

Figure S1. Obtained by C18 column in ESI⁻ mode (A) TIC of tea samples with different processing (B) TIC of QC samples (C) 3D-principal component analysis of samples.

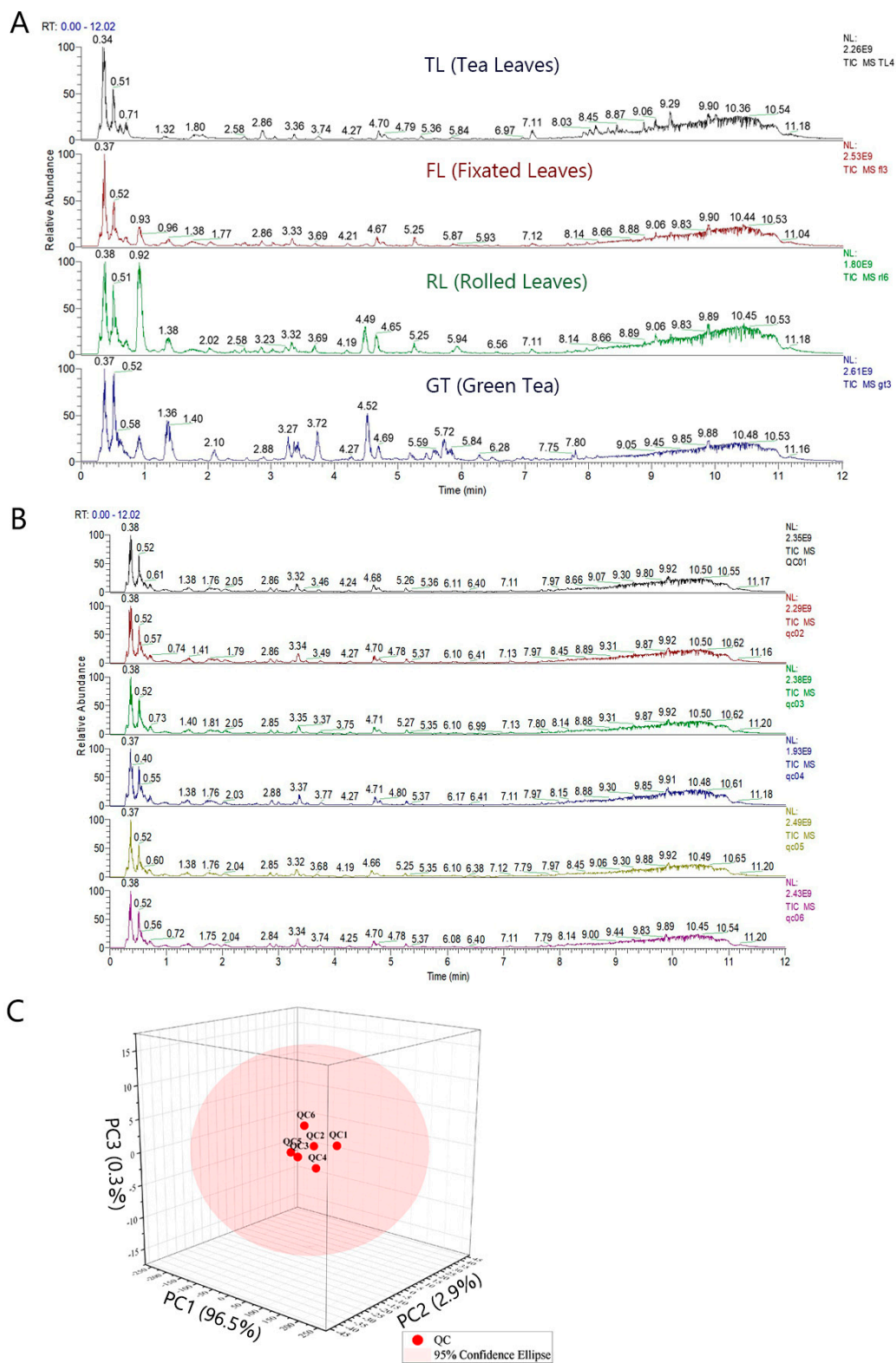


Figure S2. Obtained by HILIC column in ESI+ mode (A) TIC of tea samples with different processing (B) TIC of QC samples (C) 3D-principal component analysis of samples.

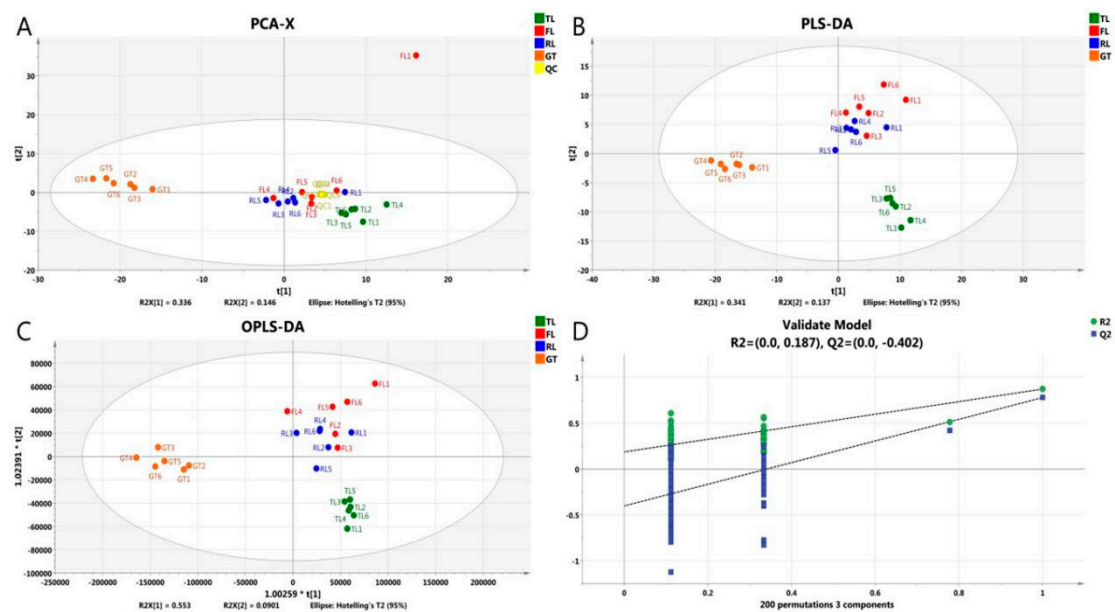


Figure S3. Multivariate statistical analyses of Rizhao green tea samples at different processing stages (C18 column, ESI-).

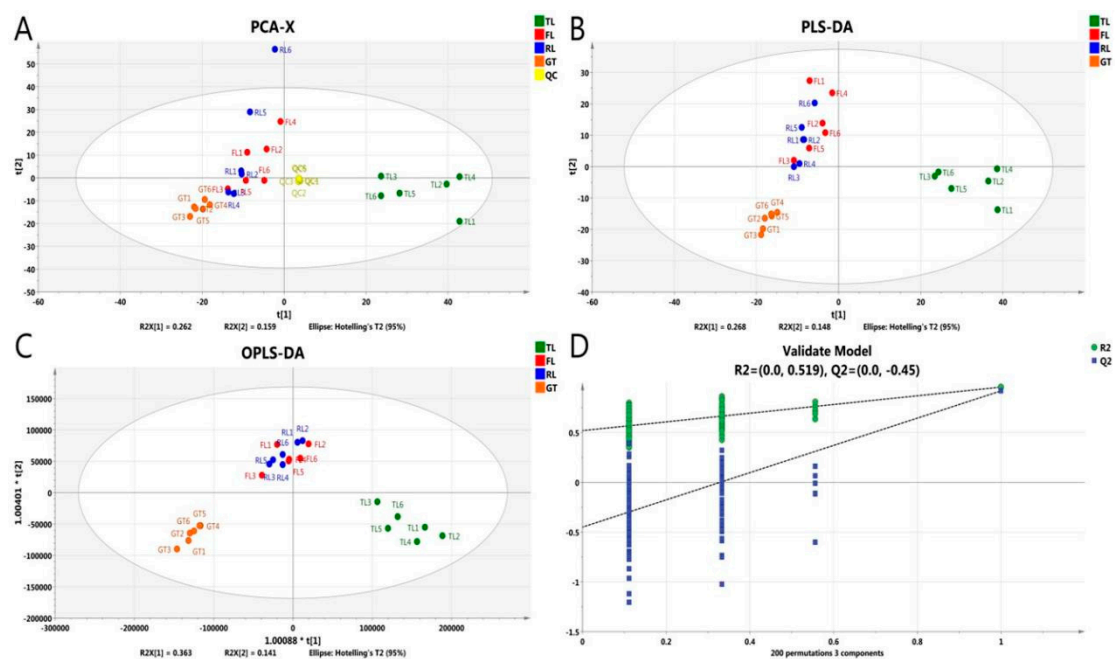


Figure S4. Multivariate statistical analyses of Rizhao green tea samples at different processing stages (Hilic column, ESI+).

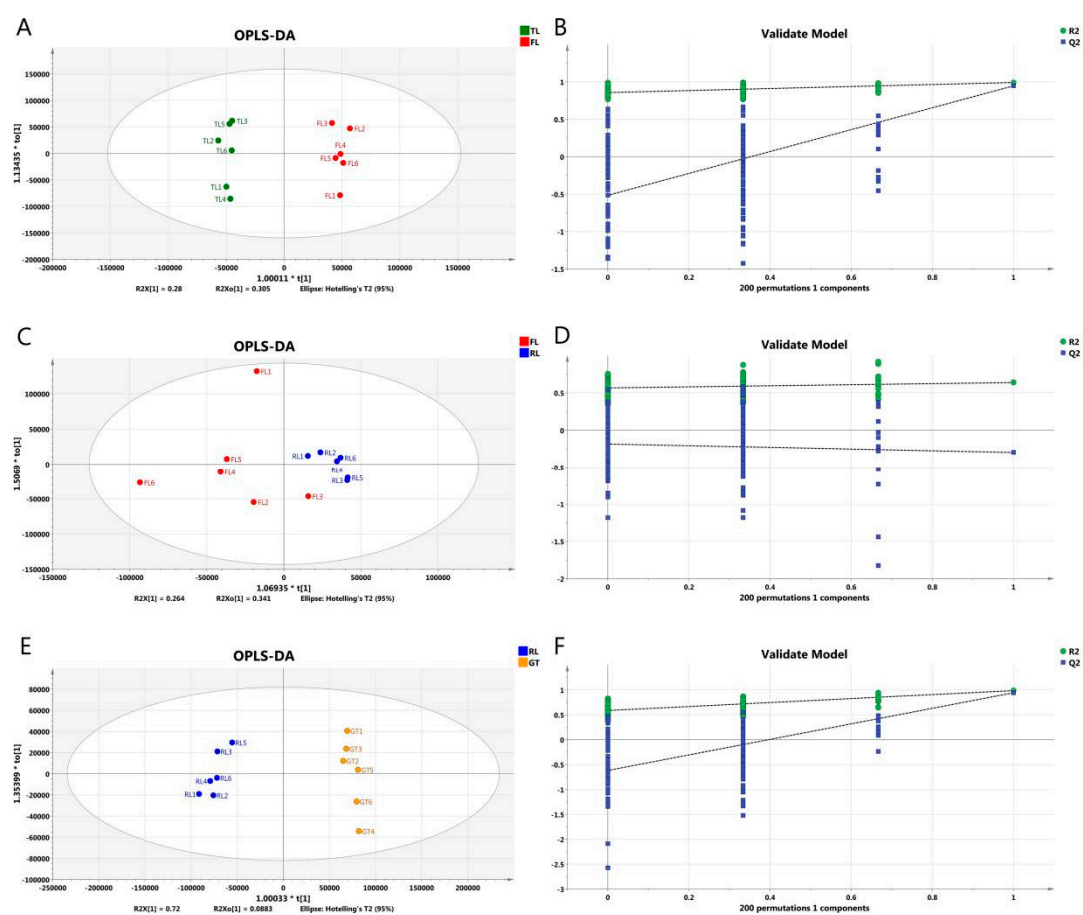


Figure S5. OPLS-DA analysis and permutation tests in samples at adjacent processing stages.

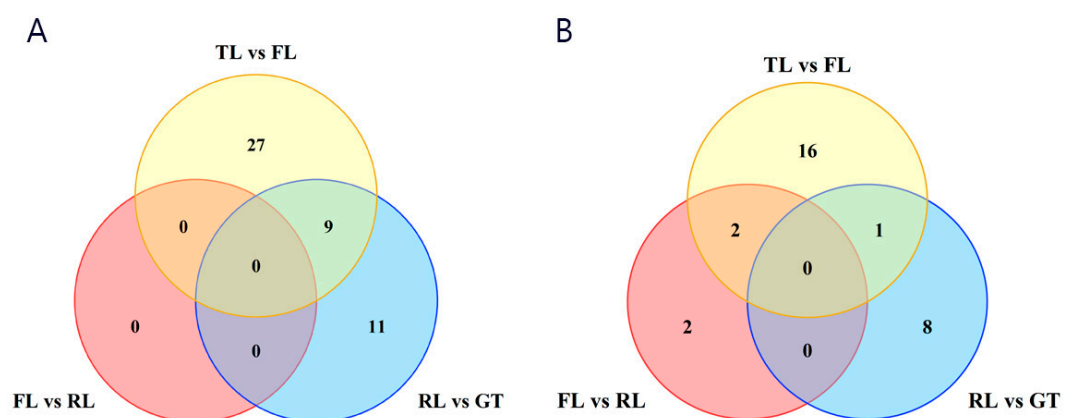


Figure S6. Venn diagram of differential metabolites of (A) C18 column in ESI⁻ mode (B) Hilic column in ESI⁺ mode.

Table S1. List of 530 non-volatile metabolites in the processing of Rizhao green tea (ESI+, C18 column).

