Table 1. Differential fecal metabolites before and after a 12-week BBr60 intervention on serum metabolism

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **MS2 score** | **mz** | **type** | **Formula** | **HMDB** | **CAS** | **KEGG ID** | **MEAN BBr60-before** | **MEAN BBr60-after** | **VIP** | **P-VALUE** | **FOLD CHANGE** |
| EDTA | 3.99 | 293.098 | POS | C10H16N2O8 | HMDB0015109 | 62-33-9 | C00284 | 0.1459 | 22.2848 | 1.7273 | 0.0002 | 152.7790 |
| Asparagine | 3.99 | 133.0607 | POS | C4H8N2O3 | HMDB0000168 | 70-47-3 | C00152 | 0.0271 | 0.0472 | 1.2708 | 0.0002 | 1.7461 |
| 1,7-Dimethylxanthine | 3.99 | 179.0575 | NEG | C7H8N4O2 | HMDB0001860 | 611-59-6 | C13747 | 1.6303 | 1.0231 | 1.0869 | 0.0296 | 0.6276 |
| Theobromine | 3.98 | 179.0575 | NEG | C7H8N4O2 | HMDB0002825 | 83-67-0 | C07480 | 1.6303 | 1.0231 | 1.0869 | 0.0296 | 0.6276 |
| gamma-Glutamylglutamine | 3.98 | 276.119 | POS | C10H17N3O6 | HMDB0011738 | 10148-81-9 | C05283 | 0.0103 | 0.0411 | 1.6214 | 0.0000 | 3.9973 |
| Citrulline | 3.98 | 176.1029 | POS | C6H13N3O3 | HMDB0000904 | 372-75-8 | C00327 | 0.0800 | 0.1292 | 1.0126 | 0.0063 | 1.6157 |
| 4-Acetamidobutyric acid | 3.98 | 144.0667 | NEG | C6H11NO3 | HMDB0003681 | 3025-96-5 | C02946 | 0.0556 | 0.0452 | 1.0599 | 0.0207 | 0.8142 |
| Levulinic acid | 3.98 | 115.0401 | NEG | C5H8O3 | HMDB0000720 | 123-76-2 |  | 0.5218 | 0.3510 | 1.6908 | 0.0000 | 0.6726 |
| Serine | 3.98 | 106.0498 | POS | C3H7NO3 | HMDB0000187 | 56-45-1 | C00065 | 0.0172 | 0.0393 | 1.4500 | 0.0003 | 2.2894 |
| Theophylline | 3.97 | 179.0575 | NEG | C7H8N4O2 | HMDB0001889 | 58-55-9 | C07130 | 1.6303 | 1.0231 | 1.0869 | 0.0296 | 0.6276 |
| Glutamate | 3.97 | 148.0605 | POS | C5H9NO4 | HMDB0000148 | 56-86-0 | C00025 | 0.0616 | 0.1412 | 1.4087 | 0.0000 | 2.2914 |
| Fumaric acid | 3.97 | 115.0039 | NEG | C4H4O4 | HMDB0000134 | 110-17-8 | C00122 | 0.0615 | 0.0396 | 1.3706 | 0.0002 | 0.6446 |
| N-Acetylcarnosine | 3.97 | 269.1244 | POS | C11H16N4O4 | HMDB0012881 | 56353-15-2 |  | 0.0074 | 0.0053 | 1.3823 | 0.0025 | 0.7146 |
| Pantothenic acid | 3.97 | 218.1035 | NEG | C9H17NO5 | HMDB0000210 | 79-83-4 | C00864 | 0.2833 | 0.2181 | 1.0975 | 0.0023 | 0.7698 |
| 9-Oxo-10(E),12(E)-octadecadienoic acid | 3.97 | 293.2121 | NEG | C18H30O3 | HMDB0004669 | 54232-58-5 | C14766 | 0.3124 | 0.1732 | 1.1096 | 0.0025 | 0.5545 |
| 13(S)-HODE | 3.97 | 295.228 | NEG | C18H32O3 | HMDB0004667 | 29623-28-7 | C14762 | 0.8103 | 0.5687 | 1.2453 | 0.0010 | 0.7019 |
| 10,13-dimethyl-17-oxo-3-sulfooxy-1,2,3,4,7,8,9,11  ,12,14,15,16-dodecahydrocyclopenta[a]phenanthrene | 3.97 | 367.1587 | NEG | C19H28O5S | HMDB0001032 | 651-48-9 | C04555 | 124.9684 | 92.4725 | 1.0703 | 0.0070 | 0.7400 |
| gamma-Glutamyllysine | 3.96 | 276.1555 | POS | C11H21N3O5 | HMDB0029154 |  |  | 0.0050 | 0.0075 | 1.3496 | 0.0004 | 1.5130 |
| trans-Aconitic acid | 3.96 | 173.0094 | NEG | C6H6O6 | HMDB0000958 | 4023-65-8 | C02341 | 0.3090 | 1.2701 | 1.9518 | 0.0000 | 4.1105 |
| cis-Aconitic acid | 3.96 | 173.0094 | NEG | C6H6O6 | HMDB0000072 | 4023-65-8 | C00417 | 0.3090 | 1.2701 | 1.9518 | 0.0000 | 4.1105 |
| Taurine | 3.96 | 124.0075 | NEG | C2H7NO3S | HMDB0000251 | 107-35-7 | C00245 | 17.8607 | 13.2360 | 1.2490 | 0.0120 | 0.7411 |
| Betaine | 3.96 | 118.086 | POS | C5H11NO2 | HMDB0000043 | 107-43-7 | C00719 | 4.2156 | 5.0657 | 1.1453 | 0.0012 | 1.2016 |
| 3-Amino-4-methylpentanoic acid | 3.96 | 130.0875 | NEG | C6H13NO2 | HMDB0245808 | 5699-54-7 |  | 9.3672 | 6.9147 | 1.2880 | 0.0012 | 0.7382 |
| Isoleucine | 3.96 | 130.0875 | NEG | C6H13NO2 | HMDB0000172 | 73-32-5 | C00407 | 9.3672 | 6.9147 | 1.2880 | 0.0012 | 0.7382 |
| Inosine | 3.96 | 269.0881 | POS | C10H12N4O5 | HMDB0000195 | 58-63-9 | C00294 | 0.0353 | 0.0193 | 1.2586 | 0.0080 | 0.5463 |
| 1-Methylinosine | 3.96 | 283.1035 | POS | C11H14N4O5 | HMDB0002721 | 2140-73-0 |  | 0.0254 | 0.0294 | 1.0441 | 0.0025 | 1.1580 |
| Taurochenodeoxycholic acid | 3.96 | 498.29 | NEG | C26H45NO6S | HMDB0000951 | 516-35-8 | C05465 | 0.9548 | 0.5889 | 1.0037 | 0.0243 | 0.6168 |
| 10-Undecenoic acid | 3.96 | 183.1392 | NEG | C11H20O2 | HMDB0033724 | 1333-28-4 | C13910 | 0.7678 | 0.4904 | 1.1294 | 0.0003 | 0.6387 |
| 3-Hydroxylauric acid | 3.96 | 197.1549 | NEG | C12H24O3 | HMDB0000387 | 45162-48-9 |  | 1.2942 | 0.8744 | 1.2303 | 0.0003 | 0.6757 |
| Denticetic-acid | 3.95 | 197.1549 | NEG | C12H22O2 | HMDB0000529 | 2430-94-6 |  | 1.2942 | 0.8744 | 1.2303 | 0.0003 | 0.6757 |
| Homoserine | 3.95 | 118.0511 | NEG | C4H9NO3 | HMDB0000719 | 672-15-1 | C00263 | 0.6086 | 0.8146 | 1.3136 | 0.0319 | 1.3384 |
| Ergothioneine | 3.95 | 230.0956 | POS | C9H15N3O2S | HMDB0003045 | 497-30-3 | C05570 | 0.0076 | 0.0147 | 1.1391 | 0.0023 | 1.9385 |
| Uric acid | 3.95 | 167.0213 | NEG | C5H4N4O3 | HMDB0000289 | 69-93-2 | C00366 | 0.5376 | 0.9378 | 1.1786 | 0.0004 | 1.7444 |
| 3-Hydroxybutyrylcarnitine (Car(4:0-O)) | 3.95 | 248.1491 | POS | C11H21NO5 | HMDB0013127 | 1469900-92-2 |  | 0.0410 | 0.0228 | 1.3803 | 0.0096 | 0.5562 |
| 5-Methyl DL-glutamate | 3.95 | 162.0761 | POS | C6H11NO4 | HMDB0061715 | 14487-45-7 |  | 0.0362 | 0.0243 | 1.5163 | 0.0000 | 0.6707 |
| Tryptophan | 3.95 | 205.0969 | POS | C11H12N2O2 | HMDB0030396 | 73-22-3 | C00078 | 0.8632 | 1.0785 | 1.0407 | 0.0027 | 1.2493 |
| Pseudouridine | 3.95 | 243.0625 | NEG | C9H12N2O6 | HMDB0000767 | 1445-07-4 | C02067 | 1.1204 | 0.9240 | 1.2271 | 0.0048 | 0.8247 |
| N,N-Diethyl-2-aminoethanol | 3.95 | 100.112 | POS | C6H15NO | HMDB0033971 | 100-37-8 |  | 0.0113 | 0.0486 | 1.6022 | 0.0000 | 4.3214 |
| 2'-O-methylcytidine | 3.95 | 258.1083 | POS | C10H15N3O5 | HMDB0242132 | 2140-72-9 |  | 0.0052 | 0.0060 | 1.3661 | 0.0004 | 1.1381 |
| Nordeoxycholic acid | 3.95 | 377.2704 | NEG | C23H38O4 | HMDB0304947 | 53608-86-9 |  | 0.0858 | 0.0590 | 1.4689 | 0.0001 | 0.6876 |
| Creatinine | 3.95 | 112.0519 | NEG | C4H7N3O | HMDB0000562 | 60-27-5 | C00791 | 0.2551 | 0.2046 | 1.3780 | 0.0026 | 0.8018 |
| 5,6-Dihydrouridine | 3.95 | 247.0923 | POS | C9H14N2O6 | HMDB0000497 | 5627-05-4 |  | 0.0061 | 0.0074 | 1.1537 | 0.0030 | 1.2068 |
| 3-Hydroxydecanoic acid | 3.95 | 187.1341 | NEG | C10H20O3 | HMDB0002203 | 19526-23-9 |  | 0.7726 | 0.5047 | 1.0849 | 0.0088 | 0.6532 |
| Valproic acid | 3.95 | 143.1079 | NEG | C8H16O2 | HMDB0001877 | 99-66-1 | C07185 | 0.5646 | 0.4778 | 1.0015 | 0.0162 | 0.8463 |
| 3-Methyl-2-oxovaleric acid | 3.95 | 129.0558 | NEG | C6H10O3 | HMDB0000491 | 1460-34-0 | C03465 | 135.4522 | 104.8729 | 1.3475 | 0.0009 | 0.7742 |
| 2-Ketocaproic acid | 3.95 | 129.0558 | NEG | C6H10O3 | HMDB0001864 | 2492-75-3 | C00902 | 135.4522 | 104.8729 | 1.3475 | 0.0009 | 0.7742 |
| 4-Methylquinolin-2-ol | 3.95 | 158.0613 | NEG | C10H9NO |  | 607-66-9 |  | 2.0079 | 1.1625 | 1.5989 | 0.0007 | 0.5790 |
| 3'-O-methylcytidine | 3.94 | 258.1083 | POS | C10H15N3O5 | HMDB0304396 | 20594-00-7 |  | 0.0052 | 0.0060 | 1.3661 | 0.0004 | 1.1381 |
| Caprylic acid | 3.94 | 143.1079 | NEG | C8H16O2 | HMDB0000482 | 124-07-2 | C06423 | 0.5646 | 0.4778 | 1.0015 | 0.0162 | 0.8463 |
| Ketoleucine | 3.94 | 129.0558 | NEG | C6H10O3 | HMDB0000695 | 816-66-0 | C00233 | 135.4522 | 104.8729 | 1.3475 | 0.0009 | 0.7742 |
| beta-Alanine | 3.94 | 88.0405 | NEG | C3H7NO2 | HMDB0000056 | 107-95-9 | C00099 | 2.9443 | 2.3777 | 1.2763 | 0.0006 | 0.8076 |
| Valine | 3.94 | 116.0718 | NEG | C5H11NO2 | HMDB0000883 | 72-18-4 | C00183 | 6.5520 | 5.1346 | 1.3824 | 0.0022 | 0.7837 |
| Imidazol-1-yl-acetic acid | 3.94 | 127.0502 | POS | C5H6N2O2 | HMDB0029736 | 22884-10-2 |  | 0.1044 | 0.4868 | 1.3705 | 0.0001 | 4.6651 |
| N-Acetyl-beta-alanine | 3.94 | 130.0511 | NEG | C5H9NO3 | HMDB0061880 | 3025-95-4 | C01073 | 0.1374 | 0.0690 | 1.1619 | 0.0004 | 0.5024 |
| Pyruvate | 3.94 | 87.0088 | NEG | C3H4O3 | HMDB0000243 | 127-17-3 | C00022 | 136.6179 | 99.5917 | 1.2218 | 0.0001 | 0.7290 |
| Lysine | 3.93 | 147.1128 | POS | C6H14N2O2 | HMDB0000182 | 56-87-1 | C00047 | 0.6402 | 0.8554 | 1.5248 | 0.0004 | 1.3361 |
| 3-methylcytidine | 3.93 | 258.1086 | POS | C10H15N3O5 | HMDB0000982 | 2140-61-6 |  | 0.0037 | 0.0045 | 1.0190 | 0.0176 | 1.2219 |
| 4-Hydroxyphenylacetic acid | 3.93 | 151.0402 | NEG | C8H8O3 | HMDB0000020 | 156-38-7 | C00642 | 0.0456 | 0.0324 | 1.0519 | 0.0207 | 0.7100 |
| Leu-Leu | 3.93 | 243.1714 | NEG | C12H24N2O3 | HMDB0028933 | 3303-31-9 | C11332 | 0.0898 | 0.0497 | 1.5008 | 0.0009 | 0.5541 |
| Ile-Leu | 3.93 | 243.1714 | NEG | C12H24N2O3 | HMDB0028911 | 26462-22-6 |  | 0.0898 | 0.0497 | 1.5008 | 0.0009 | 0.5541 |
| 2-Methylbutyrylglycine | 3.93 | 158.0824 | NEG | C7H13NO3 | HMDB0000339 | 52320-67-9 |  | 0.1059 | 0.0649 | 1.4933 | 0.0034 | 0.6130 |
| 2-Hydroxyoctanoic acid | 3.93 | 159.1028 | NEG | C8H16O3 | HMDB0000711 | 617-73-2 |  | 0.8397 | 0.5650 | 1.1681 | 0.0019 | 0.6729 |
| Citraconic acid | 3.93 | 129.0196 | NEG | C5H6O4 | HMDB0000634 | 498-23-7 | C02226 | 0.5250 | 0.3037 | 1.3855 | 0.0001 | 0.5785 |
| Acetoin | 3.93 | 87.0453 | NEG | C4H8O2 | HMDB0003243 | 513-86-0 | C00466 | 0.2368 | 0.1847 | 1.3055 | 0.0021 | 0.7802 |
| Embelin | 3.93 | 293.176 | NEG | C17H26O4 | HMDB0251767 | 550-24-3 | C10342 | 3.0092 | 2.4341 | 1.0208 | 0.0045 | 0.8089 |
| Pelargonic acid | 3.93 | 157.1236 | NEG | C9H18O2 | HMDB0000847 | 112-05-0 | C01601 | 3.1850 | 2.4304 | 1.3917 | 0.0004 | 0.7631 |
| Isoquinoline | 3.93 | 130.065 | POS | C9H7N | HMDB0034244 | 119-65-3 | C06323 | 0.0253 | 0.0147 | 1.6346 | 0.0005 | 0.5802 |
| alpha-Linolenic acid | 3.93 | 277.2177 | NEG | C18H30O2 | HMDB0001388 | 463-40-1 | C06427 | 13.7038 | 9.9151 | 1.1062 | 0.0004 | 0.7235 |
| PC(16:0/18:1(9Z)) | 3.93 | 742.5737 | POS | C42H82NO8P | HMDB0007972 |  | C13875 | 0.2324 | 0.2927 | 1.0119 | 0.0088 | 1.2592 |
| Terephthalic-Acid | 3.92 | 165.0196 | NEG | C8H6O4 | HMDB0002428 | 100-21-0 | C06337 | 0.1668 | 0.1252 | 1.2914 | 0.0096 | 0.7506 |
| Azelaic acid | 3.92 | 187.0979 | NEG | C9H16O4 | HMDB0000784 | 123-99-9 | C08261 | 0.0856 | 0.0554 | 1.6354 | 0.0007 | 0.6471 |
| LPC(17:0/0:0) | 3.92 | 510.3555 | POS | C25H52NO7P | HMDB0012108 | 50930-23-9 |  | 0.4062 | 0.6044 | 1.7623 | 0.0000 | 1.4878 |
| 3-(3-Hydroxyphenyl)propanoic acid | 3.92 | 165.0559 | NEG | C9H10O3 | HMDB0000375 | 621-54-5 | C11457 | 0.1607 | 0.1215 | 1.0292 | 0.0296 | 0.7565 |
| trans-2-Octenoic acid | 3.92 | 141.0923 | NEG | C8H14O2 | HMDB0001568 | 1871-67-6 |  | 0.5244 | 0.3713 | 1.3082 | 0.0019 | 0.7081 |
| alpha-Ketoisovaleric acid | 3.92 | 115.0402 | NEG | C5H8O3 | HMDB0000019 | 759-05-7 | C00141 | 42.4085 | 32.3576 | 1.3527 | 0.0012 | 0.7630 |
| 5,6-Dihydroxyindole | 3.92 | 148.0406 | NEG | C8H7NO2 | HMDB0004058 | 3131-52-0 | C05578 | 0.0998 | 0.0642 | 1.3638 | 0.0004 | 0.6438 |
| Capric acid | 3.92 | 171.1392 | NEG | C10H20O2 | HMDB0000511 | 334-48-5 | C01571 | 1.1614 | 0.8561 | 1.2560 | 0.0005 | 0.7372 |
| Undecanoic acid | 3.92 | 185.1549 | NEG | C11H22O2 | HMDB0000947 | 112-37-8 | C17715 | 0.3067 | 0.2019 | 1.4993 | 0.0000 | 0.6584 |
| Taurohyodeoxycholic acid | 3.91 | 498.29 | NEG | C26H45NO6S | HMDB0247202 | 386523 |  | 0.9548 | 0.5889 | 1.0037 | 0.0243 | 0.6168 |
| gamma-Linolenic acid | 3.91 | 277.2177 | NEG | C18H30O2 | HMDB0003073 | 506-26-3 | C06426 | 13.7038 | 9.9151 | 1.1062 | 0.0004 | 0.7235 |
| Phosphorylcholine | 3.91 | 184.0733 | POS | C5H15NO4P | HMDB0001565 | 3616-04-4 | C00588 | 0.0231 | 0.0394 | 1.0650 | 0.0018 | 1.7078 |
| O-Acetylserine | 3.91 | 146.046 | NEG | C5H9NO4 | HMDB0003011 | 5147-00-2 | C00979 | 0.7925 | 0.6283 | 1.4320 | 0.0199 | 0.7928 |
| N-Acetyltryptophan | 3.91 | 245.0932 | NEG | C13H14N2O3 | HMDB0013713 | 1218-34-4 | C03137 | 0.0592 | 0.0373 | 1.5387 | 0.0008 | 0.6294 |
| N2,N2-Dimethylguanosine | 3.91 | 312.1302 | POS | C12H17N5O5 | HMDB0004824 | 2140-67-2 |  | 0.0370 | 0.0436 | 1.2414 | 0.0009 | 1.1781 |
| Leu-Ile | 3.9 | 243.1714 | NEG | C12H24N2O3 | HMDB0028932 | 36077-41-5 |  | 0.0898 | 0.0497 | 1.5008 | 0.0009 | 0.5541 |
| Citric acid | 3.9 | 191.0201 | NEG | C6H8O7 | HMDB0000094 | 77-92-9 | C00158 | 0.1067 | 1.2718 | 1.2267 | 0.0263 | 11.9227 |
| Malonic acid | 3.9 | 103.0039 | NEG | C3H4O4 | HMDB0000691 | 141-82-2 | C00383 | 0.3063 | 0.2356 | 1.0794 | 0.0234 | 0.7691 |
| N-Methyl-L-asparagine | 3.9 | 127.0515 | NEG | C5H10N2O3 |  | 7175-34-0 |  | 0.0422 | 0.7850 | 1.8533 | 0.0001 | 18.5964 |
| LPC(16:0) | 3.9 | 496.3392 | POS | C24H50NO7P | HMDB0010382 | 17364-16-8 |  | 33.4970 | 50.4719 | 2.2038 | 0.0000 | 1.5068 |
| Benzoic acid | 3.9 | 121.0296 | NEG | C7H6O2 | HMDB0001870 | 65-85-0 | C00180 | 1.4314 | 1.0492 | 1.6095 | 0.0000 | 0.7330 |
| Tauroursodeoxycholic acid | 3.89 | 498.29 | NEG | C26H45NO6S | HMDB0000874 | 14605-22-2 | C16868 | 0.9548 | 0.5889 | 1.0037 | 0.0243 | 0.6168 |
| MeAIB | 3.89 | 118.0861 | POS | C5H11NO2 | HMDB0002141 | 2566-34-9 |  | 3.5884 | 3.9415 | 1.1111 | 0.0169 | 1.0984 |
| Glycolate | 3.89 | 75.0089 | NEG | C2H4O3 | HMDB0000115 | 79-14-1 | C00160 | 0.4281 | 0.3502 | 1.2746 | 0.0010 | 0.8179 |
| Allantoin | 3.89 | 157.0369 | NEG | C4H6N4O3 | HMDB0000462 | 97-59-6 | C01551 | 0.4235 | 0.2284 | 1.9105 | 0.0000 | 0.5393 |
| N-Lactoylphenylalanine | 3.89 | 236.0931 | NEG | C12H15NO4 | HMDB0062175 | 183241-73-8 |  | 0.0765 | 0.0426 | 1.3783 | 0.0029 | 0.5578 |
| 4-Ethoxybenzoic acid | 3.89 | 165.0558 | NEG | C9H10O3 |  | 619-86-3 |  | 1.9589 | 1.2518 | 1.6838 | 0.0000 | 0.6390 |
| 3-Hydroxypyruvic acid | 3.88 | 103.0039 | NEG | C3H4O4 | HMDB0001352 | 1113-60-6 | C00168 | 0.3063 | 0.2356 | 1.0794 | 0.0234 | 0.7691 |
| N,N-Dimethylarginine (ADMA) | 3.88 | 203.1502 | POS | C8H18N4O2 | HMDB0001539 | 30315-93-6 | C03626 | 0.5911 | 0.7649 | 1.2938 | 0.0004 | 1.2939 |
| 1-O-Hexadecyl-sn-glycero-3-phosphocholine (LPC(O-16:0/0:0)) | 3.88 | 482.3602 | POS | C24H52NO6P | HMDB0243890 | 52691-62-0 | C13903 | 0.5968 | 0.9721 | 2.0769 | 0.0000 | 1.6288 |
| Isobutyrylglycine | 3.88 | 144.0667 | NEG | C6H11NO3 | HMDB0000730 | 15926-18-8 |  | 0.0592 | 0.0369 | 1.5254 | 0.0000 | 0.6229 |
| PC(P-16:0/0:0) | 3.88 | 480.3449 | POS | C24H50NO6P | HMDB0010407 | 97802-53-4 |  | 0.5429 | 0.8781 | 2.0163 | 0.0000 | 1.6175 |
| Kynurenic acid | 3.88 | 188.0355 | NEG | C10H7NO3 | HMDB0000715 | 492-27-3 | C01717 | 0.4068 | 0.2684 | 1.5652 | 0.0000 | 0.6598 |
| N-Acetylalanine | 3.88 | 130.0512 | NEG | C5H9NO3 | HMDB0255053 | 139146-66-0 |  | 0.2640 | 0.2162 | 1.2892 | 0.0155 | 0.8190 |
| p-Toluquinone | 3.87 | 121.0296 | NEG | C7H6O2 |  | 553-97-9 |  | 1.4314 | 1.0492 | 1.6095 | 0.0000 | 0.7330 |
| Pipecolamide | 3.87 | 129.1022 | POS | C6H12N2O |  | 19889-77-1 | C19809 | 0.0148 | 0.0217 | 1.0043 | 0.0120 | 1.4603 |
| Ribothymidine | 3.87 | 257.078 | NEG | C10H14N2O6 | HMDB0000884 | 1463-10-1 |  | 0.3518 | 0.2887 | 1.5284 | 0.0005 | 0.8206 |
| Arabinono-1,4-lactone | 3.87 | 147.03 | NEG | C5H8O5 | HMDB0001900 | 51532-86-6 | C01114 | 0.4794 | 0.2138 | 1.7316 | 0.0000 | 0.4459 |
| Paracetamol (Drug) | 3.87 | 152.0705 | POS | C8H9NO2 | HMDB0001859 | 103-90-2 | C06804 | 0.0070 | 0.0063 | 1.1926 | 0.0001 | 0.8987 |
| N-Lactoyl-Phenylalanine | 3.86 | 236.0931 | NEG | C12H15NO4 | HMDB0062175 | 183241-73-8 |  | 0.0765 | 0.0426 | 1.3783 | 0.0029 | 0.5578 |
| Oxalic acid | 3.86 | 88.9882 | NEG | C2H2O4 | HMDB0002329 | 144-62-7 | C00209 | 0.1071 | 0.0881 | 1.0542 | 0.0076 | 0.8226 |
| Formylmethionine | 3.86 | 176.0388 | NEG | C6H11NO3S | HMDB0001015 | 4289-98-9 | C03145 | 0.2790 | 0.2341 | 1.1371 | 0.0131 | 0.8392 |
| Car(18:1) | 3.86 | 426.358 | POS | C25H47NO4 | HMDB0013337 | 13962-05-5 |  | 0.4375 | 0.5229 | 1.2723 | 0.0125 | 1.1952 |
| Ganoderic acid DM | 3.86 | 467.3158 | NEG | C30H44O4 |  | 173075-45-1 |  | 0.1352 | 0.1069 | 1.0483 | 0.0050 | 0.7907 |
| Valeric acid | 3.86 | 101.0609 | NEG | C5H10O2 | HMDB0000892 | 109-52-4 | C00803 | 0.5934 | 0.4726 | 1.2941 | 0.0043 | 0.7964 |
| Isovaleric acid | 3.85 | 101.0609 | NEG | C5H10O2 | HMDB0000718 | 503-74-2 | C08262 | 0.5934 | 0.4726 | 1.2941 | 0.0043 | 0.7964 |
| Aspartate | 3.85 | 132.0305 | NEG | C4H7NO4 | HMDB0000191 | 56-84-8 | C00049 | 0.0477 | 0.0958 | 1.1056 | 0.0013 | 2.0092 |
| Phenylacetic acid | 3.85 | 135.0453 | NEG | C8H8O2 | HMDB0000209 | 103-82-2 | C07086 | 0.0817 | 0.0570 | 1.6319 | 0.0010 | 0.6982 |
| 12-Hydroxydodecanoic acid | 3.85 | 215.1654 | NEG | C12H24O3 | HMDB0002059 | 505-95-3 | C08317 | 0.3578 | 0.2569 | 1.2195 | 0.0014 | 0.7180 |
| Pyridoxine | 3.84 | 152.0705 | POS | C8H11NO3 | HMDB0000239 | 65-23-6 | C00314 | 0.0070 | 0.0063 | 1.1926 | 0.0001 | 0.8987 |
| Malic acid | 3.84 | 133.0145 | NEG | C4H6O5 | HMDB0000744 | 6915-15-7 | C00149 | 0.2590 | 0.3855 | 1.1390 | 0.0011 | 1.4886 |
| Arachidonoylcarnitine (Car(20:4)) | 3.84 | 448.3421 | POS | C27H45NO4 | HMDB0006455 | 36816-11-2 |  | 0.0220 | 0.0291 | 1.3450 | 0.0073 | 1.3249 |
| 5-Methylcytidine | 3.83 | 258.1086 | POS | C10H15N3O5 | HMDB0000982 | 2140-61-6 |  | 0.0037 | 0.0045 | 1.0190 | 0.0176 | 1.2219 |
| Isocitric acid | 3.83 | 191.0201 | NEG | C6H8O7 | HMDB0000193 | 320-77-4 | C00311 | 0.1067 | 1.2718 | 1.2267 | 0.0263 | 11.9227 |
| Lauramine oxide | 3.83 | 230.2477 | POS | C14H31NO |  | 1643-20-5 |  | 0.2168 | 0.3495 | 2.2222 | 0.0000 | 1.6118 |
| 2,2-Dimethylsuccinic acid | 3.83 | 145.0507 | NEG | C6H10O4 | HMDB0002074 | 597-43-3 |  | 0.3861 | 0.3049 | 1.3859 | 0.0002 | 0.7898 |
| Lumichrome | 3.83 | 241.0722 | NEG | C12H10N4O2 | HMDB0254199 | 1086-80-2 | C01727 | 0.2955 | 0.1928 | 1.2553 | 0.0073 | 0.6526 |
| Phthalide | 3.83 | 135.044 | POS | C8H6O2 | HMDB0032469 | 87-41-2 | C18611 | 0.0124 | 0.0067 | 1.8407 | 0.0001 | 0.5356 |
| 3-Hydroxyphenylacetic acid | 3.82 | 151.0402 | NEG | C8H8O3 | HMDB0000440 | 621-37-4 | C05593 | 0.0456 | 0.0324 | 1.0519 | 0.0207 | 0.7100 |
| 3-Methyluridine | 3.82 | 257.078 | NEG | C10H14N2O6 | HMDB0004813 | 2140-69-4 |  | 0.3518 | 0.2887 | 1.5284 | 0.0005 | 0.8206 |
| Methylmalonic acid | 3.82 | 117.0195 | NEG | C4H6O4 | HMDB0000202 | 516-05-2 | C02170 | 0.1344 | 0.0998 | 1.3284 | 0.0169 | 0.7425 |
| Monomethyl phthalate | 3.82 | 179.0348 | NEG | C9H8O4 | HMDB0002130 | 4376-18-5 |  | 0.2337 | 0.1730 | 1.2402 | 0.0092 | 0.7405 |
| Taurodeoxycholic acid | 3.81 | 498.29 | NEG | C26H45NO6S | HMDB0000896 | 516-50-7 | C05463 | 0.9548 | 0.5889 | 1.0037 | 0.0243 | 0.6168 |
| 6-Hydroxynorleucine | 3.81 | 146.0824 | NEG | C6H13NO3 |  | 6033-32-5 |  | 0.1741 | 0.1265 | 1.5512 | 0.0000 | 0.7269 |
| 3-Methyl-1H-pyrazole-4-carbaldehyde | 3.81 | 111.0551 | POS | C5H6N2O |  | 112758-40-4 |  | 0.5123 | 0.2676 | 1.6109 | 0.0005 | 0.5223 |
| Bisindolylmaleimide I | 3.81 | 411.1852 | NEG | C25H24N4O2 | HMDB0249269 | 133052-90-1 | C11238 | 1.3747 | 1.0283 | 1.0701 | 0.0110 | 0.7480 |
| 3-Methoxyphenylacetic acid | 3.8 | 165.0559 | NEG | C9H10O3 | HMDB0059969 | 1798-09-0 |  | 0.1607 | 0.1215 | 1.0292 | 0.0296 | 0.7565 |
| 10-Hydroxydecanoic acid | 3.79 | 187.1341 | NEG | C10H20O3 | HMDB0244272 | 1679-53-4 | C02774 | 0.7726 | 0.5047 | 1.0849 | 0.0088 | 0.6532 |
| 2-Phenyllactic acid | 3.79 | 165.0558 | NEG | C9H10O3 | HMDB0142137 | 515-30-0 |  | 1.9589 | 1.2518 | 1.6838 | 0.0000 | 0.6390 |
| Butanoic acid | 3.78 | 87.0453 | NEG | C4H8O2 | HMDB0000039 | 107-92-6 | C00246 | 0.2368 | 0.1847 | 1.3055 | 0.0021 | 0.7802 |
| Ethyl 3-hydroxybenzoate | 3.78 | 165.0558 | NEG | C9H10O3 |  | 7781-98-8 |  | 1.9589 | 1.2518 | 1.6838 | 0.0000 | 0.6390 |
| Glu-Arg | 3.78 | 304.1616 | POS | C11H21N5O5 | HMDB0028813 | 7219-59-2 |  | 0.0068 | 0.0137 | 1.3855 | 0.0008 | 2.0116 |
| Gluconic acid | 3.78 | 195.0512 | NEG | C6H12O7 | HMDB0000625 | 526-95-4 | C00257 | 0.0769 | 0.1675 | 1.2972 | 0.0043 | 2.1795 |
| 4-Isopropylbenzoic acid | 3.78 | 163.0766 | NEG | C10H12O2 | HMDB0035268 | 536-66-3 | C06578 | 0.1002 | 0.0546 | 1.3373 | 0.0008 | 0.5454 |
| Ethyl 4-hydroxybenzoate | 3.77 | 165.0558 | NEG | C9H10O3 | HMDB0032573 | 120-47-8 | D01647 | 1.9589 | 1.2518 | 1.6838 | 0.0000 | 0.6390 |
| Xanthoxylin | 3.77 | 195.0663 | NEG | C10H12O4 | HMDB0029645 | 90-24-4 | C10726 | 0.2379 | 0.0713 | 1.4521 | 0.0001 | 0.2998 |
| Diacetyl | 3.77 | 85.0296 | NEG | C4H6O2 | HMDB0003407 | 431-03-8 | C00741 | 1.0297 | 0.5984 | 1.5425 | 0.0000 | 0.5811 |
| Diglycine | 3.76 | 131.0465 | NEG | C4H8N2O3 | HMDB0011733 | 556-50-3 | C02037 | 0.1770 | 0.2570 | 1.0892 | 0.0058 | 1.4522 |
| Isoxanthopterin | 3.76 | 180.0492 | POS | C6H5N5O2 | HMDB0000704 | 529-69-1 | C03975 | 0.3006 | 0.3378 | 1.0907 | 0.0070 | 1.1236 |
| 5-Oxooctanoic acid | 3.76 | 157.0871 | NEG | C8H14O3 |  | 3637-14-7 |  | 0.5312 | 0.3248 | 1.7555 | 0.0000 | 0.6114 |
| Docebenone | 3.75 | 325.1846 | NEG | C21H26O3 | HMDB0247732 | 80809-81-0 | C01349 | 18.8127 | 14.2110 | 1.1772 | 0.0100 | 0.7554 |
| Pi-Methylimidazoleacetic acid (hydrochloride) | 3.74 | 141.0659 | POS | C6H8N2O2 | HMDB0004988 | 4200-48-0 |  | 0.0055 | 0.0122 | 1.8622 | 0.0001 | 2.2029 |
| 1,3,7-Trimethyluric acid | 3.74 | 211.0826 | POS | C8H10N4O3 | HMDB0002123 | 5415-44-1 | C16361 | 0.0018 | 0.0039 | 1.2528 | 0.0000 | 2.1960 |
| Isatin | 3.74 | 146.025 | NEG | C8H5NO2 | HMDB0061933 | 1186480-61-4 | C11129 | 0.1756 | 0.0846 | 1.3696 | 0.0045 | 0.4818 |
| Caplamin | 3.73 | 130.0875 | NEG | C6H13NO2 | HMDB0001901 | 60-32-2 | C02378 | 9.3672 | 6.9147 | 1.2880 | 0.0012 | 0.7382 |
| 4-(dimethylamino)butanoate | 3.73 | 130.0875 | NEG | C6H13NO2 |  | 693-11-8 |  | 9.3672 | 6.9147 | 1.2880 | 0.0012 | 0.7382 |
