

Table S1. High-resolution electrospray ionization mass spectrometry (HR-ESI-MS) data of metabolites extracted from pomegranate anthers. Rt, retention time.

| Peak | R _t (min) | [M+NH ₄] ⁺ /[M+H] ⁺ /[M-H] ⁻ (<i>m/z</i>) | MS/MS (<i>m/z</i>) | Calculated formula | Tentative identification |
|------|----------------------|---|---|---|---|
| 1 | 0.98 | -/-/154.0621 | -/-/93.0457, 110.0722, 137.0356 | C ₆ H ₉ N ₃ O ₂ | L-histidine |
| 2 | 1.00 | -/-/146.0495 | -/-/102.0560, 128.0353 | C ₅ H ₁₀ N ₂ O ₃ | Glutamine |
| 3 | 1.03 | -/-/165.0402 | -/-/75.0086, 129.0192 | C ₆ H ₆ N ₄ O ₂ | 7-Methylxanthine |
| 4 | 1.04 | -/-/135.0371 | -/-/75.0087, 89.0244 | C ₄ H ₄ O ₅ | L-Threonic acid |
| 5 | 1.04 | -/-/341.1091 | -/-/59.0138, 71.0137, 89.0243, 101.0243, 119.0347, 179.0560, 341.1091 | C ₁₂ H ₂₂ O ₁₁ | Trehalose |
| 6 | 1.04 | -/-/377.0854 | -/-/341.1091 | C ₁₈ H ₁₈ O ₉ | Unknown |
| 7 | 1.12 | -/-/300.0489 | -/-/78.9589, 96.9694 | C ₈ H ₁₆ NO ₉ P | N-Acetyl- α -D-glucosamine 1-phosphate |
| 8 | 1.12 | -/-/179.0559 | -/-/59.0137, 75.0086, 143.0384, 161.0454 | C ₆ H ₁₂ O ₆ | D-(-)-Fructose |
| 9 | 1.12, 1.37 | - /136.02/134.014 2 | -/91.05, 119.05, 136.02/71.0138, 89.0243, 115.0036, 133.0142 | C ₄ H ₆ O ₅ | Malic acid |
| 10 | 1.14 | -/-/149.0453 | -/-/59.0138, 75.0086, 131.0348 | C ₅ H ₁₀ O ₅ | D-(-)-Arabinose |
| 11 | 1.15 | -/-/259.0294 | -/-/78.9589, 96.9692, 138.9702, 198.9908 | C ₆ H ₁₃ O ₉ P | D-Glucose 6-phosphate |
| 12 | 1.18 | -/-/439.0858 | -/-/78.9589, 96.9694 | C ₁₉ H ₂₀ O ₁₂ | Unknown |
| 13 | 1.38 | -/-/323.0283 | -/-/78.9590, 96.9694, 111.0200 | C ₉ H ₁₃ N ₂ O ₉ P | Uridine monophosphate (UMP) |
| 14 | 1.43 | -/-/188.0564 | -/-/98.0246, 114.0559, 142.0508, 144.0665 | C ₇ H ₁₁ NO ₅ | N-Acetyl-DL-glutamic acid |
| 15 | 1.54 | -/-/128.0352 | -/-/128.0352 | C ₅ H ₇ NO ₃ | 4-oxoproline |
| 16 | 1.55 | -/-/191.0197 | -/-/85.0294, 87.0086, 111.0086, 129.0193 | C ₆ H ₈ O ₇ | D-(-)-Quinic acid; Citric acid |
| 17 | 1.60 | -/-/611.1443 | -/-/128.0351, 143.0461, 306.0767 | C ₂₀ H ₃₂ N ₆ O ₁₂ S ₂ | L-Glutathione oxidized |
| 18 | 1.88 | 350.0997/- /331.0672 | 109.0287, 127.0389, 145.0495, 153.0179, 171.0285, 315.0710, /-/125.0242, 151.0035, 169.0141, 211.0247, 241.0357, 271.0451 | C ₁₃ H ₁₆ O ₁₀ | Galloyl glucoside |
| 19 | 2.25, 7.70, 8.75 | 652.1132/- /633.0740 | 259.0233, 277.0338, 303.0129, 447.0553/-/125.0241, 169.0141, 231.0295, 249.0403, 275.0198, 300.9989 | C ₂₇ H ₂₂ O ₁₈ | 6-O-galloyl-2, 3-(S)-hexahydroxydiphenoyl -D-glucose; Corilagin; Isocorilagin; Hippomanin A; Gemin D; Strictinin (galloyl |

