**Supplemental material**

# Ovicidal Effect on *Haemonchus contortus* of Extract Partitions Shrubby Plants of the Tropical Dry Forest and Potentially Active Compounds Identification by UHPLC-Q/Orbitrap/MS/MS

**Néstor Jaime Romero-Jola [1], Jaime Andrés Cubides-Cárdenas [2], Natalia Escobar [3]* and Mario J. Simirgiotis [4]**

[1] Departamento de Sanidad Animal, Facultad de Medicina Veterinaria y Zootecnia, Universidad del Tolima, Ibagué 730001, Colombia; njromeroj@ut.edu.co
[2] Grupo de Investigación e Innovación en Salud y Bienestar Animal, Laboratorio de Salud Animal y Microbiología Pecuaria, Centro de Investigación Tibaitatá, Agrosavia, Mosquera 250047, Colombia
[3] Grupo de Investigación Área Verde, Universidad de Cundinamarca, Fusagasugá 252211, Colombia
[4] Instituto de Farmacia, Facultad de Ciencias, Universidad Austral de Chile, Campus Isla Teja, Valdivia 5090000, Chile
* Correspondence: nataescobar@ucundinamarca.edu.co

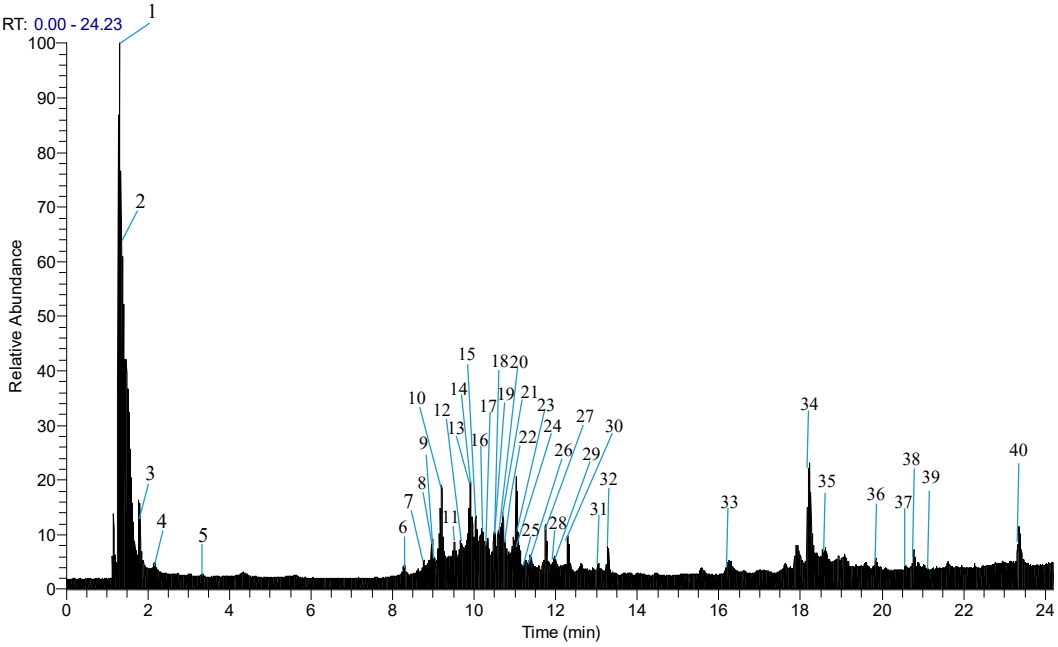



**Figure S1.** UHPLC TIC (total ion current) chromatogram of *Pithecellobium dulce* hydroethanolic extract partition

**Table S1.** Tentative identification of compounds in the hydroethanolic extract partition of *Pithecellobium dulce* by UHPLC-Q/Orbitrap/MS/ MS

| Peak | Tentative identification | [M-H]$^-$ | Retention time (min.) | Theoretical mass (*m*/*z*) | Measured mass (*m*/*z*) | Accuracy (ppm) | Other Ions (m/z)* | UV |
|---|---|---|---|---|---|---|---|---|
| 1 | Arabinonic acid | $C_5H_9O_6$ | 1.30 | 165.0399 | 165.0400 | -0,6 | 147.0295; 119.0343 | 251; 271; |
| 2 | 3-Deoxyhexonic acid | $C_6H_{11}O_6$ | 1.38 | 179.0556 | 179.0558 | -1,1 | 143.0350; 119.0341 | 268 |
| 3 | Citric acid | $C_6H_7O_7$ | 1.80 | 191.0192 | 191.0195 | -1,6 | 111.0080 | 204; 302 |
| 4 | 2,3,5,4′-Tetrahydroxystilbene 2-O-β-D-glucoside | $C_{20}H_{21}O_9$ | 2.16 | 405.1186 | 405.1172 | 3,5 | 243.0624; 179.0557; 227.0672; 163.0608 | 248; 271; 295 |
| 5 | Protocatechuic acid 4-hexoside | $C_{13}H_{15}O_9$ | 4.35 | 315.0716 | 315.0723 | -2,2 | 153.0221; 152.0165; 137.0237 | 200; 277; 300 |
| 6 | Bis(ethoxycarbonyloxymethyl) undecanedioate | $C_{19}H_{31}O_{10}$ | 8.30 | 419.1917 | 419.1926 | -2,1 | 355.0672 | 216; 276; 315 |
| 7 | Calaliukiuenoside | $C_{20}H_{35}O_{11}$ | 8.77 | 451.2179 | 451.2188 | -2,0 | 341.1093; 179.0557 | 233; 278; 315 |
| 8 | Ebuloside | $C_{21}H_{31}O_{10}$ | 8.98 | 443.1917 | 443.1925 | -1,8 | 179.0555 | 268; 323 |
| 9 | Coumaroylquinic acid | $C_{16}H_{17}O_8$ | 9.09 | 337.0923 | 337.0931 | -2,4 | 163.0396; 119.0495; 191.0557; 173.0449 | 236; 280; 349 |
| 10 | 7-Oxo-tridecanedioic acid | $C_{13}H_{21}O_5$ | 9.20 | 257.1394 | 257.1394 | 0,0 | 213.1493 | 234; 283; 357 |
| 11 | Unknow | $C_{15}H_{26}O_9N$ | 9.51 | 364.1608 | 364.1617 | -2,5 | --- | 239; 280; 356 |
| 12 | Ferulic acid-O-hexoside derivative | $C_{19}H_{29}O_{12}$ | 9.67 | 449.1659 | 449.1669 | -2,2 | 355.1038 | 239; 278; 320 |
| 13 | Hidroxydioxotridecenoic acid | $C_{13}H_{19}O_5$ | 9.90 | 255.1232 | 255.1238 | -2,4 | 211.1337; 153.0916 | 240; 278; 320 |
| 14 | Dihydroxyhexaoxohexacosanoic acid | $C_{26}H_{39}O_{10}$ | 9.90 | 511.2543 | 511.2550 | -1,4 | 465.1440; 323.1114; 255.1238; 153.0914; 211.1337 | 240; 278; 320 |
| 15 | Tetrahidroxitetraoxoicosanoic acid | $C_{20}H_{31}O_{10}$ | 10.05 | 431.1917 | 431.1926 | -2,1 | 401.1461; 387.2020 | 238; 278; 328 |
| 16 | Heptahydroxyoxohexadecanoic acid | $C_{16}H_{29}O_{10}$ | 10.20 | 381.1761 | 381.1770 | -2,4 | 351.1301 | 243; 278; 331 |
| 17 | Tetrahydroxytryoxoicosanoic acid | $C_{20}H_{33}O_{10}$ | 10.33 | 433.2074 | 433.2083 | -2,1 | 387.2028 | 241; 280; 360 |
| 18 | Unknow | $C_{10}H_{19}O_{14}$ | 10.50 | 363.0775 | 363.0759 | 4,4 | 345.1559; 144.0084; 150.0316 | 245; 276; 360 |
| 19 | Verbasoside | $C_{20}H_{29}O_{12}$ | 10.52 | 461.1659 | 461.1666 | -1,5 | 445.1718; 447.1521 | 245; 277; 360 |
| 20 | Nepetaside | $C_{16}H_{25}O_8$ | 10.59 | 345.1549 | 345.1559 | -2,9 | 327.1452; 163.0607; 183.1024; 301.1669; 289.1657; 206.0820 | 242; 280; 320 |
| 21 | Tetrahydroxytetraoxoicosanoic acid | $C_{20}H_{31}O_{10}$ | 10.71 | 431.1917 | 431.1926 | -2,1 | 389.2185; 417.2127 | 245; 271; 320 |
| 22 | Rutin | $C_{30}H_{25}O_{14}$ | 10.74 | 609.1482 | 609.1457 | 4,1 | 300.0280; 137.0248; 149.0238 | 245; 276; 323 |
| 23 | Ethyl-morroniside | $C_{19}H_{29}O_{11}$ | 11.04 | 433.1710 | 433.1719 | -2,1 | 375.1665; 179.0557; 255.1236; 417.1762 | 242; 280; 331 |
| 24 | Phloretin-di-C-hexoside | $C_{27}H_{33}O_{15}$ | 11.11 | 597.1819 | 597.1823 | -0,7 | 477.1406; 435.1284; 507.1497 | 280; 331; 368 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 25 | Quercetin-3-glucoside | $C_{21}H_{19}O_{12}$ | 11.26 | 463.0877 | 463.0886 | -1,9 | 179.0556; 163.0610; 151.0395 | 280; 331; 349 |
| 26 | Vicenin-2 | $C_{27}H_{29}O_{15}$ | 11.39 | 593.1506 | 593.1510 | -0,7 | 117.0380; 533.1301; 159.0295; 163.0401 | 282; 331; 368 |
| 27 | Luteolin 7-O-glucoside | $C_{21}H_{19}O_{11}$ | 11.76 | 447.0927 | 447.0936 | -2,0 | 151.0031; 255.0301; 107.0131 | 283; 368; 379 |
| 28 | Tridecahydroxypentadecanoic acid | $C_{15}H_{29}O_{15}$ | 11.90 | 449.1506 | 449.1490 | 3,6 | --- | 283; 368 |
| 29 | Picrocrocin | $C_{16}H_{25}O_{7}$ | 11.97 | 329.1600 | 329.1609 | -2,7 | 299.1502; 179.0555; 167.1078; 163.0607 | 283; 368 |
| 30 | Kaempferol-3-O- rhamnoside | $C_{21}H_{19}O_{10}$ | 12.30 | 431.0978 | 431.0987 | -2,1 | 255.0299; 285.0420 (kaempferol), 227.0344 | 283; 368; 379 |
| 31 | Unknow | $C_{15}H_{21}O_{8}N_{6}$ | 13.05 | 413.1501 | 413.1490 | 2,7 | --- | 275 |
| 32 | Trihydroxyhexaoxohexacosanoic acid | $C_{26}H_{39}O_{11}$ | 13.29 | 527.2492 | 527.2499 | -1,3 | 509.2393 | 225; 284 |
| 33 | Unknow | $C_{25}H_{37}O_{10}$ | 16.26 | 497.2387 | 497.2393 | -1,2 | 479.2284; 327.2177 | 283 |
| 34 | Dihydroxyhexaoxohexacosanoic acid | $C_{26}H_{39}O_{10}$ | 18.21 | 511.2543 | 511.2548 | -1,0 | 493.2444; 417.2129; 311.1686; 183.1025 | 283 |
| 35 | 2,5,8,11,14,17-Hexaoxanonadecane-3,19-diol | $C_{13}H_{27}O_{8}$ | 18.60 | 311.1706 | 311.1688 | 5,8 | 251.1481 | 283 |
| 36 | Andropanoside | $C_{26}H_{39}O_{9}$ | 19.85 | 495.2594 | 495.2602 | -1,6 | 333.2075; 317.2134; 399.2376 | 282; 328 |
| 37 | Gingerol | $C_{17}H_{25}O_{4}$ | 20.57 | 293.1753 | 293.1760 | -2,4 | 279.1636; 193.0863; 151.0756 | 280; 326 |
| 38 | Phenethyl butyrate | $C_{12}H_{15}O_{2}$ | 20.78 | 191.1072 | 191.1075 | -1,6 | --- | 278 |
| 39 | Methoxy heptaetilenglicol | $C_{15}H_{31}O_{8}$ | 21.28 | 339.2019 | 339.2002 | 5,0 | 309,2070, 325,1844 | 276 |
| 40 | Pentadecatetraenoic acid | $C_{15}H_{21}O_{2}$ | 23.38 | 233.1542 | 233.1546 | -1,7 | --- | 278 |

