|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **Class I** | **Class II** | **Formula** | **Q1 (Da)** | **Q3 (Da)** | **Molecular weight (Da)** | **Ionization**  **model** | **JDS1** | **JDS2** | **JDS3** |
| 5-Methoxyfurfural\* | Others | Aldehyde compounds | C6H6O3 | 127.04 | 53.04 | 126.0317 | [M+H]+ | 36267595 | 35299932 | 35160594 |
| Diosmetin-7-O-Neohesperidoside (Neodiosmin)\* | Flavonoids | Flavones | C28H32O15 | 609.18 | 301.08 | 608.1741 | [M+H]+ | 32524972 | 32358014 | 36902643 |
| 2-(hydroxymethyl)pyridin-3-ol | Alkaloids | Alkaloids | C6H7NO2 | 126.06 | 108.05 | 125.0477 | [M+H]+ | 36329981 | 33472771 | 31616620 |
| Diosmetin 7-O-rutinoside | Flavonoids | Flavones | C28H32O15 | 609.18 | 301.08 | 608.1741 | [M+H]+ | 32522086 | 32168502 | 35477474 |
| Ethylparaben | Phenolic acids | Phenolic acids | C9H10O3 | 165.06 | 92.03 | 166.063 | [M-H]- | 35052713 | 29160722 | 35787807 |
| 5-Hydroxymethyl-2-furaldehyde\* | Others | Aldehyde compounds | C6H6O3 | 127.04 | 53.04 | 126.0317 | [M+H]+ | 33365271 | 32433830 | 32114945 |
| Chrysoeriol-7-O-rutinoside | Flavonoids | Flavones | C28H32O15 | 607.17 | 299.05 | 608.1741 | [M-H]- | 26309165 | 34176129 | 36015489 |
| Phloroglucinol | Others | Others | C6H6O3 | 127.04 | 81.03 | 126.0317 | [M+H]+ | 32283958 | 31984623 | 31640103 |
| Swertisin | Flavonoids | Flavones | C22H22O10 | 447.13 | 297.08 | 446.1213 | [M+H]+ | 27185537 | 27288233 | 35339638 |
| 5-hydroxymethylenefural\* | Others | Others | C6H6O3 | 127.04 | 53.04 | 126.0317 | [M+H]+ | 31409951 | 28974897 | 28810520 |
| Choline | Alkaloids | Alkaloids | C5H14NO+ | 104.11 | 60.08 | 104.107 | [M]+ | 28278989 | 27521974 | 27679419 |
| Kaempferide 3-rutinoside\* | Flavonoids | Flavonols | C28H32O15 | 609.18 | 301.07 | 608.1741 | [M+H]+ | 23986921 | 22796460 | 35773096 |
| Acacetin-7-O-rutinoside (Linarin)\* | Flavonoids | Flavones | C28H32O14 | 593.19 | 285.08 | 592.1792 | [M+H]+ | 26452144 | 22435014 | 31940978 |
| 7-Methoxy-3-[1-(3-pyridyl)methylidene]-4-chromanone | Flavonoids | Other Flavonoids | C16H13NO3 | 268.1 | 136.06 | 267.0895 | [M+H]+ | 24360796 | 25230773 | 26692720 |
| Peonidin-3-O-(6''-O-p-coumaroyl)glucoside | Flavonoids | Anthocyanidins | C31H29O13+ | 609.16 | 301.07 | 609.1603 | [M]+ | 23855657 | 18004875 | 27077349 |
| 4-amino-2-methylbutanoic acid\* | Alkaloids | Alkaloids | C5H11NO2 | 118.09 | 58.07 | 117.079 | [M+H]+ | 22304182 | 21336466 | 21119946 |
| Zarzissine | Alkaloids | Alkaloids | C5H5N5 | 136.06 | 119.04 | 135.0545 | [M+H]+ | 22907584 | 18949016 | 22246549 |
| Betaine\* | Alkaloids | Alkaloids | C5H11NO2 | 118.09 | 58.07 | 117.079 | [M+H]+ | 22228385 | 20381392 | 21364825 |
| 2-Decanol\* | Others | Alcohol compounds | C10H22O | 157.16 | 157.16 | 158.1671 | [M-H]- | 20564441 | 21224592 | 21636332 |
| 6α,10α-Dihydroxy-1-oxoeremophila-7(11),8(9)-dien-12,8-olide | Terpenoids | Sesquiterpenoids | C15H18O5 | 279.12 | 149.02 | 278.1149 | [M+H]+ | 20883591 | 18954859 | 19591552 |
| 3-Hydrocinnamyl-6-CinnamylGlucose | Others | Alcohol compounds | C24H30O6 | 415.21 | 119.09 | 414.2042 | [M+H]+ | 16349112 | 29917806 | 12936997 |
| 2,5-O-Di-CinnamylSorbitol | Phenolic acids | Phenolic acids | C24H30O6 | 415.21 | 119.09 | 414.2042 | [M+H]+ | 17901629 | 28273491 | 11891717 |
| 4'-Demethyleucomin glucosyl rhamnoside\* | Flavonoids | Other Flavonoids | C28H32O14 | 593.18 | 285.08 | 592.1792 | [M+H]+ | 18045712 | 16481609 | 22366638 |
| Lidocaine | Alkaloids | Alkaloids | C14H22N2O | 235.18 | 86.1 | 234.1732 | [M+H]+ | 18731872 | 19617289 | 17823836 |
| Acacetin-7-O-neohesperidoside\* | Flavonoids | Flavones | C28H32O14 | 593.19 | 285.08 | 592.1792 | [M+H]+ | 17402692 | 14853821 | 22304277 |
