Molecular Networking Guided Investigation of The Secondary Metabolome Of Four *Morus* Species And Their in Vivo Neuroprotective Potential For The Mitigation of Alzheimer's Disease

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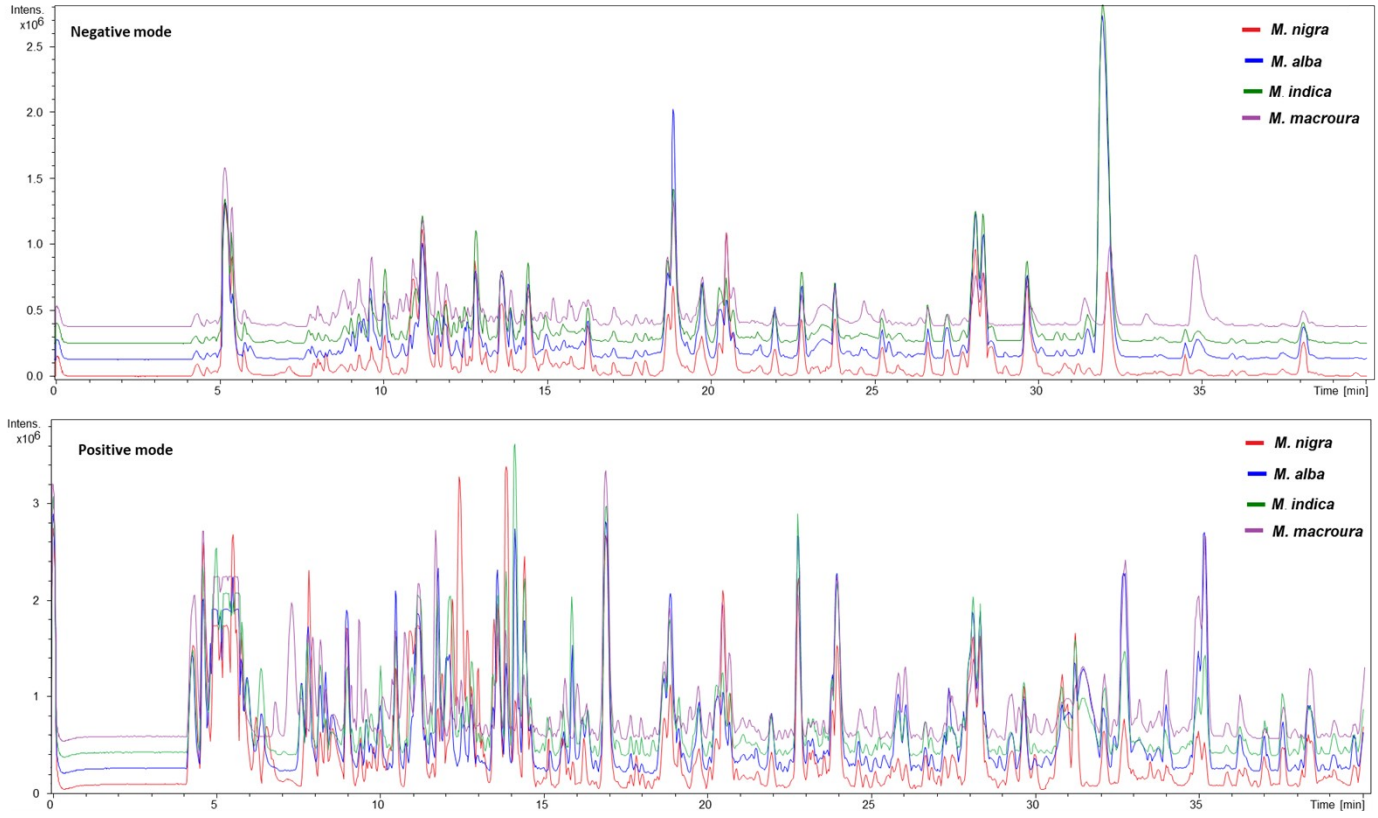
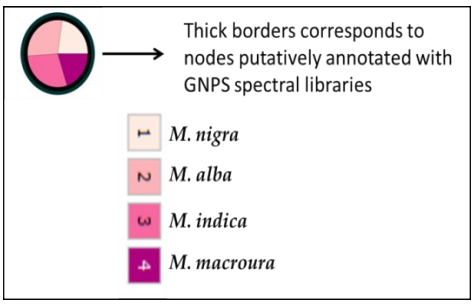
Supplementary Figures

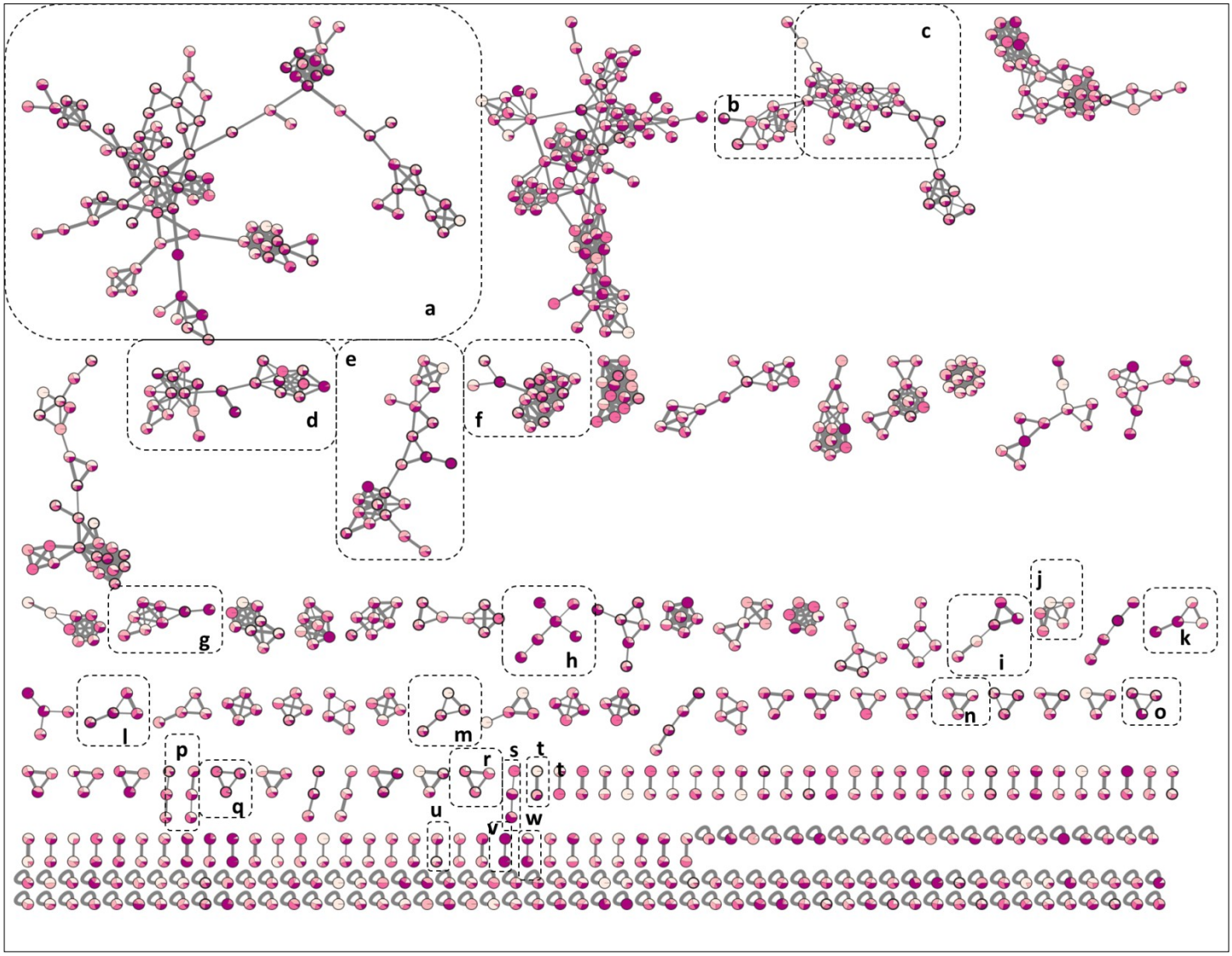
Supplementary Figure S1: Base peak chromatogram of the leaves of the studied Morus species in both ionization modes



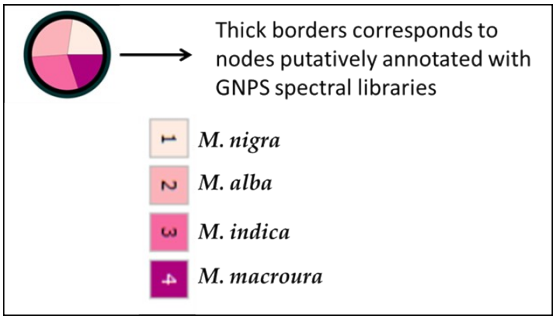
Supplementary Figure S2: Full FBMN constructed from the acquired UPLC-HRMS/MS data in the negative ionization mode of the leaves of selected *Morus* species.



