 49  | Phenolic acid            | trans-Ferulic acid                                                                  |           |             |              |
| 50  | Phenolic acid            | Hydroxy methoxy dimethylbenzoic acid *                                              |           |             |              |
| 51  | Phenolic acid            | Syringic acid                                                                       |           |             |              |
| 52  | Phenolic acid            | 3,3,4,4-Tetrahydroxy-5-oxo-cyclohexanecarboxylic acid *                             |           |             |              |
| 53  | Phenolic acid            | Hydroxyferulic acid *                                                               |           |             |              |
| 54  | Hydroxycinnamic acid     | Sinapic acid [trans-Sinapic acid]                                                   |           |             |              |
| 55  | Phenolic acid            | 2,4,6-Trihydroxy-3,5-dimethoxynbenzoic acid *                                       |           |             |              |
| 56  | Hydroxybenzoic acid      | Ellagic acid *                                                                      |           |             |              |
| 58  | Phenolic acid            | p-Coumaroylquinic acid *                                                            |           |             |              |
| 59  | Phenolic acid            | 1-[(Acetyl-l-cysteinyl)oxy]-2,3,4,5-tetrahydroxyprocyanidin-1-carboxylic acid *     |           |             |              |
| 60  | Phenolic acid            | Chlorogenic acid [3-O-Caffeoylquinic acid] *                                         |           |             |              |
| 61  | Phenolic acid            | Neochlorogenic acid [5-O-Caffeoylquinic acid]                                       |           |             |              |
| 62  | Phenolic acid            | Rosmarinic acid                                                                     |           |             |              |
| 63  | Phenolic acid            | 5-Hydroxy feruloyl hexose *                                                         |           |             |              |
| 64  | Phenolic acid            | Salvianolic acid B [Danfensuan B] *                                                |           |             |              |
| 65  | Phenolic acid            | Salvianolic acid B [Danfensuan B] *                                                |           |             |              |
| 66  | Stilbene                 | Pinosylvin *                                                                        |           |             |              |
| 67  | Stilbene                 | Resveratrol *                                                                       |           |             |              |
| 68  | Stilbene                 | 3-Hydroxyresveratrol *                                                              |           |             |              |
| 69  | Lignan                   | Pinoresinol *                                                                       |           |             |              |
| 70  | Lignan                   | Arctigenin *                                                                        |           |             |              |
| 71  | Coumarin                 | 3,4,5-Trimethoxycoumarin *                                                          |           |             |              |
| 72  | Coumarin                 | Fraxin (Fraxetin-8-O-glucoside) *                                                   |           |             |              |
| 73  | Anthocyanidin            | Anthocyanidin [cyanidin chloride; Cyanidin] *                                       |           |             |              |
| 74  | Anthocyanidin            | Petunidin *                                                                         |           |             |              |
| 75  | Anthocyanidin            | Cyanidin-3-O-glucoside [Cyanidin 3-O-beta-D-Glucoside; Kuromarin] *                 |           |             |              |
| 76  | Anthocyanidin            | Delphinidin O-pentoside *                                                           |           |             |              |
| 77  | Anthocyanidin            | Pelargonidin 3-O-(6-O-malonyl-beta-D-glucoside) *                                   |           |             |              |
| 78  | Anthocyanidin            | Cyanidin 3-(6′-Succinyl-Glucoside) *                                               |           |             |              |
| 79  | Anthocyanidin            | Delphinidin malony hexoside *                                                       |           |             |              |
| 80  | Anthocyanidin            | Cyanidin-3-O-dioxyl-glucoside *                                                    |           |             |              |
| 81  | Anthocyanidin            | Delphinidin 3,5-dihexoside *                                                       |           |             |              |
| 82  | Tannin                   | Prodelphinidin A-type *                                                             |           |             |              |
| 83  | Hydrolysable tannin      | (S)-Flavogallonic acid                                                              |           |             |              |
| No. | Class of Compounds | Identified Compounds | R. rugosa | R. davurica | R. acicularis |
|-----|--------------------|-----------------------|-----------|-------------|-------------|
| 84  | Ellagitannin       | Punicalin alpha *     |           |             |             |
| 85  | Phenylpropanoid    | Coniferin *           |           |             |             |
| 86  | Gallate ester      | Ethyl gallate *       |           |             |             |
| 87  | Gallate ester      | Beta-Glucogallin *    |           |             |             |
| 88  | Dihydrochalcone    | Phloretin [Dihydroraringenin; Phloretol] * |           |             |             |
| 89  | Flavonoid          | Diphylloside B *      |           |             |             |
| 90  | Flavonoid          | Demethylanhydrocaritin-7-O-glucopyranosyl-3-O-acylated rhamnopyranosyl-xylopyranoside * |           |             |             |

* Polyphenols identified for the first time in genus *Rosa*.

The following polyphenols are present in only *R. rugosa*: Hydroxy-methoxy (iso)flavone, Chrysoeriol, Hispidulin, Cirsiliol, 5,6,4′-Trihydroxy-7,8-dimethoxyflavone, Dihydroxytetramethoxy (iso)flavone, Pentahydroxy trimethoxy flavone, Isovitexin, Chrysin 6-C-glucoside-6′-O-deoxyhexoside, Kaempferol-3-O-α-L-rhamnoside, Naringenin, Eriodictyol-7-O-glucoside, trans-Ferulic acid, 3,3,4,4-Tetrahydroxy-5-oxo-cyclohexanecarboxylic acid, Ginkgoic acid, 1-[(Acetyl-L-cysteinyl)oxy]-2,3,4,5-tetrahydroxy cyclohexane-1-carboxylic acid, Neochlorogenic acid, Rosmarinic acid, Salvianolic acid D, Pinosylvln, Pinosesinol, 3,4,5-rimethoxy coumarin, Fraxin, Anthocyanidin [cyanidin chloride; Cyanidin], Cyanidin-3-O-dioxyl-glucoside.

The following polyphenols are present in only *R. davurica*: Chrysoeriol methyl ether, Tricin, Jaceosidin, Syringetin, Genistein C-glucoside malonylated, Diosmin, Dihydrokaempferol, Isokempferide, Isorhamnetin, Myricetin, Mearnessin, Taxifolin-O-pentoside, Kaempferol diacetyl hexoside, Kaempferol 3-O-rutinoside, Epiafzelechin, (epi)Catechin, Fustin, Hydroxy methoxy dimethylbenzoic acid, Hydroxyferulic acid, Sinapic acid, p-Coumaroylquinic acid, Salvianolic acid B, cyanidin-3-O-glucoside, Delphinidin-3-O-pentoside, Pelargonidin-3-O-(6-O-malonyl-beta-D-glucoside), Delphinidin malonyl hexoside, Delphinidin 3,5-dihexoside, (S)-Flavogallonic acid, Punicalin alpha, Coniferin.

The following polyphenols are present in only *R. acicularis*: Circinarin, Nevdensin, Morin, Rhamnetin I, Rhamnetin II, Nevdensin, Taxifolin-O-hexoside, Kaempferol 3-O-deoxyhexosylhexoside, Isorhamnetin triacetetyl hexoside, Eriodictyol, 2,4,6-Trihydroxy-3,5-dimethoxybenzoic acid, Arctigenin, Prodelphinidin A-type, Ethyl gallate, Diphylloside B.

Thus, 146 metabolome compounds were identified in the extracts of *R. rugosa*, *R. davurica*, and *R. acicularis*, many of which are characteristic of the genus *Rosa* (family Rosaceae). Of these, 115 components were identified for the first time in the genus *Rosa*. These are flavones: Chrysoeriol, Hispidulin, 5,7-Dimethoxyluteolin, Cirsimaritin, Cirsiliol, Tricin, Jaceosidin, Nevdensin, Syringetin, Isovitexin, Genistein C-glucoside malonylated, Chrysin 6-C-glucoside-6′-O-deoxyhexoside; flavanols: Dihydrokaempferol, Rhamnetin II, Kaempferol-3-O-α-L-rhamnoside, Taxifolin-O-pentoside, Taxifolin-3-O-hexoside, Isorhamnetin triacetetyl hexoside; flavan-3-ols: Epiafzelechin and Gallocatechin; flavanones: Naringenin, Fustin; phenolic acids: Caffeic acid, Citric acid, Hydroxy methoxy dimethylbenzoic acid, Hydroxyferulic acid, Ellagic acid, p-Coumaroylquinic acid, Ginkgoic acid, Salvianolic acid B, Salvianolic acid D; Salvianolic acid B; stilbenes: Pinosylvln, Resveratrol, 3-Hydroxyresveratrol; lignans: Pinoresinol, Arctigenin; coumarins: 3,4,5-Trimethoxycoumarin, Fraxin; anthocyanins Cyanidin 3-O-glucoside, Delphinidin O-pentoside, Pelargonidin 3-O-(6-O-malonyl-β-D-glucoside), Cyanidin 3-(6″-Succinyl-Glucoside), Delphinidin malonyl hexoside, Cyanidin 3-O-dioxyl-glucoside, Delphinidin 3,5-dihexoside, etc.
4. Materials and Methods

4.1. Materials

Aboveground phyto *Rosa rugosa* Thumb., *Rosa davurica* Pall., and *Rosa acicularis* Lindl. collected during expedition work on the territory of the Russian Far East, Trans-Baikal Region, and Western Siberia during the period of ripening (July–September, 2020). Phyto mass of *R. davurica* was collected on the territory of Buryatia (N 52°21'97" E 108°59'84"), in September 2020. Phyto mass of *R. rugosa* was collected on the territory of Primorsky Krai, Russia (N 42°36'10" E 131°10'55"), during the period from 10 to 20 August, 2020. Phyto mass of *R. acicularis* was collected on the territory of Kemerovo, Western Siberia (N 55°21'15" E 86°05'23"), in August 2020. All samples were morphologically authenticated according to the current standard of Pharmacopoeia of the Eurasian Economic Union [48].

The results were obtained using the equipment of the Center for Collective Use of Scientific Equipment of TSU named after G.R. Derzhavin.

4.2. Chemicals and Reagents

HPLC-grade acetonitrile was purchased from Fisher Scientific (Southborough, UK), MS-grade formic acid was from Sigma-Aldrich (Steinheim, Germany). Ultra-pure water was prepared from a SIEMENS ULTRA clear (SIEMENS water technologies, Germany), and all other chemicals were analytical grade.

4.3. Fractional Maceration

To obtain highly concentrated extracts, fractional maceration was applied. In this case, the total amount of the extractant (methyl alcohol of reagent grade) is divided into 3 parts and is consistently infused on potato with the first part, then with the second and third. The infusion time of each part of the extractant was 7 days.

4.4. Liquid Chromatography

HPLC was performed using Shimadzu LC-20 Prominence HPLC (Shimadzu, Japan), equipped with an UV-sensor and a Shodex ODP-40 4E reverse phase column to perform the separation of multicomponent mixtures. The gradient elution program was as follows: 0.01–5 min, 100% CH$_3$CN; 5–45 min, 100–25% CH$_3$CN; 45–55 min, 25–0% CH$_3$CN; control washing: 55–60 min, 0% CH$_3$CN. The entire HPLC analysis was conducted with an ESI detector at wavelengths of 230 nm and 330 nm; the temperature corresponded to 17 ºC. The injection volume was 1 mL.

