Table 1 Identification of 142 chemical constituents in *A. macrotera* by UHPLC-Q-Exactive Orbitrap MS.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak | tR | Theoretical Mass *m/z* | Experimental Mass *m/z* | Error (ppm) | Formula | MS/MS fragment(+) | MS/MS fragment(-) | Identification/Reactions | source |
| 1 | 0.85\* | 191.05611 | 191.05518 | -4.87 | C7H12O6 |  | MS2[191]:111.0074(100), 87.0073(31), 85.0281(24), 129.0180(8) | Quinic acid | L  S |
| 2 | 0.88 | 175.11895 | 175.11853 | -2.41 | C6H14N4O2 | MS2[175]:70.0657(44), 112.0869(30), 158.0925(5) |  | Arginine | L  S |
| 3 | 0.91 | 195.05102 | 195.05013 | -4.59 | C6H12O7 |  | MS2[195]:75.0073(79), 129.0181(70), 99.0074(24), 159.0287(10), 177.0393(10) | Gluconic acid | L  S |
| 4 | 0.91 | 341.10893 | 341.10855 | -1.13 | C12H22O11 |  | MS2[341]:119.0336(35), 113.0230(27), 179.0551(10), 161.0443(7) | Sucrose | L  S |
| 5 | 0.94 | 193.03537 | 193.03453 | -4.38 | C6H10O7 |  | MS2[193]:85.0280(34), 129.0180(16) | D-Galacturonic acid | L  S |
| 6 | 0.94 | 209.03029 | 209.02951 | -3.73 | C6H10O8 |  | MS2[209]:85.0281(100), 111.0440(8), 173.0088(2) | Saccharic acid | L  S |
| 7 | 0.95 | 148.06043 | 148.06013 | -2.05 | C5H9NO4 | MS2[148]:84.0459(100), 56.0508(48) |  | L-Glutamic acid | L  S |
| 8 | 0.97 | 138.05496 | 138.05469 | -1.92 | C7H7NO2 | MS2[138]:94.0656(100), 110.0604(90), 65.0394(61), 96.0449(48), 92.0500(29) |  | Trigonelline | L  S |
| 9 | 0.98\* | 133.01425 | 133.01302 | -9.22 | C4H6O5 |  | MS2[133]:115.0023(100), 71.0124(43) | Malic acid | L  S |
| 10 | 1.00\* | 145.01425 | 145.01311 | -7.84 | C5H6O5 |  | MS2[145]:57.0332(67), 127.0388(65), 101.0594(53) | α-Ketoglutaric acid | L |
| 11 | 1.00 | 173.00916 | 173.00815 | -5.84 | C6H6O6 |  | MS2[173]:111.0074(100), 85.0280(36), 154.9973(5) | Trans-Aconitic acid | L |
| 12 | 1.00 | 175.02481 | 175.02382 | -5.66 | C6H8O6 |  | MS2[175]:146.9599(100), 130.8732(1) | Ascorbic acid | L  S |
| 13 | 1.00\* | 191.01973 | 191.01880 | -4.85 | C6H8O7 |  | MS2[191]:111.0074(100), 87.0073(32), 85.0281(23) | Citric acid | L  S |
| 14 | 1.03 | 149.00916 | 149.00769 | -9.87 | C4H6O6 |  | MS2[149]:59.0125(100), 87.0073(9), 103.0388(5), 72.9917(3) | Tartaric acid | L  S |
| 15 | 1.19\* | 129.01933 | 129.01814 | -9.24 | C5H6O4 |  | MS2[129]:85.0280(100), 57.0332(27), 71.0124(17) | Citraconic acid | L  S |
| 16 | 1.19\* | 173.00916 | 173.00822 | -5.44 | C6H6O6 |  | MS2[173]:111.0074(100), 85.0280(46), 129.0181(24) | Cis-aconitic acid | L  S |
| 17 | 1.20 | 123.05529 | 123.05522 | -0.56 | C6H6N2O | MS2[123]:80.0501(100), 96.0449(49), 53.0394(40), 78.0345(11) |  | Nicotinamide | L  S |