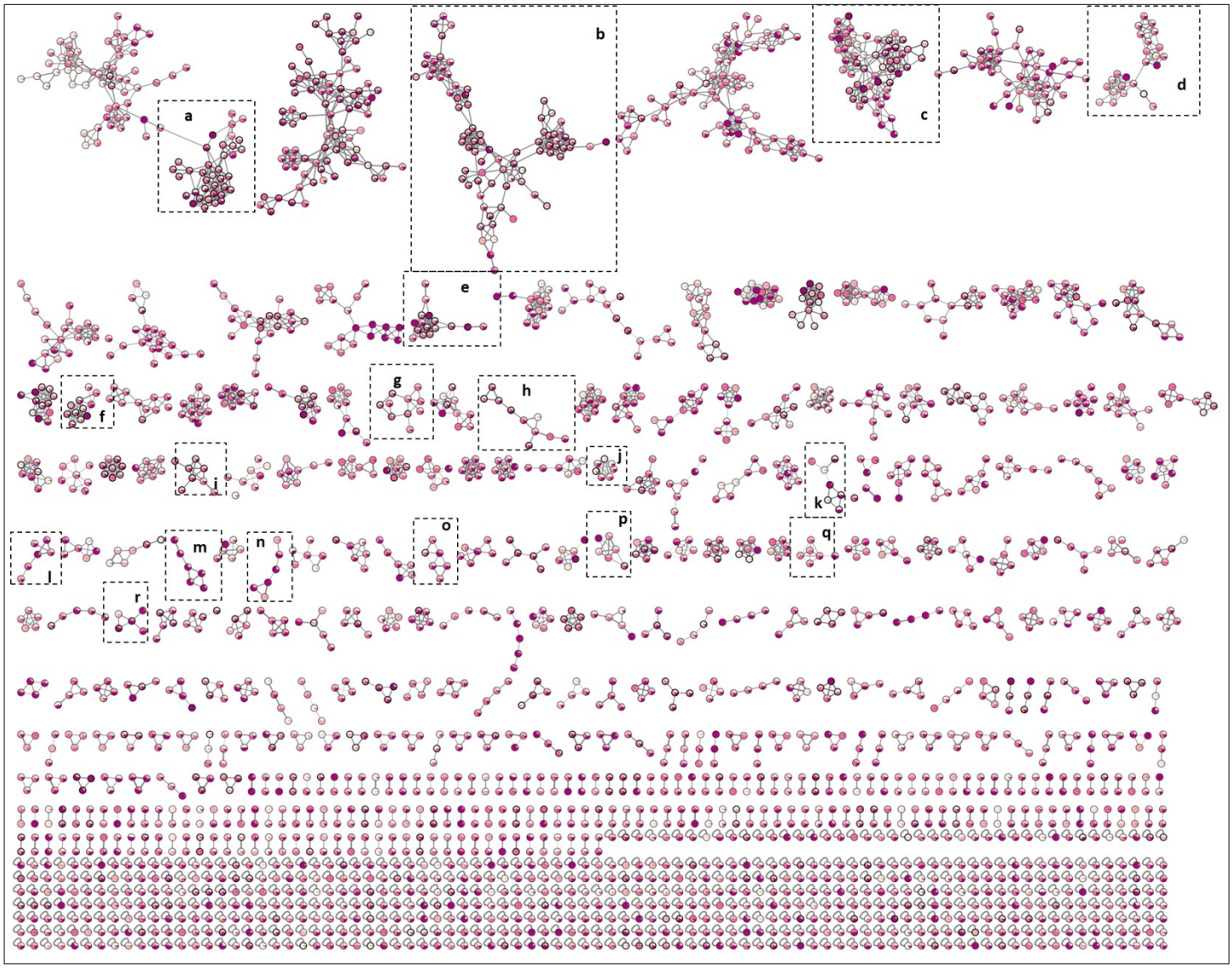
Cluster **a**: fatty acids and derivatives; **b**: flavonoid glycosides; **c**: cinnamic acid derivatives; **d**: glycosides; **e**: fatty acids and derivatives; **f**: phospholipids; **g**: benzoic acid derivatives; **h**: prenylated flavonoids; **i**: cinnamic acid derivatives, **j**:acylated flavonoid glycosides; **k**: flavonoid glycosides; **l**: coumarins; **m** & **n**: cinnamic acid derivatives; **o**: benzoic acid derivatives; **p**: prenylated flavonoids; **q**: chalcones; **r**: flavonoids; **s**: iridoid glycosides; **t**: flavonoid glycosides; **u**: lignans; **v**: prenylated flavonoids; and **w**: phenolic glycosides..



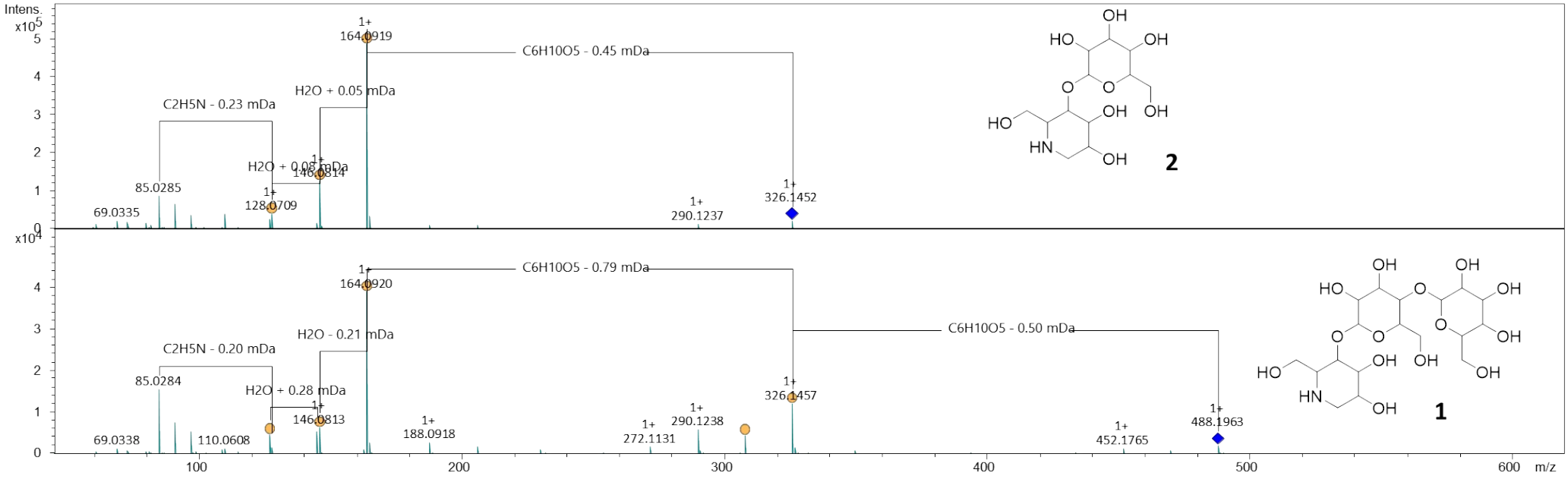
Supplementary Figure S3: Full FBMN constructed from the acquired UPLC-HRMS/MS data in the positive ionization mode of the leaves of selected *Morus* species.



