

БРЗА ИДЕНТИФИКАЦИЈА НА ПИГМЕНТИ ВО ВИНО СО ПРИМЕНА НА MALDI-TOF-MS

Масени спектрограми со MALDI TOF/TOF-MS со примена на матрикс (синапинска киселина SA) за анализа на полифеноли, пигменти, фенолни киселини, димери во црвено вино

SPE Метод (цврсто-фазан реверзна екстракција)

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МЕДИЦИНСКИ ФАКУЛТЕТ, АНАЛИТИЧКИ И БИОХЕМИСКИ ФАКУЛТЕТ-УНИВЕРЗИТЕТ
ВО ПЕЧ, РТЕ ТТК КИ, УНГАРИЈА (СЕЕРУС)

Презентацијата е фокусирана на **идентификација на антоцијани и други пигменти во црвено вино од сортата Вранец** со примена на **ласерска десорпција/јонизација со помош на матрица поврзана со масен детектор со време на прелетување (MALDI-TOF-MS)**.



ВОВЕД

- Во ова истражување беше проучуван **профилот на антоцијани и дериватизирани пигменти во црвени вина од сортата Вранец (*Vitis vinifera* L.)**, произведени во винарската визба Тиквеш, Кавадарци.
- Идентификацијата на соединенијата е извршена со примена на инструменталната техника **ласерска десорпција/јонизација со помош на матрица, поврзана со масен детектор со време на прелетување (MALDI-TOF-MS)**, по извршена **цврсто-фазна екстракција на вината, со Sep-PAK Plus C18 колони**.



ВОВЕД

- **Синапинската киселина** беше користена како матрица.
- Идентификацијата на пикови беше извршена во **позитивен мод**, врз база на таргетна фрагментација на јоните од интерес (нивните M+ сигнали).
- Со квалитативното скенирање на антоцијаните и дериватизираните пигменти со MALDI-TOF-MS, беше потврдено присуството на **глукозиди, ацетилглукозиди и p-кумароилглукозиди** во анализираните вина.



- Нашите вина се правеа од цели и мелени бобинки, а од ширата беа земени примероци во тек на ферментација и мацерација 3, 5, 7, 9, 10, 12, 15, 18 и 20 дена и по завршувањето на малолактичката ферментација.

Whole berries



Crushed berries



Основни поими во масената спектрометрија

- **MS** се базира на создавање јони од аналитот, нивна анализа според вредноста на односот маса/полнеж (m/z) и нивна детекција.
- ✓ **Јони.** Молекулски јон е наелектизирана честичка која има непарен број на електрони и се формира од молекулата (или од електронски неутрална честичка) преку додавање или отстранување на електрон.
- ✓ Фрагментен јон настанува настанува при разложување разложување на друг јон обично означува јон кој настанал со фрагментација на молекулски јон или на честичка како протонирана молекула, депротонирана молекула, јон настанат со одделување на водороден јон, молекула која содржи натриум и сл.
- ✓ Пикови. Во масената спектрометрија, пиковите ги претставуваат јоните кои се формираат во масениот спектрометар.
- **Пикот со најголем интензитет во масениот спектар се нарекува основен пик.**

Експериментален ден



ЕКСПЕРИМЕНТАЛЕН ДЕЛ

ЦЕЛОСНА АНАЛИЗА НА СИТЕ КОМПОНЕНТИ ВО БЕЛИ И ЦРВЕНИ ВИНА

SPE Метод (цврсто-фазан реверзна екстракција)

*Подготовка на примерок:

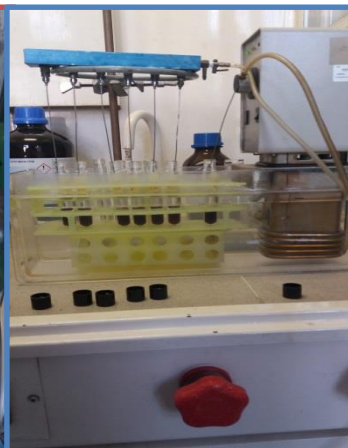
- SPE (Oasis MCX cartridges, 6 ml, 500 mg) (C18 Sep-рак)

a) Кондиционирање: 5 mL метанол и 5mL H₂O

b) Промивање: 5 ml Изопропил алкохол

c) Аплицирање на примерокот: 2 μ L

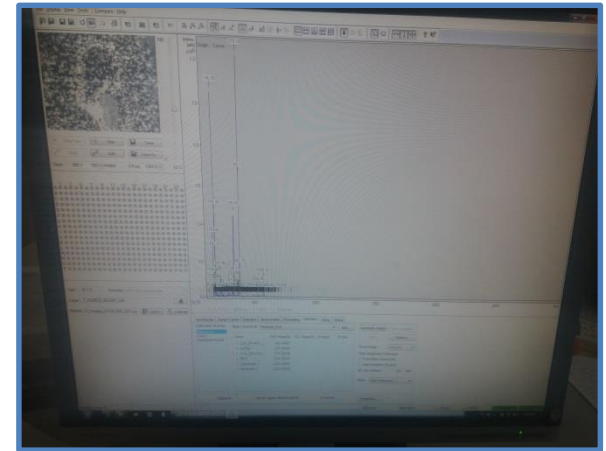
d) 100 μ L во 1.5 mL виала за HPLC анализа



MALDI TOF- MS анализа:

Основен принцип на MALDI TOF- MS:

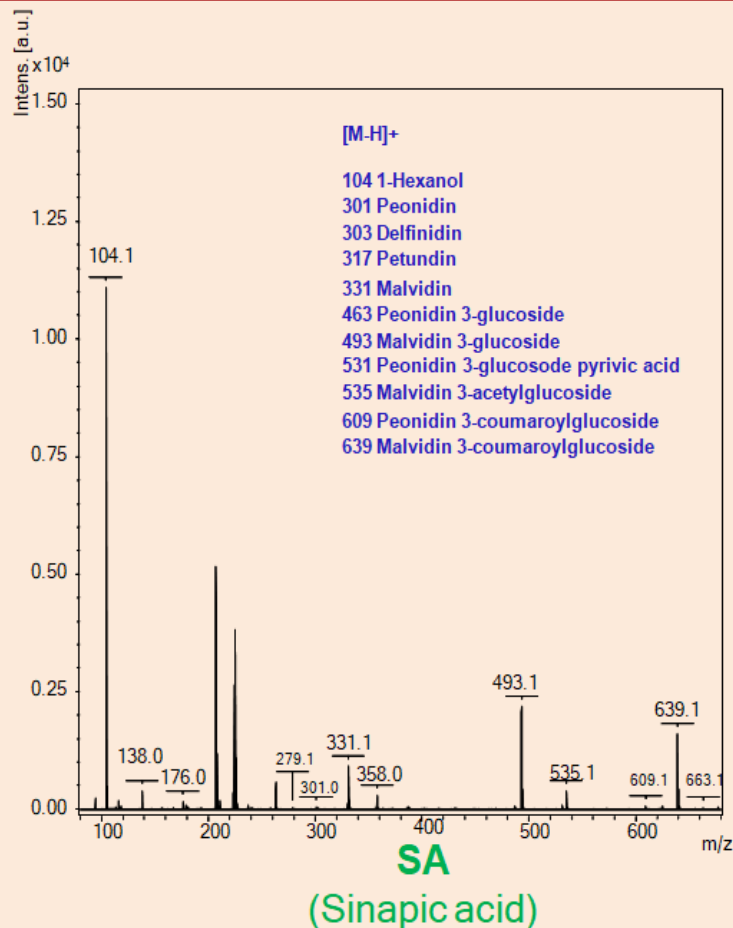
1. Подготовка на анализот со соодветна матрица (која значително го олеснува MALDI анализа создавањето на јони во гасна фаза од големи),
2. Нанесување на смесата на плочка,
3. Се остава неколку минути (2-3 мин) да се исуши растворот.



4. Подготвената плочка со примерокот се внесува во инструментот,
5. Плочката се озрачува со пулсирачки ласер, кој предизвикува разградување на молекулите од анализот и матрицот, и образување на јони,
6. Јоните одат во детекторот каде се гледа нивната маса
7. Се врши идентификација и обработка на податоците.

MALDI-TOF-MS спектри

- **MALDI-TOF-MS** е погодна техника за определување на присуство на големи молекули, со голема точност.
- Се применува за проучување на процијанидин олигомери до хептамери.
- Пиковите се идентификувани, потребна е дополнителна дообработка на секој примерок, одделно.