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|----|--|---|---------------------------|-----------------------|-----------------------|
| 1 | 1-Aminocyclopropanecarboxylic acid | C ₄ H ₇ NO ₂ | 22059-21-8 | 101.05 | -0.00022 |
| 2 | L-beta-Homoserine | C ₄ H ₉ NO ₃ | 16504-56-6 | 119.06 | -0.00014 |
| 3 | L-Cysteine | C ₃ H ₇ NO ₂ S | 52-90-4 | 121.02 | -0.00031 |
| 4 | L-Pyroglutamic acid | C ₅ H ₇ NO ₃ | 98-79-3 | 129.04 | -0.00013 |
| 5 | Pipecolic acid | C ₆ H ₁₁ NO ₂ | 535-75-1 | 129.08 | -0.00023 |
| 6 | L-Norleucine | C ₆ H ₁₃ NO ₂ | 327-57-1 | 131.09 | -0.00021 |
| 7 | N,N-Diethylglycine | C ₆ H ₁₃ NO ₂ | 1606-01-5 | 131.09 | -0.00021 |
| 8 | Aminocaproic acid | C ₆ H ₁₃ NO ₂ | 1319-82-0 | 131.09 | -0.00018 |
| 9 | Allysine | C ₆ H ₁₁ NO ₃ | 1962-83-0 | 145.07 | -0.00015 |
| 10 | Acetylserine | C ₅ H ₉ NO ₄ | 16354-58-8 | 147.05 | -0.00024 |
| 11 | 3-Methylcrotonylglycine | C ₇ H ₁₁ NO ₃ | 33008-07-0 | 157.07 | -0.00034 |
| 12 | L-Phenylalanine | C ₉ H ₁₁ NO ₂ | 63-91-2 | 165.08 | -0.00002 |
| 13 | N-Acetyl-L-leucine | C ₈ H ₁₅ NO ₃ | 1188-21-2 | 173.11 | -0.00007 |
| 14 | Boc-Glycine | C ₇ H ₁₃ NO ₄ | 4530-20-5 | 175.08 | -0.00018 |
| 15 | Ethyl methioninate | C ₇ H ₁₅ NO ₂ S | 452-95-9 | 177.08 | -0.00003 |
| 16 | DL-Tyrosine | C ₉ H ₁₁ NO ₃ | 556-03-6 | 181.07 | -0.00016 |
| 17 | 1-(Ethoxycarbonyl)proline | C ₈ H ₁₃ NO ₄ | 5700-74-3 | 187.08 | -0.00024 |
| 18 | N-Glycyl-L-leucine | C ₈ H ₁₆ N ₂ O ₃ | 869-19-2 | 188.12 | -0.00051 |
| 19 | Glycyl-L-norleucine | C ₈ H ₁₆ N ₂ O ₃ | 1504-41-2 | 188.12 | -0.00041 |
| 20 | N-Isopropyl-L-glutamine | C ₈ H ₁₆ N ₂ O ₃ | 4311-12-0 | 188.12 | -0.00002 |
| 21 | N-Acetyl-L-glutamic acid | C ₇ H ₁₁ NO ₅ | 1188-37-0 | 189.06 | 0.00015 |
| 22 | Dihydroxyphenylalanine | C ₉ H ₁₁ NO ₄ | 59-92-7 | 197.07 | -0.00022 |
| 23 | N ² ,N ² -Diethylglutamine | C ₉ H ₁₈ N ₂ O ₃ | ChemSpider ID 476314 | 202.13 | -0.00025 |
| 24 | Alanylleucine | C ₉ H ₁₈ N ₂ O ₃ | 1999-42-4 | 202.13 | -0.00019 |
| 25 | DL-Tryptophan | C ₁₁ H ₁₂ N ₂ O ₂ | 54-12-6 | 204.09 | -0.00031 |
| 26 | Cinnamoylglycine | C ₁₁ H ₁₁ NO ₃ | 16534-24-0 | 205.07 | -0.00044 |
| 27 | Val-Pro | C ₁₀ H ₁₈ N ₂ O ₃ | 20488-27-1 | 214.13 | -0.00019 |
| 28 | 2-Hydroxyoct-7-enoylglycine | C ₁₀ H ₁₇ NO ₄ | ChemSpider ID 74849653 | 215.12 | -0.00033 |
| 29 | N-(4-Oxobutyl)-L-glutamine | C ₉ H ₁₆ N ₂ O ₄ | ChemSpider ID 26332249 | 216.11 | -0.00002 |
| 30 | N-Butyl-4-methylglutamine | C ₁₀ H ₂₀ N ₂ O ₃ | ChemSpider ID 492612 | 216.15 | -0.00037 |
| 31 | Val-Val | C ₁₀ H ₂₀ N ₂ O ₃ | 3918-94-3 | 216.15 | -0.00031 |
| 32 | Boc-5-Aminopentanoic acid | C ₁₀ H ₁₉ NO ₄ | 27219-07-4 | 217.13 | -0.00036 |
| 33 | 5-Hydroxy-DL-tryptophan | C ₁₁ H ₁₂ N ₂ O ₃ | 56-69-9 | 220.08 | -0.00025 |
| 34 | 4-(Acetylamino)phenylalanine | C ₁₁ H ₁₄ N ₂ O ₃ | 24250-87-1 | 222.10 | -0.00034 |
| 35 | Gly-Phe | C ₁₁ H ₁₄ N ₂ O ₃ | 721-66-4 | 222.10 | -0.00003 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|----|---|--|---------------------------|-----------------------|-----------------------|
| 36 | Leu-pro | C ₁₁ H ₂₀ N ₂ O ₃ | 6403-35-6 | 228.15 | -0.00036 |
| 37 | 2,6-Diacetamidohexanoic acid | C ₁₀ H ₁₈ N ₂ O ₄ | 35436-74-9 | 230.13 | -0.00034 |
| 38 | Leu-Val | C ₁₁ H ₂₂ N ₂ O ₃ | 35436-83-0 | 230.16 | -0.00044 |
| 39 | Val-Leu | C ₁₁ H ₂₂ N ₂ O ₃ | 22906-55-4 | 230.16 | -0.0004 |
| 40 | Boc-L-Asparagine | C ₉ H ₁₆ N ₂ O ₅ | 7536-55-2 | 232.11 | -0.00051 |
| 41 | Threonylleucine | C ₁₀ H ₂₀ N ₂ O ₄ | 50299-12-2 | 232.14 | -0.00042 |
| 42 | Leucyl-4-hydroxyproline | C ₁₁ H ₂₀ N ₂ O ₄ | ChemSpider ID 20170035 | 244.14 | -0.00045 |
| 43 | Leu-Leu | C ₁₂ H ₂₄ N ₂ O ₃ | 3303-31-9 | 244.18 | -0.00058 |
| 44 | Leu-Gly-Gly | C ₁₀ H ₁₉ N ₃ O ₄ | 4337-37-5 | 245.14 | -0.00045 |
| 45 | Boc-7-Aminoheptanoic acid | C ₁₂ H ₂₃ NO ₄ | 60142-89-4 | 245.16 | -0.00038 |
| 46 | Boc-Lysine | C ₁₁ H ₂₂ N ₂ O ₄ | 13734-28-6 | 246.16 | -0.00046 |
| 47 | N(2)-Succinyl-L-glutamic acid | C ₉ H ₁₃ NO ₇ | 33981-72-5 | 247.07 | -0.00039 |
| 48 | Ala-Tyr | C ₁₂ H ₁₆ N ₂ O ₄ | 3061-88-9 | 252.11 | -0.00062 |
| 49 | Leu-Gln | C ₁₁ H ₂₁ N ₃ O ₄ | ChemSpider ID 3511125 | 259.15 | -0.00062 |
| 50 | Lys-Leu | C ₁₂ H ₂₅ N ₃ O ₃ | 7369-79-1 | 259.19 | -0.00061 |
| 51 | alpha-Glutamyl-4-hydroxyproline | C ₁₀ H ₁₆ N ₂ O ₆ | ChemSpider ID 35032069 | 260.10 | -0.00042 |
| 52 | L-gamma-Glutamyl-L-leucine | C ₁₁ H ₂₀ N ₂ O ₅ | 2566-39-4 | 260.14 | -0.00052 |
| 53 | Leu-Glu | C ₁₁ H ₂₀ N ₂ O ₅ | 16364-31-1 | 260.14 | -0.00051 |
| 54 | Phenylac-gln-OH | C ₁₃ H ₁₆ N ₂ O ₄ | 28047-15-6 | 264.11 | -0.0006 |
| 55 | N-Valylphenylalanine | C ₁₄ H ₂₀ N ₂ O ₃ | 75946-40-6 | 264.15 | -0.00061 |
| 56 | (2S,4S)-Hypoglycin B | C ₁₂ H ₁₈ N ₂ O ₅ | ChemSpider ID 390178 | 270.12 | -0.00067 |
| 57 | gamma-L-Glutamyl-L-glutamic acid | C ₁₀ H ₁₆ N ₂ O ₇ | 1116-22-9 | 276.10 | -0.00058 |
| 58 | Leu-Phe | C ₁₅ H ₂₂ N ₂ O ₃ | 56217-82-4 | 278.16 | -0.00068 |
| 59 | alpha-Asp-Phe | C ₁₃ H ₁₆ N ₂ O ₅ | 13433-09-5 | 280.11 | -0.00074 |
| 60 | N6-((Benzoyloxy)carbonyl)lysine | C ₁₄ H ₂₀ N ₂ O ₄ | 32302-83-3 | 280.14 | -0.00059 |
| 61 | Indoleacetylaspartate | C ₁₄ H ₁₄ N ₂ O ₅ | 2456-73-7 | 290.09 | -0.0008 |
| 62 | N-(2-Amino-3-phenylpropanoyl)glutamine | C ₁₄ H ₁₉ N ₃ O ₄ | ChemSpider ID 35032821 | 293.14 | -0.00058 |
| 63 | Aspartame | C ₁₄ H ₁₈ N ₂ O ₅ | 22839-47-0 | 294.12 | -0.00067 |
| 64 | Leucyltyrosine | C ₁₅ H ₂₂ N ₂ O ₄ | 968-21-8 | 294.16 | -0.00077 |
| 65 | Ile-Tyr | C ₁₅ H ₂₂ N ₂ O ₄ | 38579-21-4 | 294.16 | -0.00068 |
| 66 | Nicotianamine | C ₁₂ H ₂₁ N ₃ O ₆ | 34441-14-0 | 303.14 | -0.00044 |
| 67 | Tyr-Gln | C ₁₄ H ₁₉ N ₃ O ₅ | 28252-40-6 | 309.13 | -0.00083 |
| 68 | N-(tert-Butoxycarbonyl)-4-nitro-L-phenylalanine | C ₁₄ H ₁₈ N ₂ O ₆ | 33305-77-0 | 310.12 | -0.00074 |
| 69 | S-Methylglutathione | C ₁₁ H ₁₉ N ₃ O ₆ S | 2922-56-7 | 321.10 | -0.00077 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|-------------|-----------------------|-----------------------|
| 70 | (Ac)2-L-Lysyl-D-alanyl-D-alanine | C ₁₆ H ₂₈ N ₄ O ₆ | 24570-39-6 | 372.20 | -0.00092 |
| 71 | Oxidized glutathione | C ₂₀ H ₃₂ N ₆ O ₁₂ S ₂ | 121-24-4 | 612.15 | -0.00101 |
| 72 | Liquiritigenin | C ₁₅ H ₁₂ O ₄ | 578-86-9 | 256.07 | -0.00064 |
| 73 | Genistein | C ₁₅ H ₁₀ O ₅ | 446-72-0 | 270.05 | -0.00073 |
| 74 | Naringenin chalcone | C ₁₅ H ₁₂ O ₅ | 73692-50-9 | 272.07 | -0.00082 |
| 75 | Naringenin | C ₁₅ H ₁₂ O ₅ | 480-41-1 | 272.07 | -0.00068 |
| 76 | Kaempferol | C ₁₅ H ₁₀ O ₆ | 520-18-3 | 286.05 | -0.00076 |
| 77 | Luteolin | C ₁₅ H ₁₀ O ₆ | 491-70-3 | 286.05 | -0.00072 |
| 78 | Aromadendrin | C ₁₅ H ₁₂ O ₆ | 480-20-6 | 288.06 | -0.00073 |
| 79 | Tetrahydroxyflavanone | C ₁₅ H ₁₂ O ₆ | 20725-03-5 | 288.06 | -0.00071 |
| 80 | Cianidanol | C ₁₅ H ₁₄ O ₆ | 154-23-4 | 290.08 | -0.00077 |
| 81 | Quercetin | C ₁₅ H ₁₀ O ₇ | 117-39-5 | 302.04 | -0.0008 |
| 82 | 3,5,7,2',4'-Pentahydroxyflavone | C ₁₅ H ₁₀ O ₇ | 480-16-0 | 302.04 | -0.00079 |
| 83 | 2',3,5,6',7-Pentahydroxyflavanone | C ₁₅ H ₁₂ O ₇ | 80366-15-0 | 304.06 | -0.00075 |
| 84 | Myricetin | C ₁₅ H ₁₀ O ₈ | 529-44-2 | 318.04 | -0.00072 |
| 85 | Flavan-3,3',4,4',5,5',7-heptol | C ₁₅ H ₁₄ O ₈ | 491-52-1 | 322.07 | -0.00092 |
| 86 | 6-Methoxyquercetin | C ₁₆ H ₁₂ O ₈ | 519-96-0 | 332.05 | -0.00078 |
| 87 | Theogallin | C ₁₄ H ₁₆ O ₁₀ | 17365-11-6 | 344.07 | -0.00076 |
| 88 | Epiafzelechin 3-O-gallate | C ₂₂ H ₁₈ O ₉ | 108907-43-3 | 426.09 | -0.00101 |
| 89 | Isovitexin | C ₂₁ H ₂₀ O ₁₀ | 29702-25-8 | 432.10 | -0.00106 |
| 90 | Vitexin | C ₂₁ H ₂₀ O ₁₀ | 3681-93-4 | 432.10 | -0.00096 |
| 91 | Swertianolin | C ₂₀ H ₂₀ O ₁₁ | 23445-00-3 | 436.10 | -0.00081 |
| 92 | ECG | C ₂₂ H ₁₈ O ₁₀ | 1257-08-5 | 442.09 | -0.00129 |
| 93 | Trifolin | C ₂₁ H ₂₀ O ₁₁ | 23627-87-4 | 448.10 | -0.00117 |
| 94 | EGCG | C ₂₂ H ₁₈ O ₁₁ | 989-51-5 | 458.08 | -0.00113 |
| 95 | Quercetin 4'-O-glucoside | C ₂₁ H ₂₀ O ₁₂ | 20229-56-5 | 464.09 | -0.00107 |
| 96 | Quercetin-3β-D-glucoside | C ₂₁ H ₂₀ O ₁₂ | 482-35-9 | 464.09 | -0.00106 |
| 97 | Silandrin | C ₂₅ H ₂₂ O ₉ | 70815-32-6 | 466.13 | -0.00126 |
| 98 | Myricetin 3-galactoside | C ₂₁ H ₂₀ O ₁₃ | 15648-86-9 | 480.09 | -0.00099 |
| 99 | Corymboside | C ₂₆ H ₂₈ O ₁₄ | 73543-87-0 | 564.15 | -0.00118 |
| 100 | Apigenin-8-C-glucoside | C ₂₇ H ₃₀ O ₁₄ | 64820-99-1 | 578.16 | -0.00148 |
| 101 | Tiliroside | C ₃₀ H ₂₆ O ₁₃ | 20316-62-5 | 594.14 | -0.00106 |
| 102 | Kaempferol 3-O-rutinoside | C ₂₇ H ₃₀ O ₁₅ | 17650-84-9 | 594.16 | -0.00145 |
| 103 | Rutin | C ₂₇ H ₃₀ O ₁₆ | 153-18-4 | 610.15 | -0.00144 |
| 104 | Quercetin 3-O-Rhamnoside-7-O-glucoside | C ₂₇ H ₃₀ O ₁₆ | 17306-45-5 | 610.15 | -0.00137 |
| 105 | Mauritianin | C ₃₃ H ₄₀ O ₁₉ | 109008-28-8 | 740.21 | -0.0023 |
| 106 | 3,4-Dihydroxybenzaldehyde | C ₇ H ₆ O ₃ | 139-85-5 | 138.03 | -0.00032 |
| 107 | 4-Hydroxybenzoic acid | C ₇ H ₆ O ₃ | 99-96-7 | 138.03 | -0.00027 |
| 108 | Salicylic acid | C ₇ H ₆ O ₃ | 69-72-7 | 138.03 | -0.00024 |
| 109 | Protocatechuic acid | C ₇ H ₆ O ₄ | 99-50-3 | 154.03 | -0.00026 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|---------------------------|-----------------------|-----------------------|
| 110 | o-Coumaric acid | C ₉ H ₈ O ₃ | 614-60-8 | 164.05 | -0.00035 |
| 111 | 4-Hydroxycinnamic acid | C ₉ H ₈ O ₃ | 501-98-4 | 164.05 | -0.0003 |
| 112 | 4-Hydroxyphenylglyoxylic acid | C ₈ H ₆ O ₄ | 15573-67-8 | 166.03 | -0.0002 |
| 113 | 3,4-Dihydroxyphenylacetic acid | C ₈ H ₈ O ₄ | 102-32-9 | 168.04 | -0.00029 |
| 114 | Gallic acid | C ₇ H ₆ O ₅ | 149-91-7 | 170.02 | -0.00019 |
| 115 | Shikimic acid | C ₇ H ₁₀ O ₅ | 138-59-0 | 174.05 | -0.00037 |
| 116 | Caffeoquinone | C ₉ H ₆ O ₄ | 15416-77-0 | 178.03 | -0.00038 |
| 117 | 4-Methoxycinnamic acid | C ₁₀ H ₁₀ O ₃ | 830-09-1 | 178.06 | -0.00019 |
| 118 | Caffeic acid | C ₉ H ₈ O ₄ | 331-39-5 | 180.04 | -0.00025 |
| 119 | 2,5-Dihydroxyterephthalic acid | C ₈ H ₆ O ₆ | 610-92-4 | 198.02 | -0.00031 |
| 120 | Syringic acid | C ₉ H ₁₀ O ₅ | 530-57-4 | 198.05 | -0.00024 |
| 121 | 3-Acetoxycinnamic acid | C ₁₁ H ₁₀ O ₄ | 20375-42-2 | 206.06 | -0.00035 |
| | Methyl | | | | |
| 122 | 3-(2,3-dihydroxy-3-methylbutyl)-4-hydroxybenzoate | C ₁₃ H ₁₈ O ₅ | 117176-70-2 | 254.11 | -0.0005 |
| 123 | (2R,3S)-trans-Coutaric acid | C ₁₃ H ₁₂ O ₈ | 27174-06-7 | 296.05 | -0.00075 |
| 124 | Caftaric acid | C ₁₃ H ₁₂ O ₉ | 67879-58-7 | 312.05 | -0.00067 |
| 125 | Digallic acid | C ₁₄ H ₁₀ O ₉ | 536-08-3 | 322.03 | -0.00077 |
| 126 | Coniferyl ferulate | C ₂₀ H ₂₀ O ₆ | 63644-62-2 | 356.13 | -0.00088 |
| 127 | 2-(2-Carboxyethyl)-5-hydroxyphenyl hexopyranosiduronic acid | C ₁₅ H ₁₈ O ₁₀ | ChemSpider ID 74886628 | 358.09 | -0.00086 |
| 128 | Sorbic acid | C ₆ H ₈ O ₂ | 110-44-1 | 112.05 | -0.00016 |
| 129 | 7-Octene-3,5-diyn-1-ol | C ₈ H ₈ O | 114020-45-0 | 120.06 | -0.00025 |
| 130 | 9-Oxodecenoic acid | C ₁₀ H ₁₆ O ₃ | 334-20-3 | 184.11 | -0.00027 |
| 131 | 12-Aminolauric Acid | C ₁₂ H ₂₅ NO ₂ | 693-57-2 | 215.19 | -0.00039 |
| 132 | 12-Hydroxyjasmonic acid | C ₁₂ H ₁₈ O ₄ | 140631-27-2 | 226.12 | -0.00052 |
| 133 | Dodecylethanol amide | C ₁₄ H ₂₉ NO ₂ | 142-78-9 | 243.22 | -0.00044 |
| 134 | Hexadecanamide | C ₁₆ H ₃₃ NO | 629-54-9 | 255.26 | -0.00065 |
| 135 | Phloretin | C ₁₅ H ₁₄ O ₅ | 60-82-2 | 274.08 | -0.00078 |
| 136 | α-Linolenic acid | C ₁₈ H ₃₀ O ₂ | 463-40-1 | 278.22 | -0.00063 |
| 137 | Linolenelaidic acid | C ₁₈ H ₃₀ O ₂ | 28290-79-1 | 278.22 | -0.00056 |
| 138 | 12-oxo Phytodienoic acid | C ₁₈ H ₂₈ O ₃ | 85551-10-6 | 292.20 | -0.00079 |
| 139 | Methyl alpha-eleostearate | C ₁₉ H ₃₂ O ₂ | 4175-47-7 | 292.24 | -0.00076 |
| 140 | 6-Tuliposide B | C ₁₁ H ₁₈ O ₉ | 244105-18-8 | 294.09 | -0.00053 |
| 141 | Tuliposide B | C ₁₁ H ₁₈ O ₉ | 19870-33-8 | 294.09 | -0.00052 |
| 142 | 6-Gingerol | C ₁₇ H ₂₆ O ₄ | 23513-14-6 | 294.18 | -0.00063 |
| 143 | 9-oxo-10E,12Z-Octadecadienoic acid | C ₁₈ H ₃₀ O ₃ | 54232-59-6 | 294.22 | -0.0007 |
| 144 | 9-oxo-10,12-Octadecadienoic acid | C ₁₈ H ₃₀ O ₃ | 54232-58-5 | 294.22 | -0.00069 |
| 145 | Ricinelaiddic acid | C ₁₈ H ₃₄ O ₃ | 141-22-0 | 298.25 | -0.00075 |
| 146 | Palmitoyl ethanolamide | C ₁₈ H ₃₇ NO ₂ | 544-31-0 | 299.28 | -0.00066 |
| 147 | 9-J1-Phytprostane | C ₁₈ H ₂₈ O ₄ | ChemSpider ID | 308.20 | -0.0008 |