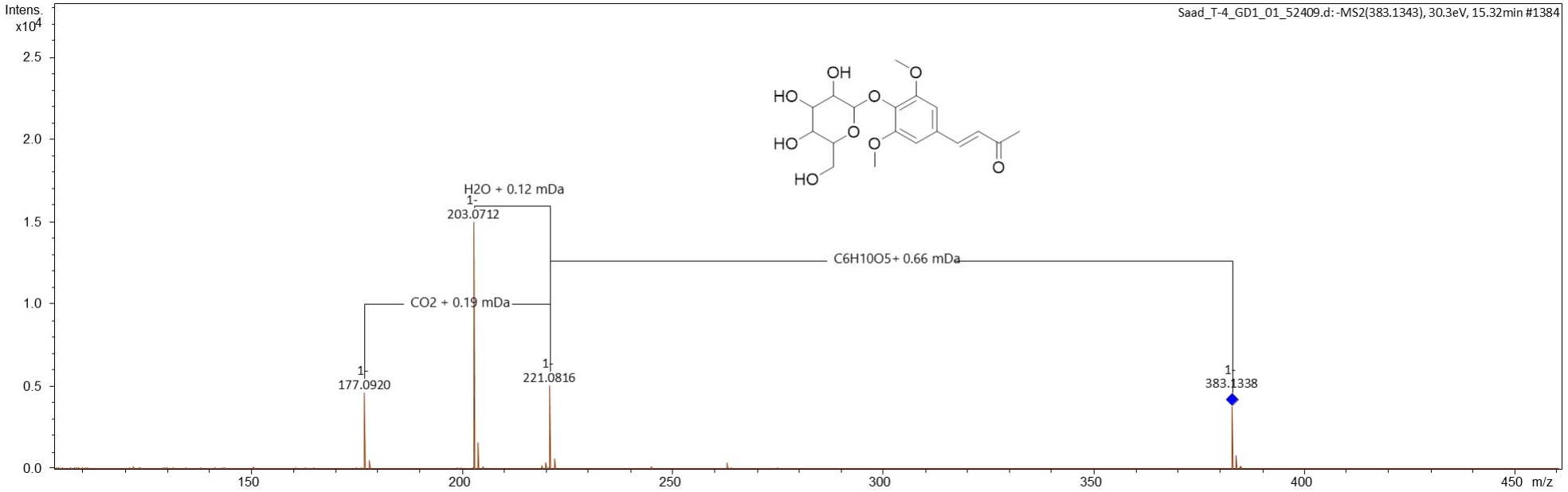
Cluster **a**: flavonoid glycosides; **b**: fatty acids and derivatives; **c**: amino acid and derivatives; **d**: peptides; **e** & **f:** cinnamic acids and derivatives; **g**: flavonoids; **h**: benzofurans; **i**: fatty acids derivatives; **j**: phospholipids, **k**: flavonoids; **l**: iminosugars; **m**: cinnamyl alcohols; **n**: chalcones; **o**: phospholipids; **p**: amino acid derivatives; **q**: peptides; **r**: flavonoids.



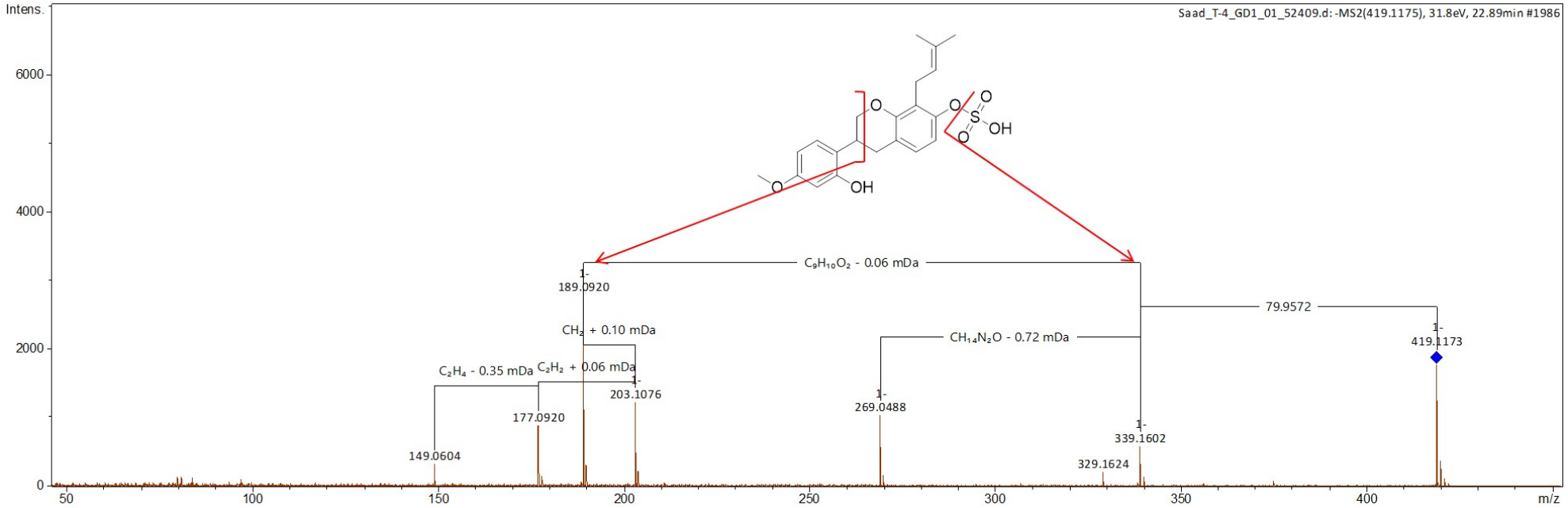
Supplementary Figure S4: MS^2 spectrum of compound 1; moranoline di-*O*-hexoside versus its mono-glycosidic analog 2: moranoline-O-hexoside



Supplementary Figure S5: MS^2 spectrum of compound 82; (Hydroxydimethoxyphenyl)butenone-*O*- hexoside



Supplementary Figure S6: MS^2 spectrum of compound 105; *O*-methylpreglabridin-*O*-sulphate



Supplementary Tables

Supplementary Table S1: Parameters set for the construction of both FBMNs through the GNPS platform

	Negative FBMN	Positive FBMN
Precursor ion mass tolerance	0.05	0.05
Fragment ion mass tolerance	0.05	0.05
Cosine score	0.7	0.7
Min shared fragments	4	4

Supplementary Table S2: Metabolites identified in the leaves of the studied *Morus* species via UPLC-HRMS/MS analysis.
-: absent, tr: traces, +: present, ++: abundant, +++: major.
***compounds previously isolated from *Morus* species, #: tentatively assigned new compounds**

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
1.	Iminosugars	Moranoline di-*O*-hexoside #	4.61			488.1979 (-1.0)	326.1457, 308.1344, **164.092**, 146.0813, 127.0395	$C_{18}H_{33}NO_{14}$	+	+	+	+	[1]
2.	Iminosugars	Moranoline-*O*-glucoside *	4.65			326.1447 (-0.5)	**164.0919**, 146.0814, 128.0709	$C_{12}H_{23}NO_9$	+	+	+	+	[1]
3.	Iminosugars	Fagomine-*O*-glucoside *	4.69			310.1498 (-0.5)	**148.097**, 130.0865, 112.0759, 97.0285, 85.0285	$C_{12}H_{23}NO_8$	+	tr	tr	+++	[2]
4.	Iminosugars	hydroxy-(hydroxymethyl)-pyrrolidinyl-*O*-glucoside *	4.70			296.1343 (-1.1)	**134.0814**, 85.0285	$C_{11}H_{21}NO_8$	+	+	+	+++	[1]

