

Supplementary

# Analysis of Antioxidant Activity and Flavonoids Metabolites in Peel and Flesh of Red-Fleshed Apple Varieties

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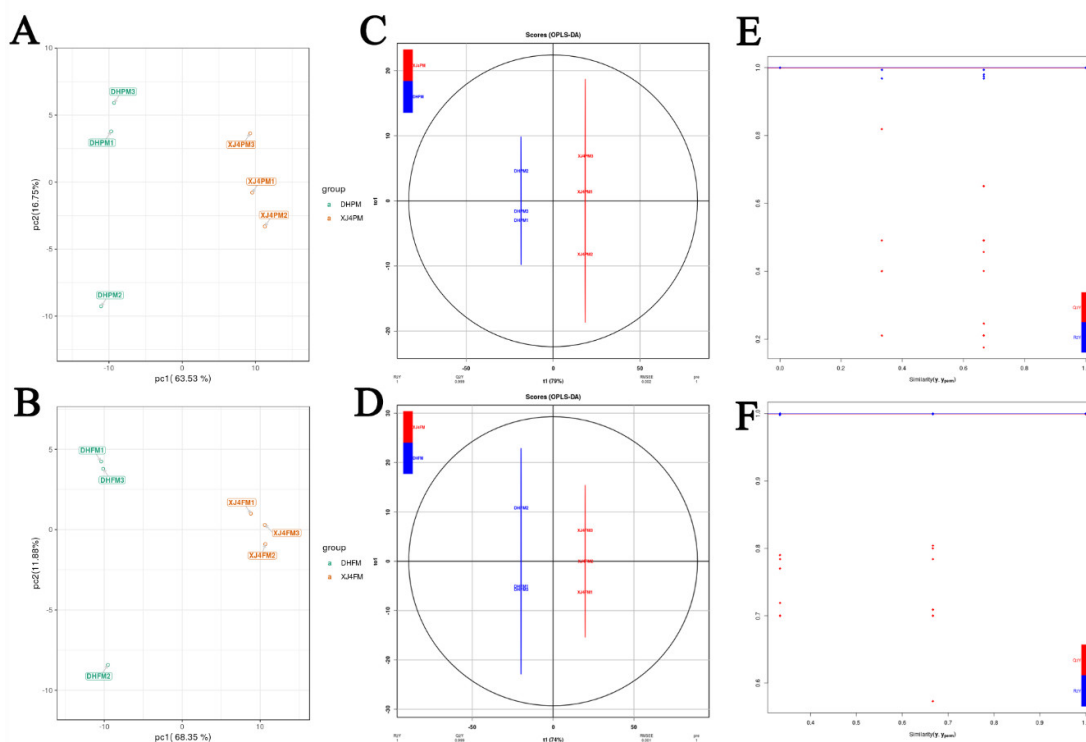
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**Figure S1.** Principle component analysis (PCA) score plot, orthogonal partial least squares-discriminant analysis (OPLS-DA) score plot and permutation test in four comparison groups. (A,B) PCA in DHPM vs. XJ4PM and DHFM vs. XJ4FM. (C,D) OPLS-DA in DHPM vs. XJ4PM and DHFM vs. XJ4FM. (E,F) Permutation test in DHPM vs. XJ4PM and DHFM vs. XJ4FM.

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**Table S1.** The differential metabolites in both DHPM vs. XJ4PM and DHFM vs. XJ4FM.