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|-----|---|---|---------------------------|-----------------------|-----------------------|
| | | | 32033755 | | |
| 148 | 8-Gingerol | C ₁₉ H ₃₀ O ₄ | 23513-08-8 | 322.21 | -0.00089 |
| 149 | Linoleoyl ethanolamide | C ₂₀ H ₃₇ NO ₂ | 68171-52-8 | 323.28 | -0.0007 |
| 150 | Oleoyl ethanolamide | C ₂₀ H ₃₉ NO ₂ | 111-58-0 | 325.30 | -0.00071 |
| 151 | 10-Nitrooleic acid | C ₁₈ H ₃₃ NO ₄ | 875685-46-4 | 327.24 | -0.00087 |
| 152 | 9-Nitro-9E-octadecenoic acid | C ₁₈ H ₃₃ NO ₄ | 875685-44-2 | 327.24 | -0.00074 |
| 153 | Glyceryl palmitate | C ₁₉ H ₃₈ O ₄ | 542-44-9 | 330.28 | -0.00084 |
| 154 | 9,10,13-Trihydroxyoctadecanoic acid | C ₁₈ H ₃₆ O ₅ | ChemSpider ID 24022689 | 332.26 | -0.00107 |
| 155 | 3-oxo-N-[(3S)-2-Oxotetrahydro-3-furanyl]hexadecanamide | C ₂₀ H ₃₅ NO ₄ | 925448-37-9 | 353.26 | -0.00119 |
| 156 | N-Oleoyl Alanine | C ₂₁ H ₃₉ NO ₃ | 745733-78-2 | 353.29 | -0.00098 |
| 157 | (5Z,13E,15R)-15-Hydroxy-16,16-dimethyl-9-oxoprostanoic acid | C ₂₂ H ₃₆ O ₄ | 53658-98-3 | 364.26 | -0.00066 |
| 158 | N-Oleoyl-L-Serine | C ₂₁ H ₃₉ NO ₄ | 1246302-99-7 | 369.29 | -0.001 |
| 159 | Brassicasterol | C ₂₈ H ₄₂ O | 516-85-8 | 394.32 | -0.00086 |
| 160 | Cholesteryl acetate | C ₂₉ H ₄₈ O ₂ | 604-35-3 | 428.36 | -0.001 |
| 161 | Halosterol B | C ₂₉ H ₄₈ O ₂ | ChemSpider ID 9808066 | 428.36 | -0.0007 |
| 162 | 1-Hexadecanoyl-sn-glycero-3-phosphoethanolamine | C ₂₁ H ₄₄ NO ₇ P | 53862-35-4 | 453.28 | -0.001 |
| 163 | 1-Palmitoylphosphatidylcholine | C ₂₄ H ₅₀ NO ₇ P | 17364-18-0 | 495.33 | -0.00119 |
| 164 | Soyacerebroside I | C ₄₀ H ₇₅ NO ₉ | 114297-20-0 | 713.54 | -0.00178 |
| 165 | L-Dilinolenoyl lecithin | C ₄₄ H ₇₆ NO ₈ P | 2701-19-1 | 777.53 | -0.00168 |
| 166 | Cytosine | C ₄ H ₅ N ₃ O | 71-30-7 | 111.04 | -0.00017 |
| 167 | 5-Formamidopyrimidine | C ₅ H ₅ N ₃ O | 56621-84-2 | 123.04 | -0.00018 |
| 168 | 5-Methylcytosine | C ₅ H ₇ N ₃ O | 554-01-8 | 125.06 | -0.0001 |
| 169 | Thymine | C ₅ H ₆ N ₂ O ₂ | 65-71-4 | 126.04 | -0.00028 |
| 170 | Adenine | C ₅ H ₅ N ₅ | 73-24-5 | 135.05 | -0.00029 |
| 171 | Hypoxanthine | C ₅ H ₄ N ₄ O | 68-94-0 | 136.04 | -0.00016 |
| 172 | Guanine | C ₅ H ₅ N ₅ O | 73-40-5 | 151.05 | -0.00018 |
| 173 | 2,6-Diamino-8-azapurine | C ₄ H ₅ N ₇ | 18620-97-8 | 151.06 | 0.00016 |
| 174 | Xanthine | C ₅ H ₄ N ₄ O ₂ | 69-89-6 | 152.03 | -0.00024 |
| 175 | 1-Methylguanine | C ₆ H ₇ N ₅ O | 938-85-2 | 165.06 | -0.0002 |
| 176 | 6-O-Methylguanine | C ₆ H ₇ N ₅ O | 20535-83-5 | 165.06 | -0.00013 |
| 177 | 1-Methylxanthine | C ₆ H ₆ N ₄ O ₂ | 6136-37-4 | 166.05 | -0.00027 |
| 178 | 7-Methylxanthine | C ₆ H ₆ N ₄ O ₂ | 552-62-5 | 166.05 | -0.00026 |
| 179 | trans-Zeatin | C ₁₀ H ₁₃ N ₅ O | 1637-39-4 | 219.11 | -0.00028 |
| 180 | 5-Methyldeoxycytidine | C ₁₀ H ₁₅ N ₃ O ₄ | 838-07-3 | 241.11 | -0.00035 |
| 181 | 1-Pentofuranosyldihydro-2,4(1H,3H)-pyrimidinedione | C ₉ H ₁₄ N ₂ O ₆ | 30100-83-5 | 246.08 | -0.00049 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|--|-------------|-----------------------|-----------------------|
| 182 | 2'-Deoxyadenosine | C ₁₀ H ₁₃ N ₅ O ₃ | 958-09-8 | 251.10 | -0.00049 |
| 183 | 1-(beta-D-Ribofuranosyl)-1,4-dihydronicotinamide | C ₁₁ H ₁₆ N ₂ O ₅ | 19132-12-8 | 256.11 | -0.00062 |
| 184 | Adenosine | C ₁₀ H ₁₃ N ₅ O ₄ | 58-61-7 | 267.10 | -0.00051 |
| 185 | 5'-Amino-5'-oxo-5'-deoxyadenosine | C ₁₀ H ₁₂ N ₆ O ₄ | 35788-21-7 | 280.09 | -0.00059 |
| 186 | 1-Methyladenosine | C ₁₁ H ₁₅ N ₅ O ₄ | 15763-06-1 | 281.11 | -0.00054 |
| 187 | 2'-O-Methyladenosine | C ₁₁ H ₁₅ N ₅ O ₄ | 2140-79-6 | 281.11 | -0.00053 |
| 188 | Guanosine | C ₁₀ H ₁₃ N ₅ O ₅ | 118-00-3 | 283.09 | -0.00059 |
| 189 | N6,N6-Dimethyladenosine | C ₁₂ H ₁₇ N ₅ O ₄ | 2620-62-4 | 295.13 | -0.00047 |
| 190 | 5'-S-Methyl-5'-thioadenosine | C ₁₁ H ₁₅ N ₅ O ₃ S | 2457-80-9 | 297.09 | -0.00063 |
| 191 | 7-Methylguanosine | C ₁₁ H ₁₅ N ₅ O ₅ | 20244-86-4 | 297.11 | -0.0007 |
| 192 | N2,N2-Dimethylguanosine | C ₁₂ H ₁₇ N ₅ O ₅ | 2140-67-2 | 311.12 | -0.00067 |
| 193 | Adenosine-3'-5'-cyclic monophosphate | C ₁₀ H ₁₂ N ₅ O ₆ P | 86594-35-6 | 329.05 | -0.00058 |
| 194 | Hypoxanthine deoxyriboside | C ₁₀ H ₁₃ N ₄ O ₇ P | 3393-18-8 | 332.05 | 0.00028 |
| 195 | Cyclic guanosine monophosphate | C ₁₀ H ₁₂ N ₅ O ₇ P | 7665-99-8 | 345.05 | -0.00062 |
| 196 | 9-Ribosylzeatin | C ₁₅ H ₂₁ N ₅ O ₅ | 15896-46-5 | 351.15 | -0.00066 |
| 197 | N6-Succinyl adenosine | C ₁₄ H ₁₇ N ₅ O ₈ | 4542-23-8 | 383.11 | -0.00104 |
| 198 | Glutaric anhydride | C ₅ H ₆ O ₃ | 108-55-4 | 114.03 | -0.0003 |
| 199 | Levulinic acid | C ₅ H ₈ O ₃ | 123-76-2 | 116.05 | -0.00009 |
| 200 | (2-Aminoethyl)phosphonic acid | C ₂ H ₈ NO ₃ P | 2041-14-7 | 125.02 | -0.00048 |
| 201 | (2S)-2-Amino-4-hexynoic acid | C ₆ H ₉ NO ₂ | 29834-76-2 | 127.06 | -0.00019 |
| 202 | 1,2,5,6-Tetrahydropyridine-3-carboxylic acid | C ₆ H ₉ NO ₂ | 498-96-4 | 127.06 | -0.00016 |
| 203 | 6-Methylnicotinic acid | C ₇ H ₇ NO ₂ | 3222-47-7 | 137.05 | -0.00015 |
| 204 | 6-oxo-Pipecolinic acid | C ₆ H ₉ NO ₃ | 3770-22-7 | 143.06 | -0.00001 |
| 205 | Tetrahydro-5-oxo-2-furanacetic acid | C ₆ H ₈ O ₄ | 60551-20-4 | 144.04 | -0.00004 |
| 206 | 4-Acetamidobutyric acid | C ₆ H ₁₁ NO ₃ | 3025-96-5 | 145.07 | -0.0001 |
| 207 | 2-Hydroxyglutaric acid | C ₅ H ₈ O ₅ | 2889-31-8 | 148.04 | 0.00011 |
| 208 | (2Z)-8-Hydroxy-2-octene-4,6-diyonic acid | C ₈ H ₆ O ₃ | 65367-65-9 | 150.03 | -0.00026 |
| 209 | 5-Aminosalicylic acid | C ₇ H ₇ NO ₃ | 89-57-6 | 153.04 | -0.00023 |
| 210 | 2-Hydrazinonicotinic acid | C ₆ H ₇ N ₃ O ₂ | 435342-14-6 | 153.05 | -0.00018 |
| 211 | Dimethyl itaconate | C ₇ H ₁₀ O ₄ | 617-52-7 | 158.06 | -0.00025 |
| 212 | Phenylbutyric acid | C ₁₀ H ₁₂ O ₂ | 1821-12-1 | 164.08 | -0.00028 |
| 213 | D-Xylonic acid | C ₅ H ₁₀ O ₆ | 4172-43-4 | 166.05 | 0.00016 |
| 214 | Acetylsalicylic acid | C ₉ H ₈ O ₄ | 50-78-2 | 180.04 | -0.00023 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|--------------------------|-----------------------|-----------------------|
| 215 | 5-Hydroxyisophthalic acid | C ₈ H ₆ O ₅ | 618-83-7 | 182.02 | -0.00024 |
| 216 | Stipitatic acid | C ₈ H ₆ O ₅ | 4440-39-5 | 182.02 | -0.00024 |
| 217 | trans-3-Indoleacrylic acid | C ₁₁ H ₉ NO ₂ | 29953-71-7 | 187.06 | -0.00029 |
| 218 | 1-(Carboxymethyl)piperidine-4-carboxylic acid | C ₈ H ₁₃ NO ₄ | 53919-19-0 | 187.08 | -0.00027 |
| 219 | 4-Hydroxyquinoline-2-carboxylic acid | C ₁₀ H ₇ NO ₃ | 492-27-3 | 189.04 | -0.00032 |
| 220 | 3-(4-Methylbenzoyl)acrylic acid | C ₁₁ H ₁₀ O ₃ | 20972-36-5 | 190.06 | -0.00025 |
| 221 | 4-(Trifluoromethyl)nicotinic acid | C ₇ H ₄ F ₃ NO ₂ | 158063-66-2 | 191.02 | -0.00037 |
| 222 | 5-Hydroxyindole-3-acetic acid | C ₁₀ H ₉ NO ₃ | 1321-73-9 | 191.06 | -0.00024 |
| 223 | 3-Oxooctahydro-4a(2H)-naphthalenecarboxylic acid | C ₁₁ H ₁₆ O ₃ | 91352-51-1 | 196.11 | -0.00033 |
| 224 | Vanillyl mandelic acid | C ₉ H ₁₀ O ₅ | 55-10-7 | 198.05 | -0.00028 |
| 225 | (2E)-3-(3,4-Dimethoxyphenyl)acrylic acid | C ₁₁ H ₁₂ O ₄ | 14737-89-4 | 208.07 | -0.00035 |
| 226 | 4-[(Ethoxycarbonyl)amino]benzoic acid | C ₁₀ H ₁₁ NO ₄ | 5180-75-6 | 209.07 | -0.00041 |
| 227 | Jasmonic acid | C ₁₂ H ₁₈ O ₃ | 6894-38-8 | 210.13 | -0.00038 |
| 228 | 2-Hydroxy-6-ketononadienedioic acid | C ₉ H ₁₀ O ₆ | ChemSpider ID 4444276 | 214.05 | -0.00039 |
| 229 | Diphenylphosphinic acid | C ₁₂ H ₁₁ O ₂ P | 1707-03-5 | 218.05 | -0.00043 |
| 230 | 4,5-Dimethoxy-2-nitrobenzoic acid | C ₉ H ₉ NO ₆ | 4998-07-6 | 227.04 | -0.00046 |
| 231 | Dimethyl succinylsuccinate | C ₁₀ H ₁₂ O ₆ | 6289-46-9 | 228.06 | -0.00034 |
| 232 | Hopantenic acid | C ₁₀ H ₁₉ NO ₅ | 18679-90-8 | 233.13 | -0.00056 |
| 233 | 3-Amino-3-(4-isopropoxy-3-methoxyphenyl)propanoic acid | C ₁₃ H ₁₉ NO ₄ | 554402-59-4 | 253.13 | -0.00049 |
| 234 | 3,4,5-Triethoxybenzoic acid | C ₁₃ H ₁₈ O ₅ | 6970-19-0 | 254.11 | -0.00065 |
| 235 | 10-Heptadecen-8-ynoic acid | C ₁₇ H ₂₈ O ₂ | 16714-84-4 | 264.21 | -0.00078 |
| 236 | 4-[2-(4-Amino-4-carboxybutanoyl)hydrazino]benzoic acid | C ₁₂ H ₁₅ N ₃ O ₅ | 69644-85-5 | 281.10 | -0.0009 |
| 237 | N-Succinyl-L-diaminopimelic acid | C ₁₁ H ₁₈ N ₂ O ₇ | 26605-36-7 | 290.11 | -0.00055 |
| 238 | (9Z,11E,13S,15Z)-13-Hydroxyoctadeca-9,11,15-trienoic acid | C ₁₈ H ₃₀ O ₃ | 87984-82-5 | 294.22 | -0.00071 |
| 239 | 2'-Deoxymugineic acid | C ₁₂ H ₂₀ N ₂ O ₇ | 74235-24-8 | 304.13 | -0.00042 |
| 240 | Imazamox | C ₁₅ H ₁₉ N ₃ O ₄ | 114311-32-9 | 305.14 | -0.00094 |
| 241 | (9Z,11E)-13-Hydroperoxyoctadeca-9,11-dienoic acid | C ₁₈ H ₃₂ O ₄ | 23017-93-8 | 312.23 | -0.00092 |
| 242 | Salicylacyl glucuronide | C ₁₃ H ₁₄ O ₉ | 29315-53-5 | 314.06 | -0.00085 |
| 243 | Luteic acid | C ₁₄ H ₈ O ₉ | 476-67-5 | 320.02 | -0.00059 |
| 244 | Ethylenediamine-N,N'-diacetic-N,N'-dipropionic acid | C ₁₂ H ₂₀ N ₂ O ₈ | 32701-19-2 | 320.12 | -0.00057 |
| 245 | (2R,9Z,12E,15Z)-2-Hydroperoxy-1 | C ₁₈ H ₃₀ O ₅ | ChemSpider ID | 326.21 | -0.00071 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|---------------------------|-----------------------|-----------------------|
| | 3-hydroxy-9,12,15-octadecatrienoic acid | | 17220740 | | |
| 246 | (2R)-2-[(7Z)-7-Hexadecen-1-yl]-3-methylenesuccinic acid | C ₂₁ H ₃₆ O ₄ | ChemSpider ID 29328054 | 352.26 | -0.00078 |
| 247 | Oxindole | C ₈ H ₇ NO | 59-48-3 | 133.05 | -0.00017 |
| 248 | Stachydrine | C ₇ H ₁₃ NO ₂ | ChemSpider ID 103115 | 143.09 | -0.0001 |
| 249 | Daechualkaloid A | C ₁₀ H ₁₃ NO ₂ | 80933-73-9 | 179.09 | -0.00019 |
| 250 | Theobromine | C ₇ H ₈ N ₄ O ₂ | 83-67-0 | 180.06 | -0.00036 |
| 251 | Theophylline | C ₇ H ₈ N ₄ O ₂ | 58-55-9 | 180.06 | -0.00033 |
| 252 | Caffeine | C ₈ H ₁₀ N ₄ O ₂ | 58-08-2 | 194.08 | -0.00035 |
| 253 | 6-Thiocaffeine | C ₈ H ₁₀ N ₄ OS | 13182-58-6 | 210.06 | -0.00029 |
| 254 | N,N-Dimethyl-5-methoxytryptamine | C ₁₃ H ₁₈ N ₂ O | 1019-45-0 | 218.14 | -0.00057 |
| 255 | Eseroline | C ₁₃ H ₁₈ N ₂ O | 469-22-7 | 218.14 | -0.00045 |
| 256 | Gentisein | C ₁₃ H ₈ O ₅ | 529-49-7 | 244.04 | -0.00057 |
| 257 | Echinatine N-oxide | C ₁₅ H ₂₅ NO ₆ | 20267-93-0 | 315.17 | -0.00079 |
| 258 | Renardine | C ₁₉ H ₂₇ NO ₆ | 2318-18-5 | 365.18 | -0.00072 |
| 259 | Jervine | C ₂₇ H ₃₉ NO ₃ | 469-59-0 | 425.29 | -0.00105 |
| 260 | Methyl gallate | C ₈ H ₈ O ₅ | 99-24-1 | 184.04 | -0.00028 |
| 261 | Ellagic acid | C ₁₄ H ₆ O ₈ | 476-66-4 | 302.01 | -0.00075 |
| 262 | Procyanidin A2 | C ₃₀ H ₂₄ O ₁₂ | 41743-41-3 | 576.13 | -0.00136 |
| 263 | Procyanidin B2 | C ₃₀ H ₂₆ O ₁₂ | 29106-49-8 | 578.14 | -0.00112 |
| 264 | Galactosamine | C ₆ H ₁₃ NO ₅ | 7535-00-4 | 179.08 | -0.00019 |
| 265 | 2-Acetamido-2,6-dideoxyglucose | C ₈ H ₁₅ NO ₅ | 40614-71-9 | 205.09 | -0.00012 |
| 266 | 2,4-Diacetamido-2,4,6-trideoxy-alpha-D-mannopyranose Methyl | C ₁₀ H ₁₈ N ₂ O ₅ | ChemSpider ID 28533246 | 246.12 | -0.00035 |
| 267 | 4,6-dideoxy-4-[(3-hydroxypropano-yl)amino]hexopyranoside | C ₁₀ H ₁₉ NO ₆ | ChemSpider ID 4928260 | 249.12 | -0.00034 |
| 268 | 1-O-Benzoylpentopyranose | C ₁₂ H ₁₄ O ₆ | ChemSpider ID 495245 | 254.08 | -0.00062 |
| 269 | (2S)-2-(beta-D-Glucopyranosyloxy)-3-methyl-3-butenenitrile | C ₁₁ H ₁₇ NO ₆ | 66871-89-4 | 259.11 | -0.00046 |
| 270 | 2(R)-Hydroxy-2-methylbutyronitrile-beta-D-glucopyranoside | C ₁₁ H ₁₉ NO ₆ | 534-67-8 | 261.12 | -0.00041 |
| 271 | 1-Deoxy-1-(hexylamino)hexitol | C ₁₂ H ₂₇ NO ₅ | ChemSpider ID 499954 | 265.19 | -0.0004 |
| 272 | (1S,5R)-5-Isopropenyl-2-methyl-2-cyclohexen-1-yl-beta-D-glucopyranoside | C ₁₆ H ₂₆ O ₆ | 113349-30-7 | 314.17 | -0.00056 |
| 273 | Methyl | C ₁₇ H ₂₄ N ₂ O ₈ | ChemSpider ID | 384.15 | -0.00118 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|--|--------------------------|-----------------------|-----------------------|
| | 2-[[{[(benzyloxy)carbonyl]amino}acetyl)amino]-2-deoxyhexopyranoside | | 511388 | | |
| 274 | 6-Acetamido-1,2,3,4-tetra-O-acetyl-6-deoxyhexopyranose | C ₁₆ H ₂₃ NO ₁₀ | ChemSpider ID 510192 | 389.13 | -0.00082 |
| 275 | (2S)-2-{[6-O-(alpha-L-Arabinopyranosyl)-beta-D-glucopyranosyl]oxy}-3-methyl-3-butenenitrile | C ₁₆ H ₂₅ NO ₁₀ | 79197-21-0 | 391.15 | -0.00083 |
| 276 | 4-O-(2-Acetamido-2-deoxy-beta-D-glucopyranosyl)-beta-D-glucopyranuronic acid | C ₁₄ H ₂₃ NO ₁₂ | 139626-60-1 | 397.12 | -0.00098 |
| 277 | 1,3,4,6-Tetra-O-acetyl-2-deoxy-2-(1-pyrrolidinyl)hexopyranose | C ₁₈ H ₂₇ NO ₉ | ChemSpider ID 499689 | 401.17 | -0.00108 |
| 278 | Methyl 2-acetamido-2-deoxy-3,6-di-O-methyl-4-O-(2,3,4,6-tetra-O-methyl-beta-D-mannopyranosyl)-beta-D-glucopyranoside | C ₂₁ H ₃₉ NO ₁₁ | ChemSpider ID 4933246 | 481.25 | -0.00112 |
| 279 | Glucosylgalactosyl hydroxylysine | C ₁₈ H ₃₄ N ₂ O ₁₃ | ChemSpider ID 109059 | 486.21 | 0.00062 |
| 280 | 2,3,4,6-Tetra-O-acetyl-1-O-[(2E)-3-(3,4-diacetoxyphenyl)-2-propenoyl]hexopyranose | C ₂₇ H ₃₀ O ₁₅ | ChemSpider ID 4524029 | 594.16 | -0.00138 |
| 281 | Pulegone | C ₁₀ H ₁₆ O | 15932-80-6 | 152.12 | -0.00024 |
| 282 | Zerumbone | C ₁₅ H ₂₂ O | 471-05-6 | 218.17 | -0.00029 |
| 283 | Caryophyllene oxide | C ₁₅ H ₂₄ O | 1139-30-6 | 220.18 | -0.00041 |
| 284 | Podolide | C ₁₉ H ₂₂ O ₅ | 55786-36-2 | 330.15 | -0.00094 |
| 285 | Gibberellin A7 | C ₁₉ H ₂₂ O ₅ | 510-75-8 | 330.15 | -0.00075 |
| 286 | Geniposide pentaacetate | C ₂₇ H ₃₄ O ₁₅ | 49776-64-9 | 598.19 | -0.00173 |
| 287 | Coumarin | C ₉ H ₆ O ₂ | 91-64-5 | 146.04 | -0.00033 |
| 288 | 8-Methylcoumarin | C ₁₀ H ₈ O ₂ | 1807-36-9 | 160.05 | 0.00014 |
| 289 | 4-Hydroxycoumarin | C ₉ H ₆ O ₃ | 1076-38-6 | 162.03 | -0.0003 |
| 290 | 7-Hydroxycoumarine | C ₉ H ₆ O ₃ | 93-35-6 | 162.03 | -0.0003 |
| 291 | Hymecromone | C ₁₀ H ₈ O ₃ | 90-33-5 | 176.05 | -0.00038 |
| 292 | Esculetin | C ₉ H ₆ O ₄ | 305-01-1 | 178.03 | -0.00038 |
| 293 | 6-Acetocoumarin | C ₁₁ H ₈ O ₃ | 1177917-22-4 | 188.05 | -0.00039 |
| 294 | 4,5,7-Trihydroxycoumarin | C ₉ H ₆ O ₅ | 17575-26-7 | 194.02 | -0.00022 |
| 295 | Scoparone | C ₁₁ H ₁₀ O ₄ | 120-08-1 | 206.06 | -0.00034 |
| 296 | Methoxsalen | C ₁₂ H ₈ O ₄ | 298-81-7 | 216.04 | -0.00032 |
| 297 | 7-Acetoxy-4-methylcoumarin | C ₁₂ H ₁₀ O ₄ | 2747-05-9 | 218.06 | -0.00029 |
| 298 | 8-Acetyl-7-hydroxy-4-methylcoumarin | C ₁₂ H ₁₀ O ₄ | 2555-29-5 | 218.06 | -0.00029 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|-------------------------|-----------------------|-----------------------|
| 299 | Urolithin D | C ₁₃ H ₈ O ₆ | 131086-98-1 | 260.03 | -0.00045 |
| 300 | (+)-Galbacin | C ₂₀ H ₂₀ O ₅ | 528-64-3 | 340.13 | -0.00075 |
| 301 | 1,4-Cyclohexadiene | C ₆ H ₈ | 628-41-1 | 80.06 | -0.00017 |
| 302 | Cyclohexene | C ₆ H ₁₀ | 110-83-8 | 82.08 | -0.00026 |
| 303 | Methyl propiolate | C ₄ H ₄ O ₂ | 922-67-8 | 84.02 | -0.00019 |
| 304 | 2-Pyrrolidone | C ₄ H ₇ NO | 616-45-5 | 85.05 | -0.00017 |
| 305 | 4-Penten-1-amine | C ₅ H ₁₁ N | 22537-07-1 | 85.09 | -0.00013 |
| 306 | Ethyl isothiocyanate | C ₃ H ₅ NS | 542-85-8 | 87.01 | -0.00018 |
| 307 | N,N-Dimethylacetamide | C ₄ H ₉ NO | 127-19-5 | 87.07 | -0.00014 |
| 308 | 1-Heptyne | C ₇ H ₁₂ | 628-71-7 | 96.09 | -0.0002 |
| 309 | Cyclopentan-1,3-dione | C ₅ H ₆ O ₂ | 3859-41-4 | 98.04 | -0.00027 |
| 310 | Phenylacetylene | C ₈ H ₆ | 536-74-3 | 102.05 | -0.00015 |
| 311 | (E)-1-Phenylmethanimine | C ₇ H ₇ N | ChemSpider ID 378751 | 105.06 | -0.00011 |
| 312 | (2E,4E)-2,4-Heptadien-6-ynal | C ₇ H ₆ O | 7200-04-6 | 106.04 | -0.0002 |
| 313 | Benzoquinone | C ₆ H ₄ O ₂ | 106-51-4 | 108.02 | -0.00021 |
| 314 | alpha-Ocimene | C ₈ H ₁₂ | 1002-35-3 | 108.09 | -0.00015 |
| 315 | Hydroquinone | C ₆ H ₆ O ₂ | 123-31-9 | 110.04 | -0.00022 |
| 316 | Diacetylene glycol | C ₆ H ₆ O ₂ | 3031-68-3 | 110.04 | -0.00018 |
| 317 | 3,5-Dimethyl-1,4-hexadiene | C ₈ H ₁₄ | 761-87-5 | 110.11 | -0.00024 |
| 318 | 1-Vinyl-2-pyrrolidone | C ₆ H ₉ NO | 88-12-0 | 111.07 | -0.00019 |
| 319 | N,N-Dimethyl-2-butyramide | C ₆ H ₉ NO | 53099-32-4 | 111.07 | -0.00015 |
| 320 | 1-Aminopyrrole-2,5-dione | C ₄ H ₄ N ₂ O ₂ | 37770-94-8 | 112.03 | -0.00021 |
| 321 | 5-Methyl-3-methylidene-oxolan-2-one | C ₆ H ₈ O ₂ | 62873-16-9 | 112.05 | -0.0002 |
| 322 | N-Acetylpyrrolidine | C ₆ H ₁₁ NO | 4030-18-6 | 113.08 | -0.0002 |
| 323 | N,N-Dimethyl-2-butenamide | C ₆ H ₁₁ NO | 14064-75-6 | 113.08 | -0.00015 |
| 324 | Butyl isothiocyanate | C ₅ H ₉ NS | 592-82-5 | 115.05 | -0.00018 |
| 325 | 3-Acetamidopropanal | C ₅ H ₉ NO ₂ | 73323-68-9 | 115.06 | -0.00018 |
| 326 | 5-(Hydroxymethyl)dihydrofuran-2(3H)-one | C ₅ H ₈ O ₃ | 10374-51-3 | 116.05 | -0.00017 |
| 327 | Indole | C ₈ H ₇ N | 120-72-9 | 117.06 | -0.00014 |
| 328 | 2,4,6-Octatriyn-1-ol | C ₈ H ₆ O | 13033-21-1 | 118.04 | -0.00011 |
| 329 | 3-Cyanophenol | C ₇ H ₅ NO | 873-62-1 | 119.04 | -0.00021 |
| 330 | 2-Methyl-5-vinylpyridine | C ₈ H ₉ N | 140-76-1 | 119.07 | -0.0002 |
| 331 | 4-Hydroxybenzaldehyde | C ₇ H ₆ O ₂ | 123-08-0 | 122.04 | -0.00033 |
| 332 | (4Z)-4-Nonen-2-yne | C ₉ H ₁₄ | 53497-78-2 | 122.11 | -0.00024 |
| 333 | Hydroxy-1,4-benzoquinone | C ₆ H ₄ O ₃ | 2474-72-8 | 124.02 | -0.00013 |
| 334 | Furan-2,5-dicarbaldehyde | C ₆ H ₄ O ₃ | 823-82-5 | 124.02 | -0.00006 |
| 335 | 1-Acetyl-1,2,3,4-tetrahydropyridine | C ₇ H ₁₁ NO | 19615-27-1 | 125.08 | -0.00025 |
| 336 | Pyrogallol | C ₆ H ₆ O ₃ | 87-66-1 | 126.03 | -0.00026 |
| 337 | 5-Hydroxy-6-methyl-2H-pyran-2-one | C ₆ H ₆ O ₃ | ChemSpider ID | 126.03 | -0.00023 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|--|-------------------------|-----------------------|-----------------------|
| | ne | | 4934394 | | |
| 338 | 4-Hydroxy-5-methyl-2-methylenefuran-3-one | C ₆ H ₆ O ₃ | 948557-12-8 | 126.03 | -0.00016 |
| 339 | 5-Methyl-3-vinyl-2-oxazolidinone | C ₆ H ₉ NO ₂ | 3395-98-0 | 127.06 | -0.00013 |
| 340 | 3-Hydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one | C ₆ H ₈ O ₃ | ChemSpider ID 461448 | 128.05 | -0.00024 |
| 341 | Methyl (2E)-4-oxo-2-pentenoate | C ₆ H ₈ O ₃ | 2833-24-1 | 128.05 | -0.0002 |
| 342 | Leucoline | C ₉ H ₇ N | 91-22-5 | 129.06 | -0.00026 |
| 343 | Diisopropylethylamine | C ₈ H ₁₉ N | 7087-68-5 | 129.15 | -0.00018 |
| 344 | Phenylpropynal | C ₉ H ₆ O | 2579-22-8 | 130.04 | -0.00021 |
| 345 | (Hydroxyethyl)methacrylate | C ₆ H ₁₀ O ₃ | 868-77-9 | 130.06 | -0.00014 |
| 346 | 3-Methylindole | C ₉ H ₉ N | 83-34-1 | 131.07 | -0.00014 |
| 347 | 3-Methylsulfolene | C ₅ H ₈ O ₂ S | 1193-10-8 | 132.02 | -0.00016 |
| 348 | Cinnamaldehyde | C ₉ H ₈ O | 104-55-2 | 132.06 | -0.00025 |
| 349 | 4-Hydroxyindole | C ₈ H ₇ NO | 2380-94-1 | 133.05 | -0.0002 |
| 350 | 1,9-Decadiyne | C ₁₀ H ₁₄ | 1720-38-3 | 134.11 | -0.0002 |
| 351 | [1,2,4]Triazolo[1,5-a]pyrimidin-7-ol | C ₅ H ₄ N ₄ O | 31592-08-2 | 136.04 | -0.00024 |
| 352 | 3-Anisaldehyde | C ₈ H ₈ O ₂ | 591-31-1 | 136.05 | -0.00025 |
| 353 | 3,4-Dihydroxystyrene | C ₈ H ₈ O ₂ | 6053-02-7 | 136.05 | -0.00021 |
| 354 | Phenyl acetate | C ₈ H ₈ O ₂ | 122-79-2 | 136.05 | -0.00015 |