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
5.	Organic acid	Quinic acid*	5.44	191.056 (0.6)	173, 127, 111, **85.0296**	193.071 (-0.5)	174.0769, 129.0550, 111.042,**8 3.0492**	$C_7H_{12}O_6$	++	+	++	+++	GNPS, [3]
6.	Phenolic glycoside	Hydroxy-dimethoxyphen yl-*O*-hexoside	5.91	331.1033 (0.4)	283.2637, 211.0244, 193.0149, 169.0137, 151.0037, **123.0449**			$C_{14}H_{20}O_9$	+++	+	+	+	
7.	Benzoic acid derivative	Dihydroxy benzoic acid-*O*-hexoside isomer I	6.06	315.072 (0.5)	**153.0193**, 109.0295	-	-	$C_{13}H_{16}O_9$	++	--	--	+++	GNPS
8.	Amino acid	*N*-[carboxy-2-methylbutyl] D-Glutamic acid isomer I	6.24			262.1289 (-1.4)	244.1182, 216.1231, 198.1122, 130.086, 118.0859, 98.0602, 81.0697	$C_{11}H_{19}NO_6$	-	++	++	-	[4]
9.	Amino acid	*N*-fructosyl phenylalanine isomer I	7.17			328.1398 (-2.1)	310.1293, 292.1184, 264.1237, **246.1132**,	$C_{15}H_{21}NO_7$	+	-	-	-	GNPS

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
							228.1023, 198.0924, 178.0862 166.0867 143.0582 132.0809, 120.081						
10.	Amino acid	*N*-[carboxy-2-methylbutyl] D-Glutamic acid isomer II	7.24			262.1289 (-1.4)	244.1182, 216.1231, 198.1122, 130.086, 118.0859, 98.0602, 81.0697	$C_{11}H_{19}NO_6$	-	tr	-	+++	
11.	Amino acid	*N*-fructosyl phenylalanine isomer II	7.31			328.1393 (0.8)	310.1293, 292.1184, 264.1237, **246.1132**, 228.1023, 198.0924, 178.0862 166.0867 143.0582 132.0809, 120.081	$C_{15}H_{21}NO_7$		-	+++	+	GNPS

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
12.	Amino acid	*N*-Benzoyl-L-aspartic acid	7.81			238.0716 (-2.3)	127.0391, 109.0286, 97.0288, **85.0286**	$C_{11}H_{11}NO_5$	++	+	+	-	[5]
13.	Phenolic glycoside	Glucogallin	7.98	331.0670 (-0.5)	283.2656, 211.025, 193.0137, **169.0143**, **151.0036**, 125.0242			$C_{13}H_{16}O_{10}$	-	+	+	++	
14.	Phenolic glycoside	dihydroxy-methoxyphenyl-*O*-hexoside (Picraquassioside D)	8.03	301.0931 (-0.6)	**139.0401**			$C_{13}H_{18}O_8$	-	tr	tr	+++	[6]
15.	Benzoic acid derivative	Dihydroxy benzoic acid-*O*-hexoside isomer II	8.23	315.0721 (0.2)	200.0553, **153.0193**, 109.0294	-	-	$C_{13}H_{16}O_9$	--	tr	++	+++	GNPS
16.	Cinnamic acid derivative	Sinapoyl-*O*-hexoside	8.36	371.098 (1.0)	**191.0561**			$C_{16}H_{20}O_{10}$	+	+	+	+	[7]

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
17.	Peptide	Glutamylvaline				247.1292 (-1.3)	184.0973 118.0867, 84.0445, **72.0808**	$C_{10}H_{18}N_2O_5$	+	++	+	+	
18.	Benzoic acid derivative	Hydroxybenzoic acid-*O*-hexoisde isomer I	8.67	299.0771 (0.5)	**137.0242**, 93.0348	-		$C_{13}H_{16}O_8$	+	+	+	+	[8]
19.	Amino acid	N^2-(4-Hydroxy-methoxybenzoyl)-D-arginine	8.82	323.1347 (4.2)	**164.0719**, 147.0447, 89.0244			$C_{14}H_{20}N_4O_5$	++	++	-	+++	[9]
20.	Cinnamic acid derivative	*O*-(*O*-hexosylcaffeoyl) quinic acid *	8.94	515.1398 (1.5)	353.0873, 315.0716, **191.056**			$C_{22}H_{28}O_{14}$	+	++	+	++	[3]
21.	Benzoic acid derivatives	Vanillic acid-*O*-hexoside	9.24	329.0876 (0.7)	283.2654, **167.035**, 152.0111, 123.0452 108.0214			$C_{14}H_{18}O_9$	+	+	+	+	GNPS, [7]
22.	Coumarin	Umbelliferone*	9.45			163.039	145.028, 135.0445, 120.0806, 117.0337, 105.0436,	$C_9H_6O_3$	+	+	+	+	[10]

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
							89.0385						
23.	Megastigmane	Megastigmanen e-epoxy-diol di-*O*-hexoside	9.69	549.2549 (0.7)	387.2023, 191.0553, **119.0349, 89.0246**			$C_{25}H_{42}O_{13}$	+	+	+	+	[11]
24.	Flavonoid-*O*-glycoside	Quercetin 3, 7 di-*O*-glucoside isomer I*	9.78	625.1412 (-0.2)	**463.0868**, 301.0348	627.1561 (-0.9)	**303.0502**	$C_{27}H_{30}O_{17}$	+	++	+	+	[12], [13]
25.	Cinnamic acid derivative	*O*-caffeoyl quinic acid isomer I*	9.79	353.0876 (0.5)	**191.0561**	355.1028 (-1.2)	**163.0392**	$C_{16}H_{18}O_9$	+	+	+	+	GNPS, [14]
26.	Benzoic acid derivative	*O*-benzoylsucrose	9.87	445.1343 (1.9)	301.0922, **139.0399**			$C_{19}H_{26}O_{12}$	+++	tr	tr	tr	[15] [16]
27.	Flavonoid-*O*-glycoside	Quercetin-*O*-hexoside –*O*-(hexosyl deoxyhexoside)	9.89	771.1988 (0)	**609.1459**, 462.0805, 301.0354	773.2134 (-1.0)	465.1033, **303.0502**	$C_{33}H_{40}O_{21}$	+	+	+++	+	[15]
28.	Amino acid	L-tryptophan – *N*- hexoside	9.95			367.1504 (-1.0)	332.1133, 303.1344, 276.1231, 258.1129, 229.0974,	$C_{17}H_{22}N_2O_7$	+	+	+	+	GNPS

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
							188.0707						
29.	Flavonoid-*O*-glycoside	Quercetin 3, 7 di-*O*-glucoside isomer II*	10.01	625.1408 (0.3)	**463.0867**, 301.0349	627.1558 (-0.4)	303.0502	$C_{27}H_{30}O_{17}$	+	+++	-	+	[12], GNPS
30.	Cinnamic acid derivative	Coumaric acid *O*-hexoside	10.22	325.0928 (0.4)	163.0399, **119.0503**	-	-	$C_{15}H_{18}O_8$	+	++	+	+	[7] SELFLOOPED
31.	Stilbene glycoside	Mulberroside E *	10.26	597.1822 (0.5) [M-H+HCOOH]$^-$	549.2539, 389.1241, **227.0714**, 189.0763			$C_{26}H_{32}O_{13}$	-	+	++	-	[17]
32.	Coumarin	Dihydroxy coumarin-O-glucoside isomer I*	10.29	339.0720 (0.5)	**177.0191**	-	-	$C_{15}H_{16}O_9$	+	-	-	+++	[17]
33.	Flavonoid glycoside	Naringenin-O-methyl ether-O-hexoside	10.30			449.1444 (-0.4)	**287.0915**, 269.0811, 241.0861	$C_{22}H_{24}O_{10}$	-	-	-	+	[18]
34.	Peptide	Pyroglutamyl - valine	10.44			229.1185 (-0.8)	183.1127, 84.0445, **72.0807**	$C_{10}H_{16}N_2O_4$	+	++	+	+	[19]

