|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MS2 componund** | **ion** | **fold-change** | ***p* value** | **VIP** | **MZ** | **RT (min)** | **MS2superclass** | **MS2class** | **KEGG code** | **Trend** |
| Pyroglutamic acid | ESI- | 0.4991 | 0.0336 | 1.9811 | 128.0 | 2.50 | Organic acids and derivatives | Carboxylic acids and derivatives | C01879 | down |
| Arachidic acid | ESI- | 0.4981 | 0.0013 | 2.0561 | 311.3 | 8.31 | Lipids and lipid-like molecules | Fatty Acyls | C06425 | down |
| Taurodeoxycholic acid | ESI- | 0.4222 | 0.0282 | 1.8883 | 498.3 | 5.96 | Lipids and lipid-like molecules | Sterol Lipids | C05463 | down |
| Glutathione, oxidized | ESI- | 0.4510 | 0.0466 | 1.6071 | 611.2 | 0.89 | Organic acids and derivatives | Carboxylic acids and derivatives | C00127 | down |
| 2-Piperidinone | ESI+ | 0.3023 | 0.0168 | 2.3494 | 100.1 | 2.44 | Organoheterocyclic compounds | Piperidines | NA | down |
| 5-Hydroxyindoleacetic acid | ESI+ | 0.2933 | 0.0125 | 2.1609 | 192.1 | 2.36 | Organoheterocyclic compounds | Indoles and derivatives | C05635 | down |
| L-Kynurenine | ESI+ | 0.2878 | 0.0165 | 2.1918 | 209.1 | 2.36 | Organic oxygen compounds | Organooxygen compounds | C00328 | down |
| Gly-Phe | ESI+ | 2.1228 | 0.0432 | 2.1897 | 223.1 | 2.45 | Organic acids and derivatives | Carboxylic acids and derivatives | NA | up |
| cis-Nerolidol | ESI+ | 0.4805 | 0.0143 | 2.0584 | 223.2 | 6.23 | Lipids and lipid-like molecules | Prenol lipids | NA | down |
| Ile-Glu | ESI+ | 0.4970 | 0.0486 | 1.6064 | 261.1 | 2.51 | Organic acids and derivatives | Carboxylic acids and derivatives | NA | down |
| Phe-Thr | ESI+ | 2.7822 | 0.0047 | 2.7017 | 267.1 | 0.83 | Organic acids and derivatives | Carboxylic acids and derivatives | NA | up |
| Linoleic acid | ESI+ | 0.3420 | 0.0328 | 2.1041 | 298.3 | 3.43 | Lipids and lipid-like molecules | Fatty Acyls | C01595 | down |
| Ethyl icosapentate | ESI+ | 0.3804 | 0.0278 | 1.7454 | 331.3 | 7.67 | Lipids and lipid-like molecules | Fatty Acyls | C16184 | down |
| Quetiapine | ESI+ | 2.4425 | 0.0046 | 1.9721 | 384.2 | 2.70 | Organoheterocyclic compounds | Benzothiazepines | C07397 | up |
| Aniline | ESI+ | 0.3457 | 0.0286 | 1.9418 | 94.1 | 2.36 | Benzenoids | Benzene and substituted derivatives | C00292 | down |
| 2-Furancarboxaldehyde | ESI+ | 0.4941 | 0.0443 | 1.4097 | 97.0 | 0.82 | Organooxygen compounds | Carbonyl compounds | C14279 | down |