| Combination name | Metabolite name                                                    | Content    |            | Fold change<br>(XJ4PM/DHPM; XJ4FM/DHFM) | VIP Grouping of specific metabolites |              |
|------------------|--------------------------------------------------------------------|------------|------------|-----------------------------------------|--------------------------------------|--------------|
|                  |                                                                    | DH         | XJ4        |                                         |                                      |              |
| ANTHOCYANIN      |                                                                    |            |            |                                         |                                      |              |
| DHPM vs. XJ4PM   | Pelargonidin 3- <i>O</i> -beta-D-glucoside (Callistephin chloride) | 9.00E + 00 | 3.14E + 07 | 3.49E + 06                              | 2.36                                 | XJ4PM        |
|                  | Cyanidin 3- <i>O</i> -malonylhexoside                              | 9.00E + 00 | 1.32E + 06 | 1.47E + 05                              | 2.1                                  | XJ4PM        |
|                  | Malvidin 3-acetyl-5-diglucoside                                    | 9.00E + 00 | 2.56E + 05 | 2.84E + 04                              | 1.93                                 | XJ4PM        |
|                  | Cyanidin 3- <i>O</i> -rutinoside (Keracyanin)                      | 9.00E + 00 | 2.40E + 05 | 2.67E + 04                              | 1.94                                 | XJ4PM        |
|                  | Pelargonidin 3- <i>O</i> -malonylhexoside                          | 9.00E + 00 | 1.63E + 04 | 1.82E + 03                              | 1.65                                 | XJ4PM        |
|                  | Cyanidin <i>O</i> -syringic acid                                   | 2.69E + 05 | 1.20E + 07 | 4.47E + 01                              | 1.19                                 | XJ4PM & DHPM |
|                  | Peonidin <i>O</i> -hexoside                                        | 4.15E + 05 | 1.66E + 07 | 4.00E + 01                              | 1.17                                 | XJ4PM & DHPM |
|                  | Peonidin 3- <i>O</i> -glucoside chloride                           | 4.46E + 05 | 1.73E + 07 | 3.87E + 01                              | 1.17                                 | XJ4PM & DHPM |
|                  | Cyanidin 3- <i>O</i> -galactoside                                  | 2.77E + 05 | 8.51E + 06 | 3.07E + 01                              | 1.13                                 | XJ4PM & DHPM |
|                  | Cyanidin 3- <i>O</i> -glucoside (Kuromanin)                        | 2.34E + 06 | 7.13E + 07 | 3.05E + 01                              | 1.13                                 | XJ4PM & DHPM |
|                  | Cyanidin 3,5- <i>O</i> -diglucoside (Cyanin)                       | 1.15E + 06 | 3.19E + 07 | 2.78E + 01                              | 1.11                                 | XJ4PM & DHPM |
| DHFM vs. XJ4FM   | Pelargonidin 3- <i>O</i> -beta-D-glucoside                         | 9.00E + 00 | 6.78E + 07 | 7.54E + 06                              | 2.16                                 | XJ4FM        |
|                  | Cyanidin 3- <i>O</i> -malonylhexoside                              | 9.00E + 00 | 1.56E + 06 | 1.74E + 05                              | 1.89                                 | XJ4FM        |
|                  | Malvidin 3-acetyl-5-diglucoside                                    | 9.00E + 00 | 1.06E + 06 | 1.17E + 05                              | 1.86                                 | XJ4FM        |
|                  | Peonidin <i>O</i> -hexoside                                        | 9.00E + 00 | 7.50E + 05 | 8.33E + 04                              | 1.83                                 | XJ4FM        |