| 18 | 1.22 | 182.08116 | 182.08084 | -1.81 | C9H11NO3 | MS2[182]:136.0756(100), 119.0491(15) |  | 1. Tyrosine | L  S |
| 19 | 1.32 | 147.06628 | 147.06526 | -6.95 | C6H12O4 |  | MS2[147]:59.0124(50), 101.0594(18), 129.0544(17) | Mevalonic acid | L  S |
| 20 | 1.32 | 191.05611 | 191.05516 | -4.98 | C7H12O6 |  | MS2[191]:111.0074(100), 87.0073(32), 85.0281(23), 129.0180(7) | Quinic acid isomer | L  S |
| 21 | 1.56\* | 169.01425 | 169.01338 | -5.13 | C7H6O5 |  | MS2[169]:125.0232(100) | Gallic acid | L |
| 22 | 1.66 | 331.06707 | 331.06720 | 0.39 | C13H16O10 |  | MS2[331]:169.0133(37), 125.0231(33) | Monogalloyl-glucose | L  S |
| 23 | 1.73 | 315.07216 | 315.07187 | -0.90 | C13H16O9 |  | MS2[315]:153.0182(100), 109.0282(13) | Protocatechuic  acid-*O*-glucoside | L  S |
| 24 | 1.83 | 373.11402 | 373.11404 | 0.05 | C16H22O10 |  | MS2[373]:123.0438(100), 193.0498(88), 149.0596(69), 89.0230(58), 61.9869(45) | Geniposidic acid | L |
| 25 | 1.85 | 164.07170 | 164.07072 | -5.98 | C9H11NO2 | MS2[166]:120.0807(100) | MS2[164]:147.0439(100), 72.0077(29), 136.9308(5), 96.9684(3) | L-Phenylalanine | L  S |
| 26 | 2.02 | 218.10339 | 218.10287 | -2.41 | C9H16O5N |  | MS2[218]:88.0389(100), 146.0810(49) | Pantothenic acid | L  S |
| 27 | 2.07 | 197.04555 | 197.04475 | -4.04 | C9H10O5 |  | MS2[197]:72.9916(5), 135.0438(3), 179.0338(3), 123.0435(2) | Danshensu | L |
| 28 | 2.07 | 315.07216 | 315.07220 | 0.14 | C13H16O9 |  | MS2[315]:153.0182(100), 109.0282(22) | Protocatechuic  acid-*O*-glucoside | L  S |
| 29 | 2.15 | 167.03498 | 167.03498 | -5.88 | C8H8O4 |  | MS2[167]:123.0438(73) | Vanillic acid | L  S |
| 30 | 2.36 | 315.10854 | 315.10849 | -0.16 | C14H20O8 |  | MS2[315]:135.0438(100), 153.0545(59), 123.0437(9) | Hydroxytyrosol Glucoside | L  S |
| 31 | 2.46 | 151.04006 | 151.03896 | -7.33 | C8H8O3 |  | MS2[151]:108.0203(3) , 93.0331(2) | Isovanillin | L  S |
| 32 | 2.46 | 153.05572 | 153.05455 | -7.63 | C8H10O3 |  | MS2[153]:123.0438(100) | Hydroxytyrosol | L  S |
| 33 | 2.55\* | 153.01933 | 153.01840 | -6.09 | C7H6O4 |  | MS2[153]:123.0438(100), 109.0281(11) | Protocatechuic acid | L  S |
| 34 | 2.60 | 167.03498 | 167.03401 | -5.82 | C8H8O4 |  | MS2[167]:137.0229(24), 123.0437(16) | Isovanillic acid | L  S |
| 35 | 3.08 | 151.04006 | 151.03894 | -7.46 | C8H8O3 |  | MS2[151]:107.0488(47), 121.0281(3) | (R)-Mandelic acid | L  S |
| 36 | 3.20 | 389.10893 | 389.10889 | -0.11 | C16H22O11 |  | MS2[389]:139.0388(100), 165.0546(66), 183.0653(50), 101.0230(19), 113.0230(13) | Deacetylasperulosidic acid | L  S |
