

Table S3. All phenolic compounds tentatively identified by LC-MS^E separated by classes and in retention time order.

| Number | Common Name | Molecular Formula | m/z (exp.) | RT (min) | Score (%) | Frag Score (%) | Frag database | Mass Error (ppm) | Isotope Similarity | Normalised abundance | | | | | | | | | | | | | | | |
|------------|--|-------------------|------------|----------|-----------|----------------|---|------------------|--------------------|----------------------|-------|--------------|--------|-------------|-------------|-------|--------------|--------|-------------|-------------|-------|--------------|--------|-------------|---|
| | | | | | | | | | | TPC | | | | | SM | | | | | US | | | | | |
| | | | | | | | | | | Carrot peel | Chard | Chayote peel | Papaya | Papaya seed | Carrot peel | Chard | Chayote peel | Papaya | Papaya seed | Carrot peel | Chard | Chayote peel | Papaya | Papaya seed | |
| FLAVONOIDS | | | | | | | | | | | | | | | | | | | | | | | | | |
| 1 | Neohesperidin | C28H34O15 | 609.1879 | 0.57 | 43.3 | 37.1 | 59.0120 (6.16%); 71.0120 (39.12%); 89.0226 (21.71%); 119.0330 (9.30%); 127.0380 (5.86%); 143.0331 (8.73%); 161.0437 (19.61%); 439.0833 (4.84%); 503.1611 (10.41%); 533.1717 (6.11%) | 8.88 | 89.46 | | | | | | | X | | X | X | X | | | | X | |
| 2 | Theaflavin | C29H24O12 | 563.1220 | 0.62 | 37.6 | 0.2 | 83.0120 (10.88%); 85.0319 (5.45%) | 4.47 | 92.76 | | | | | | | | | | X | | | | | | |
| 3 | Rhamnetin | C16H12O7 | 315.0517 | 0.69 | 37.1 | 5.0 | 123.0431 (4.14%); 159.0090 (5.56%) | 2.03 | 82.68 | | | | | | | | | X | | | | | X | | |
| 4 | Cyanidin 3-O-galactoside | C21H21O11+ | 448.1049 | 0.77 | 36.5 | 0.1 | 92.0240 (0.94%) | 8.54 | 91.78 | | | | | | | X | | X | | | | X | X | | |
| 5 | Peonidin 3-O-arabinoside | C21H21O11+ | 448.1027 | 1.41 | 41.0 | 21.4 | 330.0770 (2.89%); 341.0922 (9.16%) | 3.62 | 88.10 | | | | | | | X | | | | | | X | | | |
| 6 | Cyanidin 3-O-(6'-caffeoyl-glucoside) | C30H27O14+ | 610.1267 | 2.72 | 43.1 | 41.7 | 73.0277 (15.38%); 83.0120 (9.13%); 99.0070 (15.24%); 117.0327 (2.21%); 313.0915 (20.36%) | -9.94 | 84.84 | | | | | | | | | | X | | | | | | X |
| 7 | Cirsimaritin | C17H14O6 | 313.07014 | 2.94 | 37.8 | 0 | 0 | -5.16 | 95.03 | | | | X | | | | | | | | | | | | |
| 8 | (-)-Epigallocatechin | C15H14O7 | 305.0690 | 3.80 | 38.9 | 7.3 | 123.0432 (3.31%); 167.0331 (10.94%); 197.0437 (2.28%) | 7.47 | 95.41 | X | X | | X | X | X | X | | X | X | X | X | | | X | X |
| 9 | Kaempferol 3-O-rhamnoside | C21H19O10- | 430.0918 | 3.88 | 35.5 | 0.0 | 0 | 2.97 | 80.77 | | | | | | | X | | | | | | X | | | |
| 10 | Tectoridin | C22H22O11 | 461.1084 | 3.90 | 37.7 | 0.0 | 0 | -1.24 | 88.06 | | | | | | | | | | | | | | X | | |