|                  | Peonidin 3- <i>O</i> -glucoside chloride                           | 9.00E + 00 | 7.12E + 05 | 7.91E + 04                              | 1.83                                 | XJ4FM        |
|                  | Pelargonidin 3- <i>O</i> -malonylhexoside                          | 9.00E + 00 | 2.49E + 04 | 2.76E + 03                              | 1.53                                 | XJ4FM        |
|                  | Cyanidin 3,5- <i>O</i> -diglucoside                                | 9.27E + 04 | 4.35E + 07 | 4.69E + 02                              | 1.35                                 | XJ4FM & DHFM |
|                  | Cyanidin <i>O</i> -syringic acid                                   | 6.76E + 04 | 1.38E + 07 | 2.04E + 02                              | 1.25                                 | XJ4FM & DHFM |
|                  | Cyanidin 3- <i>O</i> -glucoside                                    | 7.30E + 05 | 7.71E + 07 | 1.06E + 02                              | 1.18                                 | XJ4FM & DHFM |
|                  | Cyanidin 3- <i>O</i> -galactoside                                  | 9.42E + 04 | 9.76E + 06 | 1.04E + 02                              | 1.17                                 | XJ4FM & DHFM |
|                  | Peonidin 3-sophoroside-5-glucoside.                                | 1.82E + 03 | 7.96E + 03 | 4.37E + 00                              | 1.00                                 | XJ4FM & DHFM |
|                  | Rosinidin <i>O</i> -hexoside                                       | 7.00E + 04 | 9.00E + 00 | 1.29E-04                                | 1.62                                 | DHFM         |
| FLAVONE          |                                                                    |            |            |                                         |                                      |              |
| DHPM vs. XJ4PM   | Selgin <i>O</i> -hexosyl- <i>O</i> -hexoside                       | 9.00E + 00 | 3.09E + 06 | 3.43E + 05                              | 2.17                                 | XJ4PM        |
|                  | Tricin <i>O</i> -saccharic acid                                    | 9.00E + 00 | 3.02E + 06 | 3.36E + 05                              | 2.16                                 | XJ4PM        |
|                  | 6- <i>C</i> -hexosyl-hesperetin <i>O</i> -hexoside                 | 9.00E + 00 | 2.41E + 06 | 2.68E + 05                              | 2.14                                 | XJ4PM        |
|                  | Luteolin 3',7-di- <i>O</i> -glucoside                              | 9.00E + 00 | 1.26E + 06 | 1.39E + 05                              | 2.09                                 | XJ4PM        |
|                  | <i>O</i> -methylChrysoeriol 5- <i>O</i> -hexoside                  | 9.00E + 00 | 1.09E + 06 | 1.22E + 05                              | 1.38                                 | XJ4PM        |

|                |                                                   |                       |            |      |              |
|----------------|---------------------------------------------------|-----------------------|------------|------|--------------|
| DHFM vs. XJ4FM | O-methylChrysoeriol 7-O-hexoside                  | 9.00E + 00 1.09E + 06 | 1.21E + 05 | 1.37 | XJ4PM        |
|                | C-hexosyl-apigenin O-hexosyl-O-hexoside           | 9.00E + 00 8.63E + 05 | 9.59E + 04 | 2.05 | XJ4PM        |
|                | Morin                                             | 9.00E + 00 7.46E + 05 | 8.29E + 04 | 2.04 | XJ4PM        |
|                | Persicoside                                       | 9.00E + 00 5.93E + 05 | 6.59E + 04 | 2.02 | XJ4PM        |
|                | Eriodictiol 6-C-hexoside 8-C-hexoside-O-hexoside  | 9.00E + 00 5.88E + 05 | 6.54E + 04 | 2.02 | XJ4PM        |
|                | Hesperetin C-hexosyl-O-hexosyl-O-hexoside         | 9.00E + 00 5.85E + 05 | 6.50E + 04 | 2.02 | XJ4PM        |
