**Supporting Information**

**Unveiling the phytochemical profile and antioxidant activity of roots from six *Polygala* species**

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**Table S1** Mass spectrometric information and the post-acquisition strategies of the chemical components in six *Polygala* species detected by UPLC-Q-TOF-MS/MS

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Pe | RT | Molecular | Measured | Calculated | Errors | ESI-MSn | Identified |  |  |  |  |  |  |  |
| ak | (min) | formula | (m/z) | (m/z) |  | （-） | compounds | Class | PT | PS | PJ | PF | PA | PG |
| 1 | 6.743 | C13H8O5 | 243.0292 | 243.0299 | 0.0007 | MS2[243]161,93 | Gentitein | Xan | - | - | - | - | √ | - |
| 2 | 4.353 | C14H64O29 | 257.0727 | 257.0528 | -0.0199 | MS2[257]223,205,195,163 | 1,3-Dihydroxyl-2-methoxanthone/1,7-Dihydroxy-3-methoxyxanthone\* | Xan | √ | - | - | √ | - | - |
| 3 | 0.379 | C14H10O6 | 273.0392 | 273.0405 | 0.0013 | MS2[273]175 | 1,3,7-Trihydroxy-2-methoxyxanthone | Xan | - | - | √ | √ | √ | √ |
| 4 | 3.086 | C15H12O6 | 287.0861 | 287.0561 | -0.0300 | MS2[287]272,259 | 1,5-Dihydroxy-2,3-dimethoxyxanthone /1,6-Dihydroxy-3,7-dimethoxyxanthone /3-Hydroxy-2,8-dimethoxyxanthone\* | Xan | √ | - | √ | - | - | - |
| 5 | 3.093 | C15H12O6 | 287.0546 | 287.0561 | 0.0015 | MS2[287]273,257 | 1,7-Dihydroxy-2,3-dimethoxyxanthone | Xan | √ | - | √ | - | - | - |
| 6 | 0.434 | C16H14O6 | 301.2064 | 301.0718 | -0.1346 | MS2[301]285,215,131 | 1-Hydroxy-3,6,7-trimethoxyxanthone /Onjixanthone I\* | Xan | - | √ | - | - | - | - |
| 7 | 7.919 | C15H12O7 | 303.1294 | 303.0510 | -0.0783 | MS2[303]273,258 | Onjixanthone II | Xan | √ | √ | - | - | - | - |
| 8 | 7.948 | C15H12O7 | 303.0503 | 303.0518 | 0.0015 | MS2[303]273,258 | 1,6,7-Trihydroxoy-2,3-dimethoxyxanthone | Xan | √ | √ | - | - | - | - |
| 9 | 7.969 | C15H12O7 | 303.0294 | 303.0520 | 0.0226 | MS2[303]273,223 | 1,3,7-Trihydroxy-2,6-dimethoxyxanthone | Xan | √ | √ | - | - | - | - |
| 10 | 3.434 | C16H14O7 | 317.1449 | 317.0686 | -0.0763 | MS2[317]287 | 6, 8-Dihydroxy-1, 2, 4-trimethoxyxanthone | Xan | √ | √ | √ | √ | √ | √ |
| 11 | 23.980 | C16H14O7 | 317.1603 | 317.0611 | -0.0992 | MS2[317]287 | 1,3-Dihydroxy-2,4,7-trimethoxyxanthone | Xan | √ | √ | √ | √ | √ | √ |
| 12 | 25.083 | C16H14O7 | 317.1765 | 317.0649 | -0.1116 | MS2[317]287 | 6,8-Dihydroxy-1,2,3-trimethoxyxanthone | Xan | √ | √ | √ | √ | √ | √ |
| 13 | 24.315 | C16H14O7 | 317.1931 | 317.0652 | -0.1279 | MS2[317]287 | 1,8-Dihydroxy-2,3,6-trimethoxyxanthone | Xan | √ | √ | √ | √ | √ | √ |
| 14 | 24.215 | C16H14O7 | 317.1593 | 317.0689 | -0.0904 | MS2[317]287 | 1,6-Dihydroxy-3,5,7-trimethoxyxanthone | Xan | √ | √ | √ | √ | √ | √ |