| 355 | 1-Decen-3-yne | C ₁₀ H ₁₆ | 33622-26-3 | 136.12 | -0.00021 |
| 356 | 1,5,9-Decatriene | C ₁₀ H ₁₆ | 13393-64-1 | 136.13 | -0.00016 |
| 357 | 6-Aminonicotinamide | C ₆ H ₇ N ₃ O | 329-89-5 | 137.06 | -0.00024 |
| 358 | (2E)-3-(1H-Imidazol-5-yl)acrylamide | C ₆ H ₇ N ₃ O | 135200-64-5 | 137.06 | -0.00017 |
| 359 | Protocatechuic aldehyde | C ₇ H ₆ O ₃ | 139-85-5 | 138.03 | -0.00027 |
| 360 | 2-Methoxyresorcinol | C ₇ H ₈ O ₃ | 29267-67-2 | 140.05 | -0.00022 |
| 361 | Ethyl 2-furoate | C ₇ H ₈ O ₃ | 1335-40-6 | 140.05 | -0.00015 |
| 362 | Lepidine | C ₁₀ H ₉ N | 491-35-0 | 143.07 | -0.00008 |
| 363 | 2-Butynophenone | C ₁₀ H ₈ O | 6710-62-9 | 144.06 | -0.00002 |
| 364 | Indole-4-carboxaldehyde | C ₉ H ₇ NO | 1074-86-8 | 145.05 | -0.00011 |
| 365 | N-(4-Hydroxy-1-methylbutyl)acetamide | C ₇ H ₁₅ NO ₂ | ChemSpider ID 471526 | 145.11 | -0.00015 |
| 366 | 3,4-Decadiene-6,8-diyne-1-ol | C ₁₀ H ₁₀ O | 6071-59-6 | 146.07 | -0.00007 |
| 367 | 3-(Methylthio)propyl isothiocyanate | C ₅ H ₉ NS ₂ | 505-79-3 | 147.02 | -0.00032 |
| 368 | Cinnamamide | C ₉ H ₉ NO | 621-79-4 | 147.07 | -0.00013 |
| 369 | 3-Methyl-1,2,3,4-tetrahydroisoquinoline | C ₁₀ H ₁₃ N | 29726-60-1 | 147.10 | -0.00021 |
| 370 | (2E)-3-(3-Hydroxyphenyl)acrylaldehyde | C ₉ H ₈ O ₂ | 26231-89-0 | 148.05 | -0.00019 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|--|---------------------------|-----------------------|-----------------------|
| 371 | 1,3-Bis(2-Hydroxyethyl)urea | C ₅ H ₁₂ N ₂ O ₃ | 15438-70-7 | 148.08 | -0.00018 |
| 372 | 2-Ethyl-2-nitro-1,3-propanediol | C ₅ H ₁₁ NO ₄ | 597-09-1 | 149.07 | -0.00005 |
| 373 | 5-Formylsalicylaldehyde | C ₈ H ₆ O ₃ | 3328-70-9 | 150.03 | -0.00027 |
| 374 | 6-Hydroxy-3-coumaranone | C ₈ H ₆ O ₃ | 6272-26-0 | 150.03 | -0.00016 |
| 375 | Vanillin | C ₈ H ₈ O ₃ | 121-33-5 | 152.05 | -0.00028 |
| 376 | Methylparaben | C ₈ H ₈ O ₃ | 99-76-3 | 152.05 | -0.00024 |
| 377 | Methyl salicylate | C ₈ H ₈ O ₃ | 119-36-8 | 152.05 | -0.00025 |
| 378 | Resacetophenone | C ₈ H ₈ O ₃ | 89-84-9 | 152.05 | -0.00019 |
| 379 | 1-Adamantanol | C ₁₀ H ₁₆ O | 768-95-6 | 152.12 | -0.00025 |
| 380 | N,N-Dimethyl-2-(2-methyl-1H-imidazol-5-yl)ethanamine | C ₈ H ₁₅ N ₃ | ChemSpider ID 476026 | 153.13 | -0.00036 |
| 381 | Triacetanamine | C ₉ H ₁₇ NO | 826-36-8 | 155.13 | -0.00027 |
| 382 | 1-Benzylimidazole | C ₁₀ H ₁₀ N ₂ | 4238-71-5 | 158.08 | -0.00014 |
| 383 | Methyl 2-morpholinoacetate | C ₇ H ₁₃ NO ₃ | 35855-10-8 | 159.09 | -0.00022 |
| 384 | 2-Morpholin-4-ylacetohydrazide | C ₆ H ₁₃ N ₃ O ₂ | 770-17-2 | 159.10 | -0.00013 |
| 385 | 4-Methoxycinnamaldehyde | C ₁₀ H ₁₀ O ₂ | 1963-36-6 | 162.07 | -0.00037 |
| 386 | Methyl cinnamate | C ₁₀ H ₁₀ O ₂ | 103-26-4 | 162.07 | -0.00028 |
| 387 | 3'-Methoxypropiofenone | C ₁₀ H ₁₂ O ₂ | 37951-49-8 | 164.08 | -0.00034 |
| 388 | Eugenol | C ₁₀ H ₁₂ O ₂ | 97-53-0 | 164.08 | -0.00027 |
| 389 | Phloracetophenone | C ₈ H ₈ O ₄ | 480-66-0 | 168.04 | -0.00025 |
| 390 | D-3,4-Dihydroxyphenylglycolaldehyde | C ₈ H ₈ O ₄ | 52819-70-2 | 168.04 | -0.00024 |
| 391 | 5-Formylfurfuryl acetate | C ₈ H ₈ O ₄ | 10551-58-3 | 168.04 | -0.00015 |
| 392 | N-Methylcyclodecanamine | C ₁₁ H ₂₃ N | 80789-66-8 | 169.18 | -0.00023 |
| 393 | Ethyl 4-amino-1-piperidinecarboxylate | C ₈ H ₁₆ N ₂ O ₂ | 58859-46-4 | 172.12 | -0.00017 |
| 394 | tert-Butyl 2-hydroxyethylmethylcarbamate | C ₈ H ₁₇ NO ₃ | 57561-39-4 | 175.12 | -0.00016 |
| 395 | 5-Benzylidihydro-2(3H)-furanone | C ₁₁ H ₁₂ O ₂ | 415902-37-3 | 176.08 | -0.00036 |
| 396 | Heptylbenzene | C ₁₃ H ₂₀ | 1078-71-3 | 176.16 | -0.00033 |
| 397 | 3-(1-Methylpyrrolidin-2-yl)pyridin-2-amine | C ₁₀ H ₁₅ N ₃ | 32726-84-4 | 177.13 | -0.00028 |
| 398 | Allyl salicylate | C ₁₀ H ₁₀ O ₃ | 10484-09-0 | 178.06 | -0.00018 |
| 399 | (E,E,E)-2,4,6-Dodecatrienal | C ₁₂ H ₁₈ O | 147217-66-1 | 178.14 | -0.00035 |
| 400 | 8-Hydroxy-6,7-dihydroisoquinoline-1,3(2H,5H)-dione | C ₉ H ₉ NO ₃ | 37704-54-4 | 179.06 | -0.00073 |
| 401 | 2-(6-Amino-1H-purin-1-yl)ethanol | C ₇ H ₉ N ₅ O | ChemSpider ID 58838095 | 179.08 | -0.00029 |
| 402 | 4-Isopropyl-7-methyl-1H-azepine-2,5-dione | C ₁₀ H ₁₃ NO ₂ | 10315-42-1 | 179.09 | -0.00045 |
| 403 | trans-Stilbene | C ₁₄ H ₁₂ | 103-30-0 | 180.09 | -0.00033 |
| 404 | Methyl (E,E,Z)-2,4,6-Decatrienoate | C ₁₁ H ₁₆ O ₂ | 51544-64-0 | 180.11 | -0.00038 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|--|---------------------------|-----------------------|-----------------------|
| 405 | 2-tert-Butyl-4-methoxyphenol | C ₁₁ H ₁₆ O ₂ | 121-00-6 | 180.11 | -0.00038 |
| 406 | 2-(2-Methylenecyclopropyl)-3-oxosuccinate | C ₈ H ₆ O ₅ | ChemSpider ID 24785550 | 182.02 | -0.00024 |
| 407 | 5-(2-Methylpropylidene)-2,4,6(1H,3H,5H)-pyrimidinetrione Ethyl | C ₈ H ₁₀ N ₂ O ₃ | 27406-43-5 | 182.07 | -0.00051 |
| 408 | 4-hydroxy-2-methylpyrimidine-5-carboxylate | C ₈ H ₁₀ N ₂ O ₃ | 53135-24-3 | 182.07 | -0.00047 |
| 409 | Mephesisin | C ₁₀ H ₁₄ O ₃ | 59-47-2 | 182.09 | -0.00026 |
| 410 | 10-Undecynoic acid | C ₁₁ H ₁₈ O ₂ | 2777-65-3 | 182.13 | -0.00029 |
| 411 | (2E)-2-Tridecene-4,6,8-triyn-1-ol | C ₁₃ H ₁₄ O | 6071-47-2 | 186.10 | -0.00032 |
| 412 | Methyl 1-acetyl-4-hydroxyprolinate | C ₈ H ₁₃ NO ₄ | ChemSpider ID 467588 | 187.08 | -0.00014 |
| 413 | Octahydro-1,6,7,8-indolizinetetrol | C ₈ H ₁₅ NO ₄ | 142393-60-0 | 189.10 | -0.00032 |
| 414 | tert-Butyl (2-amino-2-thioxoethyl)carbamate | C ₇ H ₁₄ N ₂ O ₂ S | 89226-13-1 | 190.08 | -0.00033 |
| 415 | 2,6-Dimethoxy-4-allylphenol | C ₁₁ H ₁₄ O ₃ | 6627-88-9 | 194.09 | -0.00069 |
| 416 | 2-Octanoylfuran | C ₁₂ H ₁₈ O ₂ | 5456-77-9 | 194.13 | -0.00044 |
| 417 | Sedanolid | C ₁₂ H ₁₈ O ₂ | 6415-59-4 | 194.13 | -0.0004 |
| 418 | 2-(Ethylamino)-4,5-dihydroxybenzamide | C ₉ H ₁₂ N ₂ O ₃ | 127793-87-7 | 196.08 | -0.00064 |
| 419 | 2-[2-(Benzyloxy)ethoxy]ethanol | C ₁₁ H ₁₆ O ₃ | 2050-25-1 | 196.11 | -0.00039 |
| 420 | Dibenzylamine | C ₁₄ H ₁₅ N | 103-49-1 | 197.12 | -0.00038 |
| 421 | 2-Amino-2-[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]ethanol | C ₇ H ₁₄ N ₆ O | ChemSpider ID 519465 | 198.12 | 0.00038 |
| 422 | 3,3-Dimethyl-1,5-dioxaspiro(5.5)undecan-9-one Ethyl | C ₁₁ H ₁₈ O ₃ | 69225-59-8 | 198.13 | -0.00038 |
| 423 | 5-ethoxy-4-methyl-1,3-oxazole-2-carboxylate | C ₉ H ₁₃ NO ₄ | 23429-04-1 | 199.08 | -0.00029 |
| 424 | (2Z)-2-Benzylidene-6-heptenal | C ₁₄ H ₁₆ O | ChemSpider ID 74853191 | 200.12 | -0.00024 |
| 425 | Diisopropyl diazene-1,2-dicarboxylate | C ₈ H ₁₄ N ₂ O ₄ | 2446-83-5 | 202.10 | -0.00032 |
| 426 | Xanthurenic acid | C ₁₀ H ₇ NO ₄ | 59-00-7 | 205.04 | -0.00031 |
| 427 | Ethyl methylphenylglycidate | C ₁₂ H ₁₄ O ₃ | 77-83-8 | 206.09 | -0.00037 |
| 428 | Asarone | C ₁₂ H ₁₆ O ₃ | 2883-98-9 | 208.11 | -0.00024 |
| 429 | 2-Methylene-5,10-undecadienoic acid methyl ester | C ₁₃ H ₂₀ O ₂ | 51788-60-4 | 208.15 | -0.00042 |
| 430 | 4-Heptyloxyphenol | C ₁₃ H ₂₀ O ₂ | 13037-86-0 | 208.15 | -0.00033 |
| 431 | 5-(4-Methoxyphenyl)-1,3-cyclohexanedione | C ₁₃ H ₁₄ O ₃ | 1774-12-5 | 218.09 | -0.00042 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|--------------------------|-----------------------|-----------------------|
| 432 | (4E)-6-(1,3-Benzodioxol-5-yl)-4-hexen-3-one | C ₁₃ H ₁₄ O ₃ | ChemSpider ID 4509686 | 218.09 | -0.00039 |
| 433 | D-Pantothenic acid | C ₉ H ₁₇ NO ₅ | 79-83-4 | 219.11 | -0.00033 |
| 434 | 1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone | C ₁₃ H ₁₆ O ₃ | 62458-64-4 | 220.11 | -0.00045 |
| 435 | Hexamethylcyclotrisiloxane | C ₆ H ₁₈ O ₃ Si ₃ | 541-05-9 | 222.06 | -0.00044 |
| 436 | 3-(5-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[2,3-c]pyridin-3-yl)propanoate | C ₁₁ H ₁₄ N ₂ O ₃ | ChemSpider ID 533528 | 222.10 | -0.00037 |
| 437 | N-[2-(4-Morpholinyl)ethyl]-1H-1,2,4-triazole-5-carboxamide | C ₉ H ₁₅ N ₅ O ₂ | ChemSpider ID 493565 | 225.12 | -0.0005 |
| 438 | 1-[(2,2-Dimethyl-1,3-dioxolan-4-yl)methyl]-2,4(1H,3H)-pyrimidinedione | C ₁₀ H ₁₄ N ₂ O ₄ | ChemSpider ID 3233081 | 226.09 | -0.00045 |
| 439 | 1,6-Hexanediol diacrylate | C ₁₂ H ₁₈ O ₄ | 13048-33-4 | 226.12 | -0.00052 |
| 440 | 1,8-Diazacyclotetradecan-2,9-dione | C ₁₂ H ₂₂ N ₂ O ₂ | 56403-09-9 | 226.17 | -0.00034 |
| 441 | 1,4-diazabicyclo[2.2.2]octane-2,3-dimethyl-1-carboxylate | C ₁₀ H ₁₆ N ₂ O ₄ | ChemSpider ID 519583 | 228.11 | -0.00019 |
| 442 | 5-Hydroxy-6-methoxy-7H-furo[3,2-g]chromen-7-one | C ₁₂ H ₈ O ₅ | 35779-46-5 | 232.04 | -0.00036 |
| 443 | 4-(4-Hydroxy-3-methoxyphenyl)-3,6-dihydro-1(2H)-pyridinecarbaldehyde | C ₁₃ H ₁₅ NO ₃ | ChemSpider ID 535604 | 233.10 | -0.00064 |
| 444 | 3-Hydroxy-4,5,6-trimethoxytetrahydro-2H-pyran-2-carboxamide | C ₉ H ₁₇ NO ₆ | ChemSpider ID 482310 | 235.11 | -0.00048 |
| 445 | 4-Hydroxy-4-(5-methoxy-2-nitrophenyl)-2-butanone | C ₁₁ H ₁₃ NO ₅ | 681446-84-4 | 239.08 | -0.00052 |
| 446 | 2,5-Anhydro-1-deoxy-1-(2-pyridinylamino)hexitol | C ₁₁ H ₁₆ N ₂ O ₄ | ChemSpider ID 497379 | 240.11 | -0.00036 |
| 447 | 4,5-Epoxymorphinan | C ₁₆ H ₁₉ NO | ChemSpider ID 536950 | 241.15 | -0.00066 |
| 448 | 2-[(cyclohexylcarbonyl)amino]-3-methylbutanoate | C ₁₃ H ₂₃ NO ₃ | ChemSpider ID 479972 | 241.17 | -0.0006 |
| 449 | 1-(2,4-Dideoxyhexopyranosyl)-2,4(1H,3H)-pyrimidinedione | C ₁₀ H ₁₄ N ₂ O ₅ | ChemSpider ID 506602 | 242.09 | -0.00043 |
| 450 | Dimethyl N-isobutyrylglutamate | C ₁₁ H ₁₉ NO ₅ | ChemSpider ID 469496 | 245.13 | -0.00042 |
| 451 | 2,3',4,6-Tetrahydroxybenzophenone | C ₁₃ H ₁₀ O ₅ | 26271-33-0 | 246.05 | -0.00047 |
| 452 | 2-(12-Tridecyn-1-yl)furan | C ₁₇ H ₂₆ O | 24708-33-6 | 246.20 | -0.00046 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|---------------------------|-----------------------|-----------------------|
| 453 | Podocarpin-12-ol | C ₁₇ H ₃₀ O | ChemSpider ID 503994 | 250.23 | -0.00072 |
| 454 | 6-Hydroxy-4,4,7-trimethyl-5-nitro-2-chromanone | C ₁₂ H ₁₃ NO ₅ | ChemSpider ID 538525 | 251.08 | -0.00066 |
| 455 | Mono(3-carboxypropyl) phthalate | C ₁₂ H ₁₂ O ₆ | 66851-46-5 | 252.06 | -0.00052 |
| 456 | (2Z)-3-(6,7-Dimethoxy-1,3-benzodioxol-5-yl)-2-hydroxyacrylaldehyde | C ₁₂ H ₁₂ O ₆ | ChemSpider ID 74852295 | 252.06 | -0.00035 |
| 457 | Pirimicarb-desmethyl-formamido | C ₁₁ H ₁₆ N ₄ O ₃ | 27218-04-8 | 252.12 | -0.00069 |
| 458 | 2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol | C ₁₃ H ₂₀ O ₅ | 71046-09-8 | 256.13 | -0.0007 |
| 459 | Octadecapenten-3-one | C ₁₈ H ₂₆ O | ChemSpider ID 10476703 | 258.20 | -0.00063 |
| 460 | Propyl N-(methoxycarbonyl)-N-methylglycyl-N-methylglycinate | C ₁₁ H ₂₀ N ₂ O ₅ | ChemSpider ID 4927395 | 260.14 | -0.00046 |
| 461 | Maclurin | C ₁₃ H ₁₀ O ₆ | 519-34-6 | 262.05 | -0.00052 |
| 462 | Methohexital | C ₁₄ H ₁₈ N ₂ O ₃ | 151-83-7 | 262.13 | -0.00058 |
| 463 | 1-(2-Methoxy-5-nitrobenzyl)-4-methylpiperazine | C ₁₃ H ₁₉ N ₃ O ₃ | ChemSpider ID 471676 | 265.14 | -0.0004 |
| 464 | Ethyl (2Z)-[(1,3-benzodioxol-5-ylmethyl)imino](hydroxyamino)acetate | C ₁₂ H ₁₄ N ₂ O ₅ | ChemSpider ID 4911614 | 266.09 | -0.00048 |
| 465 | (2E)-N-(4-Amino-2,3-dihydroxybutyl)-3-(4-hydroxyphenyl)acrylamide | C ₁₃ H ₁₈ N ₂ O ₄ | ChemSpider ID 59650572 | 266.13 | -0.00056 |
| 466 | Methyl 2-hydroxy-6-methyl-3-nitro-4-(2-oxopropyl)benzoate | C ₁₂ H ₁₃ NO ₆ | 89586-50-5 | 267.07 | -0.00046 |
| 467 | Rhamnopterin | C ₁₀ H ₁₃ N ₅ O ₄ | 13392-24-0 | 267.10 | -0.00057 |
| 468 | 1-Decanoyl-2,6-dimethylpiperidine | C ₁₇ H ₃₃ NO | 4629-19-0 | 267.26 | -0.00075 |
| 469 | Thiodiacetophenone | C ₁₆ H ₁₄ O ₂ S | 2461-80-5 | 270.07 | -0.00075 |
| 470 | (3E)-3-[(Methoxyacetyl)hydrazono]-N-(tetrahydro-2-furanylmethyl)butanamide | C ₁₂ H ₂₁ N ₃ O ₄ | ChemSpider ID 7871039 | 271.15 | -0.00085 |
| 471 | Di-2-pentanyl malate | C ₁₄ H ₂₆ O ₅ | ChemSpider ID 468884 | 274.18 | 0.00053 |
| 472 | 4,5,6-Trimethoxy-7H-furo[3,2-g]chromen-7-one | C ₁₄ H ₁₂ O ₆ | 18646-71-4 | 276.06 | -0.00078 |
| 473 | p-Coumaroylagmatine | C ₁₄ H ₂₀ N ₄ O ₂ | 7295-86-5 | 276.16 | -0.00059 |
| 474 | 6-Shogaol | C ₁₇ H ₂₄ O ₃ | 555-66-8 | 276.17 | -0.00061 |
| 475 | Phenyl laurate | C ₁₈ H ₂₈ O ₂ | 4228-00-6 | 276.21 | -0.00081 |
| 476 | [3-Acetyloxy-2-(acetyloxymethyl)-2-nitropropyl] acetate | C ₁₀ H ₁₅ NO ₈ | 7344-23-2 | 277.08 | -0.00091 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|--|---------------------------|-----------------------|-----------------------|
| 477 | 6,8-Dihydroxy-3-[(2S)-2-hydroxy-4-oxopentyl]-1H-isochromen-1-one | C ₁₄ H ₁₄ O ₆ | ChemSpider ID 31143389 | 278.08 | -0.00062 |
| 478 | 4-(3-Butoxy-4-methoxybenzyl)-2-imidazolidinone | C ₁₅ H ₂₂ N ₂ O ₃ | 29925-17-5 | 278.16 | -0.00068 |
| 479 | Heptyl (4-nitrophenyl)carbamate; Heptyl 4-nitrophenylcarbamate | C ₁₄ H ₂₀ N ₂ O ₄ | 92374-99-7 | 280.14 | -0.0006 |
| 480 | (2,2-Dimethyl-1,3-dioxolan-4-yl)methyl 4-nitrobenzoate | C ₁₃ H ₁₅ NO ₆ | ChemSpider ID 470054 | 281.09 | -0.00081 |
| 481 | N,N'-(2,4,5-Trimethoxy-1,3-phenylene)diacetamide | C ₁₃ H ₁₈ N ₂ O ₅ | ChemSpider ID 524502 | 282.12 | -0.00051 |
| 482 | N-Acetoxy-N-[5-(2,5-dioxo-1-pyrrolidinyl)pentyl]acetamide | C ₁₃ H ₂₀ N ₂ O ₅ | ChemSpider ID 470427 | 284.14 | -0.00045 |
| 483 | (2Z)-4,6,7-Trihydroxy-2-(4-hydroxybenzylidene)-1-benzofuran-3(2H)-one 2,5-Dioxo-1-pyrrolidinyl | C ₁₅ H ₁₀ O ₆ | ChemSpider ID 24846195 | 286.05 | -0.00072 |
| 484 | N-([(2-methyl-2-propanyl)oxy]carbonyl} alaninate Diethyl | C ₁₂ H ₁₈ N ₂ O ₆ | 3392-05-0 | 286.12 | -0.00079 |
| 485 | [amino(2-isobutrylhydrazino)methylene]malonate | C ₁₂ H ₂₁ N ₃ O ₅ | ChemSpider ID 1651360 | 287.15 | -0.00072 |
| 486 | 2-[(4-Amino-7H-pyrrolo[2,3-d]pyrimidin-7-yl)methoxy]ethyl dihydrogen phosphate | C ₉ H ₁₃ N ₄ O ₅ P | 86626-01-9 | 288.06 | 0.00047 |
| 487 | 1,5-Anhydro-1-(2,4,6-trihydroxyphenyl)hexitol Pentyl | C ₁₂ H ₁₆ O ₈ | ChemSpider ID 74886754 | 288.08 | -0.0007 |
| 488 | N-(methoxycarbonyl)-N-methylglycyl-N-methylglycinate | C ₁₃ H ₂₄ N ₂ O ₅ | ChemSpider ID 4927397 | 288.17 | -0.0009 |
| 489 | 6-Amino-1-[2-(3,4-dimethoxyphenyl)ethyl]pyrimidine-2,4(1H,3H)-dione | C ₁₄ H ₁₇ N ₃ O ₄ | 446266-76-8 | 291.12 | -0.00061 |
| 490 | 2-Acetyl-4,7,8-trihydroxy-6-methoxy-3-methyl-1,5-naphthalenedione | C ₁₄ H ₁₂ O ₇ | 1228-77-9 | 292.06 | -0.00039 |
| 491 | Methyl alpha-aspartylphenylalaninate | C ₁₄ H ₁₈ N ₂ O ₅ | 22839-65-2 | 294.12 | -0.00065 |
| 492 | Troxipide | C ₁₅ H ₂₂ N ₂ O ₄ | 30751-05-4 | 294.16 | -0.00061 |
| 493 | Disulfiram | C ₁₀ H ₂₀ N ₂ S ₄ | 97-77-8 | 296.05 | -0.00066 |
| 494 | Octamethylcyclotetrasiloxane | C ₈ H ₂₄ O ₄ Si ₄ | 556-67-2 | 296.07 | -0.00051 |
| 495 | 2,3,5,6-Tetrahydroxy-4-methoxy-N'-phenylhexanehydrazide | C ₁₃ H ₂₀ N ₂ O ₆ | 7404-33-3 | 300.13 | -0.00041 |
| 496 | 3-Hydroxy-cis-5-octenoylcarnitine | C ₁₅ H ₂₇ NO ₅ | ChemSpider ID | 301.19 | -0.00082 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|---------------------------|-----------------------|-----------------------|
| | | | 28639168 | | |
| 497 | 1,5-Dicyclopentyl-3-(2-cyclopentyl-ethyl)-2-pentene | C ₂₂ H ₃₈ | 54934-71-3 | 302.30 | -0.00076 |
| 498 | 3-(2,4,5-Trihydroxyphenyl)-4,6,7-chromanetriol | C ₁₅ H ₁₄ O ₇ | ChemSpider ID 74851598 | 306.07 | -0.00076 |
| 499 | Myristic acid diethanolamide | C ₁₈ H ₃₇ NO ₃ | 7545-23-5 | 315.28 | -0.00063 |
| 500 | 1-(4-Ethoxyphenyl)-3-(4-methyl-1-piperazinyl)-2,5-pyrrolidinedione | C ₁₇ H ₂₃ N ₃ O ₃ | 21621-46-5 | 317.17 | -0.00071 |
| 501 | 2-Aminooctadecane-1,3,4-triol Methyl | C ₁₈ H ₃₉ NO ₃ | 13552-11-9 | 317.29 | -0.00073 |
| 502 | N-[1-(4-ethoxyphenyl)-2,5-dioxo-3-pyrrolidinyl]alaninate | C ₁₆ H ₂₀ N ₂ O ₅ | 1008942-96-8 | 320.14 | -0.00076 |
| 503 | 2-sec-Butyl-4,6-dinitrophenyl isopropyl carbonate Isopropyl | C ₁₄ H ₁₈ N ₂ O ₇ | 973-21-7 | 326.11 | -0.00071 |
| 504 | 10-hydroxy-11-(4-morpholinyl)undecanoate | C ₁₈ H ₃₅ NO ₄ | ChemSpider ID 3235787 | 329.26 | -0.00098 |
| 505 | (2S,3S)-2-(Dimethylamino)-1,3-octadecanediol | C ₂₀ H ₄₃ NO ₂ | ChemSpider ID 24823237 | 329.33 | -0.00084 |
| 506 | 2-[4-(Benzyloxy)-3-ethoxyphenyl]-2-hydroxyethyl acetate Dimethyl | C ₁₉ H ₂₂ O ₅ | ChemSpider ID 490054 | 330.15 | -0.00091 |
| 507 | 4-(2,5-dimethoxyphenyl)-1,4-dihydro-3,5-pyridinedicarboxylate | C ₁₇ H ₁₉ NO ₆ | ChemSpider ID 527848 | 333.12 | -0.00084 |
| 508 | N-Benzyl-N-isopropyl-2-naphthalenesulfonamide Methyl | C ₂₀ H ₂₁ NO ₂ S | ChemSpider ID 643051 | 339.13 | 0.00158 |
| 509 | 6-(dimethylamino)octadecanoate | C ₂₁ H ₄₃ NO ₂ | 56817-90-4 | 341.33 | -0.00102 |
| 510 | 2,2'-(3,6-Dioxo-2,5-piperazinediyl)bis(N-hydroxy-N-propylacetamide) | C ₁₄ H ₂₄ N ₄ O ₆ | ChemSpider ID 477146 | 344.17 | -0.0009 |
| 511 | 3-[(3-Hydroxyundecanoyl)oxy]-4-(trimethylammonio)butanoate | C ₁₈ H ₃₅ NO ₅ | ChemSpider ID 59664326 | 345.25 | -0.00111 |
| 512 | 3-Methyl-5-(5,5,8a-trimethyl-2-methyl-7-oxodecahydro-1-naphthalenyl)pentyl acetate | C ₂₂ H ₃₆ O ₃ | ChemSpider ID 29814842 | 348.27 | -0.00062 |
| 513 | 10-Undecenyl-1-N-(cyclohexylcarboxonyl)alaninate | C ₂₁ H ₃₇ NO ₃ | ChemSpider ID 4926097 | 351.28 | -0.00081 |
| 514 | Tridecyl N-[(allyloxy)carbonyl]alaninate | C ₂₀ H ₃₇ NO ₄ | ChemSpider ID 4928205 | 355.27 | -0.00103 |
| 515 | Tetradecyl N-(ethoxycarbonyl)alaninate | C ₂₀ H ₃₉ NO ₄ | ChemSpider ID 4927832 | 357.29 | -0.00107 |
| 516 | 3-(7-Hydroxy-4b-methyl-2-methyle | C ₂₅ H ₃₄ O ₂ | ChemSpider ID | 366.26 | -0.00079 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|--|---------------------------|-----------------------|-----------------------|
| | netetradecahydro-1-phenanthrenyl)- 1-phenyl-1-propanone | | 537775 | | |
| 517 | Decamethylcyclopentasiloxane | C ₁₀ H ₃₀ O ₅ Si ₅ | 541-02-6 | 370.09 | -0.00091 |
| 518 | Riboflavin | C ₁₇ H ₂₀ N ₄ O ₆ | 83-88-5 | 376.14 | -0.00113 |
| | 1,6-Dimethyl | | | | |
| 519 | 2-O-(3,4,5-trihydroxybenzoyl)hexar ate | C ₁₅ H ₁₈ O ₁₂ | ChemSpider ID 35014325 | 390.08 | -0.00065 |
| | Tetramethyl | | | | |
| 520 | 1-tert-butyl-1,6-dihydro-6-methoxy -2,3,4,5-pyridinetetracarboxylate | C ₁₈ H ₂₅ NO ₉ | ChemSpider ID 538592 | 399.15 | -0.00092 |
| 521 | 3-Methoxy-1,2-didehydrocrinan-6,1 1-diyl diacetate | C ₂₁ H ₂₃ NO ₇ | ChemSpider ID 470632 | 401.15 | -0.00109 |
| 522 | Octyl propyl undecyl phosphate | C ₂₂ H ₄₇ O ₄ P | ChemSpider ID 4927331 | 406.32 | 0.00127 |
| 523 | 7-Dehydrocholesterol acetate | C ₂₉ H ₄₆ O ₂ | 1059-86-5 | 426.35 | -0.00099 |
| 524 | Cholesta-7,14-dien-7-yl acetate | C ₂₉ H ₄₆ O ₂ | ChemSpider ID 549949 | 426.35 | -0.00071 |
| 525 | (3beta,5beta,6beta)-5,6-Epoxyergos t-24(28)-ene-3,19-diol | C ₂₈ H ₄₆ O ₃ | ChemSpider ID 10283126 | 430.34 | -0.00101 |
| 526 | Trimazosin | C ₂₀ H ₂₉ N ₅ O ₆ | 35795-16-5 | 435.21 | -0.00202 |
| 527 | Oleanolic aldehyde | C ₃₀ H ₄₈ O ₂ | 17020-22-3 | 440.36 | -0.0011 |
| 528 | 7-Hydroxycholest-5-en-3-yl benzoate | C ₃₄ H ₅₀ O ₃ | 40824-59-7 | 506.37 | -0.00112 |
| 529 | Pheophorbide A | C ₃₅ H ₃₆ N ₄ O ₅ | 15664-29-6 | 592.27 | -0.00176 |

