

Supplementary Material

Table S1. Phenolic acids found in MS by RP-HPLC-MS/MS in negative mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|-------------------------------------|---|----------------------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| 24-methyl cholesterol ferulate | C ₃₈ H ₅₆ O ₄ | Hydroxycinnamic acid | 576,85 | 0,77 | NA | NA | NA | NA | 0,76 | 0,01 | 578,87 | -2,02 |
| Avenanthramide 2F | C ₁₇ H ₁₅ NO ₆ | Hydroxycinnamic acid | 329,3 | 18,42 | NA | NA | NA | NA | 18,65 | -0,23 | 329,3 | 0 |
| 4-glycogallic acid | C ₁₃ H ₁₆ O ₁₀ | Hydroxybenzoic acid | 332,26 | 20,92 | 20,91 | 0,01 | 332,25 | 0,01 | 20,93 | -0,01 | 332,25 | 0,01 |
| Galloyl glucosa | C ₁₃ H ₁₆ O ₁₀ | Hydroxybenzoic acid | 332,07 | 20,92 | 20,91 | 0,01 | 332,25 | -0,18 | 20,93 | -0,01 | 332,25 | -0,18 |
| Sinapine | C ₁₆ H ₂₄ NO ₅ | Hydroxycinnamic acid | 310,37 | 21,8 | 21,62 | 0,18 | 310,36 | 0,01 | NA | NA | NA | NA |
| Ellagic acid glucoside | C ₂₀ H ₁₆ O ₁₃ | Hydroxybenzoic acid | 464,34 | 22,52 | 22,51 | 0,01 | 464,32 | 0,02 | 22,53 | -0,01 | 464,32 | 0,02 |
| Protocatechuic acid 4-O-glucoside | C ₁₃ H ₁₆ O ₉ | Hydroxybenzoic acid | 316,26 | 22,29 | 22,94 | -0,65 | 316,26 | 0 | 22,97 | -0,68 | 316,26 | 0 |
| P-coumaroyl tartaric acid | C ₁₃ H ₁₂ O ₈ | Hydroxycinnamic acid | 296,23 | 23,55 | 23,57 | -0,02 | 296,23 | 0 | 23,6 | -0,05 | 296,23 | 0 |
| Caffeoyl tartaric acid | C ₁₃ H ₁₂ O ₉ | Hydroxycinnamic acid | 312,23 | 23,85 | 23,86 | -0,01 | 312,23 | 0 | 23,88 | -0,03 | 312,23 | 0 |
| 4-hydroxybenzoic acid 4-O-glucoside | C ₁₃ H ₁₆ O ₈ | Hydroxybenzoic acid | 300,26 | 25,42 | 25,44 | -0,02 | 300,26 | 0 | 25,46 | -0,04 | 300,26 | 0 |
| Ellagic acid acetyl arabinoside | C ₂₁ H ₁₆ O ₁₃ | Hydroxybenzoic acid | 476,34 | 25,59 | 25,57 | 0,02 | 476,35 | -0,01 | 25,61 | -0,02 | 476,35 | -0,01 |
| Ellagic acid acetyl-xyloside | C ₂₁ H ₁₆ O ₁₃ | Hydroxybenzoic acid | 476,34 | 25,59 | 25,57 | 0,02 | 476,35 | -0,01 | 25,61 | -0,02 | 476,35 | -0,01 |
| Feruloyl tartaric acid | C ₁₄ H ₁₄ O ₉ | Hydroxycinnamic acid | 326,26 | 28,7 | 28,7 | 0 | 326,27 | -0,01 | NA | NA | NA | NA |

NA: Not among the most abundant in the extract.