| Desaminotyrosine | 3.73 | 165.0558 | NEG | C9H10O3 | HMDB0002199 | 501-97-3 | C01744 | 1.9589 | 1.2518 | 1.6838 | 0.0000 | 0.6390 |
| 3-Hydroxyacetophenone | 3.73 | 135.0453 | NEG | C8H8O2 |  | 121-71-1 |  | 0.0817 | 0.0570 | 1.6319 | 0.0010 | 0.6982 |
| 4-Hydroxyphenylacetaldehyde | 3.73 | 135.0453 | NEG | C8H8O2 | HMDB0003767 | 7339-87-9 | C03765 | 0.0817 | 0.0570 | 1.6319 | 0.0010 | 0.6982 |
| Phosphate | 3.73 | 96.9698 | NEG | H3O4P | HMDB0001429 | 7664-38-2 | C00009 | 0.8104 | 1.1962 | 1.6067 | 0.0012 | 1.4760 |
| 7-Ketodeoxycholic acid | 3.73 | 405.2651 | NEG | C24H38O5 | HMDB0000391 | 911-40-0 | C04643 | 0.1550 | 0.1136 | 1.3231 | 0.0022 | 0.7327 |
| 3-Oxocholic acid | 3.73 | 405.2651 | NEG | C24H38O5 | HMDB0000502 | 2304-89-4 |  | 0.1550 | 0.1136 | 1.3231 | 0.0022 | 0.7327 |
| Quillaic acid | 3.73 | 485.3263 | NEG | C30H46O5 |  | 631-01-6 | C08972 | 0.0711 | 0.0505 | 1.4811 | 0.0008 | 0.7094 |
| PC(17:0/17:0) | 3.73 | 744.5894 | POS | C42H84NO8P |  | 70897-27-7 |  | 0.6935 | 0.8309 | 1.0155 | 0.0496 | 1.1982 |
| PC(16:0/18:0) | 3.73 | 744.5894 | POS | C42H84NO8P | HMDB0007970 | 59403-51-9 |  | 0.6935 | 0.8309 | 1.0155 | 0.0496 | 1.1982 |
| PC(18:0/16:0) | 3.73 | 744.5894 | POS | C42H84NO8P | HMDB0008034 | 59403-53-1 |  | 0.6935 | 0.8309 | 1.0155 | 0.0496 | 1.1982 |
| Bilirubin | 3.73 | 583.2568 | NEG | C33H36N4O6 | HMDB0000054 | 635-65-4 | C00486 | 0.7109 | 1.6438 | 1.1947 | 0.0003 | 2.3124 |
| 3-(2-Hydroxyphenyl)propanoic acid | 3.72 | 165.0559 | NEG | C9H10O3 | HMDB0033752 | 495-78-3 | C01198 | 0.1607 | 0.1215 | 1.0292 | 0.0296 | 0.7565 |
| 3-Hydroxyoctanoic acid | 3.72 | 141.0923 | NEG | C8H16O3 | HMDB0001954 | 14292-27-4 | C20793 | 0.5244 | 0.3713 | 1.3082 | 0.0019 | 0.7081 |
| 4'-Hydroxyacetophenone | 3.72 | 135.0453 | NEG | C8H8O2 |  | 99-93-4 | C10700 | 0.0817 | 0.0570 | 1.6319 | 0.0010 | 0.6982 |
| (1-Hydroxycyclohexyl)acetic acid | 3.72 | 157.0871 | NEG | C8H14O3 |  | 14399-63-4 |  | 0.5312 | 0.3248 | 1.7555 | 0.0000 | 0.6114 |
| Pyruvaldehyde | 3.72 | 71.014 | NEG | C3H4O2 | HMDB0001167 | 78-98-8 | C00546 | 3.0346 | 2.1329 | 1.8162 | 0.0000 | 0.7029 |
| Palmitoylcarnitine (Car(16:0)) | 3.72 | 400.3421 | POS | C23H45NO4 | HMDB0000222 | 2364-67-2 | C02990 | 0.2844 | 0.3900 | 1.5907 | 0.0000 | 1.3713 |
| Dihydrouracil | 3.72 | 95.0252 | NEG | C4H6N2O2 | HMDB0000076 | 504-07-4 | C00429 | 0.1872 | 0.1322 | 1.2879 | 0.0022 | 0.7061 |
| Royal jelly acid | 3.72 | 185.1184 | NEG | C10H18O3 | HMDB0244269 | 14113-05-4 |  | 1.5121 | 0.8376 | 1.2775 | 0.0006 | 0.5539 |
| Phthalic acid | 3.71 | 165.0196 | NEG | C8H6O4 | HMDB0002107 | 88-99-3 | C01606 | 0.1668 | 0.1252 | 1.2914 | 0.0096 | 0.7506 |
| Tetrahydrocorticosterone | 3.71 | 349.2386 | NEG | C21H34O4 | HMDB0000268 | 68-42-8 | C05476 | 0.1150 | 0.0882 | 1.2387 | 0.0004 | 0.7667 |
| AKBA | 3.71 | 511.3417 | NEG | C32H48O5 |  | 67416-61-9 |  | 0.0401 | 0.0328 | 1.1056 | 0.0120 | 0.8175 |
| 5-Hydroxyvalproic acid | 3.69 | 159.1028 | NEG | C8H16O3 | HMDB0013898 | 53660-23-4 | C16650 | 0.8397 | 0.5650 | 1.1681 | 0.0019 | 0.6729 |
| Bisindolylmaleimide VIII (acetate) | 3.65 | 397.1693 | NEG | C24H22N4O2 | HMDB0257261 | 125313-65-7 |  | 0.4154 | 0.3192 | 1.1119 | 0.0115 | 0.7685 |
| PC(10:0/10:0) | 3.54 | 548.3641 | POS | C28H56NO8P | HMDB0244070 | 3436-44-0 |  | 0.0038 | 0.0152 | 1.6539 | 0.0007 | 4.0202 |
| 7,3',4',5'-Tetrahydroxyflavone | 2.75 | 287.055 | POS | C15H10O6 |  |  |  | 0.0007 | 0.0346 | 1.7951 | 0.0001 | 48.8561 |
| 3-(3-Hydroxypropyl)-3,5-dihydro-4H-pyrimido[5,4-b]indol-4-one | 2.75 | 244.1081 | POS | C13H13N3O2 |  |  |  | 0.0089 | 0.0061 | 1.4733 | 0.0018 | 0.6914 |
| 1-Octadecyl-2-acetyl-sn-glycero-3-phosphocholine | 2.75 | 552.4025 | POS | C28H58NO7P |  |  |  | 0.0976 | 0.1233 | 1.3870 | 0.0007 | 1.2630 |
| [(Aminocarbonyl)amino](phenyl)acetic acid | 2.75 | 193.0619 | NEG | C9H10N2O3 |  |  |  | 0.0465 | 0.0340 | 1.3998 | 0.0001 | 0.7308 |
| cis-7-Hexadecenoic acid | 2.75 | 253.2173 | NEG | C16H30O2 | HMDB0002186 | 2416-19-5 |  | 0.1926 | 0.1400 | 1.0253 | 0.0070 | 0.7271 |
| Dihexadecyldimethylammonium cation | 2.75 | 494.5659 | POS | C34H72N |  |  |  | 0.0068 | 0.0104 | 1.6269 | 0.0000 | 1.5174 |
| HYDROCOTARNINE | 2.75 | 222.1125 | POS | C12H15NO3 | HMDB0033701 | 550-10-7 | C13534 | 0.4738 | 0.5463 | 1.1784 | 0.0026 | 1.1531 |
| N-Methylvaline | 2.75 | 132.1019 | POS | C6H13NO2 | HMDB0061716 |  |  | 0.0209 | 0.0425 | 1.5805 | 0.0052 | 2.0345 |
| Ethyldodecanoate | 2.75 | 227.2016 | NEG | C14H28O2 | HMDB0033788 | 106-33-2 |  | 0.1590 | 0.1333 | 1.0354 | 0.0162 | 0.8384 |
| PC(38:6) | 2.74 | 806.5692 | POS | C46H80NO8P |  |  |  | 0.0439 | 0.0564 | 1.3346 | 0.0050 | 1.2833 |
| PC(42:4) | 2.74 | 848.6523 | POS | C50H92NO8P |  |  |  | 0.1488 | 0.1813 | 1.3836 | 0.0014 | 1.2184 |
| N-Methyl-L-prolinamide | 2.74 | 129.1023 | POS | C6H12N2O |  |  |  | 0.0097 | 0.0684 | 1.2781 | 0.0067 | 7.0558 |
| (3-Ethyl-2-imino-2,3-dihydro-1H-benzimidazol-1-yl)acetic acid | 2.74 | 220.1079 | POS | C11H13N3O2 |  |  |  | 0.0562 | 0.0454 | 1.3465 | 0.0007 | 0.8074 |
| His-Trp | 2.74 | 342.1559 | POS | C17H19N5O3 | HMDB0028896 | 23403-90-9 |  | 0.0604 | 0.0345 | 1.6475 | 0.0017 | 0.5710 |
| 2-Methylbenzamide oxime | 2.74 | 151.0866 | POS | C8H10N2O | HMDB0341238 |  |  | 0.0143 | 0.0083 | 1.9256 | 0.0000 | 0.5767 |
| N-Methylpropionamide | 2.74 | 88.0757 | POS | C4H9NO |  |  |  | 0.0825 | 0.4499 | 1.5945 | 0.0000 | 5.4568 |
| Glycerophospho-N-palmitoylethanolamine | 2.74 | 454.2931 | POS | C21H44NO7P |  |  |  | 0.1678 | 0.2262 | 1.6325 | 0.0000 | 1.3476 |
| 1-O-Hexadecyl-2-O-(2E-butenoyl)-sn-glyceryl-3-phosphocholine | 2.74 | 550.3865 | POS | C28H56NO7P |  |  |  | 0.1252 | 0.1547 | 1.1137 | 0.0100 | 1.2361 |
| Tetraethylammonium cation | 2.74 | 130.159 | POS | C8H20N |  |  |  | 0.0093 | 0.0192 | 1.3987 | 0.0000 | 2.0681 |
| Tetrapropylammonium cation | 2.74 | 186.2215 | POS | C12H28N |  |  |  | 0.0128 | 0.0251 | 2.3115 | 0.0000 | 1.9709 |
| Tetradecylamine | 2.74 | 214.2529 | POS | C14H31N | HMDB0258887 |  |  | 0.0033 | 0.0053 | 1.9288 | 0.0000 | 1.5971 |
| 1-Hexadecylamine | 2.74 | 242.2841 | POS | C16H35N | HMDB0243891 |  |  | 0.0472 | 0.0783 | 2.2215 | 0.0000 | 1.6599 |
| 9,11-Methane-epoxyprostaglandin F1.alpha. | 2.74 | 351.2541 | NEG | C21H36O4 |  |  |  | 0.1602 | 0.1201 | 1.1617 | 0.0019 | 0.7496 |
| 3-Cyclohexyl-2-hydroxypropanoic acid | 2.74 | 171.1028 | NEG | C9H16O3 |  |  |  | 2.0128 | 1.3672 | 1.4558 | 0.0002 | 0.6793 |
| 11-Hydroxyundecanoic acid | 2.74 | 201.1497 | NEG | C11H22O3 |  |  |  | 0.1203 | 0.0719 | 1.3542 | 0.0009 | 0.5978 |
| Tetraoctylammonium cation | 2.74 | 466.5343 | POS | C32H68N |  |  |  | 0.0039 | 0.0065 | 1.9450 | 0.0000 | 1.6491 |
| Dicyclohexyl(hydroxy)acetic acid | 2.74 | 239.1654 | NEG | C14H24O3 |  |  |  | 0.3080 | 0.2102 | 1.2163 | 0.0010 | 0.6822 |
| (+)-trans-Chrysanthemic acid | 2.74 | 167.1079 | NEG | C10H16O2 |  |  |  | 0.5497 | 0.3942 | 1.2693 | 0.0035 | 0.7170 |
| 2-Cyano-L-phenylalanine | 2.74 | 191.0814 | POS | C10H10N2O2 |  |  |  | 0.0510 | 0.0246 | 1.7171 | 0.0000 | 0.4834 |
| Dodeca-2(E),4(E)-dienoic acid | 2.74 | 195.1393 | NEG | C12H20O2 | HMDB0340679 |  |  | 2.9595 | 2.0419 | 1.7924 | 0.0000 | 0.6900 |
| 2,6-Di-tert-butyl-4-(4-morpholinylmethyl)phenol | 2.74 | 306.2426 | POS | C19H31NO2 |  |  |  | 0.1219 | 1.9295 | 1.5933 | 0.0000 | 15.8232 |
| Nootkatone | 2.74 | 219.1742 | POS | C15H22O |  |  |  | 0.0522 | 0.7256 | 1.8037 | 0.0001 | 13.8972 |
| 1,5-Naphthalenediamine | 2.74 | 159.0916 | POS | C10H10N2 | HMDB0244231 |  | C19463 | 0.0302 | 0.0381 | 1.3319 | 0.0005 | 1.2640 |
| butabarbital | 2.74 | 211.1089 | NEG | C10H16N2O3 | HMDB0014382 | 125-40-6 | C07827 | 0.1428 | 0.1133 | 1.4197 | 0.0191 | 0.7936 |
| 4-Nitrobenzoic acid | 2.74 | 166.0145 | NEG | C7H5NO4 | HMDB0246532 |  | C18625 | 0.9814 | 0.7466 | 1.3379 | 0.0110 | 0.7608 |
| 9-HPODE | 2.74 | 311.2231 | NEG | C18H32O4 | HMDB0062434 | 29774-12-7 | C14827 | 0.2966 | 0.1820 | 1.7983 | 0.0000 | 0.6134 |
| 6-Pentyl-2H-pyran-2-one | 2.74 | 165.0922 | NEG | C10H14O2 | HMDB0031085 | 27593-23-3 |  | 2.7491 | 1.8153 | 1.2862 | 0.0026 | 0.6603 |
| Chlorothalonil-4-hydroxy | 2.74 | 244.9084 | NEG | C8HCl3N2O | HMDB0240624 | 28343-61-5 |  | 0.3698 | 0.2768 | 1.2162 | 0.0016 | 0.7486 |
| LPC(22:6) | 2.74 | 568.3394 | POS | C30H50NO7P |  |  |  | 0.5460 | 0.6345 | 1.2361 | 0.0162 | 1.1619 |
| PC(38:5) | 2.73 | 790.5738 | POS | C46H82NO8P |  |  |  | 0.1789 | 0.2360 | 1.3891 | 0.0120 | 1.3195 |
| 1-Amino-1-cyclobutanecarboxylic acid | 2.73 | 114.0562 | NEG | C5H9NO2 |  |  |  | 3.6298 | 2.5287 | 1.3582 | 0.0002 | 0.6966 |
| 4-Methyl-1H-pyrazole-3-carboxylic acid | 2.73 | 125.0358 | NEG | C5H6N2O2 |  |  |  | 0.0474 | 0.4155 | 1.8716 | 0.0001 | 8.7698 |
| 7H-[1,2,4]Triazolo[4,3-b][1,2,4]triazole-3,7-diamine | 2.73 | 140.068 | POS | C3H5N7 |  |  |  | 0.2652 | 0.3302 | 1.4850 | 0.0005 | 1.2451 |
| 2-Hydroxy-6-methylquinoline-3-carbaldehyde | 2.73 | 188.0704 | POS | C11H9NO2 |  |  |  | 1.2113 | 1.5695 | 1.0391 | 0.0022 | 1.2957 |
| 1-(4-Hydroxyphenyl)-2-methylaminoethanone | 2.73 | 164.0719 | NEG | C9H11NO2 |  |  |  | 5.4730 | 4.0990 | 1.5693 | 0.0002 | 0.7489 |
| 1-O-Octadecyl-sn-glyceryl-3-phosphorylcholine | 2.73 | 510.3914 | POS | C26H56NO6P | HMDB0011149 | 74430-89-0 | C04317 | 0.0834 | 0.1141 | 1.6735 | 0.0003 | 1.3675 |
| 2-(4-Oxo-4H-quinazolin-3-yl)-propanoic acid | 2.73 | 219.0762 | POS | C11H10N2O3 |  |  |  | 0.0057 | 0.0023 | 1.5849 | 0.0001 | 0.4097 |
| 2-((3aR,4S,7R,7aS)-1,3-Dioxohexahydro-1H-4,7-methanoisoindol-2(3H)-yl)propanoic acid | 2.73 | 236.093 | NEG | C12H15NO4 |  |  |  | 0.0888 | 0.0491 | 1.4263 | 0.0004 | 0.5526 |
| 4-(4-Piperidinyl)morpholine | 2.73 | 171.1491 | POS | C9H18N2O |  |  |  | 0.0243 | 0.0364 | 1.1073 | 0.0000 | 1.4940 |
| 3-Amino-4-ethylbenzenesulfonic acid | 2.73 | 200.0389 | NEG | C8H11NO3S |  |  |  | 0.0783 | 0.0556 | 1.5671 | 0.0003 | 0.7099 |
| (3-Methylbutyl)(6-methylheptan-2-yl)amine | 2.73 | 200.2371 | POS | C13H29N |  |  |  | 0.0019 | 0.0047 | 2.0656 | 0.0000 | 2.4628 |
| Ciprostene | 2.73 | 363.2543 | NEG | C22H36O4 |  |  |  | 0.4214 | 0.3094 | 1.4546 | 0.0008 | 0.7343 |
| 5-Hydroxy-2-(hydroxymethyl)pyridine | 2.73 | 124.0405 | NEG | C6H7NO2 |  |  |  | 0.1717 | 0.1209 | 1.0110 | 0.0067 | 0.7038 |
| (12Z)-9,10,11-Trihydroxyoctadec-12-enoic acid | 2.73 | 329.2336 | NEG | C18H34O5 |  |  |  | 0.7307 | 0.2874 | 1.8834 | 0.0000 | 0.3933 |
| 6-Hydroxyoctadec-4-enoic acid | 2.73 | 297.2436 | NEG | C18H34O3 |  |  |  | 0.1104 | 0.0884 | 1.2042 | 0.0058 | 0.8008 |
| 1-Hexadecyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine | 2.73 | 768.5891 | POS | C44H82NO7P |  |  |  | 1.4286 | 1.8682 | 1.4880 | 0.0009 | 1.3077 |
| 1-O-Hexadecyl-2-O-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glyceryl-3-phosphorylcholine | 2.73 | 766.5738 | POS | C44H80NO7P | HMDB0039528 | 132196-28-2 |  | 1.3560 | 1.7624 | 1.3721 | 0.0048 | 1.2997 |
| 2-(3-Methylbutoxy)acetic acid | 2.73 | 145.0871 | NEG | C7H14O3 |  |  |  | 0.2132 | 0.1575 | 1.5523 | 0.0006 | 0.7388 |
| 1-O-Hexadecyl-2-O-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glyceryl-3-phosphorylcholine | 2.73 | 792.5894 | POS | C46H82NO7P | HMDB0013409 | 132213-85-5 |  | 0.5941 | 0.7556 | 1.4131 | 0.0061 | 1.2717 |
| 1-(1Z-Octadecenyl)-2-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphocholine | 2.73 | 818.6047 | POS | C48H84NO7P | HMDB0011262 |  |  | 0.2355 | 0.2925 | 1.4184 | 0.0216 | 1.2416 |
| 3.beta.,7.alpha.-Dihydroxy-5-cholestenoic acid | 2.73 | 431.3172 | NEG | C27H44O4 |  |  |  | 0.7912 | 0.5924 | 1.3978 | 0.0003 | 0.7487 |
| N-Methyl-N-(methylsulfonyl)glycine | 2.73 | 166.0181 | NEG | C4H9NO4S |  |  |  | 3.6399 | 6.7376 | 1.3862 | 0.0005 | 1.8510 |
| 4-(1-Pyrazolyl)benzaldehyde | 2.73 | 173.0707 | POS | C10H8N2O |  |  |  | 0.0527 | 0.1039 | 1.7314 | 0.0001 | 1.9707 |
| 4-(4-Methyl-1-piperazinyl)butanoic acid | 2.73 | 187.1439 | POS | C9H18N2O2 |  |  |  | 0.0479 | 0.1604 | 1.8078 | 0.0000 | 3.3470 |
| Dexrazoxane | 2.73 | 267.1102 | NEG | C11H16N4O4 | HMDB0014524 | 24584-09-6 |  | 0.0873 | 0.0683 | 1.0508 | 0.0155 | 0.7821 |
| 4-Ethoxy-4-oxobut-2-enoic acid | 2.73 | 143.0351 | NEG | C6H8O4 | HMDB0246416 |  |  | 1.9124 | 1.4389 | 1.6779 | 0.0000 | 0.7524 |
| Mupirocin | 2.73 | 499.2917 | NEG | C26H44O9 | HMDB0014554 | 12650-69-0 | C11758 | 0.2360 | 0.1490 | 1.1214 | 0.0012 | 0.6314 |
| 2,4-dihydroxyheptadec-16-ynyl acetate | 2.73 | 325.2387 | NEG | C19H34O4 | HMDB0031048 | 24607-06-5 |  | 0.1141 | 0.0918 | 1.1847 | 0.0009 | 0.8044 |
| 1-Octadecylamine | 2.73 | 270.3153 | POS | C18H39N | HMDB0029586 | 124-30-1 |  | 0.0611 | 0.1067 | 2.2302 | 0.0000 | 1.7463 |
| D-Ribose | 2.73 | 149.0457 | NEG | C5H10O5 | HMDB0000283 | 613-83-2 | C00121 | 2.1911 | 1.1685 | 1.6182 | 0.0000 | 0.5333 |
| DIHYDROJASMONIC\_ACID | 2.73 | 211.1342 | NEG | C12H20O3 | HMDB0033601 | 98674-52-3 |  | 1.2716 | 0.9578 | 1.3415 | 0.0001 | 0.7532 |
| Pyrogallol | 2.73 | 125.0245 | NEG | C6H6O3 | HMDB0013674 | 87-66-1 | C01108 | 0.1503 | 0.1127 | 1.4229 | 0.0000 | 0.7494 |
| LPC(O-18:1) | 2.73 | 508.3759 | POS | C26H54NO6P |  |  |  | 0.2691 | 0.3597 | 1.5349 | 0.0006 | 1.3364 |
| LPC(20:4) | 2.73 | 544.3398 | POS | C28H50NO7P | HMDB0010395 |  |  | 0.0252 | 0.0880 | 1.0849 | 0.0000 | 3.4859 |
| Piperolactam A | 2.72 | 266.0816 | POS | C16H11NO3 | HMDB0033060 | 112501-42-5 |  | 0.0007 | 0.0028 | 1.6627 | 0.0088 | 4.2217 |
| 1-Pyrrolidinecarboximidamide | 2.72 | 114.1025 | POS | C5H11N3 |  |  |  | 0.0081 | 0.0229 | 1.0939 | 0.0045 | 2.8479 |
| L-Isoserine | 2.72 | 104.0355 | NEG | C3H7NO3 |  |  |  | 0.4608 | 0.7958 | 1.4685 | 0.0000 | 1.7270 |
| N-[4-(Pyridin-2-yl)-1,3-thiazol-2-yl]cyclopentanecarboxamide | 2.72 | 272.0867 | NEG | C14H15N3OS |  |  |  | 0.0244 | 0.0680 | 1.3683 | 0.0003 | 2.7913 |
| 2-Amino-5,5,5-trifluoropentanoic acid | 2.72 | 170.0436 | NEG | C5H8F3NO2 |  |  |  | 0.3941 | 0.3324 | 1.1205 | 0.0131 | 0.8434 |
| (2Z)-2-Hexadecenoic acid | 2.72 | 253.2177 | NEG | C16H30O2 |  |  |  | 0.1353 | 0.0982 | 1.0675 | 0.0029 | 0.7259 |
| Resorufin | 2.72 | 212.0351 | NEG | C12H7NO3 | HMDB0257166 |  |  | 0.0118 | 0.0074 | 1.5572 | 0.0332 | 0.6235 |
| 4-Methyloxazole-5-carboxylic acid | 2.72 | 126.0198 | NEG | C5H5NO3 |  |  |  | 0.5462 | 0.3841 | 1.3219 | 0.0001 | 0.7032 |
| Atropic acid | 2.72 | 147.0454 | NEG | C9H8O2 |  |  |  | 0.2547 | 0.1909 | 1.5483 | 0.0002 | 0.7494 |
| 5-Methyl-1H-pyrazole-3-carbaldehyde | 2.72 | 109.0408 | NEG | C5H6N2O |  |  |  | 1.3216 | 0.7188 | 1.5853 | 0.0002 | 0.5439 |
| 4-Hydroxytamoxifen | 2.72 | 386.2121 | NEG | C26H29NO2 | HMDB0060530 |  | C05011 | 0.0368 | 0.0697 | 1.1570 | 0.0000 | 1.8950 |
| Hexadecanedioic acid, 3,3,14,14-tetramethyl- | 2.72 | 341.27 | NEG | C20H38O4 | HMDB0254402 |  |  | 0.1759 | 0.1217 | 1.2614 | 0.0034 | 0.6918 |
| 9S,15S-Dihydroxy-5Z,13E-prostadienoic acid | 2.72 | 337.2387 | NEG | C20H34O4 |  |  |  | 0.1865 | 0.1321 | 1.4943 | 0.0005 | 0.7086 |
| 8-Methoxy-4-oxo-1,4-dihydroquinoline-2-carboxylic acid | 2.72 | 218.0459 | NEG | C11H9NO4 | HMDB0060426 |  | C05830 | 0.1127 | 0.0705 | 1.1627 | 0.0029 | 0.6253 |
| 1-Hexadecyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine | 2.72 | 746.6043 | POS | C42H84NO7P |  |  |  | 0.3940 | 0.4420 | 1.0190 | 0.0345 | 1.1217 |
| 3-(Aminocarbonyl)benzoic acid | 2.72 | 164.0355 | NEG | C8H7NO3 |  |  |  | 0.2041 | 0.1376 | 1.2464 | 0.0207 | 0.6739 |
| 4,5-DIDEMETHYLSIMMONDSIN | 2.72 | 344.1352 | NEG | C15H23NO8 | HMDB0041207 | 135074-86-1 |  | 0.1294 | 0.0899 | 1.6869 | 0.0000 | 0.6950 |
| LPC(O-22:1) | 2.72 | 564.4389 | POS | C30H62NO6P |  |  |  | 0.0147 | 0.0203 | 1.1010 | 0.0035 | 1.3861 |
| Eicoseneoylcarnitine (Car(20:1)) | 2.72 | 454.3896 | POS | C27H51NO4 |  |  |  | 0.0070 | 0.0105 | 1.5670 | 0.0018 | 1.5049 |
| Piperazine-N,N'-bis(2-hydroxypropanesulfonic acid) | 2.71 | 363.0898 | POS | C10H22N2O8S2 |  |  |  | 0.0310 | 0.0211 | 1.1496 | 0.0061 | 0.6821 |
| DL-2-Methylglutamic acid | 2.71 | 160.0617 | NEG | C6H11NO4 |  |  |  | 0.4135 | 0.3302 | 1.4115 | 0.0026 | 0.7987 |
| 1-Methylhydantoin | 2.71 | 115.0503 | POS | C4H6N2O2 | HMDB0003646 | 616-04-6 | C02565 | 0.0017 | 0.0512 | 1.7596 | 0.0006 | 29.5578 |
| 1-Oleoyl-2-palmitoyl-sn-glycero-3-phosphocholine | 2.71 | 760.5832 | POS | C42H82NO8P | HMDB0008100 |  |  | 0.2173 | 0.3453 | 1.5203 | 0.0041 | 1.5888 |
| 15S-Hydroperoxy-11Z,13E-eicosadienoic acid | 2.71 | 339.2545 | NEG | C20H36O4 |  |  |  | 0.1814 | 0.1329 | 1.3306 | 0.0008 | 0.7323 |
| Urushiol I | 2.71 | 319.2645 | NEG | C21H36O2 |  |  |  | 0.0923 | 0.0720 | 1.1165 | 0.0207 | 0.7801 |
| Trihydroxycholestanoic acid | 2.71 | 449.3281 | NEG | C27H46O5 | HMDB0000601 | 547-98-8 |  | 0.3869 | 0.2722 | 1.2260 | 0.0008 | 0.7036 |
| 3-Dodecyloxypropylamine | 2.71 | 244.2632 | POS | C15H33NO |  |  |  | 0.0167 | 0.0250 | 2.1903 | 0.0000 | 1.4960 |
| 2,5-Dimethyl-4-pyrimidinamine | 2.71 | 124.0868 | POS | C6H9N3 |  |  |  | 0.0156 | 0.0082 | 1.3946 | 0.0004 | 0.5289 |
| (3E,5E)-2-(4-Methoxy-4-oxobutyl)nona-3,5-dienoic acid | 2.71 | 253.1447 | NEG | C14H22O4 |  |  |  | 0.1219 | 0.0842 | 1.4136 | 0.0002 | 0.6911 |
| 5.alpha.-Pregnan-3.alpha.,17-diol-20-one 3-sulfate | 2.71 | 413.2009 | NEG | C21H34O6S |  |  |  | 6.2815 | 4.1888 | 1.2531 | 0.0007 | 0.6668 |
| 2-Methylpropanamine | 2.71 | 74.0964 | POS | C4H11N | HMDB0034198 | 78-81-9 | C02787 | 0.8213 | 2.8073 | 1.9195 | 0.0000 | 3.4182 |
| (S)-3,4-Dihydroxybutyric acid (lithium hydrate) | 2.71 | 119.0351 | NEG | C4H8O4 | HMDB0000337 | 51267-44-8 |  | 2.0820 | 1.7992 | 1.0981 | 0.0008 | 0.8642 |
| 4-Hydroxyglutamic acid | 2.71 | 144.0305 | NEG | C5H9NO5 | HMDB0002273 | 2485-33-8 | C05947 | 0.2934 | 0.1568 | 1.7596 | 0.0001 | 0.5346 |
| Isovaleramide | 2.71 | 102.0911 | POS | C5H11NO |  | 541-46-8 | D04637 | 0.0703 | 0.3402 | 1.9361 | 0.0000 | 4.8380 |
| PI(16:0/18:1) | 2.71 | 835.5325 | NEG | C43H81O13P | HMDB0009783 | 50730-13-7 | C13888 | 1.3080 | 0.8495 | 1.2309 | 0.0001 | 0.6494 |
| 2-Hydroxy-1,3-dimethyl-9H-thioxanthen-9-one | 2.7 | 255.0478 | NEG | C15H12O2S |  |  |  | 0.0099 | 0.2159 | 1.7395 | 0.0009 | 21.8835 |
| Pro-Pro | 2.7 | 213.1235 | POS | C10H16N2O3 | HMDB0011180 | 20488-28-2 |  | 0.0263 | 0.0103 | 1.7156 | 0.0000 | 0.3913 |
| 2-Amino-4,4,4-trifluorobutanoic acid | 2.7 | 156.0278 | NEG | C4H6F3NO2 |  |  |  | 0.2087 | 0.2660 | 1.0045 | 0.0001 | 1.2742 |
| His-Thr | 2.7 | 257.1243 | POS | C10H16N4O4 | HMDB0028895 | 142879-28-5 |  | 0.0059 | 0.0039 | 1.2940 | 0.0084 | 0.6724 |
| Pro-Asp | 2.7 | 229.0832 | NEG | C9H14N2O5 |  |  |  | 0.2088 | 0.1264 | 1.1112 | 0.0243 | 0.6052 |
| 2-(4-Amino-1-piperidinyl)acetamide | 2.7 | 158.1288 | POS | C7H15N3O |  |  |  | 0.0892 | 0.0657 | 1.4143 | 0.0002 | 0.7366 |
| 5-((1E,3E)-Hepta-1,3-dien-1-yl)-1,2,3-trihydroxycyclopentanecarboxylic acid | 2.7 | 255.1245 | NEG | C13H20O5 |  |  |  | 0.4267 | 0.3265 | 1.2557 | 0.0035 | 0.7650 |
| N-Methyldioctylamine | 2.7 | 256.2998 | POS | C17H37N |  |  |  | 0.0012 | 0.0025 | 1.0545 | 0.0000 | 2.0712 |
| Palmitoyleicosapentaenoyl phosphatidylcholine | 2.7 | 780.5519 | POS | C44H78NO8P |  |  |  | 1.1171 | 1.4173 | 1.3171 | 0.0016 | 1.2687 |
| (2-{[2-docosanamido-3-hydroxyoctadec-4-en-1-yl phosphonato]oxy}ethyl)trimethylazanium | 2.7 | 845.6711 | NEG | C45H91N2O6P | HMDB0012103 | 94359-12-3 |  | 0.1806 | 0.1325 | 1.0173 | 0.0011 | 0.7336 |
| PC(36:5) | 2.7 | 780.552 | POS | C44H78NO8P | HMDB0007890 |  |  | 0.0233 | 0.0346 | 1.5275 | 0.0088 | 1.4867 |
| PC(38:7) | 2.7 | 804.5517 | POS | C46H78NO8P |  |  |  | 0.0299 | 0.0350 | 1.1977 | 0.0010 | 1.1701 |
| Thr-Glu | 2.69 | 247.0937 | NEG | C9H16N2O6 |  |  |  | 0.0045 | 0.5221 | 1.8044 | 0.0003 | 115.0797 |
| 2-(Naphthalen-1-yl)-1H-1,3-benzodiazole | 2.69 | 245.1065 | POS | C17H12N2 |  |  |  | 0.0586 | 0.0403 | 1.0953 | 0.0058 | 0.6868 |
| Diisopropyl\_sulfide | 2.69 | 119.0893 | POS | C6H14S | HMDB0029579 | 625-80-9 |  | 0.2354 | 0.2773 | 1.1049 | 0.0043 | 1.1780 |
| Arg-Gly-Asp | 2.69 | 347.1682 | POS | C12H22N6O6 | HMDB0248572 |  |  | 0.0031 | 0.0144 | 1.7615 | 0.0000 | 4.5933 |
| cis-4-Hydroxycyclohexanecarboxylic acid | 2.69 | 143.0715 | NEG | C7H12O3 |  |  |  | 0.1245 | 0.0909 | 1.5404 | 0.0000 | 0.7304 |
| 1-Hexadecyl-2-(8Z,11Z,14Z-eicosatrienoyl)-sn-glycero-3-phosphocholine | 2.69 | 770.6029 | POS | C44H84NO7P |  |  |  | 0.4667 | 0.5601 | 1.1561 | 0.0131 | 1.2002 |
| 9-Hydroxyrisperidone | 2.69 | 425.2009 | NEG | C23H27FN4O3 | HMDB0015396 | 144598-75-4 |  | 0.4104 | 0.2686 | 1.0012 | 0.0234 | 0.6543 |
| 5-Isopropyl-5-methylhydantoin | 2.68 | 157.0971 | POS | C7H12N2O2 |  |  |  | 0.0186 | 0.0103 | 1.7251 | 0.0000 | 0.5530 |
| 2-Amino-3-(1H-pyrazol-1-yl)propanoic acid | 2.68 | 156.0767 | POS | C6H9N3O2 | HMDB0034267 | 2734-48-7 |  | 0.0567 | 0.2488 | 1.1989 | 0.0000 | 4.3891 |
| 1,11-Undecanedicarboxylic acid | 2.68 | 243.1604 | NEG | C13H24O4 | HMDB0002327 | 505-52-2 |  | 0.0755 | 0.0491 | 1.2173 | 0.0183 | 0.6502 |
| 1,2-Distearoyl-sn-glycero-3-phospho-(1'-rac-glycerol) | 2.68 | 777.5683 | NEG | C42H83O10P |  |  |  | 0.0798 | 0.0588 | 1.0502 | 0.0092 | 0.7366 |
| Meclizine | 2.68 | 391.1944 | POS | C25H27ClN2 | HMDB0014875 | 569-65-3 | C07116 | 0.0013 | 0.0045 | 1.7491 | 0.0000 | 3.4337 |
| LPC(O-20:0) | 2.68 | 538.4245 | POS | C28H60NO6P |  |  |  | 0.0141 | 0.0180 | 1.3844 | 0.0055 | 1.2778 |