* Daughter ions

**Compounds identified in *Pithecellobium dulce***

*Glycosylated flavonoids.*

Five glycosylated flavonoids corresponding to peaks 24, 25, 26, 27, and 30 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 24 with a [M-H]-ion *m/z* 597.1823 and daughter ions at *m/z* 477.1406, 435.1284 and 507.1497 were identified as phloretin-di-C-hexoside [1]. Peak 25 with a [M-H]-ion *m/z* 463.0886 and daughter ions at *m/z* 179.0556, 163.0610 and 151.0395 were identified as quercetin-3-glucoside [2]. Peak 26 with a [M-H]-ion *m/z* 463.0886 and daughter ions at *m/z* 593.1510 and daughter ions at *m/z* 117.0380, 533.1301, 159.0295 and 163.0401 were identified as vicenin-2 [3]. Peak 27 with a [M-H]-ion *m/z* 447.0936 and daughter ions at *m/z* 151.0031, 255.0301 and 107.0131 were identified as luteolin 7-O-glucoside [4]. Peak 30 with a [M-H]-ion *m/z* 431.0987 *and* daughter ions at *m/z* and 255.0299, 285.0420 (aglycone kaempferol), 227.0344, and 227.0344 were identified as kaempferol-3-O- rhamnoside [5].

*Flavonoids.*

One flavonoid we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 22 with a [M-H]-ion *m/z* 609.1457 and daughter ions at *m/z* 300.0280, 137.0248, and 149.0238 were identified as rutin [6]**.**

*Fatty acids*

Eleven fatty acids corresponding to peaks 10, 13, 14, 15, 16, 17, 21, 28, 32, 34 and 40 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 10 with a [M-H]-ion *m/z* 257.1394 and daughter ion at *m/z* 213.1493 were identified as 7-oxo-tridecanedioic acid. Peak 13 with a [M-H]-ion *m/z* 255.1238 and daughter ions at *m/z* 211.1337 and 153.0916 were identified as hidroxydioxotridecenoic acid. Peak 14 with a [M-H]-ion *m/z* 511.2550 and daughter ions at *m/z* 465.1440, 323.1114, 255.1238, 153.0914 and 211.1337 were identified as dihydroxyhexaoxohexacosanoic acid. Peak 15 with a [M-H]-ion *m/z* 431.1926 and daughter ions at *m/z* 401.1461 and 387.2020 were identified as tetrahidroxitetraoxoicosanoic acid. Peak 16 with a [M-H]-ion *m/z* 381.1770 and daughter ion at *m/z* 351.1301 were identified as heptahydroxyoxohexadeanoic acid. Peak 17 with a [M-H]-ion *m/z* 433.2083 and daughter ion at *m/z* 387.2028 were identified as tetrahydroxytryoxoicosanoic acid. Peak 21 with a [M-H]-ion *m/z* 431.1926 and daughter ions at *m/z* 389.2185 and 417.2127 were identified as tetrahydroxytetraoxoicosanoic acid. Peak 28 with a [M-H]-ion *m/z* 449.1490 we identified as tridecahydroxypentadecanoic acid. Peak 32 with a [M-H]-ion *m/z* 527.2499 and daughter ion at *m/z* 509.2393 were identified as trihydroxyhexaoxohexacosanoic acid. Peak 34 with a [M-H]-ion *m/z* 511.2548 and daughter ions at *m/z* 493.2444, 417.2129, 311.1686, and 183.1025 were identified as dihydroxyhexaoxohexacosanoic acid. Peak 40 with a [M-H]-ion *m/z* 233.1546 we identified as pentadecatetraenoic acid.

*Organooxygen compounds (Carbohydrates, carbohydrate conjugates, alcohols and polyols)*

Six organooxygen compounds corresponding to peaks 1, 9, 12, 19, 23, 29 and 35 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 1 with a [M-H]-ion *m/z* 165.0400 and daughter ions at *m/z* 147.0295 and 119.0343were identified as arabinonic acid. Peak 9 with a [M-H]-ion *m/* 337.0931 and daughter ions at *m/z* 163.0396, 119.0495, 191.0557 and 173.0449 were identified as coumaroylquinic acid [7] . Peak 12 with a [M-H]-ion *m/* 449.1669 and daughter ions at *m/z* 355.1038 were identified as ferulic acid-O-hexoside derivative [8]. Peak 19 with a [M-H]-ion *m/* 461.1666 and daughter ions at *m/z* 445.1718 and 447.1521 were identified as verbasoside [9]. Peak 23 with a [M-H]-ion *m/* 433.1719 and daughter ions at *m/z* 375.1665, 179.0557, 255.1236 and 417.1762 were identified as ethyl-morroniside[10]. Peak 29 with a [M-H]-ion *m/* 329.1609 and daughter ions at *m/z* 299.1502, 179.0555, 167.1078 and 163.0607 were identified as picrocrocin [11]. Peak 35 with a [M-H]-ion *m/* 311.1688 and daughter ion at *m/z* 251.1481 were identified as 2,5,8,11,14,17-Hexaoxanonadecane-3,19-diol.

*Terpene glycosides*

Two terpene glycosides compounds corresponding to peaks 20 and 36 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 20 with a [M-H]-ion *m/z* 345.1559 and daughter ions at *m/z* 327.1452, 163.0607, 183.1024, 301.1669, 289.1657 and 206.0820 were identified as nepetaside [12]. Peak 36 with a [M-H]-ion *m/z* 495.2602 and daughter ions at *m/z* 333.2075, 317.2134 and 399.2376 were identified as andropanoside [13].

*Hydroxy acids and derivatives*

One hydroxy acid compound corresponding to peak 2 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 2 with a [M-H]-ion *m/z* 179.0558 and daughter ions at *m/z* 143.0350 and 119.0341were identified as 3-Deoxyhexonic acid.

*Carboxylic acids and derivatives*

One carboxylic acid compound corresponding to peak 3 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 3 with a [M-H]-ion *m/z* 191.0195 and daughter ion at *m/z* 111.0080 were identified as citric acid [14].

*Stilbenes*

One stilbene compound corresponding to peak 4 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 4 with a [M-H]-ion *m/z* 405.1172 and daughter ion at *m/z* 243.0624, 179.0557, 227.0672 and 163.0608 were identified as 2,3,5,4′-Tetrahydroxystilbene 2-O-β-D-glucoside [15].

*Benzene and substituted derivatives*

One benzene compound corresponding to peak 5 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 5 with a [M-H]-ion *m/z* 315.0723 and daughter ion at *m/z* 153.0221, 152.0165 and 137.0237 were identified as protocatechuic acid 4-hexoside ( ). Peak 38 with a [M-H]-ion *m/z* 191.1075 we identified as phenethyl butyrate [16].