Table S2. Phenolic acids found in *MS* by RP-HPLC-MS/MS in positive mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|-----------------------------------|---|------------------------------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| Dihydrocaffeic acid | C ₉ H ₁₀ O ₄ | Hydroxyphenyl propanoic acid | 182,17 | 18,69 | 18,83 | -0,14 | 182,16 | 0,01 | 18,76 | -0,07 | 182,16 | 0,01 |
| Homovanillic acid | C ₉ H ₁₀ O ₄ | Hydroxyphenylacetic acid | 182,17 | 18,69 | 18,83 | -0,14 | 182,16 | 0,01 | 18,76 | -0,07 | 182,16 | 0,01 |
| Caffeic acid | C ₉ H ₈ O ₄ | Hydroxycinnamic acid | 180,16 | 18,75 | 18,61 | 0,14 | 180,15 | 0,01 | 18,61 | 0,14 | 180,15 | 0,01 |
| Gallic acid 4-O-glucoside | C ₁₃ H ₁₆ O ₁₀ | Hydroxybenzoic acid | 332,26 | 20,92 | 20,92 | 0 | 332,27 | -0,01 | 21 | -0,08 | 332,25 | 0,01 |
| Galloyl glucose | C ₁₃ H ₁₆ O ₁₀ | Hydroxybenzoic acid | 332,26 | 20,92 | 20,92 | 0 | 332,27 | -0,01 | 21 | -0,08 | 332,25 | 0,01 |
| Ellagic acid glucoside | C ₂₀ H ₁₆ O ₁₃ | Hydroxybenzoic acid | 464,34 | 22,52 | 22,27 | 0,25 | 464,32 | 0,02 | 22,27 | 0,25 | 464,32 | 0,02 |
| P-coumaroyl malic acid | C ₁₃ H ₁₂ O ₇ | Hydroxycinnamic acid | 280,23 | 22,56 | 22,61 | -0,05 | 280,23 | 0 | 22,59 | -0,03 | 280,23 | 0 |
| P-coumaric acid | C ₉ H ₈ O ₃ | Hydroxycinnamic acid | 164,16 | 22,67 | 22,69 | -0,02 | 164,15 | 0,01 | 22,85 | -0,18 | 164,15 | 0,01 |
| 5-O-galloylquinic acid | C ₁₄ H ₁₆ O ₁₀ | Hydroxybenzoic acid | 344,27 | 22,93 | 22,87 | 0,06 | 344,28 | -0,01 | 23,1 | -0,17 | 344,28 | -0,01 |
| Protocatechuic acid 4-O-glucoside | C ₁₃ H ₁₆ O ₉ | Hydroxybenzoic acid | 316,26 | 22,93 | 23,08 | -0,15 | 316,26 | 0 | 23,09 | -0,16 | 316,26 | 0 |
| P-coumaroyl tartaric acid | C ₁₃ H ₁₂ O ₈ | Hydroxycinnamic acid | 296,23 | 23,55 | 23,63 | -0,08 | 296,23 | 0 | 23,41 | 0,14 | 296,23 | 0 |
| 2-hydroxybenzoic acid | C ₇ H ₆ O ₃ | Hydroxybenzoic acid | 138,12 | 23,56 | 23,47 | 0,09 | 138,13 | -0,01 | 23,56 | 0 | 138,13 | -0,01 |

