Journal of Chemistry and Technologies, 2024, *32*(2), 267-275

Journal of Chemistry and Technologies

pISSN 2663-2934 (Print), ISSN 2663-2942 (Online).

journal homepage: http://chemistry.dnu.dp.ua
editorial e-mail: chem.dnu@gmail.com

UDC 543.9+581.1+582.639

CHEMOTAXONOMIC SIGNIFICANCE ASSESSMENT OF PHYTOCHEMICAL HETEROGENEITY OF THE GENUS *SORBUS* INFLORESCENCES

Yuriy V. Lykholat[1], Nina O. Khromykh[2*], Andriy O. Anishchenko[3], Oleh O. Didur[2], Svitlana D. Koptieva[3], Tetyana V. Sklyar[1], Olena V. Liashenko[1]

[1]*Oles Honchar Dnipro National University, Faculty of Biology and Ecology, 72, Nauky Ave., Dnipro, 49010, Ukraine*
[2]*Oles Honchar Dnipro National University, Biology Research Institute, 72, Nauky Ave., Dnipro, 49010, Ukraine*
[3]*Oles Honchar Dnipro National University, Faculty of Chemistry, 72, Nauky Ave., Dnipro, 49010, Ukraine*
Received 3 May 2024; accepted 17 June 2024; available online 10 July 2024

Abstract

The chemotaxonomic value of phytocompounds heterogeneity in inflorescences of different plants the same genus was tested by analyzing the phytochemical profiles of inflorescences hexane extracts of *Sorbus aria* species and three natural hybrids for which this species is the parental. Specific distribution of saturated and unsaturated fatty acids, aldehydes, alcohols, alkanes, terpenoids, nitrogen-containing and sulfur-containing compounds identified by the GC-MS was found in the floral extracts. Multivariate analysis of obtained data determined two principal components that described 84.4 % of metabolites total variance, and established the phytocompounds that corresponded to the greatest extent to the inflorescence's identity. Cluster analysis showed different relatedness levels between the parental species *S. aria* and the hybridogenic species *S. hybrida*, *S. latifolia*, and *S. intermedia*. The multivariate analysis results agree with the studied natural hybrids known genetic data, which confirms the chemotaxonomic value of the inflorescences chemical diversity and determines the prospects of such a direction of research.

Keywords: *Sorbus* L.; inflorescences; phytocompounds; multivariate analysis; chemotaxonomy.

ОЦІНКА ХЕМОТАКСОНОМІЧНОГО ЗНАЧЕННЯ ФІТОХІМІЧНОЇ ГЕТЕРОГЕННОСТІ СУЦВІТЬ РОДУ *SORBUS*

Юрій В. Лихолат[1], Ніна О. Хромих[2], Андрій О. Аніщенко[3], Олег О. Дідур[2], Світлана Д. Коптєва[3], Тетяна В. Скляр[1], Олена В. Ляшенко[1]

[1]*Дніпровський національний університет імені Олеся Гончара, біолого-екологічний факультет , 72, пр. Науки, Дніпро, 49010, Україна*
[2]*Дніпровський національний університет імені Олеся Гончара, НДІ біології, 72, пр. Науки, Дніпро, 49010, Україна*
[3]*Дніпровський національний університет імені Олеся Гончара, хімічний факультет, 72, пр. Науки, Дніпро, 49010, Україна*

Анотація

Хемотаксономічне значення гетерогенності фітосполук у суцвіттях різних рослин одного роду перевірено шляхом аналізу фітохімічних профілів гексанових екстрактів суцвіть виду *Sorbus aria* та трьох природних гібридів, для яких цей вид є батьківським. У квіткових екстрактах виявлено специфічний розподіл насичених і ненасичених жирних кислот, альдегідів, спиртів, алканів, терпеноїдів, нітрогеновмісних і сульфуровмісних сполук, ідентифікованих методом ГХ-МС. Багатофакторний аналіз отриманих даних визначив два головних компоненти, які описують 84.4 % сумарної дисперсії метаболітів, і встановив фітосполуки, що найбільшою мірою відповідають ідентичності суцвіть. Кластерний аналіз показав різні рівні спорідненості між батьківським видом та гібридогенними видами *S. hybrida*, *S. latifolia* і *S. intermedia*. Результати багатофакторного аналізу узгоджуються з відомими генетичними даними досліджуваних природних гібридів, що підтверджує хемотаксономічну цінність хімічного різноманіття суцвіть і визначає перспективність такого напряму досліджень.

Ключові слова: Sorbus L.; суцвіття; фітосполуки; багатофакторний аналіз; хемотаксономія.

**Corresponding author: e-mail: Khromykh2012@gmail.com*

doi: 10.15421/jchemtech.v32i2.303257

Journal of Chemistry and Technologies, 2024, *32*(2), 267-275

Introduction

The phytochemical composition of the genus *Sorbus* L. plants (family *Rosaceae*) is the object of intensive research today due to ethno-pharmacological information on the powerful medicinal and preventive properties of plants.[1] The genus *Sorbus* has a wide geographical distribution in the temperate zone, less in the subtropical regions of the Northern Hemisphere, where plants grow naturally or are cultivated in different climatic and edaphic conditions.[2] In particular, the best-known species *Sorbus aucuparia*, in addition to natural growth in the territory of Europe (up to the extreme north), the Caucasus and Eastern Asia, was introduced throughout the world in the temperate climate zone.[3] The species *S. aucuparia*, *Sorbus domestica* and *Sorbus torminalis* are natural on the territory of Ukraine, while some other species and hybrids were introduced and are cultivated in different regions of the country.[4] Within the genus *Sorbus*, which includes up to 250 species,[5] plants show a wide variation in vegetative and generative organs morphological features, as well as the exceptional genetic diversity due to the ability of plants to undergo introgressive hybridization followed by apomixis and polyploidy,[6] which led to a significant expansion of genotypes, hybrids and varieties of the genus *Sorbus* and complicated its taxonomy.[7]

The composition of phytocompounds extracted from plants of different *Sorbus* species and hybrids is also characterized by great chemical diversity, including saturated and unsaturated fatty acids, alcohols, aldehydes, alkanes[8] and secondary metabolites, such as phenolic acids,[9] flavonoids,[10] terpenoids[1] and nitrogenous compounds.[11] The quantitative and qualitative composition of secondary metabolites varies significantly in *Sorbus* plants, in particular the content of phenolic acids and flavonoids in leaves[12] and fruits[13] of different plant species, and even in fruits of different varieties of the same species.[10] In addition, the total content of polyphenols[7] and flavonoids[14] in leaves and inflorescences of different genotypes of the genus *Sorbus* varies greatly depending on geographic, climatic, and edaphic environmental conditions.