Антоцијани (црвени пигменти) присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Anthocyanins	Cyanidin	Anthocyanins	287.244	C15H11O6	287.055	287.0556	288.0628	286.0483	322.025
Anthocyanins	Cyanidin 3,5-O-diglucoside	Anthocyanins	611.525	C27H31O16	611.1607	611.1612	612.1685	610.1539	646.1306
Anthocyanins	Cyanidin 3-O-(6''-acetyl-galactoside)	Anthocyanins	491.422	C23H23O12	491.1184	491.119	492.1262	490.1117	526.0884
Anthocyanins	Cyanidin 3-O-(6''-acetyl-glucoside)	Anthocyanins	491.422	C23H23O12	491.1184	491.119	492.1262	490.1117	526.0884
Anthocyanins	Cyanidin 3-O-(6''-caffeoyl-glucoside)	Anthocyanins	611.527	C30H27O14	611.1395	611.1401	612.1474	610.1328	646.1095
Anthocyanins	Cyanidin 3-O-(6''-dioxalyl-glucoside)	Anthocyanins	592.416	C25H20O17	592.0695	592.07	593.0773	591.0628	627.0395
Anthocyanins	Cyanidin 3-O-(6''-malonyl-3''-glucosyl-glucoside)	Anthocyanins	697.572	C30H33O19	697.1611	697.1616	698.1689	696.1543	732.131
Anthocyanins	Cyanidin 3-O-(6''-malonyl-glucoside)	Anthocyanins	535.431	C24H23O14	535.1082	535.1088	536.1161	534.1015	570.0782
Anthocyanins	Cyanidin 3-O-(6''-p-coumaroyl-glucoside)	Anthocyanins	595.528	C30H27O13	595.1446	595.1452	596.1524	594.1379	630.1146
Anthocyanins	Cyanidin 3-O-(6''-succinyl-glucoside)	Anthocyanins	549.458	C25H25O14	549.1239	549.1244	550.1317	548.1172	584.0938
Anthocyanins	Cyanidin 3-O-arabinoside	Anthocyanins	419.359	C20H19O10	419.0973	419.0978	420.1051	418.0905	454.0672
Anthocyanins	Cyanidin 3-O-galactoside	Anthocyanins	449.385	C21H21O11	449.1078	449.1084	450.1157	448.1011	484.0778
Anthocyanins	Cyanidin 3-O-glucoside	Anthocyanins	449.385	C21H21O11	449.1078	449.1084	450.1157	448.1011	484.0778
Anthocyanins	Cyanidin 3-O-glucosyl-rutinoside	Anthocyanins	757.667	C33H41O20	757.2186	757.2191	758.2264	756.2118	792.1885
Anthocyanins	Cyanidin 3-O-rutinoside	Anthocyanins	595.526	C27H31O15	595.1657	595.1663	595.1736	594.159	630.1357
Anthocyanins	Cyanidin 3-O-sambubioside	Anthocyanins	616.952	C26H29ClO15	616.1189	616.1195	617.1268	615.1122	651.0889
Anthocyanins	Cyanidin 3-O-sambubioside 5-O-glucoside	Anthocyanins	743.64	C32H39O20	743.2029	743.2035	744.2107	742.1962	778.1729
Anthocyanins	Cyanidin 3-O-sophoroside	Anthocyanins	611.525	C27H31O16	611.1607	611.1612	612.1685	610.1539	646.1306
Anthocyanins	Cyanidin 3-O-xyloside	Anthocyanins	419.359	C20H19O10	419.0973	419.0978	420.1051	418.0905	454.0672
Anthocyanins	Cyanidin 3-O-xylosyl-rutinoside	Anthocyanins	727.641	C32H39O19	727.208	727.2086	728.2158	726.2013	762.178
Anthocyanins	Delphinidin 3,5-O-diglucoside	Anthocyanins	627.525	C27H31O17	627.1556	627.1561	628.1634	626.1488	662.1255
Anthocyanins	Delphinidin 3-O-(6''-acetyl-galactoside)	Anthocyanins	507.421	C23H23O13	507.1133	507.1139	508.1211	506.1066	542.0833
Anthocyanins	Delphinidin 3-O-(6''-acetyl-glucoside)	Anthocyanins	507.421	C23H23O13	507.1133	507.1139	508.1211	506.1066	542.0833
Anthocyanins	Delphinidin 3-O-(6''-p-coumaroyl-glucoside)	Anthocyanins	611.527	C30H27O14	611.1395	611.1401	612.1474	610.1328	646.1095
Anthocyanins	Delphinidin 3-O-arabinoside	Anthocyanins	435.358	C20H19O11	435.0922	435.0927	436.1	434.0855	470.0621
Anthocyanins	Delphinidin 3-O-feruloyl-glucoside	Anthocyanins	641.553	C31H29O15	641.1501	641.1506	642.1579	640.1434	676.12
Anthocyanins	Delphinidin 3-O-galactoside	Anthocyanins	465.384	C21H21O12	465.1028	465.1033	466.1106	464.096	500.0727
Anthocyanins	Delphinidin 3-O-glucoside	Anthocyanins	465.384	C21H21O12	465.1028	465.1033	466.1106	464.096	500.0727
Anthocyanins	Delphinidin 3-O-glucosyl-glucoside	Anthocyanins	627.525	C27H31O17	627.1556	627.1561	628.1634	626.1488	662.1255

Антоцијани (црвени пигменти) присутни во виното

Anthocyanins	Delphinidin 3-O-rutinoside	Anthocyanins	611.525	C27H31O16	611.1607	611.1612	612.1685	610.1539	646.1306
Anthocyanins	Delphinidin 3-O-sambubioside	Anthocyanins	597.499	C26H29O16	597.145	597.1456	598.1528	596.1383	632.115
Anthocyanins	Delphinidin 3-O-xyloside	Anthocyanins	435.358	C20H19O11	435.0922	435.0927	436.1	434.0855	434.08555
Anthocyanins	Malvidin 3,5-O-diglucoside	Anthocyanins	655.578	C29H35O17	655.1869	655.1874	656.1947	654.1801	690.1568
Anthocyanins	Malvidin 3-O-(6''-acetyl-galactoside)	Anthocyanins	535.474	C25H27O13	535.1446	535.1452	536.1524	534.1379	570.1146
Anthocyanins	Malvidin 3-O-(6''-acetyl-glucoside)	Anthocyanins	535.474	C25H27O13	535.1446	535.1452	536.1524	534.1379	570.1146
Anthocyanins	Malvidin 3-O-(6''-caffeoyl-glucoside)	Anthocyanins	655.58	C32H31O15	655.1657	655.1663	656.1736	654.159	690.1357
Anthocyanins	Malvidin 3-O-(6''-p-coumaroyl-glucoside)	Anthocyanins	639.58	C32H31O14	639.1708	639.1714	640.1787	638.1641	674.1408
Anthocyanins	Malvidin 3-O-arabinoside	Anthocyanins	463.411	C22H23O11	463.1235	463.1234	464.1313	462.1168	498.0934
Anthocyanins	Malvidin 3-O-galactoside	Anthocyanins	528.89	C23H25ClO12	528.1029	528.1035	529.1107	527.0962	563.0729
Anthocyanins	Malvidin 3-O-glucoside	Anthocyanins	493.437	C23H25O12	439.1341	439.1346	434.1419	492.1273	528.104
Anthocyanins	Pelargonidin	Anthocyanins	271.245	C15H11O5	271.0601	271.0606	272.0679	270.0534	306.03
Anthocyanins	Pelargonidin 3,5-O-diglucoside	Anthocyanins	630.979	C27H31ClO15	630.1346	630.1351	631.1424	629.1279	665.1045
Anthocyanins	Pelargonidin 3-O-(6''-malonyl-glucoside)	Anthocyanins	519.432	C24H23O13	519.1133	519.1139	520.1211	518.1066	554.0833
Anthocyanins	Pelargonidin 3-O-(6''-succinyl-glucoside)	Anthocyanins	533.458	C25H25O13	533.129	533.1295	534.1368	532.12222	568.0989
Anthocyanins	Pelargonidin 3-O-arabinoside	Anthocyanins	403.359	C20H19O9	403.1024	403.1029	404.1102	402.0956	438.0723
Anthocyanins	Pelargonidin 3-O-galactoside	Anthocyanins	433.385	C21H21O10	433.1129	433.1135	434.1027	432.1062	468.0829
Anthocyanins	Pelargonidin 3-O-glucoside	Anthocyanins	433.385	C21H21O10	433.1129	433.1135	434.1027	432.1062	468.0829
Anthocyanins	Pelargonidin 3-O-glucosyl-rutinoside	Anthocyanins	741.667	C33H41O19	741.2237	741.2242	742.2315	740.2169	776.1936
Anthocyanins	Pelargonidin 3-O-rutinoside	Anthocyanins	579.527	C27H31O14	579.1708	579.1714	578.1787	578.1641	614.1408
Anthocyanins	Pelargonidin 3-O-sambubioside	Anthocyanins	565.5	C26H29O14	565.1552	565.1557	566.163	564.1485	600.1251
Anthocyanins	Pelargonidin 3-O-sophoroside	Anthocyanins	595.526	C27H31O15	595.1657	595.1663	596.1736	594.459	630.1357
Anthocyanins	Peonidin	Anthocyanins	301.271	C16H13O6	301.0707	301.0712	302.0785	300.0639	336.0406
Anthocyanins	Peonidin 3-O-(6''-acetyl-galactoside)	Anthocyanins	505.448	C24H25O12	505.1341	505.1346	506.1419	504.1273	540.104
Anthocyanins	Peonidin 3-O-(6''-acetyl-glucoside)	Anthocyanins	505.448	C24H25O12	505.1341	505.1346	506.1419	504.1273	540.104
Anthocyanins	Peonidin 3-O-(6''-p-coumaroyl-glucoside)	Anthocyanins	609.554	C31H29O13	609.1603	609.1608	610.1681	608.1535	644.1302
Anthocyanins	Peonidin 3-O-arabinoside	Anthocyanins	449.385	C21H21O11	449.1078	449.1084	450.1157	448.1011	484.0778
Anthocyanins	Peonidin 3-O-galactoside	Anthocyanins	463.411	C22H23O11	463.1235	463.124	464.1313	462.1168	498.0934
Anthocyanins	Peonidin 3-O-glucoside	Anthocyanins	463.411	C22H23O11	463.1235	463.124	464.1313	462.1168	498.0934
Anthocyanins	Peonidin 3-O-rutinoside	Anthocyanins	609.553	C28H33O15	609.1814	609.1819	610.1892	608.1747	644.1513
Anthocyanins	Petunidin 3,5-O-diglucoside	Anthocyanins	641.551	C28H33O17	641.1712	641.1718	642.1791	640.1645	676.1412
Anthocyanins	Petunidin 3-O-(6''-acetyl-galactoside)	Anthocyanins	521.448	C24H25O13	521.129	521.1295	522.1368	520.1222	556.0989
Anthocyanins	Petunidin 3-O-(6''-acetyl-glucoside)	Anthocyanins	521.448	C24H25O13	521.129	521.1295	522.1368	520.1222	556.0989
Anthocyanins	Petunidin 3-O-(6''-p-coumaroyl-glucoside)	Anthocyanins	625.554	C31H29O14	625.1552	625.1557	625.163	624.1485	660.1251
Anthocyanins	Petunidin 3-O-arabinoside	Anthocyanins	449.385	C21H21O11	449.1078	449.1084	450.1157	448.1011	484.0778
Anthocyanins	Petunidin 3-O-galactoside	Anthocyanins	479.411	C22H23O12	479.1184	479.119	480.1262	478.1117	514.0884
Anthocyanins	Petunidin 3-O-glucoside	Anthocyanins	479.411	C22H23O12	479.1184	479.119	480.1262	478.1117	514.0884
Anthocyanins	Petunidin 3-O-rhamnoside	Anthocyanins	447.412	C22H23O10	447.1286	447.1291	448.1364	446.1218	482.0985
Anthocyanins	Petunidin 3-O-rutinoside	Anthocyanins	595.526	C27H31O15	595.1657	595.1663	595.1736	594.159	630.1357
Anthocyanins	Pigment A	Polymeric anthocyanins	609.554	C31H29O13	609.1603	609.1608	610.1681	608.1535	644.1302
Anthocyanins	Pinotin A	Polymeric anthocyanins	625.554	C31H29O14	625.1552	625.1557	626.163	624.1485	660.1251
Anthocyanins	Vitisin A	Polymeric anthocyanins	561.468	C26H25O14	561.1239	561.1244	562.1317	560.1172	596.0938