*Double esters*

One double ester compound corresponding to peak we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 7 with a [M-H]-ion *m/z* 419.1926 and daughter ion at *m/z* 355.0672 were identified as bis(ethoxycarbonyloxymethyl) undecanedioate.

*Carbohydrates and carbohydrate-derivatives*

One carbohydrate compound corresponding to peak 7 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 7 with a [M-H]-ion *m/z* 451.2188 and daughter ion at *m/z* 341.1093 and 179.0557 were identified as calaliukiuenoside [17].

*Terpenoids*

One terpenoid compound corresponding to peak 8 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 7 with a [M-H]-ion *m/z* 443.1925 and daughter ion at *m/z* 179.0555 were identified as ebuloside [18].

*Phenols*

One phenol compound corresponding to peak 37 we identified using UHPLC-Q/Orbitrap/MS/MS. Peak 37 with a [M-H]-ion *m/z* 293.1760 and daughter ions at *m/z* 279.1636, 193.0863 and 151.0756 were identified as gingerol [19].

*Glycol alcohols*

One glycol compound corresponding to peak 39 we identified using UHPLC- Q/Orbitrap/MS/MS. Peak 39 with a [M-H]-ion m/z 339.2002 and daughter ions at m/z 309.2070 and 325.1844 were identified as methoxy heptaetilenglicol.

*Unknown compounds*

Peaks 11, 18, 31 and 33 with a [M-H] -ions m/z 364.1617, 363.0759, 413.1490, and 497.2393 respectively correspond to unknown compounds.

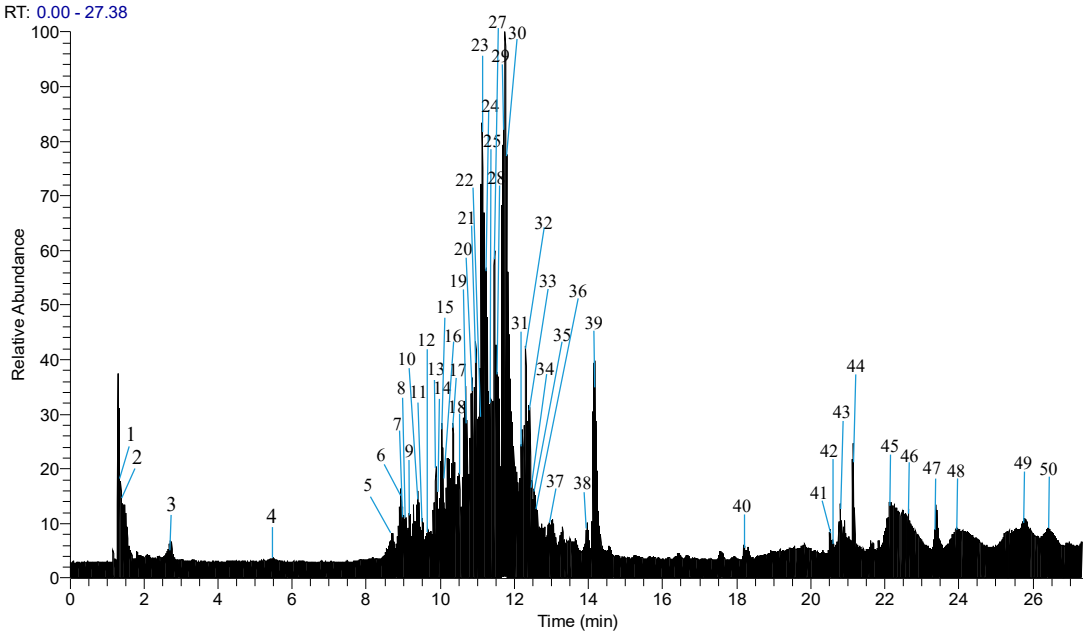



Figure S2. UHPLC TIC (total ion current) chromatogram of *Leucaena leucocephala* ethyl acetate extract partition.

**Table S2.** Tentative identification of compounds in the ethyl acetate extract partition of *Leucaena leucocephala* by UHPLC-Q/Orbitrap/MS/ MS