The phytochemical heterogeneity inherent in species and hybrids of the genus *Sorbus* has also been established within other plant genera, in particular *Prunus* genus[15] and *Actinidia* genus,[16] supporting the assumption[17] that the distribution of secondary metabolites within one genus is not random and has taxonomic value. Research in this direction gives positive results, in particular, the chemotaxonomic significance of the phytochemical heterogeneity of the volatile inflorescence components of various plants species of the genus *Chorisia* was recently shown.[18] The use of phenolic compounds of inflorescences as chemical markers made it possible to establish the relationship of some species, hybrids and varieties of the genus *Sorbus* with the structure of phenolic acids and flavonoids.[7]

We assumed that the chemical diversity of phytocompounds of other classes in plants of the genus *Sorbus* may also have marker features. The verification of the assumption was carried out on the basis of the phytochemical composition analysis of the hexane extracts of the inflorescences of *Sorbus* plants, which are genetically related. The aim of our work was to identify the chemotaxonomic value of the diversity of non-phenolic phytocompounds in the inflorescences of the *Sorbus aria* species and several natural hybrids for which this species is one of the parental forms.

Experimental

Plant Material Collection. The collection of the fully blooming inflorescences of *S. aria* (L.) Crantz., *S. latifolia* (Lam.) Pers., S*. hybrida* L., and *S. intermedia* (Ehrh.) Pers. was carried out in the Botanical Garden of Oles Honchar Dnipro National University (48°26'7" N, 35°2'34" E; Dnipro city, Ukraine) in May 2023. Plant material was packed in plastic containers, transferred to the laboratory and air-dried in the shade under room conditions.

Extraction Procedure. The extracts of inflorescences were prepared by maceration of air-dried and crushed plant material in hexane (1 : 10 w/v) during 24 h in dark with occasional stirring. Further, filtered extracts were evaporated at 40 ºC using rotary evaporator (IKA® RV 10, Germany), and the obtained solid fractions stored at 4 ºC prior to analysis.

Phytochemical Profiling. Phytochemical profiling of the hexane extracts of *Sorbus* inflorescences was made by GC-MS assay using chromatographic system Shimadzu-GC-MS (QP 2020 El, Japan) equipped with Rxi®-5ms column (30 m × 0.25 mm, film thickness 0.25 μm) containing 5 % diphenyl/95 % dimethyl polysiloxane as a fixed liquid phase. The oven temperature was programmed from 50 °C (with 2 min initial hold) to 300 °C at a rate of 15 °C per min, and kept constant at 300 °C for 5 min. The carrier gas helium passed at a total flow 28.2 and

column flow 1.2 ml/min. Injector temperature was 280 °C; sample volume was 1 μL.

The separated compounds identification was achieved based on Mass Spectrum Library 2014 for GC-MS (O2125401310) by their mass spectra comparison with those in the National Institute of Standards and Technology (NIST14.lib, NIST14s.lib) spectral database with a matching probability ≥ 80 %. The content of individual compounds was estimated using the corresponding peak area and expressed as a percentage of the total amount.

Statistical Analysis. The research was carried out in triplicate. Multivariate statistical proceeding of the obtained results was performed by principal component analysis (PCA) and multivariate scaling methods using the software package Statistica 10.1. StatSoft Inc. (USA). For this, a data matrix was prepared with rows representing the cases (i.e. plant species) and columns describing variables (i.e. phytocompound content), and the resulting data were exported to an Excel file for multivariate analysis.

PCA was used as an unsupervised method to identify statistically significant differences between the inflorescences of the studied *Sorbus* species according to the non-phenolic phytocomponent composition of the extracts. Correlation analysis was conducted to determine the character of the correlations between phytocompounds and the studied plant species and to reveal the non-phenolic constituents which determined the phytochemical identity of the inflorescences of *Sorbus* species. Cluster analysis was used to establish homogeneous groups of phytocompounds in inflorescences of different plant species and to estimate the Euclidean distance between the studied *Sorbus* species and natural hybrids.

Results and Discussion

GC-MS analysis of hexane extracts of inflorescences of the genus *Sorbus* plants allowed to identify a total of 87 chemical compounds, the distribution of which was species-specific. In the inflorescences of *S. aria*, 50 phytocompounds were identified, which accounted for 93.42 % of the total compounds amount in the extract; in the inflorescences of *S. latifolia*, 49 compounds were identified (97.87 % of the total amount), in the inflorescences of *S. intermedia* – 44 compounds (99.56 % of the total amount), and in the inflorescences of *S. hybrida* – 37 compounds (90.54 % of the total amount).

Among the identified non-phenolic phytoconstituents, some compounds were found exclusively in the inflorescences extract of one plant species out of four (Table 1).