Халкони и флавоноли присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Chalcones	Butein	Chalcones	272.253	C15H12O5	272.0679	272.0685	273.0757	271.0612	307.0379
Chalcones	Xanthohumol	Alkylchalcones	354.396	C21H22O5	345.1462	345.1467	355.154	353.1394	389.1161
Dihydrochalcones	3-Hydroxyphloretin 2'-O-glucoside	Dihydrochalcones	452.409	C21H24O11	452.1313	452.1319	453.1391	451.1246	487.1013
Dihydrochalcones	3-Hydroxyphloretin 2'-O-xylosyl-glucoside	Dihydrochalcones	584.523	C26H32O15	584.1736	584.1741	585.1814	583.1668	619.1435
Dihydrochalcones	Phloretin	Dihydrochalcones	274.269	C15H14O5	274.0836	274.0841	275.0914	273.0768	309.0535
Dihydrochalcones	Phloretin 2'-O-xylosyl-glucoside	Dihydrochalcones	568.524	C26H32O14	568.1787	568.1792	569.1865	567.1719	603.1486
Dihydrochalcones	Phloridzin	Dihydrochalcones	436.409	C21H24O10	436.1364	436.1369	437.1442	435.1297	471.1063
Dihydroflavonols	Dihydromyricetin 3-O-rhamnoside	Dihydroflavonols	466.392	C21H22O12	466.1106	466.1111	467.1184	465.1038	501.0805
Dihydroflavonols	Dihydroquercetin	Dihydroflavonols	304.252	C15H12O7	304.0578	304.0583	305.0656	303.051	339.0277
Dihydroflavonols	Dihydroquercetin 3-O-rhamnoside	Dihydroflavonols	450.393	C21H22O11	450.1157	450.1162	451.1235	449.1089	485.0856
Flavanols	(+)-Catechin	Catechins	290.268	C15H14O6	290.0785	290.079	291.0863	289.0718	325.0484
Flavanols	(+)-Catechin 3-O-gallate	Catechins	442.372	C22H18O10	442.0894	442.089	443.0973	441.0827	477.0594
Flavanols	(+)-Catechin 3-O-glucose	Catechins	452.409	C21H24O11	452.1313	452.1319	453.1391	451.1246	487.1013
Flavanols	(+)-Gallocatechin	Catechins	306.267	C15H14O7	306.0734	306.074	307.0812	305.0667	341.0434
Flavanols	(+)-Gallocatechin 3-O-gallate	Catechins	458.372	C22H18O11	485.0844	485.0849	459.0922	457.0776	493.0543
Flavanols	(-)-Epicatechin	Catechins	290.268	C15H14O6	290.0785	290.079	291.0863	289.0718	325.0484
Flavanols	(-)-Epicatechin 3-O-gallate	Catechins	442.372	C22H18O10	442.0894	442.09	443.0973	441.0827	447.0594
Flavanols	(-)-Epicatechin-(2a-7)(4a-8)-epicatechin 3-O-galactoside	Proanthocyanidin dimers	706.646	C36H34O15	706.1892	706.1898	707.197	705.1825	741.1592
Flavanols	(-)-Epigallocatechin	Catechins	306.267	C15H14O7	306.0734	306.074	307.0812	305.0667	341.0434
Flavanols	(-)-Epigallocatechin 3-O-gallate	Catechins	458.372	C22H18O11	458.0844	458.0849	459.0922	457.0776	493.0543
Flavanols	Cinnamtannin A2	Proanthocyanidin tetramers	1155.02	C60H50O24	1154.2687	1154.2692	1155.2765	1153.2619	1189.2386
Flavanols	Procyanidin dimer B1	Proanthocyanidin dimers	578.52	C30H26O12	578.1419	578.1424	579.1497	577.1351	613.1118
Flavanols	Procyanidin dimer B2	Proanthocyanidin dimers	578.52	C30H26O12	578.1419	578.1424	579.1497	577.1351	613.1118
Flavanols	Procyanidin dimer B3	Proanthocyanidin dimers	578.52	C30H26O12	578.1419	578.1424	579.1497	577.1351	613.1118
Flavanols	Procyanidin dimer B4	Proanthocyanidin dimers	578.52	C30H26O12	578.1419	578.1424	579.1497	577.1351	613.1118
Flavanols	Procyanidin dimer B5	Proanthocyanidin dimers	578.52	C30H26O12	578.1419	578.1424	579.1497	577.1351	613.1118
Flavanols	Procyanidin dimer B7	Proanthocyanidin dimers	578.52	C30H26O12	578.1419	578.1424	579.1497	577.1351	613.1118
Flavanols	Procyanidin trimer C1	Proanthocyanidin trimers	866.772	C45H38O18	866.2053	866.2058	867.2131	865.1985	901.1752
Flavanols	Procyanidin trimer C2	Proanthocyanidin trimers	866.772	C45H38O18	866.2053	866.2058	867.2131	865.1985	901.1752

Флавоноли присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Flavanols	Procyanidin trimer EEC	Proanthocyanidin trimers	866.772	C45H38O18	866.2053	866.2058	867.2131	865.1985	901.1752
Flavanols	Procyanidin trimer T2	Proanthocyanidin trimers	866.772	C45H38O18	866.2053	866.2058	867.2131	865.1985	901.1752
Flavanols	Prodelphinidin dimer B3	Proanthocyanidin dimers	610.519	C30H26O14	610.1317	610.1323	611.1395	609.125	645.1017
Flavanols	Prodelphinidin trimer C-GC-C	Proanthocyanidin trimers	882	C45H38O19	882.2002	882.2007	883.208	881.1935	917.1701
Flavanols	Prodelphinidin trimer GC-C-C	Proanthocyanidin trimers	882	C45H38O19	882.2002	882.2007	883.208	881.1935	917.1701
Flavanols	Prodelphinidin trimer GC-GC-C	Proanthocyanidin trimers	898	C45H38O20	898.1951	898.1956	899.2029	897.1884	933.165
Flavanols	Theaflavin	Theaflavins	564.494	C29H24O12	564.1262	564.1268	565.1341	563.1195	599.0962
Flavanols	Theaflavin 3'-O-gallate	Theaflavins	716.598	C36H28O16	716.1372	716.1377	717.145	715.1305	715.1071
Flavanols	Theaflavin 3,3'-O-digallate	Theaflavins	868.702	C43H32O20	868.1481	868.1487	869.156	867.1414	903.1181
Flavanols	Theaflavin 3-O-gallate	Theaflavins	716.598	C36H28O16	716.1372	716.1377	717.145	715.1305	751.1071
Flavanones	6-Geranylnaringenin	Alkylflavanones	408.487	C25H28O5	408.1931	408.1937	409.201	407.1864	443.1631
Flavanones	6-Prenylnaringenin	Alkylflavanones	340.37	C20H20O5	340.1305	340.1311	341.1384	339.1238	375.1005
Flavanones	8-Prenylnaringenin	Alkylflavanones	340.37	C20H20O5	340.1305	340.1311	341.1384	339.1238	375.1005
Flavanones	Didymin	Flavanones	594.561	C28H34O14	594.1943	594.1949	595.2021	593.1876	629.1643
Flavanones	Eriocitrin	Flavanones	596.534	C27H32O15	596.1736	596.1741	597.1814	595.1668	631.1435
Flavanones	Eriodictyol	Flavanones	288.252	C15H12O6	288.0628	288.0634	289.0707	287.0561	323.0328
Flavanones	Eriodictyol 7-O-glucoside	Flavanones	450.393	C21H22O11	450.1157	450.1162	451.1235	449.1089	485.0859
Flavanones	Hesperetin	Methoxyflavanones	302.279	C16H14O6	302.0785	302.079	303.0863	301.0718	337.0484
Flavanones	Hesperidin	Flavanones	610.561	C28H34O15	610.1892	610.1898	611.197	609.1825	645.1592
Flavanones	Isoxanthohumol	Alkylmethoxyflavanones	354.396	C21H22O5	354.1462	354.1467	355.154	353.1394	389.1161
Flavanones	Naringenin	Flavanones	272.253	C15H12O5	272.0679	272.0685	273.0757	271.0612	307.0379
Flavanones	Naringenin 7-O-glucoside	Flavanones	434.393	C21H22O10	434.1207	434.1213	435.1286	433.114	469.0907
Flavanones	Naringin	Flavanones	580.535	C27H32O14	580.1787	580.1792	581.1865	579.1719	615.1486
Flavanones	Naringin 4'-O-glucoside	Flavanones	434.393	C21H22O10	434.1207	434.1213	435.1286	433.114	469.0907
Flavanones	Naringin 6'-malonate	Flavanones	666.581	C30H34O17	666.1791	666.1796	667.1869	665.1723	701.149
Flavanones	Narirutin	Flavanones	580.535	C27H32O14	580.1787	580.1792	581.1865	579.1719	615.1486
Flavanones	Narirutin 4'-O-glucoside	Flavanones	742.675	C33H42O19	742.2315	742.232	743.2393	741.2248	777.2014
Flavanones	Neeriocitrin	Flavanones	596.534	C27H32O15	569.1736	569.1741	597.1814	595.1668	631.1435
Flavanones	Neohesperidin	Flavanones	610.561	C28H34O15	610.1892	610.1898	611.197	609.1825	645.1592

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Flavanones	Pinocembrin	Flavanones	256.253	C15H12O4	256.073	256.0736	257.0808	255.0663	291.043
Flavanones	Poncirin	Flavanones	594.561	C28H34O14	594.1943	594.1949	595.2021	593.1876	629.1643
Flavanones	Sakuranetin	Methoxyflavanones	286.279	C16H14O5	286.0836	286.0841	287.0914	285.0768	321.0535
Flavones	5,6-Dihydroxy-7,8,3',4'-tetramethoxyflavone	Methoxyflavones	374.341	C19H18O8	374.0996	374.1002	375.1074	373.0929	409.0696
Flavones	6-Hydroxyluteolin	Flavones	302.236	C15H10O7	302.0421	302.0427	303.0499	301.0354	337.0121
Flavones	6-Hydroxyluteolin 7-O-rhamnoside	Flavones	448.377	C21H20O11	448.1	448.1006	449.1078	447.0933	483.07
Flavones	7,3',4'-Trihydroxyflavone	Flavones	270.237	C15H10O5	270.0523	270.0528	271.0601	296.0455	305.0222
Flavones	7,4'-Dihydroxyflavone	Flavones	254.238	C15H10O4	254.0574	254.0579	255.0652	253.0506	289.0273
Flavones	Apigenin	Flavones	270.237	C15H10O5	270.0523	270.0528	271.0601	269.0455	305.0222
Flavones	Apigenin 6,8-C-arabinoside-C-glucoside	Flavones	564	C26H28O14	564.1474	564.1476	565.1552	563.1406	599.1173
Flavones	Apigenin 6,8-C-galactoside-C-arabinoside	Flavones	564	C26H28O14	564.1474	564.1476	565.1552	563.1406	599.1173
Flavones	Apigenin 6,8-di-C-glucoside	Flavones	594.518	C27H30O15	594.1579	594.1585	595.1657	593.1512	629.1279
Flavones	Apigenin 6-C-glucoside	Flavones	432.378	C21H20O10	432.1051	432.1056	433.1129	431.0984	467.075
Flavones	Apigenin 7-O-(6''-malonyl-apiosyl-glucoside)	Flavones	650.538	C29H30O17	650.1478	650.1483	651.1556	649.141	685.1177
Flavones	Apigenin 7-O-apiosyl-glucoside	Flavones	564.492	C26H28O14	564.1474	564.1479	565.1552	563.1406	599.1173
Flavones	Apigenin 7-O-diglucuronide	Flavones	622.485	C27H26O17	622.1165	622.117	623.1243	621.1097	657.0864
Flavones	Apigenin 7-O-glucoside	Flavones	420.41	C21H24O9	420.1415	420.142	421.1493	419.1348	455.1114
Flavones	Apigenin 7-O-glucuronide	Flavones	446.361	C21H18O11	446.0844	446.0849	447.0922	445.0776	481.0543
Flavones	Baicalein	Flavones	270.237	C15H10O5					
Flavones	Chrysin	Flavones	254.238	C15H10O4					
Flavones	Chrysoeriol 7-O-(6''-malonyl-apiosyl-glucoside)	Methoxyflavones	680.564	C30H32O18					
Flavones	Chrysoeriol 7-O-(6''-malonyl-glucoside)	Methoxyflavones	548.45	C25H24O14					
Flavones	Chrysoeriol 7-O-apiosyl-glucoside	Methoxyflavones	594.518	C27H30O15					
Flavones	Chrysoeriol 7-O-glucoside	Methoxyflavones	462.404	C22H22O11					
Flavones	Cirsilineol	Methoxyflavones	344.315	C18H16O7					
Flavones	Cirsimaritin	Methoxyflavones	314.289	C17H14O6					
Flavones	Diosmin	Methoxyflavones	608.545	C28H32O15					
Flavones	Eupatorin	Methoxyflavones	344.315	C18H16O7					
Flavones	Gardenin B	Methoxyflavones	358.342	C19H18O7					
Flavones	Geraldone	Methoxyflavones	284.263	C16H12O5					
Flavones	Hispidulin	Methoxyflavones	300.263	C16H12O6					
Flavones	Isorhoifolin	Flavones	578.519	C27H30O14					
Flavones	Jaceosidin	Methoxyflavones	330.289	C17H14O7					
Flavones	Luteolin	Flavones	286.236	C15H10O6					
Flavones	Luteolin 6-C-glucoside	Flavones	448.377	C21H20O11					
Flavones	Luteolin 7-O-(2-apiosyl-6-malonyl)-glucoside	Flavones	666.538	C29H30O18					
Flavones	Luteolin 7-O-(2-apiosyl-glucoside)	Flavones	580.492	C26H28O15					
Flavones	Luteolin 7-O-diglucuronide	Flavones	638.484	C27H26O18					
Flavones	Luteolin 7-O-glucoside	Flavones	448.377	C21H20O11					