| Peak | Tentative identification | [M-H]$^-$ | Retention time (min.) | Theoretical mass (*m/z*) | Measured mass (*m/z*) | Accuracy (ppm) | MS ions m/z)* | UV |
|---|---|---|---|---|---|---|---|---|
| 1 | Quinic acid | $C_7H_{11}O_6$ | 1.34 | 191.0556 | 191.0560 | -2,1 | 173.0452; 117.0189 | 269 |
| 2 | Syringaldehyde Syringate O derivate quinic acid. | $C_{18}H_{17}O_9$ | 1.36 | 377.0873 | 377.0861 | 3,2 | 347.0755; 349.0911 | 203; 269 |
| 3 | Gallic acid | $C_7H_5O_5$ | 2.70 | 169.0137 | 169.0139 | -1,2 | 125.0238 | 212; 271 |
| 4 | Gallocatechin isomer | $C_{15}H_{13}O_7$ | 5.49 | 305.0661 | 305.0669 | -2,6 | 153.0188; 109.0287 | 202; 263; 283 |
| 5 | Hydroxytrioxopentadecenoic acid | $C_{15}H_{21}O_6$ | 8.72 | 297.1338 | 297.1347 | -3,0 | 233.1446; 125.0236; 177.0201 | 234; 268 |
| 6 | Pentahidroxitetraoxoicosanoic acid | $C_{20}H_{31}O_{11}$ | 8.92 | 447.1866 | 447.1875 | -2,0 | 437.1589; 401.1821 | 235 |
| 7 | Hydroxytrioxotetradecanoic acid | $C_{14}H_{21}O_6$ | 9.01 | 285.1338 | 285.1346 | -2,8 | 257.1037 | 236 |
| 8 | Gallocatechin | $C_{15}H_{13}O_7$ | 9.18 | 305.0661 | 305.0670 | -3,0 | 125.0238; 137.0238; 109.0287; 139.0394; 179.0344; 167.0345 | 207; 227; 274 |
| 9 | Digalloyl glucose | $C_{20}H_{19}O_{14}$ | 9.29 | 483.0775 | 483.0783 | -1,7 | 125.0237; 169.0139; 211.0242; 271.0459; 313.0553 | 222; 278 |
| 10 | Caffeoylquinic acid | $C_{16}H_{17}O_9$ | 9.41 | 353.0873 | 353.0882 | -2,5 | 191.0559; 161.0239; 179.0344; 135.0444 | 234; 286; 325 |
| 11 | Gallic acid derivative I | $C_{17}H_{23}O_{11}$ | 9.52 | 403.1240 | 403.1251 | -2,7 | 125.0238; 177.0177; 109.0288 | 232; 279 |
| 12 | Myrsinoside A | $C_{20}H_{21}O_{12}$ | 9.67 | 453.1033 | 453.1043 | -2,2 | 123.0443; 125.0237; 167.0345; 135.0446; 313.0570 | 232; 279 |
| 13 | Trihydroxypentaoxooctadecanoic acid | $C_{18}H_{25}O_{10}$ | 9.89 | 401.1448 | 401.1458 | -2,5 | 343.1398 | 232; 278 |
| 14 | Unknow | $C_{24}H_{21}O_8$ | 9.92 | 437.1236 | 437.1224 | 2,7 | 401.1457; 179.0346 | 230; 279; 268 |
| 15 | Tetrahydroxytetraoxoicosanoic acid | $C_{20}H_{31}O_{10}$ | 10.05 | 431.1917 | 431.1925 | -1,9 | 385.1886; | 232; 275 |
| 16 | Catechin | $C_{15}H_{13}O_6$ | 10.23 | 289.0712 | 289.0720 | -2,8 | 125.0237; 137.0238; 151.0395; 165.0553; 271.0610 | 203; 227; 279 |
| 17 | Gallocatechin gallate | $C_{22}H_{17}O_{11}$ | 10.34 | 457.0771 | 457.0780 | -2,0 | 125.0237; 169.0135; 335.0775; 289.0718;; 137.0238; 109.0287 | 207; 276; 368 |
| 18 | Isorhamnetin -O-glucoside | $C_{22}H_{21}O_{12}$ | 10.50 | 477.1033 | 477.1043 | -2,1 | 151.0025; 163.0396; 300.0284 | 228; 274; 354 |
| 19 | Myricetin-3-O-hexoside | $C_{21}H_{19}O_{13}$ | 10.70 | 479.0826 | 479.0833 | -1,5 | 125.0235; 287.0190; 151.0033; 316.0230 (myricetin) | 208; 225; 264; 354 |
| 20 | Myricetin 3-arabinoside | $C_{20}H_{17}O_{12}$ | 10.85 | 449.0720 | 449.0729 | -2,0 | 125.0239; 271.0246; 316.0220 (myricetin) | 209; 226; 265; 354 |
| 21 | Rutin | $C_{27}H_{29}O_{16}^-$ | 10.96 | 609.1499 | 609.1459 | 6,6 | 151.0032; 300.0278; 137.0238 | 203; 257; 354 |
| 22 | Myricetin-3-arabinoside isomer | $C_{20}H_{17}O_{12}$ | 11.02 | 449.0720 | 449.0730 | -2,2 | 125.0238; 271.0247; 300.0286; 301.0359 | 201; 228; 269; 354 |
| 23 | Myricetin 3-O-rhamnoside (myricitrin) | $C_{21}H_{19}O_{12}$ | 11.13 | 463.0877 | 463.0884 | -1,5 | 271.0249; 316.0226; 178.9982; 151.0031; | 208; 262; 351 |
| 24 | Quercetin-3-O-glucuronide | $C_{21}H_{17}O_{13}$ | 11.26 | 477.0669 | 477.0677 | -1,7 | 301.0355; 151.0031; 285.0404; 177.0192; 125.0237 | 203; 257; 290; 353 |
| 25 | Epicatechin gallate | $C_{22}H_{17}O_{10}$ | 11.36 | 441.0822 | 441.0831 | -2,0 | 125.0237; 289.0718; 137.0239; | 202; 224; 272; 337 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 26 | Kaempferol-3-O-glucorhamnoside | $C_{27}H_{29}O_{15}$ | 11.39 | 593.1506 | 593.1509 | -0,5 | 285.0403; 125.0237; 255.0302 | 202; 224; 270; 341 |
| 27 | Quercetin 3-O-arabinoside | $C_{20}H_{17}O_{11}$ | 11.46 | 433.0771 | 433.0780 | -2,1 | 151.0031; 271.0246; 178.9982; 300.0277; 301.0356 (aglycone quercetin) | 202; 257; 286; 354 |
| 28 | Cyanidin-3-arabinoside | $C_{20}H_{19}O_{10}$ | 11.52 | 419.0978 | 419.0981 | -0,7 | 285.0414 | 202; 225; 267; 353 |
| 29 | Quercetin 3-O-pentoside | $C_{20}H_{17}O_{11}$ | 11.68 | 433.0771 | 433.0779 | -1,8 | 151.0031; 178.9982; 271.0247; 301.0351 (aglycone quercetin),; 300.0275 | 202; 257; 353 |
| 30 | Quercetin 3-O-Rhamnoside | $C_{21}H_{19}O_{11}$ | 11.76 | 447.0927 | 447.0935 | -1,8 | 151.0031; 178.9982; 255.0296; 300.0276; 301.0351 (aglycone quercetin) | 210; 257; 349 |
| 31 | Kaempferol-3-*O*-pentoside | $C_{20}H_{17}O_{10}$ | 12.21 | 417.0822 | 417.0832 | -2,4 | 255.0297; 285.0402 (aglycone kaempferol) | 228; 270; 337 |
| 32 | Luteolin-7- rhamnoside | $C_{21}H_{19}O_{10}$ | 12.31 | 431.0978 | 431.0988 | -2,3 | 255.0298; 285.0399 (aglycone luteolin); 109.0286 | 227; 266 |
| 33 | Myricetin | $C_{15}H_9O_8$ | 12.41 | 317.0297 | 317.0305 | -2,5 | 151.0031; 137.0237; | 226; 270; 368 |
| 34 | Kaempferol dimethylether Hexoside | $C_{22}H_{19}O_{12}$ | 12.54 | 475.0877 | 475.0886 | -1,9 | 125.0237; 151.0034; 137.0237; 461.0713 | 272; 367 |
| 35 | Quercetin galloyl pentoside | $C_{27}H_{21}O_{15}$ | 12.58 | 585.0880 | 585.0886 | -1,0 | 301.0356; 151.0033; 433.0781 | 271; 268 |
| 36 | Cinchonain I | $C_{24}H_{19}O_9$ | 12.65 | 451.1029 | 451.1041 | -2,7 | 341.0677; 315.0885; 287.0563; 217.0138 | 271; 368 |
| 37 | Apigenin 7-O-glucuronide | $C_{21}H_{17}O_{11}$ | 12.92 | 445.0771 | 445.0782 | -2,5 | 225.0556; 269.0453; 175.0242 | 273; 368 |
| 38 | Luteolin | $C_{15}H_9O_6$ | 13.96 | 285.0399 | 285.0408 | -3,2 | 133.0287 | 195; 221; 284 |
| 39 | Quercetin | $C_{15}H_9O_7$ | 14.17 | 301.0348 | 301.0356 | -2,7 | 107.0131; 151.0031 | 195; 220; 284; 368 |
| 40 | Quercetin pentoside derivate | $C_{24}H_{23}O_{11}$ | 18.20 | 487.1240 | 487.1248 | -1,6 | 255.0293; 271.0255; 300.0276 (aglycone quercetin) | 282 |
| 41 | Gingerol | $C_{17}H_{25}O_4$ | 20.59 | 293.1753 | 293.1761 | -2,7 | 279.1637 | 278 |
| 42 | 2,5,8,11,14,17-Hexaoxanonadecane-3,19-diol | $C_{13}H_{27}O_8$ | 20.61 | 311.1706 | 311.1690 | 5,1 | 251.1481 | 278 |
| 43 | Phenethyl butyrate | $C_{12}H_{15}O_2$ | 20.80 | 191.1072 | 191.1075 | -1,6 | 121.0653 | 278 |
| 44 | Unknow | $C_{30}H_{53}O_{14}N_6$ | 21.13 | 721.3620 | 721.3639 | -2,6 | 711.3353; | 278; 325 |
| 45 | Unknow | $C_{28}H_{43}O_{11}$ | 22.17 | 555.2805 | 555.2846 | -7,4 | --- | 275 |
| 46 | Octahidroxyheptacosapentaenoic acid | $C_{27}H_{43}O_{10}$ | 22.64 | 527.2856 | 527.2864 | -1,5 | --- | 275 |
| 47 | Pentadecatetraenoic acid | $C_{15}H_{21}O_2$ | 23.38 | 233.1542 | 233.1547 | -2,1 | 183.0119 | 278 |
| 48 | Heptaethylene glycol | $C_{14}H_{29}O_8$ | 23.94 | 325.1862 | 325.1847 | 4,6 | 309.1744; 251.1482 | 275 |
| 49 | Unknow | $C_{30}H_{41}O_{11}$ | 25.82 | 577.2649 | 577.2690 | -7,1 | --- | 275 |
| 50 | Dihydroxypentadecatetraenoic acid | $C_{15}H_{21}O_4$ | 26.39 | 265.1440 | 265.1482 | -15,8 | 249.1494; 223.0968 | 275 |

* Daughter ions

**Compounds identified in *Leucaena leucocephala***

*Flavonoid glycosides*

Sixteen glycosylated flavonoids corresponding to peaks 18, 19, 20, 21, 22, 23, 24, 26, 27,28, 29, 30, 31, 32, 34 and 40 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 18 with a [M-H]-ion *m/z* 477.1043 and daughter ions at *m/z* 151.0025, 163.0396 and 300.0284 were identified as isorhamnetin-O-glucoside [20]. Peak 19 with a [M-H]-ion *m/z* 479.0833 and daughter ions at *m/z* 125.0235, 287.0190, 151.0033 and 316.0230 (aglycone myricetin) were identified as myricetin-3-O-hexoside [21]. Peak 20 with a [M-H]-ion *m/z* 449.0729 and daughter ions at *m/z* 125.0239, 271.0246, 316.0220 (aglycone myricetin) were identified as myricetin 3-arabinoside [22]. Peak 21 with a [M-H]-ion *m/z* 609.1459 and daughter ions at *m/z* 151.0032, 300.0278 and 137.0238 were identified as rutin [23]. Peak 22 with a [M-H]-ion *m/z* 449.0730 and daughter ions at *m/z* 125.0238, 271.0247, 300.0286 and 301.0359 were identified as myricetin-3-arabinoside isomer [22]. Peak 23 with a [M-H]-ion *m/z* 463.0884 and daughter ions at *m/z* 271.0249, 316.0226, 178.9982 and 151.0031 were identified as myricetin 3-O-rhamnoside (myricitrin) [24]. Peak 24 with a [M-H]-ion *m/z* 477.0677 and daughter ions at *m/z* 301.0355, 151.0031, 285.0404, 177.0192 and 125.0237 were identified as quercetin-3-O-glucuronide [25]. Peak 26 with a [M-H]-ion *m/z* 593.1509 and daughter ions at *m/z* 285.0403, 125.0237 and 255.0302 were identified as kaempferol-3-O-glucorhamnoside [26]. Peak 27 with a [M-H]-ion *m/z* 433.0780 and daughter ions at *m/z* 151.0031, 271.0246, 178.9982, 300.0277 and 301.0356 (aglycone quercetin) were identified as quercetin 3-O-arabinoside [27] . Peak 28 with a [M-H]-ion *m/z* 419.0981 and daughter ion at *m/z* 285.0414 were identified as cyanidin-3-arabinoside [28]. Peak 29 with a [M-H]-ion *m/z* 433.0779 and daughter ions at *m/z* 151.0031, 178.9982, 271.0247, 301.0351 (aglycone quercetin) and 300.0275 were identified as quercetin 3-O-pentoside [29]. Peak 30 with a [M-H]-ion *m/z* 447.0935 and daughter ions at *m/z* 151.0031, 178.9982, 255.0296, 300.0276 and 301.0351 (aglycone quercetin) were identified as quercetin 3-O-rhamnoside [30]. Peak 31 with a [M-H]-ion *m/z* 417.0832 and daughter ions at *m/z* 255.0297 and 285.0402 (aglycone kaempferol) were identified as kaempferol-3-*O*-pentoside [31]. Peak 32 with a [M-H]-ion *m/z* 431.0988 and daughter ions at *m/z* 255.0298, 285.0399 (aglycone luteolin) and 109.0286 and were identified as luteolin-7-rhamnoside [32]. Peak 34 with a [M-H]-ion *m/z* 475.0886 and daughter ions at *m/z* 125.0237; 151.0034, 137.0237 and 461.0713 were identified as kaempferol dimethylether hexoside [33]. Peak 40 with a [M-H]-ion *m/z* 487.1248 and daughter ions at *m/z* 255.0293, 271.0255 and 300.0276 (aglycone quercetin) were identified as quercetin pentoside derivative.