Table 1

Uncommon chemical constituents of *Sorbus* inflorescences as identified by GC-MS

N	Compound Name	Formula	Content, % of total			
			S. aria	*S. hybrida*	*S. latifolia*	*S. intermedia*
1	2-Methyl-pentanol	$C_7H_{16}O$		0.19		
2	1,4-Dimethyl-benzene	C_8H_{10}			0.15	
3	Butyrolactone	$C_4H_6O_2$				0.20
4	2-Propyl-heptanol	$C_{10}H_{22}O$			0.19	
5	3-Methyl-1,6-heptadien-3-ol	$C_8H_{14}O$			0.54	
6	Tetradecane	$C_{14}H_{30}$				1.32
7	1H-Tetrazole-5-amine	CH_3N_5		0.24		
8	Isobormyl acetate	$C_{12}H_{20}O_2$	0.37			
9	2-Methyl-2-undecanethiol	$C_{12}H_{26}S$	0.29			
10	Tridecan-1-ol	$C_{13}H_{28}O$			0.67	
11	2-Hexyl-1-octanol	$C_{14}H_{30}O$			0.19	
12	D-Homo-24-nor-17-oxachola-20,22-diene-3,7,16-trione	$C_{26}H_{32}O_6$		0.20		
13	1,2-Tetradecanediol	$C_{14}H_{30}O_2$				0.17
14	Triethyl citrate	$C_{12}H_{20}O_7$	0.39			
15	Myristic acid, 9-octadecenyl ester	$C_{32}H_{62}O_2$			0.56	
16	Tetracosanol	$C_{24}H_{50}O$			0.20	
17	2-Tridecenal	$C_{13}H_{24}O$			0,19	
18	Octadecanoic acid, hydrazide	$C_{18}H_{38}N_2O$		0.32		
19	Propanoic acid, 3-mercapto-dodecyl ester	$C_{15}H_{30}O_2S$			2.45	
20	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-dien-2,8-dione	$C_{17}H_{24}O_3$			0.53	
21	Nonadecane	$C_{19}H_{40}$		4.16		
22	Eicosanoic acid (syn. Arachidic acid)	$C_{20}H_{40}O_2$			0.32	
23	Phthalic acid, dibutyl ester	$C_{16}H_{22}O_4$		1.06		
24	Tetracosanoic acid, isobutyl ester	$C_{28}H_{56}O_2$		0.25		

Journal of Chemistry and Technologies, 2024, *32*(2), 267-275

Continuation of table 1

25	8,10-Hexadecadien-1-ol	$C_{16}H_{30}O$			0.24	
26	13-Octadecenal	$C_{18}H_{34}O$			0.28	
27	Hexacontanoic acid, 18-oxo	$C_{60}H_{118}O_3$		0.28		
28	Carbonic acid, prop-1-en-2-yl tetradecyl ester	$C_{18}H_{38}O_3$		0.18		
29	Propanoic acid, 3,3-thiobis-didodecyl ester	$C_{30}H_{58}O_4S$				0.49
30	Spiroisohumulone	$C_{21}H_{30}O_5$				0.23
31	cis-9-Tetradecenoic acid, isobutyl ester	$C_{18}H_{34}O_2$				0.40
32	Undec-10-ynoic acid, tetradecyl ester	$C_{25}H_{46}O_2$			0.76	
33	1,2-Octadecanediol	$C_{18}H_{38}O_2$		1.04		
34	Cholest-1-eno-[2,1-a] naphthalene-3,4-dihydro	$C_{35}H_{52}$	3.98			
35	Cycloeucalenol acetate	$C_{32}H_{52}O_2$				2.33
36	Urs-12-ene -3-ol (syn. alpha-Amyrin)	$C_{30}H_{50}O$	0.87			
37	14-Methylcholest-7-en-3-ol	$C_{28}H_{48}O$			0.27	
	Total amount of uncommon metabolites		5.90	7.92	7.54	5.14

Since the indicated uncommon metabolites of the inflorescences of the studied *Sorbus* plants do not fully describe the data structure, they were not taken into account in the multivariate analysis, and a group of 50 phytocompounds was selected for further work, which were present in the extracts of the inflorescences of two or more species of *Sorbus* plants (Table 2).

Based on the data on the content of common phytoconstituents, a matrix was created for the multidimensional analysis of the component composition of the hexane extracts of *Sorbus* inflorescences.

Table 2

The common chemical constituents of *Sorbus* inflorescences as identified by GC-MS

N	Compound Name	Formula	Content, % of total			
			S. aria	*S. hybrida*	*S. latifolia*	*S. intermedia*
1	Butanedioic acid, 2-cyano-2,3-dimethyldecyl ester	$C_{11}H_{17}NO_4$		0.30		0.17
2	Cyclododecane	$C_{12}H_{24}$		0.23		0.17
3	8,14-Cedranoxide	$C_{15}H_{24}O$	0.28		0.38	
4	1-Methylinosine	$C_{11}H_{14}N_4O_5$	0.18	0.22		0.26
5	6-Methyloctadecane	$C_{19}H_{40}$	0.40	0.60	0.26	0.68
6	1,1-Dimethyl-2-octyl cyclobutane	$C_{14}H_{28}$	0.25	0.24		0.16
7	Oxalic acid, hexyl-2-methylphenyl ester	$C_{15}H_{20}O_4$			0.29	0.20
8	Hexadecane	$C_{16}H_{34}$	0.57		0.19	2.79
9	2-Propenoic acid, 1,2-etanediyl ester	$C_8H_{10}O_4$	2.22	1.87		1.85
10	2-Propenoic acid, pentadecyl ester	$C_{18}H_{34}O_2$	0.16		9.63	
11	13-Heptadecyn-1-ol	$C_{17}H_{32}O$	0.69	1.41		0.27
12	Heptadecane	$C_{17}H_{36}$	1.15			3.99
13	(2-Phenyl-1,3-dioxolan-4-yl)methyl-9-octadecenoate	$C_{28}H_{44}O_4$	0.21	0.27	0.46	0.39
14	Hexadecanoic acid	$C_{16}H_{32}O_2$	0.75		7.51	0.39
15	3-Chloropropionic acid, dodecyl ester	$C_{15}H_{29}ClO_2$	0.17		0.46	
16	Butyl-undecyl Phthalate	$C_{23}H_{36}O_4$	0.30			0.38
17	2-Methyltetracosane	$C_{25}H_{52}$	1.98		1.97	1.48
18	Ethyl isoallocholate (syn. cholic acid ethyl ester)	$C_{26}H_{44}O_5$	0.79		0.79	
19	Olean-12-en-3-one	$C_{30}H_{48}O$	0.62			0.86
20	(Hexahydrofarnesyl acetone)	$C_{18}H_{36}O$	0.27	0.46	0.22	0.28
21	Heneicosane	$C_{21}H_{44}$	5.66	8.58	10.28	
22	9,12-Octadecadienoic acid (Z, Z) (syn. Linoleic acid)	$C_{18}H_{32}O_2$	1.92		12.91	2.39
23	3-Hydroxydodecanoic acid	$C_{12}H_{24}O_3$	0.26		0.22	0.17
24	Trans-2-Undecen-1-ol	$C_{11}H_{22}O$	0.20	0.24		
25	Pentadecanal	$C_{15}H_{30}O$	0.73		0.27	0.59
26	Eicosane	$C_{20}H_{42}$	16.84	26.60	4.32	19.32
27	2-Dodecen-1-yl succinic anhydride	$C_{16}H_{26}O_3$	0.29		0.21	
28	Undec-10-ynoic acid, undecyl ester	$C_{22}H_{40}O_2$	0.19		0.39	
29	Heptacosane	$C_{27}H_{56}$		2.50		1.06
30	Heptadecanal	$C_{17}H_{34}O$		0.98	0.25	1.10
31	2-Methyloctacosane	$C_{29}H_{60}$	1.84	1.57		1.55
32	2-Methylhexacosane	$C_{27}H_{56}$	4.71	1.72	2.52	3.57
33	1-Heptacosanol	$C_{27}H_{56}$	0.28	0.75	0.21	0.27
34	7-Hexadecenal	$C_{16}H_{30}O$	0.73		1.77	
35	Cyclooctacosane	$C_{28}H_{56}$	0.33	1.52		0.19
36	Diisooctyl Phthalate	$C_{24}H_{38}O_4$	3.86	2.18	1.77	7.21