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|----|---------------------------|-----------------------------|---|---|---|
| | | | | | HHDP glucoside) |
| 20 | 2.27 | - /171.0288/169.0 141 | -/81.0341, 107.0130, 109.0286, 125.0233, 127.0389, 153.0180/125.0242 | C ₇ H ₆ O ₅ | Gallic acid |
| 21 | 2.29 | -/-/153.0192 | -/-/83.0138, 151.0036 | C ₇ H ₆ O ₄ | 2,4-Dihydroxybenzoic acid |
| 22 | 2.42, 4.45, 5.89, 7.12 | 502.1180/- /483.0782 | 127.0390, 153.0180, 171.0285, 297.0598, 315.0703/-/125.0243, 169.0141, 313.0565, 331.0675 | C ₂₀ H ₂₀ O ₁₄ | (Digalloyl glucoside) Gallic acid 3- <i>O</i> -β-D-(6'- <i>O</i> - galloyl)-glucopyranoside |
| 23 | 2.54 | - /345.0812/343.0 669 | -/153.0180/191.0561 | C ₁₄ H ₁₆ O ₁₀ | Unknown |
| 24 | 3.04 | -/-/295.1035 | -/-/59.0138, 71.0137, 89.0243, 101.0244, 119.0349 | C ₁₁ H ₂₀ O ₉ | Unknown |
| 25 | 4.37 | -/467.0816/- | -/153.0180/- | C ₂₀ H ₁₈ O ₁₃ | Unknown |
| 26 | 4.44 | -/-/218.1033 | -/-/88.0403, 146.0822 | C ₉ H ₁₇ NO ₅ | Pantothenic acid |
| 27 | 4.65 | -/-/325.0565 | -/-/93.0343, 125.0242, 169.0141 | C ₁₄ H ₁₄ O ₉ | Unknown |
| 28 | 4.79 | -/-/487.1098 | -/-/125.0242, 169.0141, 211.0249, 331.0672, 469.0991 | C ₂₀ H ₂₄ O ₁₄ | Galloyl-hexoside derivative |
| 29 | 5.36 | -/-/309.1193 | -/-/59.0137, 89.0243, 101.0244, 119.0349 | C ₁₂ H ₂₂ O ₉ | Unknown |
| 30 | 6.08 | -/-/203.0828 | -/-/74.0247, 116.0505, 142.0662, 159.0928 | C ₁₁ H ₁₂ N ₂ O ₂ | D-(+)-tryptophan |
| 31 | 6.26 | - /469.1339/467.1 198 | -/139.0388/125.0243, 137.0247, 167.0349, 179.0347, 219.0655, 305.0666 | C ₂₁ H ₂₄ O ₁₂ | Unknown |
| 32 | 6.65 | -/595.1439/- | -/271.0595, 433.1123/- | C ₂₇ H ₃₁ O ₁₅ ⁺ | Cyanidin-3- <i>O</i> -rutinoside |
| 33 | 6.67 | - /497.0923/495.0 784 | -/153.0180, 305.0285/191.0561, 343.0669 | C ₂₁ H ₂₀ O ₁₄ | Unknown |
| 34 | 6.74 | -/-/611.1619 | -/-/93.0345, 149.0244, 165.0190, 193.0140, 269.0453, 287.0557, 355.0678, 449.1100 | C ₂₇ H ₃₁ O ₁₆ ⁺ | Cyanidin-3,5-di- <i>O</i> -glucoside |
| 35 | 6.80 | -/-/401.1089 | -/-/134.0372, 149.0607, 178.0270, 193.0505, 355.1036 | C ₁₇ H ₂₂ O ₁₁ | Unknown |
| 36 | 6.81 | -/-/355.1035 | -/-/134.0372, 149.0606, 178.0270, 193.0505 | C ₁₆ H ₂₀ O ₉ | Unknown |
| 37 | 7.00 | - /185.0442/183.0 296 | -/126.0311, 153.0180, 171.0285/124.0164, 168.0063 | C ₈ H ₈ O ₅ | Unknown |
| 38 | 7.24, 8.47 | 804.1237/- /785.0843 | 153.0181, 259.0233, 277.0338, 303.0131, 467.0816, 617.0771, 787.1013/-/125.0244, 169.0141, 231.0297, 249.0404, 275.0198, | C ₃₄ H ₂₆ O ₂₂ | (Digalloyl HHDP glucoside) 1,2-di- <i>O</i> -galloyl-4,6- <i>O</i> -(<i>S</i>)- hexahydroxydiphenylβ-D- glucopyranoside; |

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|----|------------------------------|---------------------|--|---|---|
| | | | 300.9989 | | Tercatin/1,4-di- <i>O</i> -galloyl-3,6-(<i>R</i>)-hexahydroxydiphenyl- β -glucopyranose; TellimagrandinI; PedunculaginII |
| 39 | 7.51 | -/-/323.1346 | -/-/59.0138, 71.0137, 89.0243, 101.0243, 113.0244 | C ₁₃ H ₂₄ O ₉ | Unknown |
| 40 | 7.59 | 818.1030/-/799.0637 | 259.0233, 277.0340, 303.0131, 337.0185, 463.0507, 765.0567, 801.0789/-/300.9989, 479.0468 | C ₃₄ H ₂₄ O ₂₃ | Granatin A (Ellagic acid derivative) |
| 41 | 7.60, 8.28, 8.88, 9.15, 9.74 | 654.1290/-/635.0895 | 153.0182, 449.0721, 467.0818/-/125.0243, 169.0141, 313.0567, 465.0678, 483.0781 | C ₂₇ H ₂₄ O ₁₈ | 1,2,3-tri- <i>O</i> -galloyl- β -glucopyranose; 1,2,4-tri- <i>O</i> -galloyl- β -glucopyranose; 1,2,6-tri- <i>O</i> -galloyl- β -glucopyranose; 1,3,4-tri- <i>O</i> -galloyl- β -glucopyranose; 1,4,6-tri- <i>O</i> -galloyl- β -glucopyranose |
| 42 | 8.09 | -/-/387.1664 | -/-/163.1127 | C ₁₈ H ₂₈ O ₉ | Unknown |
| 43 | 8.29 | -/-/455.1772 | -/-/101.0607, 125.0244, 163.0611, 307.1036, 409.1716 | C ₁₈ H ₃₂ O ₁₃ | Unknown |
| 44 | 8.38 | -/-/387.1663 | -/-/59.0138, 163.1127 | C ₁₈ H ₂₈ O ₉ | Unknown |
| 45 | 8.77 | -/-/305.0700 | -/-/59.0138, 96.9599, 225.1132 | C ₈ H ₁₈ O ₁₂ | Unknown |
| 46 | 8.78 | 832.1186/-/813.0793 | 259.0233, 277.0337, 303.0126, 351.0341, 477.0647, 783.0665, 815.0907/-/300.9990, 479.0453 | C ₃₅ H ₂₆ O ₂₃ | HHDP glucoside derivative |
| 47 | 8.90 | -/-/281.1394 | -/-/171.1178, 189.1285, 237.1497 | C ₁₅ H ₂₂ O ₅ | 4-(2,7-Dihydroxy-6-methyl-2-heptanyl)-3-hydroxybenzoic acid |
| 48 | 9.04 | -/-/172.0872 | -/-/130.0872 | C ₈ H ₁₅ N O ₃ | 2-(Acetylamino)hexanoic acid |
| 49 | 9.42 | -/-/631.0581 | -/-/125.0242, 169.0142, 217.0146, 245.0089, 273.0044, 300.9990, 445.0399, 463.0523, 613.0485 | C ₂₇ H ₂₀ O ₁₈ | HHDP glucoside derivative [(-)-vescalin; castalin; terflavin D] |
| 50 | 9.46 | -/-/627.1572 | -/-/125.0242, 133.0294, 177.0192, 285.0404, 339.0726, 465.1038 | C ₂₇ H ₃₂ O ₁₇ | Unknown |
| 51 | 9.65 | 954.1190/-/935.0796 | 153.0180, 259.0235, 277.0338, 303.0129, 447.0533, 767.0712/-/275.0198, 300.9990 | C ₄₁ H ₂₈ O ₂₆ | Casuarinin |
| 52 | 9.70, 10.42 | -/-/483.0311 | -/-/125.0243, 169.0140, 247.0247, 300.9988, | C ₈ H ₂₀ O ₂₃ | (Digalloyl glucoside) Gallic acid 3- <i>O</i> - β -D-(6'- <i>O</i> - |