|                | C-hexosyl-isorhamnetin O-hexoside                 | 9.00E + 00 1.67E + 05 | 1.86E + 04 | 1.90 | XJ4PM        |
|                | Tricin 4'-O-(syringyl alcohol) ether 5-O-hexoside | 9.00E + 00 1.55E + 05 | 1.73E + 04 | 1.89 | XJ4PM        |
|                | Chrysoeriol 8-C-hexoside                          | 9.00E + 00 4.92E + 04 | 5.47E + 03 | 1.25 | XJ4PM        |
|                | Apigenin                                          | 9.00E + 00 4.38E + 04 | 4.87E + 03 | 1.22 | XJ4PM        |
|                | Acacetin                                          | 9.00E + 00 3.31E + 04 | 3.68E + 03 | 1.66 | XJ4PM        |
|                | Tricin 5-O-rutinoside                             | 9.00E + 00 1.14E + 04 | 1.26E + 03 | 1.15 | XJ4PM        |
|                | Selgin O-malonylhexoside                          | 3.92E + 05 3.01E + 07 | 7.68E + 01 | 1.30 | XJ4PM & DHPM |
|                | Liquiritin                                        | 8.43E + 04 2.43E + 06 | 2.89E + 01 | 1.00 | XJ4FM & DHFM |
|                | Apigenin 5-O-glucoside                            | 5.96E + 05 1.43E + 07 | 2.40E + 01 | 1.08 | XJ4PM & DHPM |
|                | Astilbin                                          | 3.85E + 04 7.91E + 05 | 2.06E + 01 | 1.05 | XJ4PM & DHPM |
|                | Eriodictiol C-hexosyl-O-hexoside                  | 1.25E + 05 2.30E + 06 | 1.84E + 01 | 1.60 | XJ4PM & DHPM |
|                | Chrysoeriol                                       | 2.37E + 03 3.61E + 04 | 1.52E + 01 | 1.34 | XJ4PM & DHPM |
|                | Chrysoeriol 6-C-hexoside 8-C-hexoside-O-hexoside  | 5.59E + 05 4.47E + 04 | 8.00E-02   | 1.45 | XJ4PM & DHPM |
|                | Luteolin 8-C-hexosyl-O-hexoside                   | 1.30E + 06 5.20E + 04 | 4.01E-02   | 1.01 | XJ4PM & DHPM |
|                | Baicalein-7-O-glucuronide (Baicalin)              | 5.51E + 04 9.00E + 00 | 1.63E-04   | 1.79 | DHPM         |
|                | Chrysoeriol 7-O-rutinoside                        | 9.30E + 05 9.00E + 00 | 9.67E-06   | 2.03 | DHPM         |
|                | Diosmin                                           | 2.21E + 06 9.00E + 00 | 4.08E-06   | 2.11 | DHPM         |
|                | 6-C-hexosyl-hesperetin O-hexoside                 | 9.00E + 00 7.26E + 06 | 8.06E + 05 | 2.00 | XJ4FM        |
|                | Luteolin 3',7-di-O-glucoside                      | 9.00E + 00 3.64E + 06 | 4.04E + 05 | 1.95 | XJ4FM        |
|                | Selgin O-hexosyl-O-hexoside                       | 9.00E + 00 1.98E + 06 | 2.20E + 05 | 1.91 | XJ4FM        |
|                | 8-C-hexosyl-hesperetin O-hexoside                 | 9.00E + 00 6.70E + 05 | 7.45E + 04 | 1.82 | XJ4FM        |
|                | Eriodictiol 6-C-hexoside 8-C-hexoside-O-hexoside  | 9.00E + 00 6.06E + 05 | 6.74E + 04 | 1.81 | XJ4FM        |
|                | Hesperetin C-hexosyl-O-hexosyl-O-hexoside         | 9.00E + 00 4.05E + 05 | 4.50E + 04 | 1.78 | XJ4FM        |
|                | Limocitrin O-hexoside                             | 9.00E + 00 3.43E + 05 | 3.81E + 04 | 1.77 | XJ4FM        |
|                | Chrysoeriol 8-C-hexoside                          | 9.00E + 00 2.49E + 05 | 2.76E + 04 | 1.74 | XJ4FM        |
|                | Chrysoeriol 6-C-hexoside 8-C-hexoside-O-hexoside  | 9.00E + 00 2.28E + 05 | 2.53E + 04 | 1.73 | XJ4FM        |
|                | Butin                                             | 9.00E + 00 1.82E + 05 | 2.02E + 04 | 1.71 | XJ4FM        |
|                | Eriocitrin                                        | 9.00E + 00 7.77E + 04 | 8.63E + 03 | 1.64 | XJ4FM        |

|                 |                                                   |                       |            |      |              |
|-----------------|---------------------------------------------------|-----------------------|------------|------|--------------|
|                 | Tricin <i>O</i> -saccharic acid                   | 9.00E + 00 5.43E + 04 | 6.03E + 03 | 1.60 | XJ4FM        |