| | | | | | | | | | | | | |
|-------------------------------------|---|----------------------|--------|-------|-------|-------|--------|-------|-------|-------|--------|-------|
| 3-hydroxybenzoic acid | C ₇ H ₆ O ₃ | Hydroxybenzoic acid | 138,12 | 23,56 | 23,47 | 0,09 | 138,13 | -0,01 | 23,56 | 0 | 138,13 | -0,01 |
| 4-hydroxybenzoic acid | C ₇ H ₆ O ₃ | Hydroxybenzoic acid | 138,12 | 23,56 | 23,47 | 0,09 | 138,13 | -0,01 | 23,56 | 0 | 138,13 | -0,01 |
| Vanillic acid | C ₈ H ₈ O ₄ | Hydroxybenzoic acid | 168,14 | 23,84 | 23,69 | 0,15 | 168,15 | -0,01 | 23,66 | 0,18 | 168,15 | -0,01 |
| Caffeoyl tartaric acid | C ₁₃ H ₁₂ O ₉ | Hydroxycinnamic acid | 312,23 | 23,85 | 23,64 | 0,21 | 312,22 | 0,01 | 24,08 | -0,23 | 312,22 | 0,01 |
| Sinapic acid | C ₁₁ H ₁₂ O ₅ | Hydroxycinnamic acid | 224,21 | 23,91 | 24 | -0,09 | 224,21 | 0 | 23,94 | -0,03 | 224,21 | 0 |
| Valoneic acid dilactone | C ₂₁ H ₁₀ O ₁₃ | Hydroxybenzoic acid | 470,29 | 24,04 | NA | NA | NA | NA | 24,1 | -0,06 | 470,3 | -0,01 |
| Gallic acid 3-O-gallate | C ₁₄ H ₁₀ O ₉ | Hydroxybenzoic acid | 322,22 | 24,05 | 24,28 | -0,23 | 322,22 | 0 | 23,93 | 0,12 | 322,22 | 0 |
| 4-hydroxybenzoic acid 4-O-glucoside | C ₁₃ H ₁₆ O ₈ | Hydroxybenzoic acid | 300,26 | 25,42 | 25,45 | -0,03 | 300,26 | 0 | 25,24 | 0,18 | 300,26 | 0 |
| Ellagic acid acetyl arabinoside | C ₂₁ H ₁₆ O ₁₃ | Hydroxybenzoic acid | 476,34 | 25,59 | 25,76 | -0,17 | 476,35 | -0,01 | NA | NA | NA | NA |
| Ellagic acid acetyl-xyloside | C ₂₁ H ₁₆ O ₁₃ | Hydroxybenzoic acid | 476,34 | 25,59 | 25,76 | -0,17 | 476,35 | -0,01 | NA | NA | NA | NA |
| Caffeoyl aspartic acid | C ₁₃ H ₁₃ NO ₇ | Hydroxycinnamic acid | 295,24 | 26,37 | 26,59 | -0,22 | 295,25 | -0,01 | NA | NA | NA | NA |
| Hydrocaffeic acid | C ₉ H ₈ O ₅ | Hydroxycinnamic acid | 196,16 | 26,42 | 26,62 | -0,2 | 196,15 | 0,01 | 26,42 | 0 | 196,15 | 0,01 |
| Gallic acid | C ₇ H ₆ O ₅ | Hydroxybenzoic acid | 170,12 | 26,46 | 26,59 | -0,13 | 170,12 | 0 | 26,69 | -0,23 | 170,12 | 0 |
| Ellagic acid | C ₁₄ H ₆ O ₈ | Hydroxybenzoic acid | 302,19 | 26,55 | 26,64 | -0,09 | 302,2 | -0,01 | 26,3 | 0,25 | 302,2 | -0,01 |
| Avenanthramide 2P | C ₁₆ H ₁₃ NO ₅ | Hydroxycinnamic acid | 299,28 | 26,61 | 26,67 | -0,06 | 299,27 | 0,01 | NA | NA | NA | NA |
| Caffeic acid 4-O-glucoside | C ₁₅ H ₁₈ O ₉ | Hydroxycinnamic acid | 342,29 | 26,71 | 26,65 | 0,06 | 342,3 | -0,01 | 26,78 | -0,07 | 342,31 | -0,02 |
| Caffeoyl glucose | C ₁₅ H ₁₈ O ₉ | Hydroxycinnamic acid | 342,29 | 26,71 | 26,65 | 0,06 | 342,3 | -0,01 | 26,78 | -0,07 | 342,31 | -0,02 |
| P-coumaric acid 4-O-glucoside | C ₁₅ H ₁₈ O ₈ | Hydroxycinnamic acid | 326,29 | 27,32 | 27,27 | 0,05 | 326,31 | -0,02 | 27,28 | 0,04 | 326,31 | -0,02 |
| P-coumaroylquinic acid | C ₁₆ H ₁₈ O ₈ | Hydroxycinnamic acid | 338,31 | 27,73 | 27,88 | -0,15 | 338,31 | 0 | 27,84 | -0,11 | 338,31 | 0 |

| | | | | | | | | | | | | |
|---------------------------|--|---------------------|--------|-------|-------|------|--------|---|------|-------|--------|---|
| 2,3-dihydroxybenzoic acid | C ₇ H ₆ O ₄ | Hydroxybenzoic acid | 154,12 | 35,26 | 35,25 | 0,01 | 154,12 | 0 | 35,3 | -0,04 | 154,12 | 0 |
| 2,4-dihydroxybenzoic acid | C ₇ H ₆ O ₄ | Hydroxybenzoic acid | 154,12 | 35,26 | 35,25 | 0,01 | 154,12 | 0 | 35,3 | -0,04 | 154,12 | 0 |
| 2,5-dihydroxybenzoic acid | C ₇ H ₆ O ₄ | Hydroxybenzoic acid | 154,12 | 35,26 | 35,25 | 0,01 | 154,12 | 0 | 35,3 | -0,04 | 154,12 | 0 |
| 2,6-dihydroxybenzoic acid | C ₇ H ₆ O ₄ | Hydroxybenzoic acid | 154,12 | 35,26 | 35,25 | 0,01 | 154,12 | 0 | 35,3 | -0,04 | 154,12 | 0 |
| Protocatechuic acid | C ₇ H ₆ O ₄ | Hydroxybenzoic acid | 154,12 | 35,26 | 35,25 | 0,01 | 154,12 | 0 | 35,3 | -0,04 | 154,12 | 0 |