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| | | | | | galloyl)- glucopyranoside |
| 53 | 9.74 | 986.1085/- /967.0688 | 235.0233, 275.0180, 337.0183, 799.0611/-/247.0247, 273.0042, 300.9991, 905.0679, 931.0482, 949.0594 | C ₄₁ H ₂₈ O ₂₈ | HHDP glucoside derivative |
| 54 | 9.77 | - /627.1542/625.1 412 | -/303.0494/271.0248, 300.0276 | C ₂₇ H ₃₀ O ₁₇ | Unknown |
| 55 | 9.97 | -/-/475.0335 | -/-/125.0243, 169.0140, 275.0198, 300.9991, 452.0313, 466.0285 | C ₂₄ H ₁₂ O ₁₁ | HHDP glucoside derivative |
| 56 | 10.08 | 970.1134/- /951.0739 | 277.0338, 303.0130, 337.0183, 783.0665, 953.0862/-/273.0040, 300.9989, 933.0644 | C ₄₁ H ₂₈ O ₂₇ | Granatin B (galloyl-HHDP- DHHDP-hexoside) |
| 57 | 10.09 | /-/933.0646 | /-/273.0041, 300.9990 | C ₄₁ H ₂₆ O ₂₆ | Galloylpunicalin; Castalagin |
| 58 | 10.29 | 1000.1258/- /981.0853 | 813.0759/-/245.0089, 273.0040, 300.9989, 945.0648 963.0764 | C ₄₂ H ₃₀ O ₂₈ | HHDP glucoside derivative |
| 59 | 10.45 | 820.1175/- /801.0795 | 109.0286, 153.0180, 445.0387, 615.0610, 633.0706/-/123.0088, 169.0142, 245.0089, 273.0040, 300.9990, 445.0423, 597.0524, 615.0630, 765.0571, 783.0687 | C ₃₄ H ₂₆ O ₂₃ | Puniguconin |
| 60 | 10.65 | - /956.1342/937.0 958 | -/153.0181, 277.0339, 303.0130, 599.0656, 769.0869/125.0242, 169.0141, 249.0403, 275.0198, 300.9989 | C ₄₁ H ₃₀ O ₂₆ | Punicafolin |
| 61 | 10.66 | - /611.1653/609.1 475 | -/287.0550, 449.1078/271.0250, 300.0276 | C ₂₇ H ₃₀ O ₁₆ | Rutin |
| 62 | 10.68 and 12.42 | -/-/335.0408 | -/-/183.0297 | C ₁₅ H ₁₂ O ₉ | Flurtamone |
| 63 | 10.77 | - /467.0816/465.1 039 | -/137.0232, 153.0180, 179.0336, 305.0649/109.0292, 125.0242, 133.0294, 177.0192, 193.0141, 285.0408, 303.0510, 355.0668 | C ₂₁ H ₂₂ O ₁₂ | Unknown |
| 64 | 10.79 | - /449.0719/447.0 934 | -/287.0544/285.0404 | C ₂₁ H ₂₀ O ₁₁ | Flavonoid glycoside |
| 65 | 10.85 | -/-/300.9989 | -/-/300.9990 | C ₁₄ H ₆ O ₈ | Ellagic acid |
| 66 | 10.88 | 1122.1238/- /1103.0846 | 277.0337, 303.0128, 337.0184, 481.0630, 783.0660, 935.0693/- /273.0041, 300.9989, 933.0639, 951.0739 | C ₄₈ H ₃₂ O ₃₁ | HHDP glucoside derivative |

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|----|-------|-----------------------------|--|---|---|
| 67 | 10.98 | 806.1392/- /787.0999 | 153.0180, 237.0388, 449.0707, 619.0920/-/125.0243, 169.0141, 313.0566, 465.0674, 617.0777 | C ₃₄ H ₂₈ O ₂₂ | 1,2,4,6-tetra- <i>O</i> -galloyl-β-D-glucose |
| 68 | 11.02 | -/815.0586 | -/123.0085, 169.0141, 217.0138, 245.0083, 273.0036, 300.9990. 615.0657, 765.0623, 783.0698 | C ₃₅ H ₂₈ O ₂₃ | Pedunculagin I derivative (bis-HHDP glucoside derivative) |
| 69 | 11.24 | - /483.1128/481.0 989 | -/127.0390, 153.0180, 195.0286, 312.0600/125.0243, 149.0243, 193.0142, 257.0455, 355.0670, 463.0889 | C ₂₁ H ₂₂ O ₁₃ | Unknown |
| 70 | 11.64 | - /449.0719/447.0 934 | -/287.0544/285.0404 | C ₂₁ H ₂₀ O ₁₁ | Cynaroside (Luteolin 7- <i>O</i> -glycoside); Kaempferol 4'- <i>O</i> -glucoside |
| 71 | 11.68 | 984.1292/- /965.0900 | 277.0338, 303.0130, 351.0338, 797.0815/-/245.0089, 273.0042, 300.9991 | C ₄₂ H ₃₀ O ₂₇ | Pedunculagin I derivative (Bis-HHDP glucoside derivative) |
| 72 | 11.81 | - /451.1001/449.1 093 | -/121.0285, 127.0389, 153.0180, 163.0387, 289.0700/93.0345, 117.0345, 125.0242, 149.0242, 167.0348, 193.0142, 269.0454, 287.0540, 313.0574, 355.0666 | C ₂₁ H ₂₂ O ₁₁ | Hovetrichoside C |
| 73 | 11.91 | 972.1294/- /953.0890 | 153.0180, 785.0811/-/125.0243, 169.0141, 217.0142, 245.0092, 273.0041, 300.9990, 617.0771, 767.0731, 917.0720, 935.0803 | C ₄₁ H ₃₀ O ₂₇ | Galloyl-bis-HHDP-hexoside |
| 74 | 12.28 | 958.1503/- /939.1109 | 153.0181, 771.1024/-/125.0242, 169.0141, 465.0683, 769.0901 | C ₄₁ H ₃₂ O ₂₆ | 1,2,3,4,6-penta- <i>O</i> -galloyl-β-D-glucose |
| 75 | 12.61 | 1108.1454/- /1089.1057 | 153.0180, 303.0125, 599.0649, 769.0908, 921.0995/-/125.0139, 169.0139, 275.0200, 300.9990, 937.0954 | C ₄₈ H ₃₄ O ₃₀ | HHDP glucoside derivative |
| 76 | 12.90 | - /305.0650/303.0 511 | -/137.0232, 153.0180, 179.0335/109.0293, 125.0242, 133.0294, 151.0399, 177.0191, 193.0142 | C ₁₅ H ₁₂ O ₇ | Unknown |
| 77 | 13.04 | - /273.0754/271.0 147 | -/147.0439, 153.0180, 171.0285/119.0501, 151.0037, 177.0193 | C ₁₅ H ₁₂ O ₅ | Naringenin |
| 78 | 13.05 | - /449.0719/447.0 934 | -/287.0544/285.0404 | C ₂₁ H ₂₀ O ₁₁ | Kaempferol 7- <i>O</i> -glucoside |
| 79 | 13.11 | - | -/151.0035, 271.0613, | C ₂₀ H ₁₈ O ₁₁ | Unknown |