| 15 | 24.585 | C16H14O7 | 317.1049 | 317.0679 | -0.0370 | MS2[317]287 | 3,6-Dihydroxy-1,2,7-trimethoxyxanthone | Xan | √ | √ | √ | √ | √ | √ |
| 16 | 3.952 | C17H16O7 | 331.0813 | 331.0823 | 0.0011 | MS2[331]301,295，245,235,223 | 6-Hydroxy-1,2,3,7-tetramethoxyxanthone | Xan | √ | √ | - | - | √ | √ |
| 17 | 3.904 | C17H16O7 | 331.0821 | 331.0842 | 0.0021 | MS2[331]301,293 | 2-(3,4-Dimethoxyphenyl)-3,5,7-trihydroxychroman-4-one | Xan | √ | √ | - | - | √ | √ |
| 18 | 0.457 | C12H22O11 | 341.1059 | 341.1089 | 0.0030 | MS2[341]198,179,161 | Sucrose | Oth | √ | √ | √ | √ | √ | √ |
| 19 | 4.360 | C19H18O10 | 405.1887 | 405.0822 | -0.1065 | MS2[405]357,341,315,285 | Lancerin | Xan | √ | √ | - | - | - | - |
| 20 | 4.935 | C19H18O11 | 421.3305 | 421.0776 | -0.2529 | MS2[421]205 | Mangiferin or isomer | Xan | - | - | √ | - | - | - |
| 21 | 6.005 | C20H20O11 | 435.0954 | 435.0933 | -0.0021 | MS2[435]405,399 | 7-*O*-Methylmangiferin | Xan | √ | √ | √ | - | - | - |
| 22 | 0.651 | C19H20O12 | 439.1717 | 439.0882 | -0.0835 | MS2[439]306,195,191,179 | Hydroxy-dihydromangiferin | Xan | √ | √ | - | √ | √ | √ |
| 23 | 1.242 | C19H26O13 | 461.2418 | 461.1295 | -0.1123 | MS2[461]281,239,179,137 | Sibiricose A3 | Oli | √ | √ | √ | √ | √ | √ |
| 24 | 0.444 | C17H30O15 | 473.1611 | 473.1512 | -0.0099 | MS2[473]341,131 | Galactopyranosyl-galactopyranosyl-arabinose | Oth | - | √ | √ | √ | - | - |
| 25 | 6.117 | C20H28O13 | 475.0560 | 475.1452 | 0.0892 | MS2[476]439,355,315,219,120 | Polygalatenoside D | Oli | - | - | √ | - | - | √ |
| 26 | 6.026 | C18H32O16 | 503.2291 | 503.1618 | -0.0673 | MS2[503]491,315,272,205,190,163 | Maltotriose | Oth | √ | √ | √ | √ | - | √ |
| 27 | 2.411 | C22H30O14 | 517.1561 | 517.1563 | 0.0002 | MS2[517]437 | Arillanin B | Oli | - | √ | √ | √ | √ | - |
| 28 | 2.253 | C22H30O14 | 517.3157 | 517.3229 | 0.0073 | MS2[517]193,175,160 | Sibiricose A5 | Oli | √ | √ | √ | √ | √ | √ |
| 29 | 5.257 | C24H26O14 | 537.1612 | 537.1245 | -0.0367 | MS2[537]417,405,387 | Sibiricaxanthone A | Xan | √ | √ | √ | √ | √ | √ |
| 30 | 5.278 | C24H26O14 | 537.2345 | 537.1294 | -0.1051 | MS2[537]387,315,267 | Sibiricaxanthone B | Xan | √ | √ | √ | √ | √ | √ |
| 31 | 2.566 | C23H32O15 | 547.0785 | 547.1663 | 0.0878 | MS2[547]341,299,223,205,190，175 | Sibiricose A6 | Oli | √ | √ | √ | √ | √ | √ |
| 32 | 10.442 | C23H32O15 | 547.2416 | 547.1668 | -0.0748 | MS2[547]367,295,265, 205 | Sibiricose A1 | Oli | √ | √ | √ | √ | √ | √ |
| 33 | 3.520 | C24H34O15 | 561.6109 | 561.1820 | -0.4289 | MS2[562]562,559 | Sibiricose A2 | Oli | √ | √ | √ | - | - | - |
| 34 | 5.179 | C25H28O15 | 567.1400 | 567.1397 | -0.0003 | MS2[567]345,315,272 | Polygalaxanthone III | Xan | √ | √ | √ | - | √ | √ |