NA: Not among the most abundant in the extract.

Table S3. Flavonoids found in MS by RP-HPLC-MS/MS in negative mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|----------------------------|---|--------------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| Kaempferol | C ₁₅ H ₁₀ O ₆ | Flavonol | 286,23 | 20,99 | 21,01 | -0,02 | 286,24 | -0,01 | 21,01 | -0,02 | 286,24 | -0,01 |
| Luteolin | C ₁₅ H ₁₀ O ₆ | Flavone | 286,23 | 20,99 | 21,01 | -0,02 | 286,24 | -0,01 | 21,01 | -0,02 | 286,24 | -0,01 |
| Scutellarein | C ₁₅ H ₁₀ O ₆ | Flavone | 286,24 | 20,99 | 21,01 | -0,02 | 286,24 | 0 | 21,01 | -0,02 | 286,24 | 0 |
| Cyanidin | C ₁₅ H ₁₁ O ₆ | Anthocyanin | 287,24 | 21 | 21,02 | -0,02 | 287,24 | 0 | 21 | 0 | 287,24 | 0 |
| 6-hydroxyluteolin | C ₁₅ H ₁₀ O ₇ | Flavone | 302,23 | 21,13 | 21,14 | -0,01 | 302,24 | -0,01 | 21,15 | -0,02 | 302,24 | -0,01 |
| Apigenin 7-O-glucuronide | C ₂₁ H ₁₈ O ₁₁ | Flavone | 446,4 | 22,24 | NA | NA | NA | NA | 22,26 | -0,02 | 446,36 | 0,04 |
| Cirsimaritin | C ₁₇ H ₁₄ O ₆ | Flavone | 314,29 | 22,64 | NA | NA | NA | NA | 22,63 | 0,01 | 314,29 | 0 |
| Isorhamnetin | C ₁₆ H ₁₂ O ₇ | Flavonol | 316,26 | 22,29 | 22,94 | -0,65 | 316,26 | 0 | 22,97 | -0,68 | 316,26 | 0 |
| Nepetin | C ₁₆ H ₁₂ O ₇ | Flavone | 316,26 | 22,29 | 22,94 | -0,65 | 316,26 | 0 | 22,97 | -0,68 | 316,26 | 0 |
| Ramnetin | C ₁₆ H ₁₂ O ₇ | Flavonol | 316,26 | 22,29 | 22,94 | -0,65 | 316,26 | 0 | 22,97 | -0,68 | 316,26 | 0 |
| Daidzin | C ₂₁ H ₂₀ O ₉ | Isoflavonoid | 416,38 | 24,32 | 24,3 | 0,02 | 416,38 | 0 | 24,32 | 0 | 416,38 | 0 |
| Myricetin 3-O-arabinoside | C ₂₀ H ₁₈ O ₁₂ | Flavonol | 450,35 | 25,18 | NA | NA | NA | NA | 25,16 | 0,02 | 450,36 | -0,01 |
| Hispidulin | C ₁₆ H ₁₂ O ₆ | Flavone | 300,26 | 25,42 | 25,44 | -0,02 | 300,26 | 0 | 25,46 | -0,04 | 300,26 | 0 |
| Peonidin | C ₁₆ H ₁₃ O ₆ | Anthocyanin | 301,27 | 25,42 | 25,44 | -0,02 | 301,27 | 0 | 25,46 | -0,04 | 301,27 | 0 |
| Kaempferide | C ₁₆ H ₁₁ O ₆ | Flavonol | 299,25 | 25,43 | 25,44 | -0,01 | 299,26 | -0,01 | 25,48 | -0,05 | 299,26 | -0,01 |
| Kaempferol 3-O-glucoronide | C ₂₁ H ₁₈ O ₁₂ | Flavonol | 462,36 | 25,54 | 25,56 | -0,02 | 462,36 | 0 | 25,6 | -0,06 | 462,36 | 0 |