Note: Annot. Delta Mass represents the difference between the actual measured value of molecular weight and the theoretical value.

Table S2. List of 349 non-volatile metabolites in the processing of Rizhao green tea (ESI⁻, C18 column).

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|----|---|---|-------------|-----------------------|-----------------------|
| 1 | N-Carbobenzoxo-DL-serine | C ₁₁ H ₁₃ NO ₅ | 2768-56-1 | 239.08 | 0.00003 |
| 2 | Val-Val | C ₁₀ H ₂₀ N ₂ O ₃ | 3918-94-3 | 216.15 | 0.00036 |
| 3 | N-Acetylvaline | C ₇ H ₁₃ NO ₃ | 3067-19-4 | 159.09 | 0.00004 |
| 4 | N-Acetyl-DL-tryptophan | C ₁₃ H ₁₄ N ₂ O ₃ | 87-32-1 | 246.10 | -0.00048 |
| 5 | N-Acetyl-DL-phenylalanine | C ₁₁ H ₁₃ NO ₃ | 2901-75-9 | 207.09 | -0.00024 |
| 6 | N-Acetyl-L-leucine | C ₈ H ₁₅ NO ₃ | 1188-21-2 | 173.11 | -0.00002 |
| 7 | N6-((Benzoyloxy)carbonyl)lysine | C ₁₄ H ₂₀ N ₂ O ₄ | 32302-83-3 | 280.14 | 0.00053 |
| 8 | N2-(tert-Butoxycarbonyl)glutamin | C ₁₀ H ₁₈ N ₂ O ₅ | 85535-45-1 | 246.12 | -0.00017 |
| 9 | Boc-4-Nitro-L-phenylalanine | C ₁₄ H ₁₈ N ₂ O ₆ | 33305-77-0 | 310.12 | -0.00009 |
| 10 | DL-Alanyl-DL-leucine | C ₉ H ₁₈ N ₂ O ₃ | 1638-60-4 | 202.13 | -0.00001 |
| 11 | alpha-Methyl-L-tyrosine | C ₁₀ H ₁₃ NO ₃ | 672-87-7 | 195.09 | -0.00018 |
| 12 | L-Theanine | C ₇ H ₁₄ N ₂ O ₃ | 3081-61-6 | 174.10 | -0.00045 |
| 13 | L-gamma-Glutamyl-L-leucine | C ₁₁ H ₂₀ N ₂ O ₅ | 2566-39-4 | 260.14 | 0.00008 |
| 14 | Leu-Val | C ₁₁ H ₂₂ N ₂ O ₃ | 35436-83-0 | 230.16 | -0.00016 |
| 15 | Leu-pro | C ₁₁ H ₂₀ N ₂ O ₃ | 6403-35-6 | 228.15 | 0.00033 |
| 16 | Leu-Leu | C ₁₂ H ₂₄ N ₂ O ₃ | 3303-31-9 | 244.18 | 0.00009 |
| 17 | Leu-Gly-Gly | C ₁₀ H ₁₉ N ₃ O ₄ | 4337-37-5 | 245.14 | 0.00014 |
| 18 | Hexahydrohippuric acid | C ₉ H ₁₅ NO ₃ | 32377-88-1 | 185.10 | -0.00049 |
| 19 | Gly-Phe | C ₁₁ H ₁₄ N ₂ O ₃ | 721-66-4 | 222.10 | 0.00031 |
| 20 | Gly-Leu | C ₈ H ₁₆ N ₂ O ₃ | 869-19-2 | 188.12 | 0.00033 |
| 21 | DL-Tryptophan | C ₁₁ H ₁₂ N ₂ O ₂ | 54-12-6 | 204.09 | -0.00040 |
| 22 | DL-Phenylalanine | C ₉ H ₁₁ NO ₂ | 150-30-1 | 165.08 | -0.00008 |
| 23 | Dihydroxyphenylalanine | C ₉ H ₁₁ NO ₄ | 63-84-3 | 197.07 | -0.00016 |
| 24 | Boc-Glycine | C ₇ H ₁₃ NO ₄ | 4530-20-5 | 175.08 | 0.00016 |
| 25 | Ala-Tyr | C ₁₂ H ₁₆ N ₂ O ₄ | 3061-88-9 | 252.11 | 0.00018 |
| 26 | 5-Hydroxy-DL-tryptophan | C ₁₁ H ₁₂ N ₂ O ₃ | 56-69-9 | 220.08 | -0.00004 |
| 27 | 2-Morpholinoacetic acid | C ₆ H ₁₁ NO ₃ | 3235-69-6 | 145.07 | -0.00011 |
| 28 | 1-(tert-Butoxycarbonyl)proline | C ₁₀ H ₁₇ NO ₄ | 59433-50-0 | 215.12 | 0.00012 |
| 29 | 1-(Ethoxycarbonyl)proline | C ₈ H ₁₃ NO ₄ | 5700-74-3 | 187.08 | 0.00007 |
| 30 | Methyl gallate | C ₈ H ₈ O ₅ | 99-24-1 | 184.04 | -0.00058 |
| 31 | Ellagic acid | C ₁₄ H ₆ O ₈ | 476-66-4 | 302.01 | -0.00063 |
| 32 | Procyanidin B2 | C ₃₀ H ₂₆ O ₁₂ | 29106-49-8 | 578.14 | -0.00124 |
| 33 | Gallic acid | C ₇ H ₆ O ₅ | 149-91-7 | 170.02 | -0.00041 |
| 34 | Digallic acid | C ₁₄ H ₁₀ O ₉ | 536-08-3 | 322.03 | -0.00046 |
| 35 | Epigallocatechin 3-O-(3-O-methyl)gallate | C ₂₃ H ₂₀ O ₁₁ | 83104-87-4 | 472.10 | -0.00089 |
| 36 | (-)-Epigallocatechin 3'-O-glucuronide | C ₂₁ H ₂₂ O ₁₃ | 569670-41-3 | 482.11 | -0.00003 |
| 37 | (+)-Gallocatechin | C ₁₅ H ₁₄ O ₇ | 970-73-0 | 306.07 | -0.00074 |
| 38 | (-)-Epigallocatechin gallate | C ₂₂ H ₁₈ O ₁₁ | 989-51-5 | 458.08 | -0.00118 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|----|--|--|---------------------------|-----------------------|-----------------------|
| 39 | (-)-Epiafzelechin 3-O-gallate | C ₂₂ H ₁₈ O ₉ | 108907-43-3 | 426.09 | -0.00052 |
| 40 | Epicatechin 3-O-(3-O-methylgallate) | C ₂₃ H ₂₀ O ₁₀ | 83104-86-3 | 456.11 | -0.00029 |
| 41 | (-)-Epicatechin gallate | C ₂₂ H ₁₈ O ₁₀ | 1257-08-5 | 442.09 | -0.00131 |
| 42 | Epitheaflagallin 3-O-gallate | C ₂₇ H ₂₀ O ₁₃ | 102067-92-5 | 552.09 | -0.00008 |
| 43 | Methylgallic acid-O-sulphate | C ₈ H ₈ O ₈ S | ChemSpider ID 30778507 | 263.99 | 0.00020 |
| 44 | 5-Sulfosalicylic acid | C ₇ H ₆ O ₆ S | 97-05-2 | 217.99 | 0.00005 |
| 45 | Sinapinic acid | C ₁₁ H ₁₂ O ₅ | 530-59-6 | 224.07 | -0.00033 |
| 46 | Salicylic acid | C ₇ H ₆ O ₃ | 69-72-7 | 138.03 | -0.00067 |
| 47 | Protocatechuic acid | C ₇ H ₆ O ₄ | 99-50-3 | 154.03 | -0.00054 |
| 48 | Coniferyl ferulate | C ₂₀ H ₂₀ O ₆ | 63644-62-2 | 356.13 | 0.00005 |
| 49 | Chlorogenic acid | C ₁₆ H ₁₈ O ₉ | 327-97-9 | 354.09 | -0.00043 |
| 50 | Caftaric acid | C ₁₃ H ₁₂ O ₉ | 67879-58-7 | 312.05 | 0.00030 |
| 51 | 3,4-Dihydroxyphenylpyruvic acid | C ₉ H ₈ O ₅ | 4228-66-4 | 196.04 | -0.00011 |
| 52 | 3,4-Dihydroxyphenylacetic acid | C ₈ H ₈ O ₄ | 102-32-9 | 168.04 | -0.00013 |
| 53 | Theaflavic acid | C ₂₁ H ₁₆ O ₁₀ | 30407-93-3 | 428.07 | -0.00066 |
| 54 | 2-Protocatechuoyl phloroglucinolcarboxylate | C ₁₄ H ₁₀ O ₈ | 30048-34-1 | 306.04 | -0.00021 |
| 55 | 2-Caffeoylisocitric acid | C ₁₅ H ₁₄ O ₁₀ | ChemSpider ID 4444181 | 354.06 | -0.00030 |
| 56 | (+)-Chebulic acid | C ₁₄ H ₁₂ O ₁₁ | ChemSpider ID 35014171 | 356.04 | -0.00029 |
| 57 | 4-Hydroxycinnamic acid | C ₉ H ₈ O ₃ | 501-98-4 | 164.05 | -0.00029 |
| 58 | Xanthosine | C ₁₀ H ₁₂ N ₄ O ₆ | 146-80-5 | 284.08 | -0.00001 |
| 59 | Thymidine | C ₁₀ H ₁₄ N ₂ O ₅ | 50-89-5 | 242.09 | -0.00031 |
| 60 | Succinyladenosine | C ₁₄ H ₁₇ N ₅ O ₈ | 4542-23-8 | 383.11 | 0.00035 |
| 61 | N-Acetylcytidine | C ₁₁ H ₁₅ N ₃ O ₆ | 3768-18-1 | 285.10 | 0.00030 |
| 62 | 1-Methylxanthine | C ₆ H ₆ N ₄ O ₂ | 6136-37-4 | 166.05 | -0.00018 |
| 63 | Guanine | C ₅ H ₅ N ₅ O | 73-40-5 | 151.05 | -0.00022 |
| 64 | Deoxyuridine | C ₉ H ₁₂ N ₂ O ₅ | 951-78-0 | 228.07 | 0.00024 |
| 65 | Deoxyinosine | C ₁₀ H ₁₂ N ₄ O ₄ | 890-38-0 | 252.09 | -0.00003 |
| 66 | Cyclic di-AMP | C ₂₀ H ₂₄ N ₁₀ O ₁₂ P ₂ | 54447-84-6 | 658.10 | -0.00014 |
| 67 | c-GMP-AMP | C ₂₀ H ₂₄ N ₁₀ O ₁₃ P ₂ | 849214-04-6 | 674.10 | -0.00007 |
| 68 | Arabinosylhypoxanthine | C ₁₀ H ₁₂ N ₄ O ₅ | 7013-16-3 | 268.08 | -0.00001 |
| 69 | Adenine | C ₅ H ₅ N ₅ | 73-24-5 | 135.05 | -0.00005 |
| 70 | 8-Hydroxy-2'-deoxyguanosine | C ₁₀ H ₁₃ N ₅ O ₅ | 88847-89-6 | 283.09 | -0.00041 |
| 71 | 5-Methyluridine | C ₁₀ H ₁₄ N ₂ O ₆ | 1463-10-1 | 258.09 | 0.00000 |
| 72 | Theogallin | C ₁₄ H ₁₆ O ₁₀ | 17365-11-6 | 344.07 | -0.00125 |
| 73 | Theasinensin A | C ₄₄ H ₃₄ O ₂₂ | 89064-31-3 | 914.15 | -0.00056 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|------------|-----------------------|-----------------------|
| 74 | Taxifolin | C ₁₅ H ₁₂ O ₇ | 480-18-2 | 304.06 | -0.00020 |
| 75 | Swertianolin | C ₂₀ H ₂₀ O ₁₁ | 23445-00-3 | 436.10 | -0.00017 |
| 76 | Scutellarin | C ₂₁ H ₁₈ O ₁₂ | 27740-01-8 | 462.08 | 0.00002 |
| 77 | Apigenin-7-O-rhamnoglucoside | C ₂₇ H ₃₀ O ₁₄ | 17306-46-6 | 578.16 | -0.00118 |
| 78 | Quercitrin | C ₂₁ H ₂₀ O ₁₁ | 522-12-3 | 448.10 | -0.00100 |
| 79 | Naringenin-7-O-glucoside | C ₂₁ H ₂₂ O ₁₀ | 529-55-5 | 434.12 | -0.00049 |
| 80 | Plantagoside | C ₂₁ H ₂₂ O ₁₂ | 78708-33-5 | 466.11 | -0.00065 |
| 81 | Kaempferol | C ₁₅ H ₁₀ O ₆ | 520-18-3 | 286.05 | -0.00023 |
| 82 | 3',4',5,7-Tetrahydroxyflavanone | C ₁₅ H ₁₂ O ₆ | 4049-38-1 | 288.06 | 0.00019 |
| 83 | Cianidanol | C ₁₅ H ₁₄ O ₆ | 154-23-4 | 290.08 | -0.00078 |
| 84 | 5,7,3',4'-Tetrahydroxy-3,6,8-trimethoxyflavone | C ₁₈ H ₁₆ O ₉ | 61451-85-2 | 376.08 | -0.00057 |
| 85 | 3,4,5,7,3',4',5'-Heptahydroxyflavan | C ₁₅ H ₁₄ O ₈ | 491-52-1 | 322.07 | -0.00084 |
| 86 | 4',5,7-Trihydroxyflavanone | C ₁₅ H ₁₂ O ₅ | 67604-48-2 | 272.07 | -0.00039 |
| 87 | Phloretin | C ₁₅ H ₁₄ O ₅ | 60-82-2 | 274.08 | -0.00009 |
| 88 | 6-Methoxyquercetin | C ₁₆ H ₁₂ O ₈ | 519-96-0 | 332.05 | -0.00014 |
| 89 | Kaempferol-3-O-rutinoside | C ₂₇ H ₃₀ O ₁₅ | 17650-84-9 | 594.16 | -0.00128 |
| 90 | Miquelianin | C ₂₁ H ₁₈ O ₁₃ | 22688-79-5 | 478.07 | -0.00079 |
| 91 | Kaempferol 3-arabinofuranoside | C ₂₀ H ₁₈ O ₁₀ | 5041-67-8 | 418.09 | -0.00063 |
| 92 | Isoquercetin | C ₂₁ H ₂₀ O ₁₂ | 482-35-9 | 464.09 | -0.00078 |
| 93 | Salvigenin | C ₁₈ H ₁₆ O ₆ | 19103-54-9 | 328.09 | -0.00038 |
| 94 | Gossypin | C ₂₁ H ₂₀ O ₁₃ | 652-78-8 | 480.09 | -0.00086 |
| 95 | Eucalyptin | C ₁₉ H ₁₈ O ₅ | 3122-88-1 | 326.12 | -0.00018 |
| 96 | Dihydromyricetin | C ₁₅ H ₁₂ O ₈ | 27200-12-0 | 320.05 | -0.00025 |
| 97 | Baicalin | C ₂₁ H ₁₈ O ₁₁ | 21967-41-9 | 446.08 | -0.00037 |
| 98 | Quercetin | C ₂₀ H ₁₈ O ₁₁ | 572-30-5 | 434.08 | -0.00033 |
| 99 | 3-O-alpha-L-arabinopyranoside | C ₂₁ H ₂₂ O ₁₁ | 29838-67-3 | 450.12 | -0.00053 |
| 100 | 5,7-Dihydroxy-3',4',5'-trimethoxyflavanone | C ₁₈ H ₁₈ O ₇ | 62252-10-2 | 346.11 | 0.00011 |
| 101 | Scoparone | C ₁₁ H ₁₀ O ₄ | 120-08-1 | 206.06 | -0.00033 |
| 102 | 4-Methylumbelliferyl-beta-D-glucuronide | C ₁₆ H ₁₆ O ₉ | 6160-80-1 | 352.08 | 0.00029 |
| 103 | 4-Methylumbelliferyl-beta-D-glucopyranoside | C ₁₆ H ₁₈ O ₈ | 18997-57-4 | 338.10 | -0.00089 |
| 104 | 7-Ethoxy-4-methylcoumarin | C ₁₂ H ₁₂ O ₃ | 87-05-8 | 204.08 | -0.00007 |
| 105 | 4-Hydroxycoumarin | C ₉ H ₆ O ₃ | 1076-38-6 | 162.03 | -0.00029 |
| 106 | Coumarin | C ₉ H ₆ O ₂ | 91-64-5 | 146.04 | 0.00014 |
| 107 | Aesculin | C ₁₅ H ₁₆ O ₉ | 531-75-9 | 340.08 | 0.00002 |
| 108 | 7-Ethoxycoumarin | C ₁₁ H ₁₀ O ₃ | 31005-02-4 | 190.06 | -0.00011 |
| 109 | 4-Methyl-6,7-diacetoxycoumarin | C ₁₄ H ₁₂ O ₆ | 55939-28-1 | 276.06 | -0.00016 |
| 110 | 4,5,7-Trihydroxycoumarin | C ₉ H ₆ O ₅ | 17575-26-7 | 194.02 | -0.00027 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|---------------------------|-----------------------|-----------------------|
| 111 | Vanillin | C ₈ H ₈ O ₃ | 121-33-5 | 152.05 | -0.00053 |
| 112 | Trimethyl 4-hydroxy-5-methyl-1,2,3-benzenet ricarboxylate | C ₁₃ H ₁₄ O ₇ | ChemSpider ID 538404 | 282.07 | -0.00084 |
| 113 | Triethyl 1,3,5-benzenetricarboxylate | C ₁₅ H ₁₈ O ₆ | 4105-92-4 | 294.11 | 0.00018 |
| 114 | 4-(3-Butoxy-4-methoxybenzyl)-2-i midazolidinone | C ₁₅ H ₂₂ N ₂ O ₃ | 29925-17-5 | 278.16 | 0.00033 |
| 115 | Pyrogallol | C ₆ H ₆ O ₃ | 87-66-1 | 126.03 | -0.00011 |
| 116 | Oxydi-3,1,2-propanetriyl tetrabutanoate | C ₂₂ H ₃₈ O ₉ | ChemSpider ID 479813 | 446.25 | -0.00022 |
| 117 | N-(5-Phenyl-1H-1,2,4-triazol-3-yl)b enzamide | C ₁₅ H ₁₂ N ₄ O | ChemSpider ID 495787 | 264.10 | -0.00121 |
| 118 | Monobutyrim | C ₇ H ₁₄ O ₄ | 557-25-5 | 162.09 | 0.00005 |
| 119 | 6-Methyl-5-hepten-2-one | C ₈ H ₁₄ O | 110-93-0 | 126.10 | 0.00009 |
| 120 | Lauric anhydride | C ₂₄ H ₄₆ O ₃ | 645-66-9 | 382.35 | 0.00057 |
| 121 | Methyl p-toluenesulfonate | C ₈ H ₁₀ O ₃ S | 80-48-8 | 186.04 | 0.00026 |
| 122 | Methyl alpha-aspartylphenylalaninate | C ₁₄ H ₁₈ N ₂ O ₅ | 22839-65-2 | 294.12 | 0.00064 |
| 123 | Methyl 3-hydroxydodecanoate | C ₁₃ H ₂₆ O ₃ | 72864-23-4 | 230.19 | 0.00011 |
| 124 | Methyl 3,5-di-tert-butyl-4-hydroxybenzoate | C ₁₆ H ₂₄ O ₃ | 2511-22-0 | 264.17 | 0.00011 |
| 125 | Maclurin | C ₁₃ H ₁₀ O ₆ | 519-34-6 | 262.05 | 0.00010 |
| 126 | Indole | C ₈ H ₇ N | 120-72-9 | 117.06 | -0.00004 |
| 127 | Hexyl fumarate | C ₁₆ H ₂₈ O ₄ | 19139-31-2 | 284.20 | 0.00022 |
| 128 | Heptanoic anhydride | C ₁₄ H ₂₆ O ₃ | 626-27-7 | 242.19 | 0.00016 |
| 129 | Guaiacol sulfate | C ₇ H ₈ O ₅ S | 3233-59-8 | 204.01 | 0.00008 |
| 130 | Guaiacol | C ₇ H ₈ O ₂ | 544-31-0 | 124.05 | 0.00025 |
| 131 | Diethylene glycol monolaurate | C ₁₆ H ₃₂ O ₄ | 141-20-8 | 288.23 | 0.00008 |
| 132 | 2-Hydroxyquinoline | C ₉ H ₇ NO | 59-31-4 | 145.05 | 0.00012 |
| 133 | Ethyl p-hydroxybenzoate | C ₉ H ₁₀ O ₃ | 120-47-8 | 166.06 | 0.00009 |
| 134 | Ethylene dodecanedioate | C ₁₄ H ₂₄ O ₄ | 54982-83-1 | 256.17 | 0.00013 |
| 135 | Ethyl lactate | C ₅ H ₁₀ O ₃ | 97-64-3 | 118.06 | -0.00044 |
| 136 | Ethyl cinnamate | C ₁₁ H ₁₂ O ₂ | 103-36-6 | 176.08 | 0.00008 |
| 137 | Ethyl 2-oxocyclohexanecarboxylate | C ₉ H ₁₄ O ₃ | 1655-07-8 | 170.09 | -0.00009 |
| 138 | Ethyl 2-acetylheptanoate | C ₁₁ H ₂₀ O ₃ | 24317-94-0 | 200.14 | -0.00009 |
| 139 | Epicatechin-3'-sulfate | C ₁₅ H ₁₄ O ₉ S | 1038922-77-8 | 370.04 | 0.00006 |
| 140 | 6-Nitroveratraldehyde | C ₉ H ₉ NO ₅ | 20357-25-9 | 211.05 | 0.00004 |
| 141 | Di-tert-butyl malonate | C ₁₁ H ₂₀ O ₄ | 541-16-2 | 216.14 | 0.00017 |
| 142 | Diphenol glucuronide | C ₁₂ H ₁₄ O ₈ | ChemSpider ID 30778502 | 286.07 | -0.00028 |
| 143 | Dimethyl itaconate | C ₇ H ₁₀ O ₄ | 617-52-7 | 158.06 | -0.00014 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|-------------------------|-----------------------|-----------------------|
| 144 | Dimethyl 2,3-bis(1-methoxyethoxy)succinate | C ₁₂ H ₂₂ O ₈ | ChemSpider ID 476915 | 294.13 | 0.00003 |
| 145 | Dimethyl 1,4-cyclohexanedicarboxylate | C ₁₀ H ₁₆ O ₄ | 94-60-0 | 200.10 | -0.00011 |
| 146 | Dimedone | C ₈ H ₁₂ O ₂ | 126-81-8 | 140.08 | 0.00004 |
| 147 | Diethyl tartrate | C ₈ H ₁₄ O ₆ | 13811-71-7 | 206.08 | -0.00013 |
| 148 | Diethyl phosphate | C ₄ H ₁₁ O ₄ P | 598-02-7 | 154.04 | 0.00013 |
| 149 | Diethyl malonate | C ₇ H ₁₂ O ₄ | 105-53-3 | 160.07 | 0.00011 |
| 150 | Diethyl benzoylmalonate | C ₁₄ H ₁₆ O ₅ | 1087-97-4 | 264.10 | 0.00003 |
| 151 | Dibutyl malate | C ₁₂ H ₂₂ O ₅ | 6280-99-5 | 246.15 | -0.00015 |
| 152 | Dibutyl itaconate | C ₁₃ H ₂₂ O ₄ | 2155-60-4 | 242.15 | -0.00008 |
| 153 | Dibutyl Fumarate | C ₁₂ H ₂₀ O ₄ | 105-75-9 | 228.14 | -0.00007 |
| 154 | Ethyl p-methoxycinnamate | C ₁₂ H ₁₄ O ₃ | 24393-56-4 | 206.09 | 0.00017 |
| 155 | Diallyl phthalate | C ₁₄ H ₁₄ O ₄ | 131-17-9 | 246.09 | -0.00053 |
| 156 | Coumarone | C ₈ H ₆ O | 271-89-6 | 118.04 | -0.00017 |
| 157 | Caproic anhydride | C ₁₂ H ₂₂ O ₃ | 2051-49-2 | 214.16 | -0.00010 |
| 158 | Butylphthalide | C ₁₂ H ₁₄ O ₂ | 6066-49-5 | 190.10 | -0.00011 |
| 159 | Butyl acrylate | C ₇ H ₁₂ O ₂ | 141-32-2 | 128.08 | 0.00000 |
| 160 | Bis(2-methoxyethyl) tartarate | C ₁₀ H ₁₈ O ₈ | ChemSpider ID 476785 | 266.10 | -0.00015 |
| 161 | Bis(2-butoxyethyl) adipate | C ₁₈ H ₃₄ O ₆ | 141-18-4 | 346.24 | -0.00035 |
| 162 | Benzoquinone | C ₆ H ₄ O ₂ | 106-51-4 | 108.02 | 0.00006 |
| 163 | Phenol | C ₆ H ₆ O | 108-95-2 | 94.04 | 0.00001 |
| 164 | Bellidifolin | C ₁₄ H ₁₀ O ₆ | 2798-25-6 | 274.05 | 0.00007 |
| 165 | Atranorin | C ₁₉ H ₁₈ O ₈ | 479-20-9 | 374.10 | 0.00005 |
| 166 | Ethyl benzoylacetate | C ₁₁ H ₁₂ O ₃ | 94-02-0 | 192.08 | -0.00005 |
| 167 | Acetophenone | C ₈ H ₈ O | 98-86-2 | 120.06 | -0.00003 |
| 168 | Aceglatone | C ₁₀ H ₁₀ O ₈ | 642-83-1 | 258.04 | 0.00003 |
| 169 | 7-Benzyl-2-(4-bromophenyl)-6-methylindolizine | C ₂₂ H ₁₈ BrN | ChemSpider ID 549718 | 375.06 | 0.00129 |
| 170 | 6-Oxododecanedioic acid | C ₁₂ H ₂₀ O ₅ | 4132-62-1 | 244.13 | 0.00003 |
| 171 | 6-Acetyl-4,5,7,8-tetrahydroxynaphthalene-1,2-dione | C ₁₂ H ₈ O ₇ | 3718-80-7 | 264.03 | -0.00078 |
| 172 | 5-Benzylidene-2,2-dimethyl-1,3-dioxane-4,6-dione | C ₁₃ H ₁₂ O ₄ | 1214-54-6 | 232.07 | -0.00031 |
| 173 | Spinochrome M | C ₁₂ H ₁₀ O ₆ | 2808-46-0 | 250.05 | -0.00007 |
| 174 | 4-Phenolsulfonic acid | C ₆ H ₆ O ₄ S | 98-67-9 | 174.00 | 0.00036 |
| 175 | Vanillin 4-sulfate | C ₈ H ₈ O ₆ S | 744984-09-6 | 232.00 | -0.00016 |
| 176 | 4,6-Di-tert-Butylpyrogallol | C ₁₄ H ₂₂ O ₃ | 3934-77-8 | 238.16 | 0.00006 |
| 177 | 3-Decyloxolane-2,5-dione | C ₁₄ H ₂₄ O ₃ | 18470-76-3 | 240.17 | 0.00007 |
| 178 | 3,5-Ditert-butyl-4-hydroxybenzaldehyde | C ₁₅ H ₂₂ O ₂ | 1620-98-0 | 234.16 | -0.00011 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|--------------------------|-----------------------|-----------------------|
| 179 | Schizotenuin F | C ₂₈ H ₂₄ O ₁₂ | 127498-36-6 | 552.13 | -0.00066 |