| 35 | 4.367 | C25H28O15 | 567.1360 | 567.1355 | -0.0005 | MS2[567]461,285 | Wubangziside C | Xan | √ | √ | √ | - | √ | - |
| 36 | 9.121 | C26H30O15 | 581.1942 | 581.1506 | -0.0436 | MS2[581]273,257 | Polygalaxanthone V | Xan | √ | √ | - | √ | √ | √ |
| 37 | 46.809 | C27H32O15 | 595.2945 | 595.1663 | -0.1282 | MS2[595]365 | Polygalaxanthone IV | Xan | √ | √ | √ | √ | √ | - |
| 38 | 9.690 | C27H32O16 | 611.2104 | 611.1612 | -0.0492 | MS2[611]303,287 | Polygalaxanthone VII | Xan | √ | √ | - | - | - | √ |
| 39 | 11.674 | C29H34O15 | 621.1539 | 621.1819 | 0.0280 | MS2[621]499,337 | ReinioseB/ C\* | Oli | √ | - | - | √ | - | √ |
| 40 | 11.814 | C29H34O15 | 621.5603 | 621.1825 | -0.3778 | MS2[621]598,595 | Reiniose C/B\* | Oli | √ | - | - | - | - | - |
| 41 | 7.592 | C29H34O16 | 637.2643 | 637.1774 | -0.0869 | MS2[637]547,529,461 | Sibiricaxanthone F | Xan | √ | √ | √ | - | √ | - |
| 42 | 10.597 | C30H36O16 | 651.1979 | 651.1937 | -0.0042 | MS2[651]443 | Unknown | Oli | - | √ | √ | √ | - | - |
| 43 | 10.735 | C30H36O16 | 651.2006 | 651.1925 | -0.0081 | MS2[651]443 | 3'-Sinapoyl-6-benzoylsucrose | Oli | √ | √ | - | - | √ | √ |
| 44 | 7.393 | C30H36O17 | 667.1933 | 667.1844 | -0.0089 | MS2[667]461,205 | Tenuifoliside B | Oli | √ | √ | √ | √ | √ | √ |
| 45 | 8.561 | C30H36O17 | 667.3523 | 667.1879 | -0.1644 | MS2[667]461,357,205,190,137 | Tenuifoliside B2 | Oli | - | - | √ | - | - | - |
| 46 | 2.732 | C36H56O12 | 679.3143 | 679.3694 | 0.0551 | MS2[679]547,503,461,277,167 | Tenuifiolin | Sap | √ | √ | √ | √ | - | √ |
| 47 | 11.900 | C31H38O17 | 681.2026 | 681.2031 | 0.0005 | MS2[681]443 | Tenuifoliside A | Oli | √ | √ | √ | √ | √ | √ |
| 48 | 8.763 | C32H38O17 | 693.3674 | 693.2036 | -0.1638 | MS2[693]675,601,175 | Glomeratose B | Oli | √ | √ | - | √ | √ | - |
| 49 | 8.903 | C32H38O17 | 693.3674 | 693.2036 | -0.1638 | MS2[693]675,601,175 | 3-(3,4-Dimethoxyphenylpropionyl)fructose (2→1) 6-(4-methoxycinnamyl) glucose | Oli | √ | √ | - | √ | √ | - |
| 50 | 16.069 | C32H40O18 | 711.2145 | 711.2136 | -0.0009 | MS2[711]701,665,543 | Telephiose C | Oli | √ | - | √ | - | - | √ |
| 51 | 8.298 | C33H40O18 | 723.1199 | 723.2146 | 0.0947 | MS2[723]547,493 | 1'-Sinapoyl-3'-feruloylsucrose | Oli | - | √ | - | - | - | - |
| 52 | 10.557 | C33H40O18 | 723.2148 | 723.2142 | -0.0006 | MS2[723]547,517，205 | Arillanin A | Oli | √ | √ | √ | √ | √ | √ |
| 53 | 5.921 | C33H40O18 | 723.2159 | 723.2221 | 0.0062 | MS2[723]485,335,237 | 3'-Feruloy-6-sinapoylsucrose or isomer | Oli | - | √ | - | √ | √ | - |
| 54 | 17.840 | C34H42O18 | 737.3286 | 737.2293 | -0.0993 | MS2[737]499 | Reiniose A | Oli | √ | - | - | √ | √ | √ |