*Flavonoids*

Nine flavonoids corresponding to peaks 4, 8, 16, 17, 25, 33, 36, 38 and 39 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 4 with a [M-H]-ion *m/z* 305.0669 and daughter ions at *m/z* 153.0188 and 109.0287 were identified as gallocatechin isomer [34]. Peak 8 with a [M-H]-ion *m/z* 305.0670 and daughter ions at *m/z* 125.0238, 137.0238, 109.0287, 139.0394, 179.0344 and 167.0345 were identified as gallocatechin [35]. Peak 16 with a [M-H]-ion *m/z* 289.0720 and daughter ions at *m/z* 125.0237, 137.0238, 151.0395, 165.0553, 271. 0610 were identified as catechin [36]. Peak 17 with a [M-H]-ion *m/z* 457.0780 and daughter ions at *m/z* 125.0237, 169.0135, 335.0775, 289.0718, 137.0238 and 109.0287 were identified as gallocatechin gallate [34]. Peak 25 with a [M-H]-ion *m/z* 441.0831 and daughter ions at *m/z* 125.0237, 289.0718 and 137.0239 were identified as epicatechin gallate [34]. Peak 33 with a [M-H]-ion *m/z* 317.0305 and daughter ions at *m/z* 151.0031 and 137.0237 were identified as myricetin [37]. Peak 36 with a [M-H]-ion *m/z* 451.1041 and daughter ions at *m/z* 341.0677, 315.0885, 287.0563 and 217.0138 were identified as cinchonain I [38]. Peak 38 with a [M-H]-ion *m/z* 285.0408 and daughter ion at *m/z* 133.0287 were identified as luteolin [39]. Peak 39 with a [M-H]-ion *m/z* 301.0356 and daughter ion at *m/z* 107.0131 and 151.0031 were quercetin [40].

*Fatty acids*

Eight fatty acids corresponding to peaks 5, 6, 7, 13, 15, 46, 47 and 50 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 5 with a [M-H]-ion *m/z* 297.1347 and daughter ions at *m/z* 233.1446, 125.0236 and 177.0201 were identified as hydroxytrioxopentadecenoic acid. Peak 6 with a [M-H]-ion *m/z* 447.1875 and

daughter ions at *m/z* 437.1589 and 401.1821 were identified as pentahidroxitetraoxoicosanoic acid. Peak 7 with a [M-H]-ion *m/z* 285.1346 and daughter ion at *m/z* 257.1037 were identified as hydroxytrioxotetradecanoic acid. Peak 13 with a [M-H]-ion *m/z* 401.1458 and daughter ion at *m/z* 343.1398 were identified as trihydroxypentaoxooctadecanoic acid. Peak 15 with a [M-H]-ion *m/z* 431.1925 and daughter ion at *m/z* 385.1886 were identified as tetrahydroxytetraoxoicosanoic acid. Peak 46 with a [M-H]-ion *m/z* 527.2864 we identified as octahidroxyheptacosapentaenoic acid. Peak 47 with a [M-H]-ion *m/z* 233.1547 and daughter ion at *m/z* 183.0119 were identified as pentadecatetraenoic acid. Peak 50 with a [M-H]-ion *m/z* 265.1482 and daughter ions at *m/z* 249.1494 and 223.0968 were identified as dihydroxypentadecatetraenoic acid.

*Organooxygen compounds*

Three organooxigen compounds corresponding to peaks 1, 10 and 48 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 1 with a [M-H]-ion *m/z* 191.0560 and daughter ions at *m/z* 173.0452 and 117.0189 were identified as quinic acid [41]. Peak 10 with a [M-H]-ion *m/z* 353.0882 and daughter ions at *m/z* 191.0559, 161.0239, 179.0344 and 135.0444 were identified as caffeoylquinic acid [42]. Peak 48 with a [M-H]-ion *m/z* 325.1847 and daughter ions at *m/z* 309.1744, and 251.1482 were identified as heptaethylene glycol.

*Benzene and substituted derivatives*

Three benzene and substituted derivatives compounds corresponding to peaks 3, 11 and 43 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 3 with a [M-H]-ion *m/z* 169.0139 and daughter ion at *m/z* 125.0238 were identified as gallic acid [43]. Peak 11 with a [M-H]-ion *m/z* 403.1251 and daughter ions at *m/z* 125.0238, 177.0177 and 109.0288 were identified as gallic acid derivative I . Peak 43 with a [M-H]-ion *m/z* 191.1075 and daughter ion at *m/z* 121.0653 were identified as phenethyl butyrate [16].

*Organic acids and related compounds*

One organic acid corresponding to peak 2 was identified using UHPLC-Q/Orbitrap/MS/MS. Peak 3 with a [M-H]-ion *m/z* 377.0861 and daughter ions at *m/z* 347.0755 and 349.0911were identified as syringaldehyde syringate or derivate quinic acid [44].

*Tannins*

One organic acid corresponding to peak 9 was identified using UHPLC-Q/Orbitrap/MS/MS. Peak 9 with a [M-H]-ion *m/z* 483.0783 and daughter ions at *m/z* 125.0237, 169.0139, 211.0242, 271.0459 and 313.0553 were identified as digalloyl glucose [45].

*Phenolic glycosides*

One organic acid corresponding to peak 12 was identified using UHPLC-Q/Orbitrap/MS/MS. Peak 12 with a [M-H]-ion *m/z* 453.1043 and daughter ions at *m/z* 123.0443, 125.0237, 167.0345, 135.0446 and 313.0570 were identified as myrsinoside A[46].

*Galloylated flavonoid glycoside*

One galloylated flavonoid glycoside compound corresponding to peak 35 was identified using UHPLC-Q/Orbitrap/MS/MS. Peak 35 with a [M-H]-ion *m/z* 585.0886 and daughter ions at *m/z* 301.0356, 151.0033 and 433.0781 were identified as quercetin galloyl pentoside [47].

*Flavonoid-7-o-glucuronides*

One flavonoid-7-o-glucuronide compound corresponding to peak 35 was identified using UHPLC-Q/Orbitrap/MS/MS. Peak 37 with a [M-H]-ion *m/z* 445.0782 and daughter ions at *m/z* 225.0556, 269.0453 and 175.0242 were identified as apigenin 7-O-glucuronide [48].

*Phenols*

One phenol compound corresponding to peak 41 was identified using UHPLC-Q/Orbitrap/MS/MS. Peak 41 with a [M-H]-ion *m/z* 293.1761 and daughter ion at *m/z* 279.1637 were identified as gingerol [49].

*Unknown compounds.*

Peaks 14, 44, 45 and 49 with a [M-H] -ions m/z 437.1224, 721.3639, 555.2846 and 577.2690 respectively correspond to unknown compounds.

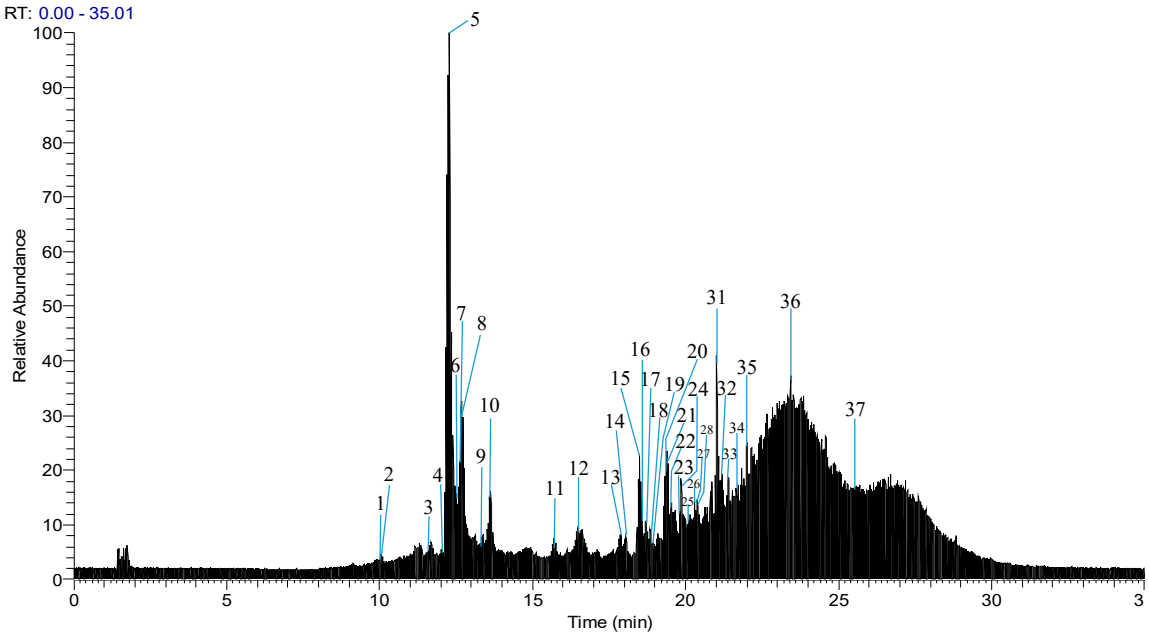



**Figure S3.** UHPLC TIC (total ion current) chromatogram of *Gliricidia sepium* dichloromethane extract partition.

**Table S3.** Tentative identification of compounds in the dichloromethane extract partition of *Gliricidia sepium* by UHPLC-Q/Orbitrap/MS/ MS