Continuation of table 2

37	Octadecanal	$C_{18}H_{36}O$	0.30	0.70	0.25	0.19
38	Tetratetracontane	$C_{44}H_{90}$	11.24	12.57	5.57	10.70
39	Nonacosane	$C_{29}H_{60}$	9.83	8.57	7.94	13.46
40	1-Octacosanol	$C_{28}H_{58}O$	3.07		5.25	1.55
41	9-Tricosene	$C_{23}H_{46}$	0.31		0.23	
42	Olean-12-ene-3,28-diol	$C_{30}H_{50}O_2$	0.34	0.35		0.46
43	1-Heptatriacontanol	$C_{37}H_{76}O$	1.34		2.29	0.89
44	1-Hentetracontanol	$C_{41}H_{84}O$	8.10	4.93		13.48
45	Triarachine	$C_{63}H_{122}O_6$	0.56		0.47	0.19
46	3,5-dehydro-6-methoxypivalate-cholest-22-ene-21-ol	$C_{33}H_{54}O_3$	0.22	0.49		
47	Lup-20(29)-en-3-ol (3. beta) (syn. Lupeol)	$C_{30}H_{50}O$	1.23	1.03	1.35	1.18
48	Urs-12-ene	$C_{30}H_{50}$	0.80		9.08	0.58
49	24-Norursa-3,12-diene	$C_{29}H_{48}$	0.91	1.74	0.30	
50	3-acetoxy-7,8-epoxylanostan-11-ol	$C_{32}H_{54}O$	0.44		0.32	
	Total		87.52	82.62	90.33	94.42

Principal component analysis (PCA) of the created matrix was performed to review the similarities and differences between the inflorescences of the studied *Sorbus* species and natural hybrids in terms of non-phenolic metabolite content. The PCA results showed the first principal component (PC 1), second principal component (PC 2) and third (PC 3) principal component that explained the total variance of the data and correlated with positive or negative loadings for the metabolites; the most significant factor loadings (> 0.7) are shown in Table 3.

Table 3

Factor loadings of the principal components according to results of the PCA analysis of phytocompounds identified in the inflorescences of *Sorbus* plants

N*	PC 1	PC 2	PC 3	N*	PC 1	PC 2	PC 3	N*	PC 1	PC 2	PC 3
1	–0.883			14	0.901			28	0.968		
2	–0.891			15	0.964			29	–0.869		
3	0.934			16		–0.971		32		–0.784	
4	–0.897			17	0.817			34	0.966		
5	–0.894			18	0.857			36		–0.923	
6	–0.786			19		–0.975		38	–0.923		
7			–0.731	20	–0.855			40	0.998		
8		–0.881		21		0.907		42	–0.837		
9	–0.776			22	0.916			43	0.991		
10	0.868			23	0.761			44		–0.832	
11	–0.796			25		–0.881		45	0.819		
12		–0.917		26	–0.989			47	0.974		
13			–0.843	27	0.734			48	0.897		

Note. * - numbering of the compounds is given in accordance with the data in the Table 2.

The first (PC 1) and the second (PC 2) principal components, which accounted for the largest percentage of the total variance of the phytocomponent content data, were selected for in-depth analysis of the correlation matrix (Fig. 1). The projection of the variables (i.e. phytocompounds) onto the factor plane gives a diagram of factor loadings (Fig. 1a), which shows that the first principal component (PC 1) and the second principal component (PC 2) described 57.41 % and 26.98 % of the total variance data respectively.

The projection of cases (i.e., plant species) onto the factor plane (Fig. 1b) demonstrates the possibility of distinguishing species of studied plants of the genus *Sorbus* based on the distribution of unique groups of non-phenolic phytocompounds inherent in the inflorescences according to the total factor load of the first principal component (PC 1) and the second principal component (PC 2).