4.5. Mass Spectrometry

MS analysis was performed on an ion trap amaZon SL (BRUKER DALTONIKS, Germany) equipped with an ESI source in negative and positive ion modes. The optimized parameters were obtained as follows: ionization source temperature: 70 ºC, gas flow: 4 L/min, nebulizer gas (atomizer): 7.3 psi, capillary voltage: 4500 V, end plate bend voltage: 1500 V, fragmentary: 280 V, collision energy: 60 eV. A four-stage ion separation mode (MS/MS mode) was implemented.

5. Conclusions

The extracts of *Rosa rugosa* Thumb., *Rosa davurica* Pall., and *Rosa acicularis* Lindl. contain a large number of polyphenolic complexes which are biologically active compounds. For the most complete and safe extraction, the method of maceration with MeOH was used. To identify target analytes in extracts, HPLC was used in combination with the ion trap. The results of a preliminary study showed the presence of 146 bioactive compounds, of which 115 were identified for the first time in the genus *Rosa* (family Rosaceae). Of these 115 chemical compounds identified for the first time in the genus *Rosa*, 70 compounds belonged to the polyphenolic group: 18 flavones, 7 flavonols, 3 flavan-3-ols, 2 flavanones, 14 phenolic acids, 3 stilbenes, 2 lignans, 2 coumarins, 9 anthocyanidins, 3 tannins, etc. The proven richness of the bioactive components of targeted extracts of *R. rugosa*, *R. davurica*, etc.
and *R. acicularis* invites extensive biotechnological and pharmaceutical research, which can make a significant contribution both in the field of functional and enriched nutrition, and in the field of cosmetology and pharmacy. It should also be noted that the variability of the genus *Rosa* (family *Rosaceae*) contributes to the selection of the most drought-resistant species and samples for household, decorative, and forest reclamation needs in the arid climatic zones of Eurasia.

It is important to note that the useful properties of the genus *Rosa* (family *Rosaceae*) are: food (*R. rugosa, R. acicularis*), perfumery (*R. acicularis, R. ecae*), nectariferous (*R. canina, R. cinnamomea*), decorative (*R. acicularis, R. rugosa*), and soil-strengthening (*R. acicularis, R. rugosa, R. spinosissima*). A wide variety of biologically active polyphenolic compounds opens up rich opportunities for the creation of new drugs, as well as bioactive additives based on extracts from the genus *Rosa*.

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**Conflicts of Interest:** The authors declare no conflict of interest.
Appendix A

Table A1. Compounds identified from the extracts of *Rosa rugosa* Thumb., *Rosa davurica* Pall., and *Rosa acicularis* Lindl. in positive and negative ionization modes by HPLC-ion trap–MS/MS.

| No. | Class of Compounds | Identified Compounds | Formula | Mass | Molecular Ion [M−H]− | Molecular Ion [M+H]+ | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|--------------------|----------------------|---------|------|----------------------|----------------------|---------------------|---------------------|---------------------|------------|
| 1   | Flavone            | Hydroxy-methoxy (iso) flavone * | C_{16}H_{12}O_{4} | 268.2641 | 269 | 252 | 221 | 190 | Propolis [31] |
| 2   | Flavone            | Apigenin [5,7-Dihydroxy-2-(4-hydroxyphenyl)-4H-Chromen-4-One] | C_{15}H_{10}O_{5} | 270.2369 | 271 | 253 | 224 | Holistic Affect [27]; Andean blueberry [28]; Stere obsolus [29]; Rose rugosa [30]; Propolis [31] |
| 3   | Flavone            | Chrysoeriol [Chryseriol] * | C_{16}H_{12}O_{6} | 300.2629 | 301 | 269; 195 | 240 | Mentha [29]; Propolis [31]; *Hedyotis diffusa* [27]; *Andean blueberry* [28]; *Stevia rebaudiana* [29]; *Mexican lupine species* [33] |
| 4   | Flavone            | Hesperidin * | C_{16}H_{12}O_{6} | 300.2629 | 301 | 269; 243; 197 | 224; 188; 153 | Mentha [29]; *Cissus japonensis* [49] |
| 5   | Flavone            | 5,7-Dimethoxy-luteolin * | C_{17}H_{14}O_{6} | 314.2895 | 313 | 212; 285; 184; 113 | 113; 145; 185 | *Syringa armeniaca* [10] |
| 6   | Flavone            | Cirsimartin [Scrophulein; 4′,5-Dihydroxy-6,7-Dimethoxyflavone; 7-Methyicapillarisin] * | C_{17}H_{14}O_{6} | 314.2895 | 315 | 300; 240; 213; 185 | 272; 227; 185; 169; 153 | *Ocimum* [19]; *Rosmarinus officinalis* [20] |
| 7   | Flavone            | Chrysoeriol methyl ether * | C_{17}H_{14}O_{6} | 314.2895 | 315 | 267; 243; 187 | 187 | *Bougainvillea* [21] |
| 8   | Flavone            | Cirsiiol * | C_{17}H_{14}O_{7} | 329 | 229 | *Bougainvillea* [21] |
| 9   | Flavone            | Trisetin [5,7,4′-trihydroxy-3′,5′-dimethoxyflavone] * | C_{17}H_{14}O_{7} | 329 | 314; 299; 229 | 299; 271 | 271; 227 | *Triticum aestivum* [22]; *millet grains* [23]; *Sasa veitchii*; *Phyllostachys nigra* [24] |
| 10  | Flavone            | Jacassinidin [5,7,4′-trihydroxy-3′,5′-dimethoxyflavone] * | C_{17}H_{14}O_{7} | 329 | 351 | 305; 185 | *Mentha* [26,50] |
| 11  | Flavone            | 5,6,4′-Trihydroxy-7,8-dimethoxyflavone * | C_{17}H_{14}O_{7} | 329 | 351 | 299; 179 | 215 | *F. glaucescens; F. herrerae* [25]; *Mentha* [26] |
| 12  | Flavone            | Nevedensin * | C_{17}H_{14}O_{7} | 344.3534 | 345 | 300; 240; 213; 185 | 272; 227; 185; 169; 153 | *Ocimum* [19]; *Mentha* [26] |
| 13  | Flavone            | Syringetin * | C_{17}H_{14}O_{7} | 341.2683 | 347 | 317; 218; 299; 258; 241; 191 | *C. edulis* [25] |
| 14  | Flavone            | Dihydroxy-trimethoxy-flavone * | C_{18}H_{16}O_{7} | 352.3136 | 355 | 377; 373; 273; 213 | 357 | *F. glaucescens; C. edulis* [25] |
| 15  | Flavone            | Pentahydroxy-trimethoxy-flavone * | C_{18}H_{16}O_{7} | 352.3136 | 355 | 277; 373; 273; 213 | 357 | *F. glaucescens; C. edulis* [25] |
| 16  | Flavone            | Isovitexin [Saponaretin; Homovitexin; Apigenin-6-C-Glucoside] * | C_{23}H_{20}O_{10} | 432.3773 | 433 | 415; 305; 243; 175; 261; 243; 191; 115 | 133 | *millet grains* [23]; *Phyllostachys nigra* [24]; *Rhus coriaria* [32] |
| 17  | Flavone            | Genistein C-glucoside malonylated * | C_{23}H_{22}O_{13} | 518.4237 | 517 | 473; 435 | 455; 413; 339 | *Mexican lupine species* [33] |
| 18  | Flavone            | Chrysin 6-C-glucoside-6″-O-deoxyhexoside * | C_{27}H_{30}O_{13} | 562.5193 | 563 | 400; 363; 259; 183; 125 | 259; 224; 214; 133 | *F. glaucescens* [25]; *Mentha* [26]; *Lemon* [39]; *Grataegi Fructus* [52] |
| 19  | Flavone            | Diosmin [Diosmetin-7-O-rutinoside; Barosmin; Diosimin] * | C_{25}H_{32}O_{15} | 608.5447 | 609 | 591; 420; 355; 269 | 285 | *Andean blueberry* [28]; *Rhus coriaria* (Sumac) [32]; *Lonicera japonica* [34]; *Potato leaves* [35]; *Rapeseed petals* [36] |
| 20  | Flavonol           | Kaempferol [5,7-Dihydroxy-2-(4-hydroxyphenyl)-4H-Chromen-4-one] | C_{15}H_{12}O_{5} | 286.2603 | 287 | 187; 227; 199; 125 | *Mexican lupine species* [33]; *Cissus japonensis* [49]; *Cissus kuekenthalii* [57]; *Cassia fascicularis* [58] |
| 21  | Flavonol           | Dihydrokaempferol [Armosakendrin; Katuranin] * | C_{15}H_{12}O_{5} | 288.2522 | 287 | 259; 183; 117 | 215 | *F. glaucescens* [25]; *Andean blueberry* [28]; *Ecklonia fraxinoides* [37]; *Cassia fascicularis* [58] |
| No. | Class of Compounds | Identified Compounds | Formula | Mass | Molecular Ion [M – H] | Molecular Ion [M + H]+ | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|-------------------|---------------------|---------|------|----------------------|------------------------|----------------------|----------------------|----------------------|-----------|
| 22  | Flavonol          | Isokaempferide [3-O-Methylkaempferol] | C_{28}H_{28}O_{14} | 500.2629 | 301 | 301 | 299; 240; 209 | 209; 240; 209 | 209; 240; 209 | Rosa rugosa [53]; Propolis [51] |
| 23  | Flavonol          | Quercetin           | C_{28}H_{26}O_{12} | 382.2397 | 305 | 289 | 263; 243 | 213; 233 | 213; 233 | Rosa rugosa [53]; Propolis [51]; Staphylococcus aureus [12] |
| 24  | Flavonol          | Morin               | C_{15}H_{14}O_{6} | 320.2357 | 301 | 289; 240; 221 | 221 | 209; 157; 127 | Rosa rugosa [53]; Red waxes [52] |
| 25  | Flavonol          | Rhamnetin I [beta-Rhamnetin; Quercetin 7-Methyl ether] | C_{28}H_{28}O_{15} | 318.2357 | 301 | 285; 235; 215; 117 | 215 | 159; 127 | Rosa rugosa [53]; Blue coriaria L. (Sumac) [52]; Propolis [51]; Myrtus communis [51]; Embelia [51]; Stevia rebaudiana [51] |
| 26  | Flavonol          | Rhamnetin II *      | C_{28}H_{28}O_{16} | 320.2397 | 317 | 165; 185; 153; 123 | 117; 123 | 117; 123 | Rosa rugosa [53]; Blue coriaria L. (Sumac) [52]; Propolis [51]; Myrtus communis [51]; Embelia [51]; Stevia rebaudiana [51] |
| 27  | Flavonol          | Isoquercetin [Isoquercetin; Quercetin 7-Methyl ether; 3-Methyl(quercetin)] | C_{26}H_{26}O_{12} | 318.2357 | 317 | 285; 244; 190; 156 | 156 | 156 | Rosa rugosa [53]; Blue coriaria L. (Sumac) [52]; Propolis [51]; Myrtus communis [51]; Embelia [51] |
| 28  | Flavonol          | Myricetin           | C_{24}H_{28}O_{14} | 318.2357 | 319 | 289; 237; 185 | 185 | 185 | Rosa rugosa [53]; Blue coriaria L. (Sumac) [52]; Propolis [51]; Myrtus communis [51]; Embelia [51] |
| 29  | Flavonol          | Meanouetin *        | C_{24}H_{28}O_{15} | 332.2617 | 331 | 287 | 287 | 287 | 287 | Rosa rugosa [53]; Blue coriaria L. (Sumac) [52]; Propolis [51]; Myrtus communis [51]; Embelia [51]; Stevia rebaudiana [51]; Eucalyptus [57] |
| 30  | Flavonol          | Kaempferol 3-O-α-l-rhamnoside * | C_{27}H_{30}O_{16} | 432.3775 | 430 | 415; 313; 243; 198 | 198 | 198 | Rosa rugosa [53]; C. edulis [23]; Andean blueberry [28] |
| 31  | Flavonol          | Ariculatrin [Quercetin 3-Alpha-1-Arabinofuranoside; Ariculatrin] | C_{27}H_{30}O_{13} | 434.3703 | 433 | 309 | 309 | 309 | 309 | Rosa rugosa [53]; C. edulis [23]; Andean blueberry [28] |
| 32  | Flavonol          | Taxifolin-3-pentoside [Dihydroquercetin pentoside] * | C_{26}H_{28}O_{14} | 436.3711 | 435 | 301; 317 | 275; 239; 192; 179; 151 | 151 | 151 | Rosa rugosa [53]; Propolis [51]; Eucalyptus Globulus [52]; Rosa rugosa [53]; C. edulis [23]; Andean blueberry [28] |
| 33  | Flavonol          | Taxifolin-3-α-l-rhamnoside [Dihydroquercetin-3-α-l-rhamnoside] * | C_{27}H_{30}O_{15} | 446.3902 | 447 | 287; 305; 324; 449 | 240; 236; 227; 202 | 202 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56] |
| 34  | Flavonol          | Kaempferol 3-deoxyhexoside | C_{26}H_{28}O_{12} | 532.4003 | 533 | 453; 353; 289 | 289; 239 | 239 | 239 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56] |
| 35  | Flavonol          | Kaempferol 3-o-nitinoside | C_{27}H_{30}O_{15} | 594.5101 | 595 | 285; 195 | 155 | 155 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56] |
| 36  | Flavonol          | Kaempferol 3-o-deoxyxylosoxyhexoside | C_{27}H_{30}O_{15} | 594.5101 | 595 | 287; 263; 165 | 155; 145 | 145 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56] |
| 37  | Flavonol          | Isoquercetin triacetyl hexoside * | C_{28}H_{32}O_{16} | 642.4929 | 645 | 445; 440; 277; 277 | 277; 277 | 277 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56]; Stevia rebaudiana [51]; Embelia [51] |
| 38  | Flavan-3-ol       | Epicatechin [epi-Atelochin] * | C_{22}H_{16}O_{3} | 274.2697 | 275 | 244; 157 | 157 | 157 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56] |
| 39  | Flavan-3-ol       | Catechin [β-Catechin] | C_{22}H_{16}O_{3} | 290.2691 | 291 | 272; 174 | 174 | 174 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56]; Stevia rebaudiana [51]; Embelia [51] |
| 40  | Flavan-3-ol       | (epi)Catechin *     | C_{22}H_{16}O_{3} | 290.2691 | 291 | 272; 117 | 117 | 117 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56]; Stevia rebaudiana [51]; Embelia [51] |
| 41  | Flavan-3-ol       | Gallatechin [-(+Gallatechin)] * | C_{22}H_{16}O_{3} | 336.2705 | 307 | 291 | 291 | 291 | Rosa rugosa [53]; Propolis [51]; Eucalyptus hirta [56]; Stevia rebaudiana [51]; Embelia [51] |
| No. | Class of Compounds | Identified Compounds | Formula | Mass | Molecular Ion [M – H] | Molecular Ion [M + H]^+ | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|-------------------|----------------------|---------|------|----------------------|------------------------|-----------------------|-----------------------|-----------------------|------------|
| 42  | Flavonone         | Naringenin [Naringtet; Naringenone] | C_{15}H_{12}O_{5} | 272.5228 | 275 | 153, 236 | 123 |
| 43  | Flavonone         | Fustin [2,3-Dihydrofistein] * | C_{15}H_{12}O_{6} | 288.2522 | 289 | 269, 140 | 179 |
| 44  | Flavonone         | Eriodictyol [3′,4′,5,7-tetrahydroxy-flavanone] | C_{15}H_{12}O_{6} | 288.2522 | 287 | 269, 241, 155, 127 | 267, 251, 223, 183, 155 | 249, 199, 155 | Rosmarinus officinalis [20]; Andean blueberry [28]; Rosa rugosa [30]; Mexican lupine species [33]; Rapeseed petals [36]; Punica granatum [65] |
| 45  | Flavonone         | Eriodictyol-7-O-glucoside [Pyracanthoside; Miscanthoside] * | C_{21}H_{22}O_{11} | 450.3928 | 449 | 269; 151 | 225 |
| 46  | Hydroxycinnamic acid | Caffeic acid * | C_{9}H_{8}O_{4} | 180.1574 | 181 | 135 | 119 |
| 47  | Phenolic acid     | Quinic acid | C_{7}H_{12}O_{6} | 192.1666 | 191 | 191, 147 | 173, 136 | 133 |
| 48  | Phenolic acid     | Citric acid [Anhydrous; Citrus] * | C_{6}H_{8}O_{7} | 192.1235 | 191 | 111, 173 | 111 |
| 49  | Phenolic acid     | trans-Ferulic acid | C_{10}H_{10}O_{4} | 194.184 | 195 | 153 | 125 |
| 50  | Phenolic acid     | Hydroxy methoxy dimethylbenzoic acid * | C_{10}H_{12}O_{4} | 196.1999 | 195 | 129 | 119 |
| 51  | Phenolic acid     | Syringic acid | C_{6}H_{12}O_{5} | 198.1727 | 199 | 157, 183, 119 | 142 |
| 52  | Phenolic acid     | 3,4,4,6-Tetrahydroxy-5-acetoxybenzoic acid * | C_{10}H_{12}O_{7} | 246.1701 | 247 | 161, 149 | 143 | 119 |
| 53  | Phenolic acid     | Hydroxyferulic acid * | C_{10}H_{12}O_{5} | 214.1634 | 215 | 195 | 129 |
| 54  | Hydroxycinnamic acid | Sinapic acid [trans-Sinapic acid] | C_{11}H_{12}O_{5} | 224.2100 | 225 | 209 | 139, 192 |
| 55  | Phenolic acid     | 2,3,4,6-Tetrahydroxy-3,5-dimethoxybenzoic acid * | C_{7}H_{12}O_{7} | 230.1915 | 231 | 191 | 127 |
| 56  | Phenolic acid     | Chlorenic acid [3-O-Caffeylquinic acid] * | C_{13}H_{12}O_{8} | 354.3087 | 355 | 191 | 173 |