| 37 | 3.23 | 285.06159 | 285.06146 | -0.46 | C12H14O8 |  | MS2[285]:152.0103(100), 153.0183(74), 108.0202(58), 109.0282(11) | Dihydroxybenzoic acid pentoside isomer | L  S |
| 38 | 3.26 | 205.09715 | 205.09680 | -1.73 | C11H12N2O2 | MS2[205]:188.0702(100), 146.0597(53) |  | L-Tryptophan | L  S |
| 39 | 3.30 | 375.12967 | 375.12949 | -0.48 | C16H24O10 |  | MS2[375]:169.0860(100), 213.0762(43), 151.0754(41), 113.0231(23) | Loganic acid | L |
| 40 | 3.34 | 299.11363 | 299.11343 | -0.66 | C14H20O7 |  | MS2[299]:59.0124(74), 101.0231(45), 119.0487(39), 113.0230(29), 137.0233(17) | Salidroside | L  S |
| 41 | 3.41 | 137.02442 | 137.02328 | -8.30 | C7H6O3 |  | MS2[137]:93.0332(2) | 4-Hydroxybenzoic acid | L  S |
| 42 | 3.49 | 175.06119 | 175.06021 | -5.64 | C7H12O5 |  | MS2[175]:146.9599(100), 115.0387(94), 85.0644(36), 113.0594(35) | 2-isopropylmalic acid | L  S |
| 43 | 3.56 | 153.01933 | 153.01820 | -7.40 | C7H6O4 |  | MS2[153]:109.0282(100), 123.0439(43), 108.0203(25) | Gentisic acid | L |
| 44 | 3.60 | 299.07724 | 299.07706 | -0.60 | C13H16O8 |  | MS2[299]:137.0231(100), 93.0332(16) | Salicylic acid-hexoside | L  S |
| 45 | 3.63 | 451.12458 | 451.12430 | -0.63 | C21H24O11 |  | MS2[451]:289.0714(100), 205.0497(6), 137.0231(3) | Catechin-glucopyranoside | L  S |
| 46 | 3.70 | 461.16645 | 461.16632 | -0.28 | C20H30O12 |  | MS2[461]:135.0439(100), 101.0231(64), 205.0709(63), 143.0338(50), 59.0125(50) | Forsythiaside E | L |
| 47 | 3.75 | 175.02481 | 175.02374 | -6.12 | C6H8O6 |  | MS2[175]:146.9599(100), 130.8732(1), 157.0494(1) | Ascorbic acid isomer | L |
| 48 | 3.93 | 341.08780 | 341.08746 | -1.01 | C15H18O9 |  | MS2[341]:179.0339(100), 135.0438(22) | CA-hexoside | L  S |
| 49 | 3.95 | 181.04954 | 181.04915 | -2.13 | C9H8O4 | MS2[181]:163.0385(100), 145.0281(11) |  | Caffeic acid isomer | L |
| 50 | 3.98 | 431.15588 | 431.15549 | -0.92 | C19H28O11 |  | MS2[431]:101.0229(20), 149.0443(14), 119.0487(8), 229.1136(5) | Osmanthuside H | L  S |
| 51 | 4.05 | 131.07136 | 131.07014 | -9.36 | C6H12O3 |  | MS2[131]:87.0437(5), 85.0644(2) | 2-hydroxyhexanoic acid or isomer | L |
| 52 | 4.19 | 323.13475 | 323.13446 | -0.91 | C13H24O9 |  | MS2[323]:89.0230(100), 101.0230(75), 59.0124(62), 119.0336(43), 113.0230(32) | Periplobiose | L  S |
| 53 | 4.24 | 167.03498 | 167.03392 | -6.36 | C8H8O4 |  | MS2[167]:137.0232(18), 123.0438(11) | Orsellinic acid | L  S |
| 54 | 4.26 | 163.04007 | 163.03886 | -7.40 | C9H8O3 |  | MS2[163]:119.0489(55) | 2-Coumaric acid | L  S |
| 55 | 4.31 | 151.04006 | 151.03893 | -7.53 | C8H8O3 |  | MS2[151]:93.0331(11), 108.0204(4) | vanillin | L  S |