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Flavones	Luteolin 7-O-glucuronide	Flavones	462.36	C21H18O12					
Flavones	Luteolin 7-O-malonyl-glucoside	Flavones	534.423	C24H22O14					
Flavones	Luteolin 7-O-rutinoside	Flavones	594.518	C27H30O15					
Flavones	Neodiosmin	Methoxyflavones	608.545	C28H32O15					
Flavones	Nepetin	Methoxyflavones	316.262	C16H12O7					
Flavones	Nobiletin	Methoxyflavones	402.395	C21H22O8					
Flavones	Pebrellin	Methoxyflavones	344.315	C18H16O7					
Flavones	Rhoifolin	Flavones	578.519	C27H30O14					
Flavones	Rhoifolin 4'-O-glucoside	Flavones	740.659	C33H40O19					
Flavones	Scutellarein	Flavones	286.236	C15H10O6					
Flavones	Sinensetin	Methoxyflavones	372.369	C20H20O7					
Flavones	Tangeretin	Methoxyflavones	372.369	C20H20O7					
Flavones	Tetramethylscutellarein	Methoxyflavones	342.343	C19H18O6					
Flavonols	3,7-Dimethylquercetin	Methoxyflavonols	330.289	C17H14O7					
Flavonols	3-Methoxynobiletin	Methoxyflavonols	432.421	C22H24O9					
Flavonols	3-Methoxysinensetin	Methoxyflavonols	402.395	C21H22O8					
Flavonols	5,3',4'-Trihydroxy-3-methoxy-6:7-methylenedioxyflavone 4'-O-glucuronide	Methoxyflavonols	520.396	C23H20O14					
Flavonols	5,4'-Dihydroxy-3,3'-dimethoxy-6:7-methylenedioxyflavone 4'-O-glucuronide	Methoxyflavonols	534.423	C24H22O14					
Flavonols	6,8-Dihydroxykaempferol	Flavonols	318.235	C15H10O8					
Flavonols	Galangin	Flavonols	270.237	C15H10O5					
Flavonols	Isorhamnetin	Methoxyflavonols	316.262	C16H12O7					
Flavonols	Isorhamnetin 3-O-galactoside	Methoxyflavonols	478.403	C22H22O12					
Flavonols	Isorhamnetin 3-O-glucoside	Methoxyflavonols	478.403	C22H22O12					
Flavonols	Isorhamnetin 3-O-glucoside 7-O-rhamnoside	Methoxyflavonols	624.544	C28H32O16					
Flavonols	Isorhamnetin 3-O-glucuronide	Methoxyflavonols	492.386	C22H20O13					
Flavonols	Isorhamnetin 3-O-rutinoside	Methoxyflavonols	462.404	C22H22O11					
Flavonols	Isorhamnetin 4'-O-glucoside	Methoxyflavonols	478.403	C22H22O12	478.1106	478.1111	479.1184	477.1038	513.0805
Flavonols	Isorhamnetin 7-O-rhamnoside	Methoxyflavonols	478.403	C22H22O12	478.1106	478.1111	479.1184	477.1038	513.0805
Flavonols	Jaceidin 4'-O-glucuronide	Methoxyflavonols	536.439	C24H24O14					
Flavonols	Kaempferide	Methoxyflavonols	299.255	C16H11O6					
Flavonols	Kaempferol	Flavonols	286.236	C15H10O6					
Flavonols	Kaempferol 3,7,4'-O-triglucoside	Flavonols	772.658	C33H40O21					
Flavonols	Kaempferol 3,7-O-diglucoside	Flavonols	610.518	C27H30O16					
Flavonols	Kaempferol 3-O-(2''-rhamnosyl-6''-acetyl-galactoside) 7-O-rhamnoside	Flavonols	784.669	C34H40O21					
Flavonols	Kaempferol 3-O-(2''-rhamnosyl-galactoside) 7-O-rhamnoside	Flavonols	740.659	C33H40O19					
Flavonols	Kaempferol 3-O-(6''-malonyl-glucoside)	Flavonols	534.423	C24H22O14					
Flavonols	Kaempferol 3-O-(6''-acetyl-galactoside) 7-O-rhamnoside	Flavonols	636.555	C29H32O16					
Flavonols	Kaempferol 3-O-acetyl-glucoside	Flavonols	490.414	C23H22O12					
Flavonols	Kaempferol 3-O-galactoside	Flavonols	448.377	C21H20O11					

Флавоноли присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Flavonols	Kaempferol 3-O-galactoside 7-O-rhamnoside	Flavonols	594.518	C27H30O15					
Flavonols	Kaempferol 3-O-glucoside	Flavonols	448.377	C21H20O11					
Flavonols	Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	756.659	C33H40O20					
Flavonols	Kaempferol 3-O-glucosyl-rhamnosyl-glucoside	Flavonols	756.659	C33H40O20					
Flavonols	Kaempferol 3-O-glucuronide	Flavonols	462.36	C21H18O12					
Flavonols	Kaempferol 3-O-rhamnoside	Flavonols	431.37	C21H19O10					
Flavonols	Kaempferol 3-O-rhamnosyl-rhamnosyl-glucoside	Flavonols	740.659	C33H40O19					
Flavonols	Kaempferol 3-O-rutinoside	Flavonols	594.518	C27H30O15					
Flavonols	Kaempferol 3-O-sophoroside	Flavonols	610.518	C27H30O16					
Flavonols	Kaempferol 3-O-sophoroside 7-O-glucoside	Flavonols	772.658	C33H40O21					
Flavonols	Kaempferol 3-O-xylosyl-glucoside	Flavonols	580.492	C26H28O15					
Flavonols	Kaempferol 3-O-xylosyl-rutinoside	Flavonols	740.659	C33H40O19					
Flavonols	Kaempferol 7-O-glucoside	Flavonols	447.369	C21H19O11					
Flavonols	Methylgalangin	Methoxyflavonols	284.263	C16H12O5					
Flavonols	Morin	Flavonols	302.236	C15H10O7					
Flavonols	Myricetin	Flavonols	318.235	C15H10O8					
Flavonols	Myricetin 3-O-arabinoside	Flavonols	450.35	C20H18O12					
Flavonols	Myricetin 3-O-galactoside	Flavonols	480.376	C21H20O13	480.0898	480.0904	481.0977	479.0831	515.0598
Flavonols	Myricetin 3-O-glucoside	Flavonols	480.376	C21H20O13	480.0898	480.0904	481.0977	479.0831	515.0598
Flavonols	Myricetin 3-O-rhamnoside	Flavonols	464.376	C21H20O12					
Flavonols	Myricetin 3-O-rutinoside	Flavonols	626.517	C27H30O17					
Flavonols	Patuletin 3-O-(2''-feruloylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside	Methoxyflavonols	964.826	C43H48O25					
Flavonols	Patuletin 3-O-glucosyl-(1->6)-[apiosyl(1->2)]-glucoside	Methoxyflavonols	788.657	C33H40O22					
Flavonols	Quercetin	Flavonols	302.236	C15H10O7					
Flavonols	Quercetin 3,4'-O-diglucoside	Flavonols	626.517	C27H30O17					
Flavonols	Quercetin 3-O-(6''-malonyl-glucoside)	Flavonols	550.422	C24H22O15					
Flavonols	Quercetin 3-O-(6''-malonyl-glucoside) 7-O-glucoside	Flavonols	712.563	C30H32O20					
Flavonols	Quercetin 3-O-(6''-acetyl-galactoside) 7-O-rhamnoside	Flavonols	652.554	C29H32O17					
Flavonols	Quercetin 3-O-acetyl-rhamnoside	Flavonols	490.414	C23H22O12					
Flavonols	Quercetin 3-O-arabinoside	Flavonols	434.35	C20H18O11					
Flavonols	Quercetin 3-O-galactoside	Flavonols	464.376	C21H20O12					
Flavonols	Quercetin 3-O-galactoside 7-O-rhamnoside	Flavonols	610.518	C27H30O16					
Flavonols	Quercetin 3-O-glucoside	Flavonols	464.376	C21H20O12					
Flavonols	Quercetin 3-O-glucosyl-rhamnosyl-galactoside	Flavonols	772.658	C33H40O21	772.2057	772.2062	773.2135	771.1989	807.1756
Flavonols	Quercetin 3-O-glucosyl-rhamnosyl-glucoside	Flavonols	772.658	C33H40O21	772.2057	772.2062	773.2135	771.1989	807.1756
Flavonols	Quercetin 3-O-glucosyl-xyloside	Flavonols	596.491	C26H28O16					
Flavonols	Quercetin 3-O-glucuronide	Flavonols	478.36	C21H18O13					
Flavonols	Quercetin 3-O-rhamnoside	Flavonols	448.377	C21H20O11					
Flavonols	Quercetin 3-O-rhamnosyl-galactoside	Flavonols	610.518	C27H30O16					