| 11 | (-)-Epicatechin | C15H14O6 | 289.06921 | 3.91 | 36.6 | 0 | 0 | -8.81 | 92.51 | X | X | | X | X | | | | | | | | | | | X |
| 12 | Kaempferide | C16H11O6- | 298.0499 | 3.94 | 36.0 | 0.0 | 0 | 5.34 | 85.99 | | | | | | | X | | X | X | | | | X | | |
| 13 | Chrysoeriol 7-O-apiosyl-glucoside | C27H30O15 | 593.1509 | 4.10 | 47.8 | 43.4 | 73.0278 (36.10%); 83.0120 (30.46%); 193.0490 (82.02%); 259.0594 (2.03%); 283.0598 (3.65%); 353.0652 (83.92%); 383.0753 (38.07%) | -0.52 | 96.46 | | | X | | | | | | X | | | | | X | | |
| 14 | Peonidin 3-O-glucoside | C22H23O11+ | 462.1182 | 4.13 | 36.3 | 0.6 | 79.0171 (6.48%); 107.0120 (22.48%) | 3.01 | 84.48 | | | | | | | | | | X | | | | | | |
| 15 | Luteolin 6-C-glucoside | C21H20O11 | 447.0898 | 4.17 | 42.8 | 29.2 | 92.0250 (2.835); 117.0327 (18.70%); 130.0288 (3.03%); 145.0276 (4.72%); 232.0548 (3.25%); 273.0394 (1.17%); 401.0846 (4.24%) | -7.70 | 93.45 | | | | X | X | | | X | X | | | | X | X | X | |
| 16 | Eriocitrin/Neoeriocitrin | C27H32O15 | 595.1664 | 4.36 | 36.9 | 0.0 | 0 | -0.66 | 84.51 | | | | | | | | | X | | | | | X | | |
| 17 | Quercetin 3-O-rhamnosyl-rhamnosyl-glucoside | C33H40O20 | 755.2042 | 4.55 | 48.5 | 54.0 | 151.0017 (4.39%); 156.0404 (3.17%); 255.0282 (5.92%); 271.0232 (9.71%); 272.0286 (2.32%); 300.0259 (100%); 301.0310 (30.02%) | 0.25 | 88.75 | | | | | X | | | | X | | | | | | | X |
| 18 | Apigenin 7-O-apiosyl-glucoside | C26H28O14 | 563.1400 | 4.60 | 51.0 | 62.0 | 117.0326 (7.03%); 267.0258 (1.76%); 282.0518 (4.75%); 283.0593 (8.76%); 297.0357 (11.04%); 309.0372 (1.30%); 311.0547 (10.09%); 323.0547 (9.63%); 324.0613 (6.21%); 325.0701 (26.84%); 353.0651 (100%); 365.0654 (18.05%); 383.0759 (70.08%); 395.0762 (5.87%); 413.0869 (6.69%); 443.0973 (12.70%); 473.1082 (8.11%) | -1.07 | 94.09 | | | | X | | | | | X | | | | | X | | |
| 19 | Genistin | C21H20O10 | 431.1012 | 4.62 | 35.2 | 0.0 | 0 | 6.45 | 83.55 | | | | | | | | | | X | | | | | | X |
| 20 | Quercetin 3-O-glucuronide | C21H18O13 | 477.0632 | 4.66 | 41.2 | 25.7 | 446.0454 (3.02%) | -8.84 | 90.24 | | | X | | | | X | | X | X | | | X | | X | |
| 21 | Luteolin 7-O-rutinoside | C27H30O15 | 593.1509 | 4.72 | 37.1 | 0.0 | 0 | -0.47 | 85.99 | | | | | X | X | | | X | | | | | | | |
| 22 | Dihydroformononetin | C16H14O4 | 269.08121 | 4.76 | 55.1 | 95.5 | 121.0274 (100%) | -2.68 | 83.25 | | | | | X | | | | | | | | X | | | |
| 23 | Apigenin 6,8-di-C-glucoside | C27H30O15 | 593.1515 | 4.82 | 37.6 | 0.0 | 0 | 0.45 | 88.36 | | | | | | | | | X | | | | | X | | |
| 24 | 4'-O-Methylepigallocatechin | C16H16O7 | 319.08228 | 4.91 | 38.1 | 0 | 0 | -0.14 | 90.86 | X | | | | X | | | | | | | | | | | |
| 25 | Apigenin 6-C-glucoside | C21H20O10 | 431.09714 | 4.99 | 56.5 | 93 | 283.0595 (78.06%); 300.0273 (100%); 301.0334 (47.81%); 311.0543 (38.98%); 359.0659 (28.68%) | -2.84 | 92.91 | | | | X | X | | | | | | | | | | | |