| 56 | 4.31\* | 289.07176 | 289.07147 | -1.02 | C15H14O6 |  | MS2[289]:109.0281(100), 123.0438(69) | Catechin | L  S |
| 57 | 4.35 | 181.04954 | 181.04921 | -1.80 | C9H8O4 | MS2[181]:163.0386(100), 145.0281(10) |  | Caffeic acid isomer | L |
| 58 | 4.38 | 285.06159 | 285.06137 | -0.77 | C12H14O8 |  | MS2[285]:153.0181(100), 152.0103(51), 108.0203(35), 109.0283(17) | Dihydroxybenzoic acid pentoside | L  S |
| 59 | 4.40 | 341.08780 | 341.08740 | -1.19 | C15H18O9 |  | MS2[341]:179.0339(100), 135.0438(20) | CA-hexoside | L  S |
| 60 | 4.66\* | 353.08781 | 353.08765 | -0.44 | C16H18O9 |  | MS2[353]:135.0438(17), 191.0552(11), 179.0340(10) | Cryptochlorogenic acid | L |
| 61 | 4.75 | 131.07136 | 131.07018 | -9.06 | C6H12O3 |  | MS2[131]:85.0644(100), 87.0437(10) | 2-hydroxyhexanoic acid or isomer | L |
| 62 | 4.75\* | 353.08781 | 353.08670 | -3.13 | C16H18O9 |  | MS2[353]:191.0552(27), 135.0439(15), 179.0340(12) | Chlorogenic acid | L |
| 63 | 4.78 | 289.07176 | 289.07083 | -3.22 | C15H14O6 |  | MS2[289]:123.0438(83), 109.0281(43) | Epicatechin | L  S |
| 64 | 4.92\* | 179.03498 | 179.03395 | -5.76 | C9H8O4 |  | MS2[179]:135.0438(100) | Caffeic acid | L  S |
| 65 | 4.94 | 517.15628 | 517.15601 | -0.52 | C22H30O14 |  | MS2[517]:193.0497(100), 134.0361(12), 149.0595(7), 178.0257(5) | Ferulic acid dihexoside | L  S |
| 66 | 4.99 | 355.10345 | 355.10324 | -0.61 | C16H20O9 |  | MS2[355]:193.0497(100), 175.0390(21), 149.0596(17), 134.0360(15), 217.0493(4) | Ferulic Acid-hexoside | L  S |
| 67 | 5.30 | 625.14102 | 625.14136 | 0.54 | C27H30O17 |  | MS2[625]:301.0348(6), 463.0860(3) | Quercetin dihexoside | L  S |
| 68 | 5.55 | 355.10345 | 355.10327 | -0.52 | C16H20O9 |  | MS2[355]:193.0497(100), 175.0390(57), 134.0359(18), 149.0596(18), 217.0499(7) | Ferulic Acid-hexoside | L  S |
| 69 | 5.69 | 163.04007 | 163.03908 | -6.06 | C9H8O3 |  | MS2[163]:119.0489(6), 135.0438(4) | 3-Coumaric acid | L  S |
| 70 | 5.82 | 449.10893 | 449.10855 | -0.86 | C21H22O11 |  | MS2[449]:125.0232(38), 151.0027(32), 285.0404(10) | Taxifolin 7-rhamnoside | L |
| 71 | 5.87 | 593.15119 | 593.15088 | -0.53 | C27H30O15 | MS2[595]:325.0699(100), 379.0804(71), 163.0386(59), 337.0697(51), 409.0908(35) | MS2[593]:353.0663(100), 383.0768(49), 473.1084(28) | Vicenin II | L  S |
| 72 | 5.89 | 167.03498 | 167.03392 | -6.36 | C8H8O4 |  | MS2[167]:152.0103(18), 108.0206(1), 123.0440(1) | 4-Methoxysalicylic acid | L  S |
| 73 | 5.89 | 355.10345 | 355.10327 | -0.52 | C16H20O9 |  | MS2[355]:193.0497(100), 175.0390(44), 149.0596(21), 134.0362(16), 217.0499(7) | Ferulic Acid-hexoside | L  S |