Флавоноли, изофлавоноиди и лигнани присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Flavonols	Quercetin 3-O-rhamnosyl-rhamnosyl-glucoside	Flavonols	756.659	C33H40O20					
Flavonols	Quercetin 3-O-rutinoside	Flavonols	610.518	C27H30O16					
Flavonols	Quercetin 3-O-sophoroside	Flavonols	626.517	C27H30O17					
Flavonols	Quercetin 3-O-xyloside	Flavonols	434.35	C20H18O11					
Flavonols	Quercetin 3-O-xylosyl-glucuronide	Flavonols	610.474	C26H26O17					
Flavonols	Quercetin 3-O-xylosyl-rutinoside	Flavonols	742.632	C32H38O20					
Flavonols	Quercetin 4'-O-glucoside	Flavonols	464.376	C21H20O12					
Flavonols	Quercetin 7,4'-O-diglucoside	Flavonols	626.517	C27H30O17					
Flavonols	Rhamnetin	Methoxyflavonols	316.262	C16H12O7					
Flavonols	Spinacetin 3-O-(2"-feruloylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside	Methoxyflavonols	978.853	C44H50O25					
Flavonols	Spinacetin 3-O-(2"-p-coumaroylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside	Methoxyflavonols	948.827	C43H48O24					
Flavonols	Spinacetin 3-O-glucosyl-(1->6)-glucoside	Methoxyflavonols	670.57	C29H34O18					
Flavonols	Spinacetin 3-O-glucosyl-(1->6)-[apiosyl(1->2)]-glucoside	Methoxyflavonols	802.684	C34H42O22					
Isoflavonoids	6"-O-Acetyldaidzin	Isoflavones	458.415	C23H22O10					
Isoflavonoids	6"-O-Acetylgenistin	Isoflavones	474.414	C23H22O11					
Isoflavonoids	6"-O-Acetylglycitin	Methoxyisoflavones	488.441	C24H24O11					
Isoflavonoids	6"-O-Malonyldaidzin	Isoflavones	502.424	C24H22O12					
Isoflavonoids	6"-O-Malonylgenistin	Isoflavones	518.424	C24H22O13					
Isoflavonoids	6"-O-Malonylglycitin	Methoxyisoflavones	532.45	C25H24O13					
Isoflavonoids	Biochanin A	Methoxyisoflavones	284.263	C16H12O5					
Isoflavonoids	Daidzein	Isoflavones	254.238	C15H10O4					
Isoflavonoids	Daidzin	Isoflavones	416.378	C21H20O9					
Isoflavonoids	Formononetin	Methoxyisoflavones	268.264	C16H12O4					
Isoflavonoids	Genistein	Isoflavones	270.237	C15H10O5					
Isoflavonoids	Genistin	Isoflavones	432.378	C21H20O10					
Isoflavonoids	Glycitein	Methoxyisoflavones	284.263	C16H12O5					
Isoflavonoids	Glycitin	Methoxyisoflavones	446.404	C22H22O10					
Lignans	1-Acetoxy-pinoresinol	Lignans	416.421	C22H24O8					
Lignans	7-Hydroxymatairesinol	Lignans	374.384	C20H22O7					
Lignans	7-Hydroxysecoisolariciresinol	Lignans	374.471	C22H30O5					
Lignans	7-Oxomatairesinol	Lignans	372.369	C20H20O7					
Lignans	Anhydro-secoisolariciresinol	Lignans	344.402	C20H24O5					
Lignans	Arctigenin	Lignans	372.412	C21H24O6					
Lignans	Conidendrin	Lignans	356.369	C20H20O6					
Lignans	Cyclolariciresinol	Lignans	360.401	C20H24O6					
Lignans	Dimethylmatairesinol	Lignans	386.438	C22H26O6					
Lignans	Episesamin	Lignans	354.353	C20H18O6					
Lignans	Episesaminol	Lignans	370.353	C20H18O7					
Lignans	Isohydroxymatairesinol	Lignans	374.384	C20H22O7					

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Lignans	Isolariciresinol	Lignans	360.401	C20H24O6	360.1567	360.1573	361.1646	359.15	395.1267
Lignans	Lariciresinol	Lignans	360.401	C20H24O6	360.1567	360.1573	361.1646	359.15	395.1267
Lignans	Lariciresinol-sesquillignan	Lignans	556.601	C30H36O10					
Lignans	Matairesinol	Lignans	358.385	C20H22O6					
Lignans	Medioresinol	Lignans	388.411	C21H24O7					
Lignans	Nortrachelogenin	Lignans	374.384	C20H22O7					
Lignans	Pinoresinol	Lignans	358.385	C20H22O6					
Lignans	Secoisolariciresinol	Lignans	365.395	C20H26O6					
Lignans	Secoisolariciresinol-sesquillignan	Lignans	558.617	C30H38O10					
Lignans	Sesamin	Lignans	354.353	C20H18O6					
Lignans	Sesaminol	Lignans	370.353	C20H18O7					
Lignans	Sesamol	Lignans	138.121	C7H6O3					
Lignans	Sesamolin	Lignans	370.353	C20H18O7					
Lignans	Sesamolinol	Lignans	372.369	C20H20O7					
Lignans	Syringaresinol	Lignans	418.437	C22H26O8					
Lignans	Todolactol A	Lignans	376.4	C20H24O7					
Lignans	Trachelogenin	Lignans	388.411	C21H24O7					
Alkylmethoxyphenols	4-Ethylguaiacol	Alkylmethoxyphenols	152.19	C9H12O2					
Alkylmethoxyphenols	4-Vinylguaiacol	Alkylmethoxyphenols	150.174	C9H10O2					
Alkylmethoxyphenols	4-Vinylsyringol	Alkylmethoxyphenols	242.27	C15H14O3					
Alkylphenols	3-Methylcatechol	Alkylphenols	124.137	C7H8O2					
Alkylphenols	4-Ethylcatechol	Alkylphenols	138.164	C8H10O2					
Alkylphenols	4-Ethylphenol	Alkylphenols	122.164	C8H10O					
Alkylphenols	4-Methylcatechol	Alkylphenols	124.137	C7H8O2					
Alkylphenols	4-Vinylphenol	Alkylphenols	120.148	C8H8O					
Alkylphenols	5-Heneicosenylresorcinol	Alkylphenols	402	C27H46O2					
Alkylphenols	5-Heneicosylresorcinol	Alkylphenols	404.669	C27H48O2					
Alkylphenols	5-Heptadecylresorcinol	Alkylphenols	348.562	C23H40O2					
Alkylphenols	5-Nonadecenylresorcinol	Alkylphenols	374	C25H42O2					
Alkylphenols	5-Nonadecylresorcinol	Alkylphenols	376.616	C25H44O2					
Alkylphenols	5-Pentacosenylresorcinol	Alkylphenols	458.759	C31H54O2					
Alkylphenols	5-Pentacosylresorcinol	Alkylphenols	460.775	C31H56O2					
Alkylphenols	5-Pentadecylresorcinol	Alkylphenols	320.509	C21H36O2					
Alkylphenols	5-Tricosenylresorcinol	Alkylphenols	430.706	C29H50O2					
Alkylphenols	5-Tricosylresorcinol	Alkylphenols	432.722	C29H52O2					
Curcuminoids	Bisdemethoxycurcumin	Curcuminoids	308.328	C19H16O4					
Curcuminoids	Curcumin	Curcuminoids	368.38	C21H20O6					
Curcuminoids	Demethoxycurcumin	Curcuminoids	338.354	C20H18O5					

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Furanocoumarins	Bergapten	Furanocoumarins	216.189	C12H8O4					
Furanocoumarins	Isopimpinellin	Furanocoumarins	246.215	C13H10O5					
Furanocoumarins	Psoralen	Furanocoumarins	186.163	C11H6O3					
Furanocoumarins	Xanthotoxin	Furanocoumarins	216.189	C12H8O4					
Hydroxybenzaldehydes	4-Hydroxybenzaldehyde	Hydroxybenzaldehydes	122.121	C7H6O2					
Hydroxybenzaldehydes	Gallic aldehyde	Hydroxybenzaldehydes	154.12	C7H6O4					
Hydroxybenzaldehydes	p-Anisaldehyde	Methoxybenzaldehydes	136.148	C8H8O2					
Hydroxybenzaldehydes	Protocatechuic aldehyde	Hydroxybenzaldehydes	138.121	C7H6O3					
Hydroxybenzaldehydes	Syringaldehyde	Methoxybenzaldehydes	182.173	C9H10O4					
Hydroxybenzaldehydes	Vanillin	Methoxybenzaldehydes	152.147	C8H8O3					
Hydroxybenzoketones	2,3-Dihydroxy-1-guaiacylpropanone	Methoxybenzoketones	212.199	C10H12O5					
Hydroxybenzoketones	3-Methoxyacetophenone	Methoxybenzoketones	150.174	C9H10O2					
Hydroxycinnamaldehydes	Ferulaldehyde	Methoxycinnamaldehydes	178.185	C10H10O3					
Hydroxycinnamaldehydes	Sinapaldehyde	Methoxycinnamaldehydes	208.211	C11H12O4					
Hydroxycoumarins	4-Hydroxycoumarin	Hydroxycoumarins	162.142	C9H6O3					
Hydroxycoumarins	Coumarin	Hydroxycoumarins	146.143	C9H6O2					
Hydroxycoumarins	Esculetin	Hydroxycoumarins	178.141	C9H6O4					
Hydroxycoumarins	Esculin	Hydroxycoumarins	340.282	C15H16O9					
Hydroxycoumarins	Mellein	Hydroxycoumarins	178.185	C10H10O3					
Hydroxycoumarins	Scopoletin	Hydroxycoumarins	192.168	C10H8O4					
Hydroxycoumarins	Umbelliferone	Hydroxycoumarins	162.142	C9H6O3					
Hydroxyphenylpropenes	2-Methoxy-5-prop-1-enylphenol	Methoxyphenylpropenes	164.201	C10H12O2					
Hydroxyphenylpropenes	Acetyl eugenol	Methoxyphenylpropenes	206.238	C12H14O3					
Hydroxyphenylpropenes	Anethole	Methoxyphenylpropenes	148.202	C10H12O					
Hydroxyphenylpropenes	Estragole	Methoxyphenylpropenes	148.202	C10H12O					
Hydroxyphenylpropenes	Eugenol	Methoxyphenylpropenes	164.201	C10H12O2					
Hydroxyphenylpropenes	[6]-Gingerol	Methoxyphenylpropenes	300.434	C17H32O4					
Methoxyphenols	Guaiacol	Methoxyphenols	124.137	C7H8O2					
Naphtoquinones	1,4-Naphtoquinone	Naphtoquinones	158.153	C10H6O2					