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
35.	Flavonoid-*O*-glycoside	Kaempferol -*O*-rutinoside--*O*-glucoside *	10.49	755.2037 (0.4)	**593.1502**, 447.0915, 285.0401	757.2192 (-0.8)	449.1081, **287.0554**	$C_{33}H_{40}O_{20}$	+	+	++	+	[15]
36.	Coumarin	Dihydroxy coumarin-*O*-glucoside isomer II*	10.55	339.0722 (-0.0)	**177.0192**	341.0867 (-0.0)	**179.0340**	$C_{15}H_{16}O_9$	+	++	++	+++	GNPS, [17]
37.	Flavonoid-*O*-glycoside	Tetrahydroxyflavanone di-*O*-hexoside isomer I	10.62	611.1607 (1.7)	447.0918, 285.0402, **241.0504**			$C_{27}H_{32}O_{16}$	-	-	+++	-	[6]
38.	Benzoic acid derivative	Hydroxybenzoic acid-*O*-hexoisde isomer II	10.77	299.0772 (0.2)	**137.0242**, 93.0347	-	-	$C_{13}H_{16}O_8$	+	++	+	+	[8]
39.	Flavonoid-*O*-glycoside	Tetrahydroxyflavanone di-*O*-hexoside isomer II	10.82	611.1612 (0.9)	447.0926, 403.1031, **241.0505**			$C_{27}H_{32}O_{16}$	-	-	+++	-	[6]
40.	Cinnamic acid derivative	*O*-caffeoyl quinic acid isomer II*	10.98	353.0877 (0.2)	**191.0561**	355.1027 (-0.9)	**163.0393**	$C_{16}H_{18}O_9$	+	+	+	+	GNPS, [14]
41.	Amino acid	Phenylglutamate	11.00			295.1294 (-1.7)	232.0969, 186.0916,	C14H18N2O5	+	++	+	+	

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
							120.0811, 84.0444						
42.	Flavonoid-*O*-glycoside	Quercetin -*O*-(rutinoside-*O*-hexoside) isomer I	11.14			773.2139 (-0.6)	**303.0504**	$C_{33}H_{40}O_{21}$	++	-	-	+	[15]
43.	Cinnamic acid derivative	*O*-caffeoyl quinic acid isomer III*	11.25	353.0877 (0.3)	**191.0561**	355.1025 (-0.5)	163.0391	$C_{16}H_{18}O_9$	+	+	+	+	GNPS, [14]
44.	Flavonoid-*O*-glycoside	Quercetin –*O*-glucosyl-*O*-rutinoside isomer II	11.28	-	**-**	773.2135 (-0.1)	**303.0503**	$C_{33}H_{40}O_{21}$	++	+	+++	++	[15]
45.	Cinnamic acid derivative	Rosmarinic acid	11.52	359.0768 (1.2)	271.0972, **242.0582**			$C_{18}H_{16}O_8$	++	+	++	+	[20]
46.	Flavonoid-*O*-glycoside	Quercetin -*O*-(di-*O*-rhamnosyl-*O*-hexoside)*	11.61	755.2032 (1.1) in neg	**300.0271**	757.2185 (0.1)	**303.0501**	$C_{33}H_{40}O_{20}$	+	+	++	+	GNPS, [21]
47.	Benzyl alcohol derivative	Benzyl -O-pentosyl-O-hexoside	11.48	401.1452 (0.4)	269.1021, 237.0758, **219.0663**, 193.0503,			$C_{18}H_{26}O_{10}$	+	+	+	+	

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
					161.0458, 101.0245								
48.	Cinnamic acid derivative	*O*-caffeoyl quinic acid isomer IV*	11.94	353.0873 (1.3)	**191.056**	355.1025 (-0.4)	163.0393	$C_{16}H_{18}O_9$	+	+	+	+	GNPS, [13]
49.	Flavonoid-*O*-glycoside	Quercetin-*O*-dihexoside *	12.05	625.1414 (-0.6)	**300.0276**	627.1556 (-0.1)	**303.0501**	$C_{27}H_{30}O_{17}$	+	+	+	+++	GNPS, [3]
50.	Flavonoid-*O*-glycoside	Kaempferol -*O*-rutinoside-*O*-rhamnoside *	12.20	739.2087 (-1.2)	**284.0324**	741.2239 (-0.3)	**287.0552**	$C_{33}H_{40}O_{19}$	+	+	++	+	GNPS, [15]
51.	Flavonoid-*O*-glycoside	Scutellarein dimethylether-*O*-sophoroside	12.48	637.1776 (-0.3)	**475.124**, 295.0610			$C_{29}H_{34}O_{16}$	-	-	-	++	[22]
52.	Flavonoid-*O*-glycoside	Quercetin-*O*-rutinoside *	12.56	609.1458 (0.5)	**300.0273**	611.1612 (-0.8)	**303.0500**	$C_{27}H_{30}O_{16}$	++	-	++	++	[23]
53.	Iridoid glycoside	*O*-hydroxybenzoyl monomelittosid e isomer I	12.60	481.1347 (0.9)	316.0219, 179.0347, 163.0397, **137.0243**			$C_{22}H_{26}O_{12}$	-	+++	+++	++	[24]
54.	Cinnamic acid derivative	*O*-coumaroyl-quinic acid	12.69	337.0926 (0.9)	**191.0559**	339.1077 (-0.9)	**147.0442**	$C_{16}H_{18}O_8$	++	+	+	+	GNPS

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
55.	Flavonoid-*O*-glycoside	Quercetin-*O*-rutinoside isomer II *	12.85	-	**-**	611.1603 (0.6)	**303.0500**	$C_{27}H_{30}O_{16}$	+	+	+	+	[23]
56.	Flavonoid-*O*-glycoside	Quercetin-*O*-glucoside *	12.84			465.1029 (-0.3)	330.2650, **303.0503**, 251.1258, 217.1229	$C_{21}H_{20}O_{12}$	++	+	++	+	[15]
57.	Lignan	Lyoniresinol-*O*-hexoside	13.06	581.2234 (-0.1)	**449.2024 , 389.1601,** 367.1030, 305.1139, 216.08761 72.0890			$C_{28}H_{38}O_{13}$	-	++	-	++	[25]
58.	Iridoid glycoside	ligstroside-*O*-hexoside	13.06	685.2353 (-0.6)	**477.1765**, 315.1238			$C_{31}H_{42}O_{17}$	-	++	tr	+++	[26]
59.	Chalcone	trimethoxy-dihydrochalcone-*O*-dihexoside isomer I #	13.09			641.2445 (-0.8)	329.1234, 299.1284, 193.0863, **167.0704**, 149.0599	$C_{30}H_{40}O_{15}$	-	+	-	-	
60.	Flavonoid-*O*-glycoside	Kaempferol-*O*-hexoside *	13.14			449.1077 (0.2)	**287.0556**, 217.1235	$C_{21}H_{20}O_{11}$	+	++	+++	+	[15]

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
61.	Flavonoid-*O*-glycoside	Kaempferol-*O*-rutinoside isomer I *	13.16	593.1507 (0.9)	**284.0324**	595.1661 (-0.6)	**287.0553**	$C_{27}H_{30}O_{15}$	+	+	+++	+	GNPS, [23]
62.	Lignan	Lariciresinol-*O*-hexoside	13.19	521.2022 (1.2)	**329.1391**			$C_{26}H_{34}O_{11}$	+++	+	+	+	GNPS, [27]
63.	Iridoid glycoside	*O*-hydroxybenzoyl monomelittoside isomer II	13.26	481.1352 (-0.1)	316.0219, 179.0347, 163.0397, **137.0243**			$C_{22}H_{26}O_{12}$	tr	+++	+++	++	[24]
64.	Cinnamic acid derivative	*O*-caffeoylquinic acid methyl ester	13.29	367.1034 (0.2)	**179.0349,** 161.0243, 135.0451			$C_{17}H_{20}O_9$	++	+	+	+	
65.	Coumarin	Dihydroxycoumarin	13.30	177.0193 (0.4)	149.0243, **133.0293,** 105.0346			$C_9H_6O_4$	+	+	+	+++	GNPS
66.	Flavonoid-*O*-glycoside	kaempferol -*O*-rutinoside isomer II*	13.54	593.1506 (1.0)	**285.0401**	595.1662 (-0.8)	**287.0552**	$C_{27}H_{30}O_{15}$	+	++	+	+	GNPS, [23]
67.	Flavonoid-*O*-glycoside	Quercetin-*O*-glucoside *	13.65	463.0879 (0.7)	**300.0274**	465.1027 (0.1)	**303.0498**	$C_{21}H_{20}O_{12}$	+	+	+	+	GNPS, [23]