| 2-(Chloromethyl)-5,6-dimethylthieno[2,3-d]pyrimidin-4-ol | 2.67 | 227.0052 | NEG | C9H9ClN2OS |  |  |  | 0.9343 | 0.5936 | 1.2128 | 0.0041 | 0.6354 |
| Valdecoxib | 2.67 | 315.0798 | POS | C16H14N2O3S | HMDB0005033 | 181695-72-7 |  | 0.0972 | 2.9250 | 1.7492 | 0.0004 | 30.0900 |
| 4-Methyl-3-(trifluoromethyl)-1H-pyrazol-5-amine | 2.67 | 166.0579 | POS | C5H6F3N3 |  |  |  | 0.0099 | 0.0146 | 1.1106 | 0.0088 | 1.4813 |
| 5-Aminopentanal | 2.67 | 102.0913 | POS | C5H11NO | HMDB0012815 |  | C12455 | 0.0632 | 0.0323 | 1.7956 | 0.0001 | 0.5118 |
| 1-Behenoyl-2-hydroxy-sn-glycero-3-phosphocholine | 2.67 | 580.4334 | POS | C30H62NO7P | HMDB0010398 |  | C04230 | 0.0257 | 0.0326 | 1.1004 | 0.0100 | 1.2705 |
| D-SEDOHEPTULOSE | 2.67 | 209.0677 | NEG | C7H14O7 | HMDB0254327 |  |  | 0.2496 | 0.3844 | 1.5043 | 0.0000 | 1.5401 |
| 6-Thioinosine | 2.67 | 283.0519 | NEG | C10H12N4O4S |  |  |  | 0.8465 | 0.6978 | 1.2809 | 0.0155 | 0.8243 |
| 3-Hydroxy-2-[(Z)-oct-2-enyl]pentanedioic acid | 2.67 | 257.1396 | NEG | C13H22O5 |  |  |  | 0.3467 | 0.2718 | 1.3890 | 0.0011 | 0.7839 |
| Thelephoric acid | 2.67 | 351.0125 | NEG | C18H8O8 | HMDB0030552 | 479-64-1 |  | 0.1144 | 0.4182 | 1.7879 | 0.0000 | 3.6565 |
| Suberohydroxamic acid | 2.66 | 203.1039 | NEG | C8H16N2O4 |  |  |  | 0.0068 | 0.0834 | 1.8289 | 0.0000 | 12.2151 |
| 2-(Aminomethyl)-4-chlorophenol | 2.66 | 156.023 | NEG | C7H8ClNO |  |  |  | 0.0074 | 0.3241 | 1.6983 | 0.0026 | 43.7294 |
| 2-Oct-7-enylpentanedioic acid | 2.66 | 241.1447 | NEG | C13H22O4 |  |  |  | 0.0509 | 0.0355 | 1.3149 | 0.0006 | 0.6969 |
| Arachidonic sulfonic acid | 2.66 | 339.2 | NEG | C19H32O3S |  |  |  | 11.0525 | 8.7894 | 1.0246 | 0.0176 | 0.7952 |
| 3-Hydroxyglutaric acid | 2.65 | 147.0301 | NEG | C5H8O5 | HMDB0000428 | 638-18-6 |  | 0.2315 | 0.1354 | 1.1123 | 0.0014 | 0.5849 |
| 4-(Pentafluorosulfanyl)aniline | 2.65 | 220.0201 | POS | C6H6F5NS |  |  |  | 0.0063 | 0.0110 | 1.6758 | 0.0004 | 1.7470 |
| 5-(2-Fluorobenzyl)-1,3-thiazol-2-amine | 2.65 | 209.0532 | POS | C10H9FN2S |  |  |  | 0.0026 | 0.1873 | 1.8675 | 0.0000 | 72.7102 |
| 2-(1-Methyl-1H-pyrazol-4-yl)-1H-benzimidazole | 2.65 | 197.0822 | NEG | C11H10N4 |  |  |  | 0.0297 | 0.0228 | 1.1869 | 0.0169 | 0.7663 |
| Phaclofen | 2.65 | 248.0236 | NEG | C9H13ClNO3P | HMDB0256382 |  |  | 0.4849 | 0.2015 | 1.3170 | 0.0000 | 0.4155 |
| Hymexazole | 2.65 | 100.0392 | POS | C4H5NO2 |  |  |  | 0.0184 | 0.0116 | 1.2230 | 0.0001 | 0.6305 |
| 5-Bromo-4-fluoro-2-hydroxybenzoic acid | 2.65 | 232.9251 | NEG | C7H4BrFO3 |  |  |  | 0.0720 | 0.0556 | 1.2038 | 0.0014 | 0.7720 |
| Artocarpin | 2.65 | 437.1937 | POS | C26H28O6 | HMDB0030849 | 7608-44-8 |  | 0.0033 | 0.0040 | 1.0960 | 0.0050 | 1.2316 |
| FA 18:3+2O | 2.65 | 309.2073 | NEG | C18H30O4 | HMDB0246689 |  |  | 0.1625 | 0.1139 | 1.4826 | 0.0001 | 0.7008 |
| LPC(19:0) | 2.65 | 538.3861 | POS | C27H56NO7P |  | 108273-88-7 |  | 0.0552 | 0.0787 | 1.7263 | 0.0000 | 1.4273 |
| N6-(1-Iminoethyl)-L-lysine | 2.64 | 188.1394 | POS | C8H17N3O2 | HMDB0249982 |  |  | 0.0291 | 0.0161 | 1.1608 | 0.0371 | 0.5543 |
| (.+/-.)-Nuarimol | 2.64 | 315.0676 | POS | C17H12ClFN2O |  |  |  | 0.0545 | 3.6656 | 1.7596 | 0.0004 | 67.2445 |
| 4-Chloro-6-propylamino-2-methylthiopyrimidine | 2.64 | 218.051 | POS | C8H12ClN3S |  |  |  | 0.0021 | 0.0052 | 1.4104 | 0.0080 | 2.4509 |
| 2-Naphthalenecarboxamide, N-[2-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)ethyl]- | 2.64 | 427.2165 | NEG | C26H28N4O2 |  |  |  | 0.4676 | 0.3253 | 1.2628 | 0.0035 | 0.6956 |
| 2-({2-[(2-Carboxyphenyl)sulfanyl]ethyl}sulfanyl)benzoic acid | 2.63 | 333.0237 | NEG | C16H14O4S2 |  |  |  | 0.0093 | 0.3911 | 1.9030 | 0.0000 | 42.0222 |
| 2-Cyano-N-(3,4-difluorophenyl)acetamide | 2.63 | 197.0532 | POS | C9H6F2N2O |  |  |  | 0.0151 | 0.3132 | 1.6352 | 0.0004 | 20.8060 |
| (2E)-4-Hydroxybut-2-enoic acid | 2.63 | 101.0245 | NEG | C4H6O3 | HMDB0003381 | 24587-49-3 |  | 2.9869 | 2.1834 | 1.7074 | 0.0000 | 0.7310 |
| o-Nitrobenzoic acid | 2.63 | 166.0146 | NEG | C7H5NO4 | HMDB0245255 |  | C16234 | 0.6214 | 0.3142 | 1.5740 | 0.0000 | 0.5055 |
| 4-{[4-(Acetyloxy)benzoyl]amino}benzoic acid | 2.63 | 298.07 | NEG | C16H13NO5 |  |  |  | 1.2709 | 0.6970 | 1.6140 | 0.0019 | 0.5484 |
| 4-Amino-2-oxo-1,2-dihydropyrimidine-5-carboxylic acid | 2.63 | 154.026 | NEG | C5H5N3O3 | HMDB0246202 |  |  | 2.4242 | 1.7342 | 1.5685 | 0.0023 | 0.7153 |
| Heptadecanoyl\_carnitine | 2.63 | 414.3578 | POS | C24H47NO4 | HMDB0006210 | 106182-29-0 |  | 0.0075 | 0.0098 | 1.1803 | 0.0006 | 1.3186 |
| PC(40:9) | 2.63 | 828.5493 | POS | C48H78NO8P |  |  |  | 0.0498 | 0.0686 | 1.8256 | 0.0000 | 1.3774 |
| LPA(0:0/18:2(9Z,12Z)) | 2.62 | 435.2506 | POS | C21H39O7P | HMDB0007852 |  |  | 0.0016 | 0.0026 | 1.2907 | 0.0000 | 1.6391 |
| 4-Chloro-N-(2-methoxy-5-methylphenyl)benzenesulfonamide | 2.62 | 310.0328 | NEG | C14H14ClNO3S |  |  |  | 0.1486 | 0.4349 | 1.3740 | 0.0000 | 2.9261 |
| 1-(3-(Trifluoromethyl)phenyl)piperazine | 2.62 | 231.1087 | POS | C11H13F3N2 | HMDB0244703 |  |  | 0.0019 | 0.0060 | 1.3016 | 0.0001 | 3.1128 |
| 5,10-Dihydro-10-phenophosphazinol 10-oxide | 2.61 | 230.0396 | NEG | C12H10NO2P |  |  |  | 0.1718 | 0.1500 | 1.5423 | 0.0010 | 0.8734 |
| Damnacanthal | 2.61 | 283.0624 | POS | C16H10O5 | HMDB0250841 |  |  | 0.0334 | 0.0223 | 1.1910 | 0.0035 | 0.6673 |
| L-Arginine ethyl ester | 2.61 | 203.1501 | POS | C8H18N4O2 |  |  |  | 0.0082 | 0.0191 | 1.0907 | 0.0263 | 2.3273 |
| 6-Fluoro-2-(trifluoromethyl)-4-quinolinol | 2.61 | 230.0253 | NEG | C10H5F4NO |  |  |  | 0.2574 | 0.1335 | 1.7365 | 0.0000 | 0.5186 |
| monolinolein | 2.61 | 393.24 | POS | C21H38O4 | HMDB0242115 |  |  | 0.0008 | 0.0016 | 1.6129 | 0.0000 | 2.0054 |
| 3,5-Dihydroxyphenylglycine | 2.61 | 182.046 | NEG | C8H9NO4 | HMDB0244908 |  |  | 0.1339 | 0.0931 | 1.1476 | 0.0006 | 0.6951 |
| PC(18:1) | 2.6 | 518.3219 | POS | C26H50NO8P |  | 56391-91-4 |  | 1.1562 | 1.5014 | 1.6164 | 0.0000 | 1.2986 |
| 3-{[(4-Fluorophenyl)sulfanyl]methyl}-1-benzofuran-2-carboxylic acid | 2.6 | 301.0352 | NEG | C16H11FO3S |  |  |  | 0.0016 | 0.0070 | 1.7827 | 0.0000 | 4.5002 |
| 2,2,5,5-Tetramethyl-2,5-dihydro-1H-imidazole-4-thiol | 2.6 | 159.0957 | POS | C7H14N2S |  |  |  | 0.0064 | 0.0245 | 1.4461 | 0.0125 | 3.8096 |
| N-Acetylglycylglycine | 2.6 | 173.057 | NEG | C6H10N2O4 |  |  |  | 0.2297 | 1.5720 | 1.4738 | 0.0034 | 6.8442 |
| 1-(2,4-Dihydroxyphenyl)-2-(4-nitrophenyl)ethanone | 2.6 | 272.0542 | NEG | C14H11NO5 |  |  |  | 0.1568 | 0.0960 | 1.3387 | 0.0084 | 0.6125 |
| 5-(4-Acetoxy-3-oxo-1-butynyl)-2,2'-bithiophene | 2.6 | 291.0122 | POS | C14H10O3S2 | HMDB0038459 | 1222-83-9 |  | 0.0143 | 0.0906 | 1.0339 | 0.0061 | 6.3488 |
| Alloimperatorin | 2.6 | 271.0925 | POS | C16H14O4 | HMDB0301848 |  | C09053 | 0.0372 | 0.0453 | 1.2266 | 0.0430 | 1.2157 |
| 4,4-Difluoro-1-phenyl-1,3-butanedione | 2.59 | 199.0574 | POS | C10H8F2O2 |  |  |  | 0.0022 | 0.0031 | 1.1053 | 0.0092 | 1.4112 |
| Prolyl-Histidine | 2.59 | 253.128 | POS | C11H16N4O3 | HMDB0029019 |  |  | 0.0043 | 0.0118 | 1.7210 | 0.0004 | 2.7532 |
| Gln-Glu | 2.58 | 274.1049 | NEG | C10H17N3O6 |  |  |  | 0.0270 | 0.0535 | 1.4850 | 0.0000 | 1.9832 |
| 4-Methyl-N-(4-methyl-2-pyridinyl)benzenesulfonamide | 2.58 | 263.0874 | POS | C13H14N2O2S |  |  |  | 0.0080 | 0.0421 | 1.1770 | 0.0006 | 5.2563 |
| Vanilpyruvic\_acid | 2.58 | 211.0593 | POS | C10H10O5 | HMDB0011714 | 1081-71-6 |  | 0.0005 | 0.0016 | 1.2620 | 0.0345 | 3.0384 |
| 1,6-Dihydroxy-3,7-dimethoxy-2-(2-hydroxy-3-methyl-3-butenyl)-8-(3-methyl-2-butenyl)-xanthone | 2.58 | 441.1887 | POS | C25H28O7 | HMDB0039915 |  |  | 0.0158 | 0.0225 | 1.3237 | 0.0105 | 1.4288 |
| Dihydrocitrinone | 2.57 | 265.0692 | NEG | C13H14O6 |  |  |  | 0.2530 | 0.1177 | 1.8430 | 0.0000 | 0.4654 |
| rac-4-Sulfoxypropranolol | 2.57 | 354.1041 | NEG | C16H21NO6S |  |  |  | 0.0176 | 0.0123 | 1.3594 | 0.0019 | 0.7009 |
| 1-Methyl-3-isobutylxanthine | 2.57 | 223.1175 | POS | C10H14N4O2 | HMDB0245912 |  | C13708 | 0.0066 | 0.0214 | 1.6068 | 0.0052 | 3.2307 |
| Nodakenitin | 2.57 | 247.0926 | POS | C14H14O4 | HMDB0302268 |  | C09278 | 0.0019 | 0.0649 | 1.5607 | 0.0025 | 34.0713 |
| 1h-indole-3-butanoic acid | 2.57 | 204.0979 | POS | C12H13NO2 | HMDB0002096 | 133-32-4 | C11284 | 0.0360 | 0.2623 | 1.4780 | 0.0014 | 7.2948 |
| 6-Nitro-1,2,3-benzotriazin-4(3H)-one | 2.56 | 191.0201 | NEG | C7H4N4O3 |  |  |  | 0.9231 | 5.1918 | 1.8654 | 0.0000 | 5.6244 |
| 4-Allyl-5-(2-methylphenyl)-4H-1,2,4-triazol-3-yl hydrosulfide | 2.56 | 232.0929 | POS | C12H13N3S |  |  |  | 0.0008 | 0.0219 | 1.7441 | 0.0000 | 25.8410 |
| (2R)-2-(2,5-Difluorophenyl)pyrrolidine | 2.56 | 184.0943 | POS | C10H11F2N |  |  |  | 0.7480 | 0.8519 | 1.1064 | 0.0080 | 1.1389 |
| 1H-Indazole-3-carboxamide, 1-(5-fluoropentyl)-N-8-quinolinyl- | 2.56 | 377.1785 | POS | C22H21FN4O |  |  |  | 0.0009 | 0.0078 | 1.7846 | 0.0000 | 8.4432 |
| 1-Hydroxy-2-naphthoic acid | 2.56 | 187.0421 | NEG | C11H8O3 | HMDB0243892 |  | C03203 | 6.3007 | 5.1829 | 1.2556 | 0.0225 | 0.8226 |
| PC(22:4(7Z,10Z,13Z,16Z)/P-18:1(9Z)) | 2.56 | 820.6224 | POS | C48H86NO7P | HMDB0008655 |  | C00157 | 0.0529 | 0.0628 | 1.0516 | 0.0191 | 1.1868 |
| DG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/0:0) | 2.56 | 615.4966 | POS | C39H66O5 | HMDB0007222 |  |  | 0.0085 | 0.0107 | 1.1065 | 0.0023 | 1.2576 |
| 5,6,7,8-Tetrahydrothieno[2,3-b]quinolin-4-amine | 2.55 | 205.0819 | POS | C11H12N2S |  |  |  | 0.0023 | 0.0557 | 1.8061 | 0.0001 | 24.0541 |
| 3-Cyano-4,7-dimethylcoumarin | 2.55 | 200.0682 | POS | C12H9NO2 |  |  |  | 0.0176 | 0.0913 | 1.6528 | 0.0000 | 5.1939 |
| Methanone, (4-ethyl-1-naphthalenyl)(5-hydroxy-1-pentyl-1H-indol-3-yl)- | 2.55 | 386.2075 | POS | C26H27NO2 |  |  |  | 0.0040 | 0.0235 | 1.8796 | 0.0000 | 5.8346 |
| threo-Syringoylglycerol | 2.55 | 245.0996 | POS | C11H16O6 | HMDB0031237 | 121748-11-6 |  | 0.0276 | 0.1126 | 1.5750 | 0.0076 | 4.0854 |
| Methyl 1-hydroxy-2-naphthoate | 2.55 | 201.0578 | NEG | C12H10O3 |  |  |  | 0.5083 | 0.3677 | 1.0087 | 0.0253 | 0.7235 |
| 5-(4-Aminophenyl)-4-phenyl-2,4-dihydro-3H-1,2,4-triazole-3-thione | 2.55 | 267.0735 | NEG | C14H12N4S |  |  |  | 0.8834 | 0.5230 | 1.4124 | 0.0073 | 0.5920 |
| N-(2-Thienylmethyl)-7H-purin-6-amine | 2.55 | 232.0637 | POS | C10H9N5S |  |  |  | 0.0059 | 0.0030 | 1.0026 | 0.0332 | 0.5116 |
| N-Docosanoyltaurine | 2.55 | 446.3362 | NEG | C24H49NO4S |  |  |  | 2.1531 | 1.6724 | 1.2828 | 0.0020 | 0.7768 |
| 3-(5-Amino-3-methyl-1H-pyrazol-1-yl)propanenitrile | 2.55 | 151.0964 | POS | C7H10N4 |  |  |  | 0.0606 | 0.0725 | 1.0276 | 0.0155 | 1.1959 |
| 16,16-Dimethylprostaglandin A2 | 2.55 | 361.2363 | NEG | C22H34O4 |  |  |  | 0.5492 | 0.4102 | 1.5140 | 0.0002 | 0.7469 |
| Triptophenolide | 2.55 | 311.1689 | NEG | C20H24O3 |  |  |  | 20.8088 | 15.5062 | 1.1919 | 0.0125 | 0.7452 |
| 8-Geranyl-7-hydroxycoumarin | 2.55 | 297.1532 | NEG | C19H22O3 |  |  |  | 8.0499 | 5.8361 | 1.2205 | 0.0110 | 0.7250 |
| Pyrazolam | 2.54 | 354.0305 | POS | C16H12BrN5 |  |  |  | 0.0029 | 0.0164 | 1.7889 | 0.0000 | 5.5971 |
| 2,5-Dimethyl-3,4-diphenyl-2,4-cyclopentadien-1-one | 2.54 | 261.1306 | POS | C19H16O |  |  |  | 0.0189 | 0.0228 | 1.5390 | 0.0001 | 1.2045 |
| Triciribine | 2.54 | 321.1311 | POS | C13H16N6O4 |  |  |  | 0.0103 | 0.0142 | 1.4401 | 0.0014 | 1.3784 |
| 1,6-Anhydro-.beta.-D-glucose | 2.54 | 161.0457 | NEG | C6H10O5 | HMDB0000640 | 498-07-7 |  | 3.5341 | 2.6041 | 1.8274 | 0.0000 | 0.7368 |
| 2-Bromo-4,6-dichlorophenol | 2.53 | 238.8704 | NEG | C6H3BrCl2O |  |  |  | 0.2020 | 0.1073 | 1.6982 | 0.0002 | 0.5311 |
| 4-(1,3-Dithiolan-2-yl)aniline | 2.53 | 198.0381 | POS | C9H11NS2 |  |  |  | 0.0049 | 0.0215 | 1.7061 | 0.0002 | 4.3731 |
| 5-(2-methoxyethylamino)-3H-1,3,4-thiadiazole-2-thione | 2.53 | 192.0244 | POS | C5H9N3OS2 |  |  |  | 0.0095 | 0.0171 | 1.3345 | 0.0000 | 1.8040 |
| 6-Hydrazino-3-pyridazinecarboxamide | 2.53 | 154.0743 | POS | C5H7N5O |  |  |  | 0.0313 | 0.1036 | 1.5708 | 0.0002 | 3.3090 |
| Benz[a]anthracen-1-ol, 8-methoxy-3-methyl- | 2.53 | 289.1258 | POS | C20H16O2 |  |  |  | 0.0092 | 0.0606 | 1.6912 | 0.0002 | 6.5627 |
| 8beta-Angeloyloxy-15-hydroxy-1alpha,10R-dimethoxy-3-oxo-11(13)-germacren-12,6alpha-olide | 2.53 | 425.2149 | POS | C22H32O8 | HMDB0039013 |  |  | 0.0054 | 0.0067 | 1.2548 | 0.0027 | 1.2456 |
| Gln-Arg | 2.53 | 301.1592 | NEG | C11H22N6O4 |  |  |  | 0.1706 | 0.1211 | 1.2435 | 0.0041 | 0.7098 |
| 1-(1H-Indol-3-yl)-2-(4-morpholinyl)-2-oxoethanone | 2.53 | 257.0965 | NEG | C14H14N2O3 |  |  |  | 0.0750 | 0.0173 | 1.1648 | 0.0000 | 0.2300 |
| 5-Amino-2-(5-amino-1,3-benzoxazol-2-yl)phenol | 2.53 | 240.075 | NEG | C13H11N3O2 |  |  |  | 0.1491 | 0.0701 | 1.3727 | 0.0032 | 0.4703 |
| 3-Hydroxy-3-(methoxycarbonyl)pentanedioic acid | 2.53 | 205.0355 | NEG | C7H10O7 |  |  |  | 0.2946 | 0.1766 | 1.1760 | 0.0162 | 0.5994 |
| 1-Allyl-6-hydroxy-2,4(1H,3H)-pyrimidinedione | 2.52 | 167.0439 | NEG | C7H8N2O3 |  |  |  | 0.2496 | 0.2287 | 1.3257 | 0.0207 | 0.9164 |
| Endothal dimethyl ester | 2.52 | 215.089 | POS | C10H14O5 |  |  |  | 0.0130 | 0.0328 | 1.4197 | 0.0037 | 2.5181 |
| 1H-Pyrrole-2,5-dione, 1-methyl-3-(1-methyl-1H-indol-3-yl)-4-(pentylamino)- | 2.52 | 326.1904 | POS | C19H23N3O2 |  |  |  | 0.0008 | 0.0030 | 1.3968 | 0.0067 | 3.7372 |
| Arachidyl\_carnitine | 2.52 | 456.4052 | POS | C27H53NO4 | HMDB0006460 |  |  | 0.0032 | 0.0062 | 1.6965 | 0.0001 | 1.9776 |
| N-[4-Nitro-3-(trifluoromethyl)phenyl]acetamide | 2.51 | 249.0458 | POS | C9H7F3N2O3 |  |  |  | 0.0004 | 0.0090 | 1.5327 | 0.0000 | 20.9763 |
| 5-(Trifluoromethyl)-2(1H)-pyridinone | 2.51 | 164.0294 | POS | C6H4F3NO |  |  |  | 0.0442 | 0.0763 | 1.4073 | 0.0003 | 1.7275 |
| Ikarugamycin | 2.51 | 477.282 | NEG | C29H38N2O4 |  |  |  | 0.5121 | 0.4187 | 1.0301 | 0.0462 | 0.8175 |
| 1-(4-Chlorophenyl)-2-[(5-methyl-4H-1,2,4-triazol-3-yl)sulfanyl]ethanone | 2.51 | 266.0179 | NEG | C11H10ClN3OS |  |  |  | 45.6486 | 24.3673 | 1.4970 | 0.0002 | 0.5338 |
| Acetyl tributyl citrate | 2.51 | 403.2329 | POS | C20H34O8 | HMDB0034159 | 77-90-7 |  | 0.0251 | 0.0358 | 1.8525 | 0.0001 | 1.4243 |
| Desisopropyldisopyramide | 2.5 | 298.1872 | POS | C18H23N3O | HMDB0061024 |  |  | 0.0100 | 0.0122 | 1.1077 | 0.0004 | 1.2207 |
| 2-(3-Carboxy-4-chlorophenyl)-1,3-dioxo-2,3-dihydro-1H-isoindole-5-carboxylic acid | 2.5 | 343.9952 | NEG | C16H8ClNO6 |  |  |  | 0.7024 | 3.4891 | 1.5622 | 0.0004 | 4.9673 |
| Altenuene | 2.5 | 291.0837 | NEG | C15H16O6 |  |  |  | 0.9607 | 96.4211 | 1.8097 | 0.0000 | 100.3638 |
| Fenarimol | 2.5 | 331.0449 | POS | C17H12Cl2N2O | HMDB0040599 |  | C11226 | 0.1247 | 5.8648 | 1.8508 | 0.0000 | 47.0418 |
| 2-(4-Morpholinyl)-4H-pyrimido[2,1-a]isoquinolin-4-one | 2.5 | 282.1195 | POS | C16H15N3O2 |  |  |  | 0.1194 | 0.1360 | 1.3666 | 0.0076 | 1.1393 |
| 3H-Benzimidazol-5-yl-[4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]pyrimidin-2-yl]amine | 2.5 | 333.1522 | POS | C17H16N8 |  |  |  | 0.0030 | 0.0285 | 1.8016 | 0.0000 | 9.6226 |
| 1-O-Hexadecyl-2-O-(N-methylcarbamoyl)-sn-glyceryl-3-phosphorylcholine | 2.5 | 539.39 | POS | C26H55N2O7P |  |  |  | 0.0162 | 0.0223 | 1.5394 | 0.0000 | 1.3757 |
| 10-Methylbenzo[g]pteridine-2,4(3H,10H)-dione | 2.5 | 227.054 | NEG | C11H8N4O2 |  |  |  | 0.1015 | 0.0655 | 1.0093 | 0.0063 | 0.6450 |
| 5-(4-Methylpiperazin-1-yl)-5-oxopentanoic acid | 2.5 | 215.1388 | POS | C10H18N2O3 |  |  |  | 0.0259 | 0.0491 | 1.3138 | 0.0010 | 1.8966 |
| Risedronic\_acid | 2.5 | 284.0091 | POS | C7H11NO7P2 | HMDB0015022 | 105462-24-6 | C08233 | 0.0470 | 0.0959 | 1.4864 | 0.0000 | 2.0389 |
| 3-(3-Hydroxy-5-methylphenoxy)-5-methylbenzene-1,2-diol | 2.49 | 245.0782 | NEG | C14H14O4 |  |  |  | 0.0828 | 0.0694 | 1.2170 | 0.0285 | 0.8383 |
| 2-[1-(Aminomethyl)cyclopentyl]acetic acid | 2.49 | 158.1174 | POS | C8H15NO2 |  |  |  | 0.0143 | 0.0262 | 1.6321 | 0.0000 | 1.8309 |
| Heptanedioic acid, 1-(2-cyclopentylidenehydrazide) | 2.48 | 241.1547 | POS | C12H20N2O3 |  |  |  | 0.0591 | 0.0699 | 1.0011 | 0.0023 | 1.1820 |
| N-Stearoyltaurine | 2.48 | 390.2735 | NEG | C20H41NO4S | HMDB0240595 | 63155-80-6 |  | 0.0998 | 0.0827 | 1.0082 | 0.0430 | 0.8287 |
| 2-Methyl-3-[(tetrahydro-2-furanylcarbonyl)amino]benzoic acid | 2.47 | 248.0929 | NEG | C13H15NO4 |  |  |  | 0.1299 | 0.0653 | 1.6991 | 0.0004 | 0.5026 |
| 7-Hydroxy-6-methoxy-3-methyl-5-(propan-2-ylidene)furo[2,3,4-de]chromen-2(5H)-one | 2.46 | 273.0732 | NEG | C15H14O5 |  |  |  | 0.0033 | 0.4256 | 1.8325 | 0.0001 | 129.2923 |
| N-.alpha.-(tert-Butoxycarbonyl)-L-proline | 2.46 | 214.1085 | NEG | C10H17NO4 |  |  |  | 0.3170 | 0.1442 | 1.6933 | 0.0000 | 0.4549 |
| PC(20:2(11Z,14Z)/18:3(9Z,12Z,15Z)) | 2.46 | 808.5828 | POS | C46H82NO8P | HMDB0008338 |  |  | 0.2044 | 0.2504 | 1.5516 | 0.0001 | 1.2255 |
| PC(18:0/18:3(6Z,9Z,12Z)) | 2.46 | 784.5819 | POS | C44H82NO8P | HMDB0008040 |  |  | 8.2381 | 10.0409 | 1.5115 | 0.0037 | 1.2188 |
| 4-[5-(7-Hydroxy-5,5,8a-trimethyl-2-methylidene-3,4,4a,6,7,8  -hexahydro-1H-naphthalen-1-yl)-3-methylpentoxy]-4-oxobutanoic acid | 2.46 | 407.2806 | NEG | C24H40O5 |  |  |  | 0.3210 | 0.2533 | 1.0032 | 0.0084 | 0.7891 |
| PC(20:2(11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z)) | 2.45 | 832.5835 | POS | C48H82NO8P | HMDB0008347 |  |  | 0.1092 | 0.1318 | 1.5846 | 0.0014 | 1.2075 |
| Xanthophyll | 2.45 | 568.427 | POS | C40H56O2 | HMDB0303013 |  |  | 0.2186 | 0.2463 | 1.1529 | 0.0125 | 1.1267 |
| Fluazifop | 2.44 | 328.0821 | POS | C15H12F3NO4 | HMDB0252322 |  | C18527 | 0.0002 | 0.0173 | 1.7854 | 0.0000 | 97.4928 |
| Harderoporphyrinogen | 2.44 | 615.315 | POS | C35H42N4O6 | HMDB0002160 | 42607-18-1 |  | 0.0016 | 0.0070 | 1.2240 | 0.0008 | 4.3326 |
| 2-Chloro-4,5-dimethoxybenzoic acid | 2.44 | 215.0145 | NEG | C9H9ClO4 |  |  |  | 1.4076 | 0.7434 | 1.7546 | 0.0000 | 0.5281 |
| Oxfendazole | 2.44 | 314.0558 | NEG | C15H13N3O3S | HMDB0031812 | 53716-50-0 |  | 0.0449 | 0.0235 | 1.4186 | 0.0003 | 0.5235 |
| (E)-5-[(1S,4aR,8aR)-2-Formyl-5,5,8a-trimethyl-1,4,4a,6  ,7,8-hexahydronaphthalen-1-yl]-3-(acetyloxymethyl)pent-2-enoic acid | 2.43 | 375.2212 | NEG | C22H32O5 |  |  |  | 0.9087 | 0.6705 | 1.4469 | 0.0001 | 0.7378 |
| Mebendazole | 2.43 | 294.0912 | NEG | C16H13N3O3 | HMDB0014781 | 31431-39-7 |  | 0.0015 | 0.1637 | 1.5344 | 0.0001 | 110.1578 |
| PC(P-18:1(9Z)/0:0) | 2.43 | 506.3601 | POS | C26H52NO6P | HMDB0010408 |  | C04230 | 0.0510 | 0.0744 | 1.5851 | 0.0000 | 1.4587 |
| Amphetamine | 2.42 | 158.0924 | POS | C9H13N | HMDB0014328 | 300-62-9 | C07514 | 0.0021 | 0.0161 | 1.8967 | 0.0000 | 7.6982 |
| DL-2,4-Diaminobutyric acid | 2.41 | 119.0814 | POS | C4H10N2O2 | HMDB0002362 | 305-62-4 |  | 0.2060 | 0.5651 | 1.6350 | 0.0006 | 2.7438 |
| Nilutamide | 2.41 | 318.0681 | POS | C12H10F3N3O4 | HMDB0014803 | 63612-50-0 | C08164 | 0.0012 | 0.0455 | 1.7869 | 0.0002 | 37.9659 |
| LysoPC(22:1(13Z)) | 2.41 | 578.4181 | POS | C30H60NO7P | HMDB0010399 |  | C04230 | 0.0075 | 0.0175 | 1.1576 | 0.0000 | 2.3402 |
| 5-(Tetradecyloxy)-2-furoic acid | 2.4 | 323.2232 | NEG | C19H32O4 |  |  |  | 0.0814 | 0.0625 | 1.3249 | 0.0002 | 0.7683 |
| PC(18:1(9Z)/18:3(9Z,12Z,15Z)) | 2.39 | 782.5693 | POS | C44H80NO8P | HMDB0008074 |  |  | 0.1121 | 0.1678 | 1.7622 | 0.0017 | 1.4975 |
| 3-[(1E,3E)-Hepta-1,3-dienyl]pentanedioic acid | 2.39 | 225.1133 | NEG | C12H18O4 |  |  |  | 0.4214 | 0.2877 | 1.5211 | 0.0000 | 0.6827 |
| PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z)) | 2.39 | 856.5825 | POS | C50H82NO8P | HMDB0008707 |  | C00157 | 0.0428 | 0.0537 | 1.5473 | 0.0012 | 1.2541 |
| (2-aminoethoxy)[2-[hexadec-9-enoyloxy]-3-[octadeca-1.11-dien-1-yloxy]propoxy]phosphinic acid | 2.38 | 698.5133 | NEG | C39H74NO7P | HMDB0011405 |  |  | 5.6665 | 3.3509 | 1.2582 | 0.0001 | 0.5913 |
| L-Erythrulose | 2.38 | 119.0351 | NEG | C4H8O4 | HMDB0006293 | 533-50-6 | C02045 | 0.7026 | 0.3097 | 1.5987 | 0.0000 | 0.4407 |
| 1-Hydroxypyrene | 2.37 | 219.0829 | POS | C16H10O | HMDB0013139 | 5315-79-7 | C14519 | 0.0143 | 0.0105 | 1.3737 | 0.0014 | 0.7313 |
| 2-(2,6-Dihydroxy-4-methoxycarbonylbenzoyl)-3-hydroxybenzoic acid | 2.37 | 331.0504 | NEG | C16H12O8 |  |  |  | 0.0844 | 0.0671 | 1.7637 | 0.0002 | 0.7957 |
| LysoPC(16:1(9Z)) | 2.37 | 494.3247 | POS | C24H48NO7P | HMDB0010383 | 76790-27-7 | C04230 | 0.9020 | 1.1658 | 1.1970 | 0.0014 | 1.2925 |
| 9,10-Dihydrojasmonic acid | 2.37 | 211.1341 | NEG | C12H20O3 |  |  |  | 0.2760 | 0.1759 | 1.4631 | 0.0005 | 0.6372 |
| PC(20:2(11Z,14Z)/18:1(9Z)) | 2.37 | 812.6161 | POS | C46H86NO8P | HMDB0008334 |  |  | 0.0380 | 0.0820 | 1.1530 | 0.0400 | 2.1557 |
| PC(20:3(5Z,8Z,11Z)/14:0) | 2.37 | 756.5536 | POS | C42H78NO8P | HMDB0008361 |  |  | 1.4406 | 1.7179 | 1.0914 | 0.0263 | 1.1925 |
| PC(20:3(5Z,8Z,11Z)/P-18:0) | 2.37 | 796.62 | POS | C46H86NO7P | HMDB0008391 |  |  | 0.8882 | 0.9847 | 1.1206 | 0.0462 | 1.1087 |
| 3-cis-Hydroxy-b,e-Caroten-3'-one | 2.37 | 551.4241 | POS | C40H54O | HMDB0002890 | 143167-27-5 |  | 0.2437 | 0.2936 | 1.3268 | 0.0142 | 1.2048 |
| Niflumic acid | 2.36 | 281.0545 | NEG | C13H9F3N2O2 | HMDB0015573 | 4394-00-7 | C13698 | 2.5902 | 2.1587 | 1.2373 | 0.0285 | 0.8334 |
| (1-Amino-3-methyl-1,3-dihydrobenzoimidazol-2-ylidene)cyanoacetic acid ethyl ester | 2.35 | 259.1153 | POS | C13H14N4O2 |  |  |  | 0.0173 | 0.0639 | 1.5926 | 0.0004 | 3.6941 |
| PC(14:0/P-18:1(9Z)) | 2.35 | 716.5566 | POS | C40H78NO7P | HMDB0007898 |  | C00157 | 0.0141 | 0.0201 | 1.0880 | 0.0067 | 1.4274 |