Терпени и тирозоли присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Naphtoquinones	Juglone	Naphtoquinones	174.153	C10H6O3					
Other polyphenols	3,4-Dihydroxyphenylglycol	Other polyphenols	170.163	C8H10O4					
Other polyphenols	Arbutin	Other polyphenols	272.251	C12H16O7					
Other polyphenols	Catechol	Other polyphenols	110.111	C6H6O2					
Other polyphenols	Coumestrol	Coumestans	268.221	C15H8O5					
Other polyphenols	Phenol	Other polyphenols	94.1112	C6H6O					
Other polyphenols	Phlorin	Other polyphenols	288.251	C12H16O8					
Other polyphenols	Pyrogallol	Other polyphenols	126.11	C6H6O3					
Phenolic terpenes	Carnosic acid	Phenolic terpenes	332.434	C20H28O4					
Phenolic terpenes	Carnosol	Phenolic terpenes	330.418	C20H26O4					
Phenolic terpenes	Carvacrol	Phenolic terpenes	150.218	C10H14O					
Phenolic terpenes	Epirosmanol	Phenolic terpenes	346.417	C20H26O5					
Phenolic terpenes	Rosmadiol	Phenolic terpenes	344.402	C20H24O5					
Phenolic terpenes	Rosmanol	Phenolic terpenes	346.417	C20H26O5					
Phenolic terpenes	Thymol	Phenolic terpenes	150.218	C10H14O					
Tyrosols	3,4-DHPEA-AC	Tyrosols	196.2	C10H12O4					
Tyrosols	3,4-DHPEA-EA	Tyrosols	378.373	C19H22O8					
Tyrosols	3,4-DHPEA-EDA	Tyrosols	320.337	C17H20O6					
Tyrosols	Demethyloleuropein	Tyrosols	526.487	C24H30O13					
Tyrosols	Hydroxytyrosol	Tyrosols	154.163	C8H10O3					
Tyrosols	Hydroxytyrosol 4-O-glucoside	Tyrosols	316.304	C14H20O8					
Tyrosols	Ligstroside	Tyrosols	524.514	C25H32O12					
Tyrosols	Ligstroside-aglycone	Tyrosols	362.374	C19H22O7					
Tyrosols	Oleoside 11-methylester	Tyrosols	404.366	C17H24O11					
Tyrosols	Oleoside dimethylester	Tyrosols	418.392	C18H26O11					
Tyrosols	Oleuropein	Tyrosols	540.514	C25H32O13					
Tyrosols	Oleuropein-aglycone	Tyrosols	378.373	C19H22O8					
Tyrosols	p-HPEA-AC	Tyrosols	180.201	C10H12O3					
Tyrosols	p-HPEA-EA	Tyrosols	362	C19H22O7					
Tyrosols	p-HPEA-EDA	Tyrosols	304.338	C17H20O5					
Tyrosols	Tyrosol	Tyrosols	138.164	C8H10O2					

Хидрокси бензоеви киселини и нивни деривати присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Hydroxybenzoic acids	2,3-Dihydroxybenzoic acid	Hydroxybenzoic acids	154.12	C7H6O4	154.0261	154.0266	155.0339	153.0193	188.996
Hydroxybenzoic acids	2,4-Dihydroxybenzoic acid	Hydroxybenzoic acids	154.12	C7H6O4	154.0261	154.0266	155.0339	153.0193	188.996
Hydroxybenzoic acids	2,6-Dihydroxybenzoic acid	Hydroxybenzoic acids	154.12	C7H6O4	154.0261	154.0266	155.0339	153.0193	188.996
Hydroxybenzoic acids	2-Hydroxybenzoic acid	Hydroxybenzoic acids	138.121	C7H6O3	138.0311	138.0317	139.039	137.0244	137.0011
Hydroxybenzoic acids	3,5-Dihydroxybenzoic acid	Hydroxybenzoic acids	154.12	C7H6O4					
Hydroxybenzoic acids	3-Hydroxybenzoic acid	Hydroxybenzoic acids	138.121	C7H6O3	138.0311	138.0317	139.039	137.0244	137.0011
Hydroxybenzoic acids	4-Hydroxybenzoic acid	Hydroxybenzoic acids	138.121	C7H6O3	138.0311	138.0317	139.039	137.0244	137.0011
Hydroxybenzoic acids	4-Hydroxybenzoic acid 4-O-glucoside	Hydroxybenzoic acids	300.261	C13H16O8					
Hydroxybenzoic acids	5-O-Galloylquinic acid	Hydroxybenzoic acids	344.271	C14H16O10					
Hydroxybenzoic acids	Benzoic acid	Hydroxybenzoic acids	122.121	C7H6O2					
Hydroxybenzoic acids	Ellagic acid	Hydroxybenzoic acid dimers	302.193	C14H6O8					
Hydroxybenzoic acids	Ellagic acid acetyl-arabinoside	Hydroxybenzoic acid dimers	476.344	C21H16O13					
Hydroxybenzoic acids	Ellagic acid acetyl-xyloside	Hydroxybenzoic acid dimers	476.344	C21H16O13					
Hydroxybenzoic acids	Ellagic acid arabinoside	Hydroxybenzoic acid dimers	434.307	C19H14O12					
Hydroxybenzoic acids	Ellagic acid glucoside	Hydroxybenzoic acid dimers	464.333	C20H16O13					
Hydroxybenzoic acids	Gallic acid	Hydroxybenzoic acids	170.12	C7H6O5					
Hydroxybenzoic acids	Gallic acid 3-O-gallate	Hydroxybenzoic acids	322.224	C14H10O9					
Hydroxybenzoic acids	Gallic acid 4-O-glucoside	Hydroxybenzoic acids	332.26	C13H16O10					
Hydroxybenzoic acids	Gallic acid ethyl ester	Hydroxybenzoic acids	198.173	C9H10O5					
Hydroxybenzoic acids	Galloyl glucose	Hydroxybenzoic acids	332.26	C13H16O10					
Hydroxybenzoic acids	Gentisic acid	Hydroxybenzoic acids	154.12	C7H6O4					
Hydroxybenzoic acids	Lambertianin C	Ellagitannins	2805.9	C123H80O78					
Hydroxybenzoic acids	Protocatechuic acid	Hydroxybenzoic acids	154.12	C7H6O4					
Hydroxybenzoic acids	Protocatechuic acid 4-O-glucoside	Hydroxybenzoic acids	316.261	C13H16O9					
Hydroxybenzoic acids	Punicalagin	Ellagitannins	1084.72	C48H28O30					
Hydroxybenzoic acids	Sanguiin H-6	Ellagitannins	1871.28	C82H54O52					
Hydroxybenzoic acids	Syringic acid	Methoxybenzoic acids	198.173	C9H10O5					
Hydroxybenzoic acids	Valoneic acid dilactone	Hydroxybenzoic acid dimers	470.296	C21H10O13					

Хидрокси циметни киселини и нивни деривати присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula	M*	M	(M+H)+	(M-H)-	(M+CL)-
Hydroxybenzoic acids	Vanillic acid	Methoxybenzoic acids	168.147	C8H8O4					
Hydroxycinnamic acids	1,2'-Disinapoyl-2-feruloylgentiobiose	Methoxycinnamic acids	930.855	C44H50O22					
Hydroxycinnamic acids	1,2,2'-Triferuloylgentiobiose	Methoxycinnamic acids	870.803	C42H46O20					
Hydroxycinnamic acids	1,2,2'-Trisinapoylgentiobiose	Methoxycinnamic acids	960.881	C45H52O23					
Hydroxycinnamic acids	1,2-Diferuloylgentiobiose	Methoxycinnamic acids	694.634	C32H38O17					
Hydroxycinnamic acids	1,2-Disinapoylgentiobiose	Methoxycinnamic acids	754.686	C34H42O19					
Hydroxycinnamic acids	1-Sinapoyl-2,2'-diferuloylgentiobiose	Methoxycinnamic acids	900.829	C43H48O21					
Hydroxycinnamic acids	1-Sinapoyl-2-feruloylgentiobiose	Methoxycinnamic acids	724.66	C33H40O18					
Hydroxycinnamic acids	2,5-di-S-Glutathionyl caftaric acid	Hydroxycinnamic acids	922.844	C33H42N6O21 S2					
Hydroxycinnamic acids	2-S-Glutathionyl caftaric acid	Hydroxycinnamic acids	617.537	C23H27N3O15 S					
Hydroxycinnamic acids	24-Methylcholestanol ferulate	Methoxycinnamic acids	578.865	C38H58O4					
Hydroxycinnamic acids	24-Methylcholesterol ferulate	Methoxycinnamic acids	576.849	C38H56O4	576.4173	576.4179	577.4251	575.4106	611.3873
Hydroxycinnamic acids	24-Methylenecholestanol ferulate	Methoxycinnamic acids	576.849	C38H56O4	576.4173	576.4179	577.4251	575.4106	611.3873
Hydroxycinnamic acids	24-Methylthosterol ferulate	Methoxycinnamic acids	576.849	C38H56O4	576.4173	576.4179	577.4251	575.4106	611.3873
Hydroxycinnamic acids	3,4-Dicaffeoylquinic acid	Hydroxycinnamic acids	516.451	C25H24O12					
Hydroxycinnamic acids	3,4-Diferuloylquinic acid	Methoxycinnamic acids	544.504	C27H28O12					
Hydroxycinnamic acids	3,5-Dicaffeoylquinic acid	Hydroxycinnamic acids	516.451	C25H24O12					
Hydroxycinnamic acids	3,5-Diferuloylquinic acid	Methoxycinnamic acids	544.504	C27H28O12					
Hydroxycinnamic acids	3-Caffeoylquinic acid	Hydroxycinnamic acids	354.309	C16H18O9					
Hydroxycinnamic acids	3-Feruloylquinic acid	Methoxycinnamic acids	368.335	C17H20O9					
Hydroxycinnamic acids	3-p-Coumaroylquinic acid	Hydroxycinnamic acids	338.309	C16H18O8					
Hydroxycinnamic acids	3-Sinapoylquinic acid	Methoxycinnamic acids	398.361	C18H22O10					
Hydroxycinnamic acids	4,5-Dicaffeoylquinic acid	Hydroxycinnamic acids	516.451	C25H24O12					
Hydroxycinnamic acids	4-Caffeoylquinic acid	Hydroxycinnamic acids	354.309	C16H18O9					