|                 | <i>O</i> -methylChrysoeriol 7- <i>O</i> -hexoside | 9.00E + 00 4.73E + 04 | 5.26E + 03 | 1.59 | XJ4FM        |
|                 | Tricin 5- <i>O</i> -rutinoside                    | 9.00E + 00 4.45E + 04 | 4.94E + 03 | 1.59 | XJ4FM        |
|                 | <i>O</i> -methylChrysoeriol 5- <i>O</i> -hexoside | 9.00E + 00 3.99E + 04 | 4.43E + 03 | 1.58 | XJ4FM        |
|                 | Apigenin                                          | 9.00E + 00 1.39E + 04 | 1.55E + 03 | 1.03 | XJ4FM        |
|                 | Chrysoeriol                                       | 9.00E + 00 7.42E + 03 | 8.25E + 02 | 1.41 | XJ4FM        |
|                 | Selgin 5- <i>O</i> -hexoside                      | 5.45E + 04 2.81E + 06 | 5.15E + 01 | 1.20 | XJ4FM & DHFM |
|                 | Apigenin <i>O</i> -hexosyl- <i>O</i> -rutinoside  | 5.41E + 03 1.27E + 05 | 2.36E + 01 | 1.30 | XJ4FM & DHFM |
|                 | Naringenin C-hexoside                             | 1.98E + 04 2.21E + 05 | 1.11E + 01 | 1.28 | XJ4FM & DHFM |
|                 | Narcissoside                                      | 6.73E + 04 2.85E + 03 | 4.23E-02   | 1.23 | XJ4FM & DHFM |
|                 | Chrysoeriol 7- <i>O</i> -rutinoside               | 1.68E + 04 9.00E + 00 | 5.37E-04   | 1.04 | DHFM         |
|                 | C-hexosyl-luteolin <i>O</i> -sinapic acid         | 2.41E + 04 9.00E + 00 | 3.74E-04   | 1.52 | DHFM         |
|                 | Luteolin C-hexoside                               | 2.42E + 04 9.00E + 00 | 3.72E-04   | 1.53 | DHFM         |
|                 | 6-C-hexosyl luteolin <i>O</i> -pentoside          | 3.15E + 04 9.00E + 00 | 2.86E-04   | 1.09 | DHFM         |
|                 | Diosmin                                           | 3.20E + 04 9.00E + 00 | 2.81E-04   | 1.08 | DHFM         |
|                 | Luteolin <i>O</i> -sinapoylhexoside               | 4.34E + 04 9.00E + 00 | 2.07E-04   | 1.58 | DHFM         |
|                 | 3- <i>O</i> -Acetylpinobanksin                    | 4.79E + 04 9.00E + 00 | 1.88E-04   | 1.53 | DHFM         |
| <b>FLAVONOL</b> |                                                   |                       |            |      |              |
| DHPM vs. XJ4PM  | Quercetin                                         | 9.00E + 00 5.59E + 05 | 6.21E + 04 | 2.02 | XJ4PM        |
|                 | Laricitrin                                        | 9.00E + 00 6.04E + 04 | 6.71E + 03 | 1.80 | XJ4PM        |
|                 | Isorhamnetin                                      | 9.00E + 00 2.26E + 04 | 2.51E + 03 | 1.70 | XJ4PM        |
|                 | Rhamnetin (7- <i>O</i> -methxyl quercetin)        | 9.00E + 00 3.26E + 03 | 3.62E + 02 | 1.47 | XJ4PM        |
|                 | Isorhamnetin <i>O</i> -acetyl-hexoside            | 7.88E + 04 6.68E + 06 | 8.47E + 01 | 1.33 | XJ4PM & DHPM |
|                 | Quercetin-3,4'- <i>O</i> -di-beta-glucopyranoside | 2.39E + 04 3.38E + 05 | 1.42E + 01 | 1.46 | XJ4PM & DHPM |
|                 | Isorhamnetin 3- <i>O</i> -neohesperidoside        | 2.21E + 05 1.02E + 04 | 4.63E-02   | 1.03 | XJ4PM & DHPM |
|                 | Quercetin 3- <i>O</i> -rutinoside (Rutin)         | 5.91E + 07 1.13E + 06 | 1.92E-02   | 1.13 | XJ4PM & DHPM |
|                 | Quercetin 7- <i>O</i> -rutinoside                 | 3.48E + 07 5.03E + 05 | 1.45E-02   | 1.17 | XJ4PM & DHPM |
|                 | Kaempferol 3- <i>O</i> -robinobioside (Biorobin)  | 1.13E + 06 1.54E + 04 | 1.37E-02   | 1.66 | XJ4PM & DHPM |
| DHFM vs. XJ4FM  | Kaempferol 3- <i>O</i> -rutinoside (Nicotiflorin) | 1.16E + 06 9.00E + 00 | 7.77E-06   | 2.08 | DHPM         |
|                 | Syringetin 3- <i>O</i> -hexoside                  | 9.00E + 00 4.68E + 05 | 5.20E + 04 | 1.79 | XJ4FM        |
|                 | Rhamnetin                                         | 9.00E + 00 5.00E + 03 | 5.56E + 02 | 1.36 | XJ4FM        |