| Peak | Tentative identification | $[M-H]^-$ | Retention time (min.) | Theoretical mass (*m/z*) | Measured mass (*m/z*) | Accuracy (ppm) | MS ions (m/z)* | UV |
|---|---|---|---|---|---|---|---|---|
| 1 | Esculetin | $C_9H_5O_4$ | 10.05 | 177.0188 | 177.0184 | 2,3 | 133.0282; 149.0234 | 260; 290 |
| 2 | Caffeic acid | $C_9H_7O_4$ | 11.15 | 179.0344 | 179.0341 | 1,7 | 135.0440 | 246; 291 |
| 3 | Dihydro-p-coumaric acid isomer | $C_9H_9O_3$ | 11.52 | 165.0552 | 165.0547 | 3,0 | 147.0141; 119.0490 | 228; 273 |
| 4 | Hydroxycoumarin | $C_9H_5O_3$ | 12.05 | 161.0239 | 161.0234 | 3,1 | 133.0283; 117.0335 | 244; 277 |
| 5 | Dihydro-p-coumaric acid | $C_9H_9O_3$ | 12.26 | 165.0552 | 165.0546 | 3,6 | 121.0648; 106.0412; 147.0440; 119.0490 | 228; 273 |
| 6 | Azelaic acid | $C_9H_{15}O_4$ | 12.49 | 187.0970 | 187.0966 | 2,1 | 121.0654; 141.0914; 143.1073; 123.0808; 171.1020 | 246; 267 |
| 7 | Derivative Tianshic Acid | $C_{12}H_{19}O_5$ | 12.60 | 243.1232 | 243.1228 | 1,6 | 225.1122; 199.1328 | 233; 276; 325 |
| 8 | p-coumaric acid | $C_{9\|}H_7O_3$ | 12.66 | 163.0395 | 163.0391 | 2,5 | 147.0440; 119.0492 | 233; 274; 325 |
| 9 | Dihydroxydioxooctadecanoic acid | $C_{18}H_{31}O_6$ | 13.34 | 343.2121 | 343.2115 | 1,7 | 327.2166 | 249 |
| 10 | N-Carbobenzyloxy-L-isoleucine | $C_{14}H_{18}O_4N$ | 13.62 | 264.1236 | 264.1232 | 1,5 | 220.1333; 246.1129 | 232; 275; 308 |
| 11 | Leu/dihydro-p-coumaric acid | $C_{15}H_{20}NO_4$ | 15.70 | 278.1392 | 278.1388 | 1,4 | 130,0866 (leucine), 119,0495, 121,0651, 165,0552 (dihydro-p-coumaric acid) | 247; 266; 329 |
| 12 | Trihydroxyoctadecadienoic acid | $C_{18}H_{31}O_5$ | 16.46 | 327.2171 | 327.2168 | 0,9 | 309.2057; 169.0856; 187.0962 | 228; 273 |
| 13 | Phe /Dihydro-p-coumaric acid | $C_{18}H_{18}NO_4$ | 17.88 | 312.1236 | 312.1232 | 1,3 | 147.0441; 119.0490; 121.0562; 164.0706 ( phenylalanine) | 247; 271; 329 |
| 14 | Dihydroxy-methoxyflavanone | $C_{16}H_{13}O_5$ | 18.03 | 285.0763 | 285.0760 | 1,1 | 109.0283; 165.0546; 271.0605; 147.0440; 177.0544 | 249; 272; 379 |
| 15 | Dihydroxydodecadienoic acid | $C_{12}H_{19}O_4$ | 18.50 | 227.1283 | 227.1279 | 1,8 | 183.1381; 165.1279; 209.1172 | 249 |
| 16 | Tianshic acid | $C_{18}H_{33}O_5$ | 18.61 | 329.2328 | 329.2324 | 1,2 | 227.1279; 167.1067; 197.1173; 215.1279; 243.1229; 311.2229 | 248; 273; |
| 17 | Dihydro-p-coumaric acid derivative I | $C_{20}H_{22}NO_5$ | 18.69 | 356.1498 | 356.1494 | 1,1 | 121.0646; 147.0440; 119.0490; 165.0547; (dihydro-p-coumaric acid); 208.0969 | 249; 273; |
| 18 | Derivative tianshic acid | $C_{18}H_{31}O_5$ | 18.85 | 327.2171 | 327.2167 | 1,2 | 301.2010; 227.1279; 197.1173; 215.1279; 243.1229; 167.1067; 311.2229 | 248; 273 |
| 19 | Hesperetin | $C_{16}H_{13}O_6$ | 19.00 | 301.0712 | 301.0709 | 1,0 | 165.0547; 273.0761; 153.0183; 135.0076 | 249; 274 |
| 20 | Dihydro-p-coumaric acid isomer | $C_9H_9O_3$ | 19.34 | 165.0552 | 165.0546 | 3,6 | 121.0646; 106.0411; 147.0439; 119.0491 | 229; 273 |
| 21 | Tianshic acid | $C_{18}H_{33}O_5$ | 19.41 | 329.2328 | 329.2324 | 1,2 | 227.1279; 197.1174; 215.1281; 243.1228; 311.2221 | 228; 237 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 22 | Dihydroxy-methoxyflavanone derivative I | $C_{21}H_{25}O_6$ | 19.55 | 373.1651 | 373.1646 | 1,3 | 121.0647; 147.0439; 165.0543; 285.0768 | 274 |
| 23 | Unknow | $C_{12}H_{15}O_5$ | 19.65 | 239.0919 | 239.0916 | 1,3 | --- | 275 |
| 24 | Dihydroxy-methoxyflavanone derivative II | $C_{21}H_{27}O_6$ | 19.86 | 375.1808 | 375.1802 | 1,6 | 121.0647; 147.0439; 165.0544 | 283; 311 |
| 25 | Hydroxy-dimethoxyisoflavan | $C_{17}H_{17}O_4$ | 20.12 | 285.1127 | 285.1122 | 1,8 | 147.0441; 107.0490 | 243; 267 |
| 26 | Dihydro-p-coumaric acid derivative II | $C_{29}H_{31}O_8$ | 20.29 | 507.2019 | 507.2007 | 2,4 | 121.0646; 165.0547; (dihydro-p-coumaric acid) 147.0440; 119.0490; | 247; 279 |
| 27 | Hydroxydioxoheptadecenoic acid | $C_{17}H_{27}O_5$ | 20.37 | 311.1858 | 311.1855 | 1,0 | 193.0863, 195.1021, 197.1169, 237.1122, 239.1278, 267,1236 | 249; 278 |
| 28 | Dihydro-p-coumaroyloctanoic acid | $C_{17}H_{23}O_5$ | 20.40 | 307.1545 | 307.1542 | 1,0 | 121.0446; 147.0441; 159.1016; 165.0545 (dihydro-p-coumaric acid) | 251; 274 |
| 29 | Dihydro-p-coumaroyl-trioxooctadecanoic acid | $C_{27}H_{39}O_7$ | 20.84 | 475.2696 | 475.2684 | 2,5 | 121.0648; 165.0544 (dihydro-p-coumaric acid); 147. 0439; 311.2217 | 248; 274 |
| 30 | Phenethyl butyrate | $C_{12}H_{15}O_2$ | 20.92 | 191.1072 | 191.1067 | 2,6 | 121.0647; | 252; 275 |
| 31 | Dihydro-p-coumaroylnonanoic acid | $C_{18}H_{25}O_5$ | 21.02 | 321.1702 | 321.1696 | 1,9 | 151.0753; 121.0647; 165.0545 (dihydro-p-coumaric acid); 173.1171 | 274 |
| 32 | Trihydroxyheptaoxotriacontadienoic acid | $C_{30}H_{45}O_{12}$ | 21.18 | 597.2919 | 597.2933 | -2,3 | ---- | 274 |
| 33 | Dihydro-p-coumaroyl hydroxytrioxooctadecanoic acid | $C_{27}H_{41}O_7$ | 21.40 | 477.2852 | 477.2840 | 2,5 | 121.0647; 165.0545 (dihydro-p-coumaric acid); 147.0442; 327.2166; 329.2321 | 274 |
| 34 | 3 ,4 -Dihydroxy cinamic acid octacosyl ester derivated | $C_{30}H_{43}O_4$ | 21.74 | 467.3161 | 467.3152 | 1,9 | 121.0647; 165.0545; 147.0441 | 274 |
| 35 | Dihydro-p-coumaroylhydroxyoxohexadecanoic acid | $C_{25}H_{39}O_6$ | 22.01 | 435.2747 | 435.2737 | 2,3 | 401.2321; 339.1986; 287.2215 | 272 |
| 36 | 3 ,4 -Dihydroxy cinamic acid octacosyl ester derivated isomer | $C_{30}H_{43}O_4$ | 23.44 | 467.3161 | 467.3149 | 2,6 | 441.2267; 325.1830 | 251; 271 |
| 37 | Octahydroxyoctacosenoic acid | $C_{28}H_{55}O_{10}$ | 25.48 | 551.3795 | 551.3720 | 13,6 | --- | 271 |