The diagram of factor loadings (scatter plot 2D) reflects the scatter of phytocompounds of *Sorbus* inflorescences as a result of the influence of the first (PC 1) and second (PC 2) principal components and characterizes the contribution of specific non-phenolic metabolites to the overall variance of the data. According to factor loadings, the first principal component correlated with the highest positive loading for octacosanol (40 in Table 2), heptatriacontanol (43), lupeol (47), 8,14-cedranoxide (3), linoleic acid (22), 2-propenoic acid, pentadecyl ester (10), ethyl isoallocholate (18), and triarachine (45), but with a significant negative loading for eicosane (26), tetratetracontane (38), methylinosine (4), 6-methyloctadecane (5) and olean-12-ene-3,28-diol (42).

Journal of Chemistry and Technologies, 2024, *32*(2), 267-275

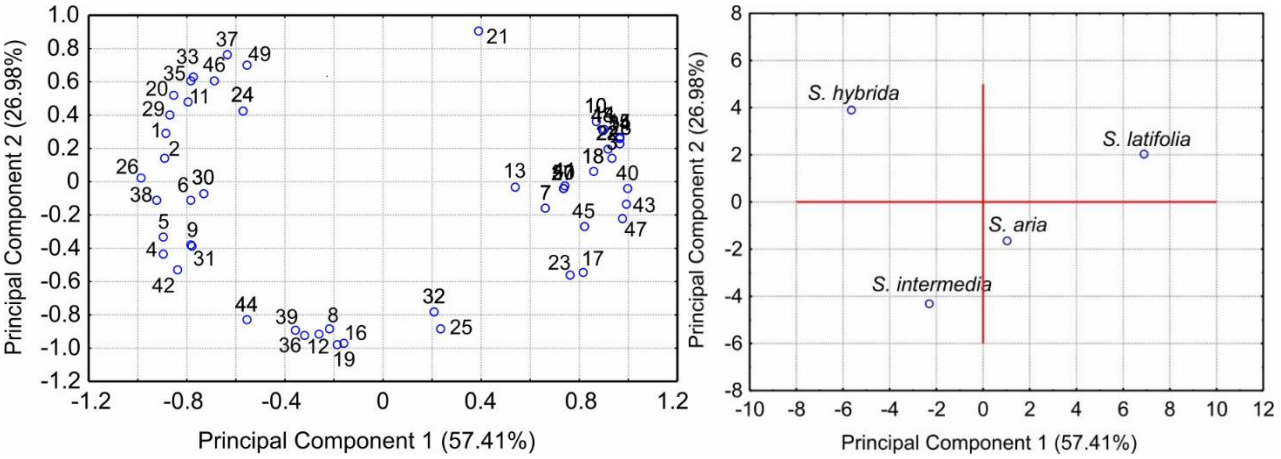

Fig. 1. PCA analysis of the phytoconstituents of *S. aria, S. latifolia, S. hybrida* and *S. intermedia* inflorescences: PCA scatter plot 2D (Fig. 1a), score plot (Fig. 1b). The different numbers in the scatter plot 2D correspond to the numbering of the phytocompounds in Table 2.

The second principal component correlated with the highest positive loading for heneicosane (21), octadecanal (37), heptacosanol (33), but with a negative loading for olean-12-en-3-one (19), butyl-undecyl phthalate (16), heptadecane (12), diisooctyl phthalate (36), and pentadecanal (25).

The results of the application of the Two-Way Joining method determined the correlation between the studied plant species and the phytoconstituents, which most significantly determined the unique nature of the non-phenolic phytochemical profile of *Sorbus* inflorescences (Fig. 2).

Cluster analysis of the dataset on the content of non-phenolic metabolites in *Sorbus* inflorescences made it possible to establish the distance of connection between the studied plants and to construct a tree diagram illustrating the degree of relationship between the natural hybrids *S. latifolia*, *S. hybrida*, *S. intermedia* and the species *S. aria*, which is one of the parental forms for the specified hybrids (Fig. 3).

According to the results of cluster analysis, the greatest distance in the composition of non-phenolic inflorescence metabolites was between *S. aria* and the hybridogenic species *S. latifolia*.

Discussing the results, it should be noted that the significant heterogeneity of the chemical composition of the non-phenolic fraction of phytocompounds in the inflorescences of *Sorbus* plants that we found is consistent with the known data on the wide variation of the spectrum of flavonoids and phenolic acids in the inflorescences of different species, hybrids and varieties of the *Sorbus* genus.[7] In our study, an attempt was made to assess the significance of the phytochemical diversity of floral non-phenolic compounds to reveal the relationship of *S. aria* and three hybridogenic forms, for which this species is one of the parents.

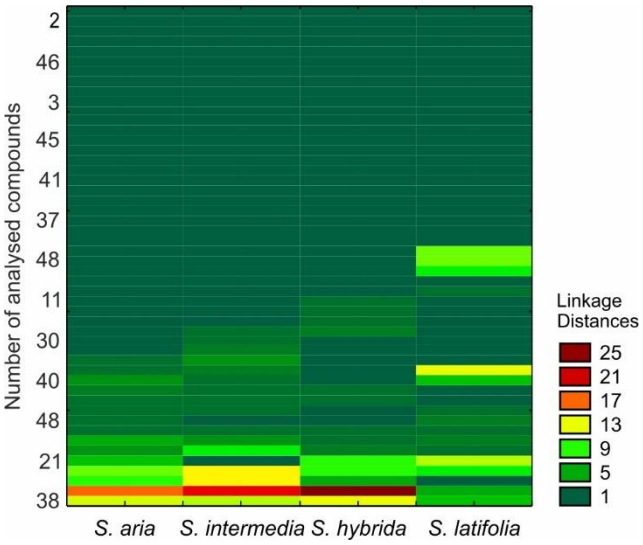

Fig. 2. Two-Way Joining correlations between phytocompounds identified in inflorescences and different *Sorbus* species. The colors from green to red on the graph represent the level of correlation (from lower to higher)

Discussing the results, it should be noted that the significant heterogeneity of the chemical composition of the non-phenolic fraction of phytocompounds in the inflorescences of *Sorbus* plants that we found is consistent with the known data on the wide variation of the spectrum of flavonoids and phenolic acids in the inflorescences of different species, hybrids and varieties of the *Sorbus* genus.[7] In our study, an attempt was made to assess the significance of the phytochemical diversity of floral non-

Journal of Chemistry and Technologies, 2024, *32*(2), 267-275

phenolic compounds to reveal the relationship of *S. aria* and three hybridogenic forms, for which this species is one of the parents.