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| | | /435.0918/433.0780 | 301.0353 | | |
| 80 | 13.32, 13.59 | -/-461.1093 | -/-255.0295, 283.0247, 298.0479, 313.0345, 446.0860 | C ₂₂ H ₂₂ O ₁₁ | Unknown |
| 81 | 13.50 | - /451.1001/449.1094 | -/121.0286, 127.0392, 153.0182, 163.0389, 289.0702/135.0451, 151.0036, 287.0562 | C ₂₁ H ₂₂ O ₁₁ | Hovetrichoside C |
| 82 | 13.71 | - /449.0719/447.0934 | -/287.0544/285.0404 | C ₂₁ H ₂₀ O ₁₁ | Flavonoid glycosides |
| 83 | 13.73 | - /465.1020/463.0885 | -/303.0497/301.0354 | C ₂₁ H ₂₀ O ₁₂ | Tricetin 4'-O-β-glucopyranoside |
| 84 | 13.82 | - /303.0494/301.0352 | -/303.0497/301.0354 | C ₁₅ H ₁₀ O ₇ | Tricetin |
| 85 | 13.96 | - /317.0652/315.0512 | -/302.0421/300.0276 | C ₁₆ H ₁₂ O ₇ | Isorhamnetin |
| 86 | 13.99 | - /479.1178/477.1039 | -/317.0053/300.0275, 315.0511 | C ₂₁ H ₂₂ O ₁₂ | 6-O-[(2E)-3-(4-Hydroxyphenyl)-2-propenoyl]-1-O-(3,4,5-trihydroxybenzoyl)hexopyranose |
| 87 | 14.66 | -/-487.0522 | -/-183.0297, 335.0410 | C ₂₂ H ₁₆ O ₁₃ | Unknown |
| 88 | 14.71 | - /289.0701/287.0562 | -/121.0285, 153.0181, 163.0388/93.0344, 117.0345, 125.0243, 193.0141 | C ₁₅ H ₁₂ O ₆ | Eriodictyol |
| 89 | 14.73 | -/-125.0243 | -/-57.0345 | C ₆ H ₆ O ₃ | Phloroglucinol |
| 90 | 14.75 | -/-193.0141 | -/-149.0243, 151.0035 | C ₉ H ₆ O ₅ | Unknown |
| 91 | 14.83 | - /419.0967/417.0830 | -/287.0543/285.0404 | C ₂₀ H ₁₈ O ₁₀ | Luteolin 3'-O-β-xylopyranoside |
| 92 | 15.30 | -/-263.1288 | -/-151.0764, 201.1280, 204.1155, 219.1390 | C ₁₅ H ₂₀ O ₄ | Abscisic acid |
| 93 | 15.80 | - /287.0545/285.0405 | -/287.0544/285.0406 | C ₁₅ H ₁₀ O ₆ | Luteolin |
| 94 | 15.98 | - /317.0650/315.0511 | -/302.0415/272.0329, 300.0275 | C ₁₆ H ₁₂ O ₇ | Isorhamnetin |
| 95 | 17.80 | - /271.0597/269.0 | -/271.0595/269.0456 | C ₁₅ H ₁₀ O ₅ | Apigenin |