*indicates the presence of a single fragment or characteristic peak.
| No. | Identifed Compounds | Formula | Mass | Molecular Ion [M – H]\(^{-}\)* | Molecular Ion [M + H]⁺ | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|---------------------|---------|------|-----------------------------|------------------------|----------------------|----------------------|----------------------|-------------|
| 61  | Phenolic acid       | Neochlorogenic acid [5-O-Caffeoylquinic acid] | C\(_{16}\)H\(_{18}\)O\(_{9}\) | 354.3087 | 353 | 173; 111 | Andean blueberry [28]; *Stevia rebaudiana* [29]; *Rosa rugosa* [30]; *Lonicera japonica* [34]; *Euphorbia hirta* [35]; Citrus maxima, *Sambucus nigra* [67] |
| 62  | Phenolic acid       | Rosmarinic acid | C\(_{18}\)H\(_{16}\)O\(_{8}\) | 360.3148 | 361 | 164; 131; 105; 104; 103 | 253; 121 | 225; 210; 179 | Rosmarinus officinalis [20]; *Mentha* [26]; *Rosa rugosa* [30]; *Mentha* [70]; Huoliisu Oral Liquid [71]; *Rosemary* [72] |
| 63  | Phenolic acid       | 5-Hydroxy feruloyl hexose * | C\(_{16}\)H\(_{20}\)O\(_{10}\) | 372.3240 | 373 | 211; 277; 354 | 175 | | millet grains [23] |
| 64  | Phenolic acid       | Salvianolic acid D * | C\(_{20}\)H\(_{18}\)O\(_{10}\) | 418.3509 | 417 | 373 | 347; 303 | | *Salvia multiorrizae* [74] |
| 65  | Phenolic acid       | Salvianolic acid B [Danfensuan B] * | C\(_{36}\)H\(_{30}\)O\(_{16}\) | 718.6138 | 719 | 521; 199 | 475 | | *Bougainvillea* [21]; *Mentha* [50]; Huoliisu Oral Liquid [71]; *Mentha* [73]; *Salvia miltiorrhiza* [74] |
| 66  | Stilbene            | Pinosylvin [3,5-Stilbenediol; Trans-3,5-Dihydroxystilbene] * | C\(_{14}\)H\(_{12}\)O\(_{2}\) | 212.2439 | 213 | 195; 171 | 143 | 127 | *Pinus resinosa* [75]; *Pinus sylvestris* [76] |
| 67  | Stilbene            | Resveratrol [trans-Resveratrol; 3,4′,5-Trihydroxystilbene; Stilbentriol] * | C\(_{14}\)H\(_{12}\)O\(_{3}\) | 228.2433 | 229 | 169; 210; 141; 115 | 141 | 113 | *A. cordifolia*; *F. glaucescens*; *F. herrerae* [25]; *Radix polygoni multiflori* [42]; *Embelia* [56]; *Vine stilbenoids* [77] |
| 68  | Stilbene            | 3-Hydroxyresveratrol [Piceatannol] * | C\(_{14}\)H\(_{12}\)O\(_{4}\) | 244.2427 | 245 | 199; 210; 141; 115 | 141 | 113 | *A. cordifolia*; *F. glaucescens*; *F. herrerae* [25]; *Radix polygoni multiflori* [42]; *Embelia* [56]; *Vine stilbenoids* [77] |
| 69  | Lignan             | Pinoresinol * | C\(_{20}\)H\(_{22}\)O\(_{6}\) | 358.3851 | 359 | 340; 208 | 322; 196 | 274; 214 | *Passiflora incarnata* [61]; *Punica granatum* [65]; *Eucommia cortex* [79]; Lignans [80] |
| 70  | Lignan             | Arctigenin * | C\(_{21}\)H\(_{24}\)O\(_{6}\) | 372.4117 | 373 | 354; 306; 283; 252; 211 | 336; 319; 289; 252; 218 | 288; 236; 197 | *Lignina* [50]; *Trichosanthes ovata* [63]; *Goyaz* [64] |
| 71  | Coumarin           | 3,4,5-Trimethoxycoumarin * | C\(_{12}\)H\(_{12}\)O\(_{5}\) | 236.2207 | 237 | 192; 206; 178 | 132 | 130; 117 | Propolis [31] |
| 72  | Coumarin           | Fraxin [Fraxin-8-O-glucoside] * | C\(_{16}\)H\(_{18}\)O\(_{10}\) | 370.3081 | 371 | 191 | 127 | *Vitis vinifera* [45]; *Actinidia* [69]; *Solanum tuberosum* [83] |
| 73  | Anthocyanidin      | Cyanidin-3-O-glucoside [Cyanidin 3-O-beta-D-Glucoside; Kuromarin] * | C\(_{21}\)H\(_{21}\)O\(_{11}\) | 449.3848 | 447 | 287; 195; 167 | 196; 163; 125 | *Triticum aestivum* [22]; *Malpighia emarginata* [84] |
| 74  | Anthocyanidin      | Delphinidin 3-O-pentoside * | C\(_{20}\)H\(_{19}\)O\(_{12}\) | 435.3583 | 435 | 305; 245 | 245; 149 | *Triticum aestivum* [22]; *Myrtus communis* [61]; *Gossypium hirsutum* [62] |
| 75  | Anthocyanidin      | Cyanidin-3-O-dioxayl-glucoside * | C\(_{31}\)H\(_{28}\)O\(_{12}\) | 593.5248 | 593 | 287; 214 | 213; 153 | *Triticum aestivum* [22]; *Myrtus communis* [61]; *Gossypium hirsutum* [62] |
| 76  | Anthocyanidin      | Delphinidin 3,5-dihexoside * | C\(_{27}\)H\(_{31}\)O\(_{17}\) | 627.5248 | 627 | 413; 227 | 227; 151 | *F. herrerae* [25]; *Andean blueberry* [28]; *Berberis microphylla* [85] |
| No. | Class of Compounds | Identified Compounds | Formula | Mass | Molecular Ion [M – H] | Molecular Ion [M + H] | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|--------------------|----------------------|---------|------|----------------------|----------------------|----------------------|----------------------|----------------------|------------|
| 82  | Tannin             | Prodelphinidin A-type*| C_{30}H_{26}O_{13} | 594.5206 | 595  | 406, 287, 245  | 241, 211, 165, 153 | 213 |                    | His cupro [45] |
| 83  | Hydrolysable tannin| Oligogallic acid      | C_{21}H_{11}O_{13} | 470.2603 | 471  | 407, 321, 247, 205 | 205, 387, 389 | 177, 151 |                    |                        |
| 84  | Ellagitannin        | Punicalin alpha*      | C_{24}H_{23}O_{12} | 782.5253 | 783  | 721, 469, 599, 531 | 596 |                    |                        |                        |
| 85  | Phenylpropanoid     | Coniferin [Coniferol; Alcohol Beta-O-Glucoside]* | C_{16}H_{22}O_{8} | 342.3411 | 343  | 240  | 183  | 127 |                        |                        |
| 86  | Gallate ester      | Ethyl gallate*        | C_{16}H_{23}O_{5} | 358.1727 | 197  | 169, 125 | 124 |                    | Bonggarviola [21]; Terminalia arjuna [46]; Euphorbica [59] |
| 87  | Gallate ester      | Beta-Glucogallin [3-O-Galloyl-Beta-D-Glucose; Monogalloyl glucose] | C_{24}H_{24}O_{12} | 668.7763 | 669 | 447, 592, 533, 483, 433, 369, 317 | 523, 484, 418, 369, 317 | 439 |                        |                        |
| 88  | Flavonoid           | Dihydrochalcone       | C_{15}H_{14}O_{5} | 274.2687 | 275  | 257, 229, 215 | 225, 239, 229, 210 |                        |                        |
| 89  | Flavonoid           | Demethylhydroxycinnam mitochondrial cinnamoylanilides | C_{24}H_{14}O_{20} | 836.7854 | 837  | 675, 603, 541, 483, 403 | 441, 341 | 341, 241 |                        |                        |
| 90  | OTHERS              | Cyclohexenecarboxylic acid | Shikimic acid [L-Schikimic acid]* | C_{7}H_{10}O_{5} | 174.1513 | 173  | 111 |                        |                        |
| 91  | Vitamin             | L-Ascorbic acid [Vitamin C] | C_{6}H_{8}O_{6} | 176.1241 | 175  | 127 |                        |                        |
| 92  | Monoterpenoid       | Methyl eugenol*       | C_{11}H_{14}O_{2} | 178.2277 | 179  | 161  | 123 |                        |                        |
| 93  | Omega-5 fatty acid  | Hydroxymyristic acid* | C_{10}H_{20}O_{2} | 204.2668 | 205  | 186, 158 | 146, 149 | 144, 138 |                        |                        |
| 94  | Essential amino acid| L-Tryptophan [L-Tryptophan; (S)-Tryptophan]* | C_{12}H_{14}N_{2}O_{2} | 204.2252 | 205  | 196, 158 | 146, 149 | 144, 138 |                        |                        |
| 95  | Sesquiterpenoid     | Caryophyllene oxide [Caryophyllene-alpha-oxide]* | C_{15}H_{20}O_{2} | 226.3000 | 227  | 161  | 147 |                        |                        |
| 96  | 3,4,5-Trimethoxyphenylacetic acid | 3,4,5-Trimethoxyphloridin-3,5-dicarboxylic acid* | C_{14}H_{12}O_{5} | 242.2599 | 243  | 127, 143, 119, 109 | 127, 117 |                        |                        |
| 97  | Omega-5 fatty acid  | Myristilic acid [2S-Tetradecanoic acid]* | C_{14}H_{26}O_{2} | 244.3040 | 245  | 199, 127 | 139 |                        |                        |
| 98  | Quassinolide        | Dehydrocostus Lactone | Dehydrocostus Lactone* | C_{15}H_{18}O_{3} | 246.2599 | 247  | 209, 127 | 139 |                        |                        |
| 99  | Germacradiene      | Costusolide* | C_{15}H_{24}O_{2} | 333.3510 | 333  | 186 | 168 |                        |                        |
| 100 | Biphenyl derivative | Randaiol* | C_{15}H_{20}O_{2} | 242.2599 | 243  | 127, 143, 119, 109 | 127, 117 |                        |                        |
| 101 | Peptide            | 5-Chloro-4-propyl-2-isourea* | C_{12}H_{22}N_{3}O_{4} | 242.2716 | 243  | 197 | 165 |                        |                        |
| 102 | Hydnocarpus acid   | Hydroxymyristic acid [2S-Hydroxymyristic acid; Alpha-Hydroxymyristic acid]* | C_{14}H_{20}O_{5} | 244.3703 | 245  | 229, 222, 213, 201 | 227, 215, 201 |                        |                        |
| No. | Identified Compounds | Formula | Mass | Molecular Ion (M+H)+ | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|----------------------|---------|------|---------------------|----------------------|----------------------|----------------------|------------|
| 104 | Medium-chain fatty acid | C_{12}H_{22}O_5 | 246.3001 | 247 | 229; 202; 174; 156 | 183; 156; 144 | 136 | F. glaucescens [23] |
| 105 | Acylic alcohol nitrile glycoside | C_{12}H_{22}NO_6 | 239.2058 | 240 | 196; 232 | 168 | 141 | Rhodiocyanoside A [93], Rhodiola rosea [94] |
| 106 | Naphthoquinone | C_{21}H_{18}O_7 | 241.1077 | 242 | 247 | 219 | Blue cornelian [92] |
| 107 | Acorus | C_{21}H_{22}NO_5 | 265.3653 | 266 | 247; 190; 166 | 166 | 141 | Magnolia officinalis [92] |
| 108 | Ribonucleoside composite of adenine (purine) | C_{24}H_{32}N_5O_4 | 267.2413 | 268 | 136 | 135 | 144 | Licorice (glycyrrhiza) [36], Huolisu Oral Liquid [71] |
| 109 | 3,4,5,8,9,10-Pentahydroxydibenzo[b,d]pyran-6-one | C_{13}H_{8}O_7 | 276.1984 | 277 | 175; 231; 259 | 131; 177 | 141 | Terminalia arjuna [46] |
| 110 | Linoleic acid amide | C_{18}H_{33}NO | 279.4607 | 280 | 262 | 244; 196; 164; 128 | 226; 196; 164 | Propolis [31], Rhus coriaria [32] |
| 111 | Oleamide | C_{18}H_{35}NO | 281.4766 | 282 | 247 | 173; 201; 145 | 222; 196; 164 | 141 | Propolis [31] |
| 112 | Terpenoid | C_{15}H_{22}O_5 | 282.3322 | 283 | 239; 265; 167 | 215 | 193; 170 | Rhodiola rosea [93], Rhodiola sacra [94] |
| 113 | Alkaloid | C_{17}H_{23}NO_3 | 289.3694 | 290 | 272; 146 | 164 | 141 | Sceletium [96] |
| 114 | Alkaloid | C_{17}H_{25}NO_3 | 291.3853 | 292 | 274; 226; 111 | 121 | 141 | A. cordifolia [25], Sceletium [96] |
| 115 | Brevifolincarboxylic acid | C_{13}H_{8}O_8 | 292.4131 | 291 | 247 | 191; 203; 191; 175; 147 | 191 | 141 | Euphorbia hirta [59] |
| 116 | Alkaloid | C_{18}H_{25}NO_3 | 303.3960 | 304 | 257; 195; 153 | 231; 149 | 213 | 141 | A. cordifolia [25] |
| 117 | Diterpenoid | C_{19}H_{18}O_4 | 310.3438 | 311 | 287; 243; 187 | 259 | 215 | 141 | Huolisu Oral Liquid [72], Salviae Miltiorrhizae [97] |
| 118 | Oxylipins | C_{18}H_{30}O_5 | 310.4284 | 309 | 291; 247; 198; 183 | 181 | 141 | Potato leaves [35] |
| 119 | Tyramines | C_{18}H_{19}NO_4 | 313.3478 | 314 | 296; 236; 175 | 222; 206; 178 | 222; 194; 168 | 141 | Rosmarinus officinalis [20], Rosemary [72], Lepechinia [102] |
| 120 | Alkaloid | C_{19}H_{25}NO_4 | 326.2986 | 325 | 270; 226; 198 | 166 | 141 | A. cordifolia [25] |
| 121 | Dihydroxy eicosatrienoic acid | C_{20}H_{34}O_5 | 328.4437 | 327 | 291; 229; 211; 125 | 183 | 141 | Phyllanthus nigricans [32], Rhinanthus tanguticus [106] |
| 122 | Oxylipins | C_{18}H_{32}O_5 | 330.4596 | 329 | 251; 209; 253; 211; 171; 179 | 273; 217; 179 | 253 | 222 | Gynaecium [36], Phyllanthus Americanus [106], Boccardi [101] |
| 123 | Alkaloid | C_{18}H_{32}O_5 | 331.4061 | 3301 | 270; 226; 198 | 166 | 141 | A. cordifolia [25] |
| 124 | Alkaloid | C_{20}H_{28}O_4 | 332.4339 | 331 | 287; 243; 187 | 259 | 215 | 141 | Rosmarinus officinalis [20], Rosemary [72], Lepechinia [102] |
| 125 | Dihydroxy eicosatrienoic acid | C_{20}H_{34}O_5 | 338.4816 | 339 | 327; 177 | 303; 274; 233 | 178; 148 | 141 | G. cyclocarpa, A. cordifolia, C. edulis [25] |
| 126 | Berberine alkaloid | C_{21}H_{22}NO_4 | 352.4037 | 353 | 330; 309; 270; 235; 195 | 317; 243; 215; 160 | 141 | Ocotea [103], Palmatina [104] |
| 127 | Unaturated fatty acid | C_{21}H_{22}NO_4 | 372.6284 | 373 | 341 | 327 | 141 | A. cordifolia, F. pottsii [15] |
| 128 | Unaturated fatty acid | C_{21}H_{22}NO_4 | 380.6474 | 381 | 363; 354; 290; 261; 231 | 342; 303; 276 | 141 | F. glaucescens [23] |
| 129 | Sterol | C_{21}H_{22}O_4 | 400.6981 | 401 | 383; 367; 337; 279 | 309; 321; 283; 249 | 262 | 141 | A. cordifolia, C. edulis [25], Oryza sativa [105] |
| 130 | Alkaloid | C_{14}H_{22}NO_5 | 407.4375 | 408 | 389 | 343; 183 | 299; 161 | Camellia kucha [98] |
Table A1. Cont.