| 180 | 2-O-Acetylmalic Anhydride | C ₆ H ₆ O ₅ | 24766-96-9 | 158.02 | -0.00048 |
| 181 | 2-Methyl-3-(2-pyridin-4-yl-thiazol-4-yl)-1H-indole | C ₁₇ H ₁₃ N ₃ S | ChemSpider ID 620846 | 291.08 | -0.00099 |
| 182 | 2-Hydroxy-6-ketononadienedioic acid | C ₉ H ₁₀ O ₆ | ChemSpider ID 4444276 | 214.05 | -0.00042 |
| 183 | 2-Acetoxy-3-[3-(4-hydroxy-phenyl)-acryloyloxy]-succinic acid | C ₁₅ H ₁₄ O ₉ | 106928-35-2 | 338.06 | -0.00042 |
| 184 | 2,7-Dimethoxynaphthalene | C ₁₂ H ₁₂ O ₂ | 3469-26-9 | 188.08 | -0.00002 |
| 185 | 1-O-Galloylglycerol | C ₁₀ H ₁₂ O ₇ | 87087-60-3 | 244.06 | -0.00044 |
| 186 | 2,3,4,5-Tetrahydroxy-N-nonylpentanamide | C ₁₄ H ₂₉ NO ₅ | ChemSpider ID 480198 | 291.20 | 0.00004 |
| 187 | 2-(4-Methoxyphenyl)-1,3-dithiolane | C ₁₀ H ₁₂ OS ₂ | 6712-20-5 | 212.03 | -0.00050 |
| 188 | 2-(2-(Benzoyloxy)propoxy)propyl benzoate | C ₂₀ H ₂₂ O ₅ | 20109-39-1 | 342.15 | -0.00046 |
| 189 | 1'-Acetoxychavicol acetate | C ₁₃ H ₁₄ O ₄ | 52946-22-2 | 234.09 | -0.00031 |
| 190 | 1,4,7,10,13-Pentaoxacyclopentadecane | C ₁₀ H ₂₀ O ₅ | 33100-27-5 | 220.13 | 0.00017 |
| 191 | 15,15'-Bi(1,4,7,10,13-pentaoxacyclohexadecane) | C ₂₂ H ₄₂ O ₁₀ | ChemSpider ID 487416 | 466.28 | -0.00029 |
| 192 | 1,6-Hexanediol diacrylate | C ₁₂ H ₁₈ O ₄ | 13048-33-4 | 226.12 | -0.00023 |
| 193 | 1,2,3,4,5,6-Heptanehexayl hexaacetate | C ₁₉ H ₂₈ O ₁₂ | ChemSpider ID 470156 | 448.16 | -0.00036 |
| 194 | 1-(4-Chloro-2-nitrophenyl)piperidine | C ₁₁ H ₁₃ ClN ₂ O ₂ | 33784-44-0 | 240.07 | 0.00032 |
| 195 | 2-Amino-2-methylpropanenitrile | C ₆ H ₁₁ NO ₄ | 19355-69-2 | 161.07 | 0.00005 |
| 196 | (Hydroxyethyl)methacrylate | C ₆ H ₁₀ O ₃ | 868-77-9 | 130.06 | 0.00018 |
| 197 | (2-Dodecen-1-yl)succinic anhydride | C ₁₆ H ₂₆ O ₃ | 19780-11-1 | 266.19 | 0.00005 |
| 198 | Riboflavin | C ₁₇ H ₂₀ N ₄ O ₆ | 83-88-5 | 376.14 | 0.00037 |
| 199 | 1,3-Dicaffeoylquinic acid | C ₂₅ H ₂₄ O ₁₂ | 30964-13-7 | 516.13 | -0.00072 |
| 200 | Hydroquinone | C ₆ H ₆ O ₂ | 123-31-9 | 110.04 | -0.00032 |
| 201 | Eugenol | C ₁₀ H ₁₂ O ₂ | 97-53-0 | 164.08 | -0.00007 |
| 202 | Curcumin II | C ₂₀ H ₁₈ O ₅ | 22608-11-3 | 338.12 | -0.00007 |
| 203 | Theophylline | C ₇ H ₈ N ₄ O ₂ | 58-55-9 | 180.06 | -0.00032 |
| 204 | Paucin | C ₂₃ H ₃₂ O ₁₀ | 26836-43-1 | 468.20 | -0.00207 |
| 205 | Vanilloloside | C ₁₄ H ₂₀ O ₈ | 74950-96-2 | 316.12 | 0.00002 |
| 206 | Sweroside | C ₁₆ H ₂₂ O ₉ | 14215-86-2 | 358.13 | -0.00036 |
| 207 | Sinapaldehyde glucoside | C ₁₇ H ₂₂ O ₉ | 154461-65-1 | 370.13 | 0.00005 |
| 208 | (2S)-2-(beta-D-Glucopyranosyloxy)-3-methyl-3-butenenitrile | C ₁₁ H ₁₇ NO ₆ | 66871-89-4 | 259.11 | -0.00023 |
| 209 | Piceid | C ₂₀ H ₂₂ O ₈ | 65914-17-2 | 390.13 | 0.00024 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|---------------------------|-----------------------|-----------------------|
| 210 | Neohesperidose | C ₁₂ H ₂₂ O ₁₀ | 17074-02-1 | 326.12 | -0.00028 |
| 211 | Methyl 2,3,6-tri-O-acetyl-4-O-octylhexopyranoside | C ₂₁ H ₃₆ O ₉ | ChemSpider ID 470432 | 432.24 | -0.00021 |
| 212 | Methyl 2,3,4-tri-O-acetyl-1-O-benzoylhexopyranuronate | C ₂₀ H ₂₂ O ₁₁ | ChemSpider ID 494836 | 438.12 | -0.00013 |
| 213 | Khellol glucoside | C ₁₉ H ₂₀ O ₁₀ | 17226-75-4 | 408.11 | -0.00016 |
| 214 | Indoxyl beta-D-glucoside | C ₁₄ H ₁₇ NO ₆ | 487-60-5 | 295.11 | -0.00059 |
| 215 | alpha-D-Mannose | C ₆ H ₁₂ O ₆ | 7296-15-3 | 180.06 | 0.00008 |
| 216 | 1-Galloyl-beta-D-glucose | C ₁₃ H ₁₆ O ₁₀ | 13405-60-2 | 332.07 | -0.00030 |
| 217 | Geranyl beta-D-glucopyranoside | C ₁₆ H ₂₈ O ₆ | 22850-13-1 | 316.19 | 0.00027 |
| 218 | Eriocitrin | C ₂₇ H ₃₂ O ₁₅ | 13463-28-0 | 596.17 | -0.00097 |
| 219 | Dihydrophaseic acid 4-O-beta-D-glucoside | C ₂₁ H ₃₂ O ₁₀ | ChemSpider ID 10160748 | 444.20 | -0.00028 |
| 220 | Caffeic acid 3-glucoside | C ₁₅ H ₁₈ O ₉ | 24959-81-7 | 342.09 | -0.00041 |
| 221 | beta-Syringin | C ₁₇ H ₂₄ O ₉ | 118-34-3 | 372.14 | -0.00017 |
| 222 | beta-D-Glucose pentaacetate | C ₁₆ H ₂₂ O ₁₁ | 604-69-3 | 390.12 | -0.00011 |
| 223 | Benzyl beta-primeveroside | C ₁₈ H ₂₆ O ₁₀ | 130622-31-0 | 402.15 | -0.00073 |
| 224 | Apiin | C ₂₆ H ₂₈ O ₁₄ | ChemSpider ID 4444321 | 564.15 | -0.00160 |
| 225 | 5,6-Bis-O-(2-oxopropyl)hexose | C ₁₂ H ₂₀ O ₈ | ChemSpider ID 468771 | 292.12 | 0.00020 |
| 226 | Dihydrocaffeic acid 3-O-glucuronide | C ₁₅ H ₁₈ O ₁₀ | 1187945-71-6 | 358.09 | -0.00025 |
| 227 | Dihydroferulic acid 4-O-glucuronide | C ₁₆ H ₂₀ O ₁₀ | 86321-28-0 | 372.11 | -0.00038 |
| 228 | 2-Methoxyphenyl 6-O-beta-D-xylopyranosyl-beta-D-glucopyranoside | C ₁₈ H ₂₆ O ₁₁ | ChemSpider ID 58837448 | 418.15 | -0.00019 |
| 229 | 2-Hydroxy-2-(4-methyl-2-oxocyclohexyl)propyl hexopyranoside | C ₁₆ H ₂₈ O ₈ | ChemSpider ID 30791612 | 348.18 | -0.00006 |
| 230 | 2-Acetyl-1,3,4-tri-O-acetyl-2-deoxypentopyranose | C ₁₃ H ₁₈ O ₈ | ChemSpider ID 470300 | 302.10 | -0.00024 |
| 231 | 2,3-Di-O-benzyl-5-O-(4-nitrobenzoyl)pentofuranose | C ₂₆ H ₂₅ NO ₈ | ChemSpider ID 488596 | 479.16 | -0.00026 |
| 232 | 2(R)-Hydroxy-2-methylbutyronitrile-beta-D-glucopyranoside | C ₁₁ H ₁₉ NO ₆ | 534-67-8 | 261.12 | -0.00007 |
| 233 | 1,6-Di-O-galloyl-beta-D-glucopyranose | C ₂₀ H ₂₀ O ₁₄ | 23363-08-8 | 484.08 | -0.00128 |
| 234 | 1,3,4,6-Tetra-O-acetyl-alpha-D-glucopyranose | C ₁₄ H ₂₀ O ₁₀ | 13036-15-2 | 348.11 | -0.00042 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|---------------------------|-----------------------|-----------------------|
| 235 | 2-Deoxy-beta-D-arabino-hexopyranose tetraacetate | C ₁₄ H ₂₀ O ₉ | 16750-06-4 | 332.11 | -0.00012 |
| 236 | 1,2-Di-O-acetyl-3,5-di-O-benzoylpenntofuranose | C ²³ H ²² O ⁹ | ChemSpider ID 494887 | 442.13 | -0.00048 |
| 237 | geniposide | C ₁₇ H ₂₄ O ₁₀ | 24512-63-8 | 388.14 | -0.00039 |
| 238 | Triptidolide | C ₂₀ H ₂₄ O ₇ | 38647-10-8 | 376.15 | -0.00030 |
| 239 | Picrotin | C ₁₅ H ₁₈ O ₇ | 21416-53-5 | 310.11 | 0.00016 |
| 240 | 20(S)-Ginsenoside | C ₃₆ H ₆₂ O ₈ | 78214-33-2 | 622.44 | -0.00131 |
| 241 | Lamiide | C ₁₇ H ₂₆ O ₁₂ | 27856-54-8 | 422.14 | -0.00016 |
| 242 | Gibberellin A7 | C ₁₉ H ₂₂ O ₅ | 510-75-8 | 330.15 | -0.00031 |
| 243 | Gibberellin A53 | C ₂₀ H ₂₈ O ₅ | 51576-08-0 | 348.19 | 0.00000 |
| 244 | Deoxyloganic acid | C ₁₆ H ₂₄ O ₉ | 22487-36-1 | 360.14 | -0.00048 |
| 245 | Brusatol | C ₂₆ H ₃₂ O ₁₁ | 14907-98-3 | 520.19 | -0.00083 |
| 246 | Artemotil | C ₁₇ H ₂₈ O ₅ | 75887-54-6 | 312.19 | -0.00009 |
| 247 | Allamandin | C ₁₅ H ₁₆ O ₇ | 51820-82-7 | 308.09 | 0.00025 |
| 248 | (+)-Gibberellic acid | C ₁₉ H ₂₂ O ₆ | 77-06-5 | 346.14 | 0.00016 |
| 249 | Sebacic acid | C ₁₀ H ₁₈ O ₄ | 111-20-6 | 202.12 | -0.00002 |
| 250 | Vanillyl mandelic acid | C ₉ H ₁₀ O ₅ | 55-10-7 | 198.05 | -0.00022 |
| 251 | Porphobilinogen | C ₁₀ H ₁₄ N ₂ O ₄ | 487-90-1 | 226.10 | 0.00010 |
| 252 | Piscidic acid | C ₁₁ H ₁₂ O ₇ | 35388-57-9 | 256.06 | 0.00002 |
| 253 | Phthalic acid | C ₈ H ₆ O ₄ | 88-99-3 | 166.03 | -0.00033 |
| 254 | Butyl levulinate | C ₉ H ₁₆ O ₃ | 2052-15-5 | 172.11 | 0.00017 |
| 255 | N-Succinyl-L-diaminopimelic acid | C ₁₁ H ₁₈ N ₂ O ₇ | 26605-36-7 | 290.11 | 0.00008 |
| 256 | 2-Naphthalen-2-yloxypropanoic acid | C ₁₃ H ₁₂ O ₃ | 10470-82-3 | 216.08 | 0.00009 |
| 257 | N,N-Diacetyllegionaminic acid | C ₁₃ H ₂₂ N ₂ O ₈ | ChemSpider ID 10179688 | 334.14 | 0.00012 |
| 258 | p-Tolyl beta-D-glucuronide | C ₁₃ H ₁₆ O ₇ | 17680-99-8 | 284.09 | 0.00074 |
| 259 | Dibenzoyl-D-tartaric acid | C ₁₈ H ₁₄ O ₈ | 17026-42-5 | 358.07 | -0.00010 |
| 260 | 3,6,9-Trioxaundecanedioic acid | C ₈ H ₁₄ O ₇ | 13887-98-4 | 222.07 | 0.00016 |
| 261 | Luteic acid | C ₁₄ H ₈ O ₉ | 476-67-5 | 320.02 | -0.00013 |
| 262 | Benzyl formate | C ₈ H ₈ O ₂ | 104-57-4 | 136.05 | 0.00006 |
| 263 | 4-[2-(4-Amino-4-carboxybutanoyl)hydrazino]benzoic acid | C ₁₂ H ₁₅ N ₃ O ₅ | 69644-85-5 | 281.10 | 0.00068 |
| 264 | 4-Hydroxyquinoline-2-carboxylic acid | C ₁₀ H ₇ NO ₃ | 492-27-3 | 189.04 | -0.00030 |
| 265 | 2-Isopropylmalic acid | C ₇ H ₁₂ O ₅ | 3237-44-3 | 176.07 | -0.00003 |
| 266 | Hopantenic acid | C ₁₀ H ₁₉ NO ₅ | 18679-90-8 | 233.13 | -0.00001 |
| 267 | Homovanillic acid | C ₉ H ₁₀ O ₄ | 306-08-1 | 182.06 | 0.00029 |
| 268 | Dimethyl succinylsuccinate | C ₁₀ H ₁₂ O ₆ | 6289-46-9 | 228.06 | 0.00005 |
| 269 | Glutaric anhydride | C ₅ H ₆ O ₃ | 108-55-4 | 114.03 | 0.00006 |
| 270 | Glutaric acid | C ₅ H ₈ O ₄ | 110-94-1 | 132.04 | -0.00009 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|---------------------------|-----------------------|-----------------------|
| 271 | Fukiic acid | C ₁₁ H ₁₂ O ₈ | 35388-56-8 | 272.05 | -0.00039 |
| 272 | D-Xylonic acid | C ₅ H ₁₀ O ₆ | 4172-43-4 | 166.05 | 0.00029 |
| 273 | D-Pantothenic acid | C ₉ H ₁₇ NO ₅ | 79-83-4 | 219.11 | -0.00031 |
| 274 | DL-Mevalonic acid | C ₆ H ₁₂ O ₄ | 150-97-0 | 148.07 | -0.00004 |
| 275 | Di-(2-ethylhexyl)phosphoric acid | C ₁₆ H ₃₅ O ₄ P | 298-07-7 | 322.23 | 0.00003 |
| 276 | D-Gluconic acid | C ₆ H ₁₂ O ₇ | 526-95-4 | 196.06 | -0.00029 |
| 277 | Cinnamic acid | C ₉ H ₈ O ₂ | 140-10-3 | 148.05 | 0.00001 |
| 278 | Chorismic acid | C ₁₀ H ₁₀ O ₆ | 617-12-9 | 226.05 | 0.00017 |
| 279 | Brassylic acid | C ₁₃ H ₂₄ O ₄ | 505-52-2 | 244.17 | -0.00021 |
| 280 | Benzoic acid | C ₇ H ₆ O ₂ | 65-85-0 | 122.04 | 0.00023 |
| 281 | Azelaic acid | C ₉ H ₁₆ O ₄ | 123-99-9 | 188.10 | -0.00004 |
| 282 | Acetylsalicylic acid | C ₉ H ₈ O ₄ | 50-78-2 | 180.04 | 0.00013 |
| 283 | 5-Methoxy-3-indoleacetate | C ₁₁ H ₁₁ NO ₃ | 3471-31-6 | 205.07 | -0.00035 |
| 284 | 5-[(3-Methoxyphenoxy)methyl]-2-furoic acid | C ₁₃ H ₁₂ O ₅ | 405897-57-6 | 248.07 | -0.00043 |
| 285 | 5,5'-Dehydrodivanillate | C ₁₆ H ₁₄ O ₈ | 2134-90-9 | 334.07 | -0.00027 |
| 286 | 5-(3,4-Dimethoxyphenyl)-2-methyl-3-furoic acid | C ₁₄ H ₁₄ O ₅ | 696627-31-3 | 262.08 | -0.00022 |
| 287 | 4-oxo-1,2-Cyclopentanedicarboxylic acid | C ₇ H ₈ O ₅ | 1703-61-3 | 172.04 | 0.00025 |
| 288 | 4-Methylsulfonylbenzoic acid | C ₈ H ₈ O ₄ S | 4052-30-6 | 200.01 | -0.00013 |
| 289 | 4-Carboxy-3-hydroxyphenyl hexopyranosiduronic acid | C ₁₃ H ₁₄ O ₁₀ | ChemSpider ID 74886630 | 330.06 | -0.00047 |
| 290 | 3-Butene-1,2,3-tricarboxylic acid | C ₇ H ₈ O ₆ | 26326-05-6 | 188.03 | 0.00030 |
| 291 | 3,8,13,17-Tetramethyl-12-vinyl-2,7,18-Porphinetripropionic acid | C ₃₅ H ₃₆ N ₄ O ₆ | 30783-27-8 | 608.26 | -0.00031 |
| 292 | 3,4-Dimethoxyhydrocinnamic acid | C ₁₁ H ₁₄ O ₄ | 2107-70-2 | 210.09 | 0.00001 |
| 293 | 3,4,5-Trimethoxyphenylacetic acid | C ₁₁ H ₁₄ O ₅ | 951-82-6 | 226.08 | -0.00002 |
| 294 | 3,4,5-Trimethoxyhydrocinnamic acid | C ₁₂ H ₁₆ O ₅ | 25173-72-2 | 240.10 | -0.00013 |
| 295 | 2-Methylcitric acid | C ₇ H ₁₀ O ₇ | 6061-96-7 | 206.04 | -0.00007 |
| 296 | 2-Furoic acid | C ₅ H ₄ O ₃ | 88-14-2 | 112.02 | -0.00015 |
| 297 | 2-Amino-4-pyrimidinecarboxylate | C ₅ H ₄ N ₃ O ₂ | ChemSpider ID 24784670 | 138.03 | 0.00058 |
| 298 | 2,5-Dihydroxyterephthalic acid | C ₈ H ₆ O ₆ | 610-92-4 | 198.02 | -0.00044 |
| 299 | 2,3,4,5-Tetramethoxybenzoic acid | C ₁₁ H ₁₄ O ₆ | 72023-44-0 | 242.08 | 0.00020 |
| 300 | 2,2-Bis(hydroxymethyl)propionic acid | C ₅ H ₁₀ O ₄ | 4767-03-7 | 134.06 | -0.00020 |
| 301 | 2-(Benzoyloxy)-3-hydroxysuccinic acid | C ₁₁ H ₁₀ O ₇ | 65621-34-3 | 254.04 | -0.00008 |
| 302 | 12-oxo Phytodienoic Acid | C ₁₈ H ₂₈ O ₃ | 67204-66-4 | 292.20 | 0.00008 |
| 303 | 10-Undecenoic acid | C ₁₁ H ₂₀ O ₂ | 112-38-9 | 184.15 | -0.00005 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|--|--------------|-----------------------|-----------------------|
| 304 | 1,3,7-Trimethyluric acid | C ₈ H ₁₀ N ₄ O ₃ | 5415-44-1 | 210.08 | 0.00019 |
| 305 | 3-Dehydroquinic acid | C ₇ H ₁₀ O ₆ | 10534-44-8 | 190.05 | 0.00011 |
| 306 | (+)-Quinic acid | C ₇ H ₁₂ O ₆ | 36413-60-2 | 192.06 | -0.00027 |
| 307 | trans-Ferulic Acid | C ₁₀ H ₁₀ O ₄ | 1135-24-6 | 194.06 | -0.00024 |
| 308 | 4-Methoxycinnamic acid | C ₁₀ H ₁₀ O ₃ | 830-09-1 | 178.06 | -0.00017 |
| 309 | 3,4-Dimethoxycinnamic acid | C ₁₁ H ₁₂ O ₄ | 2316-26-9 | 208.07 | -0.00017 |
| 310 | (2,2,6,6-Tetramethyl-4-piperidiny) acetic acid | C ₁₁ H ₂₁ NO ₂ | 34635-77-3 | 199.16 | 0.00010 |
| 311 | (+)-Absciscic acid | C ₁₅ H ₂₀ O ₄ | 7773-56-0 | 264.14 | 0.00024 |
| 312 | Shikimic acid | C ₇ H ₁₀ O ₅ | 138-59-0 | 174.05 | -0.00025 |
| 313 | pinellic acid | C ₁₈ H ₃₄ O ₅ | 97134-11-7 | 330.24 | -0.00039 |
| 314 | Phaseolic acid | C ₁₃ H ₁₂ O ₈ | 53755-04-7 | 296.05 | 0.00006 |
| 315 | Phaseic acid | C ₁₅ H ₂₀ O ₅ | 24394-14-7 | 280.13 | -0.00011 |
| 316 | Dibutyl sebacate | C ₁₈ H ₃₄ O ₄ | 109-43-3 | 314.25 | -0.00002 |
| 317 | 1-Acetoxy-2-hydroxy-16-heptadecy n-4-one | C ₁₉ H ₃₂ O ₄ | 24607-10-1 | 324.23 | 0.00002 |
| 318 | Tuliposide B | C ₁₁ H ₁₈ O ₉ | 19870-33-8 | 294.09 | -0.00013 |
| 319 | Suberic acid | C ₈ H ₁₄ O ₄ | 505-48-6 | 174.09 | 0.00006 |
| 320 | Soyacerebroside I | C ₄₀ H ₇₅ NO ₉ | 114297-20-0 | 713.54 | -0.00325 |
| 321 | Ricinelaiddic acid | C ₁₈ H ₃₄ O ₃ | 141-22-0 | 298.25 | 0.00013 |
| 322 | Methyl 2-octynoate | C ₉ H ₁₄ O ₂ | 111-12-6 | 154.10 | 0.00001 |
| 323 | 10-Hydroxy-2-decenoic acid | C ₁₀ H ₁₈ O ₃ | 14113-05-4 | 186.13 | -0.00002 |
| 324 | Phloionolic acid | C ₁₈ H ₃₆ O ₅ | 496-86-6 | 332.26 | -0.00014 |
| 325 | N-Oleoyl-L-Serine | C ₂₁ H ₃₉ NO ₄ | 1246302-99-7 | 369.29 | 0.00007 |
| 326 | 3-Hydroxydecanoic acid | C ₁₀ H ₂₀ O ₃ | 14292-26-3 | 188.14 | 0.00023 |
| 327 | 1-alpha-Linolenoylglycerol | C ₂₁ H ₃₆ O ₄ | 18465-99-1 | 352.26 | 0.00031 |
| 328 | 2-Hydroxydocosanoic acid | C ₂₂ H ₄₄ O ₃ | 13980-14-8 | 356.33 | 0.00062 |
| 329 | Linolenelaiddic acid | C ₁₈ H ₃₀ O ₂ | 28290-79-1 | 278.22 | 0.00000 |
| 330 | 16-Hydroxyhexadecanoic acid | C ₁₆ H ₃₂ O ₃ | 506-13-8 | 272.24 | 0.00008 |
| 331 | Ethyl 3-oxohexanoate | C ₈ H ₁₄ O ₃ | 3249-68-1 | 158.09 | -0.00024 |
| 332 | Dodecanedioic acid | C ₁₂ H ₂₂ O ₄ | 693-23-2 | 230.15 | -0.00009 |
| 333 | Diethyl diallylmalonate | C ₁₃ H ₂₀ O ₄ | 3195-24-2 | 240.14 | 0.00008 |
| 334 | 9-Hydroxynonanoic acid | C ₉ H ₁₈ O ₃ | 3788-56-5 | 174.13 | 0.00006 |
| 335 | 9,10-Dihydroxystearic acid | C ₁₈ H ₃₆ O ₄ | 120-87-6 | 316.26 | 0.00008 |
| 336 | 2-Hydroxytetraecosanoic acid | C ₂₄ H ₄₈ O ₃ | 544-57-0 | 384.36 | 0.00048 |
| 337 | 13-Hydroxyoctadecadienoic acid | C ₁₈ H ₃₂ O ₃ | 29623-28-7 | 296.24 | -0.00007 |
| 338 | 13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid | C ₁₉ H ₃₄ O ₅ | 150147-08-3 | 342.24 | -0.00028 |
| 339 | 13(S)-Hydroperoxylinolenic acid | C ₁₈ H ₃₀ O ₄ | 67597-26-6 | 310.21 | -0.00013 |
| 340 | 12-Hydroxyjasmonic acid glucoside | C ₁₈ H ₂₈ O ₉ | 120399-24-8 | 388.17 | -0.00016 |
| 341 | 12-Hydroxylauric acid | C ₁₂ H ₂₄ O ₃ | 505-95-3 | 216.17 | 0.00020 |
| 342 | 12-Hydroxyoctadecanoic acid | C ₁₈ H ₃₆ O ₃ | 106-14-9 | 300.27 | 0.00035 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|---------------------------|-----------------------|-----------------------|
| 343 | 12-Aminolauric Acid | C ₁₂ H ₂₅ NO ₂ | 693-57-2 | 215.19 | 0.00017 |
| 344 | (5Z,8Z)-Tetradecadienoylcarnitine | C ₂₁ H ₃₇ NO ₄ | 1469901-01-6 | 367.27 | 0.00006 |
| 345 | LPE(18:3) | C ₂₃ H ₄₂ NO ₇ P | ChemSpider ID 24769359 | 475.27 | 0.00011 |
| 346 | (10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid | C ₁₈ H ₃₂ O ₅ | 95341-44-9 | 328.22 | -0.00040 |
| 347 | Pentadecanedioic acid | C ₁₅ H ₂₈ O ₄ | 1460-18-0 | 272.20 | 0.00011 |
| 348 | N-Undecanoylglycine | C ₁₃ H ₂₅ NO ₃ | 83871-09-4 | 243.18 | -0.00069 |
| 349 | N-Lauroylglycine | C ₁₄ H ₂₇ NO ₃ | 7596-88-5 | 257.20 | -0.00014 |