| 74 | 5.96 | 175.02481 | 175.02383 | -5.61 | C6H8O6 |  | MS2[175]:146.9599(100), 130.8740(1) | Ascorbic acid isomer | L |
| 75 | 5.98 | 415.16097 | 415.15945 | -3.66 | C19H28O10 |  | MS2[415]:161.0442(100), 101.0230(4), 71.0124(2), 113.0232(1) | Phenylethanol rutin | L  S |
| 76 | 6.26\* | 163.04007 | 163.03893 | -6.98 | C9H8O3 |  | MS2[163]:119.0489(100) | 4-Coumaric acid | L  S |
| 77 | 6.28 | 415.16097 | 415.16110 | 0.31 | C19H28O10 |  | MS2[415]:101.0230(46), 71.0125(43), 113.0227(33), 161.0443(7) | Phenylethanol rutin | L  S |
| 78 | 6.28\* | 173.08193 | 173.08095 | -5.67 | C8H14O4 |  | MS2[173]:111.0801(75), 129.0908(5) | Suberic acid | L  S |
| 79 | 6.33 | 563.14062 | 563.14032 | -0.55 | C26H28O14 | MS2[565]:391.0800(100), 379.0803(95), 409.0909(91), 325.0696(75), 337.0695(51) | MS2[563]:353.067(100), 383.0771(64), 473.1086(18), 443.0978(13) | Schaftoside | L  S |
| 80 | 6.52 | 449.10893 | 449.10858 | -0.79 | C21H22O11 |  | MS2[449]:125.0232(100), 177.0550(3), 285.0405(6) | Taxifolin 7-rhamnoside | L |
| 81 | 6.63 | 755.20402 | 755.20392 | -0.13 | C33H40O20 |  | MS2[755]:300.0273(100), 301.0334(14), 178.9977(3), 151.0029(1) | Quercetin rutin rhamnoside | L  S |
| 82 | 6.74 | 173.08193 | 173.08110 | -4.81 | C8H14O4 |  | MS2[173]:111.0801(75), 129.0908(5) | Suberic acid isomer | L |
| 83 | 6.88 | 563.14062 | 563.14038 | -0.44  -1.45 | C26H28O14 | MS2[565]:379.0804(100), 325.0699(58), 337.0699(40), 397.0908(36), 349.0697(30) | MS2[563]:353.0664(100), 443.0977(57), 383.0746(51), 473.1095(31) | Isoschaftoside | L  S |
| 84 | 6.88 | 595.13046 | 595.12866 | -3.02 | C26H28O16 |  | MS2[595]:151.0024(100), 300.0270(7), 301.0347(6) | quercetin-arabinosyglucoside | L  S |
| 85 | 6.90\* | 193.05063 | 193.04959 | -5.40 | C10H10O4 |  | MS2[193]:134.0360(100), 178.0260(91), 149.0595(41), 137.0231(17) | Ferulic acid | L  S |
| 86 | 6.93 | 595.16684 | 595.16760 | 1.27 | C27H32O15 |  | MS2[595]:151.0025(100), 287.0559(61), 135.0440(17) | Eriocitrin | L  S |
| 87 | 6.95 | 609.14611 | 609.14612 | 0.02 | C27H30O16 |  | MS2[609]:300.0272(100), 301.0334(14) | Rutin isomer | L |
| 88 | 6.95 | 755.20402 | 755.20361 | -0.54 | C33H40O20 |  | MS2[755]:300.0273(100), 301.0335(13), 178.9984(3), 151.0026(2) | Quercetin rutin rhamnoside | L |
| 89 | 7.06 | 639.19306 | 639.19299 | -0.11 | C29H36O16 |  | MS2[639]:161.0232(100), 179.0340(6), 135.0438(5) | β-Hydroxyverbascoside | L  S |
| 90 | 7.11 | 449.10893 | 449.10831 | -1.39 | C21H22O11 |  | MS2[449]:151.0027(100), 125.0232(68), 285.0405(2), 177.0544(2) | Taxifolin 7-rhamnoside | L |
| 91 | 7.18 | 217.10814 | 217.10744 | -3.26 | C10H18O5 |  | MS2[217]:155.1065(39), 171.1015(26), 199.0965(5), 137.0956(4) | Epieucommiol | L  S |