Хидроксидни циметни киселини и нивни деривати присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula
Hydroxycinnamic acids	4-Feruloylquinic acid	Methoxycinnamic acids	368.335	C17H20O9
Hydroxycinnamic acids	4-p-Coumaroylquinic acid	Hydroxycinnamic acids	338.309	C16H18O8
Hydroxycinnamic acids	4-Sinapoylquinic acid	Methoxycinnamic acids	398.361	C18H22O10
Hydroxycinnamic acids	5-5'-Dehydrodiferulic acid	Methoxycinnamic acid dimers	386.352	C20H18O8
Hydroxycinnamic acids	5-8'-Benzofuran dehydrodiferulic acid	Methoxycinnamic acid dimers	386.352	C20H18O8
Hydroxycinnamic acids	5-8'-Dehydrodiferulic acid	Methoxycinnamic acid dimers	386.352	C20H18O8
Hydroxycinnamic acids	5-Caffeoylquinic acid	Hydroxycinnamic acids	354.309	C16H18O9
Hydroxycinnamic acids	5-Feruloylquinic acid	Methoxycinnamic acids	368.335	C17H20O9
Hydroxycinnamic acids	5-p-Coumaroylquinic acid	Hydroxycinnamic acids	338.309	C16H18O8
Hydroxycinnamic acids	5-Sinapoylquinic acid	Methoxycinnamic acids	398.361	C18H22O10
Hydroxycinnamic acids	8-O-4'-Dehydrodiferulic acid	Methoxycinnamic acid dimers	386.352	C20H18O8
Hydroxycinnamic acids	Avenanthramide 2c	Hydroxycinnamic acids	315.277	C16H13NO6
Hydroxycinnamic acids	Avenanthramide 2f	Methoxycinnamic acids	329.304	C17H15NO6
Hydroxycinnamic acids	Avenanthramide 2p	Hydroxycinnamic acids	299.278	C16H13NO5
Hydroxycinnamic acids	Avenanthramide K	Hydroxycinnamic acids	315.277	C16H13NO6
Hydroxycinnamic acids	Caffeic acid	Hydroxycinnamic acids	180.157	C9H8O4
Hydroxycinnamic acids	Caffeic acid 4-O-glucoside	Hydroxycinnamic acids	342.298	C15H18O9
Hydroxycinnamic acids	Caffeic acid ethyl ester	Hydroxycinnamic acids	208.211	C11H12O4
Hydroxycinnamic acids	Caffeoyl aspartic acid	Hydroxycinnamic acids	295.245	C13H13NO7
Hydroxycinnamic acids	Caffeoyl glucose	Hydroxycinnamic acids	342.298	C15H18O9
Hydroxycinnamic acids	Caffeoyl tartaric acid	Hydroxycinnamic acids	312.229	C13H12O9
Hydroxycinnamic acids	Chicoric acid	Hydroxycinnamic acids	474.371	C22H18O12
Hydroxycinnamic acids	Cinnamic acid	Hydroxycinnamic acids	148.159	C9H8O2
Hydroxycinnamic acids	Cinnamoyl glucose	Hydroxycinnamic acids	310.299	C15H18O7
Hydroxycinnamic acids	Ferulic acid	Methoxycinnamic acids	194.184	C10H10O4
Hydroxycinnamic acids	Ferulic acid 4-O-glucoside	Methoxycinnamic acids	356.325	C16H20O9
Hydroxycinnamic acids	Feruloyl glucose	Methoxycinnamic acids	356.325	C16H20O9
Hydroxycinnamic acids	Feruloyl tartaric acid	Methoxycinnamic acids	326.256	C14H14O9
Hydroxycinnamic acids	Hydroxycaffeic acid	Hydroxycinnamic acids	196.157	C9H8O5

Хидрокси циметни киселини и Стилбени присутни во виното

Polyphenol Sub-Class	Name	Family	Molecular Weight	Chemical Formula
Hydroxycinnamic acids	Isoferulic acid	Methoxycinnamic acids	194.184	C10H10O4
Hydroxycinnamic acids	m-Coumaric acid	Hydroxycinnamic acids	164.158	C9H8O3
Hydroxycinnamic acids	o-Coumaric acid	Hydroxycinnamic acids	164.158	C9H8O3
Hydroxycinnamic acids	p-Coumaric acid	Hydroxycinnamic acids	164.158	C9H8O3
Hydroxycinnamic acids	p-Coumaric acid 4-O-glucoside	Hydroxycinnamic acids	326.299	C15H18O8
Hydroxycinnamic acids	p-Coumaric acid ethyl ester	Hydroxycinnamic acids	192.211	C11H12O3
Hydroxycinnamic acids	p-Coumaroyl glucose	Hydroxycinnamic acids	326.299	C15H18O8
Hydroxycinnamic acids	p-Coumaroyl glycolic acid	Hydroxycinnamic acids	222.194	C11H10O5
Hydroxycinnamic acids	p-Coumaroyl malic acid	Hydroxycinnamic acids	280.23	C13H12O7
Hydroxycinnamic acids	p-Coumaroyl tartaric acid	Hydroxycinnamic acids	296.23	C13H12O8
Hydroxycinnamic acids	p-Coumaroyl tartaric acid glucosidic ester	Hydroxycinnamic acids	474	
Hydroxycinnamic acids	p-Coumaroyl tyrosine	Hydroxycinnamic acids	327.331	C18H17NO5
Hydroxycinnamic acids	p-Coumaroylquinic acid	Hydroxycinnamic acids	338.309	C16H18O8
Hydroxycinnamic acids	Rosmarinic acid	Hydroxycinnamic acids	360.315	C18H16O8
Hydroxycinnamic acids	Schottenol ferulate	Methoxycinnamic acids	590.875	C39H58O4
Hydroxycinnamic acids	Sinapic acid	Methoxycinnamic acids	224.21	C11H12O5
Hydroxycinnamic acids	Sinapine	Methoxycinnamic acids	310.366	C16H24NO5
Hydroxycinnamic acids	Sitosterol ferulate	Methoxycinnamic acids	590.875	C39H58O4
Hydroxycinnamic acids	Stigmasterol ferulate	Methoxycinnamic acids	592.891	C39H60O4
Hydroxycinnamic acids	Verbascoside	Hydroxycinnamic acids	624.587	C29H36O15
Hydroxyphenylacetic acids	3,4-Dihydroxyphenylacetic acid	Hydroxyphenylacetic acids	168.147	C8H8O4
Hydroxyphenylacetic acids	4-Hydroxyphenylacetic acid	Hydroxyphenylacetic acids	152.147	C8H8O3
Hydroxyphenylacetic acids	Homovanillic acid	Methoxyphenylacetic acids	182.173	C9H10O4
Hydroxyphenylacetic acids	Homoveratric acid	Methoxyphenylacetic acids	196.2	C10H12O4
Hydroxyphenylacetic acids	Methoxyphenylacetic acid	Methoxyphenylacetic acids	166.174	C9H10O3
Hydroxyphenylpropanoic acids	Dihydro-p-coumaric acid	Hydroxyphenylpropanoic acids	166.174	C9H10O3
Hydroxyphenylpropanoic acids	Dihydrocaffeic acid	Hydroxyphenylpropanoic acids	182.173	C9H10O4
Stilbenes	d-Viniferin	Stilbene dimers	454.471	C28H22O6
Stilbenes	e-Viniferin	Stilbene dimers	454.471	C28H22O6
Stilbenes	Pallidol	Stilbene dimers	454.471	C28H22O6
Stilbenes	Piceatannol	Stilbenes	244.243	C14H12O4
Stilbenes	Piceatannol 3-O-glucoside	Stilbenes	406.383	C20H22O9
Stilbenes	Pinosylvin	Stilbenes	212.244	C14H12O2
Stilbenes	Pterostilbene	Stilbenes	256.296	C16H16O3
Stilbenes	Resveratrol	Stilbenes	228.243	C14H12O3
Stilbenes	Resveratrol 3-O-glucoside	Stilbenes	390.384	C20H22O8
Stilbenes	Resveratrol 5-O-glucoside	Stilbenes	390.384	C20H22O8

compound	rt (min)	ESI (-)		ESI (+)		Oxygen candidate biomarkers			Iron candidate biomarkers			
		m/z	error (ppm)	m/z	error (ppm)	pre-MLF ESI+	post-MLF ESI+	pre-MLF ESI-	pre-MLF ESI+	pre-MLF ESI-	post-MLF ESI+	post-MLF ESI-
peonidin 3-(6'-acetyl)-glucoside*	29.20	503.1195	0.00	505.1360	-3.96							
malvidin 3-glucoside ethyl-galocatechin	29.26	-		825.2221	1.94	x						
peonidin 3-glucoside ethyl-catechin	29.69	-		779.2200	-2.44							
malvidin 3-glucoside ethyl-catechin	29.71	-		809.2290	-0.37	x						
malvidin 3-glucoside ethyl-catechin	30.14	-		809.2300	-1.61	x					x	
peonidin 3-glucoside ethyl-catechin	30.40	-		779.2192	-1.41							
malvidin 3-(6'-p-coumaroyl)-glucoside 4-vinylcatechol	31.59	-		771.4451	-4.15	x						
carboxypyranol malvidin 3-(6'-p-coumaroyl)-glucoside	31.66	-		707.1607	0.00	x					x	
cyanidin 3-(6'-p-coumaroyl)-glucoside	31.70	-		595.1440	1.04							
petunidin 3-(6'-p-coumaroyl)-glucoside	31.76	-		625.1552	0.00							
malvidin 3-(6'-p-coumaroyl)-glucoside 4-vinylsyringol	31.90	-		787.1868	1.52	x						x
malvidin 3-(6'-p-coumaroyl)-glucoside*	32.40	637.1559	-0.47	639.1710	-0.26						x	
carboxypyranol petunidin 3-(6'-p-coumaroyl)-glucoside	32.54	-		693.1478	4.04	x						
pyranol malvidin 3-(6'-p-coumaroyl)-glucoside	32.73	-		663.1720	-1.73				x			
peonidin 3-(6'-p-coumaroyl)-glucoside*	32.97	607.1459	0.33	609.1600	0.49							
carboxypyranol malvidin 3-(6'-acetyl)-glucoside	33.66	-		603.1579	3.98				x			
malvidin 3-(6'-p-coumaroyl)-glucoside ethyl-catechin	33.73	-		955.2649	0.63				x			
petunidin 3-glucoside 4-vinylcatechol	33.82	-		611.1395	0.00							
petunidin 3-glucoside-4-vinylphenol	34.76	-		595.1440	1.04	x						
malvidin 3-glucoside 4-vinylcatechol	35.23	-		625.1552	-0.13	x						
xanthilium salt	35.82	-		619.1439	1.13	x						
malvidin 3-glucoside 4-vinylphenol	36.11	-		609.1600	0.49							
malvidin 3-glucoside 4-vinylsyringol	36.24	-		669.1528	-2.09	x						
malvidin 3-glucoside 4-vinylguaiacol	36.39	-		639.1710	-0.26	x						
peonidin 3-(6'-p-coumaroyl)-glucoside 4-vinylphenol	37.50	-		725.1857	1.10	x						
malvidin 3-(6'-p-coumaroyl)-glucoside 4-vinylphenol	37.90	-		755.1954	2.65							
tannins												
proanthocyanidin type B dimer ^a	11.22	593.1240	0.00	-							x	
prodelphinidin type B dimer ^b	11.46	609.124	1.64	611.1380	2.50	x				x		
carboxymethine-flavanol dimers	12.08	635.1430	-3.78	-					x			
procyanidin type B trimer ^c	12.99	865.2121	-4.16	867.2136	-0.58						x	
carboxymethine-flavanol dimers	13.23	635.1455	-0.79	-				x				