| 55 | 2.372 | C35H36O18 | 743.1217 | 743.1829 | 0.0612 | MS2[743]731,727 | Unknown | Oli | √ | - | - | - | - | - |
| 56 | 5.932 | C34H40O19 | 751.3131 | 751.2086 | -0.1045 | MS2[751]465,427,315,272 | Glomeratose E | Oli | - | - | √ | √ | √ | √ |
| 57 | 9.363 | C34H42O19 | 753.1604 | 753.2247 | 0.0643 | MS2[753]631,581,273 | Sibiricose A4 | Oli | √ | √ | √ | √ | √ | √ |
| 58 | 9.366 | C34H42O19 | 753.2266 | 753.2258 | -0.0008 | MS2[753]611,553,545 | 3,6'-Disinapoylsucrose | Oli | - | √ | - | - | - | - |
| 59 | 14.308 | C35H44O19 | 767.4602 | 767.2399 | -0.2203 | MS2[767]529,265,223，205 | Tenuifolioside C | Oli | √ | √ | √ | √ | √ | √ |
| 60 | 8.858 | C36H44O20 | 795.2121 | 795.2347 | 0.0226 | MS2[795]753,629,509,465 | 3-Acetyl-3',6-O-disinapoylsucrose | Oli | - | - | √ | - | - | - |
| 61 | 16.145 | C37H44O20 | 807.2368 | 807.2341 | -0.0027 | MS2[807]237,175 | Unknown | Sap | √ | √ | - | - | - | - |
| 62 | 18.505 | C39H46O21 | 849.3311 | 849.3830 | 0.0519 | MS2[849]819,779 | Unknown | Oth | √ | - | - | √ | - | - |
| 63 | 24.443 | C40H46O21 | 861.2534 | 861.2459 | -0.0075 | MS2[861]473,257 | Unknown | Oli | √ | √ | - | √ | √ | - |
| 64 | 3.441 | C41H48O22 | 891.3143 | 891.2559 | -0.0584 | MS2[891]861,753 | Tenuifoliside E | Oli | - | - | √ | - | - | √ |
| 65 | 8.532 | C40H52O24 | 915.7362 | 915.2776 | -0.4586 | MS2[915]651,561 | Reiniose F | Oli | √ | √ | √ | √ | √ | √ |
| 66 | 1.441 | C48H76O20 | 971.4835 | 971.4857 | 0.0022 | MS2[971]962 | Polygalasaponin XIV or isomer | Sap | √ | - | √ | - | - | - |
| 67 | 6.153 | C48H78O20 | 973.4192 | 973.5008 | 0.0816 | MS2[973]861,794,771 | Polygalasaponin VI | Sap | - | - | √ | - | - | - |
| 68 | 16.640 | C53H84O24 | 1103.4472 | 1103.5269 | 0.0797 | MS2[1103]957 | PolygalasaponinXXVIII | Sap | - | - | √ | √ | √ | √ |
| 69 | 6.467 | C54H86O24 | 1117.5446 | 1117.5431 | -0.0015 | MS2[1118]1093,1074 | Polygalasapion XXIV | Sap | √ | - | - | - | - | √ |
| 70 | 18.372 | C54H64O29 | 1175.3846 | 1175.3455 | -0.0391 | MS2[1175]1104,999,879 | Glomeratose F | Oli | √ | √ | √ | - | √ | √ |
| 71 | 14.102 | C55H68O31 | 1223.3968 | 1223.3672 | -0.0296 | MS2[1223]1077 | Tenuifoliose S | Oli | √ | √ | √ | √ | - | - |
| 72 | 22.534 | C53H70O33 | 1233.4521 | 1233.3727 | -0.0794 | MS2[1233]1203 | TenuifolioseV | Oli | - | √ | - | - | - | - |
| 73 | 31.448 | C58H92O28 | 1235.4486 | 1235.5691 | 0.1205 | MS2[1235]1205 | Arilloside B | Sap | √ | √ | - | - | √ | - |
| 74 | 31.462 | C58H92O28 | 1235.4238 | 1235.5702 | 0.1464 | MS2[1235]1205 | Arillatanoside A | Sap | √ | √ | - | - | - | - |
| 75 | 31.483 | C58H92O28 | 1235.4286 | 1235.5736 | 0.1450 | MS2[1235]1205 | Polygalasaponin XXII | Sap | √ | √ | - | - | - | √ |