| Oseltamivir acid | 2.34 | 283.1663 | NEG | C14H24N2O4 |  |  |  | 0.0479 | 0.0228 | 1.1262 | 0.0061 | 0.4767 |
| 2-(Dipentylamino)-2-(hydroxymethyl)-1,3-propanediol | 2.34 | 262.2375 | POS | C14H31NO3 |  |  |  | 0.0260 | 0.0097 | 2.2056 | 0.0000 | 0.3717 |
| honokiol | 2.34 | 267.1439 | POS | C18H18O2 | HMDB0253212 |  | C10630 | 0.0049 | 0.0221 | 1.6557 | 0.0003 | 4.5003 |
| PC(22:4(7Z,10Z,13Z,16Z)/P-18:0) | 2.34 | 822.636 | POS | C48H88NO7P | HMDB0008653 |  |  | 0.2409 | 0.2819 | 1.3202 | 0.0063 | 1.1703 |
| 2,6-Cyclolycopene-1,5-diol | 2.33 | 570.44 | POS | C40H58O2 | HMDB0034902 | 223744-29-4 |  | 0.0448 | 0.0714 | 1.7477 | 0.0000 | 1.5958 |
| 1-(10Z-Heptadecenoyl)-sn-glycero-3-phospho-(1'-rac-glycerol) | 2.33 | 495.2793 | NEG | C23H45O9P |  |  |  | 0.2583 | 0.1861 | 1.1487 | 0.0009 | 0.7203 |
| Demethoxycurcumin | 2.33 | 337.1113 | NEG | C20H18O5 | HMDB0033801 | 22608-11-3 |  | 0.1033 | 0.0630 | 1.7270 | 0.0001 | 0.6095 |
| 4-tert-Butyl-N-(4-nitrophenyl)benzamide | 2.32 | 299.139 | POS | C17H18N2O3 |  |  |  | 0.0057 | 0.0138 | 1.3893 | 0.0002 | 2.4475 |
| Nitrotyrosine | 2.31 | 225.0495 | NEG | C9H10N2O5 | HMDB0001904 | 3604-79-3 |  | 0.0081 | 0.0230 | 1.4411 | 0.0004 | 2.8514 |
| (3-Oxo-2-piperazinyl)acetic acid | 2.31 | 159.0764 | POS | C6H10N2O3 |  |  |  | 0.0022 | 0.0063 | 1.6683 | 0.0000 | 2.8460 |
| 3-Amino-5,6-dimethyl-2-pyrazinecarboxylic acid | 2.3 | 168.0767 | POS | C7H9N3O2 |  |  |  | 0.0160 | 0.2098 | 1.7861 | 0.0000 | 13.1501 |
| 3-Hydroxy-6-methylheptyl 2-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranoside | 2.3 | 469.2271 | NEG | C20H38O12 |  |  |  | 0.0911 | 0.0609 | 1.3582 | 0.0010 | 0.6685 |
| PI(16:1(9Z)/18:1(9Z)) | 2.29 | 835.533 | POS | C43H79O13P | HMDB0009801 |  | C00626 | 0.0120 | 0.0083 | 1.0295 | 0.0007 | 0.6931 |
| 1-Anilino-3-(3,6-dibromo-9H-carbazol-9-yl)-2-propanol | 2.26 | 472.9858 | POS | C21H18Br2N2O |  |  |  | 0.0009 | 0.0051 | 1.6599 | 0.0001 | 5.6173 |
| 2-Hexylbutanedioic acid | 2.26 | 201.1135 | NEG | C10H18O4 |  |  |  | 0.0566 | 0.0446 | 1.2593 | 0.0162 | 0.7870 |
| N-(4-Methylphenyl)-N'-(6-methyl-2-pyridinyl)thiourea | 2.26 | 256.0912 | NEG | C14H15N3S |  |  |  | 0.0162 | 0.0076 | 1.0058 | 0.0002 | 0.4703 |
| Okaramine D | 2.26 | 581.2409 | NEG | C33H34N4O6 |  |  |  | 0.0653 | 0.0554 | 1.2480 | 0.0207 | 0.8484 |
| CPA(18:2(9Z,12Z)/0:0) | 2.26 | 417.2397 | POS | C21H37O6P | HMDB0007007 |  |  | 0.0007 | 0.0013 | 1.3364 | 0.0000 | 1.7447 |
| Eplerenone | 2.26 | 415.2116 | POS | C24H30O6 | HMDB0014838 | 107724-20-9 | C12512 | 0.0024 | 0.0034 | 1.3433 | 0.0005 | 1.3857 |
| Erythronolactone | 2.26 | 117.0195 | NEG | C4H6O4 | HMDB0000349 | 17675-99-9 |  | 0.8519 | 0.5941 | 1.6444 | 0.0005 | 0.6973 |
| Nitrofurazone | 2.26 | 197.0316 | NEG | C6H6N4O4 | HMDB0014480 | 59-87-0 | C08042 | 178.9130 | 128.7669 | 1.5809 | 0.0045 | 0.7197 |
| 3-Oxocyclobutanecarboxylic acid | 2.25 | 113.0246 | NEG | C5H6O3 |  |  |  | 2.8816 | 2.1514 | 1.6191 | 0.0000 | 0.7466 |
| N-Acetylglucosaminylasparagine | 2.25 | 334.1258 | NEG | C12H21N3O8 |  |  |  | 0.1064 | 0.8729 | 1.2232 | 0.0000 | 8.2031 |
| 5-[(2-Chlorophenoxy)methyl]-4-methyl-4H-1,2,4-triazole-3-thiol | 2.25 | 254.0159 | NEG | C10H10ClN3OS |  |  |  | 0.0813 | 0.0442 | 1.0355 | 0.0462 | 0.5441 |
| (E)-2-Cyano-1-(tert-pentyl)guanidine | 2.25 | 155.1291 | POS | C7H14N4 |  |  |  | 0.0237 | 0.0170 | 1.2025 | 0.0004 | 0.7180 |
| (2S)-2-[(2R,3S,7R,8R,8aS)-2,3,4'-Trihydroxy-4,4,7,8a-tetramethyl  -6'-oxospiro[2,3,4a,5,6,7-hexahydro-1H-naphthalene-8,2  '-3,8-dihydrofuro[2,3-e]isoindole]-7'-yl]-3-methylbutanoic acid | 2.25 | 502.2799 | POS | C28H39NO7 |  |  |  | 0.0018 | 0.0066 | 1.5923 | 0.0000 | 3.7573 |
| 4-(4-Morpholinyl)-1,3,5-triazin-2-ylamine | 2.25 | 182.1036 | POS | C7H11N5O |  |  |  | 0.0220 | 0.0193 | 1.0154 | 0.0253 | 0.8745 |
| (R)-N-[1-[4-(2,4-Dimethoxybenzyl)-5-phenethyl-4H-1  ,2,4-triazol-3-yl]-2-(1H-indol-3-yl)ethyl]picolinamide | 2.25 | 587.2766 | POS | C35H34N6O3 | HMDB0253735 |  |  | 0.0171 | 0.0692 | 1.3798 | 0.0000 | 4.0574 |
| N-Cyclohexyl-N'-(tetrahydro-2-furanylmethyl)urea | 2.25 | 227.1753 | POS | C12H22N2O2 |  |  |  | 0.0279 | 0.0354 | 1.0349 | 0.0067 | 1.2696 |
| Methoxyfenozide | 2.25 | 369.2122 | POS | C22H28N2O3 | HMDB0254547 |  | C18525 | 0.0009 | 0.0037 | 1.8972 | 0.0000 | 4.0353 |
| Putative Phenylalanine conjugated chenodeoxycholic acid | 2.25 | 540.3663 | POS | C33H49NO5 | HMDB0242391 |  |  | 0.0294 | 0.0391 | 1.4977 | 0.0001 | 1.3310 |
| ISOPALMITIC ACID | 2.25 | 255.233 | NEG | C16H32O2 | HMDB0031068 | 4669-02-7 |  | 2.7204 | 2.2933 | 1.1648 | 0.0169 | 0.8430 |
| Lormetazepam | 2.24 | 335.0378 | POS | C16H12Cl2N2O2 | HMDB0041919 | 848-75-9 |  | 0.0024 | 0.1252 | 1.8651 | 0.0000 | 51.9290 |
| 4-(3-Methyl-5-oxo-4,5-dihydro-1H-pyrazol-1-yl)benzoic acid | 2.24 | 217.0618 | NEG | C11H10N2O3 |  |  |  | 0.1519 | 0.0787 | 1.5716 | 0.0001 | 0.5179 |
| N1-[3-(Benzyloxy)benzyl]-1H-tetrazole-1,5-diamine | 2.24 | 297.1477 | POS | C15H16N6O |  |  |  | 0.0138 | 0.0296 | 1.0341 | 0.0002 | 2.1389 |
| 13,14-dihydro-PGE1 | 2.24 | 357.2651 | POS | C20H36O5 | HMDB0002689 | 19313-28-1 |  | 0.0021 | 0.0013 | 1.0351 | 0.0319 | 0.6353 |
| 2-{[(2-Oxo-2H-chromen-3-yl)carbonyl]amino}benzoic acid | 2.23 | 310.0705 | POS | C17H11NO5 |  |  |  | 0.0003 | 0.0064 | 1.1223 | 0.0009 | 19.7568 |
| N-Phenyl-N'-(3-pyridinylmethyl)thiourea | 2.23 | 242.076 | NEG | C13H13N3S |  |  |  | 0.0046 | 0.0035 | 1.3401 | 0.0026 | 0.7640 |
| 5-[2-Chloro-5-(trifluoromethyl)anilino]-5-oxopentanoic acid | 2.23 | 308.0311 | NEG | C12H11ClF3NO3 |  |  |  | 0.1735 | 0.1399 | 1.0919 | 0.0125 | 0.8063 |
| Emodin-8-Beta-D-Glucoside | 2.23 | 471.0695 | POS | C21H20O10 | HMDB0303798 |  |  | 0.0005 | 0.0007 | 1.0113 | 0.0216 | 1.4513 |
| Streptozocin | 2.23 | 266.0976 | POS | C8H15N3O7 | HMDB0014572 | 18883-66-4 | C07313 | 0.1757 | 0.1961 | 1.0875 | 0.0088 | 1.1160 |
| Bromhexine | 2.22 | 375.0056 | POS | C14H20Br2N2 |  |  |  | 0.0009 | 0.0020 | 1.1905 | 0.0162 | 2.2883 |
| Taxifolin | 2.22 | 303.0504 | NEG | C15H12O7 | HMDB0303943 |  | C01617 | 0.0464 | 0.0258 | 1.0864 | 0.0025 | 0.5568 |
| (2-aminoethoxy)[2-[octadec-9-enoyloxy]-3-[octadeca-1  .11-dien-1-yloxy]propoxy]phosphinic acid | 2.22 | 726.5441 | NEG | C41H78NO7P | HMDB0011408 |  |  | 7.0918 | 3.9526 | 1.4517 | 0.0000 | 0.5573 |
| SM\_C16:1 | 2.22 | 716.5776 | POS | C40H80N2O6P | HMDB0029216 |  |  | 0.0525 | 0.0629 | 1.3411 | 0.0234 | 1.1970 |
| 1-[6-Chloro-5-(trifluoromethoxy)-1H-benzimidazol-2-yl]-1H-pyrazole-4-carboxylic acid | 2.21 | 347.0127 | POS | C12H6ClF3N4O3 |  |  |  | 0.0047 | 0.0424 | 1.5336 | 0.0004 | 9.0471 |
| N-Acetylsulfamethoxazole | 2.21 | 296.0659 | POS | C12H13N3O4S | HMDB0013854 | 21312-10-7 | C13061 | 0.0077 | 0.0275 | 1.6085 | 0.0000 | 3.5617 |
| Neohancoside D | 2.21 | 547.1694 | NEG | C23H32O15 |  |  |  | 0.2546 | 0.1692 | 1.6890 | 0.0000 | 0.6647 |
| 2-[(2-Fluorophenyl)amino]acetohydrazide | 2.21 | 182.0762 | NEG | C8H10FN3O |  |  |  | 0.2422 | 0.1958 | 1.4134 | 0.0009 | 0.8086 |
| 2-amino-3-({hydroxy[2-(icosanoyloxy)-3-[octadec-11-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid | 2.21 | 816.5764 | NEG | C44H84NO10P | HMDB0112392 |  |  | 49.7330 | 41.5500 | 1.0207 | 0.0076 | 0.8355 |
| 2,4-DIHYDROXYPTERIDINE | 2.21 | 163.0251 | NEG | C6H4N4O2 | HMDB0254198 |  | C03212 | 0.0803 | 0.0491 | 1.6755 | 0.0003 | 0.6109 |
| S-Sulforaphene | 2.21 | 176.1393 | POS | C6H9NOS2 | HMDB0031573 | 2404-46-8 |  | 0.0262 | 0.0373 | 1.4247 | 0.0000 | 1.4214 |
| Convallatoxin | 2.21 | 551.2867 | POS | C29H42O10 | HMDB0034362 | 5822-57-1 |  | 0.0015 | 0.0043 | 1.6086 | 0.0000 | 2.7876 |
| 7-Hydroxy-3-(4-methoxyphenoxy)-2-(trifluoromethyl)-4H-chromen-4-one | 2.2 | 351.0497 | NEG | C17H11F3O5 |  |  |  | 0.0781 | 0.1084 | 1.0087 | 0.0332 | 1.3874 |
| Fenazaflor | 2.2 | 374.9922 | POS | C15H7Cl2F3N2O2 |  |  |  | 0.0010 | 0.0033 | 1.2375 | 0.0020 | 3.1772 |
| 3-[[(5-Methyl-1,3,4-thiadiazol-2-yl)thio]methyl]coumarilic acid | 2.2 | 307.0195 | POS | C13H10N2O3S2 |  |  |  | 0.0015 | 0.0021 | 1.2011 | 0.0005 | 1.4269 |
| trans-Epoxysuccinyl-L-leucylamido(4-guanidino)butane | 2.2 | 358.2072 | POS | C15H27N5O5 |  |  |  | 0.0073 | 0.0143 | 1.3438 | 0.0088 | 1.9561 |
| Aurintricarboxylic acid | 2.2 | 421.0604 | NEG | C22H14O9 | HMDB0248731 |  |  | 1.2942 | 0.7617 | 1.0406 | 0.0115 | 0.5885 |
| Fenhexamid | 2.2 | 300.0576 | NEG | C14H17Cl2NO2 | HMDB0252201 |  | C18593 | 0.0982 | 0.0683 | 1.6845 | 0.0000 | 0.6963 |
| (22E,24R)-Stigmasta-4,22-diene-3,6-dione | 2.2 | 425.3456 | POS | C29H44O2 | HMDB0038656 | 50868-51-4 |  | 0.0993 | 0.1203 | 1.0422 | 0.0058 | 1.2112 |
| arctiin | 2.19 | 533.2051 | NEG | C27H34O11 | HMDB0301809 | 20362-31-6 | C16915 | 0.0119 | 0.0067 | 1.5110 | 0.0029 | 0.5628 |
| Linalool\_oxide\_D\_3-[apiosyl-(1->6)-glucoside] | 2.19 | 465.2306 | POS | C21H36O11 | HMDB0031367 |  |  | 0.0002 | 0.0010 | 1.3944 | 0.0003 | 4.1115 |
| Benzophenone-4 | 2.19 | 307.0299 | NEG | C14H12O6S | HMDB0258614 |  |  | 0.6498 | 0.4897 | 1.2839 | 0.0019 | 0.7536 |
| Sulprophos sulfoxide | 2.18 | 339.0342 | POS | C12H19O3PS3 |  |  |  | 0.0033 | 0.0118 | 1.7272 | 0.0008 | 3.5650 |
| Lys-His | 2.18 | 284.1704 | POS | C12H21N5O3 |  |  |  | 0.0040 | 0.0180 | 1.6065 | 0.0005 | 4.5473 |
| Benazepril | 2.18 | 423.1957 | NEG | C24H28N2O5 | HMDB0014682 | 86541-75-5 | C06843 | 0.0198 | 0.0125 | 1.6286 | 0.0032 | 0.6349 |
| Ethyl 3-(trifluoromethyl)-1H-pyrazole-5-carboxylate | 2.17 | 207.0366 | NEG | C7H7F3N2O2 |  |  |  | 0.0039 | 0.0249 | 1.7853 | 0.0000 | 6.3695 |
| Chicoric acid | 2.17 | 473.0747 | NEG | C22H18O12 | HMDB0002375 | 70831-56-0 | C10437 | 0.0954 | 0.0761 | 1.7862 | 0.0012 | 0.7978 |
| Dopamine 4-.beta.-D-glucuronide | 2.17 | 328.1075 | NEG | C14H19NO8 |  |  |  | 2.0903 | 1.6784 | 1.1036 | 0.0006 | 0.8029 |
| N-(4-Chlorobenzyl)-9H-purin-6-amine | 2.17 | 258.0566 | NEG | C12H10ClN5 |  |  |  | 0.1594 | 0.1257 | 1.1944 | 0.0125 | 0.7888 |
| apigetrin | 2.17 | 431.1007 | NEG | C21H20O10 | HMDB0037340 | 578-74-5 | C04608 | 0.0167 | 0.0113 | 1.3430 | 0.0183 | 0.6780 |
| 3-Hydroxystigmast-5-en-7-one | 2.17 | 429.3772 | POS | C29H48O2 | HMDB0034422 | 2034-74-4 |  | 0.0231 | 0.0384 | 1.7929 | 0.0000 | 1.6586 |
| 5-Azacytidine | 2.16 | 243.0753 | NEG | C8H12N4O5 |  |  |  | 0.0044 | 0.0029 | 1.1571 | 0.0015 | 0.6630 |
| His-Tyr | 2.16 | 319.1365 | POS | C15H18N4O4 | HMDB0028897 | 35979-00-1 |  | 0.0066 | 0.0190 | 1.5918 | 0.0005 | 2.8743 |
| 1,7-Dioxa-4,10-diazacyclododecane | 2.15 | 175.143 | POS | C8H18N2O2 |  |  |  | 0.0983 | 0.1728 | 1.4391 | 0.0009 | 1.7574 |
| 4-Benzyloxy-3-iodo-5-methoxybenzaldehyde | 2.15 | 369.0005 | POS | C15H13IO3 |  |  |  | 0.0004 | 0.0092 | 1.8438 | 0.0000 | 21.1761 |
| Cirsimaritin | 2.15 | 313.0738 | NEG | C17H14O6 | HMDB0250276 |  | C17785 | 0.0477 | 0.0021 | 1.5220 | 0.0002 | 0.0447 |
| {4-[(Phenoxyacetyl)amino]phenyl}acetic acid | 2.15 | 284.091 | NEG | C16H15NO4 |  |  |  | 0.0512 | 0.0857 | 1.1604 | 0.0000 | 1.6754 |
| Gallomyricitrin | 2.14 | 615.1033 | NEG | C28H24O16 |  |  |  | 0.0322 | 0.0209 | 1.0792 | 0.0125 | 0.6511 |
| 3-(3-Nitrophenyl)-5-(2-phenylethyl)-1,2,4-oxadiazole | 2.13 | 296.1051 | POS | C16H13N3O3 |  |  |  | 0.0003 | 0.0353 | 1.7705 | 0.0008 | 136.7837 |
| Epalrestat | 2.13 | 320.0387 | POS | C15H13NO3S2 |  |  |  | 0.0069 | 0.0257 | 1.0653 | 0.0010 | 3.7461 |
| Sulfamethoxazole | 2.13 | 252.0466 | NEG | C10H11N3O3S | HMDB0015150 | 723-46-6 | C07315 | 0.0574 | 0.0434 | 1.2355 | 0.0016 | 0.7561 |
| Gentamicin | 2.13 | 478.3285 | POS | C21H43N5O7 | HMDB0014936 | 1403-66-3 |  | 0.0191 | 0.0276 | 1.1715 | 0.0010 | 1.4418 |
| 2-(2-Bromo-4,5-dimethoxyphenyl)-6,7-dimethoxy-1-naphthol | 2.12 | 417.0387 | NEG | C20H19BrO5 |  |  |  | 0.0222 | 0.0311 | 1.3017 | 0.0026 | 1.3998 |
| Methyl 2-hydroxy-3,5-dinitrobenzoate | 2.12 | 241.0122 | NEG | C8H6N2O7 |  |  |  | 0.0730 | 0.0503 | 1.0322 | 0.0285 | 0.6882 |
| liriodenine | 2.12 | 298.0526 | POS | C17H9NO3 | HMDB0301844 |  | C09567 | 0.0057 | 0.0098 | 1.4154 | 0.0000 | 1.7240 |
| Florfenicol | 2.12 | 358.0105 | POS | C12H14Cl2FNO4S | HMDB0252314 |  |  | 0.0006 | 0.0498 | 1.7621 | 0.0000 | 87.6896 |
| 4-Bromo-1-(4-morpholinosulfonylphenyl)pyrazole | 2.11 | 371.9975 | POS | C13H14BrN3O3S |  |  |  | 0.0126 | 0.0493 | 1.0807 | 0.0061 | 3.9242 |
| Phe-His | 2.11 | 303.1417 | POS | C15H18N4O3 | HMDB0028997 | 33367-37-2 |  | 0.0074 | 0.0317 | 1.6372 | 0.0003 | 4.2809 |
| Fusarochromanone | 2.11 | 293.1528 | POS | C15H20N2O4 | HMDB0033514 | 104653-89-6 |  | 0.0007 | 0.0010 | 1.0724 | 0.0052 | 1.4436 |
| 4H-1,2,4-Triazole-3-sulfonamide | 2.1 | 146.9968 | NEG | C2H4N4O2S |  |  |  | 0.1278 | 0.0905 | 1.0564 | 0.0014 | 0.7081 |
| (1S)-2-Amino-1-(4-chlorophenyl)-1-[4-(1H-pyrazol-4-yl)phenyl]ethanol | 2.09 | 312.094 | NEG | C17H16ClN3O |  |  |  | 0.0151 | 0.0554 | 1.6614 | 0.0000 | 3.6627 |
| 5-Hydroxy-2-{[(4-nitrophenoxy)acetyl]amino}benzoic acid | 2.09 | 331.061 | NEG | C15H12N2O7 |  |  |  | 0.2130 | 0.1666 | 1.3830 | 0.0001 | 0.7823 |
| Propyl gallate | 2.08 | 211.0589 | NEG | C10H12O5 | HMDB0033835 | 121-79-9 | C11155 | 0.4927 | 0.3972 | 1.2520 | 0.0030 | 0.8062 |
| 1-(4-Chlorophenyl)-3,5-dimethyl-1H-pyrazole-4-carboxylic acid | 2.07 | 249.0471 | NEG | C12H11ClN2O2 |  |  |  | 0.1661 | 0.1434 | 1.6143 | 0.0029 | 0.8636 |
| 5'-Hydroxytenoxicam | 2.07 | 354.0257 | POS | C13H11N3O5S2 | HMDB0014098 |  |  | 0.0002 | 0.0012 | 1.4309 | 0.0001 | 5.9237 |
| Corynanthin | 2.07 | 372.223 | POS | C21H26N2O3 | HMDB0250478 |  |  | 0.0043 | 0.0316 | 1.8590 | 0.0000 | 7.3315 |
| Serine-Cholic Acid | 2.07 | 460.3116 | POS | C27H45NO7 | HMDB0242388 |  |  | 0.0074 | 0.0422 | 1.8295 | 0.0003 | 5.7446 |
| 4-Imidazolidineheptanoic acid, 3-[(2-cyclohexyl-2-hydroxyethyl)amino]-2,5-dioxo-1-(phenylmethyl)- | 2.06 | 460.2752 | POS | C25H37N3O5 | HMDB0249489 |  |  | 0.0022 | 0.0099 | 1.7947 | 0.0001 | 4.5073 |
| Swertiamarin | 2.06 | 419.1145 | NEG | C16H22O10 | HMDB0258644 |  |  | 0.0531 | 0.0308 | 1.6616 | 0.0001 | 0.5795 |
| Lanceoloside A | 2.05 | 391.1082 | NEG | C19H20O9 |  |  |  | 0.0452 | 0.0303 | 1.4762 | 0.0176 | 0.6694 |
| (1,3-Benzothiazol-2-ylsulfonyl)acetic acid | 2.05 | 255.9713 | NEG | C9H7NO4S2 |  |  |  | 0.0462 | 0.1367 | 1.6718 | 0.0000 | 2.9549 |
| Mebeverine | 2.05 | 430.2649 | POS | C25H35NO5 | HMDB0254388 |  |  | 0.0052 | 0.0320 | 1.8773 | 0.0000 | 6.1598 |
| Procaterol | 2.04 | 291.1665 | POS | C16H22N2O3 | HMDB0015453 | 72332-33-3 |  | 0.0013 | 0.0032 | 1.2041 | 0.0076 | 2.4440 |
| Aspochalasin D | 2.02 | 402.2696 | POS | C24H35NO4 |  |  |  | 0.0061 | 0.0456 | 1.7046 | 0.0003 | 7.4286 |
| gamma-Amino-gamma-cyanobutanoate | 1.99 | 129.0659 | POS | C5H8N2O2 |  |  |  | 0.1760 | 1.9425 | 1.7232 | 0.0005 | 11.0393 |
| N-Acetylneuraminate | 1.95 | 308.0989 | NEG | C11H19NO9 | HMDB0000230 | 131-48-6 | C00270 | 9.5199 | 7.4239 | 1.5576 | 0.0120 | 0.7798 |
| (R)-S-Lactoylglutathione | 1.94 | 416.053 | NEG | C13H21N3O8S |  |  |  | 0.2005 | 0.1595 | 1.3829 | 0.0008 | 0.7955 |
| M324T174 | 1.94 | 324.094 | NEG | C9H15NO8 |  |  |  | 0.9489 | 0.6848 | 1.7067 | 0.0000 | 0.7217 |
| (2S)-2-Isopropyl-3-oxosuccinate | 1.9 | 173.0458 | NEG | C7H10O5 |  |  |  | 0.1678 | 0.0336 | 1.1312 | 0.0030 | 0.2003 |
| M211T175 | 1.89 | 211.0014 | NEG | C5H11O8P |  |  |  | 0.0467 | 0.0363 | 1.1837 | 0.0169 | 0.7785 |
| M243T127 | 1.88 | 243.018 | NEG | C6H12O8S |  |  |  | 0.0529 | 0.0373 | 1.0143 | 0.0032 | 0.7052 |
| Ethanolamine phosphate | 1.87 | 200.0333 | NEG | C2H8NO4P | HMDB0000224 | 1071-23-4 | C00346 | 0.0513 | 0.0740 | 1.1804 | 0.0015 | 1.4424 |
| 4-Guanidinobutanal | 1.87 | 130.0974 | POS | C5H11N3O |  |  |  | 0.6471 | 0.4422 | 1.4796 | 0.0001 | 0.6834 |
| 5-Hydroxyisourate | 1.87 | 165.0055 | NEG | C5H4N4O4 |  |  |  | 1.2624 | 0.9622 | 1.3773 | 0.0096 | 0.7622 |
| M513T53 | 1.87 | 513.4167 | NEG | C28H54O4 |  |  |  | 0.1922 | 0.1290 | 1.0584 | 0.0022 | 0.6711 |
| Sebacic acid | 1.85 | 201.1133 | NEG | C10H18O4 | HMDB0000792 | 111-20-6 | C08277 | 0.0929 | 0.0585 | 1.4837 | 0.0001 | 0.6297 |
| UDP-N-acetyl-D-mannosaminouronate | 1.85 | 637.0809 | NEG | C17H25N3O18P2 |  |  |  | 0.0294 | 0.0220 | 1.5044 | 0.0110 | 0.7488 |
| UDP-3-ketoglucose | 1.84 | 580.0593 | NEG | C15H22N2O17P2 |  |  |  | 0.1050 | 0.0781 | 1.3976 | 0.0002 | 0.7438 |
| Formamidopyrimidine nucleoside triphosphate | 1.82 | 579.9702 | POS | C10H18N5O15P3 |  |  |  | 0.2265 | 0.2529 | 1.3583 | 0.0048 | 1.1166 |
| 5-Hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate | 1.81 | 201.0257 | NEG | C5H6N4O5 |  |  |  | 0.0110 | 0.0344 | 1.2029 | 0.0073 | 3.1366 |
| M255T209 | 1.81 | 254.9827 | POS | C6H8O10S |  |  |  | 0.2396 | 0.2756 | 1.7016 | 0.0001 | 1.1504 |
| M87T134 | 1.81 | 87.009 | NEG | C3H4O3 |  |  |  | 0.2851 | 0.2237 | 1.4722 | 0.0263 | 0.7844 |
| P1,P4-Bis(5'-uridyl) tetraphosphate | 1.79 | 849.0102 | NEG | C18H26N4O23P4 |  |  |  | 0.0067 | 0.0040 | 1.4563 | 0.0021 | 0.5973 |
| M213T111\_1 | 1.79 | 213.0173 | NEG | C7H12O5 |  |  |  | 1.5255 | 0.7737 | 1.6588 | 0.0000 | 0.5072 |
| M246T207 | 1.78 | 246.0324 | POS | C5H8O8S |  |  |  | 0.0092 | 0.0161 | 1.3286 | 0.0003 | 1.7599 |
| 1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide | 1.77 | 349.0552 | POS | C10H15N4O9P |  |  |  | 0.0004 | 0.0491 | 1.5945 | 0.0002 | 124.5226 |
| L-2-Amino-3-oxobutanoic acid | 1.77 | 98.0249 | NEG | C4H7NO3 |  |  |  | 3.8062 | 2.4008 | 1.5337 | 0.0274 | 0.6308 |
| M282T176 | 1.77 | 282.083 | NEG | C9H14O9 |  |  |  | 0.0517 | 0.4077 | 1.5759 | 0.0027 | 7.8857 |
| 3-Sulfino-L-alanine | 1.76 | 212.0292 | NEG | C3H7NO4S |  |  |  | 0.0027 | 0.0111 | 1.6803 | 0.0010 | 4.1720 |
| M505T253 | 1.76 | 505.0407 | NEG | C10H16N4O12P2 |  |  |  | 0.0033 | 0.1013 | 1.7335 | 0.0005 | 30.4497 |
| 2,5-Dioxopiperazine | 1.75 | 95.0252 | NEG | C4H6N2O2 |  |  |  | 0.1216 | 0.0686 | 1.6472 | 0.0007 | 0.5639 |
| M209T209 | 1.75 | 209.0044 | NEG | C7H8O6 |  |  |  | 0.4632 | 0.3857 | 1.0376 | 0.0253 | 0.8327 |
| UDP | 1.74 | 403.0002 | NEG | C9H14N2O12P2 | HMDB0000295 | 58-98-0 | C00015 | 0.1421 | 0.2435 | 1.5974 | 0.0007 | 1.7134 |
| 2-Aminobut-2-enoate | 1.74 | 137.9964 | NEG | C4H7NO2 |  |  |  | 0.0680 | 0.0748 | 1.0833 | 0.0385 | 1.0991 |
| D-Glucosaminate-6-phosphate | 1.73 | 334.05 | NEG | C6H14NO9P |  |  |  | 0.1598 | 0.1138 | 1.1508 | 0.0002 | 0.7121 |
| M642T230 | 1.73 | 641.9981 | NEG | C18H24NO18PS |  |  |  | 0.0051 | 0.0035 | 1.3099 | 0.0115 | 0.6801 |
| 3-Sulfinylpyruvate | 1.71 | 172.9581 | NEG | C3H4O5S |  |  |  | 0.1846 | 0.1354 | 1.1759 | 0.0115 | 0.7335 |
| N-Feruloylglycine | 1.71 | 272.0539 | NEG | C12H13NO5 |  |  |  | 0.7219 | 0.4292 | 1.6334 | 0.0035 | 0.5945 |
| M202T112 | 1.71 | 202.0382 | NEG | C7H6O6 |  |  |  | 0.7396 | 0.5973 | 1.2925 | 0.0043 | 0.8075 |
| 4-Carboxy-4-hydroxy-2-oxoadipate | 1.7 | 256.966 | NEG | C7H8O8 |  |  |  | 0.0980 | 0.2918 | 1.6622 | 0.0000 | 2.9763 |
| 2-Hydroxy-2,4-pentadienoate | 1.7 | 113.0246 | NEG | C5H6O3 |  |  |  | 1.4424 | 0.8689 | 1.5494 | 0.0001 | 0.6024 |
| M149T198 | 1.69 | 149.0459 | NEG | C5H10O5 |  |  |  | 0.1065 | 0.0691 | 1.7049 | 0.0023 | 0.6489 |
| GDP-glucose | 1.65 | 586.0666 | NEG | C16H25N5O16P2 |  |  |  | 0.0066 | 0.0054 | 1.1068 | 0.0120 | 0.8102 |
| M708T231 | 1.65 | 707.9698 | NEG | C15H24N5O19P3 |  |  |  | 0.0034 | 0.0059 | 1.5651 | 0.0006 | 1.7097 |
| Pyrimidine 5'-nucleotide | 1.64 | 309.0683 | NEG | C9H14N2O7P |  |  |  | 0.1933 | 0.1726 | 1.3439 | 0.0191 | 0.8931 |
| Methylimidazole acetaldehyde | 1.62 | 125.0709 | POS | C6H8N2O |  |  |  | 0.0803 | 0.0486 | 1.0203 | 0.0063 | 0.6053 |
| Nicotinamide D-ribonucleotide | 1.61 | 315.0419 | NEG | C11H15N2O8P |  |  |  | 0.8215 | 2.2330 | 1.6431 | 0.0003 | 2.7180 |
| M347T238 | 1.61 | 347.0035 | NEG | C10H14O11 |  |  |  | 0.2507 | 1.6914 | 1.1515 | 0.0027 | 6.7456 |
| M643T213 | 1.6 | 642.9811 | NEG | C15H22N2O20P2S |  |  |  | 0.0605 | 0.0457 | 1.0848 | 0.0012 | 0.7555 |
| M401T210 | 1.58 | 401.0426 | NEG | C12H20O14S |  |  |  | 0.1179 | 0.0937 | 1.0040 | 0.0050 | 0.7942 |
| M228T85\_2 | 1.58 | 228.0283 | NEG | C10H9NO4 |  |  |  | 0.4754 | 0.2592 | 1.7461 | 0.0000 | 0.5452 |
| Imidazole-4-acetate | 1.57 | 144.0768 | POS | C5H6N2O2 | HMDB0002024 | 645-65-8 | C02835 | 0.0101 | 0.0611 | 1.5168 | 0.0007 | 6.0318 |
| N2-Succinyl-L-arginine | 1.53 | 255.1079 | NEG | C10H18N4O5 |  |  |  | 0.2664 | 0.1717 | 1.6194 | 0.0004 | 0.6445 |
| M455T209 | 1.52 | 455.0141 | NEG | C12H19O15P |  |  |  | 1.5328 | 1.1971 | 1.4283 | 0.0045 | 0.7810 |
| M573T85 | 1.5 | 573.395 | NEG | C30H53O9 |  |  |  | 0.1471 | 0.1027 | 1.4728 | 0.0004 | 0.6981 |
| N5-Phenyl-L-glutamine | 1.47 | 221.0933 | NEG | C11H14N2O3 |  |  |  | 0.0475 | 0.0196 | 1.4839 | 0.0000 | 0.4118 |
| M132T202 | 1.47 | 132.0669 | NEG | C5H11NO3 |  |  |  | 0.0162 | 0.0123 | 1.3173 | 0.0035 | 0.7575 |
| M186T205 | 1.46 | 186.0177 | NEG | C5H11NO4 |  |  |  | 0.0079 | 0.0188 | 1.6719 | 0.0014 | 2.3812 |
| D-Glycerate | 1.45 | 144.9847 | POS | C3H6O4 |  |  |  | 0.0563 | 0.0653 | 1.0386 | 0.0243 | 1.1603 |
| M213T89\_1 | 1.44 | 213.0175 | NEG | C7H12O5 |  |  |  | 4.1252 | 2.4241 | 1.7024 | 0.0001 | 0.5876 |
| 3-Cyano-L-alanine | 1.43 | 153.0061 | POS | C4H6N2O2 |  |  |  | 0.0001 | 0.0016 | 1.7432 | 0.0001 | 13.2861 |
| 3-Indoleacetonitrile | 1.42 | 177.0407 | NEG | C10H8N2 |  |  |  | 1.1754 | 0.6620 | 1.5662 | 0.0000 | 0.5632 |