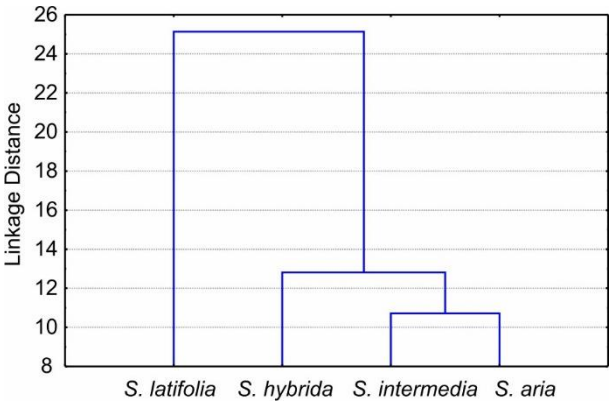

Fig. 3. Tree Diagram indicating Euclidean distances between the studied *Sorbus* species

According to the results of PCA, certain groups of phytocompounds from a total pool of 50 metabolites had the strongest correlation with differences between inflorescences of *Sorbus* plants. In *S. aria* inflorescences, heptatriacontanol, lupeol, octacosanol, triarachine, 2-methyltetracosane, 3-hydroxydodecanoic acid, pentadecanal, and 2-methylhexacosane (a metabolite known as a pheromone is probably synthesized by plants to attract pollinating insects[19]) had the greatest influence on the uniqueness of the phytochemical composition. Taking into account the results of the Two-Way Joining analysis, it can be assumed that heptatriacontanol, octacosanol and pentadecanal determined the species identity of *S. aria*, while tetratetracontane and octadecanal were responsible for its relatedness with *S. hybrida* and *S. intermedia* and the detachment of these three species from *S latifolia*.

Regarding the inflorescences of *S. latifolia*, PCA identified the most significant metabolites 2-propenoic acid, pentadecyl ester and linoleic acid (which have, respectively, antimicrobial[20] and repellent[21] properties), 7-hexadecenal, heneicosane, hexadecanoic acid, urs-12-ene, undec-10-ynoic acid, undecyl ester, 3-chloropropionic acid, dodecyl ester, 8,14-cedranoxide, and ethyl isoallocholate. According to Two-Way Joining analysis, 7-hexadecenal, heneicosane, and urs-12-ene most strongly distinguished *S. latifolia* from other species.

The uniqueness of the phytochemical composition of *S. hybrida* inflorescences, according to PCA, was determined by such metabolites as octadecanal, heptacosanol, 24-norursa-3,12-diene, hexahydrofarnesyl acetone (the last two compounds have antimicrobial properties[22-23]) 3,5-dehydro-6-methoxypivalate-cholest-22-ene-21-ol, cyclooctacosane, heptacosane (exhibits the properties of a pheromone[21]), 13-heptadecynol, butanedioic acid, 2-cyano-2,3-dimethyldecyl ester and cyclododecane. Based on the results of the Two-Way Joining analysis, heptacosanol, cyclooctacosane, and 13-heptadecynol can be identified as marker compounds of *S. hybrida* inflorescences, while heneicosane indicates affinity with *S. latifolia*.

The metabolites olean-12-ene-3,28-diol, hentetracontanol, methylinosine, nonacosane (metabolites which have attractive properties[21]), diisooctyl phthalate, 2-methyloctacosane, heptadecane, 2-propenoic acid, 1,2-ethanediyl ester, 6-methyloctadecane and tetratetracontane made the greatest contribution to the phytochemical differences of the *S. intermedia* inflorescences. According to Two-Way Joining analysis, diisooctyl phthalate and 2-methyloctacosane determined the identity of *S. intermedia*, while tetratetracontane indicated relatedness with *S. aria* and *S. hybrida*.

Similar groups of non-phenolic marker phytocompounds were established among the volatile metabolites of the inflorescences of the genus *Chorisia* plants, and included, in particular, linalool, phytane, 2-heptadecanone, hexahydro-farnesylacetone, heneicosane and tetracontane.[18]

However, the general pool of non-phenolic phytocompounds of *Sorbus* inflorescences included the metabolites that had no significant effect on the differences between species, for example, 9-tricosene, 3-acetoxy-7,8-epoxylanostan-11-ol, 2-dodecen-1-yl succinic anhydride, trans-2-undecenol, (2-phenyl-1,3 - dioxolan-4-yl) methyl-9-octadecenoate, oxalic acid, hexyl-2-methylphenyl ester, butyl-undecyl phthalate, and olean-12-en-3-one. The different significance of the *Sorbus* floral phytocompounds is consistent with the notion[24] that within a given taxon, one group of secondary metabolites is usually dominant, and several secondary components are often added to a certain number of major compounds.

The Euclidean distances between the studied *Sorbus* species determined by cluster analysis show the greatest relatedness between the species *S. aria* and the natural hybrid *S. intermedia*, smaller affinity between *S. aria* and *S. hybrida*, and the smallest affinity between *S. aria* and *S. latifolia*. To assess the relevance of the established dependence, the obtained results

were compared with known data on the genetic composition of hybridogenic taxa of the genus *Sorbus*. The species *S. hybrida* is known to have formed as a result of natural hybridization between the species *S. aucuparia* and the natural triple hybrid *S.* intermedia.[25] Regarding *S. intermedia*, it is believed that the most likely evolutionary scenario for the formation of this natural hybrid could have occurred through three-parent (*S. aria*, *S. aucuparia* and *S. torminalis*) hybridization.[6] Finally, the species *S. latifolia* is a natural hybrid between the two species *S. aria* and *S.* torminalis.[26] Therefore, the heterogeneity of the phytochemical composition of Sorbus inflorescences may reflect the heterogeneous genetic composition of the studied natural hybrids.