| 76 | 8.964 | C59H94O28 | 1249.5850 | 1249.5854 | 0.0004 | MS2[1250]1217,1158 | Onjisaponin TF | Sap | - | - | √ | - | - | - |
| 77 | 13.620 | C56H70O32 | 1253.3512 | 1253.3798 | 0.0286 | MS2[1253]1077 | Tenuifoliose T | Oli | - | - | √ | - | - | - |
| 78 | 14.593 | C56H70O32 | 1253.4512 | 1253.3766 | -0.0746 | MS2[1253]1077 | Tricornose K | Oli | √ | - | - | - | √ | √ |
| 79 | 45.505 | C59H92O29 | 1263.5950 | 1263.5646 | -0.0304 | MS2[1264]1232 | OnjisaponinMF | Sap | - | - | - | - | - | √ |
| 80 | 45.065 | C59H94O29 | 1265.4223 | 1265.3850 | -0.0373 | MS2[1265]1250,1174 | Polygalasaponin XVI/DesacylsenegasaponinB\* | Sap | - | - | - | - | √ | - |
| 81 | 15.321 | C57H70O32 | 1265.3843 | 1265.3766 | -0.0077 | MS2[1265]1119 | Tenuifoliose K | Oli | √ | √ | √ | - | √ | √ |
| 82 | 52.513 | C57H72O33 | 1283.3851 | 1283.3883 | 0.0032 | MS2[1283]1253,1245 | Tenuifoliose X | Oli | √ | - | - | √ | - | √ |
| 83 | 52.899 | C57H72O33 | 1283.0372 | 1283.3919 | 0.3547 | MS2[1283]1253,1245 | Senegose D | Oli | √ | - | - | √ | - | - |
| 84 | 11.729 | C58H72O33 | 1295.3878 | 1295.3872 | -0.0006 | MS2[1295]1165,1147,1087 | Senegose K | Oli | - | √ | - | - | - | - |
| 85 | 11.744 | C58H72O33 | 1295.3883 | 1295.3873 | -0.0010 | MS2[1295]1119 | TenuifolioseC2 | Oli | - | √ | - | - | - | - |
| 86 | 11.779 | C58H72O33 | 1295.3829 | 1295.3872 | 0.0043 | MS2[1295]1119,1087,795 | Tenuifoliose E/C\* | Oli | - | √ | - | - | - | - |
| 87 | 15.748 | C58H72O33 | 1295.4205 | 1295.3896 | -0.0309 | MS2[1295]1119 | Tenuifoliose C/E\* | Oli | √ | √ | - | - | - | - |
| 88 | 15.558 | C58H74O33 | 1297.4205 | 1297.4040 | -0.0165 | MS2[1297]1119,958 | Tricornose I | Oli | - | - | - | √ | √ | √ |
| 89 | 16.467 | C59H72O33 | 1307.5212 | 1307.3872 | -0.1340 | MS2 [1307]1265 | Tenuifoliose J | Oli | √ | √ | √ | - | √ | - |
| 90 | 20.185 | C59H72O33 | 1307.5463 | 1307.3883 | -0.1580 | MS2[1307]1161 | Tenuifoliose I | Oli | √ | √ | √ | - | √ | - |
| 91 | 17.573 | C61H96O30 | 1308.4688 | 1307.5908 | -0.8780 | MS2[1308]1130 | PolygalasaponinXXXVII | Sap | - | - | - | √ | - | - |
| 92 | 29.672 | C65H96O28 | 1323.3630 | 1323.6010 | 0.2380 | MS2[1323]1292 | Onjisaponin TH | Sap | - | √ | - | √ | √ | - |
| 93 | 16.218 | C59H74O34 | 1325.7630 | 1325.3983 | -0.3647 | MS2[1325]1149 | Tenuifoliose P、senegoseB/C\* | Oli | √ | - | - | - | - | - |
| 94 | 13.148 | C60H74O34 | 1337.4599 | 1337.3988 | -0.0611 | MS2[1337]1161,1295 | Tenuifoliose D | Oli | √ | √ | - | - | √ | - |
| 95 | 16.948 | C60H74O34 | 1337.3581 | 1337.3978 | 0.0397 | MS2[1337]1295 | Tenuifoliose B | Oli | √ | √ | - | - | - | - |
| 96 | 15.086 | C61H74O34 | 1349.3710 | 1349.3978 | 0.0268 | MS2[1349]1223 | Tenuifoliose H | Oli | √ | √ | - | - | - | - |