| 92 | 7.26 | 181.04954 | 181.04918 | -1.96 | C9H8O4 | MS2[181]:163.0386(100), 145.0281(11) |  | Caffeic acid isomer | L |
| 93 | 7.29\* | 137.02442 | 137.02322 | -8.74 | C7H6O3 |  | MS2[137]:93.0331(100) | Salicylic acid | L  S |
| 94 | 7.29\* | 609.14611 | 609.14594 | -0.28 | C27H30O16 |  | MS2[609]:300.0273(100), 301.0346(59) | Rutin | L  S |
| 95 | 7.34 | 623.19814 | 623.19812 | -0.04 | C29H36O15 |  | MS2[623]:161.0232(100), 461.1450(23), 135.0438(6), 179.0341(6) | Verbascoside | L  S |
| 96 | 7.40\* | 301.03537 | 301.03482 | -1.85 | C15H10O7 | MS2[303]:153.0184(49), 137.0235(44), 229.0497(42), 257.0446(27), 165.0184(23) | MS2[301]:151.0025(100), 178.9976(62), 121.0282(17) | Quercetin | L  S |
| 97 | 7.45\* | 463.08820 | 463.08835 | 0.33 | C21H20O12 | MS2[465]:303.0493(100) | MS2[463]:300.0271(100), 301.0344(54), 271.0240(3) | Isoquercitrin | L  S |
| 98 | 7.50\* | 593.15119 | 593.15063 | -0.95 | C27H30O15 | MS2[595]:287.0543(100) | MS2[593]:285.0401(100) | Kaempferol-3-O-neohesperidoside | L  S |
| 99 | 7.55 | 181.04954 | 181.04906 | -2.62 | C9H8O4 | MS2[181]:163.0386(100), 145.0281(12) |  | Caffeic acid isomer | L |
| 100 | 7.56 | 477.14023 | 477.13968 | -1.16 | C23H26O11 | MS2[479]:163.0387(100) | MS2[477]:161.0234(100), 135.0439(7), 315.1084(5), 221.0443(1), 323.0770(1) | Calceolarioside B | L  S |
| 101 | 7.59\* | 515.11950 | 515.11523 | -8.29 | C25H24O12 |  | MS2[515]:135.0439(5), 179.0334(3) | Isochlorogenic acid B | L |
| 102 | 7.70\* | 447.09328 | 447.09396 | 1.51 | C21H20O11 | MS2[449]:287.0555(18) | MS2[447]:285.0401(100) | Luteolin 7-O-D-glucoside | L  S |
| 103 | 7.77 | 623.19814 | 623.19904 | 1.44 | C29H36O15 |  | MS2[623]:161.0233(100), 179.0340(8), 135.0437(4), 461.1484(1) | Isoverbascoside | L  S |
| 104 | 8.03 | 623.16176 | 623.15649 | -8.45 | C28H32O16 |  | MS2[623]:161.0233(100), 315.0511(8), 145.0284(6), 163.0393(2) | Isorhamnetin-3-O-nehesperidine | L |
| 105 | 8.10\* | 447.09328 | 447.09323 | -0.12 | C21H20O11 | MS2[449]:287.0555(100) | MS2[447]:285.0401(100) | Kaempferol-7-O-glucoside | L  S |
| 106 | 8.12 | 433.07763 | 433.07745 | -0.43 | C20H18O11 |  | MS2[433]:300.0272(100), 301.0338(26), 271.0237(2) | Quercetin pentoside | L  S |
| 107 | 8.14\* | 187.09758 | 187.09671 | -4.66 | C9H16O4 |  | MS2[187]:97.0647(100), 123.0805(60), 57.0333(51), 125.0960(37), 95.0489(34) | Azelaic acid | L  S |
| 108 | 8.28 | 579.20831 | 579.20782 | -0.85 | C28H36O13 |  | MS2[579]:181.0495(100), 417.1549(22), 402.1315(12), 166.0260(11), 387.1083(2) | Syringaresinol-4’-  *O*-glucopyranoside | L  S |
