Table S4. Phytochemical profile of homogenized at 100 MPa lulo juice by high resolution LC-MS / MS

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Homogenized 100 MPa** | | | | | | |
| **Compound name** | **RT (min)** | **M/Z experimental** | **Teoric mass** | **MS/MS fragments** | **Molecular Formula** | **Error (ppm)** |
| **Hydroxycinnamic acids [M − H] ¯** | | | | | | |
| Cis-3-Caffeoylquinic acid | 12.93 | 353.0877 | 353.0878 | 190/84 | C16H18O9 | -0.4 |
| Trans-5-Caffeoylquinic acid | 12.93 | 353.0877 | 353.0878 | 354/353 | C16H18O9 | -0.4 |
| Cis-5-Caffeoylquinic acid | 12.93 | 353.0877 | 353.0878 | 190/84 | C16H18O9 | -0.4 |
| Trans-3-Caffeoylquinic acid | 12.93 | 353.0878 | 353.0877 | 190/84 | C16H18O9 | -0.4 |
| 1-Caffeoylquinic acid | 12.93 | 353.0878 | 353.0877 | 190/84 | C16H18O9 | -0.4 |
| 5-Caffeoylquinic acid | 12.93 | 353.0877 | 353.0878 | 190/84 | C16H18O9 | -0.4 |
| 3-Caffeoylquinic acid | 12.93 | 353.0878 | 353.0877 | 190/84 | C16H18O9 | -0.4 |
| 4-Caffeoylquinic acid | 12.93 | 353.0877 | 353.0878 | 190/84 | C16H18O9 | -0.4 |
| p-Coumaric acid 4-O-glucoside | 12.95 | 325.093 | 325.0929 | 199/144/142//116 | C15H18O8 | 0.5 |
| p-Coumaroyl glucose | 12.95 | 325.093 | 325.0929 | 199/144/142//116 | C15H18O8 | 0.5 |
| Caffeic acid | 13.33 | 179.0351 | 179.035 | 134/133/108/88 | C9H8O4 | 0.4 |
| Trans-Caffeic acid | 13.33 | 179.0351 | 179.035 | 134/133/108/88 | C9H8O4 | 0.4 |
| Cis-Caffeic acid | 13.33 | 179.0351 | 179.035 | 134/133/108/88 | C9H8O4 | 0.4 |
| Ferulic acid 4-O-glucoside | 13.56 | 355.1035 | 355.103 | 174/159/131 | C16H20O9 | -1.8 |
| Feruloyl glucose | 13.56 | 355.1035 | 355.103 | 174/159/131 | C16H20O9 | -1.3 |
| 4-Hydroxybenzaldehyde | 14.27 | 121.0296 | 121.0295 | 91 | C7H6O2 | 0.6 |
| p-Coumaroylquinic acid | 14.7 | 337.0929 | 337.0926 | 190/172/162/118/116/92 | C15H18O8 | -0.9 |
| 3-p-Coumaroylquinic acid | 14.7 | 337.0929 | 337.0926 | 189/172/162/118/116/92 | C16H18O7 | -0.9 |
| 4-p-Coumaroylquinic acid | 14.7 | 337.0929 | 337.0926 | 190/172/162/118/116/92 | C16H18O8 | -0.9 |
| 5-p-Coumaroylquinic acid | 14.7 | 337.0929 | 337.0926 | 190/172/162/118/116/92 | C16H18O8 | -0.9 |
| **Flavonoids [M − H] ¯** |  |  |  |  |  |  |
| Kaempferol 3,7-O-diglucoside | 16.0 | 609.1466 | 609.1461 | 299/270 | C27H30O16 | 0.8 |
| Kaempferol 3-O-sophoroside | 16.0 | 609.1466 | 609.1461 | 299/270 | C27H30O16 | 0.8 |
| *Table x (continued)* |  |  |  |  |  |  |
| Compound name | RT (min) | M/Z experimental | Teoric mass | MS/MS fragments | Molecular fornula | Error (ppm) |
| Quercetin 3-O-rutinoside | 16.0 | 609.1466 | 609.1461 | 299/270 | C27H30O16 | 0.8 |
| Quercetin 3-O-galactoside 7-O-rhamnoside | 16.0 | 609.1466 | 609.1461 | 299/270 | C27H30O16 | 0.8 |
| Kaempferol 3-O-galactoside 7-O-rhamnoside | 16.4 | 593.1512 | 593.1512 | 283/254 | C27H30O15 | 0 |