| 97 | 13.018 | C61H76O35 | 1367.3954 | 1367.4083 | 0.0129 | MS2[1367]1307,1205,1161 | Reiniose I | Oli | - | √ | - | - | - | - |
| 98 | 13.029 | C61H76O35 | 1367.4099 | 1367.4094 | -0.0005 | MS2[1367]1337 | Senegose A | Oli | - | √ | - | - | - | - |
| 99 | 18.048 | C61H76O35 | 1367.4773 | 1367.4139 | -0.0634 | MS2[1367]1337 | Tenuifoliose O | Oli | √ | √ | - | - | - | - |
| 100 | 19.103 | C62H76O35 | 1379.4282 | 1379.4083 | -0.0199 | MS2[1379]1203,1337 | Tenuifoliose A/A2\* | Oli | √ | √ | - | - | - | - |
| 101 | 18.422 | C64H100O32 | 1379.8894 | 1379.6114 | -0.2780 | MS2[1380]1307,1175 | Onjisaponin TG | Sap | √ | √ | - | - | - | - |
| 102 | 14.956 | C64H102O32 | 1381.6282 | 1381.6281 | -0.0001 | MS2[1381]1351 | Polygalasaponin XIX | Sap | √ | - | √ | - | - | √ |
| 103 | 16.834 | C64H102O33 | 1397.6061 | 1397.6315 | 0.0254 | MS2[1398]1235,1103 | Arilloside D | Sap | √ | - | - | - | - | - |
| 104 | 16.855 | C64H102O33 | 1397.6361 | 1397.6225 | -0.0136 | MS2[1398]1235,1103 | Polygalasaponin XXIX | Sap | √ | - | - | √ | - | - |
| 105 | 19.374 | C63H78O36 | 1409.4764 | 1409.4189 | -0.0575 | MS2[1409]1233 | OnjisaponinY | Sap | √ | √ | - | - | - | - |
| 106 | 19.495 | C63H78O36 | 1409.4484 | 1409.3832 | -0.0652 | MS2[1409]1221,1201 | Tenuifoliose N | Oli | √ | √ | - | - | - | - |
| 107 | 16.841 | C64H100O34 | 1411.7932 | 1411.6018 | -0.1914 | MS2[1412]1412 | Desacylsenegin III | Sap | √ | - | √ | √ | - | - |
| 108 | 23.751 | C69H102O31 | 1425.3450 | 1425.6327 | 0.2877 | MS2[1425]1395 | Senegasaponin B | Sap | - | - | - | √ | - | √ |
| 109 | 45.045 | C65H114O34 | 1427.3205 | 1427.6191 | 0.2986 | MS2[1427]1397 | Unknown | Sap | √ | √ | √ | - | √ | √ |
| 110 | 17.500 | C66H104O34 | 1439.6355 | 1439.6331 | -0.0024 | MS2[1440]1019 | Arilloside E | Sap | - | √ | √ | - | - | - |
| 111 | 12.787 | C67H78O35 | 1441.5328 | 1441.4246 | -0.1082 | MS2[1442]753,643 | Glomeratose G | Oli | - | - | √ | - | - | √ |
| 112 | 13.048 | C65H82O37 | 1453.4470 | 1453.4462 | -0.0008 | MS2[1453]1337,1307,1161,653 | Tenuifoliose M | Oli | √ | √ | √ | √ | - | - |
| 113 | 13.063 | C65H82O37 | 1453.4980 | 1453.4451 | -0.0529 | MS2[1453]1337,1307,1161,653 | Tenuifoliose Q | Oli | √ | √ | - | - | - | - |
| 114 | 32.266 | C68H80O35 | 1455.6439 | 1455.6312 | -0.0127 | MS2[1456]1429 | OnjisaponinTH | Sap | √ | √ | √ | - | √ | √ |
| 115 | 32.401 | C68H80O35 | 1455.6946 | 1455.4402 | -0.2544 | MS2[1456]1151 | SeneginII/onjisaponin G\* | Sap | √ | √ | √ | - | - | √ |
| 116 | 15.915 | C71H106O32 | 1469.4555 | 1469.6583 | 0.2028 | MS2[1469]1222 | Onjisaponin Z | Sap | - | √ | - | - | √ | √ |