| 26 | Apigenin 7-O-neohesperidoside | C27H30O14 | 577.1556 | 5.01 | 48.7 | 56.4 | 116.0490 (84.87%); 353.0653 (18.57%) | -1.23 | 88.48 | | | | X | X | | | | X | | | | | X | | |
| 27 | 5,7-Dihydroxyflavanone/Isoliquiritigenin/Dihydrodadszein | C15H12O4 | 255.0653 | 5.11 | 36.0 | 0.0 | 0 | -3.76 | 84.17 | | | | | | | | | | | | | | | | X |
| 28 | Not id compound I | C16H12O6 | 299.05583 | 5.18 | 38.6 | 0 | 0 | -0.95 | 94.22 | | | X | | | X | | | | | | | | | | |
| 29 | Quercetin 3-O-rutinoside | C27H30O16 | 609.1461 | 5.24 | 48.2 | 44.3 | 255.0284 (7.89%); 263.0582 (100%); 271.0232 (21.35%); 301.0326 (42.46%) | 0.00 | 96.89 | | | | | X | | | | | | | | X | | | |
| 30 | Petrellin | C19H18O8 | 373.0950 | 5.38 | 37.4 | 0.0 | 0 | 5.76 | 93.81 | | | | | | | | | | X | | | | | | |
| 31 | Gardenin B | C19H18O7 | 357.0969 | 5.43 | 36.1 | 0.0 | 0 | -3.12 | 83.93 | | | | | | | | | | X | | | | | | |
| 32 | Apigenin 7-O-rutinoside | C27H30O14 | 577.1561 | 5.46 | 44.0 | 32.7 | 59.0118 (27.31%); 158.0593 (100%); 353.0651 (89.60%) | -0.32 | 87.79 | | | | | | | | | X | | | | | X | | |
| 33 | Eriodictyol | C15H12O6 | 287.0548 | 5.47 | 42.0 | 18.4 | 59.0118 (32.92%); 241.0493 (46.14%) | -4.41 | 96.51 | | | X | | | X | | | | | | | | | | X |
| 34 | Phlorein | C15H14O5 | 273.0755 | 5.49 | 41.0 | 26.4 | 241.0493 (43.98%) | -4.84 | 83.95 | | | X | | | X | | | | | | | | | | X |
| 35 | Glycitin | C22H22O10 | 445.1133 | 5.53 | 39.0 | 8.1 | 117.0331 (17.47%); 309.0611 (1.90%) | -1.52 | 88.68 | | | | | | | X | | | | | | X | | X | |
| 36 | Eupatorin/Cirsilineol | C18H16O7 | 343.0847 | 5.63 | 36.9 | 0.0 | 0 | 6.79 | 91.98 | | | | | | | | | | | | | | | | X |
| 37 | Not id compounds II | C16H12O6 | 299.05569 | 5.63 | 57.6 | 97.7 | 269.0443 (100%) | -1.39 | 91.95 | | | X | | | | | | | | | | | | | |

[illegible]

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|-------------------|---------------------------------|-----------|-----------|------|-------|------|---|--------|-------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 94 | Benzoic acid | C7H6O2 | 121.0285 | 3.35 | 38.0 | 0.0 | 0 | -8.12 | 99.23 | X | X | X | X | X | | | | | | | | | | |
| 95 | 5-Caffeoylquinic acid | C16H18O9 | 353.0864 | 3.41 | 45.1 | 33.3 | 85.0276 (4.53%); 87.0069 (1.29%); 127.0381 (1.82%); 135.0431 (1.83%); 161.0224 (2.50%); 173.0437 (1.26%); 191.0543 (100%) | -3.91 | 96.87 | X | X | | | | X | X | | X | X | | | | | |
| 96 | 4-Hydroxymandelic acid | C8H8O4 | 167.03415 | 3.42 | 55.5 | 92.1 | 125.0244 (100%) | -4.98 | 91.19 | | X | | | X | | | | | | | | | | |
| 97 | 3-Hydroxyphenylacetic acid | C8H8O3 | 151.03887 | 3.44 | 52.1 | 77.0 | 125.0244 (100%) | -7.89 | 92.06 | | X | X | X | X | | | | | | | | | | |