| No. | Class of Compounds | Identified Compounds | Formula | Mass (M – H) | Molecular Ion (M + H) | 2 Fragmentation MS/MS | 3 Fragmentation MS/MS | 4 Fragmentation MS/MS | References |
|-----|-------------------|----------------------|---------|--------------|----------------------|----------------------|----------------------|----------------------|------------|
| 131 | Sterol            | Stigmasterol [*]     | C_{29}H_{48}O_{4} | 412.6908     | 413                 | 305                  | 189                  |                      | Rhus coriaria [32]; Hedyotis diffusa [27]; Olive leaves [26] |
| 132 | Iridoid monoterpenoid | Dihydrosoraflanate [*] | C_{22}H_{32}O_{8} | 424.8947     | 425                 | 360; 281             | 309; 235             |                      | Rhoea coriaria [90]; Hedyotis polyphylla [109] |
| 133 | Steroid           | Sterol [*]           | C_{27}H_{44}O_{2} | 408.6847     | 409                 |                      |                      |                      |                        |
| 134 | Triterpenoid      | Betulinic acid [*]   | C_{30}H_{44}O_{3} | 452.6686     | 453                 | 437; 387; 245        | 176; 305; 316; 213   |                      | Rhus coriaria [32]; Hedyotis polyphylla [90] |
| 135 | Triterpenoid      | Pesticide [*]        | C_{25}H_{34}O_{2} | 472.6997     | 473                 |                      |                      |                      |                        |
| 136 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 137 | Triterpenoid      | Betulinic acid [*]   | C_{30}H_{44}O_{3} | 452.6686     | 453                 |                      |                      |                      |                        |
| 138 | Triterpenoid      | Betulinic acid [*]   | C_{30}H_{44}O_{3} | 452.6686     | 453                 |                      |                      |                      |                        |
| 139 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 140 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 141 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 142 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 143 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 144 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 145 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |
| 146 | Steroid           | Sterol [*]           | C_{29}H_{48}O_{4} | 412.6908     | 413                 |                      |                      |                      |                        |