| Isorhamnetin 3-O-glucoside 7-O-rhamnoside | 16.57 | 623.1625 | 623.1618 | 313/298/270 | C27H30O16 | 1.2 |
| Isorhamnetin 3-O-rutinoside | 16.57 | 623.1625 | 623.1618 | 313/298/270 | C28H32O16 | 1.2 |
| Kaempferol 3-O-glucoside | 17.3 | 447.0933 | 447.0929 | - | C21H20O11 | -0.9 |
| 3,7-Dimethylquercetin | 18.79 | 329.0666 | 329.0667 | - | C17H14O7 | -0.2 |
| **Phenolic acids [M − H] ¯** |  |  |  |  |  |  |
| 2-Hydroxybenzoic acid | 11.33 | 137.0245 | 137.0244 | 107/96/91 | C7H6O3 | 0.5 |
| 3-Hydroxybenzoic acid | 11.33 | 137.0245 | 137.0244 | 107/96/91 | C7H6O3 | 0.5 |
| 4-Hydroxybenzoic acid | 11.33 | 137.0245 | 137.0244 | 107/96/91 | C7H6O3 | 0.5 |
| 4-Hydroxybenzoic acid 4-O-glucoside | 12.82 | 299.0773 | 299.0772 | 136/92 | C13H16O8 | 0.2 |
| Benzoic acid | 14.27 | 121.0296 | 121.0295 | 91 | C7H6O2 | 0.6 |
| **Other phenolics** **[M − H] ¯** |  |  |  |  |  |  |
| Protocatechuic aldehyde | 11.33 | 137.0245 | 137.0244 | 107/96/91 | C7H6O3 | 0.5 |
| Sesamol | 11.33 | 137.0244 | 137.0245 | 107/96/91 | C7H6O3 | 0.5 |
| 4-Hydroxycoumarin | 12.88 | 161.0245 | 161.0244 | - | C9H6O3 | 0.5 |
| Umbelliferone | 12.88 | 161.0245 | 161.0244 | 88 | C9H6O3 | 0.5 |
| Coumarin | 12.94 | 145.0296 | 145.0295 | 116/115/87 | C9H6O2 | 0.6 |
| 3,4-Dihydroxyphenyl-2-oxypropanoic acid | 13.33 | 179.035 | 179.0351 | 134/133/108/133/88 | C9H8O4 | 0.4 |
| 4-Hydroxybenzaldehyde | 14.06 | 121.0295 | 121.0296 | 91 | C7H6O2 | 0.7 |
| 4-Hydroxyphenylacetic acid | 15.28 | 151.0401 | 151.0401 | - | C8H8O3 | 0.2 |
| **Flavanones** **[M − H] ¯** | | | | | | |
| Naringin 4-O-glucoside | 14.24 | 741.2254 | 741.2248 | 208/193/178 | C33H42O19 | 0.9 |
| Neoeriocitrin | 16.27 | 595.1674 | 595.1668 | - | C27H32O15 | 0.9 |
| *Table x (continued)* |  |  |  |  |  |  |
| **Compound name** | **RT (min)** | **M/Z experimental** | **Teoric mass** | **MS/MS fragments** | **Molecular fornula** | **Error (ppm)** |
| Neohesperidin | 17.01 | 609.1831 | 609.1825 | 300 | C28H34O15 | 0.9 |
| Hesperidin | 17.01 | 609.1831 | 609.1825 | 300 | C28H34O15 | 0.9 |
| Hesperetin | 17.03 | 301.0716 | 301.0718 | - | C16H14O6 | -0.5 |
| **Flavones [M − H] ¯** | | | | | | |
| Apigenin 6,8-di-C-glucoside | 16.4 | 593.1512 | 593.1512 | 283/254 | C27H30O15 | 0 |
| Luteolin 7-O-rutinoside | 16.4 | 593.1512 | 593.1512 | 283/254 | C27H30O15 | 0 |
| Luteolin 4-O-glucoside | 17.3 | 447.0933 | 447.0929 | - | C21H20O11 | -0.9 |
| Luteolin 6-C-glucoside | 17.3 | 447.0933 | 447.0929 | - | C21H20O11 | -0.9 |
| Luteolin 7-O-glucoside | 17.3 | 447.0929 | 447.0933 | - | C21H20O11 | -0.9 |
| Luteolin 8-C-glucoside | 17.3 | 447.0929 | 447.0933 | - | C21H20O11 | -0.9 |
| **Dhydrochalcones [M − H] ¯** | | | | | | |
| Phloridzin | 17.42 | 435.1297 | 435.1297 | 178/166/155/122/100/84 | C21H24O10 | 0 |