| 98 | Vanillic acid | C10H12O5 | 211.0594 | 3.51 | 41.8 | 25.9 | 168.0768 (35.97%) | -8.47 | 92.41 | | | | X | | | | X | | | | | | | |
| 99 | 3-Feruloylquinic acid | C17H20O9 | 367.1025 | 3.59 | 45.4 | 31.2 | 117.0332 (18.38%); 155.0329 (12.09%); 193.0493 (100%) | -2.69 | 98.92 | X | X | | | | X | X | | | | X | X | | | |
| 100 | Phenylacetic acid | C8H8O2 | 135.0448 | 3.60 | 39.3 | 0.0 | 0 | -2.55 | 99.76 | X | X | X | X | X | | | | | | | | | | |
| 101 | Dihydroxybenzoic acid isomer IV | C7H6O4 | 153.0189 | 3.64 | 39.1 | 0.0 | 0 | -3.04 | 98.92 | | X | X | X | X | | | | | | | | | | |
| 102 | Feruloyl glucose | C16H20O9 | 355.1026 | 3.64 | 35.9 | 0.0 | 0 | -2.40 | 82.21 | X | X | | | | | | | | | | | | | |
| 103 | 2,3,4-Trihydroxybenzoic acid | C7H6O5 | 169.01409 | 3.65 | 47.5 | 44.9 | 113.0239 (60.82%) | -0.91 | 93.55 | | X | | | X | | | | | | | | | | |
| 104 | Phenacetyl glycine | C10H11NO3 | 192.0648 | 3.72 | 37.6 | 0.0 | 0 | -9.48 | 98.31 | | | | | | | | X | X | | | | | | X |
| 105 | Caffeoylquinic acid isomer III | C16H18O9 | 353.08644 | 3.75 | 56.6 | 98.1 | 191.0562 (100%) | -3.86 | 89.62 | X | | | | | | | | | | | | | | |
| 106 | Dihydroferulic acid | C10H12O4 | 195.0646 | 3.86 | 36.4 | 4.8 | 73.0277 (100%); 83.0120 (76.95%) | -8.40 | 86.50 | | | | | | | | X | | | | | | | |
| 107 | 4-p-Coumaroylquinic acid | C16H18O8 | 337.09195 | 3.92 | 57.9 | 98.0 | 119.0508 (24.03%); 191.0561 (100%) | -2.77 | 94.52 | X | X | | | | | | | | | | | | | |
| 108 | Homovanillic acid | C9H10O4 | 181.05063 | 3.96 | 38.2 | 0.0 | 0 | 0.00 | 90.88 | X | | | | | | | | | | | | | | |
| 109 | O-Methylgallic acid isomer II | C8H8O5 | 183.0281 | 4.20 | 37.5 | 0.0 | 0 | -10.00 | 98.50 | | X | | | | | | X | | | | | | | X |
| 110 | m-Coumaric acid | C9H8O3 | 163.03939 | 4.31 | 37.3 | 0.0 | 0 | -4.11 | 91.24 | X | | X | X | X | | | | | | | | | | |
| 111 | Rosmarinic acid | C18H16O8 | 359.0792 | 4.32 | 38.5 | 14.2 | 135.0431 (100%); 239.0548 (34.16%) | 5.49 | 84.62 | X | | | | | | | X | | | | | | | |
| 112 | p-Coumaric acid | C9H8O3 | 163.03972 | 4.58 | 58.1 | 96.2 | 119.0510 (100%) | -2.15 | 96.94 | X | X | X | X | X | | | | | | | | | | |
| 113 | Cinnamic acid | C9H8O2 | 147.0452 | 4.62 | 39.7 | 0.0 | 0 | 0.35 | 98.71 | X | | X | X | X | X | | | | | | | | | |
| 114 | Ethyl caffeate | C11H12O4 | 207.06478 | 4.69 | 35.9 | 0.0 | 0 | -7.21 | 87.87 | | X | X | | | | | | | | | | | | |
| 115 | Isoferulic acid | C10H10O4 | 193.05006 | 5.03 | 57.0 | 90.2 | 130.0422 (100%); 133.0286 (25.06%) | -2.95 | 98.48 | X | X | X | X | X | | | | | | | | | | |
| 116 | Kaempferol 3-O-rutinoside | C27H30O15 | 593.1509 | 5.26 | 37.0 | 4.7 | 283.0234 (4.97%) | -0.43 | 80.70 | | | | | | | | X | | | | | | | |