| | | | | | | | | | | | | |
|--------------------------|---|--------------|--------|-------|-------|-------|--------|-------|-------|-------|--------|-------|
| Luteolin 7-O-glucuronide | C ₂₁ H ₁₈ O ₁₂ | Flavone | 462,36 | 25,54 | 25,56 | -0,02 | 462,36 | 0 | 25,6 | -0,06 | 462,36 | 0 |
| Isoxanthohumol | C ₂₁ H ₂₂ O ₅ | Flavonone | 354,39 | 25,83 | 25,98 | -0,15 | 354,39 | 0 | 26,02 | -0,19 | 354,39 | 0 |
| Xanthohumol | C ₂₁ H ₂₂ O ₅ | Chalcone | 354,39 | 25,83 | 25,98 | -0,15 | 354,39 | 0 | 26,02 | -0,19 | 354,39 | 0 |
| 6,8-Dihydroxykaempferol | C ₁₅ H ₁₀ O ₈ | Flavonol | 318,24 | 26,59 | NA | NA | NA | NA | 26,65 | -0,06 | 318,24 | 0 |
| Myricetin | C ₁₅ H ₁₀ O ₈ | Flavonol | 318,24 | 26,59 | NA | NA | NA | NA | 26,65 | -0,06 | 318,24 | 0 |
| Morin | C ₁₅ H ₁₀ O ₇ | Flavonol | 302,24 | 27,38 | 27,36 | 0,02 | 302,22 | 0,02 | 27,43 | -0,05 | 302,22 | 0,02 |
| 6-Prenylnaringenin | C ₂₀ H ₂₀ O ₅ | Flavonol | 340,36 | 28,64 | 28,67 | -0,03 | 340,38 | -0,02 | 28,85 | -0,21 | 340,38 | -0,02 |
| 8-Prenylnaringenin | C ₂₀ H ₂₀ O ₅ | Flavonol | 340,36 | 28,64 | 28,67 | -0,03 | 340,38 | -0,02 | 28,85 | -0,21 | 340,38 | -0,02 |
| Daidzein | C ₁₅ H ₁₀ O ₄ | Isoflavonoid | 254,34 | 29,85 | 29,92 | -0,07 | 254,22 | 0,12 | NA | NA | NA | NA |

NA: Not among the most abundant in the extract.