We believe that the principal components (PC 1 and PC 2) that determined the dispersion of the non-phenolic inflorescence compounds of *Sorbus* natural hybrids are due to the contribution and interaction of parental forms. In this case, the largest conditional proportion of the parental species *S. torminalis* may correspond to the greatest distance of *S. latifolia* from the second parental species *S. aria*. The complex hybridization of *S. intermedia* and *S. hybrida* resulted in a decrease in the conditional share of *S. torminalis* in their genetic composition, which corresponds to the greater relatedness of these natural hybrids with the parental species *S. aria*. Today, the taxonomy of the genus *Sorbus* L. is far from being finalized, however, in a new taxonomic system built on the basis of molecular phylogenetic analysis, it is proposed to separate the genus *Aria* (Pers.) Host and introduce the hybridogenic species *S. intermedia* and *S. latifolia* into its composition.[4,27] Thus, the results of the multivariate analysis of non-phenolic phytocompounds of *Sorbus* inflorescences are consistent with the data obtained using other methods, which testifies to the chemotaxonomic significance of phytochemical profiling and the expediency of this line of research.

Conclusion

The GC-MS analysis of the component composition of flower hexane extracts of *S. aria* species and *S. latifolia, S. hybrida* and *S. intermedia* made it possible to identify a total of 87 non-phenolic compounds of different chemical classes, including saturated and unsaturated fatty acids and their derivatives (esters, aldehydes, alcohols, alkanes), terpenes and terpenoids (sterols), nitrogen-containing and sulfur-containing compounds. The assessment of the chemotaxonomic value of the revealed significant heterogeneity of the phytochemical profiles of inflorescences of different plant species within the same genus was carried out using the tools of multivariate analysis, which determined the first (PC 1) and the second (PC 2) principal components, which determined, respectively, 57.41 % and 26 .98 % of the total variance of the data. The groups of non-phenolic phytocompounds were established, which determined the uniqueness of the phytochemical composition of the inflorescences of the studied *Sorbus* species and corresponded to their identity to the greatest extent. The highest level of relatedness between the parental species *S. aria* and the natural hybrid *S. intermedia*, the lower relatedness between *S. aria* and *S. hybrida*, and the lowest relatedness between *S. aria* and *S. latifolia* are consistent with the known genetic characteristics of the studied hybridogenic species. The chemometric analysis of the phytochemical composition of non-phenolic compounds of the inflorescences of the genus *Sorbus* showed suitability for the differentiation of species and the assessment of their relatedness.

References

[1] Arvinte, O.M.; Senila, L.; Becze, A.; Amariei, S. (2023). Rowanberry – A Source of Bioactive Compounds and Their Biopharmaceutical Properties. *Plants* (Basel). *12*(18), 3225. https://doi.org/10.3390/plants12183225

[2] Li, M.; Tetsuo, O.T.; Gao, Y.D.; Xu, B.; Zhu, Z.M.; Ju, W.B.; Gao, X.F. (2017). Molecular phylogenetics and historical biogeography of *Sorbus* sensu stricto (Rosaceae). *Mol Phylogenet Evol.*, *111,* 76–86. https://doi.org/10.1016/j.ympev.2017.03.018.

[3] Olszewska, M.A.; Kolodziejczyk-Czepas, J.; Rutkowska, M.; Magiera, A.; Michel, P.; Rejman, M.W.; Nowak, P.; Owczarek, A. (2019). The Effect of Standardized Flower Extracts of *Sorbus aucuparia* L. on Proinflammatory Enzymes, Multiple Oxidants, and Oxidative/Nitrative Damage of Human Plasma Components In Vitro. *Oxidative Medicine and Cellular Longevity*, 9746358. https://doi.org/10.1155/2019/9746358.

[4] Fedoronchuk, M. M. (2017). Taxa of Rosaceae of the Ukrainian flora: position in a new system of the family according to molecular phylogenetic data. *Ukr. Bot. J.*, *4*(1), 3–15. https://doi.org/10.15407/ukrbotj74.01.003

[5] Sołtys, A.; Galanty, A.; Podolak, I. (2020). Ethnopharmacologically important but underestimated genus *Sorbus*: a comprehensive review. *Phytochem. Rev., 19*, 491–526. https://doi.org/10.1007/s11101-020-09674-9

[6] Németh, C.; Papp, N.; Nosková, J.; Höhn, M. (2020). Speciation by triparental hybridization in genus *Sorbus*

(Rosaceae). *Biologia Futura*, *71*, 209–222. https://doi.org/10.1007/s42977-020-00003-x

[7] Zymone, K.; Raudone, L.; Žvikas, V.; Jakštas, V.; Janulis, V. (2022). Phytoprofiling of *Sorbus* L. Inflorescences: A Valuable and Promising Resource for Phenolics. *Plants* (Basel), *11*(24), 3421. https://doi.org/10.3390/plants11243421

[8] Lykholat, Y. V.; Khromykh, N. O.; Liashenko, O. V.; Sklyar, T. V.; Anishchenko, A. O.; Balalaiev, O. K.; Holubieva, T. A.; Lykholat, T. Y. (2023). Phytochemical profiles and antimicrobial activity of the inflorescences of *Sorbus domestica*, *S. aucuparia*, and *S. torminalis*. *Biosyst. Divers*., *31*(3), 290–296. https://doi.org/10.15421/012333

[9] Tahirovic, A.; Mehic, E.; Kjosevski, N.; Bašic, N. (2019). Phenolics content and antioxidant activity of three *Sorbus* species. *Bulletin of Chemists and Technologists of Bosnia and Herzegovina*, *53*, 15–21. https://doi.org/10.35666/ghtbh.2019.03

[10] Orsavová, J.; Juríková, T.; Bednaříková, R.; Mlček, J. (2023). Total phenolic and total flavonoid content, individual phenolic compounds and antioxidant activity in sweet rowanberry cultivars. *Antioxidants*, *12*(4), 913. https://doi.org/10.3390/antiox12040913

[11] Sarv, V.; Venskutonis, P.R.; Bhat, R. (2020). The *Sorbus* spp. – Underutilised Plants for Foods and Nutraceuticals: Review on Polyphenolic Phytochemicals and Antioxidant Potential. *Antioxidants*, *9*(9), 813. https://doi.org/10.3390/antiox9090813.