Полифенолни компоненти присутни во виното

compound	ESI (-)			ESI (+)		Oxygen candidate biomarkers			Iron candidate biomarkers			
	rt (min)	m/z	error (ppm)	m/z	error (ppm)	pre-MLF ESI+	post-MLF ESI+	pre-MLF ESI-	pre-MLF ESI+	pre-MLF ESI-	post-MLF ESI+	post-MLF ESI-
prodelphinidin type B dimer ^b	13.86	-		611.1395	0.00							
procyanidin type B trimer digallate	14.03	1169.2190	-7.27	-				x				
procyanidin type D ^d	14.05	863.6815	1.62	-				x				
proanthocyanidin type B dimer ^a	14.09	593.1294	1.01	595.1435	1.85							
galocatechin*	14.51	305.0663	1.31	307.0801	3.58							
proanthocyanidin type B dimer ^a	14.90	593.1296	0.67	595.1435	1.85	x						
proanthocyanidin type B dimer ^a	15.22	593.1263	1.18	595.1435	1.85							
procyanidin type B trimer digallate	15.85	1169.2163	-3.59	-				x				
procyanidin type B trimer digallate	16.30	1169.2155	-3.59	-								
proanthocyanidin type B dimer ^a	16.44	593.1334	-4.05	595.1435	1.85							
proanthocyanidin type B tetramer ^a	16.60	1169.2663	-3.59	-								
procyanidin type A dimer ^c	16.83	-		577.1360	-3.47	x						
procyanidin B3*	16.86	577.1346	0.87	579.1500	-0.52	x						
prodelphinidin type B dimer ^b	17.03	-		611.1380	2.50	x						
procyanidin B1*	17.29	577.1343	1.39	579.1480	2.94						x	
procyanidin type B tetramer ^c	17.45	1153.2643	-2.08	-				x				
procyanidin type B trimer ^c	17.55	865.1995	-0.69	867.2136	-0.58							
proanthocyanidin type B dimer ^a	17.74	593.1327	-2.87	595.1440	1.01							
procyanidin type B trimer ^c	18.36	865.1995	-0.69	867.2136	-0.58			x	x			
procyanidin type B trimer digallate	18.45	-		1171.2732	1.54	x						
epigallocatechin*	18.50	305.0666	0.33	307.0809	0.98						x	
procyanidin B4*	18.50	577.1354	-0.52	579.1490	1.21							
catechin*	18.70	289.0710	2.42	291.0865	-0.69							
proanthocyanidin type B dimer ^a	18.87	593.1327	-4.55	595.1435	1.85							
procyanidin type B dimer ^c	19.19	577.1389	1.38	-				x				
proanthocyanidin type B dimer ^a	19.48	593.1235	4.21	595.1440	1.01							
procyanidin B2*	19.92	577.1356	-0.87	579.1506	-1.55		x				x	
procyanidin type B trimer ^c	21.20	865.2030	-4.05	-				x				
proanthocyanidin type B tetramer ^a	21.26	1169.2639	-2.82	-								
procyanidin type B trimer ^c	21.47	865.2004	-4.51	867.2130	0.12			x				
procyanidin type B dimer ^c	21.70	577.1356	-0.87	-								
epicatechin*	22.23	289.0722	-1.73	291.0869	-2.06				x			
(-)-epicatechin gallate*	24.86	441.0448	4.76	-				x				

Полифенолни киселини присутни во виното детерминирани со ESI во позитивен и негативен мод

compound	rt (min)	ESI (-)		ESI (+)		Oxygen candidate biomarkers			Iron candidate biomarkers			
		m/z	error (ppm)	m/z	error (ppm)	pre-MLF ESI+	post-MLF ESI+	pre-MLF ESI-	pre-MLF ESI+	pre-MLF ESI-	post-MLF ESI+	post-MLF ESI-
phenolic acids												
gallic acid*	9.00	169.0139	2.37	-			x					x
protocatechuic acid*	13.90	153.0166	-1.96	155.0340	0.65							
2,6 dihydroxybenzoic*	16.90	153.0195	1.31	-								
vanillic acid*	20.30	167.0351	1.20	-								
syringic acid*	21.90	197.0449	-3.04	-								
benzoic acid*	26.20	-		123.0456	0.00							
ellagic acid*	30.39	300.9977	4.32	303.0135	0.00			x				
ethyl gallate*	23.04	197.0460	2.54	199.0595	3.01							
ethyl caffate*	32.10	207.0635	3.86	209.0800	3.96							
cinnamics												
cis-caftaric acid	14.37	311.0409	-1.48	335.0378	-1.49							
trans-caftaric acid*	15.50	311.0395	-0.32	335.0378	-1.49	x						
cis-coutaric acid	17.46	295.0495	-2.03	-								
trans-coutaric acid	18.23	295.0495	-2.03	-				x				
cis-fertaric acid	19.46	325.0561	1.23	-								
trans-fertaric acid	19.76	325.0561	0.31	-								
caffeic acid*	20.70	179.0326	2.23	163.0390	-0.61	x		x				
rosmarinic acid	21.46	359.0962	3.06							x		
vanillic acid*	21.66	-		169.0498	-1.77	x						
dicafeoyl tartaric	22.01	-		474.0871	0.00	x						
p-cumaric acid*	24.30	163.0383	4.91	147.0446	0.00							
ethyl p-coumarate	35.21	191.0714	0.37	193.0859	0.00			x				

Органски киселини присутни во виното детерминирани со ESI во позитивен и негативен мод

compound	rt (min)	ESI (-)		ESI (+)		Oxygen candidate biomarkers			Iron candidate biomarkers			
		m/z	error (ppm)	m/z	error (ppm)	pre-MLF ESI+	post-MLF ESI+	pre-MLF ESI-	pre-MLF ESI+	pre-MLF ESI-	post-MLF ESI+	post-MLF ESI-
organic acids												
glucuronic acid*	1.27	193.0349	2.59	-								
mucic acid*	1.30	209.0299	1.91	-								
glutamic acid*	1.30	-		148.0594	0.00							
L-saccharopine*	1.35	275.1235	0.00	277.1369	0.00							
L-threonic acid*	1.40	135.0296	2.22	-								
2-keto-d-gluconic acid*	1.40	193.0341	6.73	-								
D-gluconic acid*	1.40	195.0488	6.15	-				x				
galacturonic acid*	1.40	193.0336	4.14	217.0325	-2.76							
5-keto-D-gluconic acid*	1.44	193.0340	2.07	-								
tartaric acid*	1.52	149.0051	0.67	-								
glycolic acid*	1.60	75.0086	2.67	-								
glyceric acid*	1.60	105.0190	2.85	-								
dehydroascorbic acid*	1.74	173.0093	-0.58	-								
pyruvic acid*	1.78	97.0088	0.00	-								
malic acid*	2.01	133.0119	0.00	322.9698	0.00			x				
ascorbic acid*	2.37	175.0224	0.00	-								
2-ketoglutaric acid*	2.40	145.0139	2.07	-								
lactic acid*	2.50	89.0236	-2.25	-					x			
maleic acid*	2.90	115.0025	1.74	-								
ribonic acid or hydroxy-glutaric acid*	3.16	147.0149	2.44	-								
citric acid*	3.92	191.0166	0.52	-								
propionic acid*	4.63	73.0295	0.00									
succinic acid*	4.95	117.0177	-3.42	-		x		x				
citramalic acid*	5.17	147.0278	0.68	-								
pantothenic acid*	14.30	218.1029	0.00	220.1176	0.00							
adipic acid*	15.50	145.0502	2.76	169.0457	2.37							
m-hydroxybenzoic acid*	17.50	-		139.0391	0.00							
isopropyl malic acid*	18.13	175.0604	4.57	199.0584	-1.51							
abscisic acid*	31.30	263.1292	-1.14	247.1335	-0.40					x		

Амино киселини, амини, јаглехидрати присутни во виното детерминирани со ESI во позитивен и негативен мод

compound	rt (min)	ESI (-)		ESI (+)		Oxygen candidate biomarkers			Iron candidate biomarkers			
		m/z	error (ppm)	m/z	error (ppm)	pre-MLF ESI+	post-MLF ESI+	pre-MLF ESI-	pre-MLF ESI+	pre-MLF ESI-	post-MLF ESI+	post-MLF ESI-
amino acids												
histidine*	1.20	-		156.0765	1.92	x						
arginine*	1.20	-		175.1197	-4.00	x						
glycine*	1.20	-		203.0529	0.00							
alanine*	1.30	-		90.0559	-3.33							
homoserine*	1.30	-		120.0650	4.16							
threonine*	1.30	-		120.0650	4.16							
L-glutamine*	1.30	-		130.0400	0.77							
proline*	1.59	114.0548	1.75	116.0705	0.50		x					
valine*	2.20	-		72.0809	0.00							
norvaline*	2.20	-		72.0809	0.00							
leucine*	4.96	130.0871	3.07	86.0964	0.00			x				
phenylalanine*	11.50	164.0683	4.33	120.0753	0.00							
tryptophan*	16.00	203.0818	3.94	188.0710	0.00	x						
amines												
spermidine*	1.02	-		146.1650	-1.20							
agmatine*	1.03	-		131.1291	0.00	x						
L-cystathionine*	1.22	221.0600	0.90	-								
propylamine*	1.35	-		60.0805	4.99							
gaba*	1.40	-		104.0713	-3.84							
uridine*	7.01	243.0623	-2.05	-								
3 indolelactic acid*	24.60	204.0661	2.45	206.0812	0.00							
tryptophol*	26.20	-		162.0913	-3.08							
carbohydrates												
hexol*	1.24	179.0556	-2.79	-								
hexol*	1.40	-		183.0877	-3.82							
pentose*	1.40	149.0448	4.70	-								
hexose*	1.40	179.0556	-2.79	203.0554	-3.94							
hexose*	1.45	-		203.0554	0.00							
trehalose*	1.50	341.1078	-3.22	325.1114	0.00							
quinic acid*	1.61	191.0706	-4.20	-								
raffinose*	2.14	503.1609	1.59	-		x			x			

ЗАКЛУЧОЦИ

ПРИМЕНА НА НАПРЕДНА АНАЛИТИЧКА ТЕХНИКА:

- MALDI-TOF-MS - идентификација и структурна карактеризација на големи и непознати молекули
 - **Вината од сортата Вранец, со (интензивна темно-црвена и рубин боја) и имаат највисока содржина на:**
 - ✓ Антоцијани,
 - ✓ Витисински пираноантоцијани
 - ✓ Хидроксифенилни пираноантоцијани
 - ✓ Фенолни киселини
 - ✓ Стилбени
 - ❖ Во текот на зреењето:
 - ✓ Антоцијаните се намалуваат (конверзија на антоцијаните во дериватизирани пигменти, како резултат на полимеризација, преципитација)
- Познавањето и примената на овие и дополнителни истражувања, се основа за воведување на високо-квалитетни врвни вина и нови брендови, произведени без недостатоци и аномалии, кои ќе бидат конкурентни на европските и светски саеми, натпревари и пазари.

БЛАГОДАРНОСТ

МЕДИЦИНСКИ ФАКУЛТЕТ, АНАЛИТИЧКИ И БИОХЕМИСКИ
ФАКУЛТЕТ-УНИВЕРЗИТЕТ ВО ПЕЧ, РТЕ ТТК КИ, УНГАРИЈА (СЕЕРУС)



CEEPUS CII-HU-0010-03-0809
“Learning and Teaching Bioanalysis”

Рецс СЕЕРУС канцеларија
Скорје СЕЕРУС канцеларија

Универзитет „Гоце Делчев“ – Штип, Штип СЕЕРУС канцеларија



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