Table S4. Flavonoids found in MS by RP-HPLC-MS/MS in positive mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | HAE | | | | RAE | | | | |
|------------------------------|--|-----------------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | Expected Retention Time (s) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| Kaempferol | C ₁₅ H ₁₀ O ₆ | Flavonol | 286,23 | 20,99 | 21,23 | -0,24 | 286,24 | -0,01 | 21,12 | -0,13 | 286,24 | -0,01 |
| Luteolin | C ₁₅ H ₁₀ O ₆ | Flavone | 286,23 | 20,99 | 21,23 | -0,24 | 286,24 | -0,01 | 21,12 | -0,13 | 286,24 | -0,01 |
| Scutellarein | C ₁₅ H ₁₀ O ₆ | Flavone | 286,24 | 20,99 | 21,23 | -0,24 | 286,24 | 0 | 21,12 | -0,13 | 286,24 | 0 |
| Cyanidin | C ₁₅ H ₁₁ O ₆ | Anthocyanin | 287,24 | 21 | 21,02 | -0,02 | 287,24 | 0 | 21,24 | -0,24 | 287,24 | 0 |
| 6-hydroxyluteolin | C ₁₅ H ₁₀ O ₇ | Flavone | 302,23 | 21,13 | 21,18 | -0,05 | 302,23 | 0 | 21,18 | -0,05 | 302,23 | 0 |
| Isorhamnetin | C ₁₆ H ₁₂ O ₇ | Flavonol | 316,26 | 22,93 | 23,08 | -0,15 | 316,26 | 0 | 23,09 | -0,16 | 316,26 | 0 |
| Nepetin | C ₁₆ H ₁₂ O ₇ | Flavone | 316,26 | 22,93 | 23,08 | -0,15 | 316,26 | 0 | 23,09 | -0,16 | 316,26 | 0 |
| Ramnetin | C ₁₆ H ₁₂ O ₇ | Flavonol | 316,26 | 22,93 | 23,08 | -0,15 | 316,26 | 0 | 23,09 | -0,16 | 316,26 | 0 |
| Daidzin | C ₂₁ H ₂₀ O ₉ | Isoflavonoid | 416,38 | 24,32 | 24,28 | 0,04 | 416,37 | 0,01 | 24,26 | 0,06 | 416,37 | 0,01 |
| Phoretin | C ₁₅ H ₁₄ O ₅ | Dihydrochalcone | 274,27 | 24,92 | 25,05 | -0,13 | 274,26 | 0,01 | 25,05 | -0,13 | 274,26 | 0,01 |
| Eriodictyol | C ₁₅ H ₁₂ O ₆ | Flavonone | 288,25 | 24,96 | 25,01 | -0,05 | 288,25 | 0 | 24,89 | 0,07 | 288,25 | 0 |
| Sakuranetin | C ₁₆ H ₁₄ O ₅ | Flavonone | 286,27 | 25,26 | 25,49 | -0,23 | 286,27 | 0 | 25,41 | -0,15 | 286,27 | 0 |
| Hispidulin | C ₁₆ H ₁₂ O ₆ | Flavone | 300,26 | 25,42 | 25,45 | -0,03 | 300,26 | 0 | 25,24 | 0,18 | 300,26 | 0 |
| Peonidin | C ₁₆ H ₁₃ O ₆ | Anthocyanin | 301,27 | 25,42 | 25,41 | 0,01 | 301,27 | 0 | 25,41 | 0,01 | 301,27 | 0 |
| Kaempferide | C ₁₆ H ₁₁ O ₆ | Flavonol | 299,25 | 25,43 | 25,44 | -0,01 | 299,26 | -0,01 | 25,67 | -0,24 | 299,26 | -0,01 |
| Pelargonidin 3-O-arabinoside | C ₂₀ H ₁₉ O ₉ | Anthocyanin | 403,36 | 25,52 | 25,45 | 0,07 | 403,36 | 0 | 25,36 | 0,16 | 403,36 | 0 |

| | | | | | | | | | | | | |
|------------------------------|---|--------------|--------|-------|-------|-------|--------|-------|-------|-------|--------|-------|
| Kaempferol 3-O-glucuronide | C ₂₁ H ₁₈ O ₁₂ | Flavonol | 462,36 | 25,54 | 25,62 | -0,08 | 462,37 | -0,01 | 25,29 | 0,25 | 462,37 | -0,01 |
| Luteolin 7-O-glucuronide | C ₂₁ H ₁₈ O ₁₂ | Flavone | 462,36 | 25,54 | 25,62 | -0,08 | 462,37 | -0,01 | 25,29 | 0,25 | 462,37 | -0,01 |
| Isoxanthohumol | C ₂₁ H ₂₂ O ₅ | Flavonone | 354,39 | 25,83 | NA | NA | NA | NA | 25,88 | -0,05 | 354,41 | -0,02 |
| Xanthohumol | C ₂₁ H ₂₂ O ₅ | Chalcone | 354,39 | 25,83 | NA | NA | NA | NA | 25,88 | -0,05 | 354,41 | -0,02 |
| Myricetin | C ₁₅ H ₁₀ O ₈ | Flavonol | 318,24 | 26,59 | 26,68 | -0,09 | 318,23 | 0,01 | 26,62 | -0,03 | 318,23 | 0,01 |
| Delphinidin 3-O-arabinoside | C ₂₀ H ₁₉ O ₁₁ | Anthocyanin | 435,36 | 26,93 | 27,06 | -0,13 | 435,35 | 0,01 | 26,86 | 0,07 | 435,35 | 0,01 |
| Biochanin A | C ₁₆ H ₁₂ O ₅ | Isoflavonoid | 284,26 | 27,17 | 27,1 | 0,07 | 284,27 | -0,01 | 27,37 | -0,2 | 284,27 | -0,01 |
| Geraldone | C ₁₆ H ₁₂ O ₅ | Flavone | 284,26 | 27,17 | 27,1 | 0,07 | 284,27 | -0,01 | 27,37 | -0,2 | 284,27 | -0,01 |
| Glycitein | C ₁₆ H ₁₂ O ₅ | Isoflavonoid | 284,26 | 27,17 | 27,1 | 0,07 | 284,27 | -0,01 | 27,37 | -0,2 | 284,27 | -0,01 |
| Methylgalangin | C ₁₆ H ₁₂ O ₅ | Flavonol | 284,26 | 27,17 | 27,1 | 0,07 | 284,27 | -0,01 | 27,37 | -0,2 | 284,27 | -0,01 |
| Morin | C ₁₅ H ₁₀ O ₇ | Flavonol | 302,24 | 27,38 | 27,39 | -0,01 | 302,22 | 0,02 | 27,3 | 0,08 | 302,23 | 0,01 |
| Isoharmnetin 3-O-glucuronide | C ₂₂ H ₂₀ O ₁₃ | Flavonol | 492,39 | 27,7 | 27,71 | -0,01 | 492,38 | 0,01 | NA | NA | NA | NA |
| 6"-O-acetylglycitin | C ₂₄ H ₂₄ O ₁₁ | Isoflavonoid | 488,44 | 27,97 | 27,84 | 0,13 | 488,44 | 0 | 27,8 | 0,17 | 488,44 | 0 |
| 6"-O-malonylgenistin | C ₂₄ H ₂₂ O ₁₃ | Isoflavonoid | 518,42 | 29,64 | NA | NA | NA | NA | 29,43 | 0,21 | 518,42 | 0 |