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| | | 456 | | | |
| 96 | 18.20 | - /275.0910/273.0 769 | -/107.0494/119.0499, 123.0451, 167.0348 | C ₁₅ H ₁₄ O ₅ | Phloretin |
| 97 | 18.30 | - /301.0701/299.0 561 | -/286.0465/256.0377, 284.0327 | C ₁₆ H ₁₂ O ₆ | Unknown |
| 98 | 18.71 | - /331.0805/327.2 178 | -/315.0495, 331.0809/171.1026, 211.1339, 229.1444 | C ₁₈ H ₃₂ O ₅ | Corchorifatty acid F |
| 99 | 19.74 | -/-/457.1720 | -/-/125.0244, 169.0142 | C ₂₁ H ₃₀ O ₁₁ | Unknown |
| 100 | 19.88 | -/-/401.0878 | -/-/121.0294, 225.0558, 313.0725 | C ₂₀ H ₁₈ O ₉ | Unknown |
| 101 | 19.95 | -/-/329.2334 | -/-/171.1026, 211.1340, 229.1444 | C ₁₈ H ₃₄ O ₅ | (15Z)-9,12,13-Trihydroxy-15-octadecenoic acid |
| 102 | 21.49 | -/-/643.2777 | -/-/136.0767, 190.0507, 339.1352, 611.2536 | C ₃₄ H ₄₄ O ₁₂ | Unknown |
| 103 | 21.68 | -/-/293.1759 | -/-/221.1546, 236.1053 | C ₁₇ H ₂₆ O ₄ | Unknown |
| 104 | 21.70 | - /489.2850/487.3 434 | -/147.0441/487.3434 | C ₃₀ H ₄₈ O ₅ | Asiatic acid |
| 105 | 21.86 | -/-/309.1709 | -/-/162.1049, 219.1753, 281.1758 | C ₁₇ H ₂₆ O ₅ | Unknown |
| 106 | 21.92 | -/-/239.1289 | -/-/154.0635, 167.1440, 195.1390 | C ₁₃ H ₂₀ O ₄ | Unknown |
| 107 | 22.13 | -/-/473.3639 | -/-/473.3638 | C ₃₀ H ₅₀ O ₄ | Punicanolic acid |
| 108 | 22.62 | -/-/471.3483 | -/-/471.3481 | C ₃₀ H ₄₈ O ₄ | Unknown |
| 109 | 22.71 | - /279.0930/277.1 444 | -/149.0232/121.0293, 127.1127, 134.0372 | C ₁₆ H ₂₂ O ₄ | Mono(2-ethylhexyl) phthalate |
| 110 | 23.09 | -/-/452.2784 | -/-/255.2330 | C ₂₁ H ₄₄ NO ₇ P | Glycerophospho-N-palmitoyl ethanolamine |
| 111 | 23.05 | -/-/265.1479 | -/-/96.9600 | C ₁₂ H ₂₆ O ₄ S | Dodecyl sulfate |
| 112 | 23.35 | -/-/347.1714 | -/-/217.0713, 301.1661 | C ₁₆ H ₂₈ O ₈ | Unknown |
| 113 | 23.94 | - /457.3675/455.3 532 | -/95.0800, 189.1637, 261.1845, 393.3515, 411.3629, 439.3566/455.3533 | C ₃₀ H ₄₈ O ₃ | Ursolic acid; Oleanolic acid; Hydroxyurs-12-en-23-oic acid |
| 114 | 24.11 | -/-/339.2331 | -/-/163.1129 | C ₂₃ H ₃₂ O ₂ | 2,2'-methylenebis(4-methyl-6-tert-butylphenol) |
| 115 | 24.37 | -/-/271.2279 | -/-/225.2223 | C ₁₆ H ₃₂ O ₃ | 16-hydroxyhexadecanoic acid |

Table S2. High-resolution electrospray ionization mass spectrometry (HR-ESI-MS) data of metabolites extracted from pomegranate petals. Rt, retention time.

| Peak | R _t (min) | [M+NH ₄] ⁺ /[M+H] ⁺ /[M-H] ⁻ (m/z) | MS/MS (m/z) | Calculated formula | Tentative identification |
|------|----------------------|--|---|---|---------------------------------|
| 1 | 1.01 | -/-/181.0715 | -/-/59.0137, 71.0137, 89.0243, 101.0242, 119.0347, 131.0349, 163.0610, 181.0716 | C ₆ H ₁₄ O ₆ | D-(-)-mannitol |
| 2 | 1.03 | -/-/135.0297 | -/-/75.0087, 89.0244 | C ₄ H ₈ O ₅ | L-Threonic acid |
| 3 | 1.03 | -/-/146.0458 | -/-/102.059, 128.0352 | C ₅ H ₉ N O ₄ | L-Glutamic acid |
| 4 | 1.04 | -/-/341.1091 | -/-/59.0138, 71.0137, 89.0243, 101.0243, 119.0347, 179.0560, 341.1091 | C ₁₂ H ₂₂ O ₁₁ | Trehalose |
| 5 | 1.04 | -/-/165.0402 | -/-/75.0086, 129.0192 | C ₆ H ₆ N ₄ O ₂ | 7-Methylxanthine |
| 6 | 1.04 | -/381.0788/- | -/381.0784/- | C ₁₇ H ₁₆ O ₁₀ | Unknown |
| 7 | 1.06 | -/-/377.0853 | -/-/341.1091 | C ₁₈ H ₁₈ O ₉ | Unknown |
| 8 | 1.06 | -/-/179.0559 | -/-/59.0138, 75.0086, 143.0349, 161.0454 | C ₆ H ₁₂ O ₆ | D-(-)-Fructose |
| 9 | 1.09 | -/-/149.0453 | -/-/59.0138, 75.0086, 131.0348 | C ₅ H ₁₀ O ₅ | D-(-)-Arabinose |
| 10 | 1.14 | -/-/259.0294 | -/78.9589, 96.9692, 138.9702, 198.9908 | C ₆ H ₁₃ O ₉ P | D-Glucose 6-phosphate |
| 11 | 1.23 | -/-/439.0858 | -/-/78.9589, 96.9694 | C ₁₉ H ₂₀ O ₁₂ | Unknown |
| 12 | 1.30 | -/136.02/134.0142 | -/91.05, 119.05, 136.02/71.0138, 89.0243, 115.0036, 133.0142 | C ₄ H ₆ O ₅ | Malic acid |
| 13 | 1.53 | -/-/481.0627 | -/-/275.0198, 300.9989 | C ₂₀ H ₁₈ O ₁₄ | HHDP glucoside derivative |
| 14 | 1.58 | -/-/191.0197 | -/-/85.0294, 87.0086, 111.0086, 129.0193 | C ₆ H ₈ O ₇ | D-(-)-Quinic acid ; Citric acid |
| 15 | 1.71 | -/-/645.1889 | -/-/71.0137, 113.0243 | C ₂₄ H ₃₈ O ₂₀ | Unknown |
| 16 | 1.81, 7.12 | -/315.0710/- | -/153.0180/- | C ₁₃ H ₁₄ O ₉ | Unknown |
| 17 | 1.87 | 350.0997/- /331.0670 | 109.0287, 127.0389, 145.0495, 153.0179, 171.0285, 315.0710/- /125.0242, 151.0036, 169.0140, 211.0246, 271.0454 | C ₁₃ H ₁₆ O ₁₀ | Galloyl glucoside |
| 18 | 2.26 | - /171.0288/169.01 41 | -/81.0341, 107.0130, 109.0286, 125.0233, 127.0389, 153.0180/125.0242 | C ₇ H ₆ O ₅ | Gallic acid |
| 19 | 2.27 | -/-/777.2307 | -/-/113.0242 | C ₂₉ H ₄₆ O ₂₄ | Unknown |
| 20 | 2.57 | - /345.0814/343.06 70 | -/153.0180/191.0560 | C ₁₄ H ₁₆ O ₁₀ | Unknown |
| 21 | 4.45 | -/-/218.1033 | -/-/88.0403, 146.0822 | C ₉ H ₁₇ NO ₅ | Pantothenic acid |
| 22 | 4.46 | -/-/325.0565 | -/-/93.0343, 125.0242, 169.0141 | C ₁₄ H ₁₄ O ₉ | Unknown |
| 23 | 4.79 | -/-/487.1096 | -/-/125.0242, 169.0140, 211.0250, | C ₂₀ H ₂₄ O ₁₄ | Galloyl-hexoside derivative |