| 117 | Trans-ferulic acid | C10H10O4 | 193.0489 | 5.36 | 37.6 | 0.0 | 0 | -8.75 | 97.52 | | | | | | | | X | X | X | | | X | X | X |
| 118 | Dicafeoylquinic acid isomer I | C25H24O12 | 515.1199 | 5.51 | 42.8 | 24.1 | 161.0224 (22.64%) | 0.78 | 90.98 | X | | | | | | | | | | | | | | |
| 119 | Ferulic acid | C10H10O4 | 193.0490 | 5.53 | 42.0 | 21.7 | 117.0331 (100%) | -8.59 | 97.67 | X | X | X | X | X | | | X | X | X | X | X | X | X | X |
| 120 | Sinapic acid | C11H12O5 | 223.0598 | 5.56 | 46.1 | 40.2 | 121.0282 (66.82%); 149.0230 (100%); 166.0253 (5.33%); 167.0330 (54.78%) | -6.35 | 97.63 | | X | | X | | | | X | | X | | | X | | X |
| 121 | Dicafeoylquinic acid isomer II | C25H24O12 | 515.1200 | 5.66 | 41.1 | 8.2 | 161.0234 (3.54%) | 0.90 | 98.21 | X | | | | | | | | | | | | | | |
| 122 | Hippuric acid | C9H9NO3 | 178.0497 | 5.68 | 35.4 | 0.0 | 0 | -7.12 | 85.15 | | | | | | | | X | | | | | | | |
| 123 | Dihydro-p-coumaric acid | C9H10O3 | 165.05481 | 5.90 | 38.3 | 0.0 | 0 | -5.45 | 97.53 | X | | | | | | | | | | | | | | |
| 124 | 4-Hydroxybenzoic acid | C7H6O3 | 137.0238 | 5.92 | 50.5 | 58.1 | 92.0257 (80.05%); 119.0122 (100%) | -4.30 | 99.49 | X | X | X | X | X | X | | | X | | | | | | X |
| 125 | Dicafeoylquinic acid isomer III | C25H24O12 | 515.1199 | 6.03 | 50.7 | 56.8 | 135.0446 (59.78%); 179.0346 (73.43%); 353.0872 (5.26%) | 0.74 | 97.37 | X | | | | | | | | | | | | | | |
| 126 | Dicafeoylquinic acid isomer IV | C25H24O12 | 515.1186 | 6.29 | 44.1 | 25.0 | 135.0431 (41.76%); 179.0330 (67.93%); 353.0865 (9.38%) | -1.77 | 97.62 | | | | | | X | | | | | | X | | | |
| 127 | Danshensu | C9H10O5 | 197.0457 | 7.16 | 40.6 | 14.4 | 141.0542 (7.46%); 144.0440 (15.20%); 154.0642 (10.18%); 156.0439 (19.05%); 172.0392 (7.65%) | 0.76 | 89.58 | | | | | | | | X | | | | | | | |
| 128 | Caffeic acid | C9H8O4 | 179.0346 | 7.67 | 56.8 | 87.7 | 135.0445 (100%) | -1.94 | 98.56 | X | X | X | X | X | X | | | | | | | | | |
| 129 | Cinnamoyl glucose | C15H18O7 | 309.1004 | 8.87 | 37.1 | 10.9 | 85.0281 (39.49%); 265.0528 (5.77%); 267.0901 (17.29%); 295.0854 (9.94%) | 7.78 | 83.51 | | | | | | | | X | | | | | | | |
| OTHER POLYPHENOLS | | | | | | | | | | | | | | | | | | | | | | | | |
| 130 | Hydroxytyrosol | C8H10O3 | 153.05473 | 1.08 | 36.7 | 0 | 0 | -6.42 | 91.04 | | | | | X | X | | | | | | | | | |
| 131 | 4-Vinylphenol | C8H8O | 119.04967 | 1.10 | 37.2 | 0 | 0 | -4.73 | 91.47 | | X | | | X | X | | | | | | | | | |
| 132 | Oleuropein | C25H32O13 | 539.1718 | 1.12 | 38.3 | 8.8 | 118.0284 (0.82%); 134.0593 (32.88%); 175.0400 (1.56%); 206.0447 (2.69%); 212.0668 (2.23%); 242.0769 (3.12%) | -9.58 | 93.05 | | | | | | | | | X | | | | | | |
| 133 | Curcumin | C21H20O6 | 367.1162 | 1.24 | 36.7 | 3.1 | 83.0120 (4.58%); 97.0277 (17.17%) | -6.82 | 87.90 | | | | | | | | | X | | | | | | |