NA: Not among the most abundant in the extract.

Table S5. Stilbenes found in *MS* by RP-HPLC-MS/MS in negative mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|-------------|--|----------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| Resveratrol | C ₁₄ H ₁₂ O ₃ | Stilbene | 228,24 | 23,83 | 23,58 | 0,25 | 228,23 | 0,01 | NA | NA | NA | NA |

NA: Not among the most abundant in the extract.

Table S6. Stilbenes found in *MS* by RP-HPLC-MS/MS in positive mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|---------------|--|----------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| Resveratrol | C ₁₄ H ₁₂ O ₃ | Stilbene | 228,24 | 23,83 | 23,71 | 0,12 | 228,23 | 0,01 | 23,58 | 0,25 | 228,23 | 0,01 |
| Pterostilbene | C ₁₆ H ₁₆ O ₃ | Stilbene | 256,29 | 24,18 | 24,18 | 0 | 256,3 | -0,01 | NA | NA | NA | NA |

NA: Not among the most abundant in the extract.

Table S7. Other polyphenol compounds found in *MS* by RP-HPLC-MS/MS in negative mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|--------------------------|--|-----------------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| 5-heneicosenylresorcinol | C ₂₇ H ₄₆ O ₂ | Alkylphenol | 402,7 | 0,86 | 0,94 | -0,08 | 401,99 | 0,71 | NA | NA | NA | NA |
| Esculin | C ₁₅ H ₁₆ O ₉ | Hydroxycoumarin | 340,28 | 26,37 | NA | NA | NA | NA | 26,39 | -0,02 | 340,29 | -0,01 |

NA: Not among the most abundant in the extract.

Table S8. Other polyphenol compounds found in MS by RP-HPLC-MS/MS in positive mode.