| | | | | | |
|----|------------------------|-----------------------------|---|--|---|
| | | | 331.0663, 469.0993 | | |
| 24 | 4.99 | -/-/299.0771 | -/-/59.0137, 71.0137, 89.0242, 101.0242, 119.0349, 137.0243, 179.0348, 239.0564 | C ₁₃ H ₁₆ O ₈ | Unknown |
| 25 | 5.45 | -/-/315.0722 | -/-/125.0238, 151.0037, 169.0138 | C ₁₃ H ₁₆ O ₉ | Galloyl-hexoside derivative |
| 26 | 6.54 | -/-/315.0511 | -/-/153.0192 | C ₁₃ H ₁₆ O ₉ | Unknown |
| 27 | 6.62 | -/595.1650/- | -/271.0594, 433.1121/- | C ₂₇ H ₃₁ O ₁₅ ⁺ | Cyanidin-3- <i>O</i> -rutinose |
| 28 | 6.63 | -/-/611.1616 | -/-/93.0344, 149.0242, 165.0191, 193.0141, 269.0456, 287.0561, 355.0671, 449.1091 | C ₂₇ H ₃₁ O ₁₆ ⁺ | Cyanidin-3,5-di- <i>O</i> -glucoside |
| 29 | 6.99 | - /185.0442/183.02 97 | -/126.0311, 153.0180, 171.0285/124.0164, 168.0063 | C ₈ H ₆ O ₅ | Unknown |
| 30 | 7.01 | -/-/957.0849 | -/-/275.0198, 300.9989 | C ₄₀ H ₃₀ O ₂₈ | HHDP glucoside derivative |
| 31 | 7.09 | -/-/483.0782 | -/-/125.0243, 169.0141, 211.0247, 271.0459, 313.0561, 331.0685 | C ₂₀ H ₂₀ O ₁₄ | Galloyl-hexoside derivative |
| 32 | 7.30, 8.53 | 804.1237/- /785.0848 | 153.0181, 259.0233, 277.0338, 303.0131, 467.0816, 617.0771, 787.1013/-/125.0242, 169.0140, 231.0297, 249.0403, 275.0198, 300.9989 | C ₃₄ H ₂₆ O ₂₂ | 1,2-di- <i>O</i> -galloyl-4,6- <i>O</i> -(<i>S</i>)-hexahydroxydiphenyl-β-D-glucopyranoside; Tercatain/1,4-di- <i>O</i> -galloyl-3,6-(<i>R</i>)-hexahydroxydiphenyl-β-glucopyranose; TellimagrandinI; PedunculaginII |
| 33 | 7.62 | 818.1035/- /799.0640 | 259.0233, 277.0340, 303.0131, 337.0185, 463.0507, 765.0567, 801.0789/-/300.9989, 479.0467 | C ₃₄ H ₂₄ O ₂₃ | Granatin A (Ellagic acid derivative) |
| 34 | 7.67 | 652.1132/- /633.0738 | 259.0233, 277.0338, 303.0129, 447.0553/-/169.0140, 249.0404, 275.0195, 300.9988 | C ₂₇ H ₂₂ O ₁₈ | 6- <i>O</i> -galloyl-2, 3-(<i>S</i>) - hexahydroxydiphenyl -D-glucose; Corilagin; Isocorilagin; Hippomanin A; Gemin D; Strictinin (galloyl HHDP glucoside) |
| 35 | 8.27, 8.87, 9.69 | 654.1293/- /635.0891 | -153.0182, 449.0721, 467.0818/-/125.0242, 169.0141, 313.0566, 465.0673 | C ₂₇ H ₂₄ O ₁₈ | 1,2,3-tri- <i>O</i> -galloyl-β-glucopyranose; 1,2,4-tri- <i>O</i> -galloyl-β-glucopyranose; 1,2,6-tri- <i>O</i> -galloyl-β-glucopyranose; 1,3,4-tri- <i>O</i> -galloyl-β-glucopyranose; 1,4,6-tri- <i>O</i> -galloyl-β-glucopyranose |
| 36 | 8.48, | -/433.1127/- | -/271.0594/- | C ₂₁ H ₂₀ O ₁₀ | Unknown |