| 134 | 3,4-Dihydroxyphenylglycol | C8H10O4 | 169.0495 | 1.67 | 37.9 | 0.0 | 0 | -6.52 | 96.67 | | | | | | | | | | | | | X | | X |
| 135 | Catechol | C6H6O2 | 109.02891 | 1.78 | 38.1 | 0 | 0 | -5.42 | 96.82 | | X | | | X | | | | | | | | | | |
| 136 | Salvianolic acid D | C11H10O6 | 237.0391 | 2.23 | 44.4 | 35.9 | 181.0123 (100%) | -5.57 | 92.34 | | | | | | | | | X | | | | | | X |
| 137 | Pyrogallol | C6H6O3 | 125.0235 | 2.50 | 38.4 | 2.8 | 79.0185 (3.68%) | -7.42 | 97.71 | | X | X | X | X | X | | | X | | | | | | X |
| 138 | Methylcatechol isomer I | C7H8O2 | 123.04527 | 2.51 | 39.6 | 0 | 0 | 0.92 | 99.21 | | X | | | X | | | | | | | | | | |
| 139 | Syringaldehyde | C9H10O4 | 181.0489 | 2.92 | 38.5 | 12.0 | 116.0488 (100%) | -9.61 | 91.14 | X | | X | | | | | X | X | | X | X | X | X | X |
| 140 | Protocatechuic aldehyde | C7H6O3 | 137.0237 | 2.93 | 55.2 | 83.6 | 108.0217 (93.03%); 123.0455 (100%) | -5.47 | 98.84 | X | X | X | X | X | X | | | | | | | | | |
| 141 | Resacetophenone | C8H8O3 | 151.03886 | 2.94 | 55.5 | 91.5 | 108.0217 (93.03%); 123.0455 (100%) | -7.95 | 94.78 | | | | X | | | | | | | | | | | |
| 142 | Acetyl eugenol | C12H14O3 | 205.0866 | 2.94 | 37.3 | 0.0 | 0 | -2.04 | 88.88 | | | | | | | | X | | | | | | | |
| 143 | Isopimpinellin | C13H10O5 | 245.04432 | 3.05 | 36 | 0 | 0 | -4.98 | 85.81 | | | | X | | | | | | | | | | | |
| 144 | Myricenic Acid | C9H6O3 | 161.02443 | 3.19 | 50.9 | 57.5 | 133.0297 (40.60%); 134.0368 (15.40%); 135.0450 (67.22%) | 0.10 | 97.03 | X | | | | | | | | | | | | | | |
| 145 | Methylcatechol isomer II | C7H8O2 | 123.04432 | 3.26 | 51.8 | 69 | 108.0214 (100%) | -6.69 | 97.84 | | X | | | X | | | | | | | | | | |
| 146 | 5-Tricosylresorcinol | C29H52O2 | 431.3867 | 3.26 | 36.90 | 8.46 | 109.0272 (64.72%); 119.0487 (100%) | -6.33 | 83.42 | | | | | | | | X | X | | | X | | | |
| 147 | Oleoside dimethylester | C18H26O11 | 417.1398 | 3.32 | 38.4 | 0.0 | 0 | -0.93 | 93.26 | | | | | | | | | X | | | | | | |
| 148 | [6]-Gingerol | C17H32O4 | 299.2204 | 3.36 | 34.7 | 0.0 | 0 | -7.97 | 82.19 | | | | | | | | | | X | | | | | X |
| 149 | Esculetin | C9H6O4 | 177.01857 | 3.54 | 38.1 | 0 | 0 | -4.26 | 95.69 | X | X | X | X | X | | | | | | | | | | |
| 150 | 6,7-Furanocoumarin | C11H6O3 | 185.0259 | 3.54 | 37.6 | 8.7 | 145.0278 (10.48%) | 7.74 | 88.21 | | | | | | | | | | X | | | | | |
| 151 | Coumarin | C9H6O2 | 145.0306 | 3.60 | 40.0 | 16.3 | 117.0332 (57.38%) | 7.33 | 92.09 | X | X | | | X | X | | | | | | | | | X |
| 152 | Scopoletin | C10H8O4 | 191.0332 | 3.60 | 40.7 | 14.3 | 97.0276 (15.77%); 99.0432 (33.71%) | -9.36 | 99.45 | | | X | | | | | X | | X | X | | | | X |
| 153 | Arbutin | C12H16O7 | 271.0812 | 3.91 | 39.8 | 6.0 | 141.0170 (0.74%) | -4.10 | 97.71 | | X | | | | | | X | | | | X | | X | |

