**Supplementary File 6.** List of glucosinolate compounds, determined by exact mass, fragmentation patterns, and retention time. Asterisks (\*) indicate compounds confirmed by commercial standards.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| # | Systematic short name | Systematic name (- glucosinolate) | Common name | Class | Molecular formula | Retention time | [M-H]- | MS fragments |
| 1 | 3MTP | 3-methylthiopropyl | Glucoiberverin | Aliphatic | C11H21NO9S3 | 3.16 | 406.0300 | 259.013, 241.001, 195.033, 96.960 |
| 2 | 3MSI | 3-methylsulfinylpropyl\* | Glucoiberin | Aliphatic | C11H21NO10S3 | 1.86 | 422.0249 | 358.02761, 259.014, 195.034, 96.961 |
| 3 | 2OH | 2-hydroxypropyl | - | Aliphatic | C10H19NO10S2 | 1.76 | 376.0372 | 259.013, 195.034, 96.960 |
| 4 | 2PRO | 2-propenyl\* | Sinigrin | Aliphatic | C10H17NO9S2 | 2.33 | 358.0266 | 259.013, 241.003, 195.033, 96.960 |
| 5 | 3MSO | 3-methylsulfonylpropyl\* | Glucocheirolin | Aliphatic | C11H21NO11S3 | 2.06 | 438.0198 | 259.013, 241.002, 195.033, 96.960 |
| 6 | 3MSO’ | *3-methylsulfonylpropyl isomer* |  | Aliphatic | C11H21NO11S3 | 1.75 | 438.0202 | 96.961 |
| 7 | 1MP | 1-methylpropyl | - | Aliphatic | C11H21NO9S2 | 3.13 | 374.0579 | 96.961 |
| 8 | 2MP | 2-methylpropyl | - | Aliphatic | C11H21NO9S2 | 3.21 | 374.0579 | 96.960 |
| 9 | 4MTB | 4-methylthiobutyl | Glucoerucin | Aliphatic | C12H23NO9S3 | 3.69 | 420.0456 | 96.960 |
| 10 | 4MSI | 4-methylsulfinylbutyl | Glucoraphanin | Aliphatic | C12H23NO10S3 | 2.03 | 436.0405 | 372.0431, 259.013, 195.034, 96.961 |
| 11 | 4BUT | 3-butenyl | Gluconapin | Aliphatic | C11H19NO9S2 | 2.90 | 372.0423 | 96.960 |
| 12 | NMB | n-methylbutyl | - | Aliphatic | C12H23NO9S2 | 3.96 | 388.0736 | 96.960 |
| 13 | 4MSO | 4-methylsulfonylbutyl | Glucoerysolin | Aliphatic | C12H23NO11S3 | 2.24 | 452.0355 | 96.961 |
| 14 | OH4MSO | 3-hydroxy-4-methylsulfonylbutyl | - | Aliphatic | C12H23NO12S3 | 1.99 | 468.0304 | 259.013, 195.033, 96.961 |
| 15 | 5MTP | 5-methylthiopentyl | Glucoberteroin | Aliphatic | C13H25NO9S3 | 4.31 | 434.0613 | 96.961 |
| 16 | 5MSI | 5-methylsulfinylpentyl | Glucoalyssin | Aliphatic | C13H25NO10S3 | 2.32 | 450.0562 | 386.0591, 259.013, 96.961 |
| 17 | 5MSO | 5-methylsulfonylpentyl | - | Aliphatic | C13H25NO11S3 | 2.55 | 466.0511 | 259.013, 241.004, 195.033, 96.961 |
| 18 | OH5MSO | 3-hydroxy-5-methylsulfonylpentyl | - | Aliphatic | C13H25NO12S3 | 2.11 | 482.0460 | 259.013, 195.033, 96.961 |
| 19 | 6MSI | 6-methylsulfinylhexyl | Glucohesperin | Aliphatic | C14H27NO10S3 | 2.69 | 464.0719 | 400.0751, 259.013. 96.960 |
| 20 | 6MSO | 6-methylsulfonylhexyl | - | Aliphatic | C14H27NO11S3 | 2.99 | 480.0668 | 259.013, 195.033,96.960 |
| 21 | OH6MSO | 3-hydroxy-6-methylsulfonylhexyl | - | Aliphatic | C14H27NO12S3 | 2.31 | 496.0617 | 259.013, 96.960 |
| 22 | 3MECOP | 3-methoxycarbonylpropyl | Glucoerypestrin | Carboxylic | C12H21NO11S2 | 2.75 | 418.0477 | 259.013, 195.033, 96.961 |
| 23 | I3M | indol-3-ylmethyl | Glucobrassicin | Indole | C16H20N2O9S2 | 4.00 | 447.0532 | 96.960 |
| 24 | 4OHI3M | 4-hydroxy-indol-3-ylmethyl | 4-Hydroxyglucobrassicin | Indole | C16H20N2O10S2 | 3.37 | 463.0481 | 259.013, 96.961 |
| 25 | 4MEI3M | 4-methoxy-indol-3-ylmethyl | 4-Methoxyglucobrassicin | Indole | C17H22N2O10S2 | 4.39 | 477.0637 | 96.961 |

1 [M-CH4OS-H]-