* Daughter ions

**Compounds identified in *Gliricidia seipium***

*Phenylpropanoids*

Eleven phenylpropanoids compounds corresponding to peaks 3, 5, 11, 13, 17, 20, 26, 28, 29, 31, 33, and 35 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 3 with a [M-H]-ion *m/z* 165.0547 and daughter ions at *m/z* 147.0141 and 119.0490 were identified as dihydro-p-coumaric acid isomer [50]. Peak 5 with a [M-H]-ion *m/z* 165.0546 and daughter ions at *m/z* 121.0648, 106.0412, 147.0440 and 119.0490 were identified as dihydro-p-coumaric acid [50]. Peak 11 with a [M-H]-ion *m/z* 278.1388 *and* daughter ions at *m/z* 130.0866 (leucine), 119.0495, 121.0651, 165.0552 (dihydro-p-coumaric acid) were identified as Leu/dihydro-p-coumaric acid. Peak 13 with a [M-H]-ion *m/z* 312.1232 *and* daughter ions at *m/z* 147.0441, 119.0490, 121.0562 and 164.0706 (phenylalanine) were identified as Phe /Dihydro-p-coumaric acid. Peak 17 with a [M-H]-ion *m/z* 356.1494 *and* daughter ions at *m/z* 121.0646, 147.0440, 119.0490, 165.0547, (dihydro-p-coumaric acid) and 208.0969 were identified as dihydro-p-coumaric acid derivative I. Peak 20 with a [M-H]-ion *m/z* 165.0546 and daughter ions at *m/z* 121.0646, 106.0411, 147.0439 and 119.0491 *were* identified as dihydro-p-coumaric acid isomer [50]. Peak 26 with a [M-H]-ion *m/z* 507.2007 and daughter ions at *m/z* 121.0646, 165.0547, (dihydro-p-coumaric acid), 147.0440 and 119.0490 *were* identified as dihydro-p-coumaric acid derivative II. Peak 28 with a [M-H]-ion *m/z* 307.1542 and daughter ions at *m/z* 121.0446, 147.0441, 159.1016 and 165.0545 (dihydro-p-coumaric acid) were identified as dihydro-p-coumaroyloctaoic acid. Peak 29 with a [M-H]-ion *m/z* 475.2684 and daughter ions at *m/z* 121.0648, 165.0544 (dihydro-p-coumaric acid), 147. 0439 and 311.2217 *were* identified as dihydro-p-coumaroyl-trioxooctadecanoic acid. Peak 31 with a [M-H]-ion *m/z* 321.1696 and daughter ions at *m/z* 151.0753, 121.0647, 165.0545 (dihydro-p-coumaric acid) and 173.1171 *were* identified as dihydro-p-coumaroylnonanoic acid. Peak 33 with a [M-H]-ion *m/z* 477.2840 and daughter ions at *m/z* 121.0647, 165.0545 (dihydro-p-coumaric acid), 147.0442, 327.2166 and 329.2321 *were* identified as dihydro-p-coumaroyl hydroxytrioxooctadecanoic acid. Peak 35 with a [M-H]-ion *m/z* 435.2737 and daughter ions at *m/z* 401.2321, 339.1986 and 287.2215 *were* identified as dihydro-p-coumaroyl hydroxytrioxooctadecanoic acid.

*Fatty acids*

Seven fatty acid compounds corresponding to peaks 6, 7, 9, 12, 15, 16, 18, 21, 27, 32 and 37 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 6 with a [M-H]-ion *m/z* 187.0966 and daughter ions at *m/z* 121.0654, 141.0914, 143.1073, 123.0808 and 171.1020 were identified as azelaic acid [51]. Peak 7 with a [M-H]-ion *m/z* 243.1228 and daughter ions at *m/z* 225.1122 and 199.1328 were identified as derivative tianshic acid. Peak 9 with a [M-H]-ion *m/z* 343.2115 and daughter ion at *m/z* 327.2166 were identified as dihydroxydioxooctadecanoic acid [52]. Peak 12 with a [M-H]-ion *m/z* 327.2168 and daughter ion at *m/z* 309.2057, 169.0856 and 187.0962 were identified as trihydroxyoctadecadienoic acid [52, 53]. Peak 15 with a [M-H]-ion *m/z* 227.1279 and daughter ion at *m/z* 183.1381, 165.1279 and 209.1172 were identified as dihydroxydodecadienoic acid. Peak 16 with a [M-H]-ion *m/z* 329.2324 and daughter ion at *m/z* 227.1279, 167.1067, 197.1173, 215.1279, 243.1229 and 311.2229 were identified as tianshic acid [54]. Peak 18 with a [M-H]-ion *m/z* 327.2167 and daughter ion at *m/z* 301.2010, 227.1279, 197.1173, 215.1279, 243.1229, 167.1067 and 311.2229 were identified as derivative tianshic acid. Peak 21 with a [M-H]-ion *m/z* 329.2324 and daughter ion at *m/z* 227.1279, 197.1174, 215.1281, 243.1228 and 311.2221 were identified as tianshic acid [ 54]. Peak 27 with a [M-H]-ion *m/z* 311.1855 and daughter ion at *m/z* 193.0863, 195.1021, 197.1169, 237.1122, 239.1278 and 267.1236 were identified as hydroxydioxoheptadecenoic acid. Peak 32 with a [M-H]-ion *m/z* 597.2933 was identified as trihydroxyheptaoxotriacontadienoic acid. Peak 37 with a [M-H]-ion *m/z* 551.3720 was identified as octahydroxyoctacosenoic acid.

*Cinnamic acids and derivatives*

Four cinnamic acid and derivatives compounds corresponding to peaks 2, 8, 34, and 36 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 2 with a [M-H]-ion *m/z* 179.0341 and daughter ion at *m/z* 135.0440 were identified as caffeic acid [55]. Peak 2 with a [M-H]-ion *m/z* 163.0391 and daughter ion at *m/z* 147.0440 and 119.0492 were identified as p-coumaric acid [56]. Peak 34 with a [M-H]-ion *m/z* 467.3152 and daughter ions at *m/z* 121.0647, 165.0545 and 147.0441 *were* identified as 3,4 -dihydroxy cinamic acid octacosyl ester derivated.

Peak 36 with a [M-H]-ion *m/z* 467.3149 and daughter ions at *m/z* 441.2267 and 325.1830 were identified as 3,4 -dihydroxy cinamic acid octacosyl ester derivated isomer.

*Coumarins and derivatives*

Two coumarins and derivatives compounds corresponding to peaks 1 and 4 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 1 with a [M-H]-ion *m/z* 177.0184 and daughter ions at *m/z* 133.0282 and 149.0234 were identified as esculetin [57]. Peak 4 with a [M-H]-ion *m/z* 161.0234 and daughter ions at *m/z* 133.0283 and 117.0335 were identified as hydroxycoumarin [58].

*Flavonoids*

Five flavonoids compounds corresponding to peaks 14, 19, 22 24 and 25 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 14 with a [M-H]-ion *m/z* 285.0760 and daughter ions at *m/z* 109.0283, 165.0546, 271.0605, 147.0440 and 177.0544 were identified as dihydroxy-methoxyflavanone [59]. Peak 19 with a [M-H]-ion *m/z* 301.0709 and daughter ions at *m/z* 165.0547, 273.0761, 153.0183 and 135.0076 were identified as hesperetin [60]. Peak 22 with a [M-H]-ion *m/z* 373.1646 and daughter ions at *m/z* 121.0647, 147.0439, 165.0543 and 285.0768 were identified as dihydroxy-methoxyflavanone derivative I. Peak 24 with a [M-H]-ion *m/z* 375.1802 and daughter ions at *m/z* 121.0647, 147.0439 and 165.0544 were identified as dihydroxy-methoxyflavanone derivative II. Peak 25 with a [M-H]-ion *m/z* 285.1122 and daughter ions at *m/z* 147.0441 and 107.0490 were identified as dihydroxy-methoxyflavanone derivative II.

*Amino acids, peptides and analogs*

One peptide and analog compound corresponding to peak 10 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 10 with a [M-H]-ion *m/z* 264.1232 and daughter ions at *m/z* 220.1333 and 246.1129 were identified as N-Carbobenzyloxy-L-isoleucine.

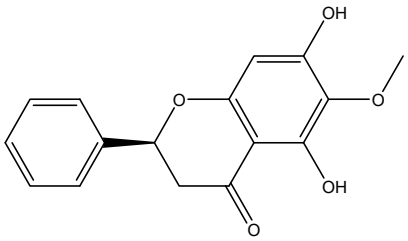
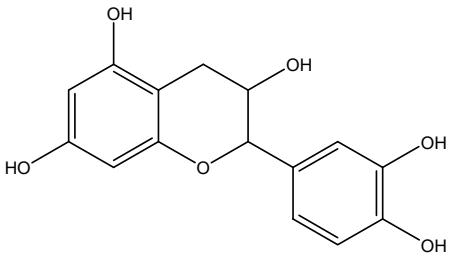
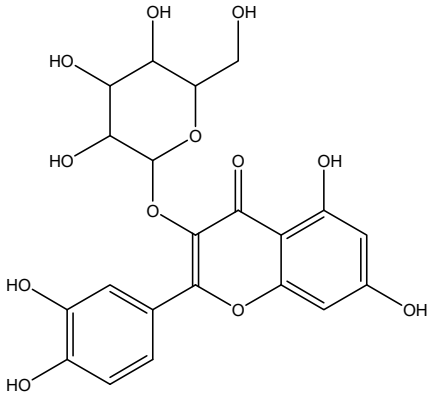
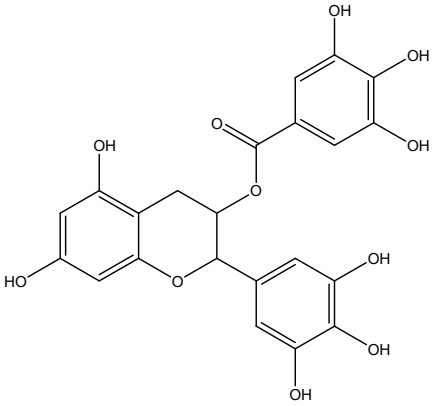
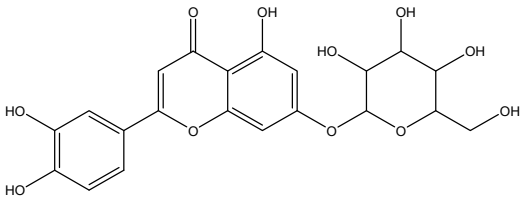
*Fatty acid esters*

One benzene and substituted derivative compound corresponding to peak 30 were identified using UHPLC-Q/Orbitrap/MS/MS. Peak 30 with a [M-H]-ion *m/z* 191.1067 and daughter ion at *m/z* 121.0647 were identified as phenethyl butyrate [16].