| M577T46 | 1.33 | 577.3752 | NEG | C33H54O8 |  |  |  | 0.6573 | 0.4633 | 1.0507 | 0.0055 | 0.7048 |
| 2-Aminomalonate semialdehyde | 1.31 | 84.0053 | NEG | C3H5NO3 |  |  |  | 0.0394 | 0.0313 | 1.2951 | 0.0358 | 0.7944 |
| (3S)-2-Oxo-3-phenylbutanoate | 1.31 | 199.0381 | NEG | C10H10O3 |  |  |  | 0.2366 | 0.2061 | 1.1330 | 0.0319 | 0.8713 |
| 4-Hydroxy-L-glutamate | 1.3 | 179.0666 | NEG | C5H9NO5 |  |  |  | 0.1004 | 0.0741 | 1.6074 | 0.0000 | 0.7377 |
| Lithocholic acid | 1.29 | 435.312 | NEG | C24H40O3 | HMDB0000761 | 434-13-9 | C03990 | 1.0748 | 0.7851 | 1.1703 | 0.0037 | 0.7305 |
| 4-Aminobutyraldehyde | 1.28 | 175.1439 | POS | C4H9NO |  |  |  | 0.0044 | 0.0214 | 1.4060 | 0.0006 | 4.8835 |
| N-Succinyl-L-glutamate 5-semialdehyde | 1.26 | 290.0885 | NEG | C9H13NO6 |  |  |  | 0.0127 | 0.0080 | 1.3366 | 0.0052 | 0.6301 |
| Cellobionate | 1.25 | 357.1095 | NEG | C12H22O12 |  |  |  | 0.0371 | 0.0225 | 1.4635 | 0.0000 | 0.6063 |
| 2-Chlorobenzoate | 1.25 | 172.0205 | NEG | C7H5ClO2 |  |  |  | 0.0186 | 0.0114 | 1.7386 | 0.0001 | 0.6117 |
| M243T162\_1 | 1.24 | 243.0625 | NEG | C9H9NO6 |  |  |  | 0.0507 | 0.0411 | 1.1084 | 0.0041 | 0.8099 |
| Oxamate | 1.19 | 109.9919 | NEG | C2H3NO3 |  | 471-47-6 | C01444 | 0.0180 | 0.0137 | 1.3437 | 0.0319 | 0.7611 |
| M305T170 | 1.12 | 305.0392 | NEG | C10H14N2O7S |  |  |  | 0.0293 | 0.0229 | 1.1316 | 0.0043 | 0.7822 |

Table 2. KEGG Enrichment data matrix before and after a 12-week BBr60 intervention on serum metabolism

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pathway** | **Description** | **Compounds.(dem)** | **Percent** | **Rich\_factor** | **p\_value** | **up\_nums** | **down\_nums** | **DA\_score** |
| hsa05230 | Central carbon metabolism in cancer | C00152;C00065;C00025;C00122;C00407;C00078;C00183;C00022;C00158;C00049;C00149;C00311 | 11.76470588 | 0.324324324 | 1.21578E-11 | 8 | 4 | 0.333333333 |
| hsa04974 | Protein digestion and absorption | C00152;C00065;C00025;C00407;C00078;C00099;C00183;C00047;C08262;C00049;C00246 | 10.78431373 | 0.234042553 | 4.53213E-09 | 6 | 5 | 0.090909091 |
| hsa01230 | Biosynthesis of amino acids | C00152;C00327;C00065;C00025;C00407;C00263;C00078;C00233;C00183;C00022;C00047;C00141;C00979;C00158;C00049;C00311 | 15.68627451 | 0.125 | 1.93E-08 | 10 | 6 | 0.25 |
| hsa00630 | Glyoxylate and dicarboxylate metabolism | C00065;C00025;C00417;C00022;C00158;C00160;C00168;C00209;C00149;C00311 | 9.803921569 | 0.15625 | 1.35367E-06 | 6 | 4 | 0.2 |
| hsa00770 | Pantothenate and CoA biosynthesis | C00864;C00099;C00183;C00022;C00141;C00049;C00429 | 6.862745098 | 0.233333333 | 3.5023E-06 | 1 | 6 | -0.714285714 |
| hsa00020 | Citrate cycle (TCA cycle) | C00122;C00417;C00022;C00158;C00149;C00311 | 5.882352941 | 0.3 | 3.67694E-06 | 4 | 2 | 0.333333333 |
| hsa01200 | Carbon metabolism | C00065;C00025;C00122;C00022;C00979;C00158;C00160;C00168;C00049;C00149;C00311;C00257 | 11.76470588 | 0.107142857 | 7.00E-06 | 7 | 5 | 0.166666667 |
| hsa00290 | Valine, leucine and isoleucine biosynthesis | C00407;C00233;C00183;C00022;C02226;C00141 | 5.882352941 | 0.260869565 | 9.05721E-06 | 0 | 6 | -1 |
| hsa00260 | Glycine, serine and threonine metabolism | C00065;C00719;C00263;C00078;C00022;C00168;C00049;C00546 | 7.843137255 | 0.166666667 | 1.00095E-05 | 5 | 3 | 0.25 |
| hsa00970 | Aminoacyl-tRNA biosynthesis | C00152;C00065;C00025;C00407;C00078;C00183;C00047;C00049 | 7.843137255 | 0.153846154 | 1.85091E-05 | 6 | 2 | 0.5 |
| hsa01210 | 2-Oxocarboxylic acid metabolism | C00025;C00417;C00407;C00078;C00233;C00183;C00022;C00047;C02226;C00141;C00158;C00049;C00311 | 12.74509804 | 0.090277778 | 1.88892E-05 | 7 | 6 | 0.076923077 |
| hsa00250 | Alanine, aspartate and glutamate metabolism | C00152;C00025;C00122;C00022;C00158;C00049 | 5.882352941 | 0.214285714 | 3.08065E-05 | 4 | 2 | 0.333333333 |
| hsa04978 | Mineral absorption | C00152;C00065;C00407;C00078;C00183;C00009 | 5.882352941 | 0.206896552 | 3.81292E-05 | 4 | 2 | 0.333333333 |
| hsa02010 | ABC transporters | C00065;C00025;C00245;C00719;C00407;C00294;C00183;C00047;C00049;C00009;C01606;C00121 | 11.76470588 | 0.086956522 | 5.89042E-05 | 6 | 6 | 0 |
| hsa00410 | beta-Alanine metabolism | C00864;C00099;C01073;C00383;C00049;C00429 | 5.882352941 | 0.1875 | 6.88042E-05 | 1 | 5 | -0.666666667 |
| hsa00360 | Phenylalanine metabolism | C00122;C00022;C00642;C11457;C07086;C05593;C01198 | 6.862745098 | 0.142857143 | 0.000103478 | 0 | 7 | -1 |
| hsa04922 | Glucagon signaling pathway | C00122;C00022;C00158;C00149;C00311 | 4.901960784 | 0.192307692 | 0.000253759 | 3 | 2 | 0.2 |
| hsa00591 | Linoleic acid metabolism | C14766;C14762;C06426;C00157;C14827 | 4.901960784 | 0.178571429 | 0.000365614 | 1 | 4 | -0.6 |
| hsa00232 | Caffeine metabolism | C13747;C07480;C07130;C16361 | 3.921568627 | 0.181818182 | 0.001370458 | 1 | 3 | -0.5 |
| hsa05211 | Renal cell carcinoma | C00122;C00149 | 1.960784314 | 0.666666667 | 0.001528787 | 1 | 1 | 0 |
| hsa00220 | Arginine biosynthesis | C00327;C00025;C00122;C00049 | 3.921568627 | 0.173913043 | 0.001630116 | 3 | 1 | 0.5 |
| hsa05231 | Choline metabolism in cancer | C00588;C00157;C04230 | 2.941176471 | 0.272727273 | 0.001673735 | 3 | 0 | 1 |
| hsa00280 | Valine, leucine and isoleucine degradation | C00407;C00233;C00183;C00141;C02170 | 4.901960784 | 0.119047619 | 0.002456367 | 0 | 5 | -1 |
| hsa00240 | Pyrimidine metabolism | C02067;C00099;C00383;C02170;C00429;C00015 | 5.882352941 | 0.09375 | 0.003154118 | 1 | 5 | -0.666666667 |
| hsa00270 | Cysteine and methionine metabolism | C00065;C00263;C00022;C00979;C03145;C00049 | 5.882352941 | 0.089552239 | 0.00397337 | 3 | 3 | 0 |
| hsa00650 | Butanoate metabolism | C00025;C00122;C00022;C00246;C00741 | 4.901960784 | 0.106382979 | 0.004047687 | 1 | 4 | -0.6 |
| hsa00330 | Arginine and proline metabolism | C02946;C00025;C00791;C00022;C02565;C05947 | 5.882352941 | 0.086956522 | 0.004600999 | 2 | 4 | -0.333333333 |
| hsa00620 | Pyruvate metabolism | C00122;C00022;C00149;C00546 | 3.921568627 | 0.125 | 0.005655607 | 1 | 3 | -0.5 |
| hsa01100 | Metabolic pathways | C00152;C13747;C07480;C00327;C02946;C00065;C07130;C00025;C00122;C00864;C04555;C02341;C00417;C00245;C00719;C00407;C00294;C00263;C05570;C00366;C00078;C02067;C00791;C06423;C00233;C00099;C00183;C00022;C00047;C00642;C02226;C06427;C06337;C11457;C00141;C05578;C01571;C06426;C00588;C00979;C00158;C00383;C00180;C00160;C00168;C01717;C01114;C00209;C00049;C07086;C00314;C00149;C00311;C05593;C02170;C00246;C00257;C06578;C02378;C01744;C03765;C08972;C00486;C01198;C10700;C00546;C00429;C01606;C00157;C14827;C04317;C00121;C02565;C05947;C12455;C03203;C01617;C00270;C00346;C00015;C02835;C01444 | 80.39215686 | 0.026675342 | 0.005947198 | 25 | 57 | -0.390243902 |
| hsa04976 | Bile secretion | C04555;C05465;C00366;C07185;C06804;C00486;C03990 | 6.862745098 | 0.072164948 | 0.006323254 | 2 | 5 | -0.428571429 |
| hsa04080 | Neuroactive ligand-receptor interaction | C00025;C00245;C00099;C00049;C00015 | 4.901960784 | 0.094339623 | 0.006798125 | 3 | 2 | 0.2 |
| hsa00920 | Sulfur metabolism | C00065;C00245;C00263;C00979 | 3.921568627 | 0.117647059 | 0.007043927 | 2 | 2 | 0 |
| hsa00350 | Tyrosine metabolism | C00122;C00022;C00642;C05578;C05593;C03765 | 5.882352941 | 0.076923077 | 0.008360454 | 0 | 6 | -1 |
| hsa00564 | Glycerophospholipid metabolism | C00065;C00588;C00157;C04230;C00346 | 4.901960784 | 0.089285714 | 0.008574818 | 5 | 0 | 1 |
| hsa01240 | Biosynthesis of cofactors | C00065;C00025;C00864;C00078;C06423;C00099;C00183;C00022;C00141;C00158;C00049;C00314;C00311;C00015 | 13.7254902 | 0.042682927 | 0.016148657 | 7 | 7 | 0 |
| hsa00430 | Taurine and hypotaurine metabolism | C00025;C00245;C00022 | 2.941176471 | 0.125 | 0.016555811 | 1 | 2 | -0.333333333 |
| hsa00785 | Lipoic acid metabolism | C06423;C00233;C00022;C00141 | 3.921568627 | 0.090909091 | 0.017333642 | 0 | 4 | -1 |
| hsa00470 | D-Amino acid metabolism | C00065;C00025;C00022;C00047;C00049 | 4.901960784 | 0.072463768 | 0.019999034 | 4 | 1 | 0.6 |
| hsa00340 | Histidine metabolism | C00025;C05570;C00049;C02835 | 3.921568627 | 0.085106383 | 0.021624659 | 4 | 0 | 1 |
| hsa00190 | Oxidative phosphorylation | C00122;C00009 | 1.960784314 | 0.166666667 | 0.029405942 | 1 | 1 | 0 |
| hsa04742 | Taste transduction | C00025;C00158;C00149 | 2.941176471 | 0.09375 | 0.035591953 | 3 | 0 | 1 |
| hsa04071 | Sphingolipid signaling pathway | C00065;C00346 | 1.960784314 | 0.133333333 | 0.044755505 | 2 | 0 | 1 |
| hsa00030 | Pentose phosphate pathway | C00022;C00257;C00121 | 2.941176471 | 0.081081081 | 0.05140534 | 1 | 2 | -0.333333333 |
| hsa04964 | Proximal tubule bicarbonate reclamation | C00025;C00149 | 1.960784314 | 0.117647059 | 0.056290232 | 2 | 0 | 1 |
| hsa00640 | Propanoate metabolism | C00099;C02170;C00546 | 2.941176471 | 0.073170732 | 0.066109887 | 0 | 3 | -1 |
| hsa04723 | Retrograde endocannabinoid signaling | C00025;C00157 | 1.960784314 | 0.105263158 | 0.068734586 | 2 | 0 | 1 |
| hsa00563 | Glycosylphosphatidylinositol (GPI)-anchor biosynthesis | C00346 | 0.980392157 | 0.25 | 0.088360496 | 1 | 0 | 1 |
| hsa04068 | FoxO signaling pathway | C00025 | 0.980392157 | 0.2 | 0.109214326 | 1 | 0 | 1 |
| hsa03320 | PPAR signaling pathway | C14762 | 0.980392157 | 0.2 | 0.109214326 | 0 | 1 | -1 |
| hsa05016 | Huntington disease | C00025 | 0.980392157 | 0.166666667 | 0.129595694 | 1 | 0 | 1 |
| hsa04930 | Type II diabetes mellitus | C00022 | 0.980392157 | 0.166666667 | 0.129595694 | 0 | 1 | -1 |
| hsa00760 | Nicotinate and nicotinamide metabolism | C00122;C00022;C00049 | 2.941176471 | 0.054545455 | 0.130074666 | 1 | 2 | -0.333333333 |
| hsa00061 | Fatty acid biosynthesis | C06423;C01571;C00383 | 2.941176471 | 0.051724138 | 0.145897452 | 0 | 3 | -1 |
| hsa04720 | Long-term potentiation | C00025 | 0.980392157 | 0.142857143 | 0.149515201 | 1 | 0 | 1 |
| hsa05017 | Spinocerebellar ataxia | C00025 | 0.980392157 | 0.142857143 | 0.149515201 | 1 | 0 | 1 |
| hsa05030 | Cocaine addiction | C00025 | 0.980392157 | 0.142857143 | 0.149515201 | 1 | 0 | 1 |
| hsa05033 | Nicotine addiction | C00025 | 0.980392157 | 0.142857143 | 0.149515201 | 1 | 0 | 1 |
| hsa05200 | Pathways in cancer | C00122;C00149 | 1.960784314 | 0.064516129 | 0.157170939 | 1 | 1 | 0 |
| hsa05022 | Pathways of neurodegeneration - multiple diseases | C00025;C00009 | 1.960784314 | 0.0625 | 0.165276204 | 2 | 0 | 1 |
| hsa04724 | Glutamatergic synapse | C00025 | 0.980392157 | 0.125 | 0.16898321 | 1 | 0 | 1 |
| hsa05143 | African trypanosomiasis | C00078 | 0.980392157 | 0.125 | 0.16898321 | 1 | 0 | 1 |
| hsa04727 | GABAergic synapse | C00025 | 0.980392157 | 0.111111111 | 0.188009857 | 1 | 0 | 1 |
| hsa04730 | Long-term depression | C00025 | 0.980392157 | 0.111111111 | 0.188009857 | 1 | 0 | 1 |
| hsa04713 | Circadian entrainment | C00025 | 0.980392157 | 0.111111111 | 0.188009857 | 1 | 0 | 1 |
| hsa05031 | Amphetamine addiction | C00025 | 0.980392157 | 0.111111111 | 0.188009857 | 1 | 0 | 1 |
| hsa00600 | Sphingolipid metabolism | C00065;C00346 | 1.960784314 | 0.057142857 | 0.189998325 | 2 | 0 | 1 |
| hsa00230 | Purine metabolism | C00294;C00366;C00209;C01444 | 3.921568627 | 0.03960396 | 0.198999621 | 1 | 3 | -0.5 |
| hsa04979 | Cholesterol metabolism | C05465 | 0.980392157 | 0.1 | 0.206605051 | 0 | 1 | -1 |
| hsa05034 | Alcoholism | C00025 | 0.980392157 | 0.1 | 0.206605051 | 1 | 0 | 1 |
| hsa05415 | Diabetic cardiomyopathy | C00022;C00546 | 1.960784314 | 0.051282051 | 0.223649957 | 0 | 2 | -1 |
| hsa04122 | Sulfur relay system | C00979 | 0.980392157 | 0.090909091 | 0.224778481 | 0 | 1 | -1 |
| hsa04072 | Phospholipase D signaling pathway | C00025 | 0.980392157 | 0.090909091 | 0.224778481 | 1 | 0 | 1 |
| hsa04540 | Gap junction | C00025 | 0.980392157 | 0.090909091 | 0.224778481 | 1 | 0 | 1 |
| hsa04928 | Parathyroid hormone synthesis, secretion and action | C00009 | 0.980392157 | 0.090909091 | 0.224778481 | 1 | 0 | 1 |
| hsa04911 | Insulin secretion | C00022 | 0.980392157 | 0.083333333 | 0.242539621 | 0 | 1 | -1 |
| hsa04721 | Synaptic vesicle cycle | C00025 | 0.980392157 | 0.083333333 | 0.242539621 | 1 | 0 | 1 |
| hsa00592 | alpha-Linolenic acid metabolism | C06427;C00157 | 1.960784314 | 0.045454545 | 0.266274718 | 1 | 1 | 0 |
| hsa05131 | Shigellosis | C00407 | 0.980392157 | 0.071428571 | 0.276861876 | 0 | 1 | -1 |
| hsa05014 | Amyotrophic lateral sclerosis | C00025 | 0.980392157 | 0.071428571 | 0.276861876 | 1 | 0 | 1 |
| hsa00120 | Primary bile acid biosynthesis | C00245;C05465 | 1.960784314 | 0.042553191 | 0.291900129 | 0 | 2 | -1 |
| hsa04066 | HIF-1 signaling pathway | C00022 | 0.980392157 | 0.066666667 | 0.293440902 | 0 | 1 | -1 |
| hsa00380 | Tryptophan metabolism | C00078;C01717;C05830 | 2.941176471 | 0.036144578 | 0.294782712 | 1 | 2 | -0.333333333 |
| hsa00982 | Drug metabolism - cytochrome P450 | C07185;C16650;C05011 | 2.941176471 | 0.034482759 | 0.320019218 | 1 | 2 | -0.333333333 |
| hsa04931 | Insulin resistance | C00022 | 0.980392157 | 0.052631579 | 0.356076152 | 0 | 1 | -1 |
| hsa00310 | Lysine degradation | C00047;C12455 | 1.960784314 | 0.035714286 | 0.367751976 | 1 | 1 | 0 |
| hsa00910 | Nitrogen metabolism | C00025 | 0.980392157 | 0.05 | 0.370855682 | 1 | 0 | 1 |
| hsa00053 | Ascorbate and aldarate metabolism | C00022;C01114 | 1.960784314 | 0.035087719 | 0.376013744 | 0 | 2 | -1 |
| hsa01232 | Nucleotide metabolism | C00294;C00015 | 1.960784314 | 0.034482759 | 0.384232183 | 1 | 1 | 0 |
| hsa04148 | Efferocytosis | C04230 | 0.980392157 | 0.047619048 | 0.385299238 | 1 | 0 | 1 |
| hsa04152 | AMPK signaling pathway | C00022 | 0.980392157 | 0.045454545 | 0.399414384 | 0 | 1 | -1 |
| hsa00740 | Riboflavin metabolism | C01727 | 0.980392157 | 0.041666667 | 0.426688859 | 0 | 1 | -1 |
| hsa00565 | Ether lipid metabolism | C04317 | 0.980392157 | 0.04 | 0.439862488 | 1 | 0 | 1 |
| hsa04024 | cAMP signaling pathway | C20793 | 0.980392157 | 0.04 | 0.439862488 | 0 | 1 | -1 |
| hsa05012 | Parkinson disease | C00009 | 0.980392157 | 0.038461538 | 0.452736311 | 1 | 0 | 1 |
| hsa04973 | Carbohydrate digestion and absorption | C00246 | 0.980392157 | 0.037037037 | 0.465317085 | 0 | 1 | -1 |
| hsa00750 | Vitamin B6 metabolism | C00314 | 0.980392157 | 0.034482759 | 0.489625766 | 0 | 1 | -1 |
| hsa00780 | Biotin metabolism | C00047 | 0.980392157 | 0.034482759 | 0.489625766 | 1 | 0 | 1 |
| hsa04216 | Ferroptosis | C00025 | 0.980392157 | 0.034482759 | 0.489625766 | 1 | 0 | 1 |
| hsa01040 | Biosynthesis of unsaturated fatty acids | C06427;C06426 | 1.960784314 | 0.027027027 | 0.508283984 | 0 | 2 | -1 |
| hsa00010 | Glycolysis / Gluconeogenesis | C00022 | 0.980392157 | 0.032258065 | 0.512839628 | 0 | 1 | -1 |
| hsa00730 | Thiamine metabolism | C00022 | 0.980392157 | 0.032258065 | 0.512839628 | 0 | 1 | -1 |
| hsa00400 | Phenylalanine, tyrosine and tryptophan biosynthesis | C00078 | 0.980392157 | 0.028571429 | 0.556176111 | 1 | 0 | 1 |
| hsa00480 | Glutathione metabolism | C00025 | 0.980392157 | 0.026315789 | 0.586152398 | 1 | 0 | 1 |
| hsa04977 | Vitamin digestion and absorption | C00864 | 0.980392157 | 0.023809524 | 0.623023409 | 0 | 1 | -1 |
| hsa04726 | Serotonergic synapse | C00078 | 0.980392157 | 0.023809524 | 0.623023409 | 1 | 0 | 1 |
| hsa00900 | Terpenoid backbone biosynthesis | C00022 | 0.980392157 | 0.02173913 | 0.656638805 | 0 | 1 | -1 |
| hsa00140 | Steroid hormone biosynthesis | C04555;C05476 | 1.960784314 | 0.01980198 | 0.677932343 | 0 | 2 | -1 |
| hsa00071 | Fatty acid degradation | C02990 | 0.980392157 | 0.02 | 0.687283452 | 1 | 0 | 1 |
| hsa00440 | Phosphonate and phosphinate metabolism | C00022 | 0.980392157 | 0.017857143 | 0.728243163 | 0 | 1 | -1 |
| hsa00040 | Pentose and glucuronate interconversions | C00022 | 0.980392157 | 0.016949153 | 0.74668332 | 0 | 1 | -1 |
| hsa01212 | Fatty acid metabolism | C00383;C02990 | 1.960784314 | 0.016393443 | 0.774657761 | 1 | 1 | 0 |
| hsa00590 | Arachidonic acid metabolism | C00157 | 0.980392157 | 0.012658228 | 0.84162737 | 1 | 0 | 1 |
| hsa00524 | Neomycin, kanamycin and gentamicin biosynthesis | C00025 | 0.980392157 | 0.012345679 | 0.848911989 | 1 | 0 | 1 |
| hsa00860 | Porphyrin metabolism | C00025;C00486 | 1.960784314 | 0.013513514 | 0.858835683 | 2 | 0 | 1 |
| hsa00520 | Amino sugar and nucleotide sugar metabolism | C00270 | 0.980392157 | 0.008474576 | 0.937021879 | 0 | 1 | -1 |
| hsa01250 | Biosynthesis of nucleotide sugars | C00270 | 0.980392157 | 0.005 | 0.991186791 | 0 | 1 | -1 |

DA score, Differential Abundance Score

Table 3. Differential fecal metabolites before and after a 12-week BBr60 intervention

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **MS2 score** | **mz** | **type** | **Formula** | **HMDB** | **CAS** | **KEGG ID** | **MEAN BBr60-before** | **MEAN BBr60-after** | **VIP** | **P-VALUE** | **FOLD CHANGE** |
| Cholic acid | 4.0000 | 391.2844 | POS | C24H40O5 | HMDB0000619 | 81-25-4 | C00695 | 0.0532 | 0.0237 | 1.6886 | 0.0446 | 0.4463 |
| Maltose | 3.9900 | 365.1054 | POS | C12H22O11 | HMDB0000163 | 69-79-4 | C00208 | 0.3513 | 0.2193 | 1.2474 | 0.0225 | 0.6243 |
| N-Acetylgalactosamine | 3.9900 | 220.0827 | NEG | C8H15NO6 | HMDB0006480 | 14131-60-3 | C05021 | 1.7753 | 0.9365 | 2.1698 | 0.0030 | 0.5275 |
| Val-Val | 3.9900 | 215.1401 | NEG | C10H20N2O3 | HMDB0029140 | 3918-94-3 |  | 8.3660 | 4.8582 | 2.2877 | 0.0415 | 0.5807 |
| Ile-Leu | 3.9900 | 245.1860 | POS | C12H24N2O3 | HMDB0028911 | 26462-22-6 |  | 6.2610 | 4.3123 | 2.0255 | 0.0332 | 0.6888 |
| 6-(Dimethylamino)purine | 3.9900 | 164.0931 | POS | C7H9N5 | HMDB0000473 | 938-55-6 |  | 0.0618 | 0.0314 | 1.8235 | 0.0479 | 0.5091 |
| 12-Hydroxystearic acid | 3.9900 | 299.2592 | NEG | C18H36O3 | HMDB0061706 | 106-14-9 |  | 74.4455 | 85.2251 | 1.3585 | 0.0274 | 1.1448 |
| Methionine sulfoxide | 3.9800 | 166.0532 | POS | C5H11NO3S | HMDB0002005 | 62697-73-8 | C02989 | 0.1009 | 0.0669 | 1.9816 | 0.0002 | 0.6635 |
| Methionine | 3.9800 | 150.0583 | POS | C5H11NO2S | HMDB0033951 | 59-51-8 | C01733 | 0.5877 | 0.4092 | 2.5163 | 0.0100 | 0.6962 |
| Isoleucine | 3.9800 | 130.0874 | NEG | C6H13NO2 | HMDB0000172 | 73-32-5 | C00407 | 17.5515 | 9.3707 | 2.5394 | 0.0162 | 0.5339 |
| Phenylalanine | 3.9800 | 166.0862 | POS | C9H11NO2 | HMDB0000159 | 63-91-2 | C00079 | 2.0962 | 1.2527 | 2.4078 | 0.0345 | 0.5976 |
| Glycohyodeoxycholic acid | 3.9800 | 448.3071 | NEG | C26H43NO5 | HMDB0255669 | 13042-33-6 |  | 8.3912 | 2.1521 | 1.9702 | 0.0067 | 0.2565 |
| Thymine | 3.9800 | 125.0357 | NEG | C5H6N2O2 | HMDB0000262 | 65-71-4 | C00178 | 11.6132 | 5.7528 | 2.2004 | 0.0070 | 0.4954 |
| Serine | 3.9800 | 106.0498 | POS | C3H7NO3 | HMDB0000187 | 56-45-1 | C00065 | 0.0603 | 0.0503 | 1.9588 | 0.0307 | 0.8349 |
| N-Acetylglucosamine | 3.9700 | 220.0827 | NEG | C8H15NO6 | HMDB0062641 | 7512-17-6 | C00140 | 1.7753 | 0.9365 | 2.1698 | 0.0030 | 0.5275 |
| 3-Amino-4-methylpentanoic acid | 3.9700 | 130.0874 | NEG | C6H13NO2 | HMDB0245808 | 5699-54-7 |  | 17.5515 | 9.3707 | 2.5394 | 0.0162 | 0.5339 |
| Arg-Phe | 3.9700 | 322.1871 | POS | C15H23N5O3 | HMDB0028716 | 2047-13-4 |  | 0.0540 | 0.0376 | 2.1496 | 0.0136 | 0.6962 |
| Taurine | 3.9700 | 124.0075 | NEG | C2H7NO3S | HMDB0000251 | 107-35-7 | C00245 | 21.6038 | 9.8224 | 1.6736 | 0.0063 | 0.4547 |
| Tryptophan | 3.9700 | 205.0971 | POS | C11H12N2O2 | HMDB0030396 | 73-22-3 | C00078 | 0.3690 | 0.1462 | 2.1467 | 0.0446 | 0.3963 |
| 1-Methyl-6-oxo-1,6-dihydropyridine-3-carboxylic acid | 3.9700 | 152.0355 | NEG | C7H7NO3 |  | 3719-45-7 |  | 0.1232 | 0.1908 | 1.1561 | 0.0496 | 1.5492 |
| Deoxyguanosine | 3.9700 | 268.1042 | POS | C10H13N5O4 | HMDB0000085 | 961-07-9 | C00330 | 0.0312 | 0.0200 | 1.8353 | 0.0446 | 0.6413 |
| 4-Ethoxybenzoic acid | 3.9700 | 147.0453 | NEG | C9H10O3 |  | 619-86-3 |  | 0.7528 | 0.3663 | 2.7377 | 0.0010 | 0.4866 |
| 13(S)-HODE | 3.9700 | 295.2278 | NEG | C18H32O3 | HMDB0004667 | 29623-28-7 | C14762 | 5.4585 | 2.9070 | 2.4281 | 0.0017 | 0.5326 |
| Linoleic acid | 3.9700 | 279.2330 | NEG | C18H32O2 | HMDB0000673 | 60-33-3 | C01595 | 340.7685 | 153.5564 | 2.5076 | 0.0004 | 0.4506 |
| Docosapentaenoic acid (DPA) | 3.9700 | 329.2486 | NEG | C22H34O2 | HMDB0006528 | 2234-74-4 | C16513 | 3.3747 | 1.5833 | 1.6198 | 0.0430 | 0.4692 |
| Trehalose | 3.9600 | 365.1054 | POS | C12H22O11 | HMDB0000975 | 99-20-7 | C01083 | 0.3513 | 0.2193 | 1.2474 | 0.0225 | 0.6243 |
| Leu-Ile | 3.9600 | 245.1860 | POS | C12H24N2O3 | HMDB0028932 | 36077-41-5 |  | 6.2610 | 4.3123 | 2.0255 | 0.0332 | 0.6888 |
| 9-Ethyladenine | 3.9600 | 164.0931 | POS | C7H9N5 |  | 2715-68-6 |  | 0.0618 | 0.0314 | 1.8235 | 0.0479 | 0.5091 |
| 2-Hydroxystearic acid | 3.9600 | 299.2592 | NEG | C18H36O3 | HMDB0062549 | 26531-80-6 | C03045 | 74.4455 | 85.2251 | 1.3585 | 0.0274 | 1.1448 |
| Glu-Arg | 3.9600 | 304.1617 | POS | C11H21N5O5 | HMDB0028813 | 7219-59-2 |  | 0.0470 | 0.0283 | 1.7187 | 0.0345 | 0.6013 |
| Threonic acid | 3.9600 | 135.0300 | NEG | C4H8O5 | HMDB0062620 | 7306-96-9 | C01620 | 0.4363 | 0.4113 | 1.4378 | 0.0332 | 0.9425 |
| Glycocholic acid | 3.9600 | 466.3164 | POS | C26H43NO6 | HMDB0000138 | 475-31-0 | C01921 | 0.1538 | 0.0289 | 1.8981 | 0.0332 | 0.1879 |
| Glycoursodeoxycholic acid | 3.9600 | 450.3215 | POS | C26H43NO5 | HMDB0000708 | 64480-66-6 |  | 0.2798 | 0.0737 | 1.7713 | 0.0216 | 0.2635 |