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
68.	Lignan	Syringaresinol-*O*-hexoside	13.95	579.2079 (0.7)	**417.1551**, 181.0506			$C_{28}H_{36}O_{13}$	+	++	+	+	GNPS
69.	Megastigmane	Oxo -ionol O-hexoside	13.99			371.2063 (0.2)	255.0655, 227.0704, **209.1539**, 191.1433, 165.1277, 137.0959	$C_{19}H_{30}O_7$	+	++	+	+	[28]
70.	Acylated flavonoid glycoside	Quercetin-*O*-(-*O*-malonyl) hexoside*	14.06			551.1032 (0.0)	**303.0503,** 127.0391	$C_{24}H_{22}O_{15}$	+++	++	+	-	[15]
71.	Chromone derivative	Hydroxy-isopropylchromanone-*O*-hexoside	14.07	383.1346 (0.4)	**221.0819**, 177.0921	-	-	$C_{18}H_{24}O_9$	tr	tr	tr	+++	[29]
72.	Cinnamic acid derivative	Di-*O*-caffeoylquinic acid isomer I *	14.22	515.118 (2.0)	353,335,191,**179**,173,161,135			$C_{25}H_{24}O_{12}$	+	+	+	+	[3]
73.	Flavonoid-*O*-glycoside	Kaempferol-*O*-glucoside *	14.47	447.093 (0.6)	**284.0327**	449.1078 (0.1)	287.0553	$C_{21}H_{20}O_{11}$	+	+	+	+	GNPS, [15]
74.	Benzoic acid	Dihydroxy	14.60	153.0192	**109.0296**,	155.0341	**137.0235**	$C_7H_6O_4$	+	+	++	++	GNPS, [3]

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
	derivative	benzoic acid*		(0.9)	67.0192	(-1.3)							
75.	Acylated flavonoid glycoside	Quercetin-*O*-(*O*-acetyl)hexoside *	14.82			507.1137 (-0.7)	**303.0505,** 187.0606, 81.0335	$C_{23}H_{22}O_{13}$	+	+	+	-	[30]
76.	Chalcone	trimethoxy-dihydrochalcone -*O*-dihexoside isomer II #	14.88			641.2444 (-0.6)	329.1234, 299.1284, 193.0863, **167.0704**, 149.0599	$C_{30}H_{40}O_{15}$	-	-	-	+	
77.	Cinnamic acid derivative	Di-*O*-caffeoylquinic acid isomer II	14.89	515.1186 (1.7)	353.087, **191.0558,** 179.0347	517.1343 (-0.4)	319.081, **163.0391**	$C_{25}H_{24}O_{12}$	++	-	++	+	[3]
78.	Acylated flavonoid glycoside	Kaempferol-*O*-(*O*-malonyl hexoside) isomer I *	15.04			535.1085 (-0.5)	**287.0555**	$C_{24}H_{22}O_{14}$					[15], GNPS
79.	Acylated flavonoid glycoside	Kaempferol-*O*-(*O*-acetyl hexoside) isomer I*	15.05 (2.1)	489.1028 (2.1)	**284.0322**, 255.0295, 229.0500, 191.0568			$C_{23}H_{22}O_{12}$	++	+	+	-	[3]
80.	Acylated flavonoid	Kaempferol -*O*-(*O*-malonyl hexoside)	15.08			535.1087 (-0.9)	**287.0554**	$C_{24}H_{22}O_{14}$	++	+	+	-	[15], GNPS

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
	glycoside	isomer II											
81.	Cinnamic acid	Couamric acid*	15.29	163.0396 (2.9)	**119.0499**			$C_9H_8O_3$	+	+	+	+	GNPS, [3]
82.	Phenolic glycoside	(Hydroxy-dimethoxyphenyl) butenone-*O*-hexoside #	15.35	383.1344	221.0817, **203.0712,** 177.0919			$C_{18}H_{24}O_9$	+	+	tr	+++	
83.	Chalcone	trimethoxy dihydro chalcone-*O*-hexoside	15.68			479.1914 (-0.4)	299.1284, 193.0863, **167.0704**, 149.0599	$C_{24}H_{30}O_{10}$	-	+	tr	+++	[31]
84.	Cinnamyl alcohols	Caffeoyl alcohol	15.70			167.0704 (-1.0)	**149.0601**, 131.0495, 121.0651 103.0545	C9H10O3	-	+	-	+++	
85.	Iridoid glycoside	Ligstroside	15.72	523.1817 (0.8)	**315.1238**, 179.0713			$C_{25}H_{32}O_{12}$	-	+	tr	+++	
86.	Cinnamic acid derivative	Di-*O*-caffeoylquinic acid isomer III	15.80	515.118 (2.6)	**353**,335,191,179,173,155,137			$C_{25}H_{24}O_{12}$	+	+	+	+	[3]
87.	Acylated flavonoid	Kaempferol-*O*-(*O*-	15.90	489.1030	327.2175, 309.2068,	491.1188	**287.0556**, 187.0613,	$C_{23}H_{22}O_{12}$	++	+	+	tr	[3]

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
	glycoside	acetylhexoside) isomer II*		(1.7)	285.033, **284.0324**, 255.0293, 89.0240	(-0.7)	109.0285						
88.	Coumarin	hydroxycoumarin*	16.32			163.0391 (-0.7)	148.0512, 135.0445, 119.0493 **107.0494**, 91.0544, 79.0542	$C_9H_6O_3$	+	+	+	+++	[10]
89.	Cinnamyl alcohol	Coniferyl alcohol*	16.34			181.0861 (-0.7)	**163.0755, 105.0701**	$C_{10}H_{12}O_3$	+	tr	tr	+++	[32]
90.	Flavonoid glycoside	Methoxylhydroxyethyl-hydroxylflavane-*O*-hexoside *	16.38	477.1764 (0.4)	**315.1235**, 193.0868, 135.0452			$C_{24}H_{30}O_{10}$	+++	+	++	+++	[33]
91.	Prenylated flavonoids	Preglabridin-*O*-hexoside	16.83	487.1971 (0.6)	343.2134, 325.1452, 243.1230, **203.1078**, 189.0918, 135.0451			$C_{26}H_{32}O_9$	-	tr	tr	+	
92.	Terpene	Loliolide*	16.93			197.1174	179.1071, 161.0965,	$C_{11}H_{16}O_3$	+				[32]

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
	lactone					(-0.8)	**133.1015**, 107.0857						
93.	Cinnamic acid derivative	Methyl caffeate*	17.71	193.0507 (-0.3)	161.0242, **134.0373**			$C_{10}H_{10}O_4$	++	+	+	++	GNPS, [34]
94.	Benzoic acid derivatives	Vanillyl vanillate-*O*-hexoside	17.81	465.1401 (0.2)	**257.0818**, 242.0587			$C_{22}H_{26}O_{11}$	tr	tr	+	+++	[35]
95.	Lignan	Lanicepside A	18.11	537.1974 (0.6)	480.3102, **329.1396**, 255.2326, 193.0870, 149.0607			$C_{36}H_{34}O_{12}$	tr	tr	+	+++	[36]
96.	Aryl-benzofuran	Moracin M*	18.19	241.0508 (-0.5)	199.0400, 157.0296			$C_{14}H_{10}O_4$	+	+	+++	+++	[37]
97.	Flavonoid	Tetrahydroxy flavone *	18.37	285.0404 (0.3)	267.0291, 241.0504, 151.0036, 125.024	287.0554 (-1.2)	**153.0185,** 135.0441	$C_{15}H_{10}O_6$	+	+	+	+	GNPS, [38]
98.	Fatty acid	8-oxononanoate (isomer 1)	18.73			173.1175 (-1.4)	109.1012, 81.0699, **67.0542**	$C_9H_{16}O_3$	++	++	++	+	
99.	Benzoic acid	Hydroxybenzoic	18.77	137.0243	**93.0347**	-	-	$C_7H_6O_3$	+	+	+	+	GNPS