[12] Gaivelyte, K.; Jakstas, V.; Razukas, A.; Janulis, V. (2013). Variation in the contents of neochlorogenic acid, chlorogenic acid and three quercetin glycosides in leaves and fruits of rowan (*Sorbus*) species and varieties from collections in Lithuania. *Nat Prod Commun*., *8*(8), 1105–1110. https://pubmed.ncbi.nlm.nih.gov/24079179/

[13] Mikulić-Petkovsek, M.; Krska, B.; Kiprovski, B.; Veberic, R. (2017). Bioactive components and antioxidant capacity of fruits from nine *Sorbus* genotypes. *J Food Sci*., *82*(3), 647–658. https://doi.org/10.1111/1750-3841.13643

[14] Bailie, A.; Renaut, S.; Ubalijoro, E.; Guerrero-Analco, J.A.; Saleem, A.; Haddad, P.; Arnason, J.T.; Johns, T.; Cuerrier, A. (2016). Phytogeographic and genetic variation in *Sorbus*, a traditional antidiabetic medicine – adaptation in action in both a plant and a discipline. *Peer J*., *4*, e2645. https://doi.org/10.7717/peerj.2645

[15] Khromykh, N.O.; Anishchenko A.A.; Didur O.O.; Gaponov A.A.; Kabar A.M.; Lykholat T.Y. (2020). Cuticular wax composition of mature leaves of species and hybrids of the genus *Prunus* differing in resistance to clasterosporium disease. *Biosyst. Divers*., *28*(4), 370–375. http://dx.doi.org/10.15421/012047

[16] Khromykh N.O.; Didur O.O.; Sklyar T.V.; Davydov V R.; Lavrentieva K.V.; Lykholat T.Y. (2022). Phytochemical profiles, antioxidant and antimicrobial activity of *Actinidia polygama* and *A. arguta* fruits and leaves. *Biosyst. Divers.*, *30*(1), 39–45. https://doi.org/10.15421/012205

[17] Wink, M. (2003). Evolution of secondary metabolites from an ecological and molecular phylogenetic perspective. *Phytochemistry, 64*, 3–19. https://doi.org/10.1016/S0031-9422(03)00300-5

[18] Fahim, J. R.; Darwish, A. G.; Zawily, A. L. I.; Wells, J.; Abourehab, M. A. S.; Desoukey, S. Y.; Attia, E. Z.; (2023). Exploring the volatile metabolites of three *Chorisia* species: Comparative headspace GC–MS, multivariate chemometrics, chemotaxonomic significance, and anti-SARS-CoV-2 potential. *Saudi Pharmaceutical Journal*, *31*(5), 706–726. https://doi.org/10.1016%2Fj.jsps.2023.03.012

[19] Spikes, A. E.; Pashen, M. A.; Millar, J. G.; Moreira, J. A.; Hamel, P. B.; Schiff, N. M.; Ginzel, M. D. (2010). First contact pheromone identified for a longhorned beetle (Coleoptera: Cerambycidae) in the subfamily Prioninae. *J Chem Ecol.*, *36*(9), 943–954. https://doi.org/10.1007/s10886-010-9837-8

[20] Mujeeb, F.; Bajpai, P.; Pathak, N. (2014). Phytochemical evaluation, antimicrobial activity, and determination of bioactive components from leaves of *Aegle marmelos***.** *BioMed Research International*, *2014*, 497606. https://doi.org/10.1155/2014/497606.

[21] "The Pherobase: Database of Pheromones and Semiochemicals". El-Sayed, 2023. http://www.pherobase.com/

[22] Ullah, O.; Shah, M.; Ur Rehman, N.; Ullah, S.; Al-Sabahi, J. N.; Alam, T.; Khan, A.; Khan, N. A.; Rafiq, N.; Bilal, S.; Al-Harrasi A. (2022). Aroma Profile and Biological Effects of *Ochradenus arabicus* Essential Oils: A Comparative Study of Stem, Flowers, and Leaves. *Molecules***.** *27*(16), 5197. https://doi.org/10.3390/molecules27165197.

[23] Xu, Z.; Gao, P.; Liu, D.; Song, W;, Zhu, L.; Liu, X. (2022). Chemical Composition and In Vitro Antioxidant Activity of *Sida rhombifolia* L. Volatile Organic Compounds. *Molecules*, *27*(20), 7067. https://doi.org/10.3390%2Fmolecules27207067

[24] Al-Hajj, N. O. M., Wang, H., Gasmalla, M. A. A.; Ma, C., Thabit, R., Rahman, M. R. T., Tang, Y. (2014). Chemical Composition and Antioxidant Activity of the Essential Oil of *Pulicaria Inuloides*. *Journal of Food and Nutrition Research*, *2*(5), 221–227. https://DOI:10.12691/jfnr-2-5-3

[25] Fitzgerald, H.; Helpdesk, G. N. (2020). Nordic Crop Wild Relative (CWR) Checklist. Version 1.16. Nordic Genetic Resource Center (NORDGEN). *Sorbus hybrida*. https://doi.org/10.15468/itkype

[26] Sennikov, A.; Kurrtto, A. A. (2017). Phylogenetic checklist of Sorbus s.l. (Rosaceae) in Europe. *Memoranda Soc Fauna Flora Fennica*,*93*, 1–78. https://www.researchgate.net/publication/317784825

[27] Fedoronchuk, M. M. (2022). Checklist of flora of Ukraine. 4: Rosaceae family (Rosales, Angiosperms)]. *Chornomors'k. bot. z.*, 18*(4)*, 305–349. https://dx.doi.org/10.32999%2Fksu1990-553X%2F2022-18-4-1