| Uracil | 3.9600 | 111.0201 | NEG | C4H4N2O2 | HMDB0000300 | 66-22-8 | C00106 | 48.7970 | 28.9972 | 2.8264 | 0.0029 | 0.5942 |
| Aminopicoline | 3.9600 | 109.0760 | POS | C6H8N2 | HMDB0246517 | 695-34-1 |  | 0.0438 | 0.0650 | 1.3147 | 0.0430 | 1.4852 |
| 3-Amino-4-hydroxybenzoic acid | 3.9500 | 154.0499 | POS | C7H7NO3 | HMDB0304941 | 1571-72-8 | C12115 | 0.0543 | 0.0775 | 1.3245 | 0.0105 | 1.4276 |
| 2-Keto-3-deoxygalactonic acid | 3.9500 | 177.0406 | NEG | C6H10O6 | HMDB0001353 | 17510-99-5 | C01216 | 5.0672 | 1.6048 | 2.7506 | 0.0005 | 0.3167 |
| Pro-Phe | 3.9500 | 263.1391 | POS | C14H18N2O3 | HMDB0011179 | 13589-02-1 |  | 0.1902 | 0.1178 | 2.6399 | 0.0061 | 0.6192 |
| Phe-Val | 3.9500 | 265.1548 | POS | C14H20N2O3 | HMDB0029008 | 3918-90-9 |  | 0.8931 | 0.5016 | 2.4264 | 0.0048 | 0.5616 |
| Deoxyinosine | 3.9500 | 251.0786 | NEG | C10H12N4O4 | HMDB0000071 | 890-38-0 | C05512 | 36.8536 | 23.2784 | 2.3826 | 0.0234 | 0.6316 |
| Guvacoline (hydrochloride) | 3.9500 | 142.0863 | POS | C7H11NO2 |  | 6197-39-3 | C16821 | 0.0199 | 0.0327 | 1.6822 | 0.0100 | 1.6440 |
| 2-Ketobutyric acid | 3.9500 | 101.0245 | NEG | C4H6O3 | HMDB0000005 | 600-18-0 | C00109 | 2.8774 | 2.1203 | 1.2716 | 0.0004 | 0.7369 |
| Sphingosine | 3.9500 | 300.2897 | POS | C18H37NO2 | HMDB0000252 | 123-78-4 | C00319 | 16.6441 | 7.3454 | 2.0589 | 0.0274 | 0.4413 |
| NAE(18:2) | 3.9500 | 324.2898 | POS | C20H37NO2 | HMDB0012252 | 68171-52-8 |  | 3.6243 | 0.8938 | 1.7824 | 0.0110 | 0.2466 |
| NAE(18:3(6Z,9Z,12Z)) | 3.9500 | 322.2742 | POS | C20H35NO2 | HMDB0013624 | 150314-37-7 |  | 0.2720 | 0.1074 | 1.8234 | 0.0162 | 0.3947 |
| Leucine | 3.9400 | 130.0874 | NEG | C6H13NO2 | HMDB0062203 | 61-90-5 | C00123 | 17.5515 | 9.3707 | 2.5394 | 0.0162 | 0.5339 |
| 2,5-Dimethylpyrazine | 3.9400 | 109.0760 | POS | C6H8N2 | HMDB0035289 | 123-32-0 |  | 0.0438 | 0.0650 | 1.3147 | 0.0430 | 1.4852 |
| 2-Ethylpyrazine | 3.9400 | 109.0760 | POS | C6H8N2 | HMDB0031849 | 13925-00-3 |  | 0.0438 | 0.0650 | 1.3147 | 0.0430 | 1.4852 |
| 2,6-Dimethylpyrazine | 3.9400 | 109.0760 | POS | C6H8N2 | HMDB0035248 | 108-50-9 |  | 0.0438 | 0.0650 | 1.3147 | 0.0430 | 1.4852 |
| NAE(18:3(9Z,12Z,15Z)) | 3.9400 | 322.2742 | POS | C20H35NO2 | HMDB0013624 | 57086-93-8 |  | 0.2720 | 0.1074 | 1.8234 | 0.0162 | 0.3947 |
| Glycylleucine | 3.9400 | 187.1088 | NEG | C8H16N2O3 | HMDB0000759 | 869-19-2 | C02155 | 8.1926 | 4.7497 | 2.8699 | 0.0073 | 0.5798 |
| Phe-Pro | 3.9400 | 261.1246 | NEG | C14H18N2O3 | HMDB0011177 | 7669-65-0 |  | 0.5159 | 0.3060 | 2.7009 | 0.0115 | 0.5930 |
| Sucralose (Xenobiotic) | 3.9400 | 395.0075 | NEG | C12H19Cl3O8 | HMDB0031554 | 56038-13-2 | C12285 | 7.1305 | 24.1409 | 1.9757 | 0.0005 | 3.3856 |
| 2-Methyltetrahydrofuran-3-one | 3.9400 | 99.0452 | NEG | C5H8O2 | HMDB0031178 | 3188-00-9 |  | 1.0987 | 0.4557 | 2.4508 | 0.0003 | 0.4147 |
| 2,3-Pentanedione | 3.9400 | 99.0452 | NEG | C5H8O2 | HMDB0031598 | 600-14-6 |  | 1.0987 | 0.4557 | 2.4508 | 0.0003 | 0.4147 |
| 3-Methyl-2-oxovaleric acid | 3.9400 | 129.0558 | NEG | C6H10O3 | HMDB0000491 | 1460-34-0 | C03465 | 36.2015 | 14.7338 | 2.9023 | 0.0000 | 0.4070 |
| Hydroxytyrosol | 3.9400 | 153.0558 | NEG | C8H10O3 | HMDB0005784 | 10597-60-1 |  | 0.4296 | 0.1265 | 1.7651 | 0.0191 | 0.2946 |
| NAE(16:0) | 3.9400 | 300.2899 | POS | C18H37NO2 | HMDB0002100 | 544-31-0 | C16512 | 3.3480 | 1.5507 | 2.2726 | 0.0023 | 0.4632 |
| 3-Methylbut-2-enoic acid | 3.9300 | 99.0452 | NEG | C5H8O2 | HMDB0000509 | 541-47-9 |  | 1.0987 | 0.4557 | 2.4508 | 0.0003 | 0.4147 |
| Ketoleucine | 3.9300 | 129.0558 | NEG | C6H10O3 | HMDB0000695 | 816-66-0 | C00233 | 36.2015 | 14.7338 | 2.9023 | 0.0000 | 0.4070 |
| 2-Ketocaproic acid | 3.9300 | 129.0558 | NEG | C6H10O3 | HMDB0001864 | 2492-75-3 | C00902 | 36.2015 | 14.7338 | 2.9023 | 0.0000 | 0.4070 |
| N-Methyl-L-asparagine | 3.9300 | 147.0765 | POS | C5H10N2O3 |  | 7175-34-0 |  | 0.1892 | 0.1006 | 2.0197 | 0.0052 | 0.5315 |
| Gly-Phe | 3.9300 | 221.0930 | NEG | C11H14N2O3 | HMDB0028848 | 721-66-4 |  | 0.3688 | 0.2333 | 2.3410 | 0.0307 | 0.6325 |
| N-Acetylmannosamine | 3.9300 | 222.0973 | POS | C8H15NO6 | HMDB0001129 | 3615-17-6 | C00645 | 0.1091 | 0.0722 | 1.8594 | 0.0055 | 0.6615 |
| 2-Ethyl-2-hydroxybutyric acid | 3.9300 | 131.0715 | NEG | C6H12O3 | HMDB0001975 | 3639-21-2 |  | 61.6185 | 18.0582 | 2.5376 | 0.0003 | 0.2931 |
| 2-Hydroxyhexanoic acid | 3.9300 | 131.0715 | NEG | C6H12O3 | HMDB0001624 | 6064-63-7 |  | 61.6185 | 18.0582 | 2.5376 | 0.0003 | 0.2931 |
| Thymidine | 3.9300 | 241.0830 | NEG | C10H14N2O5 | HMDB0000273 | 50-89-5 | C00214 | 11.3832 | 5.9458 | 2.6149 | 0.0039 | 0.5223 |
| Arabinono-1,4-lactone | 3.9300 | 147.0300 | NEG | C5H8O5 | HMDB0001900 | 51532-86-6 | C01114 | 1.0633 | 0.5686 | 1.0296 | 0.0319 | 0.5347 |
| alpha-Ketoisovaleric acid | 3.9300 | 115.0401 | NEG | C5H8O3 | HMDB0000019 | 759-05-7 | C00141 | 17.5087 | 6.9740 | 2.8580 | 0.0000 | 0.3983 |
| Norleucine | 3.9200 | 130.0874 | NEG | C6H13NO2 | HMDB0251526 | 104809-14-5 | C01933 | 17.5515 | 9.3707 | 2.5394 | 0.0162 | 0.5339 |
| Glutamine | 3.9200 | 145.0619 | NEG | C5H10N2O3 | HMDB0000641 | 56-85-9 | C00064 | 0.5875 | 0.3009 | 2.5039 | 0.0034 | 0.5122 |
| 2-Hydroxy-3-methylbutyric acid | 3.9200 | 117.0558 | NEG | C5H10O3 | HMDB0000407 | 4026-18-0 |  | 48.1401 | 13.5910 | 2.1321 | 0.0016 | 0.2823 |
| 5-Aminosalicylic Acid | 3.9100 | 152.0355 | NEG | C7H7NO3 | HMDB0014389 | 89-57-6 | D00377|C07138 | 0.1232 | 0.1908 | 1.1561 | 0.0496 | 1.5492 |
| Dethiobiotin | 3.9100 | 213.1245 | NEG | C10H18N2O3 | HMDB0003581 | 533-48-2 | C01909 | 0.6775 | 0.4134 | 2.6269 | 0.0169 | 0.6101 |
| Nicotinamide riboside (NR) | 3.9000 | 255.0976 | POS | C11H15N2O5 | HMDB0000855 | 1341-23-7 | C03150 | 0.0849 | 0.1295 | 1.3265 | 0.0234 | 1.5247 |
| Glyco-gamma-muricholic acid | 3.9000 | 464.3020 | NEG | C26H43NO6 | HMDB0240607 | 32747-08-3 |  | 4.9789 | 0.7902 | 2.0783 | 0.0039 | 0.1587 |
| Acamprosate (calcium) | 3.9000 | 180.0339 | NEG | C5H11NO4S | HMDB0014797 | 77337-76-9 | D07058 | 0.7973 | 0.4069 | 1.4703 | 0.0199 | 0.5104 |
| Indoleacetic acid | 3.9000 | 174.0561 | NEG | C10H9NO2 | HMDB0000197 | 87-51-4 | C00954 | 0.9157 | 1.7802 | 1.3231 | 0.0136 | 1.9442 |
| gamma-Glutamylphenylalanine | 3.9000 | 293.1145 | NEG | C14H18N2O5 | HMDB0000594 | 7432-24-8 |  | 0.2801 | 0.1621 | 2.3846 | 0.0253 | 0.5788 |
| Hydroxyisocaproic acid | 3.8900 | 131.0715 | NEG | C6H12O3 | HMDB0000665 | 498-36-2 | C03264 | 61.6185 | 18.0582 | 2.5376 | 0.0003 | 0.2931 |
| Indolelactic acid | 3.8900 | 204.0666 | NEG | C11H11NO3 | HMDB0000671 | 1821-52-9 | C02043 | 4.9035 | 3.8014 | 1.4725 | 0.0479 | 0.7752 |
| 2'-Deoxyuridine | 3.8900 | 227.0674 | NEG | C9H12N2O5 | HMDB0000012 | 951-78-0 | C00526 | 6.7566 | 4.3303 | 2.3856 | 0.0216 | 0.6409 |
| Melibiose | 3.8800 | 365.1054 | POS | C12H22O11 | HMDB0000048 | 60033-03-6 | C05402 | 0.3513 | 0.2193 | 1.2474 | 0.0225 | 0.6243 |
| Homocarnosine | 3.8800 | 239.1152 | NEG | C10H16N4O3 | HMDB0000745 | 3650-73-5 | C00884 | 0.4069 | 1.3205 | 1.3847 | 0.0430 | 3.2455 |
| Formylmethionine | 3.8800 | 176.0389 | NEG | C6H11NO3S | HMDB0001015 | 4289-98-9 | C03145 | 2.0316 | 1.0372 | 2.1440 | 0.0076 | 0.5106 |
| Hydroxyphenyllactic acid | 3.8800 | 181.0508 | NEG | C9H10O4 | HMDB0000755 | 306-23-0 | C03672 | 10.7216 | 6.2335 | 2.6402 | 0.0006 | 0.5814 |
| Catechin | 3.8800 | 289.0719 | NEG | C15H14O6 | HMDB0002780 | 154-23-4 | C06562 | 2.2607 | 1.2419 | 1.9801 | 0.0008 | 0.5493 |
| 2-Hydroxy-2-methylbutyric acid | 3.8700 | 117.0558 | NEG | C5H10O3 | HMDB0001987 | 3739-30-8 |  | 48.1401 | 13.5910 | 2.1321 | 0.0016 | 0.2823 |
| Glyco-beta-muricholic acid | 3.8600 | 464.3020 | NEG | C26H43NO6 | HMDB0240607 | 66225-78-3 |  | 4.9789 | 0.7902 | 2.0783 | 0.0039 | 0.1587 |
| Taurohyodeoxycholic acid | 3.8600 | 498.2900 | NEG | C26H45NO6S | HMDB0247202 | 386523 |  | 29.3999 | 45.5254 | 1.6126 | 0.0225 | 1.5485 |
| Nipecotic acid | 3.8500 | 130.0863 | POS | C6H11NO2 | HMDB0255618 | 498-95-3 |  | 0.0354 | 0.0595 | 1.4880 | 0.0162 | 1.6797 |
| Car(18:1) | 3.8500 | 426.3582 | POS | C25H47NO4 | HMDB0013337 | 13962-05-5 |  | 0.5189 | 0.2433 | 1.6449 | 0.0253 | 0.4690 |
| MES | 3.8500 | 194.0496 | NEG | C6H13NO4S | HMDB0246678 | 4432-31-9 |  | 0.5644 | 1.5587 | 1.2647 | 0.0105 | 2.7615 |
| Ferulate | 3.8500 | 193.0506 | NEG | C10H10O4 | HMDB0000954 | 537-98-4 | C01494 | 6.2274 | 3.1033 | 1.9908 | 0.0045 | 0.4983 |
| Prunasin | 3.8500 | 296.1131 | POS | C14H17NO6 | HMDB0034934 | 99-18-3 | C00844 | 0.0529 | 0.1598 | 1.3629 | 0.0234 | 3.0227 |
| 3-Methyladenine | 3.8400 | 150.0761 | POS | C6H7N5 | HMDB0011600 | 5142-23-4 | C00913 | 0.0698 | 0.0488 | 2.0574 | 0.0400 | 0.6989 |
| 4-Hydroxyphenylpyruvic acid | 3.8400 | 179.0350 | NEG | C9H8O4 | HMDB0000707 | 156-39-8 | C01179 | 4.9774 | 2.4819 | 2.1105 | 0.0009 | 0.4986 |
| Glycodeoxycholic acid | 3.8300 | 450.3215 | POS | C26H43NO5 | HMDB0000631 | 360-65-6|16409-34-0 | C05464 | 0.2798 | 0.0737 | 1.7713 | 0.0216 | 0.2635 |
| 2-Methylhippuric acid | 3.8200 | 192.0668 | NEG | C10H11NO3 | HMDB0011723 | 27115-50-0 |  | 0.3295 | 1.1630 | 1.9030 | 0.0014 | 3.5300 |
| Tosufloxacin (tosylate hydrate) | 3.8200 | 405.1185 | POS | C19H15F3N4O3 |  | 1400591-39-0 | D02317 | 0.2490 | 0.0632 | 1.8037 | 0.0063 | 0.2537 |
| Glycochenodeoxycholic acid | 3.8100 | 450.3215 | POS | C26H43NO5 | HMDB0014642 | 13311-84-7 | C07653 | 0.2798 | 0.0737 | 1.7713 | 0.0216 | 0.2635 |
| 3-Cresol | 3.8000 | 107.0503 | NEG | C7H8O | HMDB0002048 | 108-39-4 | C01467 | 0.1910 | 0.0637 | 2.3918 | 0.0000 | 0.3333 |
| 2-Methylphenol | 3.8000 | 107.0503 | NEG | C7H8O | HMDB0002055 | 95-48-7 | C01542 | 0.1910 | 0.0637 | 2.3918 | 0.0000 | 0.3333 |
| Carbidopa | 3.8000 | 209.0920 | POS | C10H14N2O4 | HMDB0014336 | 28860-95-9 |  | 0.0171 | 0.0222 | 1.9026 | 0.0319 | 1.2955 |
| Ethyl 3-hydroxybenzoate | 3.7900 | 165.0558 | NEG | C9H10O3 |  | 7781-98-8 |  | 14.7074 | 6.4068 | 2.9806 | 0.0001 | 0.4356 |
| 2-Phenyllactic acid | 3.7900 | 165.0558 | NEG | C9H10O3 | HMDB0142137 | 515-30-0 |  | 14.7074 | 6.4068 | 2.9806 | 0.0001 | 0.4356 |
| Ethyl 4-hydroxybenzoate | 3.7800 | 165.0558 | NEG | C9H10O3 | HMDB0032573 | 120-47-8 | D01647 | 14.7074 | 6.4068 | 2.9806 | 0.0001 | 0.4356 |
| Butyllactate | 3.7800 | 145.0871 | NEG | C7H14O3 | HMDB0040254 | 138-22-7 |  | 0.4504 | 0.2115 | 2.2097 | 0.0006 | 0.4695 |
| 5-Oxooctanoic acid | 3.7700 | 157.0871 | NEG | C8H14O3 |  | 3637-14-7 |  | 0.6333 | 0.4467 | 1.8862 | 0.0274 | 0.7054 |
| 11-Dehydrocorticosterone | 3.7700 | 325.1843 | NEG | C21H28O4 | HMDB0004029 | 72-23-1 | C05490 | 21.2603 | 33.1523 | 1.3550 | 0.0006 | 1.5594 |
| Taurodeoxycholic acid | 3.7600 | 498.2900 | NEG | C26H45NO6S | HMDB0000896 | 516-50-7 | C05463 | 29.3999 | 45.5254 | 1.6126 | 0.0225 | 1.5485 |
| Docebenone | 3.7600 | 325.1843 | NEG | C21H26O3 | HMDB0247732 | 80809-81-0 | C01349 | 21.2603 | 33.1523 | 1.3550 | 0.0006 | 1.5594 |
| Monoethylglycinexylidide (MEGX) | 3.7500 | 189.1386 | POS | C12H18N2O | HMDB0060656 | 7728-40-7 | C16561 | 0.0083 | 0.0273 | 1.6183 | 0.0234 | 3.2834 |
| PC(16:0/20:4) | 3.7400 | 782.5689 | POS | C44H80NO8P | HMDB0007982 | 35418-58-7 |  | 0.9094 | 0.4111 | 1.2486 | 0.0263 | 0.4520 |
| Isoferulic acid | 3.7300 | 193.0506 | NEG | C10H10O4 | HMDB0000955 | 25522-33-2 | C10470 | 6.2274 | 3.1033 | 1.9908 | 0.0045 | 0.4983 |
| Desaminotyrosine | 3.7300 | 165.0558 | NEG | C9H10O3 | HMDB0002199 | 501-97-3 | C01744 | 14.7074 | 6.4068 | 2.9806 | 0.0001 | 0.4356 |
| Pyruvaldehyde | 3.7300 | 71.0139 | NEG | C3H4O2 | HMDB0001167 | 78-98-8 | C00546 | 3.6726 | 1.8524 | 1.2163 | 0.0307 | 0.5044 |
| Palmitoylcarnitine (Car(16:0)) | 3.7300 | 400.3424 | POS | C23H45NO4 | HMDB0000222 | 2364-67-2 | C02990 | 0.8759 | 0.3913 | 1.4405 | 0.0296 | 0.4468 |
| Phenylephrine | 3.7300 | 168.1019 | POS | C9H13NO2 | HMDB0002182 | 59-42-7 | C07441 | 0.0310 | 0.0886 | 1.5951 | 0.0041 | 2.8565 |
| 2,2,6,6-Tetramethyl-4-piperidinyl 2-methylacrylate | 3.7300 | 226.1802 | POS | C13H23NO2 |  | 31582-45-3 |  | 0.0433 | 0.0657 | 2.6390 | 0.0001 | 1.5167 |
| 3,5-Dimethoxycinnamic acid | 3.7300 | 207.0662 | NEG | C11H12O4 |  | 16909-11-8 |  | 10.0683 | 5.2897 | 1.1988 | 0.0063 | 0.5254 |
| (1-Hydroxycyclohexyl)acetic acid | 3.7200 | 157.0871 | NEG | C8H14O3 |  | 14399-63-4 |  | 0.6333 | 0.4467 | 1.8862 | 0.0274 | 0.7054 |
| Homovanillic acid | 3.7200 | 181.0508 | NEG | C9H10O4 | HMDB0000118 | 306-08-1 | C05582 | 7.5206 | 3.5563 | 1.3999 | 0.0176 | 0.4729 |
| Triamterene | 3.6600 | 254.1136 | POS | C12H11N7 | HMDB0001940 | 396-01-0 | D00386 | 0.0565 | 0.0959 | 1.7931 | 0.0048 | 1.6981 |
| Tazarotene | 3.6200 | 352.1393 | POS | C21H21NO2S | HMDB0014937 | 118292-40-3 | C12531 | 0.0754 | 0.1663 | 1.7723 | 0.0162 | 2.2047 |
| 5-Hydroxytryptophan | 3.6100 | 219.0807 | NEG | C11H12N2O3 | HMDB0000472 | 4350-09-8 | C00643 | 0.2788 | 0.1452 | 1.8944 | 0.0345 | 0.5206 |
| 4-Hydroxyderricin | 3.4900 | 339.1551 | POS | C21H22O4 |  | 55912-03-3 |  | 0.0498 | 0.1382 | 1.7229 | 0.0073 | 2.7765 |
| 4-(N-Methylacetamido)benzoic acid | 2.7500 | 194.0812 | POS | C10H11NO3 |  |  |  | 0.0415 | 0.0289 | 1.0130 | 0.0285 | 0.6957 |
| 2,8-Diazaspiro[5.5]undecane-1,7-dione | 2.7500 | 183.1128 | POS | C9H14N2O2 |  |  |  | 0.0504 | 0.0693 | 1.7691 | 0.0088 | 1.3749 |
| 4-(Dimethylamino)phenylalanine | 2.7500 | 209.1285 | POS | C11H16N2O2 |  |  |  | 0.0229 | 0.0371 | 1.4664 | 0.0041 | 1.6168 |
| Ile-Asn | 2.7500 | 246.1448 | POS | C10H19N3O4 |  |  |  | 0.0809 | 0.0601 | 2.1510 | 0.0296 | 0.7427 |
| Pro-Ile | 2.7500 | 227.1401 | NEG | C11H20N2O3 | HMDB0304810 |  |  | 1.2341 | 0.7840 | 2.5978 | 0.0155 | 0.6353 |
| Ile-Pro | 2.7500 | 229.1547 | POS | C11H20N2O3 | HMDB0011174 | 37462-92-3 |  | 0.3804 | 0.2453 | 2.5852 | 0.0039 | 0.6451 |
| 8-Methylquinolin-2(1H)-one | 2.7500 | 160.0757 | POS | C10H9NO |  |  |  | 0.0104 | 0.0315 | 1.1511 | 0.0274 | 3.0181 |
| Mepirizole | 2.7500 | 235.1190 | POS | C11H14N4O2 | HMDB0254454 |  |  | 0.1675 | 0.2335 | 1.3045 | 0.0345 | 1.3935 |
| 2,3-Dihydroxy  -3-(2-hydroxypropan-2-yl)-8a-methyl-1,2,3a,4,5,8-hexahydroazulene-6-carboxylic acid | 2.7500 | 283.1552 | NEG | C15H24O5 |  |  |  | 0.9969 | 2.0705 | 1.0593 | 0.0149 | 2.0770 |
| 7-Nitro-2,3,4,5-tetrahydro-1H-1-benzazepin-2-one | 2.7500 | 207.0764 | POS | C10H10N2O3 |  |  |  | 0.0093 | 0.0152 | 1.7022 | 0.0076 | 1.6345 |
| Brucine | 2.7500 | 395.1965 | POS | C23H26N2O4 | HMDB0249406 |  |  | 0.0073 | 0.0574 | 1.8947 | 0.0021 | 7.8724 |
| L-Tyrosine, O-(1,1-dimethylethyl)- | 2.7500 | 236.1292 | NEG | C13H19NO3 |  |  |  | 0.2382 | 1.2366 | 1.4444 | 0.0125 | 5.1904 |
| 1-Aminocyclopentanecarboxylic acid ethyl ester | 2.7500 | 158.1176 | POS | C8H15NO2 |  |  |  | 0.0584 | 0.1759 | 1.4845 | 0.0385 | 3.0119 |
| Harmane | 2.7500 | 183.0917 | POS | C12H10N2 | HMDB0035196 | 486-84-0 | C09209 | 0.1785 | 0.3244 | 1.5069 | 0.0371 | 1.8174 |
| PC(36:5) | 2.7500 | 780.5539 | POS | C44H78NO8P | HMDB0007890 |  |  | 0.0208 | 0.0101 | 1.6652 | 0.0018 | 0.4842 |
| L-Isoserine | 2.7400 | 104.0354 | NEG | C3H7NO3 |  |  |  | 0.6980 | 0.5414 | 2.3434 | 0.0253 | 0.7756 |
| L-trans-5-Hydroxy-2-piperidinecarboxylic\_acid | 2.7400 | 146.0812 | POS | C6H11NO3 | HMDB0029426 | 50439-45-7 |  | 0.5045 | 0.2166 | 1.5395 | 0.0285 | 0.4293 |
| Ser-Val | 2.7400 | 203.1037 | NEG | C8H16N2O4 |  |  |  | 2.7145 | 1.6395 | 2.4456 | 0.0319 | 0.6040 |
| Tyr-Pro | 2.7400 | 279.1340 | POS | C14H18N2O4 |  |  |  | 0.0425 | 0.0269 | 2.0777 | 0.0092 | 0.6342 |
| Val-Pro | 2.7400 | 215.1390 | POS | C10H18N2O3 | HMDB0029135 | 20488-27-1 |  | 0.0928 | 0.0691 | 2.4276 | 0.0169 | 0.7443 |
| 1-Isopropyl-1H-benzimidazole-5-carboxylic acid | 2.7400 | 203.0826 | NEG | C11H12N2O2 |  |  |  | 3.9958 | 1.4497 | 2.3744 | 0.0479 | 0.3628 |
| 2-Hydroxy-6-methylquinoline-3-carbaldehyde | 2.7400 | 188.0706 | POS | C11H9NO2 |  |  |  | 0.5271 | 0.2056 | 2.1942 | 0.0371 | 0.3900 |
| 1-(4-Hydroxyphenyl)-2-methylaminoethanone | 2.7400 | 164.0718 | NEG | C9H11NO2 |  |  |  | 14.6351 | 7.4369 | 2.5772 | 0.0285 | 0.5082 |
| 4-Methylcatechol | 2.7400 | 123.0452 | NEG | C7H8O2 | HMDB0000873 | 452-86-8 | C06730 | 0.7496 | 0.2180 | 1.7237 | 0.0061 | 0.2909 |
| Thr-Val-Leu | 2.7400 | 332.2182 | POS | C15H29N3O5 |  |  |  | 0.1751 | 0.1253 | 2.3526 | 0.0162 | 0.7154 |
| 4,5-Dimethyl-1,3-benzenediol | 2.7400 | 137.0609 | NEG | C8H10O2 |  |  |  | 0.5562 | 0.2816 | 1.4828 | 0.0052 | 0.5062 |
| Ile-Gly-Ile | 2.7400 | 300.1929 | NEG | C14H27N3O4 |  |  |  | 1.3097 | 0.8012 | 2.3160 | 0.0234 | 0.6118 |
| Isocytosine | 2.7400 | 112.0505 | POS | C4H5N3O |  |  |  | 0.3413 | 0.2464 | 2.0586 | 0.0446 | 0.7220 |
| 2-Hydroxybenzaldehyde [(E)-(2-hydroxyphenyl)methylidene]hydrazone | 2.7400 | 241.0971 | POS | C14H12N2O2 |  |  |  | 0.0949 | 0.1251 | 1.5565 | 0.0285 | 1.3187 |
| 8-Oxoadenine | 2.7400 | 152.0568 | POS | C5H5N5O | HMDB0000542 | 21149-26-8 |  | 0.1917 | 0.1198 | 1.3258 | 0.0319 | 0.6248 |
| 1,1-Dimethyl-4-phenylpiperazin-1-ium cation | 2.7400 | 191.1542 | POS | C12H19N2 |  |  |  | 0.0450 | 0.0772 | 1.1436 | 0.0285 | 1.7141 |
| 4-[(Propan-2-yl)carbamoyl]benzoic acid | 2.7400 | 206.0824 | NEG | C11H13NO3 | HMDB0060608 |  |  | 0.3702 | 1.5087 | 1.2249 | 0.0149 | 4.0755 |
| Normorphine | 2.7400 | 272.1280 | POS | C16H17NO3 | HMDB0041959 | 466-97-7 | C11785 | 0.0496 | 0.4833 | 2.4971 | 0.0000 | 9.7476 |
| Propachlor ESA | 2.7400 | 256.0648 | NEG | C11H15NO4S |  |  |  | 0.3909 | 0.8691 | 2.3890 | 0.0002 | 2.2236 |
| Citbrasine | 2.7400 | 332.1131 | POS | C17H17NO6 | HMDB0037797 | 86680-34-4 |  | 0.0252 | 0.1450 | 1.7853 | 0.0058 | 5.7548 |
| 5-Methylisoxazol-3-amine | 2.7400 | 99.0552 | POS | C4H6N2O |  |  |  | 0.0922 | 0.1144 | 1.3136 | 0.0125 | 1.2404 |
| Bufexamac | 2.7400 | 222.1136 | NEG | C12H17NO3 | HMDB0341139 |  |  | 0.7992 | 4.3654 | 1.5564 | 0.0446 | 5.4622 |
| Dodemorph | 2.7400 | 282.2792 | POS | C18H35NO |  |  |  | 7.0992 | 3.1161 | 1.9856 | 0.0199 | 0.4389 |
| 4-Chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carbaldehyde | 2.7400 | 179.9971 | NEG | C7H4ClN3O |  |  |  | 1.4626 | 9.2710 | 1.4718 | 0.0037 | 6.3385 |
| 7-Hydroxychromanone | 2.7400 | 163.0402 | NEG | C9H8O3 |  |  |  | 3.7900 | 1.3715 | 2.8002 | 0.0000 | 0.3619 |
| RICININE | 2.7400 | 182.0924 | POS | C8H8N2O2 | HMDB0042006 | 524-40-3 | C01526 | 0.1189 | 0.1493 | 1.3604 | 0.0430 | 1.2557 |
| E-(gamma-Glutamyl)-lysine | 2.7400 | 274.1409 | NEG | C11H21N3O5 | HMDB0003869 | 17105-15-6 |  | 0.8292 | 0.4464 | 2.4752 | 0.0169 | 0.5384 |
| 2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID | 2.7400 | 149.0279 | NEG | C5H10O3S | HMDB0037115 | 120-91-2 |  | 9.8602 | 2.9723 | 1.9867 | 0.0020 | 0.3014 |
| butabarbital | 2.7400 | 213.1234 | POS | C10H16N2O3 | HMDB0014382 | 125-40-6 | C07827 | 0.0626 | 0.1317 | 2.0075 | 0.0063 | 2.1033 |
| 9-HPODE | 2.7400 | 311.2229 | NEG | C18H32O4 | HMDB0062434 | 29774-12-7 | C14827 | 2.9651 | 1.5264 | 1.9603 | 0.0332 | 0.5148 |
| Metaproterenol | 2.7400 | 212.1282 | POS | C11H17NO3 | HMDB0014954 | 586-06-1 | C07144 | 0.0951 | 0.2538 | 2.5325 | 0.0001 | 2.6679 |
| Gabapentin | 2.7400 | 172.1333 | POS | C9H17NO2 | HMDB0005015 | 60142-96-3 |  | 0.1431 | 0.1983 | 2.2002 | 0.0058 | 1.3853 |
| Octenoylcarnitine (Car(8:1)) | 2.7300 | 286.2013 | POS | C15H27NO4 | HMDB0240750 |  |  | 0.0161 | 0.0379 | 1.6527 | 0.0012 | 2.3517 |
| Thr-Glu | 2.7300 | 249.1082 | POS | C9H16N2O6 |  |  |  | 0.0302 | 0.0239 | 2.1393 | 0.0296 | 0.7909 |
| Arg-Leu | 2.7300 | 288.2030 | POS | C12H25N5O3 |  |  |  | 0.1707 | 0.0872 | 2.4418 | 0.0037 | 0.5111 |
| His-Leu | 2.7300 | 267.1462 | NEG | C12H20N4O3 | HMDB0028889 | 7763-65-7 | C05010 | 0.5357 | 0.2927 | 2.2917 | 0.0307 | 0.5463 |
| Ile-Gln | 2.7300 | 258.1459 | NEG | C11H21N3O4 |  |  |  | 2.9669 | 1.5678 | 2.7959 | 0.0067 | 0.5284 |
| Leu-Gly | 2.7300 | 189.1234 | POS | C8H16N2O3 | HMDB0028929 |  |  | 0.2912 | 0.1934 | 2.5504 | 0.0125 | 0.6641 |
| 5,5-Dimethyl-3-(4-nitrobenzyl)-2,4-imidazolidinedione | 2.7300 | 262.0835 | NEG | C12H13N3O4 |  |  |  | 0.0940 | 0.1725 | 1.6783 | 0.0030 | 1.8362 |
| Threoninyl-Proline | 2.7300 | 217.1183 | POS | C9H16N2O4 | HMDB0341432 |  |  | 0.0158 | 0.0323 | 1.6975 | 0.0100 | 2.0521 |
| Val-Phe | 2.7300 | 263.1402 | NEG | C14H20N2O3 |  |  |  | 2.8442 | 1.8746 | 2.1357 | 0.0274 | 0.6591 |
| 3-(3-Hydroxyphenyl)propionic acid sulfate | 2.7300 | 245.0127 | NEG | C9H10O6S | HMDB0094710 |  |  | 14.9121 | 9.8512 | 1.5744 | 0.0176 | 0.6606 |
| 2,3-Dihydroxy-3-methylbutyric acid | 2.7300 | 133.0507 | NEG | C5H10O4 | HMDB0341247 |  | C04039 | 83.9494 | 38.1414 | 1.4784 | 0.0120 | 0.4543 |
| (2E,4E,10Z)-N-(2-Methylpropyl)hexadeca-2,4,10-trienamide | 2.7300 | 306.2789 | POS | C20H35NO |  |  |  | 0.0389 | 0.0197 | 1.2628 | 0.0142 | 0.5056 |
| N-Methyl-N-(methylsulfonyl)glycine | 2.7300 | 166.0181 | NEG | C4H9NO4S |  |  |  | 52.5633 | 18.4494 | 1.5634 | 0.0234 | 0.3510 |
| Ethyl sulfate | 2.7300 | 124.9915 | NEG | C2H6O4S | HMDB0031233 | 540-82-9 |  | 125.2975 | 14.7518 | 1.6030 | 0.0035 | 0.1177 |
| (12Z)-9,10,11-Trihydroxyoctadec-12-enoic acid | 2.7300 | 329.2335 | NEG | C18H34O5 |  |  |  | 12.8359 | 7.1772 | 1.7466 | 0.0131 | 0.5592 |
| alpha-Keto-gamma-(methylthio)butyric\_acid | 2.7300 | 147.0122 | NEG | C5H8O3S | HMDB0001553 | 583-92-6 | C01180 | 1.8088 | 0.6446 | 2.7903 | 0.0000 | 0.3563 |