Note: Annot. Delta Mass represents the difference between the actual measured value of molecular weight and the theoretical value.

Table S3. List of 206 non-volatile metabolites in the processing of Rizhao green tea (ESI+, Hilic column).

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|----|--|--|-------------------------|-----------------------|-----------------------|
| 1 | N ² -Acetyl-N-methyllysineamide | C ₉ H ₁₉ N ₃ O ₂ | ChemSpider ID 485364 | 201.15 | -0.00033 |
| 2 | N ² -(tert-Butoxycarbonyl)glutamine | C ₁₀ H ₁₈ N ₂ O ₅ | 85535-45-1 | 246.12 | -0.00041 |
| 3 | N-Acetylvaline | C ₇ H ₁₃ NO ₃ | 3067-19-4 | 159.09 | -0.00013 |
| 4 | N-Acetyl-L-leucine | C ₈ H ₁₅ NO ₃ | 1188-21-2 | 173.11 | -0.00012 |
| 5 | N-Acetyl-L-aspartic acid | C ₆ H ₉ NO ₅ | 997-55-7 | 175.05 | -0.00020 |
| 6 | L-alpha-Aspartyl-D-phenylalanine methyl ester | C ₁₄ H ₁₈ N ₂ O ₅ | 22839-65-2 | 294.12 | -0.00029 |
| 7 | Leu-Pro | C ₁₁ H ₂₀ N ₂ O ₃ | 6403-35-6 | 228.15 | -0.00030 |
| 8 | L-Theanine | C ₇ H ₁₄ N ₂ O ₃ | 3081-61-6 | 174.10 | -0.00018 |
| 9 | L-Pyroglutamic acid | C ₅ H ₇ NO ₃ | 98-79-3 | 129.04 | -0.00006 |
| 10 | L-Proline | C ₅ H ₉ NO ₂ | 147-85-3 | 115.06 | -0.00020 |
| 11 | L-Valine | C ₅ H ₁₁ NO ₂ | 72-18-4 | 117.08 | -0.00032 |
| 12 | L-Leucine | C ₆ H ₁₃ NO ₂ | 61-90-5 | 131.09 | -0.00029 |
| 13 | Homocysteine | C ₇ H ₁₃ NO ₂ | 2756-85-6 | 143.09 | -0.00027 |
| 14 | Gly-Leu | C ₈ H ₁₆ N ₂ O ₃ | 869-19-2 | 188.12 | -0.00030 |
| 15 | Ethyl DL-methionate | C ₇ H ₁₅ NO ₂ S | 452-95-9 | 177.08 | -0.00020 |
| 16 | Boc-Glycine | C ₇ H ₁₃ NO ₄ | 4530-20-5 | 175.08 | -0.00005 |
| 17 | Acetyl-L-proline | C ₇ H ₁₁ NO ₃ | 68-95-1 | 157.07 | -0.00018 |
| 18 | 5-Hydroxy-DL-tryptophan | C ₁₁ H ₁₂ N ₂ O ₃ | 56-69-9 | 220.08 | -0.00042 |
| 19 | 2-Morpholinoacetic acid | C ₆ H ₁₁ NO ₃ | 3235-69-6 | 145.07 | -0.00027 |
| 20 | N-tert-Butoxycarbonyl-DL-proline | C ₁₀ H ₁₇ NO ₄ | 59433-50-0 | 215.12 | -0.00021 |
| 21 | N-Ethoxycarbonyl-L-proline | C ₈ H ₁₃ NO ₄ | 5700-74-3 | 187.08 | 0.00018 |
| 22 | Hydroginkgolic acid | C ₂₂ H ₃₆ O ₃ | 16611-84-0 | 348.27 | -0.00068 |
| 23 | Uracil | C ₄ H ₄ N ₂ O ₂ | 66-22-8 | 112.03 | -0.00023 |
| 24 | trans-Zeatin | C ₁₀ H ₁₃ N ₅ O | 1637-39-4 | 219.11 | -0.00025 |
| 25 | 4-Amino-5-hydroxymethyl-2-methylpyrimidine | C ₆ H ₉ N ₃ O | 73-67-6 | 139.07 | -0.00018 |
| 26 | Thymine | C ₅ H ₆ N ₂ O ₂ | 65-71-4 | 126.04 | -0.00019 |
| 27 | Xanthine | C ₅ H ₄ N ₄ O ₂ | 69-89-6 | 152.03 | -0.00010 |
| 28 | Purine | C ₅ H ₄ N ₄ | 120-73-0 | 120.04 | -0.00018 |
| 29 | N6-Methyladenosine | C ₁₁ H ₁₅ N ₅ O ₄ | 1867-73-8 | 281.11 | -0.00061 |
| 30 | N,N-Dimethyladenine | C ₇ H ₉ N ₅ | 938-55-6 | 163.09 | -0.00014 |
| 31 | 1-Methylxanthine | C ₆ H ₆ N ₄ O ₂ | 6136-37-4 | 166.05 | -0.00028 |
| 32 | Hypoxanthine | C ₅ H ₄ N ₄ O | 68-94-0 | 136.04 | -0.00027 |
| 33 | Cytosine | C ₄ H ₅ N ₃ O | 71-30-7 | 111.04 | -0.00021 |
| 34 | 5'-Deoxy-5'-methylthioadenosine | C ₁₁ H ₁₅ N ₅ O ₃ S | 2457-80-9 | 297.09 | -0.00050 |
| 35 | Adenine | C ₅ H ₅ N ₅ | 73-24-5 | 135.05 | -0.00031 |
| 36 | 9-(2-Hydroxypropyl)adenine | C ₈ H ₁₁ N ₅ O | 14047-26-8 | 193.10 | -0.00021 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|----|-------------------------------------|---|------------|-----------------------|-----------------------|
| 37 | 8-Hydroxyguanine | C ₅ H ₅ N ₅ O ₂ | 5614-64-2 | 167.04 | -0.00016 |
| 38 | 6-O-Methylguanine | C ₆ H ₇ N ₅ O | 20535-83-5 | 165.06 | -0.00012 |
| 39 | 5-Methylcytosine | C ₅ H ₇ N ₃ O | 554-01-8 | 125.06 | -0.00016 |
| 40 | 3-Methyladenine | C ₆ H ₇ N ₅ | 5142-23-4 | 149.07 | -0.00017 |
| 41 | N9-Hydroxyethyladenine | C ₇ H ₉ N ₅ O | 707-99-3 | 179.08 | -0.00032 |
| 42 | 2'-Deoxyadenosine | C ₁₀ H ₁₃ N ₅ O ₃ | 958-09-8 | 251.10 | -0.00040 |
| 43 | 3,4,5,7,3',4',5'-Heptahydroxyflavan | C ₁₅ H ₁₄ O ₈ | 491-52-1 | 322.07 | -0.00048 |
| 44 | Quercitrin | C ₂₁ H ₂₀ O ₁₁ | 522-12-3 | 448.10 | -0.00081 |
| 45 | Kaempferol | C ₁₅ H ₁₀ O ₆ | 520-18-3 | 286.05 | -0.00063 |
| 46 | 3',4',5,7-Tetrahydroxyflavanone | C ₁₅ H ₁₂ O ₆ | 4049-38-1 | 288.06 | -0.00063 |
| 47 | (+)-Catechin | C ₁₅ H ₁₄ O ₆ | 154-23-4 | 290.08 | -0.00062 |
| 48 | (+)-Procyanidin B2 | C ₃₀ H ₂₆ O ₁₂ | 29106-49-8 | 578.14 | -0.00053 |
| 49 | N,N-Diethyl-4-nitroaniline | C ₁₀ H ₁₄ N ₂ O ₂ | 2216-15-1 | 194.11 | -0.00009 |
| 50 | Vanillin | C ₈ H ₈ O ₃ | 121-33-5 | 152.05 | -0.00016 |
| 51 | L-Valinol | C ₅ H ₁₃ NO | 2026-48-4 | 103.10 | -0.00029 |
| 52 | Methyl propiolate | C ₄ H ₄ O ₂ | 922-67-8 | 84.02 | -0.00019 |
| 53 | Trimethylamine N-oxide | C ₃ H ₉ NO | 1184-78-7 | 75.07 | -0.00008 |
| 54 | 2,2,6,6-Tetramethyl-4-piperidinone | C ₉ H ₁₇ NO | 826-36-8 | 155.13 | -0.00013 |
| 55 | 1-Methylpiperazine | C ₅ H ₁₂ N ₂ | 109-01-3 | 100.10 | -0.00012 |
| 56 | Ethyl piperazine-1-carboxylate | C ₇ H ₁₄ N ₂ O ₂ | 120-43-4 | 158.11 | -0.00012 |
| 57 | Thiodiglycol | C ₄ H ₁₀ O ₂ S | 111-48-8 | 122.04 | -0.00019 |
| 58 | Tetralin | C ₁₀ H ₁₂ | 119-64-2 | 132.09 | -0.00016 |
| 59 | Tetraethylene glycol dimethyl ether | C ₁₀ H ₂₂ O ₅ | 143-24-8 | 222.15 | -0.00026 |
| 60 | N-Boc-N-methyl-aminoethanol | C ₈ H ₁₇ NO ₃ | 57561-39-4 | 175.12 | -0.00019 |
| 61 | 4-Methyl-5-thiazoleethanol | C ₆ H ₉ NOS | 137-00-8 | 143.04 | -0.00014 |
| 62 | Succinimide | C ₄ H ₅ NO ₂ | 123-56-8 | 99.03 | -0.00015 |
| 63 | 4-Acetoxytyrene | C ₁₀ H ₁₀ O ₂ | 2628-16-2 | 162.07 | -0.00030 |
| 64 | Pentaethylene glycol | C ₁₀ H ₂₂ O ₆ | 4792-15-8 | 238.14 | -0.00039 |
| 65 | Tetraethylene glycol | C ₈ H ₁₈ O ₅ | 112-60-7 | 194.12 | -0.00024 |
| 66 | p-Anisoin | C ₁₆ H ₁₆ O ₄ | 119-52-8 | 272.10 | -0.00059 |
| 67 | Octylamine | C ₈ H ₁₉ N | 111-86-4 | 129.15 | -0.00012 |
| 68 | Octinoxate | C ₁₈ H ₂₆ O ₃ | 5466-77-3 | 290.19 | -0.00076 |
| 69 | 3-Acetyldindole | C ₁₀ H ₉ NO | 703-80-0 | 159.07 | -0.00016 |
| 70 | N-Nitropyrrolidine | C ₄ H ₈ N ₂ O | 930-55-2 | 100.06 | -0.00019 |
| 71 | N-Isopropylacrylamide | C ₆ H ₁₁ NO | 2210-25-5 | 113.08 | -0.00029 |
| 72 | Decylamine | C ₁₀ H ₂₃ N | 2016-57-1 | 157.18 | -0.00005 |
| 73 | N-Methylhomoveratrylamine | C ₁₁ H ₁₇ NO ₂ | 3490-06-0 | 195.13 | -0.00012 |
| 74 | N,N-Dimethylacetamide | C ₄ H ₉ NO | 127-19-5 | 87.07 | -0.00011 |
| 75 | N,N-Dibutylethanolamine | C ₁₀ H ₂₃ NO | 102-81-8 | 173.18 | -0.00017 |
| 76 | N-Lauryldiethanolamine | C ₁₆ H ₃₅ NO ₂ | 1541-67-9 | 273.27 | -0.00061 |
| 77 | Methyl ricinoleate | C ₁₉ H ₃₆ O ₃ | 141-24-2 | 312.27 | -0.00063 |
| 78 | Methyl | C ₂₁ H ₄₃ NO ₂ | 56817-90-4 | 341.33 | -0.00062 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|--|------------|-----------------------|-----------------------|
| | 6-(dimethylamino)octadecanoate | | | | |
| 79 | Piperidine-2,6-dione | C ₅ H ₇ NO ₂ | 1121-89-7 | 113.05 | -0.00010 |
| 80 | Laurylamine | C ₁₂ H ₂₇ N | 124-22-1 | 185.21 | -0.00018 |
| 81 | Laurophenone | C ₁₈ H ₂₈ O | 1674-38-0 | 260.21 | -0.00038 |
| 82 | Lauramide | C ₁₂ H ₂₅ NO | 1120-16-7 | 199.19 | -0.00031 |
| 83 | 4-Piperidinecarboxamide | C ₆ H ₁₂ N ₂ O | 39546-32-2 | 128.09 | -0.00019 |
| 84 | Indole | C ₈ H ₇ N | 120-72-9 | 117.06 | -0.00021 |
| 85 | Heptaethylene Glycol | C ₁₄ H ₃₀ O ₈ | 5617-32-3 | 326.19 | -0.00052 |
| 86 | 1-Methylcyclohexanol | C ₈ H ₁₂ O | 590-67-0 | 124.09 | -0.00019 |
| 87 | 2-Hydroxyquinoline | C ₉ H ₇ NO | 59-31-4 | 145.05 | -0.00015 |
| | Ethyl | | | | |
| 88 | 4-hydroxy-2-methylpyrimidine-5-carboxylate | C ₈ H ₁₀ N ₂ O ₃ | 53135-24-3 | 182.07 | -0.00046 |
| 89 | Ethyl 2-oxocyclohexanecarboxylate | C ₉ H ₁₄ O ₃ | 1655-07-8 | 170.09 | -0.00031 |
| 90 | Ethyl 2-(hydroxyimino)-3-oxobutanoate | C ₆ H ₉ NO ₄ | 5408-04-8 | 159.05 | -0.00018 |
| 91 | 2,6-Ditert-butyl-4-(hydroxymethyl)phenol | C ₁₅ H ₂₄ O ₂ | 88-26-6 | 236.18 | -0.00043 |
| 92 | N,N-Dimethylformamide | C ₃ H ₇ NO | 68-12-2 | 73.05 | -0.00011 |
| 93 | Dimethyl N-acetyl-L-aspartate | C ₈ H ₁₃ NO ₅ | 57289-64-2 | 203.08 | -0.00015 |
| 94 | Dimethyl 2-methylenesuccinate | C ₇ H ₁₀ O ₄ | 617-52-7 | 158.06 | -0.00012 |
| 95 | Diisopropyl sulfite | C ₆ H ₁₄ O ₃ S | 4773-13-1 | 166.07 | -0.00009 |
| | Diethyl | | | | |
| 96 | 4-oxo-4H-quinolizine-1,3-dicarboxylate | C ₁₅ H ₁₅ NO ₅ | 54401-76-2 | 289.09 | -0.00068 |
| 97 | Dielaoidylphosphatidylcholine | C ₄₄ H ₈₄ NO ₈ P | 52088-89-8 | 785.59 | -0.00342 |
| 98 | Choline O-Sulfate | C ₅ H ₁₃ NO ₄ S | 4858-96-2 | 183.06 | -0.00031 |
| 99 | Caprylic diethanolamide | C ₁₂ H ₂₅ NO ₃ | 3077-30-3 | 231.18 | -0.00038 |
| 100 | Butyl Sulfite | C ₈ H ₁₈ O ₃ S | 626-85-7 | 194.10 | -0.00056 |
| 101 | Butyl cyclohexyl phthalate | C ₁₈ H ₂₄ O ₄ | 84-64-0 | 304.17 | -0.00064 |
| 102 | Butoxytriglycol | C ₁₀ H ₂₂ O ₄ | 143-22-6 | 206.15 | -0.00018 |
| 103 | Ethyl benzoylacetate | C ₁₁ H ₁₂ O ₃ | 94-02-0 | 192.08 | -0.00021 |
| 104 | Acetophenone | C ₈ H ₈ O | 98-86-2 | 120.06 | -0.00023 |
| 105 | 4-Heptyloxyphenol | C ₁₃ H ₂₀ O ₂ | 13037-86-0 | 208.15 | -0.00030 |
| 106 | 6-Hydroxymethyl-7,8-dihydropterin | C ₇ H ₉ N ₅ O ₂ | 3672-03-5 | 195.08 | -0.00003 |
| 107 | 6,7-Dimethylpterin | C ₈ H ₉ N ₅ O | 611-55-2 | 191.08 | -0.00020 |
| 108 | 5-Hydroxyindole | C ₈ H ₇ NO | 1953-54-4 | 133.05 | -0.00004 |
| 109 | 5-(4-Methoxyphenyl)-1,3-cyclohexanedione | C ₁₃ H ₁₄ O ₃ | 1774-12-5 | 218.09 | -0.00054 |
| 110 | 4-Vinylpyridine | C ₇ H ₇ N | 100-43-6 | 105.06 | -0.00016 |
| 111 | 4-Nitroaniline | C ₆ H ₆ N ₂ O ₂ | 100-01-6 | 138.04 | -0.00017 |
| 112 | p-Anisidine | C ₇ H ₉ NO | 104-94-9 | 123.07 | 0.00008 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|---|---------------------------|-----------------------|-----------------------|
| 113 | 4-Aminophenol | C ₆ H ₇ NO | 123-30-8 | 109.05 | -0.00014 |
| 114 | 4,6-Di-tert-butylpyrogallol | C ₁₄ H ₂₂ O ₃ | 3934-77-8 | 238.16 | -0.00043 |
| 115 | 3-Methyl-5-pyrazolone | C ₄ H ₆ N ₂ O | 108-26-9 | 98.05 | -0.00013 |
| 116 | 5-Methyl-3,4-dihydropyrazole-2-carboxamide | C ₅ H ₉ N ₃ O | 17014-30-1 | 127.07 | -0.00023 |
| 117 | 3-Ethyl-o-xylene | C ₁₀ H ₁₄ | 933-98-2 | 134.11 | -0.00022 |
| 118 | 2-tert-Butyl-4-methoxyphenol | C ₁₁ H ₁₆ O ₂ | 121-00-6 | 180.11 | -0.00025 |
| 119 | 3-Amino-benzamide | C ₇ H ₈ N ₂ O | 3544-24-9 | 136.06 | -0.00011 |
| 120 | 3-Hydroxyundecanoyl carnitine | C ₁₈ H ₃₅ NO ₅ | ChemSpider ID 59664326 | 345.25 | -0.00071 |
| 121 | 3,5-Ditert-butyl-4-hydroxybenzonitrile | C ₁₅ H ₂₁ NO | 1988-88-1 | 231.16 | -0.00048 |
| 122 | 3,5-Ditert-butyl-4-hydroxybenzaldehyde | C ₁₅ H ₂₂ O ₂ | 1620-98-0 | 234.16 | -0.00053 |
| 123 | 3,5-Dimethoxybenzohydrazide | C ₉ H ₁₂ N ₂ O ₃ | 51707-38-1 | 196.08 | -0.00060 |
| 124 | 3,5-Ditert-butyl-4-hydroxyacetophenone | C ₁₆ H ₂₄ O ₂ | 14035-33-7 | 248.18 | -0.00038 |
| 125 | 2-Pyrrolidone | C ₄ H ₇ NO | 616-45-5 | 85.05 | -0.00014 |
| 126 | 2-Morpholinoacetonitrile | C ₆ H ₁₀ N ₂ O | 5807-02-3 | 126.08 | -0.00019 |
| 127 | 2-Methoxy-5-nitrophenol | C ₇ H ₇ NO ₄ | 636-93-1 | 169.04 | -0.00023 |
| 128 | 2-Amino-1-(piperidin-1-yl)propan-1-one | C ₈ H ₁₆ N ₂ O | 805974-19-0 | 156.13 | -0.00013 |
| 129 | 2-Amino-1,3,4-octadecanetriol | C ₁₈ H ₃₉ NO ₃ | 13552-11-9 | 317.29 | -0.00052 |
| 130 | N-Methylmoranoline | C ₇ H ₁₅ NO ₄ | 69567-10-8 | 177.10 | -0.00010 |
| 131 | 2,4,6-Triaminotoluene | C ₇ H ₁₁ N ₃ | 88-02-8 | 137.10 | -0.00013 |
| 132 | 1-Vinyl-2-pyrrolidone | C ₆ H ₉ NO | 88-12-0 | 111.07 | -0.00023 |
| 133 | 1-Methyl-4-nitrosopiperazine | C ₅ H ₁₁ N ₃ O | 16339-07-4 | 129.09 | -0.00017 |
| 134 | 4-Amino-1-carbethoxypiperidine | C ₈ H ₁₆ N ₂ O ₂ | 58859-46-4 | 172.12 | -0.00019 |
| 135 | 1-Boc-piperazine | C ₉ H ₁₈ N ₂ O ₂ | 57260-71-6 | 186.14 | -0.00030 |
| 136 | 1-Boc-3-piperidinol | C ₁₀ H ₁₉ NO ₃ | 85275-45-2 | 201.14 | -0.00026 |
| 137 | 1,8,15,22-Tetraazacyclooctacosane-2,9,16,23-tetrone | C ₂₄ H ₄₄ N ₄ O ₄ | 5834-63-9 | 452.34 | -0.00103 |
| 138 | 1,6-Hexanediol diacrylate | C ₁₂ H ₁₈ O ₄ | 13048-33-4 | 226.12 | -0.00048 |
| 139 | 1,3,5-Norcaratriene | C ₇ H ₆ | 4646-69-9 | 90.05 | -0.00017 |
| 140 | 1,1-Bis(morpholino)ethylene | C ₁₀ H ₁₈ N ₂ O ₂ | 14212-87-4 | 198.14 | -0.00020 |
| 141 | Diisopropyl diazene-1,2-dicarboxylate | C ₈ H ₁₄ N ₂ O ₄ | 2446-83-5 | 202.10 | -0.00015 |
| 142 | Yomogiartemin | C ₁₇ H ₂₀ O ₇ | 69684-72-6 | 336.12 | -0.00059 |
| 143 | Pyridoxal | C ₈ H ₉ NO ₃ | 66-72-8 | 167.06 | -0.00021 |
| 144 | (+)-Riboflavin | C ₁₇ H ₂₀ N ₄ O ₆ | 83-88-5 | 376.14 | -0.00072 |
| 145 | Niacin | C ₆ H ₅ NO ₂ | 59-67-6 | 123.03 | -0.00008 |
| 146 | Nicotinamide | C ₆ H ₆ N ₂ O | 98-92-0 | 122.05 | -0.00024 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|--|---|----------------------|-----------------------|-----------------------|
| 147 | Dopamine | C ₈ H ₁₁ NO ₂ | 51-61-6 | 153.08 | -0.00019 |
| 148 | Theophylline | C ₇ H ₈ N ₄ O ₂ | 58-55-9 | 180.06 | -0.00034 |
| 149 | Terminaline | C ₂₃ H ₄₁ NO ₂ | 15112-49-9 | 363.31 | -0.00080 |
| 150 | 4-Butyrobetaine | C ₇ H ₁₅ NO ₂ | ChemSpider ID 705 | 145.11 | -0.00025 |
| 151 | Oxyphylline | C ₉ H ₁₂ N ₄ O ₃ | 519-37-9 | 224.09 | -0.00027 |
| 152 | Caffeine | C ₈ H ₁₀ N ₄ O ₂ | 58-08-2 | 194.08 | -0.00034 |
| 153 | Arecoline | C ₈ H ₁₃ NO ₂ | 63-75-2 | 155.09 | -0.00015 |
| 154 | Sorbic acid | C ₆ H ₈ O ₂ | 110-44-1 | 112.05 | -0.00018 |
| 155 | Quinolinic acid | C ₇ H ₅ NO ₄ | 89-00-9 | 167.02 | -0.00014 |
| 156 | Pheophorbide A | C ₃₅ H ₃₆ N ₄ O ₅ | 15664-29-6 | 592.27 | -0.00134 |
| 157 | 4-Hexyloxybenzoic acid | C ₁₃ H ₁₈ O ₃ | 1142-39-8 | 222.13 | -0.00040 |
| 158 | Oxamide | C ₂ H ₄ N ₂ O ₂ | 471-46-5 | 88.03 | -0.00011 |
| 159 | Indole-3-acetic acid | C ₁₀ H ₉ NO ₂ | 87-51-4 | 175.06 | -0.00019 |
| 160 | gamma-Aminobutyric acid | C ₄ H ₉ NO ₂ | 56-12-2 | 103.06 | -0.00015 |
| 161 | Boc-GABA | C ₉ H ₁₇ NO ₄ | 57294-38-9 | 203.12 | -0.00023 |
| 162 | Guvacine | C ₆ H ₉ NO ₂ | 498-96-4 | 127.06 | -0.00025 |
| 163 | Gibberellin A7 | C ₁₉ H ₂₂ O ₅ | 510-75-8 | 330.15 | -0.00068 |
| 164 | Alantolactone | C ₁₅ H ₂₀ O ₂ | 546-43-0 | 232.15 | -0.00054 |
| 165 | Coumarin | C ₉ H ₆ O ₂ | 91-64-5 | 146.04 | -0.00016 |
| 166 | Butyl levulinate | C ₉ H ₁₆ O ₃ | 2052-15-5 | 172.11 | -0.00023 |
| 167 | Benzyl formate | C ₈ H ₈ O ₂ | 104-57-4 | 136.05 | -0.00017 |
| 168 | D-Pantothenic acid | C ₉ H ₁₇ NO ₅ | 79-83-4 | 219.11 | -0.00024 |
| 169 | Chrysanthemic acid | C ₁₀ H ₁₆ O ₂ | 10453-89-1 | 168.11 | -0.00027 |
| 170 | Aminolevulinic acid | C ₅ H ₉ NO ₃ | 106-60-5 | 131.06 | -0.00008 |
| 171 | 1-Aminocyclopropanecarboxylic acid | C ₄ H ₇ NO ₂ | 22059-21-8 | 101.05 | -0.00017 |
| 172 | 4-Aminobenzoic acid | C ₇ H ₇ NO ₂ | 150-13-0 | 137.05 | -0.00012 |
| 173 | 3-Methylglutaryl carnitine | C ₁₃ H ₂₃ NO ₆ | 102673-95-0 | 289.15 | 0.00079 |
| 174 | Dibutyl sebacate | C ₁₈ H ₃₄ O ₄ | 109-43-3 | 314.25 | -0.00036 |
| 175 | 1-Acetoxy-2-hydroxy-16-heptadecy n-4-one | C ₁₉ H ₃₂ O ₄ | 24607-10-1 | 324.23 | -0.00063 |
| 176 | (E)-12-Oxo-10-dodecanoic acid | C ₁₂ H ₂₀ O ₃ | 65410-38-0 | 212.14 | -0.00037 |
| 177 | Tetrahydrodeoxycorticosterone | C ₂₁ H ₃₄ O ₃ | 567-02-2 | 334.25 | -0.00071 |
| 178 | Soyacerebroside I | C ₄₀ H ₇₅ NO ₉ | 114297-20-0 | 713.54 | -0.00154 |
| 179 | Ricinelaic acid | C ₁₈ H ₃₄ O ₃ | 540-12-5 | 298.25 | -0.00050 |
| 180 | Methyl 2-octynoate | C ₉ H ₁₄ O ₂ | 111-12-6 | 154.10 | -0.00042 |
| 181 | 1-alpha-Linolenoyl-2-linoleoyl-phosphatidylcholine | C ₄₄ H ₇₈ NO ₈ P | 8002-43-5 | 779.54 | -0.00153 |
| 182 | L-alpha-1-Palmitoyl-2-linoleoylphosphatidylcholine | C ₄₂ H ₈₀ NO ₈ P | 17708-90-6 | 757.56 | -0.00076 |
| 183 | Palmitoyl alanine | C ₁₉ H ₃₇ NO ₃ | 56255-31-3 | 327.28 | -0.00093 |