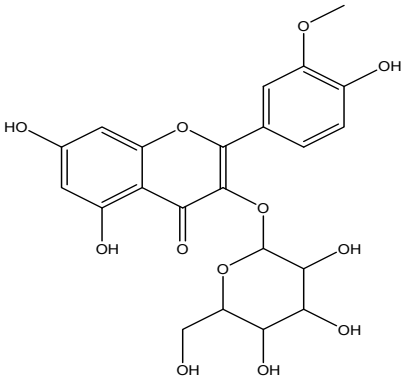
*Unknown compounds.*

Peak 23 with a [M-H] -ion m/z 239.0916 correspond to unknown compound.

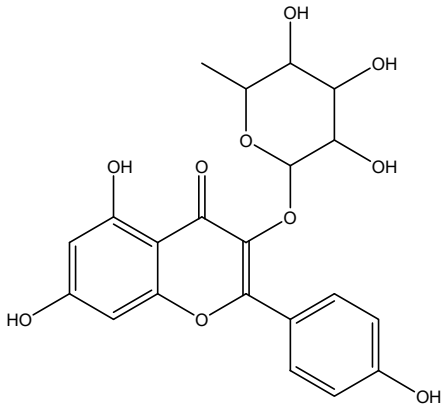
**Table S4. Chemical structures of the compounds with potential AA identified**

| Metabolites | *G. sepium* | *L. leucocephala* | *P. dulce* |
|---|---|---|---|
| **Flavonoids** |  Dihydroxymethoxy flavanone |  Catechin |  Quercetin-3-glucoside |
| |  Gallocatechin gallate |  Luteolin 7-O-glucoside | |

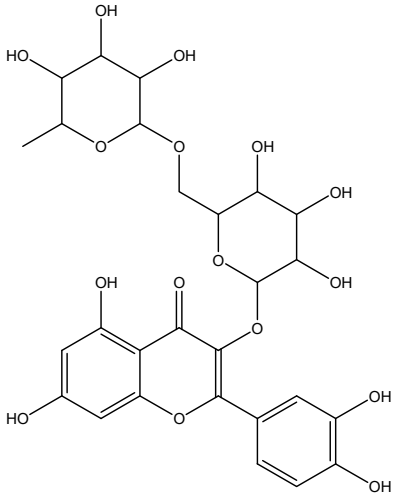
**Flavonoids**



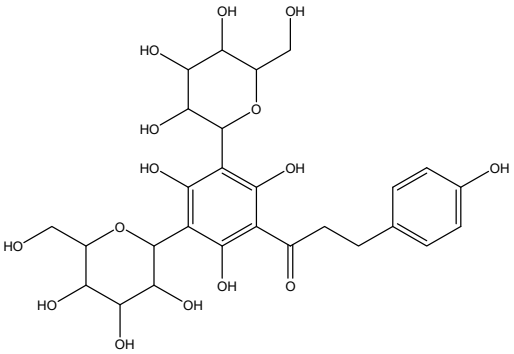
Isorhamnetin-O-glucoside



Kaempferol-3-O- rhamnoside

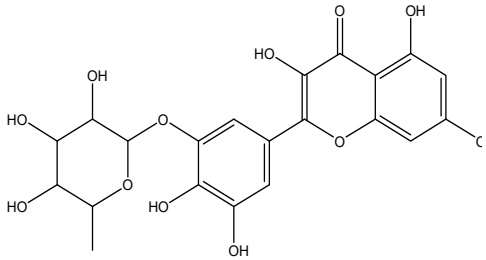


Rutin

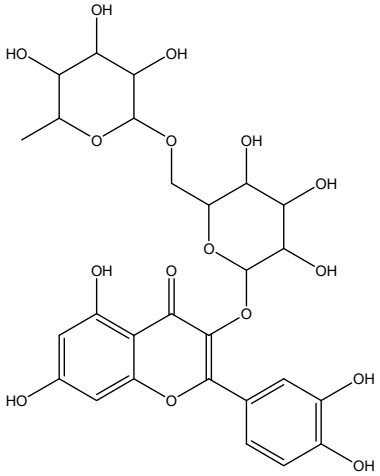


Phloretin-di-C-hexoside

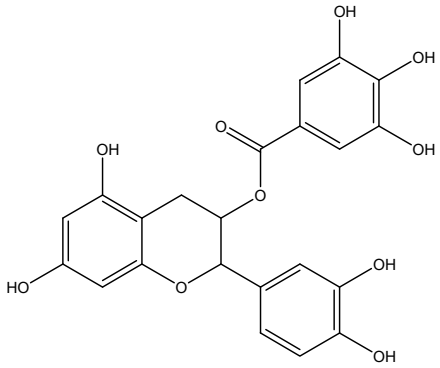
**Flavonoids**



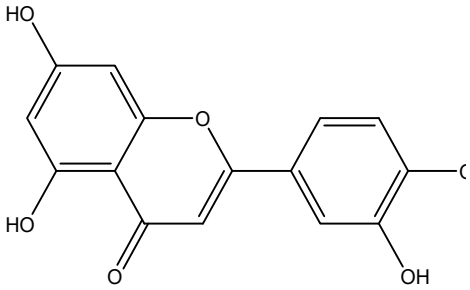
Myricetin 3-O-rhamnoside



Rutin

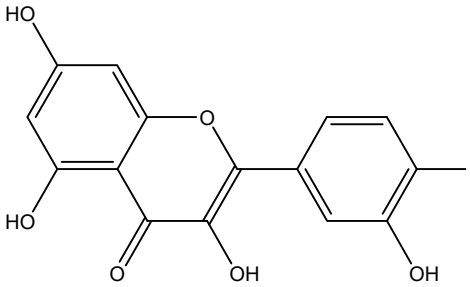


Epicatechin gallate



Luteolin

**Flavonoids**




Quercetin

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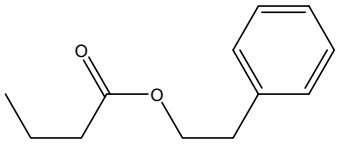
**Fatty acid esters**




Phenethyl butyrate

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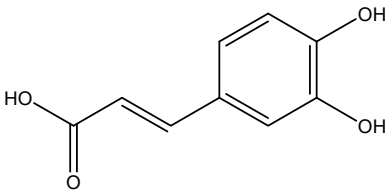
**Hydroxycinnamic acids**




Caffeic acid

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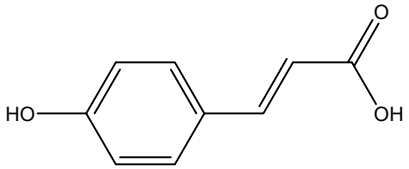


p-coumáric acid

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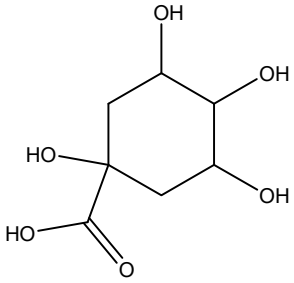
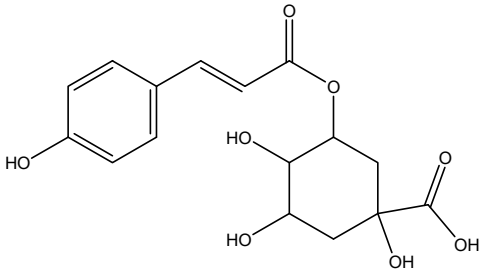
**Organooxygenated compounds**




Qunic acid




Coumaroylquinic acid

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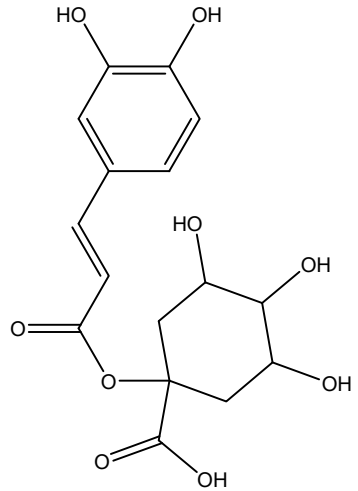

Caffeoylquinic acid

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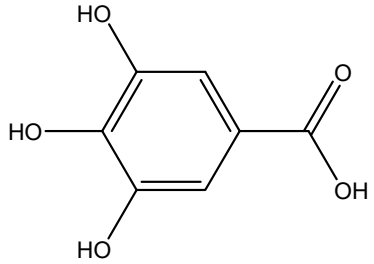
**Benzene and substituted derivatives**



Gallic acid

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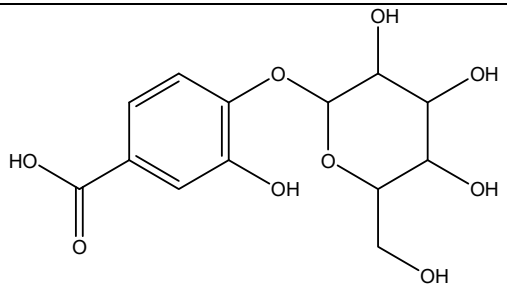
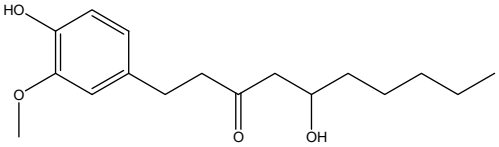
| | |
|---|---|
| **Phenolic glycosides** |  <br>Protocatechuic acid 4-hexoside |
| **Phenols** |  <br>Gingerol |

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