| 117 | 10.914 | C67H106O35 | 1469.8177 | 1469.6437 | -0.1740 | MS2[1470]1308,1097,1061 | Polygalasaponin XXXXII | Sap | - | √ | √ | - | - | √ |
| 118 | 13.098 | C66H84O38 | 1483.0972 | 1483.4557 | 0.3585 | MS2[1483]1453,1337,1307,1161 | Tenuifoliose G | Oli | √ | √ | - | - | √ | - |
| 119 | 13.440 | C71H106O33 | 1485.4339 | 1485.6533 | 0.2194 | MS2[1485]1238,679,287 | Onjisaponin E | Sap | - | - | √ | - | √ | - |
| 120 | 15.065 | C67H84O38 | 1495.3064 | 1495.4557 | 0.1493 | MS2[1495]1349 | Tenuifoliose L | Oli | √ | - | - | - | - | - |
| 121 | 13.112 | C34H42O19 | 1507.3190 | 1507.4568 | 0.1378 | MS2[1507]1420,1354,1148 | 3,6’-Disinapoyl sucrose | Oth | - | √ | - | - | √ | √ |
| 122 | 12.607 | C69H108O36 | 1511.3190 | 1511.6437 | 0.3247 | MS2[1511]904 | Reinioside F | Sap | √ | - | √ | - | - | - |
| 123 | 19.331 | C67H86O39 | 1513.9326 | 1513.4667 | -0.4659 | MS2[1513]1367 | Tenuifoliose W | Oli | √ | - | √ | √ | √ | - |
| 124 | 18.857 | C68H86O39 | 1525.8528 | 1525.6668 | -0.1860 | MS2[1526]1337 | Onjisaponion TE | Oli | √ | √ | - | - | - | - |
| 125 | 14.992 | C68H86O39 | 1525.9490 | 1525.4662 | -0.4828 | MS2[1525]1495,1379,1349,1203 | Tenuifoliose F | Oli | √ | √ | √ | - | - | - |
| 126 | 14.688 | C74H110O34 | 1541.4565 | 1541.6800 | 0.2235 | MS2[1541]1511 | Onjisaponin H | Sap | √ | √ | √ | - | √ | - |
| 127 | 53.453 | C74H110O35 | 1557.1086 | 1557.1755 | 0.0669 | MS2[1557]1506,1436 | SenegasaponinA | Sap | √ | - | - | - | - | - |
| 128 | 41.322 | C75H112O35 | 1572.4461 | 1571.6906 | -0.7555 | MS2[1572]1558 | Onjisaponin B | Sap | √ | √ | - | √ | - | √ |
| 129 | 54.001 | C75H110O36 | 1585.2409 | 1585.2794 | 0.0385 | MS2[1585]1566,1516 | Unknown | Sap | √ | - | - | - | - | - |
| 130 | 22.698 | C75H112O36 | 1587.4208 | 1587.4861 | 0.0653 | MS2[1587]1559 | Onjisaponin F | Sap | √ | √ | √ | √ | - | √ |
| 131 | 43.810 | C75H112O36 | 1588.2409 | 1587.6855 | -0.5554 | MS2[1588]1456 | Onjisaponin Wg | Sap | √ | - | √ | √ | - | √ |
| 132 | 34.786 | C76H112O36 | 1599.6883 | 1599.6805 | -0.0078 | MS2[1600]962,889 | Onjisaponin Gg/K\* | Sap | √ | √ | - | - | - | - |
| 133 | 34.822 | C76H112O36 | 1599.9565 | 1599.6855 | -0.2710 | MS2[1600]962,889 | Onjisaponin K/Gg\* | Sap | √ | √ | - | - | - | - |
| 134 | 33.250 | C76H114O36 | 1601.3883 | 1601.7110 | 0.3227 | MS2[1601]1310 | Unknown | Sap | √ | - | - | √ | - | - |
| 135 | 38.441 | C76H114O37 | 1617.4275 | 1617.6966 | 0.2691 | MS2[1617]198.163,100 | Onjisaponin R | Sap | √ | √ | - | √ | √ | √ |
| 136 | 15.670 | C77H122O41 | 1629.2464 | 1629.6955 | 0.4491 | MS2[1629]1599 | Senegasaponin C | Sap | √ | - | - | - | - | √ |
| 137 | 44.216 | C77H116O37 | 1631.4275 | 1631.7117 | 0.2842 | MS2[1631]1498,1396,1324 | Onjisaponin O | Sap | - | √ | √ | √ | - | √ |