| NO | Name | Formula | CAS | Molecular Weight (Da) | Annot.Delta Mass (Da) |
|-----|---|--|---------------------------|-----------------------|-----------------------|
| 184 | 1-alpha-Linolenoylglycerol | C ₂₁ H ₃₆ O ₄ | 18465-99-1 | 352.26 | -0.00072 |
| 185 | Linolenelaidic acid | C ₁₈ H ₃₀ O ₂ | 28290-79-1 | 278.22 | -0.00048 |
| 186 | L-alpha-Palmitin | C ₁₉ H ₃₈ O ₄ | 32899-41-5 | 330.28 | -0.00083 |
| 187 | Embelin | C ₁₇ H ₂₆ O ₄ | 550-24-3 | 294.18 | -0.00043 |
| 188 | 10-Nitrooleic acid | C ₁₈ H ₃₃ NO ₄ | 88127-53-1 | 327.24 | -0.00074 |
| 189 | Biacetyl | C ₄ H ₆ O ₂ | 431-03-8 | 86.04 | -0.00010 |
| 190 | Adipamide | C ₆ H ₁₂ N ₂ O ₂ | 628-94-4 | 144.09 | -0.00013 |
| 191 | A-12(13)-EpODE | C ₁₈ H ₃₀ O ₃ | ChemSpider ID 17220744 | 294.22 | -0.00065 |
| 192 | 2-Hexenoylcarnitine | C ₁₃ H ₂₃ NO ₄ | 99452-58-1 | 257.16 | -0.00054 |
| 193 | 13-Hydroxyoctadecadienoic acid | C ₁₈ H ₃₂ O ₃ | 29623-28-7 | 296.23 | -0.00068 |
| 194 | 13(S)-Hydroperoxylinoleic acid | C ₁₈ H ₃₂ O ₄ | 33964-75-9 | 312.23 | -0.00075 |
| 195 | 13(S)-HpOTrE;13-Hydroperoxy-9,11E,15Z-octadecatrienoic acid | C ₁₈ H ₃₀ O ₄ | ChemSpider ID 4445993 | 310.21 | -0.00072 |
| 196 | 12-Oxo phytodienoic acid | C ₁₈ H ₂₈ O ₃ | 85551-10-6 | 292.20 | -0.00066 |
| 197 | 12-Aminolauric Acid | C ₁₂ H ₂₅ NO ₂ | 693-57-2 | 215.19 | -0.00026 |
| 198 | 10-Gingerol | C ₂₁ H ₃₄ O ₄ | 23513-15-7 | 350.25 | -0.00059 |
| 199 | PC(16:0/18:3(6Z,9Z,12Z)) | C ₄₂ H ₇₈ NO ₈ P | 203393-39-9 | 755.55 | -0.00039 |
| 200 | PC(18:1(9Z)/18:2(9Z,12Z)) | C ₄₄ H ₈₂ NO ₈ P | 17041-44-0 | 783.57 | -0.00381 |
| 201 | PE(18:2(9Z,12Z)/0:0) | C ₂₃ H ₄₄ NO ₇ P | 85046-18-0 | 477.28 | -0.00079 |
| 202 | PE(16:0/20:4) | C ₄₁ H ₇₄ NO ₈ P | 70812-59-8 | 739.51 | -0.00149 |
| 203 | PE(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)) | C ₄₁ H ₇₂ NO ₈ P | ChemSpider ID 24768558 | 737.50 | -0.00123 |
| 204 | (10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid | C ₁₈ H ₃₂ O ₅ | 95341-44-9 | 328.22 | -0.00060 |
| 205 | N-Undecanoylglycine | C ₁₃ H ₂₅ NO ₃ | 83871-09-4 | 243.18 | -0.00025 |
| 206 | 7-epi-JasmonicAcid | C ₁₂ H ₁₈ O ₃ | 62653-85-4 | 210.13 | -0.00028 |

Note: Annot. Delta Mass represents the difference between the actual measured value of molecular weight and the theoretical value.

Table S4-1. Load matrix of principal components (C18 column, ESI+).

| Name | Principal component | |
|--|---------------------|--------|
| | 1 | 2 |
| Pipecolic acid | 9.151 | -0.521 |
| L-Norleucine | 2.297 | 2.304 |
| N,N-Diethylglycine | 0.688 | -0.821 |
| Allysine | -0.257 | -0.641 |
| Ethyl methioninate | -0.336 | 0.705 |
| L-alpha-Glutamyl-L-hydroxyproline | -0.454 | 0.246 |
| Cianidanol | -0.224 | 1.095 |
| Quercetin | -0.660 | 0.315 |
| Myricetin | -0.822 | -0.198 |
| 6-Methoxyquercetin | -0.762 | 0.038 |
| ECG | -0.316 | 2.546 |
| EGCG | -0.237 | 3.102 |
| 3,4-Dihydroxybenzaldehyde | -0.201 | 2.642 |
| Protocatechuic acid | -0.467 | -0.637 |
| 3,4-Dihydroxyphenylacetic acid | -0.725 | 0.185 |
| Gallic acid | -0.779 | -0.035 |
| Phloretin | -0.448 | -0.417 |
| 12-OPDA | -0.622 | -0.616 |
| 9-KODE | -0.700 | -0.598 |
| 9-Oxo-ODE | -0.785 | -0.594 |
| 9-J1-Phytostane | -0.836 | -0.590 |
| Linoleoyl ethanolamide | -0.646 | -0.612 |
| PC(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z)) | -0.550 | -0.488 |
| Guanine | 3.365 | -0.315 |
| 1-Methylxanthine | -0.429 | -0.591 |
| 2'-Deoxyadenosine | -0.500 | -0.601 |
| Guanosine | 1.858 | -0.384 |
| 5'-S-Methyl-5'-thioadenosine | -0.388 | 0.537 |
| (2S)-2-Amino-4-hexynoic acid | -0.433 | -0.624 |
| (E)-8-Hydroxy-2-octene-4,6-dienoic acid | -0.806 | -0.113 |
| 2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate | -0.745 | -0.561 |
| N-Succinyl-L,L-2,6-diaminopimelate | -0.731 | -0.422 |
| Luteic acid | -0.773 | 0.075 |
| Stachydrine | 0.443 | -0.729 |
| Methyl gallate | -0.666 | 0.069 |
| Ellagic acid | -0.828 | -0.334 |
| Procyanidin B2 | -0.830 | -0.348 |
| 4-Hydroxycoumarin | -0.464 | -0.652 |
| 1-Vinyl-2-pyrrolidone | 0.568 | -0.744 |
| N-Acetylpyrrolidine | -0.317 | -0.665 |
| 4-Hydroxybenzaldehyde | -0.397 | 2.073 |

| Name | Principal component | |
|--------------------------------|---------------------|--------|
| | 1 | 2 |
| 2-Hydroxy-1,4-benzoquinone | -0.509 | -0.447 |
| 5-Formylsalicylaldehyde | -0.747 | 0.123 |
| 3,4-Dihydroxymandelaldehyde | -0.785 | -0.551 |
| Allyl salicylate | -0.780 | -0.569 |
| Rhamnopterin | 1.181 | 0.105 |
| Di-2-pentanyl malate | -0.585 | -0.513 |
| Pheophorbide A | 2.988 | -0.230 |
| Initial eigenvalue | 2.770 | 0.946 |
| Variance contribution rate (%) | 69.243 | 23.650 |

Table S4-2. Load matrix of principal components (C18 column, ESI-).

| Name | Principal component | |
|---|---------------------|--------|
| | 1 | 2 |
| L-Theanine | 10.433 | -1.369 |
| Methyl gallate | 0.839 | 1.193 |
| Ellagic acid | 0.114 | 0.473 |
| Gallic acid | -0.724 | 0.039 |
| Digallic acid | -0.585 | -0.206 |
| (-)-Epigallocatechin gallate | -0.142 | 1.215 |
| (-)-Epiafzelechin 3-O-gallate | -0.709 | 0.084 |
| (-)-Epicatechin gallate | 0.337 | 2.069 |
| Salicylic acid | 0.831 | 1.186 |
| Protocatechuic acid | 0.346 | -0.885 |
| 3,4-Dihydroxyphenylacetic acid | -0.677 | -0.154 |
| Theaflavic acid | -0.714 | -0.131 |
| 4-Hydroxycinnamic acid | 0.647 | -0.522 |
| Theogallin | -0.083 | 0.677 |
| 3',4',5,7-Tetrahydroxyflavanone | -0.651 | -0.088 |
| Cianidanol | 4.212 | 1.209 |
| 2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-3,6,8-trimethoxy-4H-chromen-4-one | -0.736 | 0.027 |
| 3,4,5,7,3',4',5'-Heptahydroxyflavan | 0.472 | -0.737 |
| Phloretin | -0.577 | -0.188 |
| Gossypin | -0.732 | 0.039 |
| Dihydromyricetin | -0.708 | -0.112 |
| 4-Methyl-6,7-diacetoxycoumarin | -0.462 | -0.265 |
| Trimethyl 4-hydroxy-5-methyl-1,2,3-benzenetricarboxylate | -0.001 | -0.229 |
| Lauric anhydride | -0.687 | -0.069 |
| Bis(2-butoxyethyl) adipate | -0.114 | -0.024 |
| 6-Acetyl-4,5,7,8-tetrahydroxynaphthalene-1,2-dione | 0.114 | -0.825 |
| 2-Hydroxy-6-ketononadienedioic acid | -0.527 | -0.220 |
| 2-Acetoxy-3-[3-(4-hydroxy-phenyl)-acryloyloxy]-succinic acid | -0.734 | -0.108 |
| '-Acetoxychavicol acetate | -0.680 | -0.146 |
| 1,2,3,4,5,6-Heptanehexayl hexaacetate | -0.710 | -0.034 |
| Hydroquinone | -0.481 | -0.278 |
| Benzyl beta-primeveroside | -0.689 | -0.023 |
| Apiin | -0.014 | -0.240 |
| 1,6-Di-O-galloyl-b-D-glucopyranose | -0.552 | 0.372 |
| 20(S)-Ginsenoside | -0.578 | -0.157 |
| Fukiic acid | -0.629 | -0.120 |
| 5,5'-Dehydrodivanillate | -0.669 | -0.077 |
| 2-Amino-4-pyrimidinecarboxylate | 0.399 | -0.407 |
| 2,5-Dihydroxyterephthalic acid | -0.035 | -0.432 |

| Name | Principal component | |
|---|---------------------|--------|
| | 1 | 2 |
| 12-oxo Phytodienoic Acid | -0.461 | -0.058 |
| pinellic acid | -0.371 | -0.058 |
| Phaseolic acid | -0.732 | -0.115 |
| 16-Hydroxyhexadecanoic acid | -0.523 | -0.042 |
| 13-Hydroxyoctadecadienoic acid | -0.510 | -0.070 |
| 13(S)-Hydroperoxylinolenic acid | -0.335 | -0.082 |
| 12-Hydroxyoctadecanoic acid | -0.718 | -0.071 |
| (10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid | -0.497 | -0.040 |
| Initial eigenvalue | 3.083 | 0.716 |
| Variance contribution rate (%) | 77.069 | 17.907 |

Table S4-3. Load matrix of principal components (Hilic column, ESI+).

| Name | Principal component | |
|------------------------------------|---------------------|--------|
| | 1 | 2 |
| L-Leucine | 1.739 | -0.540 |
| Homocycloleucine | -0.740 | 0.034 |
| Acetyl-L-proline | -0.796 | 0.041 |
| 2-Morpholinoacetic acid | -0.701 | 0.033 |
| N6-Methyladenosine | -0.750 | 0.044 |
| 1-Methylxanthine | -0.784 | 0.043 |
| Hypoxanthin | 0.562 | -0.260 |
| Cytosine | -0.496 | -0.022 |
| Adenine | 6.427 | -2.477 |
| Thiodiglycol | -0.764 | 0.046 |
| Octinoxate | -0.666 | 0.036 |
| N-Isopropylacrylamide | 0.225 | -0.196 |
| Laurophenone | -0.804 | 0.050 |
| Choline O-Sulfate | 1.469 | -0.689 |
| 1-Vinyl-2-pyrrolidone | -0.694 | 0.057 |
| 1,3,5-Norcaratriene | 5.186 | 3.353 |
| Niacin | -0.705 | 0.026 |
| Nicotinamide | -0.559 | 0.103 |
| Theophylline | -0.495 | 0.005 |
| 4-Butyrobetaine | -0.783 | 0.048 |
| Pheophorbide A | -0.503 | -0.097 |
| Boc-GABA | -0.787 | 0.048 |
| Guvacine | -0.702 | 0.033 |
| 1-Aminocyclopropanecarboxylic acid | -0.772 | 0.166 |
| 1-alpha-Linolenoylglycerol | -0.736 | 0.040 |
| Embelin | -0.762 | 0.029 |
| A-12(13)-EpODE | -0.339 | -0.007 |
| 13(S)-HpOTrE | -0.796 | 0.049 |
| 12-Oxo phytodienoic acid | -0.475 | 0.002 |
| Initial eigenvalue | 3.108 | 0.767 |
| Variance contribution rate (%) | 77.694 | 19.168 |