| Name | Molecular Formula | Subclass | Expected Mass (m/z) | Expected Retention Time (s) | HAE | | | | RAE | | | |
|---------------------------|--|---------------------|---------------------|-----------------------------|--------------------|------------------------------|---------------------|----------------------|--------------------|------------------------------|---------------------|----------------------|
| | | | | | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) | Retention Time (s) | Retention Time Variation (s) | Observed Mass (m/z) | Mass Variation (m/z) |
| Psoralen | C ₁₁ H ₆ O ₃ | Furanocoumarin | 186,16 | 1 | NA | NA | NA | NA | 0,9 | 0,1 | 186,17 | -0,01 |
| Pyrogallol | C ₆ H ₆ O ₃ | Other polyphenol | 126,11 | 1,05 | 1,04 | 0,01 | 126,11 | 0 | 1,07 | -0,02 | 126,11 | 0 |
| Scopoletin | C ₁₀ H ₈ O ₄ | Hydroxycoumarin | 192,16 | 7,98 | 7,86 | 0,12 | 192,16 | 0 | 8,2 | -0,22 | 192,16 | 0 |
| 3,4-dihydroxyphenylglycol | C ₈ H ₁₀ O ₄ | Other polyphenol | 170,16 | 12,87 | 12,67 | 0,2 | 170,17 | -0,01 | 13,04 | -0,17 | 170,17 | -0,01 |
| Syringaldehyde | C ₉ H ₁₀ O ₄ | Hydroxybenzaldehyde | 182,17 | 18,69 | 18,83 | -0,14 | 182,16 | 0,01 | 18,76 | -0,07 | 182,16 | 0,01 |
| Coumestrol | C ₁₅ H ₈ O ₅ | Other polyphenol | 268,22 | 20,84 | 21,05 | -0,21 | 268,23 | -0,01 | NE | NE | NE | NE |
| 4-hydroxycoumarin | C ₉ H ₆ O ₃ | Hydroxycoumarin | 162,44 | 21,13 | 20,97 | 0,16 | 162,14 | 0,3 | 21,36 | -0,23 | 162,14 | 0,3 |
| Protocatechuic aldehyde | C ₇ H ₆ O ₃ | Hydroxybenzaldehyde | 138,12 | 23,56 | 23,47 | 0,09 | 138,13 | -0,01 | 23,56 | 0 | 138,13 | -0,01 |
| 1,4-Naphthoquinone | C ₁₀ H ₆ O ₂ | Naphthoquinone | 158,15 | 23,83 | 23,8 | 0,03 | 158,15 | 0 | 23,86 | -0,03 | 158,15 | 0 |
| Juglone | C ₁₀ H ₆ O ₃ | Naphthoquinone | 174,15 | 23,94 | 24,05 | -0,11 | 174,15 | 0 | NA | NA | NA | NA |
| 3-methylcatechol | C ₇ H ₈ O ₂ | Alkylphenol | 124,14 | 24,89 | 24,97 | -0,08 | 124,12 | 0,02 | 24,99 | -0,1 | 124,12 | 0,02 |
| 4-methylcatechol | C ₇ H ₈ O ₂ | Alkylphenol | 124,14 | 24,89 | 24,97 | -0,08 | 124,12 | 0,02 | 24,99 | -0,1 | 124,12 | 0,02 |
| Guaiacol | C ₇ H ₈ O ₂ | Methoxyphenol | 124,14 | 24,89 | 24,97 | -0,08 | 124,12 | 0,02 | 24,99 | -0,1 | 124,12 | 0,02 |
| Phlorin | C ₁₂ H ₁₆ O ₈ | Other polyphenol | 288,25 | 24,96 | 25,01 | -0,05 | 288,25 | 0 | 24,89 | 0,07 | 288,25 | 0 |
| Esculetin | C ₉ H ₆ O ₄ | Hydroxycoumarin | 178,14 | 25 | 25,22 | -0,22 | 178,13 | 0,01 | 24,87 | 0,13 | 178,13 | 0,01 |

| | | | | | | | | | | | | |
|-----------------|--|----------------------|--------|-------|-------|-------|--------|------|-------|-------|--------|------|
| Catechol | C ₆ H ₆ O ₂ | Other polyphenol | 110,11 | 26,13 | 25,96 | 0,17 | 110,1 | 0,01 | 26,15 | -0,02 | 110,1 | 0,01 |
| Esculin | C ₁₅ H ₁₆ O ₉ | Hydroxybenzaldehyde | 340,28 | 26,37 | 26,43 | -0,06 | 340,28 | 0 | 26,43 | -0,06 | 340,28 | 0 |
| Gallic aldehyde | C ₇ H ₆ O ₄ | Hhidroxibenzaldehído | 154,12 | 35,26 | 35,25 | 0,01 | 154,12 | 0 | 35,3 | -0,04 | 154,12 | 0 |
| Isopimpinelin | C ₁₃ H ₁₀ O ₅ | Furanocoumarin | 246,21 | 47,38 | 47,28 | 0,1 | 246,21 | 0 | 47,51 | -0,13 | 246,21 | 0 |

NA: Not among the most abundant in the extract.