| 3-Chloroaniline | Alkaloids | Alkaloids | C6H6ClN | 128.03 | 93.06 | 127.0189 | [M+H]+ | 17084174 | 17099828 | 20313282 |
| 4-Hydroxybenzoate | Phenolic acids | Phenolic acids | C7H6O3 | 137.02 | 93.03 | 138.0317 | [M-H]- | 19458978 | 15523474 | 18795881 |
| Dibutyl phthalate | Phenolic acids | Phenolic acids | C16H22O4 | 279.16 | 149.02 | 278.1518 | [M+H]+ | 17819947 | 18720634 | 16930306 |
| Des-O-Methyllasiodiplodin | Others | Lactones | C16H22O4 | 279.16 | 149.03 | 278.1518 | [M+H]+ | 17996145 | 17414390 | 17792530 |
| 7-{[(2S,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-{[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}oxan-2-yl]oxy}-5-hydroxy-2-(4-methoxyphenyl)chromen-4-one\* | Flavonoids | Flavones | C28H32O14 | 593.19 | 285.08 | 592.1792 | [M+H]+ | 17189483 | 14262154 | 21478992 |
| triptobenzene D | Terpenoids | Ditepenoids | C20H26O2 | 297.18 | 297.18 | 298.1933 | [M-H]- | 18396096 | 13847323 | 17575344 |
| 2-Methylpyrrolidine-2-carboxylic acid | Alkaloids | Alkaloids | C6H11NO2 | 130.09 | 84.09 | 129.079 | [M+H]+ | 16547912 | 16172408 | 15608534 |
| 1-Decanol\* | Others | Alcohol compounds | C10H22O | 157.16 | 157.16 | 158.1671 | [M-H]- | 14764753 | 15441061 | 16413551 |
| 3,4-Dihydroxybenzaldehyde | Others | Aldehyde compounds | C7H6O3 | 137.02 | 93.04 | 138.0317 | [M-H]- | 15680772 | 14316842 | 16494649 |
| N-(3-hydroxy-4-methoxyphenethyl)-4-hydroxybutanamide | Alkaloids | Alkaloids | C14H21NO4 | 268.15 | 136.06 | 267.1471 | [M+H]+ | 15202246 | 14945783 | 15237357 |
| Lauryldiethanolamine | Others | Others | C16H35NO2 | 274.28 | 88.08 | 273.2668 | [M+H]+ | 14232286 | 13305054 | 13816417 |
| Chrysoeriol-6-C-rhamnoside-7-O-rhamnoside | Flavonoids | Flavones | C28H32O14 | 593.18 | 447.13 | 592.1792 | [M+H]+ | 13781142 | 9760379.2 | 14512549 |
| Phyllanthusiin E | Others | Others | C13H8O8 | 291.01 | 247.03 | 292.0214 | [M-H]- | 11812246 | 10635809 | 15140620 |
| 1,2,3,4-Tetrahydro-3-carboxy-2-carboline | Alkaloids | Alkaloids | C12H12N2O2 | 217.1 | 144.08 | 216.0899 | [M+H]+ | 12051354 | 11335894 | 14006184 |
| Norephedrin 3-O-(2''-Phenylpropanyl)Glucoside | Alkaloids | Phenolamine | C24H33NO6 | 432.24 | 119.09 | 431.2308 | [M+H]+ | 11219128 | 17125932 | 8220743.7 |
| 6-Demethoxy-4'-O-methylcapillarisin rhamnosyl glucoside | Others | Chromone | C28H32O15 | 607.16 | 299.06 | 608.1741 | [M-H]- | 11885772 | 10067873 | 14170398 |
| 8-(5-Hydroxy-2,6,6-Trimethylcyclohex-2-En-1-Yl)-6-Methyloct-5-En-2-one | Terpenoids | Sesquiterpenoids | C18H30O2 | 279.23 | 81.07 | 278.2246 | [M+H]+ | 13304099 | 8701393.4 | 12724689 |
| 9-hydroxy-8-{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-1H,3H-naphtho[2,3-c]furan-1-one | Others | Others | C18H18O9 | 377.09 | 341.11 | 378.0951 | [M-H]- | 11595587 | 10952868 | 11708653 |
| Tanaphillin | Terpenoids | Sesquiterpenoids | C15H18O5 | 279.12 | 149.02 | 278.1154 | [M+H]+ | 10910552 | 10889169 | 12213310 |
| 2,6-Dimethyl-7-octene-2,3,6-triol | Terpenoids | Monoterpenoids | C10H20O3 | 187.13 | 97.06 | 188.1412 | [M-H]- | 11149188 | 11447867 | 11389462 |
| 8,10-Diethyllobelionol | Alkaloids | Piperidine alkaloids | C14H27NO2 | 242.22 | 170.15 | 241.2042 | [M+H]+ | 11283203 | 10173765 | 10575193 |
| Sulfo jasmonate | Others | Others | C12H18O7S | 305.07 | 96.96 | 306.0773 | [M-H]- | 8658722 | 11472677 | 11350265 |
| 2-Piperidone | Alkaloids | Piperidine alkaloids | C5H9NO | 100.08 | 56.05 | 99.0684 | [M+H]+ | 10925922 | 10634282 | 9890080.8 |
| Inokosterone\* | Steroids | Steroid | C27H44O7 | 481.32 | 445.3 | 480.3087 | [M+H]+ | 9170516.7 | 10674071 | 11239035 |