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|-----------|---------------------------------|----------|-----------|-------|------|------|------------------------------------|-------|-------|---|---|---|---|---|---|---|---|---|---|---|---|
| 154 | Phenol | C6H6O | 93.035067 | 3.94 | 38.5 | 0 | 0 | 5.09 | 98.56 | | X | X | | X | | | | | | | |
| 155 | Umbelliferone | C9H6O3 | 161.02442 | 3.96 | 39.3 | 0 | 0 | 0.01 | 96.61 | X | X | | X | | | | | | | | |
| 156 | Vanillin | C8H8O3 | 151.03954 | 4.46 | 38 | 0 | 0 | -3.47 | 93.86 | X | X | X | | | | | | | | | |
| 157 | Ferulaldehyde/Mellein | C10H10O3 | 177.0564 | 4.49 | 37.7 | 0 | 0 | 3.83 | 93.22 | | X | | | | | | | | | | |
| 158 | Esculin | C15H16O9 | 339.07091 | 5.28 | 48.3 | 50.8 | 121.0289 (100%); 149.0237 (84.01%) | -3.67 | 95.21 | | X | | | | | | | | | | |
| 159 | Sinapaldehyde | C11H12O4 | 207.06658 | 5.90 | 38.3 | 0 | 0 | 1.44 | 93.11 | X | | | | | | | | | | | |
| 160 | Coumestrol | C15H8O5 | 267.0319 | 6.45 | 35.1 | 0.0 | 0 | 7.64 | 84.01 | | | | | | | | X | | | | X |
| 161 | 4-Hydroxybenzaldehyde | C7H6O2 | 121.0290 | 7.55 | 57.8 | 94.9 | 92.0263 (100%) | -3.91 | 98.89 | X | X | X | X | X | | | | | | | X |
| 162 | Demethoxycurcumin | C20H18O5 | 337.10822 | 11.12 | 38 | 0 | 0 | 0.21 | 90.31 | X | | | | | | | | | | | X |
| 163 | Carnosol | C20H26O4 | 329.1745 | 12.23 | 37.9 | 0.0 | 0 | -4.12 | 94.29 | | | | | | | X | | | | X | |
| LIGNANS | | | | | | | | | | | | | | | | | | | | | |
| 164 | Sesaminol/Episesaminol I | C20H18O7 | 369.0979 | 1.71 | 38.7 | 0.0 | 0 | -0.31 | 93.76 | | | | | | X | X | | X | | X | X |
| 165 | Enterolactone | C18H18O4 | 297.1158 | 11.37 | 34.4 | 0.0 | 0 | 8.50 | 81.44 | | | | | | | X | | | | | |
| 166 | 1-Acetoxypinoresinol | C22H24O8 | 415.1365 | 3.57 | 35.6 | 5.3 | 135.0430 (100%) | -8.05 | 81.86 | | | | | | | X | | | X | | |
| 167 | Schisantherin A | C30H32O9 | 535.2024 | 4.06 | 35.9 | 0.0 | 0 | 9.34 | 89.60 | | | | | | | | X | | | | |
| 168 | Sesaminol/Episesaminol II | C20H18O7 | 369.0945 | 4.40 | 34.5 | 0.0 | 0 | -9.29 | 82.79 | | | | | X | | | | X | | X | |
| 169 | Dimethylmatairesinol/Gomisin M2 | C22H26O6 | 385.1621 | 5.29 | 35.7 | 0.0 | 0 | -9.24 | 88.57 | | | | | | | | X | | | | |
| STILBENES | | | | | | | | | | | | | | | | | | | | | |
| 170 | Viniferin/Pallidol | C28H22O6 | 453.1352 | 4.64 | 36.1 | 0.0 | 0 | 1.84 | 82.55 | | | | | | | | X | | | | |
| 171 | Resveratrol 3-O-glucoside | C20H22O8 | 389.1230 | 5.40 | 39.7 | 10.9 | 265.0731 (5.83%) | -2.99 | 91.02 | | | | | | X | X | X | | X | X | X |
| 172 | Piccatannol | C14H12O4 | 243.0648 | 6.08 | 37.9 | 0.0 | 0 | -5.91 | 96.22 | | X | | | X | | | | | | | X |

m/z = mass/charge. Bold represent reference standards.