| LPC(22:6) | 2.7300 | 568.3403 | POS | C30H50NO7P |  |  |  | 0.0030 | 0.0017 | 1.5191 | 0.0243 | 0.5695 |
| Linoleoylcarnitine (Car(18:2)) | 2.7300 | 424.3425 | POS | C25H45NO4 | HMDB0241541 | 36816-10-1 |  | 0.3264 | 0.1223 | 1.9284 | 0.0045 | 0.3746 |
| Arg-Pro | 2.7200 | 272.1719 | POS | C11H21N5O3 | HMDB0028717 | 2418-69-1 |  | 0.2577 | 0.2057 | 2.2618 | 0.0216 | 0.7982 |
| Gly-Arg | 2.7200 | 232.1406 | POS | C8H17N5O3 |  |  |  | 0.1296 | 0.0888 | 2.1233 | 0.0199 | 0.6854 |
| Glu-Val | 2.7200 | 245.1143 | NEG | C10H18N2O5 | HMDB0028832 | 5879-06-1 |  | 2.4348 | 1.6725 | 2.3189 | 0.0371 | 0.6869 |
| Salicylaldehyde | 2.7200 | 123.0440 | POS | C7H6O2 | HMDB0034170 | 90-02-8 | C06202 | 0.0196 | 0.0121 | 2.3682 | 0.0023 | 0.6162 |
| Hemiphloin | 2.7200 | 433.1141 | NEG | C21H22O10 |  |  |  | 0.6201 | 0.1834 | 2.0295 | 0.0080 | 0.2957 |
| Atropic acid | 2.7200 | 147.0453 | NEG | C9H8O2 |  |  |  | 0.6291 | 0.3177 | 2.5722 | 0.0307 | 0.5049 |
| Leu-Gly-Leu | 2.7200 | 300.1930 | NEG | C14H27N3O4 |  |  |  | 1.4659 | 0.7618 | 2.8929 | 0.0037 | 0.5197 |
| Echinocystic acid 3-glucoside | 2.7200 | 633.4017 | NEG | C36H58O9 |  |  |  | 0.4324 | 0.1311 | 2.3082 | 0.0253 | 0.3031 |
| 1-Hydroxy-N-(3-nitrophenyl)-2-naphthamide | 2.7200 | 307.0728 | NEG | C17H12N2O4 |  |  |  | 0.5676 | 0.6877 | 1.1003 | 0.0479 | 1.2115 |
| L-Tyrosinamide | 2.7200 | 181.0972 | POS | C9H12N2O2 |  |  |  | 0.0352 | 0.0743 | 1.5820 | 0.0063 | 2.1115 |
| Azelnidipine | 2.7200 | 583.2550 | POS | C33H34N4O6 | HMDB0248792 |  |  | 0.0183 | 0.0628 | 2.4573 | 0.0000 | 3.4266 |
| Aigialomycin D | 2.7200 | 333.1348 | NEG | C18H22O6 |  |  |  | 2.2068 | 2.5762 | 1.5765 | 0.0149 | 1.1674 |
| 5beta-Pregnane-3alpha,17alpha,20alpha-triol | 2.7200 | 337.2738 | POS | C21H36O3 | HMDB0006070 | 27178-64-9 |  | 0.0524 | 0.0289 | 1.9177 | 0.0023 | 0.5513 |
| 9Z,11E,13E-Octadecatrienoic acid methyl ester | 2.7200 | 293.2476 | POS | C19H32O2 |  |  |  | 0.1987 | 0.0901 | 2.1847 | 0.0115 | 0.4537 |
| Methocarbamol | 2.7200 | 242.1023 | POS | C11H15NO5 | HMDB0014567 | 532-03-6 |  | 0.0485 | 0.0816 | 1.3662 | 0.0183 | 1.6807 |
| Creatine, ethyl ester | 2.7100 | 160.1082 | POS | C6H13N3O2 | HMDB0250523 |  |  | 0.0214 | 0.0427 | 1.5234 | 0.0076 | 1.9927 |
| 5-(4-Chlorobenzyl)-1,3,4-oxadiazol-2-amine | 2.7100 | 210.0431 | POS | C9H8ClN3O |  |  |  | 0.0098 | 0.0141 | 1.4779 | 0.0183 | 1.4328 |
| Asn-Ile | 2.7100 | 244.1302 | NEG | C10H19N3O4 |  |  |  | 2.0128 | 1.1019 | 2.6232 | 0.0183 | 0.5474 |
| Homoarecoline | 2.7100 | 170.1176 | POS | C9H15NO2 | HMDB0038321 | 28125-84-0 |  | 0.0163 | 0.0231 | 2.0332 | 0.0025 | 1.4164 |
| 7-Methyladenine | 2.7100 | 150.0770 | POS | C6H7N5 | HMDB0011614 | 935-69-3 | C02241 | 0.0730 | 0.0536 | 2.0941 | 0.0496 | 0.7350 |
| Diethyl 2,4-dimethylpyrrole-3,5-dicarboxylate | 2.7100 | 238.1086 | NEG | C12H17NO4 |  |  |  | 0.5590 | 0.9560 | 1.5613 | 0.0055 | 1.7101 |
| Tripropylene glycol | 2.7100 | 193.1439 | POS | C9H20O4 |  |  |  | 0.0143 | 0.0197 | 1.5727 | 0.0162 | 1.3799 |
| 4-Acetamidophenol sulfate | 2.7100 | 230.0129 | NEG | C8H9NO5S | HMDB0059911 | 10066-90-7 |  | 0.3247 | 0.1796 | 1.7851 | 0.0319 | 0.5532 |
| Glabrone | 2.7100 | 359.0909 | POS | C20H16O5 | HMDB0029533 | 60008-02-8 |  | 0.0444 | 0.0182 | 1.4470 | 0.0032 | 0.4092 |
| Cholic acid/Muricholic acid, isoleucine-conjugated | 2.7100 | 520.3647 | NEG | C30H51NO6 |  |  |  | 0.4426 | 0.0790 | 2.2915 | 0.0385 | 0.1784 |
| Methanone, [1-(6-fluorohexyl)-1H-indol-3-yl]-1-naphthalenyl- | 2.7000 | 374.1922 | POS | C25H24FNO |  |  |  | 0.0076 | 0.0169 | 1.7567 | 0.0043 | 2.2285 |
| Lys-Pro | 2.7000 | 244.1657 | POS | C11H21N3O3 | HMDB0028959 | 52766-27-5 |  | 0.2922 | 0.1940 | 2.2101 | 0.0207 | 0.6637 |
| Sulfoacetic acid | 2.7000 | 138.9708 | NEG | C2H4O5S | HMDB0258590 |  | C14179 | 0.3559 | 0.5139 | 1.1259 | 0.0136 | 1.4440 |
| PS(16:0/16:0) | 2.7000 | 736.5126 | POS | C38H74NO10P | HMDB0000614 | 40290-42-4 |  | 0.0364 | 0.0117 | 1.4622 | 0.0371 | 0.3208 |
| 3-(1-Methyl-4-morpholinopyrazolo[3,4-d]pyrimidin-6-yl)phenol | 2.7000 | 312.1445 | POS | C16H17N5O2 |  |  |  | 0.1672 | 0.0366 | 1.7130 | 0.0358 | 0.2192 |
| N-Benzyl-D-serine | 2.7000 | 194.0823 | NEG | C10H13NO3 |  |  |  | 0.4069 | 2.3329 | 1.6861 | 0.0035 | 5.7340 |
| 3-(2,5-Dioxo-1-pyrrolidinyl)benzoic acid | 2.7000 | 218.0458 | NEG | C11H9NO4 |  |  |  | 1.4909 | 0.6988 | 2.5901 | 0.0001 | 0.4687 |
| DL-Threonine methyl ester | 2.7000 | 134.0812 | POS | C5H11NO3 | HMDB0341314 |  |  | 0.0781 | 0.0355 | 1.6941 | 0.0131 | 0.4547 |
| Isoleucylvaline | 2.7000 | 231.1703 | POS | C11H22N2O3 | HMDB0028920 |  |  | 6.2449 | 4.2051 | 2.1505 | 0.0285 | 0.6734 |
| Pesticide3\_Fenobucarb\_C12H17NO2\_Bassa | 2.7000 | 208.1333 | POS | C12H17NO2 | HMDB0252205 |  | C14425 | 0.0130 | 0.0676 | 2.7522 | 0.0002 | 5.2087 |
| 1-(beta-D-Ribofuranosyl)-1,4-dihydronicotinamide | 2.7000 | 257.1133 | POS | C11H16N2O5 | HMDB0011648 |  | C15497 | 0.1776 | 0.4668 | 1.9689 | 0.0025 | 2.6281 |
| Oleoylcarnitine (Car(18:1)) | 2.7000 | 426.3583 | POS | C25H47NO4 | HMDB0094687 | 13962-05-5 |  | 0.0952 | 0.0387 | 1.4525 | 0.0243 | 0.4066 |
| Lys-Ala | 2.6900 | 218.1501 | POS | C9H19N3O3 | HMDB0028944 | 17043-71-9 |  | 0.2884 | 0.2111 | 2.0287 | 0.0216 | 0.7320 |
| Lys-Thr | 2.6900 | 248.1607 | POS | C10H21N3O4 | HMDB0028961 | 97791-84-9 |  | 0.0412 | 0.0264 | 2.2175 | 0.0120 | 0.6399 |
| 3-Dehydroshikimic acid | 2.6900 | 171.0300 | NEG | C7H8O5 |  |  |  | 0.3511 | 0.1411 | 2.3089 | 0.0027 | 0.4018 |
| N5-(1-Iminoethyl)-L-ornithine | 2.6900 | 174.1237 | POS | C7H15N3O2 |  |  |  | 0.0988 | 0.0406 | 1.2988 | 0.0371 | 0.4109 |
| 5-O-Demethylnobiletin | 2.6900 | 389.1235 | POS | C20H20O8 | HMDB0037571 | 2174-59-6 |  | 0.3344 | 0.0623 | 1.8675 | 0.0142 | 0.1863 |
| 5-[[17-(5,6-dihydroxy-6-methylheptan-2-yl)-3,12-dihydroxy-4,4,10,13,14  -pentamethyl-2,3,5,6,7,11,12,15,16,17  -decahydro-1H-cyclopenta[a]phenanthren-2-yl]oxy]-3-hydroxy-3-methyl-5-oxopentanoic acid | 2.6900 | 635.4163 | NEG | C36H60O9 | HMDB0036438 | 126882-55-1 |  | 0.1343 | 0.0678 | 2.4967 | 0.0149 | 0.5048 |
| DEOXYCORTICOSTERONE ACETATE | 2.6900 | 395.2175 | POS | C23H32O4 | HMDB0251003 |  |  | 0.0150 | 0.0951 | 1.7848 | 0.0034 | 6.3273 |
| Methanone, (4-ethyl-1-naphthalenyl)[1-(5-fluoropentyl)-1H-indol-3-yl]- | 2.6800 | 388.2082 | POS | C26H26FNO | HMDB0259633 |  |  | 0.0038 | 0.0062 | 1.6148 | 0.0012 | 1.6433 |
| Methanone, [1-(3-fluoropentyl)-1H-indol-3-yl]-1-naphthalenyl- | 2.6800 | 360.1769 | POS | C24H22FNO |  |  |  | 0.0197 | 0.0493 | 1.5885 | 0.0253 | 2.5044 |
| Isoleucyl-Histidine | 2.6800 | 269.1609 | POS | C12H20N4O3 | HMDB0028909 |  |  | 0.1709 | 0.1042 | 2.4385 | 0.0216 | 0.6096 |
| 2,6-Diamino-4-hydroxy-5-N-methylformamidopyrimidine | 2.6800 | 184.0831 | POS | C6H9N5O2 | HMDB0011657 | 77440-13-2 | C04744 | 0.0606 | 0.0316 | 1.7080 | 0.0216 | 0.5210 |
| Valyl-Proline | 2.6800 | 215.1390 | POS | C10H18N2O3 |  |  |  | 0.0234 | 0.0345 | 1.2883 | 0.0332 | 1.4748 |
| 1H-Imidazole-4,5-dicarbohydrazide | 2.6800 | 183.0642 | NEG | C5H8N6O2 |  |  |  | 0.3319 | 0.4788 | 1.3337 | 0.0155 | 1.4426 |
| 2-Amino-6,7-diphenyl-4(3H)-pteridinone | 2.6800 | 316.1181 | POS | C18H13N5O |  |  |  | 0.0396 | 0.2322 | 1.7785 | 0.0142 | 5.8680 |
| N-Cyclopentyl-2-(1-piperazinyl)-4-quinazolinamine | 2.6800 | 298.2014 | POS | C17H23N5 |  |  |  | 0.0886 | 0.1545 | 1.0463 | 0.0191 | 1.7443 |
| Piperlonguminine | 2.6800 | 274.1439 | POS | C16H19NO3 | HMDB0030187 | 5950-12-9 |  | 0.5080 | 0.1798 | 1.3624 | 0.0307 | 0.3539 |
| 15-Keto-protaglandin\_F2alpha | 2.6800 | 375.2125 | POS | C20H32O5 | HMDB0004240 | 35850-13-6 | C05960 | 0.0294 | 0.0443 | 1.6472 | 0.0021 | 1.5100 |
| Zidovudine | 2.6800 | 266.0895 | NEG | C10H13N5O4 | HMDB0014638 | 30516-87-1 | C07210 | 0.6590 | 0.3621 | 2.3985 | 0.0063 | 0.5494 |
| 2-Amino-3,8-dimethylimidazo-[4,5-f]quinoxaline (MeIQx) | 2.6800 | 214.1077 | POS | C11H11N5 | HMDB0029864 | 77500-04-0 | C19255 | 0.0619 | 0.1083 | 1.7722 | 0.0358 | 1.7502 |
| Carbendazim | 2.6700 | 192.0767 | POS | C9H9N3O2 | HMDB0031769 | 10605-21-7 | C10897 | 0.0144 | 0.0281 | 1.3189 | 0.0019 | 1.9521 |
| Eglumegad | 2.6700 | 184.0616 | NEG | C8H11NO4 |  |  |  | 4.0709 | 6.0627 | 1.7363 | 0.0027 | 1.4893 |
| Methyl 4-(9H-purin-6-ylamino)benzoate | 2.6700 | 270.0973 | POS | C13H11N5O2 |  |  |  | 0.0438 | 0.1455 | 1.8148 | 0.0073 | 3.3245 |
| Gardenin | 2.6700 | 419.1340 | POS | C21H22O9 |  |  |  | 1.1853 | 0.1474 | 2.0284 | 0.0063 | 0.1244 |
| 7-Hydroxy-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-6-pteridinecarbaldehyde | 2.6600 | 235.0460 | NEG | C9H8N4O4 |  |  |  | 0.3268 | 0.1569 | 1.7564 | 0.0253 | 0.4801 |
| Diisopropyl\_sulfide | 2.6600 | 119.0896 | POS | C6H14S | HMDB0029579 | 625-80-9 |  | 0.1359 | 0.0990 | 2.1507 | 0.0234 | 0.7284 |
| 2-[(6-Ethoxy-4-methyl-2-quinazolinyl)amino]-5,6-dihydro-4-pyrimidinol | 2.6600 | 300.1443 | POS | C15H17N5O2 |  |  |  | 0.0198 | 0.0929 | 2.7982 | 0.0000 | 4.6874 |
| 2-[(4-Amino-6-anilino-1,3,5-triazin-2-yl)methoxy]benzaldehyde | 2.6600 | 322.1288 | POS | C17H15N5O2 |  |  |  | 0.0304 | 0.0540 | 1.7548 | 0.0183 | 1.7744 |
| Arachidonic sulfonic acid | 2.6600 | 339.1997 | NEG | C19H32O3S |  |  |  | 15.7767 | 23.4454 | 1.2765 | 0.0012 | 1.4861 |
| Isoleucyl-Threonine | 2.6600 | 233.1496 | POS | C10H20N2O4 | HMDB0028917 |  |  | 0.4209 | 0.2454 | 2.3095 | 0.0199 | 0.5829 |
| Tenuazonic acid | 2.6500 | 198.1114 | POS | C10H15NO3 |  |  |  | 0.0124 | 0.0230 | 1.4657 | 0.0120 | 1.8601 |
| Arg-Val | 2.6500 | 274.1874 | POS | C11H23N5O3 | HMDB0028722 | 2896-20-0 |  | 0.1107 | 0.0833 | 1.9557 | 0.0063 | 0.7519 |
| Dovitinib | 2.6500 | 393.1811 | POS | C21H21FN6O | HMDB0251597 |  |  | 0.0050 | 0.0215 | 2.2378 | 0.0004 | 4.2733 |
| Difenoxuron | 2.6500 | 287.1391 | POS | C16H18N2O3 |  |  |  | 0.0940 | 0.1471 | 1.3110 | 0.0110 | 1.5656 |
| 2-(4-Nitrophenyl)butyric acid | 2.6400 | 210.0762 | POS | C10H11NO4 |  |  |  | 0.0155 | 0.0301 | 1.8365 | 0.0142 | 1.9486 |
| 3-Cyano-7-hydroxycoumarin | 2.6400 | 188.0354 | POS | C10H5NO3 |  |  |  | 0.0171 | 0.0089 | 2.3987 | 0.0017 | 0.5221 |
| 3-Fluoro-4-(4-thiomorpholinyl)aniline | 2.6400 | 213.0869 | POS | C10H13FN2S |  |  |  | 0.0235 | 0.0404 | 1.8706 | 0.0076 | 1.7215 |
| 4-(2-Hydroxyethyl)piperazin-2-one | 2.6400 | 145.0973 | POS | C6H12N2O2 |  |  |  | 0.0193 | 0.0261 | 1.0155 | 0.0345 | 1.3526 |
| .delta.-Octalactone | 2.6400 | 143.1067 | POS | C8H14O2 | HMDB0038310 |  |  | 0.0251 | 0.0324 | 1.3386 | 0.0216 | 1.2908 |
| 1-O-Hexadecyl-2-O-(2E-butenoyl)-sn-glyceryl-3-phosphocholine | 2.6300 | 550.3863 | POS | C28H56NO7P |  |  |  | 0.0336 | 0.0169 | 1.9703 | 0.0332 | 0.5030 |
| Methanone, [1-(5-fluoro-4-hydroxypentyl)-1H-indol-3-yl](4-methyl-1-naphthalenyl)- | 2.6200 | 390.1871 | POS | C25H24FNO2 |  |  |  | 0.0124 | 0.0211 | 1.6144 | 0.0096 | 1.7020 |
| Pergolide sulfone | 2.6200 | 347.1814 | POS | C19H26N2O2S |  |  |  | 0.0427 | 0.0893 | 1.6922 | 0.0100 | 2.0930 |
| Lysine conjugated deoxycholic acid putative | 2.6200 | 521.3949 | POS | C30H52N2O5 | HMDB0242400 |  |  | 0.0199 | 0.0077 | 2.0801 | 0.0120 | 0.3889 |
| Isoquinoline, 5-[[(2S)-hexahydro-2-methyl-1H-1,4-diazepin-1-yl]sulfonyl]-4-methyl- | 2.6100 | 320.1454 | POS | C16H21N3O2S |  |  |  | 0.1287 | 0.2004 | 1.2899 | 0.0307 | 1.5566 |
| 3-(1-Hydroxymethyl-1-propenyl)pentanedioic\_acid | 2.6100 | 203.0914 | POS | C9H14O5 | HMDB0033092 |  |  | 0.0758 | 0.0406 | 1.2826 | 0.0243 | 0.5357 |
| 3-(2-Keto-1-methyl-3H-imidazo[4,5-b]pyridin-6-yl)benzamide | 2.6100 | 267.0907 | NEG | C14H12N4O2 |  |  |  | 4.1370 | 1.7809 | 2.2347 | 0.0332 | 0.4305 |
| Dulxanthone\_C | 2.6000 | 425.1922 | POS | C25H28O6 | HMDB0031917 | 4178-45-4 |  | 0.0067 | 0.0112 | 2.0435 | 0.0029 | 1.6823 |
| 2-(2,3-Dimethylphenyl)-7-methyl-1,2,4-triazaspiro[4.5]decane-3-thione | 2.6000 | 288.1565 | NEG | C16H23N3S |  |  |  | 1.9577 | 0.8754 | 2.8859 | 0.0058 | 0.4472 |
| 2-[(2R,3S,7R,8R,8aS)-2,3,4'-Trihydroxy-4,4,7,8a-tetramethyl-6'-oxospiro  [2,3,4a,5,6,7-hexahydro-1H-naphthalene-8,2'-3,8-dihydrofuro[2,3-e]isoindole]-7'-yl]-3-methylpentanoic acid | 2.6000 | 514.2847 | NEG | C29H41NO7 |  |  |  | 4.0246 | 4.1599 | 1.6251 | 0.0234 | 1.0336 |
| 17-Acetoxygrindelic acid | 2.6000 | 377.2367 | NEG | C22H34O5 |  |  |  | 1.1016 | 0.8163 | 1.7365 | 0.0084 | 0.7411 |
| 17-Methylene-4-androsten-3-one | 2.6000 | 285.2214 | POS | C20H28O |  |  |  | 0.0419 | 0.0666 | 1.1646 | 0.0142 | 1.5904 |
| PGF1alpha | 2.6000 | 379.2490 | POS | C20H36O5 | HMDB0002685 | 745-62-0 | C06475 | 0.0635 | 0.1947 | 1.4552 | 0.0120 | 3.0639 |
| 2-Propenethioamide, 3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-cyano-, (2E)- | 2.5900 | 317.1710 | POS | C18H24N2OS |  |  |  | 0.0214 | 0.0470 | 1.7803 | 0.0080 | 2.1963 |
| Lysyl-Glycine | 2.5900 | 204.1343 | POS | C8H17N3O3 | HMDB0304784 |  |  | 0.0707 | 0.0507 | 2.4872 | 0.0063 | 0.7167 |
| Promethazine sulfoxide | 2.5900 | 301.1397 | POS | C17H20N2OS | HMDB0247377 |  |  | 0.0448 | 0.0774 | 2.0785 | 0.0105 | 1.7254 |
| Alprazolam | 2.5900 | 309.0871 | POS | C17H13ClN4 | HMDB0014548 | 28981-97-7 | C06817 | 0.0752 | 0.1146 | 1.5233 | 0.0274 | 1.5244 |
| 1-Methoxy-N-(4-methylbenzyl)-2-propanamine | 2.5900 | 194.1540 | POS | C12H19NO |  |  |  | 0.0071 | 0.0334 | 1.9651 | 0.0004 | 4.7279 |
| Angelicolide | 2.5900 | 381.2025 | POS | C24H28O4 | HMDB0029317 | 90826-58-7 |  | 0.0194 | 0.1012 | 1.8634 | 0.0039 | 5.2258 |
| 5-[(Z)-5-Hydroxy-3-methylpent-3-enyl]-1,4a-dimethyl-6-methylidene  -3,4,5,7,8,8a-hexahydro-2H-naphthalene-1-carboxylic acid | 2.5900 | 321.2426 | POS | C20H32O3 |  |  |  | 0.1042 | 0.0752 | 1.1047 | 0.0496 | 0.7215 |
| DG(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)/0:0) | 2.5900 | 615.4982 | POS | C39H66O5 | HMDB0007333 |  |  | 0.0601 | 0.0432 | 1.4027 | 0.0125 | 0.7191 |
| N-Benzyl-2-naphthalenesulfonamide | 2.5800 | 296.0780 | NEG | C17H15NO2S |  |  |  | 0.0695 | 0.1079 | 1.1238 | 0.0385 | 1.5525 |
| 2-(Benzoylamino)-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylic acid | 2.5800 | 300.0728 | NEG | C16H15NO3S |  |  |  | 0.0852 | 0.1697 | 1.5753 | 0.0225 | 1.9911 |
| Mardepodect | 2.5800 | 393.1687 | POS | C25H20N4O | HMDB0256365 |  |  | 0.0080 | 0.0153 | 2.2222 | 0.0012 | 1.9037 |
| (E)-2'-Geranyl-3',4',7-trihydroxyflavanone | 2.5800 | 409.1970 | POS | C25H28O5 | HMDB0040317 | 113866-90-3 |  | 0.0131 | 0.0220 | 2.0081 | 0.0021 | 1.6774 |
| N,N-Dimethyl-4-(6-methylbenzo[d]thiazol-2-yl)aniline | 2.5800 | 269.1134 | POS | C16H16N2S |  |  |  | 0.0605 | 0.0908 | 1.6915 | 0.0084 | 1.5015 |
| Dehydrogingerdione | 2.5800 | 345.2105 | NEG | C21H30O4 | HMDB0029476 | 82206-04-0 |  | 1.6106 | 0.9901 | 2.0087 | 0.0084 | 0.6147 |
| Nervobscurine | 2.5700 | 383.1924 | POS | C22H26N2O4 |  |  |  | 0.0104 | 0.0236 | 1.5423 | 0.0016 | 2.2604 |
| Mulberrofuran\_A | 2.5700 | 393.2019 | POS | C25H28O4 | HMDB0033656 | 68978-04-1 | C08846 | 0.0084 | 0.0199 | 1.8824 | 0.0055 | 2.3727 |
| Licochalcone A | 2.5700 | 337.1409 | NEG | C21H22O4 |  |  |  | 0.1466 | 0.5819 | 1.6223 | 0.0115 | 3.9705 |
| 2,2'-(3-(Trifluoromethyl)phenylazanediyl)diethanol | 2.5700 | 250.1045 | POS | C11H14F3NO2 |  |  |  | 1.1071 | 0.4224 | 1.9778 | 0.0012 | 0.3816 |
| Triptophenolide | 2.5700 | 311.1687 | NEG | C20H24O3 |  |  |  | 20.4262 | 34.4241 | 1.5527 | 0.0004 | 1.6853 |
| PC(33:1) | 2.5600 | 728.5670 | POS | C41H80NO8P |  |  |  | 0.1334 | 0.0384 | 1.3413 | 0.0021 | 0.2879 |
| Rutamarin | 2.5600 | 357.1659 | POS | C21H24O5 | HMDB0030666 | 14882-94-1 | C09308 | 0.0202 | 0.0322 | 1.6233 | 0.0479 | 1.5993 |
| 1-(4-Nitrophenyl)-3-phenyl-1H-pyrazol-5-ylamine | 2.5600 | 281.1064 | POS | C15H12N4O2 |  |  |  | 0.0237 | 0.0162 | 1.5087 | 0.0243 | 0.6826 |
| Quinoline, 4-[6-[4-(1-piperazinyl)phenyl]pyrazolo[1,5-a]pyrimidin-3-yl]- | 2.5500 | 407.2027 | POS | C25H22N6 | HMDB0244322 |  |  | 0.0025 | 0.0042 | 1.7159 | 0.0169 | 1.6959 |
| (6R,12aS,12bS,13R)-8,9-Dimethoxy-5,6-dihydro-3H,4H-6,12b,12a  -(propane[1,1,3]triyl)-3a,10b-diazabenzo[7,8]cycloocta[1,2,3-cd]inden-11(12H)-one | 2.5500 | 353.1819 | POS | C21H24N2O3 |  |  |  | 0.0068 | 0.0108 | 1.0258 | 0.0415 | 1.5994 |
| 4-[(2,2-Diphenylacetyl)oxy]-1,1-dimethylpiperidinium cation | 2.5500 | 324.1920 | POS | C21H26NO2 |  |  |  | 0.0307 | 0.0522 | 1.1444 | 0.0199 | 1.7038 |
| N-(Naphthalen-2-yl)-2-sulfanylacetamide | 2.5500 | 216.0514 | NEG | C12H11NOS |  |  |  | 0.4615 | 0.6942 | 1.5151 | 0.0263 | 1.5041 |
| 12-Methoxy-8,11,13-abietatrien-20,11-olide | 2.5500 | 329.2072 | POS | C21H28O3 | HMDB0038391 |  |  | 0.0065 | 0.0110 | 1.5683 | 0.0207 | 1.6928 |
| Methanone, [1-(2-hydroxypentyl)-1H-indol-3-yl](2,2,3,3-tetramethylcyclopropyl)- | 2.5500 | 328.2232 | POS | C21H29NO2 |  |  |  | 0.0777 | 0.0463 | 2.6643 | 0.0016 | 0.5963 |
| 1-Acetylpiperidine-2-carboxylic acid | 2.5500 | 172.0969 | POS | C8H13NO3 |  |  |  | 0.0340 | 0.0503 | 2.0840 | 0.0061 | 1.4817 |
| 5-Hydroxymethyltolterodine | 2.5500 | 342.2389 | POS | C22H31NO2 | HMDB0013973 |  |  | 0.0948 | 0.0456 | 2.2048 | 0.0055 | 0.4806 |
| 2,4-Dodecadienamide, N-(p-hydroxyphenethyl)-, (E,E)- | 2.5500 | 314.2088 | NEG | C20H29NO2 |  |  |  | 0.9419 | 0.4616 | 2.4495 | 0.0105 | 0.4901 |
| N-(.alpha.-Linolenoyl)tyrosine | 2.5500 | 440.2771 | NEG | C27H39NO4 |  |  |  | 0.6524 | 0.3778 | 1.4101 | 0.0073 | 0.5790 |
| 1-(2-Chloro-4-nitrophenyl)-3-methylpiperazine | 2.5500 | 256.0818 | POS | C11H14ClN3O2 |  |  |  | 0.0261 | 0.1167 | 1.8668 | 0.0043 | 4.4735 |
| 1-Monolinolenin | 2.5500 | 353.2688 | POS | C21H36O4 |  |  |  | 0.0741 | 0.0578 | 1.5294 | 0.0371 | 0.7796 |
| Apixaban | 2.5500 | 460.2025 | POS | C25H25N5O4 | HMDB0248515 |  |  | 0.0259 | 0.0137 | 1.3183 | 0.0176 | 0.5289 |
| Nateglinide | 2.5500 | 316.1879 | NEG | C19H27NO3 | HMDB0014869 | 105816-04-4 | C12508 | 1.3493 | 0.7507 | 2.8035 | 0.0039 | 0.5563 |
| 3-(1,1-Dimethyl-2-propenyl)-8-(3-methyl-2-butenyl)xanthyletin | 2.5400 | 365.2070 | POS | C24H28O3 | HMDB0030730 | 30310-55-5 |  | 0.0145 | 0.0698 | 1.2151 | 0.0296 | 4.8294 |
| .beta.-Alanine, N-[2-(2-pyridinyl)-6-(1,2,4,5-tetrahydro-3H-3-benzazepin  -3-yl)-4-pyrimidinyl]-, ethyl ester | 2.5300 | 418.2183 | POS | C24H27N5O2 | HMDB0252948 |  |  | 0.0017 | 0.0039 | 1.5192 | 0.0191 | 2.3314 |
| 6-Ketoestriol | 2.5300 | 303.1553 | POS | C18H22O4 | HMDB0000530 | 7323-86-6 |  | 0.0441 | 0.0671 | 1.6422 | 0.0105 | 1.5212 |
| Galdosol | 2.5300 | 345.1661 | POS | C20H24O5 |  |  |  | 0.0375 | 0.0366 | 1.3310 | 0.0183 | 0.9754 |
| Cryptotanshinone | 2.5300 | 297.1445 | POS | C19H20O3 |  |  |  | 0.1346 | 0.8867 | 1.6224 | 0.0110 | 6.5853 |
| Duloxetine | 2.5300 | 298.1287 | POS | C18H19NOS | HMDB0014619 | 136434-34-9 |  | 0.2687 | 1.0155 | 1.9755 | 0.0045 | 3.7797 |
| Paynantheine | 2.5300 | 397.2121 | POS | C23H28N2O4 |  |  |  | 0.1120 | 1.2407 | 2.0342 | 0.0004 | 11.0783 |
| 5-Chloro-2-(4-propionyl-1-piperazinyl)aniline | 2.5300 | 268.1181 | POS | C13H18ClN3O |  |  |  | 0.0819 | 0.5046 | 2.0075 | 0.0019 | 6.1633 |
| Nalbuphine | 2.5300 | 358.1966 | POS | C21H27NO4 | HMDB0014982 | 20594-83-6 | C07251 | 0.0078 | 0.0155 | 1.3511 | 0.0207 | 1.9804 |
| Fostamatinib | 2.5300 | 579.1485 | NEG | C23H26FN6O9P | HMDB0252469 | 901119-35-5 | D09347 | 0.0353 | 0.0149 | 1.8559 | 0.0385 | 0.4213 |
| (3aS,5S,11bR,E)-12-Ethylidene-1,2,3a,4,5,7-hexahydro-3,5-ethanopyrrolo  [2,3-d]carbazole-6-carbaldehyde | 2.5200 | 293.1612 | POS | C19H20N2O |  |  |  | 0.0160 | 0.0253 | 1.3370 | 0.0274 | 1.5833 |
| (-)-Epigallocatechin | 2.5200 | 305.0702 | NEG | C15H14O7 | HMDB0038361 | 970-74-1 | C12136 | 12.3492 | 3.7730 | 2.0780 | 0.0149 | 0.3055 |
| Midafotel | 2.5200 | 249.0616 | NEG | C8H15N2O5P |  |  |  | 0.8875 | 1.5275 | 1.1595 | 0.0216 | 1.7211 |
| vesnarinone | 2.5200 | 396.1970 | POS | C22H25N3O4 | HMDB0042059 | 81840-15-5 |  | 0.0123 | 0.0518 | 1.3913 | 0.0131 | 4.2131 |
| DG(20:3(8Z,11Z,14Z)/14:1(9Z)/0:0) | 2.5200 | 589.4821 | POS | C37H64O5 | HMDB0007473 |  |  | 0.3077 | 0.0908 | 2.9251 | 0.0000 | 0.2951 |
| Tri(butoxyethyl)phosphate | 2.5200 | 399.2465 | POS | C18H39O7P | HMDB0259275 |  | C14446 | 0.0659 | 0.3995 | 1.5574 | 0.0067 | 6.0626 |
| N.alpha.-Benzoyl-DL-arginine-4-nitroanilide | 2.5100 | 399.1762 | POS | C19H22N6O4 | HMDB0249046 |  |  | 0.0073 | 0.0115 | 1.5047 | 0.0358 | 1.5756 |
| 4-Hydroxycyclofenil | 2.5100 | 295.1300 | NEG | C19H20O3 |  |  |  | 0.5792 | 3.6423 | 1.6036 | 0.0058 | 6.2890 |
| (S)-Edulinine | 2.5100 | 292.1546 | POS | C16H21NO4 | HMDB0030178 | 27495-36-9 |  | 0.0693 | 0.0263 | 1.8553 | 0.0021 | 0.3797 |
| Ethyl 3-(piperidin-4-yl)propanoate | 2.5100 | 186.1490 | POS | C10H19NO2 |  |  |  | 0.0120 | 0.0153 | 1.9925 | 0.0496 | 1.2743 |
| gamma-L-Glutamyl-L-pipecolic\_acid | 2.5100 | 259.1290 | POS | C11H18N2O5 | HMDB0038614 |  |  | 0.1042 | 0.1673 | 1.3644 | 0.0345 | 1.6055 |
| Beta-Ecdysterone | 2.5100 | 503.2828 | POS | C27H44O7 | HMDB0030180 | 5289-74-7 |  | 0.0062 | 0.0053 | 1.9927 | 0.0446 | 0.8507 |
| 8-Hydroxycarvedilol | 2.5000 | 423.1975 | POS | C24H26N2O5 | HMDB0013946 |  |  | 0.0037 | 0.0090 | 2.1004 | 0.0142 | 2.3994 |
| N-(3-Chloro-4-methylphenyl)-4-nitrobenzamide | 2.5000 | 291.0492 | POS | C14H11ClN2O3 |  |  |  | 0.0381 | 0.0240 | 2.2674 | 0.0096 | 0.6295 |
| 4-[2-(2,6-dimethoxy-4-prop-2-enylphenoxy)-1-hydroxypropyl]-2-methoxyphenol | 2.4900 | 375.1764 | POS | C21H26O6 | HMDB0039248 | 52190-21-3 |  | 0.0313 | 0.0530 | 1.9987 | 0.0076 | 1.6920 |