| | | | | | |
|----|-----------------|-----------------------------|---|---|---|
| | 13.07 | | | | |
| 37 | 8.73 | 832.1191/- /813.0797 | 259.0233, 277.0337, 303.0126, 351.0341, 477.0647, 783.0665, 815.0907/-/300.9989, 479.0470 | C ₃₅ H ₂₆ O ₂₃ | HHDP glucoside derivative |
| 38 | 8.83 | -/-/305.0700 | -/-/59.0138, 96.9599, 225.1132 | C ₈ H ₁₈ O ₁₂ | Unknown |
| 39 | 8.89, 9.70 | -/467.0819/- | -/153.0179/- | C ₂₀ H ₁₈ O ₁₃ | Unknown |
| 40 | 9.11 | - /451.1225/449.10 93 | -/121.0284, 289.0699/125.0242, 259.0610, 287.0562, 421.1139 | C ₂₁ H ₂₂ O ₁₁ | Hovetrichoside C |
| 41 | 9.26 | -/-/329.0878 | -/-/123.0450, 167.0348 | C ₁₄ H ₁₈ O ₉ | Unknown |
| 42 | 9.43 | -/-/631.0580 | -/-/125.0242, 169.0141, 217.0139, 245.0090, 273.0041, 300.9988, 445.0415, 463.0515, 613.0463 | C ₂₇ H ₂₀ O ₁₈ | HHDP glucoside derivative [(-)-vescalin; castalin; terflavin D] |
| 43 | 9.47 | - /449.0719/447.09 33 | -/287.0544/165.0191, 285.0404, 327.0722 | C ₂₁ H ₂₀ O ₁₁ | Flavonoid glycosides |
| 44 | 9.53 | 646.1968/- /627.1567 | 95.0495, 121.0284, 139.0388, 167.0337, 305.0648/-/139.0399, 165.0191, 345.0826, 447.0933 | C ₂₇ H ₃₂ O ₁₇ | Unknown |
| 45 | 9.71, 10.39 | 986.1091/- /967.0685 | 235.0233, 275.0180, 337.0183, 799.0611/-/247.0246, 273.0040, 300.9989, 905.0681, 931.0482, 949.0578 | C ₄₁ H ₂₈ O ₂₈ | HHDP glucoside derivative |
| 46 | 9.79 | - /611.1653/609.14 75 | -/287.0550, 449.1078/285.0403, 447.0932 | C ₂₇ H ₃₀ O ₁₆ | Rutin |
| 47 | 10.14 | 820.1189/- /801.0789 | 109.0286, 153.0180, 445.0387, 615.0610, 633.0706/-/123.0086, 169.0142, 245.0089, 273.0039, 300.9988, 445.0423, 597.0524, 615.0630, 765.0580, 783.0685 | C ₃₄ H ₂₆ O ₂₃ | Punigluconin |
| 48 | 10.15 | 970.1136/- /951.0737 | 277.0338, 303.0130, 337.0183, 783.0665, 953.0862/-/273.0040, 300.9988, 933.0644 | C ₄₁ H ₂₈ O ₂₇ | Granatin B (galloyl-HHDP- DHHDP-hexoside) |
| 49 | 10.37, 12.28 | 1000.1258/- /981.0852 | 813.0759/-/245.0089, 273.0040, 300.9988, 945.0665, 963.0736 | C ₄₂ H ₃₀ O ₂₈ | HHDP glucoside derivative |
| 50 | 10.55, 11.14 | 1144.1307/- /1125.0906 | 109.0286, 153.0181, 221.0075, 337.0183, 449.0366, 957.0822/- /247.0246, 273.0041, 300.9988, 907.0856, 933.0618, 949.0560, 1081.0951 | C ₄₇ H ₃₄ O ₃₃ | HHDP glucoside derivative |
| 51 | 10.78 | 1128.1356/- | 221.0076, 303.0128, 941.0868/- | C ₄₇ H ₃₄ O ₃₂ | bis-HHDP glucoside |

| | | | | | |
|----|-----------------|-----------------------------|---|---|---|
| | | /1109.0951 | /275.0197, 300.9988, 633.0724, 935.0798 | | derivative |
| 52 | 10.97 | -/-497.3349 | -/-433.3182, 451.3292 | C ₂₄ H ₅₀ O ₁₀ | Unknown |
| 53 | 11.00 | -/453.3429/- | -/100.1124, 210.1485, 435.3331/- | C ₂₃ H ₄₈ O ₈ | Unknown |
| 54 | 11.08 | 834.1350/- /815.0955 | 81.0341, 109.0286, 153.0179, 445.0390, 615.0604, 647.0864/- /123.0085, 169.0141, 217.0138, 245.0089, 273.0042, 300.9990. 615.0608, 765.0570, 783.0682 | C ₃₅ H ₂₈ O ₂₃ | Pedunculagin I derivative (bis-HHDP glucoside derivative) |
| 55 | 11.21 | 806.1392/- /787.1005 | 153.0180, 237.0388, 449.0707, 619.0920/-/125.0243, 169.0141, 313.0580, 465.0677, 617.0788 | C ₃₄ H ₂₈ O ₂₂ | 1,2,4,6-tetra- <i>O</i> -galloyl- β -D- glucose |
| 56 | 11.62 | 984.1292/- /965.0898 | 277.0338, 303.0130, 351.0338, 797.0815/-/245.0089, 273.0041, 300.9989 | C ₄₂ H ₃₀ O ₂₇ | Pedunculagin I derivative (Bis-HHDP glucoside derivative) |
| 57 | 11.89 | 972.1292/- /953.0889 | 153.0180, 785.0811/-/125.0243, 169.0141, 217.0142, 245.0092, 273.0041, 300.9990, 617.0811, 767.0731, 917.0720, 935.0793 | C ₄₁ H ₃₀ O ₂₇ | Galloyl-bis-HHDP-hexoside |
| 58 | 12.06, 12.64 | 680.1086/- /661.0690 | 69.0342, 127.0390, 153.0178, 245.0071, 305.0286, 331.0076, 349.0176, 475.0492, 493.0602/- /217.0146, 303.0143, 491.0478 | C ₂₈ H ₂₂ O ₁₉ | Unknown |
| 59 | 12.24 | -/-441.1980 | -/-101.0243, 263.1496, 395.1918 | C ₁₈ H ₃₄ O ₁₂ | Unknown |
| 60 | 12.25 | -/-395.1923 | -/-101.0243, 113.0244, 161.0452, 263.1502 | C ₁₇ H ₃₂ O ₁₀ | Unknown |
| 61 | 12.55 | - /449.1072/447.09 36 | -/287.0544/227.0349, 255.0297, 284.0326, 285.0401 | C ₂₁ H ₂₀ O ₁₁ | Astragaline (Kaempferol -3- <i>O</i> -glucoside) |
| 62 | 13.14 | - /433.1127/431.09 85 | -/271.0595/268.0376, 269.0454 | C ₂₁ H ₂₀ O ₁₀ | Apigenin 4'- <i>O</i> - β - glucopyranoside |
| 63 | 13.88 | -/-455.2136 | -/-71.0137, 101.0243, 277.1653,409.2078 | C ₁₉ H ₃₆ O ₁₂ | Unknown |
| 64 | 14.73 | - /289.0701/287.05 61 | -/121.0285, 153.0181, 163.0388/93.0344, 117.0342, 125.0243, 167.0351, 193.0141 | C ₁₅ H ₁₂ O ₆ | Eriodictyol |
| 65 | 15.02 | -/-435.1299 | -/-167.0348, 273.0769, 297.0772 | C ₂₁ H ₂₄ O ₁₀ | Phlorizin |
| 66 | 15.11 | -/-515.1772 | -/-125.0241, 169.0140, 201.1132,225.1135, 243.1235, 363.1662 | C ₂₃ H ₃₂ O ₁₃ | Unknown |
| 67 | 16.18 | -/-569.3182 | -/-287.2227, 449.2758, 523.3090 | C ₂₆ H ₅₀ O ₁₃ | Unknown |
| 68 | 18.74 | -/-615.2659 | -/-125.0241, 169.0137, 283.1910, | C ₂₉ H ₄₄ O ₁₄ | Unknown |