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
		acid		(1.2)									
100.	Megastigmane	Megastigmatrienone *	19.69			191.1435 (1.1)	173.1317, 135.0803, 109.1013, 91.0544, 81.0696, 67.054	$C_{13}H_{18}O$	+	-	+	+	[39]
101.	Cinnamic acid derivative	Salvianolic acid F	19.97	313.0711 (2.3)	**295.0611**, 179.0348			C17H14O6	-	tr	tr	+++	[25]
102.	Flavonoids	methoxy-hydroxyethyl-dihydroxyflavane	21.18	315.1242 (-1.2)	193.068, 175.0768, **135.0452**, 109.0297			$C_{18}H_{20}O_5$	+	tr	-	+++	[40]
103.	Chalcone	Trihydroxy methoxy chalcone	22.11	285.0767 (0.5)	**270.053**, 255.0294, 227.035			$C_{16}H_{14}O_5$	tr	tr	+++	tr	[41]
104.	Chalcone	Trihydroxychalcone	22.39	255.0663 (-0.1)	**240.0426,** 212.0479, 196.0524			$C_{15}H_{12}O_4$	tr	tr	+++	tr	
105.	Sulfated prenylated flavonoid	O-Methylpreglabridin-*O*-sulphate #	22.96	419.117	339.1599, 269.0486, 203.1078, **189.0919**,			$C_{21}H_{24}O_7S$	-	++	+	+++	

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
					177.092, 149.0608								
106.	Prenylated flavonoid	Morusyunnansin F*	23.47	325.1446 (-0.2)	**203.1080**, 189.0920, 177.0923, 135.0451			$C_{20}H_{22}O_4$	tr	+	++	+++	[42]
107.	Prenylated flavonoid	Artocarpesin *	24.40	353.1033 (-0.6)	335.0926, **283.0607**, 219.0663, 149.0245			$C_{20}H_{18}O_6$	-	tr	tr	+++	[43]
108.	Flavonoid	Hexamethoxy flavone	24.74			403.1392 (-1.2)	388.1164, **373.0929**	$C_{21}H_{22}O_8$	+++	+	-	+++	GNPS
109.	Flavonoid	Tetramethoxyflavone	25.02	-		343.1181 (-1.5)	328.0945, **313.0718**, 299.0919, 282.0887	$C_{19}H_{18}O_6$	+++	+	+	+++	GNPS
110.	Glycerolipid	Glyceryl Palmitate	26.62			331.2845 (-0.7)	313.2744, 299.1624, 257.2486, 239.2369, 137.1325, 123.117, 109.1013,	$C_{19}H_{38}O_4$	+++	++	-	-	

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
							95.0855, 85.1013, **71.0856**						
111.	Chalcone	Dihydroxy methoxy chalcone	26.47	269.0819 (0.1)	**254.0583**, 239.0351, 226.0623, 211.0399			$C_{16}H_{14}O_4$	tr	tr	+++	tr	[44]
112.	Flavonoid	Pentamethoxyfl avone	26.41			373.1286 (-1.1)	358.1045, **343.0813**, 325.0705	$C_{20}H_{20}O_7$	+++	-	+	+++	GNPS
113.	Prenylated flavonoid	Mulberrin * (Kuwanon C)	26.49	421.1652 (1.2)	352.0952, **299.1290**, 109.0295			$C_{25}H_{26}O_6$	tr	+	+++	-	[13],
114.	Aryl-benzofuran	Artoindonesiani n O*	26.93	323.1289	265.0525, 201.0935, **135.0457**			$C_{20}H_{20}O_4$	tr	+	+	++	[34]
115.	Glycerolipid	Monolinolenin	27.14			353.2691 (-1.2)	**261.2213**, 243.2104, 187.1477, 173.1334, 149.1333, 135.1168, 121.1013, 107.0855,	$C_{21}H_{36}O_4$	+	+	+	+	GNPS

	Compound Class	name	RT	M-H	MS^2	M+H	MS^2	Formula	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	Reference
							95.0855, 81.0699, 67.0543						
116.	Prenylated flavonoid	Dihydroxymethoxyl-prenylflavan*	27.32	339.1604 (-0.6)	215.1078, **203.1079**, 177.0924, 149.061			$C_{21}H_{24}O_4$	tr	++	+	+++	[10]
117.	Fatty acid amide	*N*-palmitoyl lysine	27.4			385.3426 (-0.4)	345.2034, 310.3109, 292.3016, 268.3, 261.2215, 243.2113, 219.1721, 187.1479, 163.1491, 149.1325, 123.117, 109.101, 95.0856, 81.07, 60.0442	$C_{22}H_{44}N_2O_3$	+	+	+	+	
118.	Prenylated flavonoid	(Iso)bavachin	27.80	323.1287 (0.6)	293.1756, **203.0717, 119.0499**			$C_{20}H_{20}O_4$	+	++	++	+	[45], GNPS

	Compound Class	**name**	**RT**	**M-H**	**MS²**	**M+H**	**MS²**	**Formula**	*M. nigra*	*M. alba*	*M. indica*	*M. macr-oura*	**Reference**
119.	phospholipid	Linoleoyl-sn-glycero-3-phosphocholine	27.87			520.3401 (2.0)	502.3301, 337.2747, 258.1107, 184.0737, 104.1071	$C_{26}H_{50}NO_7P$	+++	-	-	-	GNPS, [7]
120.	Prenylated flavonoid	Prenylapigenin	27.88	337.1082 (-0.3)	**203.0715**, 133.0293			$C_{20}H_{18}O_5$	tr	-	tr	+++	
121.	Aryl-benzofuran	Mulberrofuran U*	28.45	647.2290 (-0.6)	469.1286, **359.0927**, 227.0721, 177.0924			$C_{39}H_{36}O_9$	tr	+++	tr	+++	[46]
122.	Phospholipid	2-palmitoyllysophosphatidylcholine	31.42			496.3402 (-0.8)	478.3294, 313.2743, 184.0736, 104.1072	$C_{24}H_{51}NO_7P$	+++	-	+	-	GNPS, [7]