* Compounds identified for the first time in genus *Rosa.*
References

1. Thomas, E.; Vandebroek, I.; Sanca, S.; van Damme, P. Cultural Significance of Medicinal Plant Families and Species among Quechua Farmers in Apillapampa, Bolivia. J. Ethnopharmacol. 2009, 122, 60–67. [CrossRef] [PubMed]

2. Sultana, A.; Hossain, M.J.; Kuddus, M.R.; Rashid, M.A.; Zahan, M.S.; Mitra, S.; Roy, A.; Alam, S.; Sarker, M.M.R.; Naina Mohamed, I. Ethnobotanical Uses, Phytochemistry, Toxicology, and Pharmacological Properties of Euphorbia neriifolia Linn. against Infectious Diseases: A Comprehensive Review. Molecules 2022, 27, 4374. [CrossRef] [PubMed]

3. Abidullah, S.; Rauf, A.; Khan, S.W.; Ayaz, A.; Liaquat, F.; Saqib, S. A Comprehensive Review on Distribution, Pharmacological Uses and Biological Activities of Argyrolobium Roseum (Cambess.). J.auba. Spach. Acta Ecol. Sin. 2021, 42, 198–205. [CrossRef]

4. Das, R.; Mitra, S.; Tareq, A.M.; Emran, T.B.; Hossain, M.J.; Alqahtani, A.M.; Alghazwani, Y.; Dhama, K.; Simal-Gandara, J. Medicinal plants used against hepatic disorders in Bangladesh: A comprehensive review. J. Ethnopharmacol. 2022, 282, 114588. [CrossRef]

5. Mitra, S.; Lami, M.S.; Uddin, T.M.; Das, R.; Islam, F.; Anjum, J.; Hossain, M.J.; Emran, T.B. Prospective multipractical roles and pharmacological potential of dietary flavonoid narirutin. Biomed. Pharmacother. 2022, 150, 112932. [CrossRef]

6. Demain, A.L.; Fang, A. The Natural Functions of Secondary Metabolites. In History of Modern Biotechnology, 1st ed.; Springer: Berlin/Heidelberg, Germany, 2000; pp. 1–39.

7. Wink, M. Modes of Action of Herbal Medicines and Plant Secondary Metabolites. Medicines 2015, 2, 251–286. [CrossRef]

8. Anjum, J.; Mitra, S.; Das, R.; Alam, R.; Mojumder, A.; Emran, T.B.; Islam, F.; Rauf, A.; Hossain, M.J.; Aljohani, A.S.; et al. A renewed concept on the MAPK signaling pathway in cancers: Polyphenols as a choice of therapeutics. Pharmacol. Res. 2019, 2019, 99, 5350–5357. [CrossRef]

9. Campanini, E. Dizionario di Fitoterapia e Piante Medicinali, 2nd ed.; Tecniche Nuove: Milano, Italy, 2006; pp. 566–571.

10. Ieri, F.; Innocenti, M.; Possieri, L.; Gallori, S. Phenolic composition of “bud extracts” of Ribes nigrum L., Rosa canina L. and Tilia tomentosa M. J. Pharmaceut. Analus. 2015, 11, 1–9. [CrossRef]

11. Yang, Y.; Zhang, J-J.; Zhou, Q.; Wang, L.; Huang, W.; Wang, R. Effect of ultrasonic and ball-milling treatment on cell wall, nutrients, and antioxidant capacity of rose (Rosa rugosa) bee pollen, and identification of bioactive components. J. Sci. Food Agric. 2019, 199, 0530–0537. [CrossRef]

12. Hashidoko, Y. The phytochemistry of Rosa rugosa. Phytochemistry 1996, 43, 535–549. [CrossRef]

13. Lattanzio, F.; Greco, E.; Carretta, D.; Cervellati, R.; Govoni, P.; Speroni, E. In vivo anti-inflammatory effect of Rosa canina L. extract. J. Ethnopharmacol. 2011, 137, 880–885. [CrossRef] [PubMed]

14. Gurbuz, I.; Ustun, O.; Yesilada, E.; Sezik, E.; Kutsal, O. Anti-ulcerogenic activity of some plants used as folk remedy in Turkey. Ethnopharmacol. 2003, 88, 93–97. [CrossRef]

15. Ninomiya, K.; Matsuda, H.; Kubo, M.; Morikawa, T.; Nishida, N.; Yoshikawa, M. Potent anti-obese principle from Rosa canina: Structural requirements and mode of action of trans-tiliroside. Bioorganic Med. Chem. Lett. 2007, 17, 3059–3064. [CrossRef] [PubMed]

16. Chrubasik, C.; Roufogalis, B.D.; Muller-Lander, U.; Chrubasik, S. A Systematic Review on the Rosa canina Effect and Efficacy Profiles. Phytother. Res. 2008, 22, 725–733. [CrossRef] [PubMed]

17. Schwager, J.; Richard, N.; Schoop, R.; Wolfram, S. A Novel Rose Hip Preparation with Enhanced Anti-Inflammatory and Chondroprotective Effects. Mediat. Inflamm. 2014, 2014, 105710. [CrossRef] [PubMed]

18. Fathoni, A.; Saepudin, E.; Cahyana, A.H.; Rahayu, D.U.C.; Haib, J. Identification of nonvolatile compounds in clove (Syzygium aromaticum) from Manado. AIP Conf. Proc. 2016, 1862, 030079. [CrossRef]

19. Pandey, R.; Kumar, B. HPLC-QTOF–MS/MS-based rapid screening of phenolics and triterpenic acids in leaf extracts of Ocimum species and their interspecies variation. J. Liq. Chromatogr. Relat. Tech. 2016, 39, 225–238. [CrossRef]

20. Mena, P.; Cirilini, M.; Tassotti, M.; Herrlinger, K.A.; Dall’Asta, C.; Del Rio, D. Phytochemical Profiling of Flavonoids, Phenolic Acids, Terpenoids, and Volatile Fraction of a Rosemary (Rosmarinus officinalis L.) Extract. Molecules 2016, 21, 1576. [CrossRef]

21. El-Sayed, M.A.; Abbass, F.A.; Refaat, S.; El-Shafae, A.M.; Fikry, E. UPLC-ESI-MS/MS Profile of The Ethyl Acetate Fraction of Aerial Parts of Bougainvillea ‘Scarlett O’Hara’ Cultivated in Egypt. J. Chem. 2021, 64, 22. [CrossRef]

22. Sharma, M.; Sandhir, R.; Singh, A.; Kumar, P.; Mishra, A.; Jachak, S.; Singh, S.P.; Singh, J.; Roy, J. Comparison analysis of phenolic compound characterization and their biosynthesis genes between two diverse bread wheat (Triticum aestivum) varieties differing for chapatti (unleavened flat bread) quality. Front. Plant. Sci. 2016, 2016, 7, 1870. [CrossRef]

23. Chandrasekara, A.; Shahidi, F. Determination of antioxidant activity in free and hydrolyzed fractions of millet grains and characterization of their phenolic profiles by HPLC-DAD-ESI-MSn. J. Funct. Foods 2011, 3, 144–158. [CrossRef]

