

|                                         | Coef. (95% CI)         | P      |
|-----------------------------------------|------------------------|--------|
| <b>Total phenols</b>                    | 121.9 (101.3 to 142.5) | <0.001 |
| <b>Secoiridoids</b>                     | 120.2 (100.2 To 140.3) | <0.001 |
| Oleuropein                              | 0.008 (-0.004 To 0.02) | 0.19   |
| Oleuropein derivatives                  |                        |        |
| Oleuropein der I                        | -12.2 (-14.3 To -10.2) | <0.001 |
| Oleuropein der II                       | 1.50 (1.34 To 1.66)    | <0.001 |
| Oleuropein der III                      | 1.24 (1.06 To 1.42)    | <0.001 |
| me-3,4-DHPEA-EA                         | 0.48 (0.40 To 0.56)    | <0.001 |
| Hydroxy oleuropein aglycone I (HOA I)   | 0.30 (0.16 To 0.42)    | <0.001 |
| Hydroxy oleuropein aglycone II (HOA II) | 0.58 (0.30 To 0.85)    | <0.001 |
| HDCM OA                                 | 2.95 (1.48 To 4.43)    | <0.001 |
| 3,4-DHPEA-EA I                          | 2.41 (2.00 To 2.81)    | <0.001 |
| 3,4-DHPEA-EA II                         | 2.69 (2.41 To 2.97)    | <0.001 |
| Lactone                                 | -0.14 (-0.21 To -0.06) | <0.001 |
| Ligstroside derivatives                 |                        |        |
| Ligstroside I                           | 7.38 (7.19 To 9.57)    | <0.001 |
| Ligstroside II                          | 17.5 (15.7 To 19.4)    | <0.001 |
| Ligstroside III                         | 21.0 (17.6 To 24.4)    | <0.001 |
| Oleocanthal                             | 58.8 (42.9 To 74.8)    | <0.001 |
| Elenolic acid                           | 15.3 (11.0 To 19.6)    | <0.001 |
| Elenolic acid derivatives               |                        |        |
| Hydroxyelenolic acid                    | 0.40 (-0.2 To 1.01)    | 0.2    |
| <b>Flavones</b>                         | 1.98 (-0.05 To 4.01)   | 0.06   |
| Luteolin                                | 2.67 (0.94 To 4.40)    | 0.003  |
| Apigenin                                | -0.69 (-1.10 To -0.28) | 0.001  |
| <b>Phenolic alcohols</b>                | 0.96 (0.26 To 1.66)    | 0.007  |
| Hydroxytyrosol                          | -0.01 (-0.02 To 0.01)  | 0.41   |
| Dihydroxytyrosol                        | 0.11 (0.05 To 0.16)    | <0.001 |
| 3,4-DHPEA-AC                            | 0.86 (0.18 To 1.53)    | 0.01   |
| <b>Lignans</b>                          | -0.33 (-0.37 To -0.28) | <0.001 |
| Pinoresinol                             | -0.33 (-0.37 To -0.28) | <0.001 |
| <b>Phenolic acids</b>                   | -0.95 (-1.25 To -0.65) | <0.001 |
| Ferulic acid                            | -0.01 (-0.02 To -0.01) | <0.001 |
| p-coumaric acid                         | -0.37 (-0.53 To -0.21) | <0.001 |
| Vanillic acid                           | -0.57 (-0.72 To -0.42) | <0.001 |

Table s 1. GLM model adjusted for ripeness (conventional vs. organic).

| Phenolic compounds                      | m/z     | DP   | FP   | EP  | CE  | RT    |
|-----------------------------------------|---------|------|------|-----|-----|-------|
| Oleuropein                              | 539/275 | -30  | -140 | -10 | -30 | 7.68  |
| Oleuropein der I                        | 377/241 | -30  | -140 | -10 | -30 | 9.14  |
| Oleuropein der II                       | 377/307 | -30  | -140 | -10 | -30 | 8.64  |
| Oleuropein der III                      | 377/307 | -30  | -140 | -10 | -30 | 10.32 |
| me-3,4-DHPEA-EA                         | 391/255 | -30  | -140 | -10 | -30 | 11.2  |
| Hydroxy oleuropein aglycone I (HOA I)   | 393/257 | -30  | -140 | -10 | -30 | 7.6   |
| Hydroxy oleuropein aglycone II (HOA II) | 393/257 | -30  | -140 | -10 | -30 | 8.8   |
| HDCM OA                                 | 335/199 | -30  | -140 | -10 | -30 | 7.32  |
| 3,4-DHPEA-EA I                          | 377/307 | -30  | -140 | -10 | -30 | 10    |
| 3,4-DHPEA-EA II                         | 377/307 | -30  | -140 | -10 | -30 | 7.91  |
| Lactone                                 | 321/185 | -40  | -250 | -10 | -20 | 7.16  |
| Ligstroside I                           | 361/291 | -30  | -140 | -10 | -30 | 9.01  |
| Ligstroside II                          | 361/291 | -30  | -140 | -10 | -30 | 10    |
| Ligstroside III                         | 361/291 | -30  | -140 | -10 | -30 | 11.2  |
| Oleocanthal                             | 303/285 | -40  | -170 | -5  | -10 | 5.92  |
| Elenolic acid                           | 241/127 | -30  | -140 | -10 | -30 | 6.31  |
| Hydroxyelenolic acid                    | 257/137 | -30  | -140 | -10 | -30 | 6.02  |
| Luteolin                                | 285/133 | -100 | -340 | -10 | -50 | 8.15  |
| Apigenin                                | 269/117 | -70  | -200 | -10 | -50 | 9.11  |
| Hydroxytyrosol                          | 153/123 | -40  | -250 | -10 | -20 | 1.13  |
| Dihydroxytyrosol                        | 169/125 | -40  | -250 | -10 | -20 | 1.09  |
| 3,4-DHPEA-AC                            | 195/180 | -30  | -140 | -10 | -30 | 5.69  |
| Pinoresinol                             | 357/151 | -60  | -180 | -8  | -25 | 8.58  |
| Ferulic acid                            | 193/134 | -40  | -170 | -10 | -20 | 5.15  |
| <i>p</i> -coumaric acid                 | 163/119 | -40  | -150 | -10 | -25 | 4.27  |
| Vanillic acid                           | 167/123 | -30  | -200 | -10 | -30 | 2.56  |

DP: declustering potential; FP: focusing potential; EP: entrance potential; CE: collision energy; RT: retention time

Table s 2. Multiple reaction Monitoring conditions for the polyphenols