| 109 | 8.35\* | 193.05063 | 193.04976 | -4.52 | C10H10O4 |  | MS2[193]:134.0361(7), 137.0231(4), 178.0257(3) | Isoferulic acid | L  S |
| 110 | 8.38 | 579.17083 | 579.17004 | -1.37 | C27H30O14 | MS2[579]:271.0594(100) |  | Rhoifolin | L |
| 111 | 8.44 | 447.09328 | 447.09241 | -1.96 | C21H20O11 | MS2[449]:287.0555(100) | MS2[447]:285.0401(100) | Kaempferol-7-O-  glucoside | L  S |
| 112 | 8.48 | 623.16176 | 623.15948 | -3.65 | C28H32O16 |  | MS2[623]:161.0233(100), 315.0511(8), 300.0281(1) | Narcissoside | L |
| 113 | 8.50 | 181.04954 | 181.04910 | -2.40 | C9H8O4 | MS2[181]:163.0386(100), 145.0282(9) |  | Caffeic acid isomer | L |
| 114 | 8.57 | 301.07176 | 301.07181 | 0.16 | C16H14O6 |  | MS2[301]:151.0025(100) | Hesperetin isomer | L |
| 115 | 8.62 | 593.18758 | 593.18884 | 2.13 | C28H34O14 |  | MS2[593]:113.0230(100), 85.0281(36), 111.0074(15), 161.0446(7) | Poncirin | L  S |
| 116 | 8.85 | 447.09328 | 447.09286 | -0.95 | C21H20O11 | MS2[449]:287.0544(100), 303.0492(19) | MS2[447]:285.0400(100), 300.0272(29), 301.0341(9) | Quercetol-7-O-  rhamnoside | L  S |
| 117 | 9.07 | 607.16684 | 607.16681 | -0.05 | C28H32O15 | MS2[609]:301.0699(100), 302.0732(10) | MS2[607]:299.0558(100), 284.0323(13) | Neodiosmin | L  S |
| 118 | 9.46 | 447.09328 | 447.09314 | -0.32 | C21H20O11 | MS2[449]:287.0543(100), 303.0491(17) | MS2[447]:285.0402(100), 300.0271(12), 301.0345(8) | Quercetol-7-O-  rhamnoside | L  S |
| 119 | 9.76 | 447.09328 | 447.09299 | -0.66 | C21H20O11 | MS2[449]:317.0650(100), 287.0545(35) | MS2[447]:285.0400(100), 314.0429(75), 299.0192(66), 300.0258(15), 315.0490(13) | Quercetin-3-  rhamnoside | L  S |
| 120 | 10.06\* | 263.12888 | 263.12863 | -0.96 | C15H20O4 |  | MS2[263]:219.1383(100), 151.0752(62), 204.1147(54), 152.0835(37), 139.0753(35) | Abscisic acid | L  S |
| 121 | 10.23\* | 287.05611 | 287.05594 | -0.60 | C15H12O6 |  | MS2[287]:151.0025(100), 135.0439(64) | Eriodictyol | L  S |
| 122 | 10.82 | 201.11323 | 201.11243 | -3.99 | C10H18O4 |  | MS2[201]:139.1116(100), 183.1016(40) | 3-tert-Butylpropionic acid | L  S |
| 123 | 12.19 | 283.06119 | 283.06094 | -0.9 | C16H12O5 |  | MS2[283]:268.0375(77) | Calycosin | L |
| 124 | 12.22 | 301.03537 | 301.03516 | -0.72 | C15H10O7 | MS2[303]:153.0182(100), 137.0234(77), 229.0495(64), 257.0445(36), 165.0183(21) | MS2[301]:151.0025(100), 178.9975(56), 121.0281(17) | Quercetin isomer | L |
| 125 | 12.26\* | 285.04046 | 285.04025 | -0.74 | C15H10O6 | MS2[287]:153.0177(26), 135.0437(13) | MS2[285]:133.0284(100), 151.0027(34), 107.0126(20), 149.0235(17), 175.0393(16) | Luteolin | L |