24. Van Hoyweghen, L.; De Bosscher, K.; HaegeMAN, G.; DeForces, D.; Heyerick, A. In Vitro Inhibition of the Transcription Factor NF-κB and Cyclooxygenase by Bamboo Extracts. Phytother. Res. 2014, 28, 224–230. [CrossRef] [PubMed]

25. Hamed, A.R.; El-Hawary, S.S.; Ibrahim, R.M.; Abdelmohsen, U.R.; El-Halawany, A.M. Identification of Chemopreventive Components from Halopyrethys Belonging to Aizoaceae and Cactaceae Through LC/MS–Bioassay Guided Approach. J. Chrom. Sci. 2021, 59, 618–626. [CrossRef] [PubMed]

26. Xu, L.L.; Xu, J.J.; Zhong, K.R.; Shang, Z.P.; Wang, F.; Wang, R.F.; Liu, B. Analysis of non-volatile chemical constituents of Menthae Haplocalycis herba by ultra-high performance liquid chromatography—High resolution mass spectrometry. Molecules 2017, 22, 1756. [CrossRef] [PubMed]
27. Chen, X.; Zhu, P.; Liu, B.; Wei, L.; Xu, Y. Simultaneous determination of fourteen compounds of Hedychium diffusum Willd extract in rats by UHPLC-MS/MS method: Application to pharmacokinetics and tissue distribution study. J. Pharmaceut. Biomed. Analys. 2018, 159, 490–512. [CrossRef]

28. Aita, S.E.; Capirotti, A.L.; Cavaliere, C.; Cerrato, A.; Giannelli Moneta, B.; Montone, C.M.; Piovesana, S.; Lagana, A. Andean Blueberry of the Genus Distelirgma: A High-Resolution Mass Spectrometric Approach for the Comprehensive Characterization of Phenolic Compounds. Separrations 2021, 8, 58. [CrossRef]

29. Lee, S.Y.; Shaari, K. LC–MS metabolomics analysis of Stevia rebaudiana Bertoni leaves cultivated in Malaysia in relation to different developmental stages. Phytochem. Analys. 2021, 33, 249–261. [CrossRef]

30. Olech, M.; Pietrzak, W.; Nowak, R. Characterization of Free and Bound Phenolic Acids and Flavonoid Aglycones in Rosa rugosa Thumb. Leaves and Achenes Using LC–ESI–MS/MS–MRM Methods. Molecules 2020, 25, 1804. [CrossRef]

31. Belmehdi, O.; Bouyahya, A.; Jòzses, J.E.K.Ó.; Czàkòy, Z.; Zengin, G.; Sót, G.; Elbaaboua, A.; Senhajj, N.S.; Abrini, J. Synergistic interaction between propolis extract, essential oils, and antibiotics against Staphylococcus epidermidis and mexitillin resistant Staphylococcus aureus. Int. J. Second Metab. 2021, 8, 195–213. [CrossRef]

32. Abu-Reidah, I.M.; Ali-Shtayeh, M.S.; Jamous, R.M.; Arroa-Roman, D.; Segura-Carretero, A. HPLC–DAD–ESI-MS/MS screening of bioactive compounds from Rhus coriaria (Sumac) fruits. Food Chem. 2015, 166, 179–191. [CrossRef]

33. Wojakowska, A.; Piasek, A.; Garcia-Lopez, P.M.; Zamora-Natera, F.; Krajewski, P.; Marczak, L.; Kachlicki, P.; Stobiacki, M. Structural analysis and profiling of phenolic secondary metabolites of Mexican lupine species using LC–MS techniques. Phytochemistry 2013, 92, 71–86. [CrossRef]

34. Cai, Z.; Wang, C.; Zou, L.; Liu, X.; Chen, J.; Tan, M.; Mei, Y.; Wei, L. Comparison of Multiple Bioactive Constituents in the Flower and the Caulis of Lonicer a japonica Based on UPLC-QTRAP/MS/MS Combined with Multivariate Statistical Analysis. Molecules 2019, 24, 1936. [CrossRef]

35. Rodriguez-Perez, C.; Gomez-Caravaca, A.M.; Guerra-Hernandez, E.; Cerretani, L.; Garcia-Villanovoa, B.; Verardo, V. Comprehensive metabolite profiling of Solanum tuberosum L. (potato) leaves T by HPLC-ESI-QTOF-MS. Molecules 2018, 112, 390–399. [CrossRef]

36. Yin, N.-W.; Wang, S.-X.; Jia, L.-D.; Zhu, M.-C.; Yang, J.; Zhou, B.-J.; Yin, J.-M.; Li, J.-N.; et al. Identification and Characterization of Major Constituents in Different-Colored Rapeseed Petals by UPLC–HESI–MS/MS. Agric. Food Chem. 2019, 67, 11053–11065. [CrossRef] [PubMed]

37. Seukep, A.J.; Zhang, Y.-L.; Xu, Y.-B.; Guo, M.-Q. In Vitro Antibacterial and Antiproliferative Potential of Echinops lanceolatus Mattf. (Asteraceae) and Identification of Potential Bioactive Compounds. Pharmaceuticals 2020, 13, 59. [CrossRef] [PubMed]

38. Qin, D.; Wang, Q.; Li, H.; Jiang, X.; Fang, K.; Wang, Q.; Li, B.; Pan, C.; Wu, H. Identification of key metabolites based on non-targeted metabolomics and chemometrics analyses provides insights into bitterness in Kucha [Camellia kucha (Chang et Wang) Chang]. Food Res. Int. 2020, 138, 109789. [CrossRef] [PubMed]

39. Spinola, V.; Pinto, J.; Castilho, P.C. Identification and quantification of phenolic compounds of selected fruits from Madeira Island by HPLC-DAD-ESI-MSn and screening for their antioxidant activity. Food Chem. 2015, 173, 14–30. [CrossRef] [PubMed]

40. Nijat, D.; Lu, C.-F.; Lu, J.-J.; Abdulla, R.; Hasan, A.; Aidarhan, N.; Aisa, H.A. Spectrum-effect relationship between UPLC fingerprints and antidiabetic and antioxidant activities of Rosa rugosa. J. Chromatogr. B 2021, 1179, 496–507. [CrossRef] [PubMed]

41. D’Urso, G.; Saras, G.; Lai, C.; Pizza, C.; Montoro, P. LC-MS based metabolomics study of different parts of myrtle berry from Sardinia (Italy). J. Berry Res. 2017, 7, 217–229. [CrossRef]

42. Zhu, Z.-W.; Li, J.; Gao, X.-M.; Amponsem, E.; Kang, L.-Y.; Hu, L.-M.; Zhang, B.-L.; Chang, Y.-X. Simultaneous determination of stilbenes, phenolic acids, flavonoids and anthraquinones in Radix polygoni multiflori by LC–MS/MS. J. Pharmaceut. Biomed. Analys. 2012, 62, 162–166. [CrossRef]

43. De Freitas, M.A.; Silva Alves, A.I.; Andrade, J.C.; Leite-Andrade, M.C.; Lucas dos Santos, A.T.; de Oliveira, T.F.; dos Santos, F.; Silva Buonafina, M.D. Evaluation of the Antifungal Activity of the Licania rigida Leaf Ethanolic Extract against Biofilms Formed by Candida Sp. Isolates in Acrylic Resin Discs. Antibiotics 2019, 8, 250. [CrossRef]

44. Zakharenko, A.M.; Razgonova, M.P.; Pikula, K.S.; Golokhvast, K.S. Simultaneous determination of 78 compounds of Echinops roseus extract using supercritical CO2-extraction and HPLC-ESI-MS/MS spectrometry. Biochem. Res. Int. 2021, 2021, 995749. [CrossRef] [PubMed]

45. Gouto, P.; Singh, R.K.; Cortez, I. Phytochemical A Reference List of Phenolic Compounds (Including Stilbenes) in Grapewine (Vitis vinifera L.) Roots, Woods, Canes, Stems, and Leaves. Antioxidants. 2020, 9, 398. [CrossRef] [PubMed]

46. Singh, J.; Kumar, S.; Rathi, B.; Bhrara, K.; Chhikara, B.S. Therapeutic analysis of Terminalia arjuna plant extracts in combinations with different metal nanoparticles. J. Mater. NanoSci. 2015, 2, 1–7.

47. Gu, D.; Yang, Y.; Bakri, M.; Chen, Q.; Xin, X.; Aisa, H.A. A LC–QTOF–MS/MS Application to Investigate Chemical Compositions in a Fraction with Protein Tyrosine Phosphatase 1B Inhibitory Activity from Rosa Rugosa Flowers. Phytochem. Anal. 2013, 24, 661–670. [CrossRef] [PubMed]

48. Pharmacopoeia of the Eurasian Economic Union, Approved by Decision of the Board of the Eurasian Economic Commission No. 100 Dated 11 August 2020. Available online: http://www.eurasiancommission.org/ru/act/tenreg/depextreg/LSM/Documents/\%D0%A4\%D0%B0\%D1%80\%D0%BC\%D0%B0\%D0%BA\%D0%BE\%D0%BF\%D0%B5\%D1%8F\%20\%D0%A1\%D0%BE\%D1%8E\%D0%B7\%D0%B0\%D0%91\%D0%98.pdf (accessed on 1 January 2020).
49. Zhang, Z.; Jia, P.; Zhang, X.; Zhang, Q.; Yang, H.; Shi, H.; Zhang, L. LC-MS/MS determination and pharmacokinetic study of seven flavonoids in rat plasma after oral administration of Cirsium japonicum DC. extract. J. Ethnopharmacol. 2014, 158, 66–75. [CrossRef]

50. Marzouk, M.M.; Hussein, S.R.; Elkhateeb, A.; El-shabrawy, M.; Abdel-Hameed, E.-S.S.; Kawashy, S.T. Comparative study of Mentha species growing wild in Egypt: LC-ESI-MS analysis and chemosystematic significance. J. Appl. Pharm. Sci. 2018, 8, 116–122.

51. Ozarowski, M.; Piapek, A.; Paszal-Jaworska, A.; de Chaves, D.S.A.; Romanik, A.; Ryczynska, M.; Gryszczyńska, A.; Sawiakowska, A.; Kachlicki, P.; Mikolajczak, P.L.; et al. Comparison of bioactive compounds content in leaf extracts of Passiflora incarnata, P. caerulea and P. alata and in vitro cytotoxic potential on leukemia cell lines. Braz. J. Pharmacol. 2018, 28, 179–191. [CrossRef]

52. Huang, Y.; Yao, P.; Leung, K.W.; Wang, H.; Kong, X.P.; Wang, L.; Dong, T.T.X.; Chen, Y.; Tsim, K.W.K. The Yin-Yang Property of Chinese Medicinal Herbs Relates to the Non-Oxidative Activity: An Illustration Using Spleen-Meridian Herbs. Front. Pharmacol. 2018, 9, 1304. [CrossRef]

53. Sun, J.; Liang, F.; Bin, Y.; Li, D.; Pan, C. Screening Non-colored Phenolics in Red Wines using Liquid Chromatography/Ultraviolet and Mass Spectrometry/Mass Spectrometry Libraries. Molecules 2007, 12, 679–693. [CrossRef]

54. Engels, C.; Gräter, D.; Esquivel, P.; Jiménez, V.M.; Gänzle, M.G.; Schieber, A. Characterization of phenolic compounds in jocote (Spondias purpurea L.) peels by ultra-high-performance liquid chromatography/electrospray ionization mass spectrometry. Food Res. Int. 2012, 46, 557–562.