| 138 | 34.362 | C78H116O38 | 1659.5477 | 1659.1000 | -0.4477 | MS2[1660]1494,1296 | Polygalasaponin XLV | Sap | √ | - | √ | - | - | - |
| 139 | 43.291 | C79H118O38 | 1673.7212 | 1673.7228 | 0.0016 | MS2[1674]1542 | Polygalasaponin XXXII | Sap | √ | - | - | - | - | - |
| 140 | 43.366 | C79H118O38 | 1673.8225 | 1673.7223 | -0.1002 | MS2[1674]1486,1470 | Tenuifoside A | Sap | √ | - | - | - | - | - |
| 141 | 43.431 | C76H118O41 | 1686.0000 | 1685.7071 | -0.2929 | MS2[1686]1674 | Onjisaponin Ng | Sap | √ | √ | √ | - | - | - |
| 142 | 15.463 | C79H118O39 | 1689.3487 | 1689.7328 | 0.3841 | MS2[1689]1543,1325 | MyrtifoliosideA1 | Sap | √ | - | - | - | - | - |
| 143 | 38.915 | C80H120O39 | 1703.6912 | 1703.7329 | 0.0417 | MS2[1704]1588,851 | Senegin IV | Sap | √ | √ | - | √ | √ | √ |
| 144 | 39.086 | C80H120O39 | 1703.7315 | 1703.7334 | 0.0019 | MS2[1704]1588,851 | Onjisaponin A | Sap | √ | √ | - | √ | √ | √ |
| 145 | 43.996 | C81H120O40 | 1731.5855 | 1731.7278 | 0.1423 | MS2[1732]1600,1410 | Onjisaponin W | Sap | √ | √ | √ | - | - | √ |
| 146 | 44.046 | C81H120O40 | 1731.7270 | 1731.7283 | 0.0013 | MS2[1732]1600 | Onjisaponin Fg | Sap | √ | √ | - | - | - | √ |
| 147 | 32.665 | C81H122O40 | 1733.4855 | 1733.7440 | 0.2585 | MS2[1733]958 | Onjisaponin S | Sap | √ | √ | - | - | √ | √ |
| 148 | 30.394 | C82H122O41 | 1762.3658 | 1761.7388 | -0.6270 | MS2[1762]1618 | Onjisaponin V | Sap | √ | √ | - | - | - | √ |
| 149 | 30.650 | C82H122O41 | 1762.1863 | 1761.7384 | -0.4479 | MS2[1762]1618 | Onjisaponin Vg | Sap | √ | √ | - | - | - | √ |
| 150 | 34.267 | C83H124O42 | 1791.3788 | 1791.7489 | 0.3701 | MS2[1791]1567 | Onjisaponin T | Sap | √ | - | - | - | - | √ |
| 151 | 43.532 | C85H126O42 | 1817.9973 | 1817.7646 | -0.2327 | MS2[1818]1686 | Onjisaponin J | Sap | √ | √ | - | - | - | - |
| 152 | 37.184 | C86H128O43 | 1847.7829 | 1847.9955 | 0.2126 | MS2[1848]1780,1734 | Onjisaponin L | Sap | - | √ | - | - | - | - |
| 153 | 44.360 | C87H130O44 | 1877.6660 | 1877.7851 | 0.1191 | MS2[1877]1732 | Onjisaponin Sg | Sap | √ | √ | - | - | - | √ |
| 154 | 36.066 | C87H130O45 | 1893.5631 | 1893.7806 | 0.2175 | MS2[1894]1851 | Onjisaponin Ug/X\* | Sap | - | √ | - | - | - | - |

Note\*: trace characterized, Xan: Xanthones, Oli: Oligosaccharide esters, Sap: Saponins, Oth: Other chemicals, √: contain, -: exclusive.

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**Figure S1** Screening of differential metabolites between PT and the remaining five *Polygala* species (A, PS vs. PT; B, PJ vs. PT; C, PF vs. PT; D,FG vs. PT; and E, PA vs. PT, the criteria was set to satisfy VIP values≥1, Fold change≥2, *p*≤0.05).