

Chemical analysis of *C. intybus* leaf extract using UPLC-TOF-MS negative mode (ESI-)

| Compound | Adducts | Formula | m/z | Mass Error (ppm) |
|-------------------------------------|-----------|-----------|----------|------------------|
| benzoic acid | M-H | C7H6O3 | 137.0249 | 3.6490 |
| gallic acid | M-H | C7H6O5 | 137.0250 | 4.3788 |
| glutamic acid | M-H | C5H9NO4 | 146.0454 | -3.4236 |
| tartaric acid | M-H | C4H6O6 | 149.0089 | -2.0133 |
| p-coumaric acid | M-H | C9H8O3 | 163.0397 | -1.9721 |
| caffeic acid | M-H | C9H8O4 | 179.0344 | -3.3513 |
| Quinic acid | M-H | C7H12O6 | 191.0563 | 1.0468 |
| Sinapinic acid | M-H | C11H12O5 | 205.0605 | -3.1382 |
| Apigenin | M-H | C15H10O5 | 270.0519 | -3.3327 |
| 4-Hydroxybenzoyl glucose | M-H | C13H16O8 | 299.0765 | -2.3405 |
| 4-Hydroxybenzoic acid 4-O-glucoside | M-H | C13H16O8 | 299.0765 | -2.3405 |
| Quercitin | M-H | C15H10O7 | 301.0349 | -1.6609 |
| Caftaric acid | M-H | C13H12O9 | 304.0411 | 0.6430 |
| Chlorogenic acid isomers | M-H | C16H18O9 | 353.0882 | 1.1329 |
| Syringin | M-H, 2M-H | C17H24O9 | 371.1342 | -0.9281 |
| Kaempferol-7-O-glucoside | M-H, 2M-H | C21H20O11 | 447.0926 | -1.5657 |
| Kaempferol-3O-glucoside | M-H | C21H20O12 | 447.0926 | -1.5657 |
| Luteolin-7-O-glucopyranoside | M-H | C21H20O13 | 447.0926 | -1.5657 |
| Chicoric acid | M-H, 2M-H | C22H18O12 | 473.0729 | 0.8455 |
| Quercitin-3-glucuronide | M-H | C21H18O13 | 477.0684 | 1.8865 |
| Dicaffeoyl quinic acid isomers | M-H | C25H24O12 | 515.1203 | 1.5530 |
| Rutin | M-H | C27H30O16 | 609.1439 | -3.6116 |