55. Rafsanjany, N.; Senker, J.; Brandt, S.; Dobrindt, U.; Hensel, A. In Vivo Consumption of Cranberry Exerts ex Vivo Antiadhesive Activity against FimH-Dominated Uropathogenic Escherichia coli: A Combined in Vivo, ex Vivo, and in Vitro Study of an Extract from Vaccinium macrocarpon. J. Agric. Food Chem. 2015, 63, 8804–8818. [CrossRef] [PubMed]

56. Vijayan, K.P.R.; Raghu, A.V. Tentative characterization of phenolic compounds in three species of the genus Embelia by liquid chromatography coupled with mass spectrometry analysis. Spectrosc. Lett. 2019, 52, 653–670. [CrossRef]

57. Santos, S.A.O.; Freire, C.S.R.; Domingues, M.R.M.; Silvestre, A.J.D.; Neto, C.P. Characterization of Phenolic Components in Polar Extracts of Eucalyptus globulus Labill. Bark by High-Performance Liquid Chromatography-Mass Spectrometry. Agric. Food Chem. 2011, 59, 9386–9393. [CrossRef] [PubMed]

58. Sobeh, M.; Mahmoud, M.F.; Abdelfattah, M.A.O.; Cheng, H.; El-Shazly, A.M.; Wink, M. A proanthocyanidin-rich extract from Rubus ulmifolius Activities of Cold Water, Hot Water, and Methanol Extracts, and Their Respective Ethyl Acetate Fractions, from Rubus ulmifolius. Molecules 2017, 22, 1832. [CrossRef]

59. Mekam, P.N.; Martini, S.; Nguefack, J.; Tagliazucchi, D.; Stefani, E. Phenolic compounds profile of water and ethanol extracts of Euphorbia hirta L. leaves showing antioxidant and antifungal properties. South Afr. J. Bot. 2019, 127, 319–332. [CrossRef]

60. Pan, M.; Lei, Z.; Qiang, N.; Zhang, H. A Strategy Based on GC-MS/MS, UPLC-MS/MS and Virtual Molecular Docking for Development of an Innovative Pressurized Liquid Extraction Procedure by Response Surface Methodology to Recover Bioactive Compounds from Carao Tree Seeds. Foods 2021, 10, 398. [CrossRef] [PubMed]

61. Da Silva, L.P.; Pereira, E.; Pires, T.C.S.P.; Alves, M.J.; Pereira, O.R.; Barros, L.; Ferreira, I.C.F.R. Rubus ulmifolius Schott fruits: A detailed study of its nutritional, chemical and bioactive properties. Food Res. Int. 2019, 119, 34–43. [CrossRef] [PubMed]

62. Marcia Fuentes, J.A.; Lopez-Salas, L.; Borras-Linares, I.; Navarro-Alarcon, M.; Segura-Carretero, A.; Lozano-Sanchez, J. Development of an Innovative Pressurized Liquid Extraction Procedure by Response Surface Methodology to Recover Bioactive Compounds from Liqueurs from Rose Petals (Rosa rugosa). Molecules 2017, 22, 1832. [CrossRef]

63. Cendrowski, A.; Sichisz, I.; Kielszlek, M.; Kolniak-Ostek, J.; Mitek, M. UPLC-PDA-Q/TOF-MS Profile of Polyphenolic Compounds of Liqueurs from Rosaceae. J. Agric. Food Chem. 2019, 67, 5277–5287. [CrossRef]

64. Viera, M.N.; Winterhalter, P.; Jerz, G. Flavonoids from the flowers of Impatiens glandulifera Royle isolated by high performance countercurrent chromatography. Phytochem. Anal. 2016, 27, 116–125. [CrossRef] [PubMed]

65. Barros, L.; Duenas, M.; Carvalho, A.M.; Ferreira, I.C.F.R.; Santos-Buelga, C. Characterization of phenolic compounds in flowers of Cirsium japonicum DC. extract. J. Ethnopharmacol. 2014, 158, 66–75. [CrossRef]

66. Kim, S.; Oh, S.; Noh, H.B.; Ji, S.; Lee, S.H.; Koo, J.M.; Choi, C.W.; Jhun, H.P. In Vitro Antioxidant and Anti-Propionibacterium acnes Activities of Cold Water, Hot Water, and Methanol Extracts, and Their Respective Ethyl Acetate Fractions, from Sanguisorba officinalis L. Roots. Molecules 2018, 23, 3001. [CrossRef]

67. Chen, Y.; Cai, X.; Li, G.; He, X.; Yu, X.; Yu, X.; Xiao, Q.; Xiang, Z.; Wang, C. Chemical constituents of radix Actinidia chinensis planch by UPLC-QTOF–MS. Biomedical Chromatography. Biomed. Chromatogr. 2021, 35, e5103. [CrossRef]

68. Chen, X.; Zhang, S.; Xuan, Z.; Ge, D.; Chen, X.; Zhang, J.; Wang, Q.; Wu, Y.; Liu, B. The Phenolic Fraction of Mentha haplocalyx and Its Constituent Linarin Ameliorate Inflammatory Response through Inactivation of NF-kB and MAPKs in Lipopolysaccharide-Induced RAW264.7 Cells. Molecules 2017, 22, 811. [CrossRef]
71. Yin, Y.; Zhang, K.; Wei, L.; Chen, D.; Chen, Q.; Jiao, M.; Li, X.; Huang, J.; Gong, Z.; Kang, N.; et al. The Molecular Mechanism of Antioxidation of Huolisu Oral Liquid Based on Serum Analysis and Network Analysis. *Front. Pharma*. 2021, 12, 710976. [CrossRef] [PubMed]

72. Romo Vaquero, M.; Garcia Villalba, R.; Larrosa, M.; Yáñez-Gascón, M.J.; Fromentin, E.; Flanagan, J.; Roller, M.; Tomás-Barberán, F.A.; Espín, J.C.; García-Conesa, M.T. Bioavailability of the major bioactive diterpenoids in a rosemary extract: Metabolic profile in the intestine, liver, plasma, and brain of Zucker rats. *Mol. Nutr. Food Res.* 2013, 57, 1834–1846. [CrossRef]

73. Cirlini, M.; Mena, P.; Tassotti, M.; Herrlinger, K.A.; Nieman, K.M.; Dall’Asta, C.; Del Rio, D. Phenolic and volatile composition of a dry spearmint (*Mentha spicata L.*) extract. *Molecules* 2016, 21, 1007. [CrossRef] [PubMed]

74. Jiang, R.-W.; Lau, K.-M.; Hon, P.-M.; Mak, T.C.W.; Woo, K.-S.; Fung, K.-P. Chemistry and Biological Activities of Caffeic Acid Derivatives from *Salvia miltiorrhiza*. *Curr. Med. Chem.* 2005, 12, 237–246. [CrossRef] [PubMed]

75. Simard, F.; Legault, J.; Lavoie, S.; Mshvildadze, V.; Pichette, A. Isolation and Identification of Cytotoxic Compounds from the Wood of *Pinus resinosa*. *Phytotax.* 2008, 22, 919–922. [CrossRef] [PubMed]

76. Ekeberg, D.; Flate, P.-O.; Eikenes, M.; Fongen, M.; Naess-Andresen, C.F. Qualitative and quantitative determination of extractives in heartwood of Scots pine (*Pinus sylvestris L.*) by gas chromatography. *J. Chromatogr. A* 2006, 1109, 267–272. [CrossRef] [PubMed]

77. Moss, R.; Mao, Q.; Taylor, D.; Saucier, C. Investigation of monomeric and oligomeric wine stilbenoids in red wines by ultra-high-performance liquid chromatography/electrospray ionization quadrupole time-of-flight mass spectrometry. *Rapid Commun. Mass Spectrom.* 2013, 27, 1815–1827. [CrossRef]

78. Rezaire, A.; Robinson, J.C.; Bereau, D.; Verbaere, A.; Sommerer, N.; Khan, M.K.; Durand, P.; Prost, E.; Fils-Lycaon, B. Amazonian palm *Oenocarpus bataua* (“patawa”): Chemical and biological antioxidant activity—Phytochemical composition. *Food Chem.* 2014, 149, 62–70. [CrossRef]

79. Hu, E.; An, J.; Li, W.; Zhang, Z.; Chen, W.; Wang, C.; Wang, Z. UPLC-MS/MS determination and gender-related pharmacokinetic study of five active ingredients in rat plasma after oral administration of *Eucommia cortex* extract. *J. Ethnopharmacol.* 2015, 169, 145–155. [CrossRef]

80. Eklund, P.C.; Backman, M.J.; Kronberg, L.A.; Smeds, A.I.; Sjoholm, R.E. Identification of lignans by liquid chromatography-electrospray ionization ion-trap mass spectrometry. *J. Mass Spectr.* 2008, 43, 97–107. [CrossRef]

81. Dinelli, G.; Marotti, I.; Bosi, S.; Benedettelli, S.; Ghiselli, L.; Cortacero-Ramirez, S.; Carrasco-Pancorbo, A.; Segura-Carretero, A.; Fernandez-Gutierrez, A. Lignan profile in seeds of modern and old Italian soft wheat (*Triticum aestivum* L.) cultivars as revealed by CE-MS analyses. *Electrophoresis* 2007, 28, 4212–4219. [CrossRef]

82. Michalak, B.; Filipak, A.; Chomicki, P.; Pyza, M.; Wozniak, M.; Zyzynska-Granica, B.; Piwowarski, J.P.; Kicel, A.; Olszewska, M.A.; Kiss, A.K. Lignans From *Forsythia x Intermedia* Leaves and Flowers Attenuate the Pro-inflammatory Function of Leukocytes and Their Interaction With Endothelial Cells. *Front. Pharmacol.* 2018, 9, 401. [CrossRef]

83. Oertel, A.; Matros, A.; Hartmann, A.; Arapitsas, P.; Dehmer, K.J.; Martens, S.; Mock, H.P. Metabolite profiling of red and blue potatoes revealed cultivar and tissue specific patterns for anthocyanins and other polyphenols. *Planta* 2017, 246, 281–297. [CrossRef]

84. Vera de Rosso, V.; Hillebrand, S.; Cuevas Montilla, E.; Bobbio, F.O.; Winterhalter, P.; Mercadante, A.Z. Determination of anthocyanins from acerola (*Malpighia emarginata* DC.) and ac-ai (*Euterpe oleracea* Mart.) by HPLC–PDA–MS/MS. *J. Food Composit. Analys.* 2008, 21, 291–299. [CrossRef]