|                 | Myricetin 3- <i>O</i> -rhamnoside (Myricitrin)    | 1.93E + 05 1.21E + 07 | 6.28E + 01 | 1.11 | XJ4FM & DHFM |
|                 | methylQuercetin <i>O</i> -hexoside                | 3.64E + 04 1.89E + 06 | 5.20E + 01 | 1.20 | XJ4FM & DHFM |
|                 | Myricetin 3- <i>O</i> -galactoside                | 4.83E + 04 1.55E + 06 | 3.21E + 01 | 1.02 | XJ4FM & DHFM |

|                   |                                                          |                       |            |      |              |
|-------------------|----------------------------------------------------------|-----------------------|------------|------|--------------|
|                   | Isorhamnetin 3- <i>O</i> -neohesperidoside               | 1.08E + 04 9.00E + 00 | 8.33E-04   | 1.01 | DHFM         |
|                   | Kaempferol 3- <i>O</i> -robinobioside                    | 3.84E + 04 9.00E + 00 | 2.34E-04   | 1.10 | DHFM         |
|                   | Syringetin                                               | 6.33E + 04 9.00E + 00 | 1.42E-04   | 1.60 | DHFM         |
| <b>FLAVANONE</b>  |                                                          |                       |            |      |              |
| DHPM vs. XJ4PM    | Hesperetin <i>O</i> -malonylhexoside                     | 9.00E + 00 1.22E + 05 | 1.35E + 04 | 1.87 | XJ4PM        |
|                   | Phloretin                                                | 3.12E + 05 6.77E + 06 | 2.17E + 01 | 1.06 | XJ4PM & DHPM |
|                   | Hesperetin 7- <i>O</i> -neohesperidoside (Neohesperidin) | 1.39E + 07 1.87E + 05 | 1.35E-02   | 1.21 | XJ4PM & DHPM |
| DHFM vs. XJ4FM    | Naringenin                                               | 9.00E + 00 1.92E + 05 | 2.13E + 04 | 1.72 | XJ4FM        |
|                   | Hesperetin <i>O</i> -malonylhexoside                     | 9.00E + 00 1.55E + 05 | 1.72E + 04 | 1.70 | XJ4FM        |
|                   | Naringenin 7- <i>O</i> -neohesperidoside (Naringin)      | 9.00E + 00 9.60E + 04 | 1.07E + 04 | 1.66 | XJ4FM        |
|                   | Hesperetin <i>O</i> -Glucuronic acid                     | 9.00E + 00 4.25E + 04 | 4.72E + 03 | 1.58 | XJ4FM        |
|                   | Isosakuranetin-7-neohesperidoside (Poncirin)             | 1.02E + 03 1.16E + 04 | 1.14E + 01 | 1.11 | XJ4FM & DHFM |
| <b>ISOFLAVONE</b> |                                                          |                       |            |      |              |
| DHPM vs. XJ4PM    | Genistein 7- <i>O</i> -Glucoside (Genistin)              | 9.00E + 00 1.87E + 05 | 2.08E + 04 | 1.92 | XJ4PM        |
|                   | Prunetin                                                 | 1.03E + 03 3.49E + 04 | 3.40E + 01 | 1.31 | XJ4PM & DHPM |
| DHFM vs. XJ4FM    | Rotenone                                                 | 9.00E + 00 4.27E + 04 | 4.74E + 03 | 1.58 | XJ4FM        |
|                   | Genistein 7- <i>O</i> -Glucoside                         | 9.00E + 00 2.79E + 04 | 3.10E + 03 | 1.08 | XJ4FM        |
|                   | Glycitein                                                | 9.00E + 00 9.10E + 03 | 1.01E + 03 | 1.43 | XJ4FM        |
|                   | Calycosin                                                | 9.00E + 00 6.75E + 03 | 7.50E + 02 | 1.40 | XJ4FM        |
| <b>POLYPHENOL</b> |                                                          |                       |            |      |              |
| DHPM vs. XJ4PM    | Gallocatechin-gallocatechin                              | 6.36E + 05 1.96E + 07 | 3.09E + 01 | 1.12 | XJ4PM & DHPM |
|                   | (-)-Epiafzelechin                                        | 3.27E + 03 1.67E + 04 | 5.10E + 00 | 1.19 | XJ4PM & DHPM |
| DHFM vs. XJ4FM    | Gallocatechin-gallocatechin                              | 9.00E + 00 2.90E + 07 | 3.23E + 06 | 2.11 | XJ4FM        |
|                   | (-)-Epiafzelechin                                        | 1.69E + 03 4.47E + 04 | 2.64E + 01 | 1.25 | XJ4FM & DHFM |