| 126 | 12.86 | 301.07176 | 301.07138 | -1.27 | C16H14O6 |  | MS2[301]:151.0025(100) | Hesperetin | L |
| 127 | 12.92 | 373.12818 | 373.12759 | -4.52 | C20H20O7 | MS2[373]:312.0981(81), 327.0851(80), 343.0802(72), 357.0958(34) |  | sinensetin | L |
| 128 | 13.22 | 269.04555 | 269.04559 | 0.16 | C15H10O5 |  | MS2[269]:117.0333(100), 151.0026(38), 149.0234(30), 107.0126(28), 159.0442(9) | Genistein | L  S |
| 129 | 13.24 | 299.09250 | 299.09213 | -1.23 | C17H16O5 |  | MS2[299]:284.0324(100), 179.0340(13), 135.0440(3) | Farrerol | L |
| 130 | 13.31\* | 285.04046 | 285.04025 | -0.74 | C15H10O6 | MS2[287]:81.0702(73), 121.1009(31), 153.0177(29) | MS2[285]:133.0285(100), 151.0028(34), 107.0127(27), 175.0394(16), 149.0236(16) | Kaempferol | L  S |
| 131 | 13.38 | 299.05611 | 299.05600 | -0.37 | C16H12O6 |  | MS2[299]:284.0324(100) | Chrysoeriol | L  S |
| 132 | 13.43\* | 315.05103 | 315.05099 | -0.11 | C16H12O7 |  | MS2[315]:300.0272(100), 151.0026(2) | Isorhamnetin | L |
| 133 | 13.92 | 299.05611 | 299.05582 | -0.97 | C16H12O6 |  | MS2[299]:284.0323(66) | Chrysoeriol isomer | L  S |
| 134 | 14.37 | 283.06119 | 283.06094 | -0.91 | C16H12O5 |  | MS2[283]:268.0375(84) | Genkwanin | L  S |
| 135 | 14.41 | 373.12818 | 373.12723 | -2.54 | C20H20O7 | MS2[373]:312.0981(81), 327.0851(80), 343.0802(72), 357.0958(34) |  | Isosinensetin | L  S |
| 136 | 14.53 | 311.22278 | 311.22275 | -0.10 | C18H32O4 |  | MS2[311]:293.1757(28), 275.1653(3) | Dihydroxyoctadecadienoic acid | L  S |
| 137 | 14.90 | 389.12309 | 389.12195 | -2.94 | C20H20O8 | MS2[389]:356.0880(20), 374.0984(14), 359.0751(8) |  | Demethylnobiletin | L  S |
| 138 | 14.91 | 487.34289 | 487.34259 | -0.63 | C30H48O5 | MS2[489]:201.1634(100), 205.1583(79), 187.1477(43), 147.1166(38) | MS2[487]:469.3320(14) | Tormentic acid | L  S |
| 139 | 15.03 | 311.22278 | 311.22281 | 0.09 | C18H32O4 |  | MS2[311]:293.2119(33), 275.2020(8) | Dihydroxyoctadecadienoic acid isomer | L  S |
| 140 | 15.77 | 389.12309 | 389.12213 | -2.48 | C20H20O8 | MS2[389]:374.0986(44), 359.0753(23), 356.0887(5) |  | Demethylnobiletin isomer | L  S |
| 141 | 16.45 | 277.21730 | 277.21695  279.23120 | -1.27 | C18H30O2 | MS2[279]:95.0858(100), 81.0703(98), 67.0548(67), 109.1013(42), 123.1167(26) | MS2[277]:234.1860(100), 134.8934(7), 121.0283(2) | α-Linolenic acid isomer | L  S |
| 142 | 19.33 | 277.21730 | 277.21692 | 0.59 | C18H30O2 | MS2[279]:81.0703(100), 95.0858(92), 109.1013(71), 67.0548(65), 123.1167(51) | MS2[277]:134.8934(100), 121.0282(46), 234.1857(20) | α-Linolenic acid | L  S |

\* identified by comparison with reference standards.

L: leaves; S: stems.