References

1. Asano, N., et al., *N-containing sugars fromMorus alba and their glycosidase inhibitory activities.* Carbohydrate research, 1994. **259**(2): p. 243-255.
2. Nojima, H., et al., *Antihyperglycemic effects of N-containing sugars from Xanthocercis zambesiaca, Morus bombycis, Aglaonema treubii, and Castanospermum australe in streptozotocin-diabetic mice.* Journal of Natural Products, 1998. **61**(3): p. 397-400.
3. Mena, P., et al., *Phytochemical evaluation of eight white (Morus alba L.) and black (Morus nigra L.) mulberry clones grown in Spain based on UHPLC-ESI-MSn metabolomic profiles.* Food research international, 2016. **89**: p. 1116-1122.
4. Fushiya, S., et al., *New opine type amino acids from a poisonous mushroom, Clitocybe acromelalga.* Tetrahedron, 1996. **52**(3): p. 877-886.
5. Naznin, M., et al., *Metabolite profiling of Nymphaea rubra (Burm. f.) flower extracts using cyclic ion mobility–mass spectrometry and their associated biological activities.* Food Chemistry, 2023. **404**: p. 134544.
6. Winekenstädde, D., et al., *Phytochemical profile of the aerial parts of Sedum sediforme and anti-inflammatory activity of myricitrin.* Natural Product Communications, 2015. **10**(1): p. 1934578X1501000122.
7. Hegazi, N.M., et al., *Molecular networking leveraging the secondary metabolomes space of Halophila stipulaceae (Forsk.) Aschers. and Thalassia hemprichii (Ehrenb. ex Solms) Asch. in tandem with their chemosystematics and antidiabetic potentials.* 2021. **19**(5): p. 279.
8. Ragheb, A.Y., et al., *MS/MS-based molecular networking for mapping the chemical diversity of the pulp and peel extracts from Citrus japonica Thunb.; in vivo evaluation of their anti-inflammatory and anti-ulcer potential.* Scientific African, 2023: p. e01672.
9. Li, J.L., et al., *PPAR-γ agonistic metabolites from the ascidian Herdmania momus.* Journal of natural products, 2012. **75**(12): p. 2082-2087.
10. Doi, K., et al., *Studies on the constituents of the leaves of Morus alba L.* Chemical and pharmaceutical bulletin, 2001. **49**(2): p. 151-153.
11. Kanchanapoom, T., H. Otsuka, and S. Ruchirawat, *Megastigmane glucosides from Equisetum debile and E. diffusum.* Chemical and Pharmaceutical Bulletin, 2007. **55**(8): p. 1277-1280.
12. Kim, S.Y., et al., *Two flavonoids from the leaves of Mours alba induce differentiation of the human promyelocytic leukemia (HL-60) cell line.* 2000. **23**(4): p. 451-455.
13. Zhou, Q.Y.-J., et al., *LC-MS Metabolite Profiling and the Hypoglycemic Activity of Morus alba L. Extracts.* 2022. **27**(17): p. 5360.
14. Sánchez-Salcedo, E.M., et al., *(Poly) phenolic fingerprint and chemometric analysis of white (Morus alba L.) and black (Morus nigra L.) mulberry leaves by using a non-targeted UHPLC–MS approach.* Food chemistry, 2016. **212**: p. 250-255.
15. Ju, W.-T., et al., *Qualitative and quantitative analysis of flavonoids from 12 species of Korean mulberry leaves.* Journal of food science and Technology, 2018. **55**(5): p. 1789-1796.
16. Lu, M., et al., *Comparative chemical profiling of three TCM drugs in the Paeoniaceae family by UPLC-MS/MS combined with chemometric methods.* Biochemical Systematics and Ecology, 2019. **83**: p. 121-129.
17. Piao, S.J., et al., *New stilbene, benzofuran, and coumarin glycosides from Morus alba.* 2009. **92**(3): p. 579-587.
18. Mohammadi, M. and N. Kharazian, *Untargeted metabolomics study and identification of potential biomarkers in the six sections of the genus Stachys L.(Lamiaceae) using HPLC-MQ-API-MS/MS.* Phytochemical Analysis, 2022. **33**(6): p. 915-942.
19. Susanna, D., R.M. Balakrishnan, and J.P. Ettiyappan, *Comprehensive insight into the extract optimization, phytochemical profiling, and biological evaluation of the medicinal plant Nothapodytes foetida.* Biocatalysis and Agricultural Biotechnology, 2022. **42**: p. 102365.
20. Dey, P.K., A. Goswami, and A. Mitra, *A new targeted approach of postharvest accumulation of anthocyanin in fragrant leaves of Melissa officinalis L.* Industrial Crops and Products, 2023. **196**: p. 116479.
21. Zhong, Y.-M., et al., *Rapid analysis and identification of the main constituents in Patrinia scabiosaefolia Fisch. by UPLC/Q-TOF-MS/MS.* Acta Chromatographica, 2017. **29**(2): p. 267-277.
22. Zhang, L.-Q., et al., *Two new flavonoid glycosides isolated from the fruits of Catalpa ovata.* Pharmacognosy Magazine, 2020. **16**(72).

23. Pawlowska, A.M., et al., *Quali-quantitative analyses of flavonoids of Morus nigra L. and Morus alba L.(Moraceae) fruits.* 2008. **56**(9): p. 3377-3380.
24. Cheng, C., et al., *A new isoflavonoid from the rhizomes of Cyperus rotundus.* Asian Journal of Chemistry, 2014. **26**(13): p. 3967-3970.
25. Wang, S., et al., *Integration of LC/MS-based molecular networking and molecular docking allows in-depth annotation and prediction of the metabolome: A study of Salvia miltiorrhiza Bunge.* Industrial Crops and Products, 2022. **186**: p. 115298.
26. Boyer, L., et al., *Lignans and secoiridoids from the root bark of Chionanthus virginicus L.: isolation, identification and HPLC analysis.* Phytochemical Analysis: An International Journal of Plant Chemical and Biochemical Techniques, 2005. **16**(5): p. 375-379.
27. Li, C., et al., *A novel strategy by integrating chemical profiling, molecular networking, chemical isolation, and activity evaluation to target isolation of potential anti-ACE2 candidates in Forsythiae Fructus.* Phytomedicine, 2022. **96**: p. 153888.
28. Matsunami, K., et al., *Absolute configuration of (+)-pinoresinol 4-O-[6 ″-O-galloyl]-β-d-glucopyranoside, macarangiosides E, and F isolated from the leaves of Macaranga tanarius.* Phytochemistry, 2009. **70**(10): p. 1277-1285.
29. Tanaka, Y., et al., *New chromanone and acylphloroglucinol glycosides from the bracts of hops.* 2012. **5**(3): p. 514-518.
30. Hegazi, N.M., et al., *Authentication of saffron spice accessions from its common substitutes via a multiplex approach of UV/VIS fingerprints and UPLC/MS using molecular networking and chemometrics.* 2022. **367**: p. 130739.
31. Tan, H., et al., *Antioxidant and LC-QToF-MS/MS analysis of polyphenols in polar and non-polar extracts from Strobilanthes crispus and Clinacanthus nutans.* International Food Research Journal, 2020. **27**(5).
32. Hunyadi, A., et al., *In vitro anti-diabetic activity and chemical characterization of an apolar fraction of Morus alba leaf water extract.* Phytotherapy Research, 2013. **27**(6): p. 847-851.
33. Han, W.-L., et al., *Three new flavane glucosides from the leaves of Morus wittiorum.* Journal of Asian natural products research, 2010. **12**(8): p. 680-684.
34. Wang, Y., et al., *Chemical components of the fruits of Morus nigra Linn.: Methyl caffeate as a potential anticancer agent by targeting 3-phosphoglycerate dehydrogenase.* Journal of Agricultural and Food Chemistry, 2021. **69**(42): p. 12433-12444.
35. Zhang, A.-L., et al., *Phenolic and Triterpene Glycosides from the Stems of Ilex l itseaefolia.* Journal of natural products, 2005. **68**(10): p. 1531-1535.
36. Wu, R., et al., *Rapid characterization of chemical constituents and metabolites of Qi-Jing-Sheng-Bai granule by using UHPLC–Q-TOF-MS.* Journal of Separation Science, 2018. **41**(9): p. 1960-1972.
37. Rivière, C., et al., *Polyphenols from the stems of Morus alba and their inhibitory activity against nitric oxide production by lipopolysaccharide-activated microglia.* Fitoterapia, 2014. **97**: p. 253-260.
38. Jeong, S.H., et al., *Tyrosinase inhibitory polyphenols from roots of Morus lhou.* Journal of agricultural and food chemistry, 2009. **57**(4): p. 1195-1203.
39. Fadil, H.A.E., et al., *The palliative effect of mulberry leaf and olive leaf ethanolic extracts on hepatic CYP2E1 and caspase-3 immunoexpression and oxidative damage induced by paracetamol in male rats.* Environmental Science and Pollution Research, 2023: p. 1-18.
40. Zhang, H.-R., et al., *Antioxidant flavan derivatives from the leaves of Morus alba.* Phytochemistry Letters, 2019. **29**: p. 84-90.
41. Mativandlela, S.P., et al., *Antimycobacterial flavonoids from the leaf extract of Galenia africana.* Journal of natural products, 2009. **72**(12): p. 2169-2171.
42. Kim, J.Y., et al., *Chemical profiles and hypoglycemic activities of mulberry leaf extracts vary with ethanol concentration.* Food Science and Biotechnology, 2013. **22**: p. 1-5.
43. Kapche, G.D., et al., *Prenylated arylbenzofuran derivatives from Morus mesozygia with antioxidant activity.* Phytochemistry, 2009. **70**(2): p. 216-221.
44. Xia, M., et al., *Characterization of Chemical Constituents of Oxytropis microphylla (Pall.) DC. by Ultra-High-Performance Liquid Chromatography Coupled with Quadrupole-Time-of Flight Tandem Mass Spectrometry.* Separations, 2022. **9**(10): p. 297.

45. Zhang, Y., et al., *A novel strategy integrating gas phase fractionation with staggered mass range and LC-MS/MS molecular network for comprehensive metabolites profiling of Gui Ling Ji in rats.* Journal of Pharmaceutical and Biomedical Analysis, 2023. **222**: p. 115092.
46. Choi, Y.-J., et al., *Metabolomic analysis of Morus cultivar root extracts and their ameliorative effect on testosterone-induced prostate enlargement in Sprague-Dawley rats.* International Journal of Molecular Sciences, 2020. **21**(4): p. 1435.