| | | | | | |
|----|-------|-----------------------------|--|--|---|
| | | | 301.2025 | | |
| 69 | 19.87 | -/-/401.0876 | -/-/121.0293, 225.0553, 313.0717 | C ₂₀ H ₁₈ O ₉ | Unknown |
| 70 | 19.98 | -/-/357.0616 | -/-/121.0293, 357.0617 | C ₁₈ H ₁₄ O ₈ | Unknown |
| 71 | 21.40 | -/-/503.3378 | -/-/503.3378 | C ₃₀ H ₄₈ O ₆ | Arjungenin |
| 72 | 21.50 | -/-/549.3436 | -/-/503.3377 | C ₃₁ H ₅₀ O ₈ | Unknown |
| 73 | 21.72 | - /489.2850/487.34 27 | -/147.0441/487.3430 | C ₃₀ H ₄₈ O ₅ | Asiatic acid |
| 74 | 21.82 | -/-/309.1707 | -/-/162.1049, 219.1753, 281.1758 | C ₁₇ H ₂₆ O ₅ | Unknown |
| 75 | 21.90 | -/-/239.1289 | -/-/154.0635, 167.1440, 195.1390 | C ₁₃ H ₂₀ O ₄ | Unknown |
| 76 | 22.13 | -/-/473.3637 | -/-/473.3638 | C ₃₀ H ₅₀ O ₄ | Punicanolic acid |
| 77 | 22.29 | -/-/485.3275 | -/-/455.3180 | C ₃₀ H ₄₆ O ₅ | Unknown |
| 78 | 22.64 | -/-/471.3482 | -/-/471.3481 | C ₃₀ H ₄₈ O ₄ | Unknown |
| 79 | 22.70 | - /279.0930/277.14 44 | -/149.0232/121.0293, 127.1127, 134.0372 | C ₁₆ H ₂₂ O ₄ | Mono(2-ethylhexyl) phthalate |
| 80 | 23.09 | -/-/452.2784 | -/-/255.2330 | C ₂₁ H ₄₄ NO ₇ P | Glycerophospho-N-palmitoyl ethanolamine |
| 81 | 23.31 | -/-/265.1479 | -/-/96.9600 | C ₁₂ H ₂₆ O ₄ S | Dodecyl sulfate |
| 82 | 23.36 | -/-/347.1713 | -/-/217.0713, 301.1661 | C ₁₆ H ₂₈ O ₈ | Unknown |
| 83 | 23.94 | -/-/455.3530 | -/-/455.3532 | C ₃₀ H ₄₈ O ₃ | Ursolic acid; Oleanolic acid |
| 84 | 24.11 | -/-/339.2325 | -/-/163.1129 | C ₂₃ H ₃₂ O ₂ | 2,2'-methylenebis(4-methyl- 6-tert-butylphenol |
| 85 | 25.17 | -/-/325.1842 | -/-/183.0118 | C ₁₈ H ₃₀ O ₃ S | 4-Dodecylbenzenesulfonic acid |

Table S3. Summary of RNAseq data.

| Sample | Raw reads | Raw bases (bp) | Clean reads | Clean bases (bp) | Error rate (%) | Q20 (%) | Q30 (%) |
|------------|-----------|-------------------|----------------|---------------------|-------------------|------------|------------|
| Pg_anther2 | 42350106 | 6394866006 | 42102446 | 6337271438 | 0.00208 | 97.07 | 92.62 |
| Pg_anther4 | 41708934 | 6298049034 | 41225410 | 6212382316 | 0.008355 | 95.08 | 88.76 |
| Pg_anther9 | 45340278 | 6846381978 | 44964900 | 6773780416 | 0.008987 | 95.62 | 89.75 |
| Pg_petal2 | 44916484 | 6782389084 | 44659014 | 6722178230 | 0.002313 | 97.04 | 92.72 |
| Pg_petal4 | 46465480 | 7016287480 | 45870616 | 6910089572 | 0.00677 | 95.22 | 89 |
| Pg_petal9 | 42646274 | 6439587374 | 42198864 | 6355860646 | 0.007268 | 95.61 | 89.71 |

Table S4. RNAseq mapped reads and distributions.

| Sample | Total mapped | Multiple mapped | Uniquely mapped | Gene | Exon | Intergenic |
|------------|----------------------|--------------------|----------------------|----------------------|----------------------|---------------------|
| Pg_anther2 | 39009104 (92.65%) | 1931146 (4.95%) | 37077958 (95.05%) | 32475642 (87.59%) | 31859470 (98.10%) | 4602316 (12.41%) |
| Pg_anther4 | 36046221 (87.44%) | 2695755 (7.48%) | 33350466 (92.52%) | 28592716 (85.73%) | 28135489 (98.40%) | 4757750 (14.27%) |
| Pg_anther9 | 39758843 (88.42%) | 2133951 (5.37%) | 37624892 (94.63%) | 32581483 (86.60%) | 31490897 (96.65%) | 5043409 (13.40%) |
| Pg_petal2 | 41098186 (92.03%) | 3642607 (8.86%) | 37455579 (91.14%) | 31020157 (82.82%) | 30016225 (96.76%) | 6435422 (17.18%) |
| Pg_petal4 | 40602543 (88.52%) | 2110683 (5.20%) | 38491860 (94.80%) | 33369330 (86.69%) | 32170512 (96.41%) | 5122530 (13.31%) |
| Pg_petal9 | 37710951 (89.36%) | 2682376 (7.11%) | 35028575 (92.89%) | 29780137 (85.02%) | 28765272 (96.59%) | 5248438 (14.98%) |