85. Ruiz, A.; Hermosín-Gutiérrez, I.; Vergara, C.; von Baer, D.; Zapata, M.; Hitschfeld, A.; Obando, L.; Mardones, C. Anthocyanin profiles in south Patagonian wild berries by HPLC-DAD-ESI-MS/MS. *Food Res. Int.* 2013, 51, 706–713. [CrossRef]

86. Diretto, G.; Jin, X.; Capell, T.; Zhu, C.; Gomez-Gomez, L. Differential accumulation of pelargonidin glycosides in petals at three different developmental stages of the orange-flowered gentian (*Gentiana lutea* L. var. *aurantiaca*). *PloS ONE* 2019, 14, e021062. [CrossRef] [PubMed]

87. Garg, M.; Chawla, M.; Chunduri, V.; Kumar, R.; Sharma, S.; Sharma, N.K.; Kaur, N.; Kumar, A.; Mundey, J.K.; Saini, M.K.; et al. Transfer of grain colors to elite wheat cultivars and their characterization. *J. Cereal Sci.* 2016, 71, 138–144. [CrossRef]

88. Nakamura, S.; Li, X.; Matsuda, H.; Yoshikawa, M. Bioactive constituents from Chinese natural medicines. XXVIII. Chemical structures of acyclic alcohol glycosides from the roots of *Rhodiola crenulata*. *Chem. Pharm. Bull.* 2008, 56, 536–540. [CrossRef] [PubMed]

89. Fan, Z.; Wang, Y.; Yang, M.; Cao, J.; Khan, A.; Cheng, G. UHPLC-ESI-HRMS/MS analysis on phenolic compositions of different *E* *t*ea *t*e *a* extracts and their antioxidant and cytotoxic potential activities. *Food Chem.* 2020, 318, 126512. [CrossRef]

90. Suarez Montenegro, Z.J.; Alvarez-Rivera, G.; Mendiol, J.A.; Ibanez, E.; Cifuentes, A. Extraction and Mass Spectrometric Characterization of Terpenes Recovered from Olive Leaves Using a New Adsorbent-Assisted Supercritical CO2 Process. *Front. Food Sci.* 2021, 10, 1301. [CrossRef]

91. Zhang, J.; Gao, W.; Liu, Z.; Zhang, Z. Identification and Simultaneous Determination of Twelve Active Components in the Methanol Extract of Traditional Medicine Weichang’an Pill by HPLC-DAD-ESI-MS/MS. *Iran. J. Pharmaceut. Res.* 2013, 12, 15–24.

92. Guo, K.; Tong, C.; Fu, Q.; Xu, J.; Shi, S.; Xiao, Y. Identification of minor lignans, alkaloids, and phenylpropanoid glycosides in *Magnolia officinalis* by HPLC-DAD-QTOF-MS/MS. *J. Pharmaceut. Biomed. Analys.* 2019, 170, 153–160. [CrossRef]

93. Van Diermen, D.; Marston, A.; Bravo, J.; Reist, M.; Carrupt, P.A.; Hostettmann, K. Monoamine oxidase inhibition by *Rhodiola rosea* L. roots. *J. Ethnopharmacol.* 2009, 122, 397–401. [CrossRef]
Appl. Sci. 2022, 12, 9401

94. Ohsugi, M.; Fan, W.; Hase, K.; Xiong, Q.; Tezuka, Y.; Komatsu, K.; Namba, T.; Saitoh, T.; Tazawa, K.; Kadota, S. Active-oxygen scavenging activity of traditional nourishing-tonic herbal medicines and active constituents of *Rhodiola* *sacra*. *J. Ethnopharmacol.* 1999, 67, 111–119. [CrossRef]

95. Kim, K.H.; Park, Y.J.; Jang, H.J.; Lee, S.J.; Lee, S.; Yun, B.S.; Lee, S.W.; Rho, M.C. Rugosic acid A, derived from *Rosa rugosa* Thumb., is novel inhibitory agent for NF-κB and IL-6/STAT3 axis in acute lung injury model. *Phytother. Res.* 2020, 34, 3200–3210. [CrossRef] [PubMed]

96. Patnala, S.; Kanfer, I. Medicinal use of *Scelotium*; Characterization of Phytochemical Components of *Scelotium* Plant Species using HPLC with UV and Electrospray Ionization—Tandem Mass Spectroscopy. *J. Pharm. Pharmacol.* 2015, 18, 414–423. [CrossRef]

97. Yang, S.T.; Xu, X.; Rui, W.; Guo, J.; Feng, Y.F. UPLC/Q-TOF-MS Analysis for Identification of Hydrophilic Phenolics and Lipophilic Diterpenoids from Radix *Salviae Miltiorrhizae*. *Acta Chromatogr.* 2015, 27, 711–726. [CrossRef]

98. Xie, J.; Ding, C.; Ge, Q.; Zhou, Z.; Zhi, X. Simultaneous determination of ginkgolides A, B, C and bilobalide in plasma by LC–MS/MS and its application to the pharmacokinetic study of *Ginkgo biloba* extract in rats. *J. Chromatogr. B* 2008, 864, 87–94. [CrossRef]

99. Xiao, J.; Wang, T.; Li, P.; Liu, R.; Li, Q.; Bi, K. Development of two step liquid–liquid extraction tandem UHPLC–MS/MS method for the simultaneous determination of Ginkgo flavonoids, terpene lactones and nimodipine in rat plasma: Application to the pharmacokinetic study of the combination of Ginkgo biloba dispersible tablets and Nimodipine tablets. *J. Chromatogr. B* 2016, 1028, 33–41.

100. Looren-Martinez, E.J.; Spinola, V.; Gouveia, S.; Castilho, P.C. HPLC-ESI-MSn characterization of phenolic compounds, terpenoid saponins, and other minor compounds in *Bituminaria bituminosa*. *Ind. Crops Prod.* 2015, 69, 80–90. [CrossRef]

101. Park, S.K.; Ha, J.S.; Kim, J.M.; Kang, J.Y.; Lee, D.S.; Guo, T.J.; Lee, U.; Kim, D.-O.; Heo, H.J. Antiinflammatory Effect of Broccoli (*Brassica oleracea var. italica*) Leaves on Amyloid Beta (Aβ1–42)-Induced Learning and Memory Impairment. *J. Agric. Food. Chem.* 2016, 64, 3353–3361. [CrossRef]

102. Serrano, C.A.; Villena, G.K.; Rodriguez, E.F. Phytochemical profile and rosmarinic acid purification from two Peruvian *Lepechinia* Willd. species (*Salviae, Mentheae, Lamiacae*). *Sci. Rep.* 2021, 11, 7260. [CrossRef]

103. Ozarowski, M.; Piasecka, A.; Paszel-Jaworska, A.; de Chaves, D.S.A.; Romaniuk, A.; Rybczynska, M.; Gryszczynska, A.; Savikowska, A.; Kachlicki, P.; Mikolajczak, P.L.; et al. Acetylcholinesterase inhibitory activities and bioguided fractionation of the *Ocotea percoriacea* extracts: HPLC-DAD-MS/MS characterization and molecular modeling of their alkaloids in the active fraction. *Comput. Biol. Chem.* 2019, 83, 107129.

104. Yang, L.; Meng, X.; Yu, X.; Kuang, H. Simultaneous determination of anemoside B4, phellodendrine, berberine, palmatine, okubonone, esculin, esculetin in rat plasma by UPLC–ESI–MS/MS and its application to a comparative pharmacokinetic study in normal and ulcerative colitis rats. *J. Pharm. Biomed. Analys.* 2017, 134, 43–52. [CrossRef] [PubMed]

105. Seekhaw, P.; Mahatheeranont, S.; Sookwong, P.; Luangkamin, S.; Na Lampang Neonplab, A.; Puangsombat, P. Phytochemical Constituents of Thai Dark Purple Glutinous Rice Bran Extract [Cultivar Luem Pua (*Oryza sativa* L.)]. *Chiang Mai J. Sci.* 2018, 45, 1383–1395.

106. Wu, Y.; Xu, J.; He, Y.; Shi, M.; Han, X.; Li, W.; Zhang, X.; Wen, X. Metabolic Profiling of *Pitaya* (*Hylocereus polyrhizus*) during Fruit Development and Maturation. *Molecules* 2019, 24, 1114. [CrossRef] [PubMed]

107. Sut, S.; Zengin, G.; Maggi, F.; Malagoli, M.; Dall’Acqua, S. Triterpene Acid and Phenolics from Ancient Apples of Friuli Venezia Giulia as Nutraceutical Ingredients: LC-MS Study and In Vitro Activities. *Molecules* 2019, 24, 1109. [CrossRef]

108. D’Abrosca, B.; Fiorentino, A.; Monaco, P.; Oriano, P.; Pacifico, S. Annuurco acid: A new antioxidant ursane triterpene from fruits of cv. Annuurco apple. *Food Chem.* 2006, 98, 285–290.

109. Liu, H.; Lai, H.; Jia, X.; Liu, J.; Zhang, Z.; Li, Y.; Zhang, J.; Song, J.; Wu, C.; Zhang, B.; et al. Comprehensive chemical analysis of *Schisandra chinensis* by HPLC-DAD-MS combined with chemometrics. *Phytochemistry* 2013, 20, 1135–1143. [CrossRef] [PubMed]

110. Razgonova, M.; Zakharenko, A.; Pikula, K.; Kim, E.; Chernyshev, V.; Ercisli, S.; Cravotto, G.; Golokhvast, K. Rapid Mass Spectrometric Study of a Supercritical CO2-extract from Woody Liana *Schisandra chinensis* by HPLC-ESI-MS/MS. *Molecules* 2020, 25, 2689.

111. Lara-Abía, S.; Lobo-Rodrigo, G.; Welti-Chanes, J.; Pilar Cano, M. Carotenoid and Carotenoid Ester Profile and Their Deposition in Plastids in Fruits of New *Papaya* (*Carica papaya* L.) Varieties from the Canary Islands. *Foods* 2021, 10, 434. [CrossRef]

112. Etzbach, L.; Pfeiffer, A.; Weber, F.; Schieber, A. Characterization of carotenoid profiles in goldenberry (*Physalis peruviana* L.) fruits at various ripening stages and in different plant tissues by HPLC-DADPCI-MSn. *Food Chem.* 2018, 245, 508–517.

113. Al-Yafeai, A.; Malarski, A.; Bohm, V. Characterization of carotenoids and vitamin E in *R. rugosa* and *R. cantina*: Comparative analysis. *Food Chem.* 2018, 242, 435–442. [PubMed]

114. Petry, F.C.; Mercadante, A.Z. Composition by LC-MS/MS of New Carotenoid Esters in Mango and Citrus. *J. Agric. Food Chem.* 2016, 64, 8207–8224. [CrossRef] [PubMed]

115. van Breemen, R.B.; Canjura, F.L.; Schwartz, S.J. Identification of Chlorophyll Derivatives by Mass Spectrometry. *J. Agric. Food Chem.* 1991, 39, 1452–1456. [CrossRef]