| 1,3,5-Tris(4-hydroxyphenyl)benzene | 2.4900 | 355.1291 | POS | C24H18O3 |  |  |  | 0.0161 | 0.1502 | 1.7942 | 0.0030 | 9.3532 |
| Isopentenyladenine | 2.4900 | 202.1085 | NEG | C10H13N5 | HMDB0245646 |  | C04083 | 0.2883 | 0.1422 | 1.4347 | 0.0307 | 0.4932 |
| Dihydroferuperine | 2.4800 | 290.1710 | POS | C17H23NO3 | HMDB0040700 | 77795-17-6 |  | 0.0361 | 0.0270 | 2.1353 | 0.0216 | 0.7495 |
| Piracetam | 2.4800 | 143.0815 | POS | C6H10N2O2 | HMDB0256585 |  |  | 0.0669 | 0.0709 | 1.3903 | 0.0296 | 1.0594 |
| Ginkgolic Acid C17-1 | 2.4800 | 375.2895 | POS | C24H38O3 | HMDB0038522 | 111047-30-4 |  | 0.2461 | 0.1429 | 1.7661 | 0.0462 | 0.5807 |
| PA(22:0/20:5(5Z,8Z,11Z,14Z,17Z)) | 2.4800 | 779.5605 | POS | C45H79O8P | HMDB0115258 |  |  | 0.0144 | 0.0075 | 1.5200 | 0.0084 | 0.5246 |
| N-[2-(4-Prenyloxyphenyl)ethyl]tiglamide | 2.4700 | 288.1918 | POS | C18H25NO2 | HMDB0041142 | 172837-74-0 |  | 0.0677 | 0.0434 | 2.6975 | 0.0030 | 0.6408 |
| Dicyclomine | 2.4700 | 310.2740 | POS | C19H35NO2 | HMDB0014942 | 77-19-0 | C06951 | 0.1018 | 0.0476 | 1.8081 | 0.0253 | 0.4671 |
| (R)-2-Hydroxysterculic\_acid | 2.4700 | 311.2583 | POS | C19H34O3 | HMDB0031060 | 14602-38-1 |  | 0.0723 | 0.0369 | 2.0450 | 0.0061 | 0.5110 |
| N-[4-(4-Ethylpiperazin-1-yl)phenyl]benzo[g]quinolin-4-amine | 2.4600 | 383.2286 | POS | C25H26N4 |  |  |  | 0.0115 | 0.0168 | 1.1916 | 0.0274 | 1.4551 |
| Erianin | 2.4600 | 319.1512 | POS | C18H22O5 | HMDB0251918 |  |  | 0.1012 | 0.2117 | 1.4545 | 0.0149 | 2.0922 |
| Pectenotoxin\_2 | 2.4500 | 859.4966 | POS | C47H70O14 | HMDB0033491 | 97564-91-5 |  | 0.0067 | 0.0080 | 1.1502 | 0.0155 | 1.1915 |
| 3-Methyl-5-pentyl-2-furannonanoic\_acid | 2.4500 | 309.2426 | POS | C19H32O3 | HMDB0031091 | 57818-39-0 |  | 0.0616 | 0.0523 | 1.6206 | 0.0183 | 0.8491 |
| Cembratetraene-16,2:19,6-diolide | 2.4400 | 329.1710 | POS | C20H24O4 |  |  |  | 0.0187 | 0.0332 | 2.2864 | 0.0061 | 1.7770 |
| Cys-Tyr | 2.4400 | 283.0784 | NEG | C12H16N2O4S |  |  |  | 6.0920 | 3.7376 | 1.7346 | 0.0169 | 0.6135 |
| N-Pentadecanoyl-L-homoserine lactone | 2.4300 | 326.2690 | POS | C19H35NO3 |  |  |  | 0.0156 | 0.0080 | 1.6589 | 0.0446 | 0.5124 |
| Arnamiol | 2.4100 | 451.1918 | POS | C24H31ClO6 | HMDB0035062 | 102092-23-9 |  | 0.0017 | 0.0025 | 1.2591 | 0.0430 | 1.4658 |
| Kiwiionoside | 2.4100 | 407.2294 | POS | C19H34O9 | HMDB0038691 | 141897-12-3 |  | 0.0025 | 0.0043 | 1.6044 | 0.0136 | 1.7521 |
| Queuosine | 2.4000 | 410.1668 | POS | C17H23N5O7 | HMDB0011596 | 57072-36-3 |  | 0.0053 | 0.0094 | 1.4515 | 0.0017 | 1.7755 |
| 4,5-Dihydro-2-methylthiazole | 2.4000 | 102.0372 | POS | C4H7NS | HMDB0029555 | 2346-00-1 |  | 0.0038 | 0.0020 | 2.2114 | 0.0019 | 0.5332 |
| 3-(1-Isobutyl-1H-tetraazol-5-yl)aniline | 2.3900 | 218.1389 | POS | C11H15N5 |  |  |  | 0.0380 | 0.0402 | 1.0444 | 0.0285 | 1.0586 |
| 4-[(3,4,5-Trimethoxybenzoyl)amino]butanoic acid | 2.3900 | 296.1144 | NEG | C14H19NO6 |  |  |  | 2.0902 | 8.5090 | 1.6981 | 0.0100 | 4.0709 |
| Glycochenodeoxycholic\_acid\_3-glucuronide | 2.3900 | 626.3549 | POS | C32H51NO11 | HMDB0002579 | 79254-98-1 | C03033 | 0.0025 | 0.0048 | 1.3429 | 0.0332 | 1.9044 |
| Tsugaric\_acid\_A\_21-glucosyl\_ester | 2.3800 | 661.4371 | POS | C38H60O9 | HMDB0033425 | 205119-13-7 |  | 0.0172 | 0.0092 | 2.0582 | 0.0155 | 0.5380 |
| a-L-Fucopyranosyl-(1->2)-b-D-galactopyranosyl-(1->2)-D-xylose | 2.3800 | 459.1739 | POS | C17H30O14 | HMDB0041222 | 130136-27-5 |  | 0.0004 | 0.0012 | 2.4107 | 0.0008 | 2.7324 |
| O-t-Butyl-L-threonine methyl ester | 2.3700 | 190.1438 | POS | C9H19NO3 |  |  |  | 0.7214 | 0.5190 | 1.0918 | 0.0142 | 0.7194 |
| N-[1-Oxo-3-(4-oxo-1,2,3-benzotriazin-3(4H)-yl)propyl]glycine | 2.3700 | 275.0774 | NEG | C12H12N4O4 |  |  |  | 0.4533 | 0.7178 | 1.1509 | 0.0169 | 1.5834 |
| Phlorin | 2.3700 | 287.0775 | NEG | C12H16O8 |  |  |  | 1.0901 | 1.9409 | 1.3814 | 0.0142 | 1.7805 |
| Desmethyleneparoxetine | 2.3700 | 316.1350 | NEG | C18H20FNO3 |  |  |  | 20.9895 | 13.9435 | 1.7629 | 0.0415 | 0.6643 |
| N-Hexadecanoyl-L-homoserine lactone | 2.3700 | 340.2847 | POS | C20H37NO3 |  |  |  | 0.1422 | 0.0827 | 1.6744 | 0.0088 | 0.5817 |
| 3-(1H-Benzimidazol-2-yl)propanohydrazide | 2.3600 | 203.0925 | NEG | C10H12N4O |  |  |  | 0.2963 | 0.1948 | 1.7869 | 0.0183 | 0.6574 |
| 2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphoserine | 2.3600 | 762.5335 | POS | C40H76NO10P | HMDB0012357 |  |  | 0.0101 | 0.0038 | 1.5379 | 0.0149 | 0.3722 |
| Thyrotropin-Releasing Hormone | 2.3500 | 363.1764 | POS | C16H22N6O4 | HMDB0259062 |  |  | 0.1197 | 0.1936 | 1.4095 | 0.0496 | 1.6172 |
| (R)-4-((1R,3S,5S,7R,8S,9S,10S,12S,13R,14S,17R)-1,3,7,12-tetrahydroxy  -10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanoic acid | 2.3500 | 407.2793 | POS | C24H40O6 | HMDB0000307 | 80875-94-1 |  | 1.4668 | 0.7688 | 1.2417 | 0.0234 | 0.5241 |
| PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z)) | 2.3500 | 830.5778 | POS | C48H80NO8P | HMDB0008730 |  | C00157 | 1.3351 | 0.6981 | 1.2628 | 0.0446 | 0.5229 |
| 4-((N-(4-((N-Acetylvalylvalyl)amino)-3-hydroxy-6-methylheptanoyl)  alanyl)amino)-2,4,5,6-tetradeoxy-6-methylheptonic acid | 2.3300 | 660.4101 | POS | C31H57N5O10 |  |  |  | 0.0059 | 0.0260 | 1.3784 | 0.0100 | 4.4193 |
| PC(14:1(9Z)/16:1(9Z)) | 2.3300 | 702.4997 | POS | C38H72NO8P | HMDB0007903 |  |  | 0.0233 | 0.0413 | 1.6661 | 0.0004 | 1.7730 |
| Kinetin | 2.3300 | 214.0722 | NEG | C10H9N5O | HMDB0012245 | 525-79-1 | C08272 | 0.2538 | 0.3492 | 1.6072 | 0.0105 | 1.3760 |
| Muzanzagenin | 2.3200 | 443.2728 | POS | C27H38O5 | HMDB0032601 | 197080-19-6 |  | 0.0785 | 0.3860 | 1.2769 | 0.0149 | 4.9179 |
| 1,25-Dihydroxyvitamin\_D3-26,23-lactone | 2.3200 | 445.2885 | POS | C27H40O5 | HMDB0000969 | 81203-50-1 |  | 0.0350 | 0.2009 | 1.8963 | 0.0007 | 5.7435 |
| 10'-apo-beta-carotenal | 2.3100 | 377.2801 | POS | C27H36O | HMDB0059605 | 640-49-3 |  | 0.8881 | 0.4809 | 1.1823 | 0.0345 | 0.5415 |
| Carnosol | 2.3100 | 353.1710 | POS | C20H26O4 | HMDB0002121 | 5957-80-2 | C09069 | 0.0649 | 0.2462 | 1.6957 | 0.0155 | 3.7915 |
| N6-2-(4-Aminophenyl)ethyladenosine | 2.3000 | 387.1764 | POS | C18H22N6O4 |  |  |  | 0.0112 | 0.0245 | 2.1374 | 0.0018 | 2.1905 |
| Oleic acid 2,6-diisopropylanilide | 2.3000 | 442.4006 | POS | C30H51NO |  |  |  | 0.0086 | 0.0042 | 1.1932 | 0.0169 | 0.4856 |
| 2-Oleoyl-1-stearoyl-sn-glycero-3-phosphoserine | 2.3000 | 790.5526 | POS | C42H80NO10P | HMDB0010163 | 124262-93-7 | C02737 | 0.0046 | 0.0064 | 2.1329 | 0.0005 | 1.3688 |
| 15-Ketofluprostenol | 2.3000 | 457.1771 | POS | C23H27F3O6 |  |  |  | 0.0021 | 0.0028 | 1.4384 | 0.0371 | 1.3201 |
| Kendomycin | 2.3000 | 487.2990 | POS | C29H42O6 |  |  |  | 0.0502 | 0.2108 | 1.4196 | 0.0199 | 4.2022 |
| Bufotenine\_O-glucoside | 2.3000 | 367.1864 | POS | C18H26N2O6 | HMDB0029564 | 64656-15-1 |  | 0.2408 | 0.7030 | 1.5882 | 0.0136 | 2.9196 |
| Clobetasol | 2.3000 | 411.1718 | POS | C22H28ClFO4 | HMDB0015148 | 25122-46-7 |  | 0.0015 | 0.0025 | 1.8593 | 0.0183 | 1.7439 |
| DG(20:4(5Z,8Z,11Z,14Z)/14:1(9Z)/0:0) | 2.3000 | 587.4673 | POS | C37H62O5 | HMDB0007502 |  |  | 0.1292 | 0.0403 | 2.8598 | 0.0001 | 0.3122 |
| Mitragynine | 2.2900 | 399.2280 | POS | C23H30N2O4 | HMDB0041933 | 6202-22-8 | C09226 | 0.0524 | 0.6262 | 1.6419 | 0.0020 | 11.9450 |
| 3-Oxocyclobutanecarboxylic acid | 2.2800 | 113.0244 | NEG | C5H6O3 |  |  |  | 0.8740 | 0.5591 | 1.1945 | 0.0332 | 0.6397 |
| Panaxydiol | 2.2800 | 261.1809 | POS | C17H24O2 | HMDB0304717 |  |  | 0.0263 | 0.0659 | 1.7140 | 0.0191 | 2.5112 |
| (22E,\_24x)-Ergosta-4,6,8,22-tetraen-3-one | 2.2800 | 393.3116 | POS | C28H40O | HMDB0030898 | 194721-75-0 |  | 0.0913 | 0.0570 | 1.0698 | 0.0496 | 0.6247 |
| L-Thyronine | 2.2800 | 272.0930 | NEG | C15H15NO4 | HMDB0000667 | 1596-67-4 |  | 1.0700 | 1.9468 | 2.0692 | 0.0012 | 1.8194 |
| .beta.-Hydroxyphenylalanine | 2.2700 | 180.0667 | NEG | C9H11NO3 | HMDB0244981 |  |  | 5.3239 | 2.9547 | 2.4683 | 0.0415 | 0.5550 |
| 3-Hydroxymugineic\_acid | 2.2700 | 337.1266 | POS | C12H20N2O9 | HMDB0033927 | 74235-23-7 |  | 0.0095 | 0.1402 | 1.6162 | 0.0029 | 14.7774 |
| LACTULOSE | 2.2700 | 360.1504 | POS | C12H22O11 | HMDB0000740 | 4618-18-2 | C07064 | 0.2087 | 0.1188 | 1.4310 | 0.0131 | 0.5695 |
| Tacrolimus | 2.2700 | 804.4879 | POS | C44H69NO12 | HMDB0015002 | 104987-11-3 |  | 0.0670 | 0.3813 | 1.1745 | 0.0319 | 5.6940 |
| Dimethyl\_3-methoxy-4-oxo-5-(8,11,14-pentadecatrienyl)-2-hexenedioate | 2.2700 | 421.2594 | POS | C24H36O6 | HMDB0032099 |  |  | 0.0944 | 0.4240 | 1.4000 | 0.0149 | 4.4921 |
| Metalaxyl | 2.2600 | 280.1544 | POS | C15H21NO4 | HMDB0031802 |  | C10947 | 0.1628 | 0.0178 | 1.4934 | 0.0142 | 0.1095 |
| Canthaxanthin | 2.2600 | 564.4005 | POS | C40H52O2 | HMDB0003154 | 514-78-3 | C08583 | 0.0361 | 0.0119 | 1.6677 | 0.0225 | 0.3303 |
| Glycerol\_trihexanoate | 2.2600 | 387.2718 | POS | C21H38O6 | HMDB0031125 | 621-70-5 |  | 0.0432 | 0.0234 | 2.2713 | 0.0131 | 0.5421 |
| Fenoldopam | 2.2600 | 304.0708 | NEG | C16H16ClNO3 | HMDB0014938 | 67227-57-0 | C07693 | 3.1125 | 1.3447 | 2.0470 | 0.0061 | 0.4320 |
| Flibanserin | 2.2500 | 391.1713 | POS | C20H21F3N4O | HMDB0252304 |  |  | 0.0449 | 0.0798 | 1.8561 | 0.0371 | 1.7779 |
| Hexanamide, N-[(1S,2R,3E)-2-hydroxy-1-(hydroxymethyl)-3-heptadecen  -1-yl]-6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- | 2.2500 | 576.3761 | POS | C30H49N5O6 |  |  |  | 0.0761 | 0.0411 | 2.1802 | 0.0307 | 0.5398 |
| Solacauline | 2.2500 | 824.4851 | POS | C43H69NO14 | HMDB0029373 |  |  | 0.0235 | 0.1208 | 1.1546 | 0.0274 | 5.1357 |
| 1-Methyl-3-(trifluoromethyl)benzo[c][1,8]naphthyridin-6(5H)-one | 2.2500 | 277.0591 | NEG | C14H9F3N2O |  |  |  | 0.6163 | 0.3447 | 2.1095 | 0.0415 | 0.5593 |
| 3-(1-Hydroxy-3-methylbutyl)-6-(2-hydroxy-4-methyl-6-(((pentofuranosyl  -(1->3)pentopyranosyl-(1->4)pentopyranosyl)oxy)methyl)phenoxy)-2-methoxybenzoic acid | 2.2500 | 785.2852 | NEG | C36H50O19 |  |  |  | 1.3885 | 3.7480 | 1.7465 | 0.0039 | 2.6994 |
| Ethyl 3-(N-butylacetamido)propionate | 2.2500 | 216.1595 | POS | C11H21NO3 | HMDB0246904 |  | C18830 | 0.0770 | 0.2034 | 1.0410 | 0.0462 | 2.6417 |
| N1,N3-Bis(4-methylphenyl)malonamide | 2.2400 | 283.1400 | POS | C17H18N2O2 |  |  |  | 0.0238 | 0.0415 | 1.2730 | 0.0234 | 1.7453 |
| (1S,3R,4R,5R)-3-(((2E)-3-(2-(3,4-Dihydroxyphenyl)-7-hydroxy-3-(methoxycarbonyl)  -2,3-dihydro-1-benzofuran-5-yl)prop-2-enoyl)oxy)-1,4,5-trihydroxycyclohexanecarboxylic acid | 2.2400 | 545.1295 | NEG | C26H26O13 |  |  |  | 0.1188 | 0.0467 | 2.7402 | 0.0020 | 0.3933 |
| Ionomycin | 2.2400 | 709.5149 | POS | C41H72O9 |  |  |  | 0.0300 | 0.0594 | 2.0331 | 0.0006 | 1.9775 |
| 3-{[(1Z)-4-(4-Hydroxyphenyl)phthalazin-1(2H)-ylidene]amino}phenol | 2.2300 | 328.1072 | NEG | C20H15N3O2 |  |  |  | 2.6267 | 1.1146 | 2.8171 | 0.0096 | 0.4243 |
| 1-Phenylicosane-1,3-dione | 2.2300 | 387.3221 | POS | C26H42O2 | HMDB0032925 | 58446-52-9 |  | 0.0189 | 0.0146 | 1.5614 | 0.0199 | 0.7709 |
| Carebastine | 2.2300 | 500.2759 | POS | C32H37NO4 |  |  |  | 0.0806 | 0.0248 | 2.1816 | 0.0020 | 0.3080 |
| Methyl 2-(3,5-dichloro-2-hydroxy-6-methoxy-4-methylbenzoyl)-3,5-dihydroxybenzoate | 2.2300 | 399.0013 | NEG | C17H14Cl2O7 |  |  |  | 2.0233 | 6.9281 | 1.8771 | 0.0005 | 3.4241 |
| (7'R,8'R)-4,7'-Epoxy-3'-methoxy-4',5,9,9'-lignanetetrol\_9'-glucoside | 2.2300 | 509.1991 | POS | C25H32O11 | HMDB0038710 |  |  | 0.0371 | 0.0103 | 2.9781 | 0.0001 | 0.2781 |
| (3beta,23E)-3-Hydroxy-27-norcycloart-23-en-25-one | 2.2200 | 427.3615 | POS | C29H46O2 | HMDB0037382 | 132943-49-8 |  | 0.1443 | 0.0667 | 1.7253 | 0.0155 | 0.4622 |
| PC(16:1(9Z)/14:1(9Z)) | 2.2200 | 702.5008 | POS | C38H72NO8P | HMDB0007999 |  |  | 0.0079 | 0.0122 | 1.6761 | 0.0055 | 1.5358 |
| Vitamin K1 2,3-epoxide | 2.2000 | 467.3483 | POS | C31H46O3 |  |  |  | 0.0839 | 0.0254 | 1.7618 | 0.0496 | 0.3024 |
| PS(14:1(9Z)/14:1(9Z)) | 2.2000 | 676.4117 | POS | C34H62NO10P | HMDB0012342 |  |  | 0.0028 | 0.0128 | 1.4657 | 0.0115 | 4.6322 |
| Ciprofibrate | 2.2000 | 287.0230 | NEG | C13H14Cl2O3 | HMDB0250268 |  |  | 8.5402 | 4.2861 | 1.7643 | 0.0073 | 0.5019 |
| Armillatin | 2.2000 | 611.4269 | POS | C38H58O6 | HMDB0038743 | 139051-17-5 |  | 0.0179 | 0.0069 | 2.3076 | 0.0084 | 0.3833 |
| 5-(10,13-Nonadecadienyl)-1,3-benzenediol | 2.2000 | 373.3063 | POS | C25H40O2 | HMDB0039867 | 189562-02-5 |  | 0.0732 | 0.0459 | 1.3903 | 0.0400 | 0.6271 |
| DOCOSANOL | 2.2000 | 365.3165 | POS | C22H46O | HMDB0014770 | 30303-65-2 |  | 0.2926 | 0.1423 | 1.3266 | 0.0052 | 0.4863 |
| Murrayazolinine | 2.2000 | 350.2076 | POS | C23H27NO2 | HMDB0030183 | 49620-01-1 |  | 0.0553 | 0.0392 | 2.1041 | 0.0496 | 0.7083 |
| (S)-(-)-Perillyl\_alcohol | 2.2000 | 135.1169 | POS | C10H16O | HMDB0036087 | 57717-97-2 |  | 0.0145 | 0.0198 | 1.3879 | 0.0479 | 1.3591 |
| Myrtucommulone B | 2.1900 | 415.2100 | POS | C24H30O6 |  |  |  | 0.0153 | 0.0290 | 1.8133 | 0.0296 | 1.8975 |
| 4-((1E)-3-(2,4-Dihydroxyphenyl)-3-oxoprop-1-en-1-yl)phenyl 6  -O-((2E)-3-(4-hydroxyphenyl)prop-2-enoyl)-.beta.-D-glucopyranoside | 2.1900 | 563.1528 | NEG | C30H28O11 |  |  |  | 0.0418 | 0.0136 | 2.4134 | 0.0004 | 0.3242 |
| 2-Acetylthiazole | 2.1900 | 128.0178 | POS | C5H5NOS | HMDB0032964 | 24295-03-2 |  | 0.0258 | 0.0144 | 1.2311 | 0.0319 | 0.5600 |
| Neferine | 2.1900 | 625.3230 | POS | C38H44N2O6 | HMDB0034104 | 2292-16-2 |  | 0.0068 | 0.0154 | 1.7659 | 0.0131 | 2.2526 |
| 1H-Indole-3-carboxamide, 1-(5-fluoropentyl)-N-2-naphthalenyl- | 2.1800 | 375.1916 | POS | C24H23FN2O |  |  |  | 0.0121 | 0.0241 | 1.3839 | 0.0010 | 1.9943 |
| 4'-Methoxymucidin | 2.1800 | 289.1396 | POS | C17H20O4 | HMDB0030019 | 86421-33-2 |  | 0.0238 | 0.0357 | 1.2490 | 0.0371 | 1.5025 |
| (22E,24R)-Stigmasta-4,22-diene-3,6-dione | 2.1800 | 425.3460 | POS | C29H44O2 | HMDB0038656 | 50868-51-4 |  | 0.0863 | 0.0372 | 1.4213 | 0.0462 | 0.4308 |
| PS(14:1(9Z)/18:4(6Z,9Z,12Z,15Z)) | 2.1700 | 726.4423 | POS | C38H64NO10P | HMDB0112309 |  |  | 0.0033 | 0.0105 | 1.1721 | 0.0358 | 3.1580 |
| LysoPC(22:4(7Z,10Z,13Z,16Z)) | 2.1700 | 572.3793 | POS | C30H54NO7P | HMDB0010401 |  | C04230 | 0.0076 | 0.0055 | 2.5423 | 0.0076 | 0.7241 |
| 4-Hydroxyphenyl 3,6-bis-O-((2E)-3-(1-hydroxy-4-oxocyclohexa  -2,5-dien-1-yl)prop-2-enoyl)-.beta.-D-glucopyranoside | 2.1600 | 595.1426 | NEG | C30H28O13 |  |  |  | 0.0438 | 0.0134 | 2.0132 | 0.0002 | 0.3057 |
| 2,6-Dichloro-N-(3-methoxypropyl)benzamide | 2.1600 | 262.0381 | POS | C11H13Cl2NO2 |  |  |  | 0.0241 | 0.0151 | 1.4615 | 0.0183 | 0.6275 |
| Hexyl 6-O-pentopyranosylhexopyranoside | 2.1600 | 395.1976 | NEG | C17H32O10 |  |  |  | 0.3208 | 1.6590 | 1.6131 | 0.0025 | 5.1714 |
| Racemoramide | 2.1500 | 393.2499 | POS | C25H32N2O2 | HMDB0251099 |  |  | 0.0110 | 0.0078 | 2.0170 | 0.0149 | 0.7037 |
| (-)-Bilobalide | 2.1500 | 325.0889 | NEG | C15H18O8 | HMDB0242203 |  |  | 0.5612 | 0.3590 | 1.5465 | 0.0415 | 0.6396 |
| 3,3'-Disulfanediylbis(2-(2,2,2-trifluoroacetamido)propanoic acid) | 2.1400 | 430.9843 | NEG | C10H10F6N2O6S2 |  |  |  | 2.3601 | 5.1162 | 1.7000 | 0.0041 | 2.1678 |
| Ascofuranone | 2.1300 | 421.1808 | POS | C23H29ClO5 |  |  |  | 0.0034 | 0.0051 | 1.3726 | 0.0496 | 1.5052 |
| 1-(3,4-Dihydroxy-5-methoxyphenyl)-7-(3,4-dihydroxyphenyl)heptan-3-one | 2.1300 | 359.1460 | NEG | C20H24O6 |  |  |  | 2.5315 | 0.4806 | 3.1044 | 0.0000 | 0.1899 |
| 5-O-Desmethyldonepezil | 2.1200 | 366.2025 | POS | C23H27NO3 | HMDB0013958 |  |  | 0.0560 | 0.0368 | 2.1264 | 0.0385 | 0.6569 |
| Alnuside A | 2.1200 | 461.1854 | NEG | C24H30O9 |  |  |  | 0.3011 | 0.4354 | 1.1934 | 0.0307 | 1.4460 |
| Trimebutine | 2.1200 | 388.2081 | POS | C22H29NO5 | HMDB0259230 |  |  | 0.0109 | 0.0225 | 2.0231 | 0.0035 | 2.0617 |
| Reserpine | 2.1200 | 609.3279 | POS | C33H40N2O9 | HMDB0014351 | 50-55-5 | C06539 | 0.0224 | 0.0443 | 1.5083 | 0.0462 | 1.9800 |
| N-Butylscopolaminium cation | 2.1100 | 360.2129 | POS | C21H30NO4 |  |  |  | 0.0419 | 0.0267 | 2.4944 | 0.0084 | 0.6388 |
| Prostaglandin A2-biotin | 2.1100 | 645.3986 | POS | C35H56N4O5S |  |  |  | 0.0066 | 0.0317 | 1.1144 | 0.0125 | 4.8077 |
| 2,4-Dihydroxy-1-methyl-8-methylidene-13-oxododecahydro-4a,1  -(epoxymethano)-7,9a-methanobenzo[a]azulene-10-carboxylic acid | 2.1100 | 347.1462 | NEG | C19H24O6 |  |  |  | 0.6846 | 0.5933 | 1.4129 | 0.0479 | 0.8667 |
| Lactupicrin | 2.1100 | 409.1257 | NEG | C23H22O7 |  |  |  | 0.8512 | 0.4494 | 1.7478 | 0.0479 | 0.5280 |
| Ramipril | 2.1100 | 417.2462 | POS | C23H32N2O5 | HMDB0014324 | 87333-19-5 |  | 0.0228 | 0.0148 | 1.9922 | 0.0120 | 0.6494 |
| Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[trans-4  -(methylamino)cyclohexyl]-N-[[3-(4-pyridinyl)phenyl]methyl]- | 2.1000 | 490.1770 | POS | C28H28ClN3OS |  |  |  | 0.0052 | 0.0027 | 1.8833 | 0.0055 | 0.5123 |
| Vaccinoside | 2.1000 | 535.1519 | NEG | C25H28O13 |  |  |  | 0.4784 | 0.2486 | 1.3058 | 0.0136 | 0.5196 |
| 1-Hexadecyl-2-azelaoyl-sn-glycero-3-phosphocholine | 2.1000 | 652.4614 | POS | C33H66NO9P |  |  |  | 0.0991 | 0.0340 | 2.0664 | 0.0199 | 0.3432 |
| N-(1-Amino-3,3-dimethyl-1-oxobutan-2-yl)-1-pentyl-1H-indole-3-carboxamide | 2.0900 | 344.2281 | POS | C20H29N3O2 |  |  |  | 0.0439 | 0.0698 | 1.6032 | 0.0136 | 1.5912 |
| Syringolin C | 2.0800 | 506.3055 | NEG | C25H41N5O6 |  |  |  | 0.6287 | 0.1762 | 1.8629 | 0.0430 | 0.2803 |
| Isomucronulatol | 2.0800 | 301.1042 | NEG | C17H18O5 |  |  |  | 3.5585 | 1.7406 | 2.6378 | 0.0034 | 0.4891 |
| Momordicoside\_D | 2.0800 | 783.4803 | POS | C42H70O13 | HMDB0035011 | 78887-73-7 |  | 0.0068 | 0.0417 | 1.2025 | 0.0055 | 6.1650 |
| Acetamide, N-[2-[5-(acetyloxy)-3,6-dimethoxy-1-phenanthrenyl]ethyl]-N-methyl- | 2.0700 | 396.1863 | POS | C23H25NO5 |  |  |  | 0.0020 | 0.0146 | 1.7088 | 0.0430 | 7.2154 |
| Erlotinib | 2.0700 | 394.1717 | POS | C22H23N3O4 | HMDB0014671 | 183321-74-6 |  | 0.0041 | 0.0080 | 1.8549 | 0.0120 | 1.9277 |
| 1H-Indazole-3-carboxamide, N-[1-(aminocarbonyl)-2,2-dimethylpropyl]-1-pentyl- | 2.0600 | 345.2244 | POS | C19H28N4O2 |  |  |  | 0.0641 | 0.0399 | 2.0695 | 0.0080 | 0.6218 |
| Glutathione ethyl ester | 2.0600 | 336.1264 | POS | C12H21N3O6S | HMDB0252819 |  |  | 0.0089 | 0.6695 | 1.8748 | 0.0183 | 75.2606 |
| Fellutamide B | 2.0500 | 556.3632 | POS | C27H49N5O7 |  |  |  | 0.0834 | 0.0195 | 2.2449 | 0.0400 | 0.2341 |
| 4-Methoxybenzyl\_O-(2-sulfoglucoside) | 2.0500 | 381.0795 | POS | C14H20O10S | HMDB0034754 |  |  | 0.1269 | 0.0858 | 1.1440 | 0.0479 | 0.6764 |
| Piperidolate | 2.0400 | 324.1917 | POS | C21H25NO2 |  |  |  | 0.0228 | 0.0380 | 1.1801 | 0.0319 | 1.6684 |
| (2-aminoethoxy)[2-[octadec-9-enoyloxy]-3-[octadeca-1.11-dien-1-yloxy]propoxy]phosphinic acid | 2.0400 | 726.5327 | NEG | C41H78NO7P | HMDB0011408 |  |  | 0.0469 | 0.0085 | 1.7909 | 0.0115 | 0.1813 |
| Dye X-5432-26C | 2.0300 | 400.1356 | NEG | C23H19N3O4 |  |  |  | 0.0196 | 0.0262 | 1.1703 | 0.0110 | 1.3363 |
| 2-{[((2Z)-4-Phenyl-1,3-thiazol-2(3H)-ylidene)amino]carbonyl}benzoic acid | 2.0100 | 323.0543 | NEG | C17H12N2O3S |  |  |  | 2.5667 | 5.8826 | 1.9186 | 0.0041 | 2.2919 |
| M553T166 | 1.9100 | 553.3386 | NEG | C30H50O9 |  |  |  | 0.4020 | 0.2586 | 2.5411 | 0.0191 | 0.6432 |
| M549T86 | 1.9100 | 549.3067 | NEG | C30H48O10 |  |  |  | 0.3291 | 0.2070 | 2.1510 | 0.0496 | 0.6291 |
| M196T99 | 1.8600 | 196.0616 | NEG | C9H11NO4 |  |  |  | 0.8641 | 1.3722 | 1.6049 | 0.0100 | 1.5881 |
| 3-Methyl-L-tyrosine | 1.8300 | 196.0969 | POS | C10H13NO3 |  |  |  | 0.0377 | 0.0641 | 1.4588 | 0.0479 | 1.7013 |
| M240T97 | 1.7600 | 240.0867 | POS | C11H10O5 |  |  |  | 0.2957 | 0.4065 | 1.3017 | 0.0191 | 1.3747 |
| M147T70 | 1.7600 | 147.0664 | NEG | C4H8O2 |  |  |  | 41.4285 | 24.7816 | 1.3449 | 0.0084 | 0.5982 |
| Ectoine | 1.7500 | 160.1081 | POS | C6H10N2O2 | HMDB0240650 | 96702-03-3 | C06231 | 0.0250 | 0.0405 | 1.2223 | 0.0207 | 1.6199 |
| M611T221 | 1.7500 | 611.1373 | NEG | C21H30N6O12S |  |  |  | 0.0285 | 0.0103 | 1.8997 | 0.0048 | 0.3623 |
| M464T177 | 1.7000 | 464.1081 | NEG | C16H21N5O10 |  |  |  | 0.8353 | 0.3385 | 1.6594 | 0.0183 | 0.4053 |
| 2'''-N-Acetyl-6'''-deamino-6'''-hydroxyparomomycin II | 1.6800 | 676.3269 | POS | C25H46N4O16 |  |  |  | 0.0024 | 0.0049 | 1.5130 | 0.0430 | 2.0412 |
| 5-Acetamidopentanoate | 1.6500 | 180.0668 | NEG | C7H13NO3 |  |  |  | 1.5557 | 4.3388 | 1.7637 | 0.0025 | 2.7890 |
| M319T152\_1 | 1.6500 | 319.1149 | NEG | C10H16N2O6 |  |  |  | 1.3839 | 0.6964 | 1.9855 | 0.0400 | 0.5032 |
| M505T114 | 1.6100 | 505.3017 | NEG | C26H40NO5 |  |  |  | 2.5657 | 0.7438 | 1.5831 | 0.0415 | 0.2899 |
| M215T104 | 1.6000 | 215.0563 | NEG | C7H14O6 |  |  |  | 2.0613 | 2.8096 | 1.4714 | 0.0076 | 1.3630 |
| N5-Hydroxy-L-ornithine | 1.5600 | 131.0816 | POS | C5H12N2O3 |  |  |  | 0.0329 | 0.0386 | 1.5610 | 0.0243 | 1.1736 |
| M338T153 | 1.5600 | 338.1461 | NEG | C16H25N2O7 |  |  |  | 0.4683 | 0.2011 | 1.6548 | 0.0253 | 0.4294 |
| M245T168 | 1.5300 | 245.0433 | NEG | C5H11NO7S |  |  |  | 2.1622 | 1.3152 | 2.2618 | 0.0253 | 0.6083 |
| (3S,4S)-3-Hydroxytetradecane-1,3,4-tricarboxylate | 1.5000 | 367.1723 | NEG | C17H30O7 |  |  |  | 3.6210 | 1.3793 | 2.6565 | 0.0115 | 0.3809 |
| M254T158 | 1.4900 | 254.1137 | POS | C11H12N2O4 |  |  |  | 0.0145 | 0.0238 | 2.3878 | 0.0012 | 1.6367 |
| M611T175 | 1.4600 | 611.3633 | NEG | C32H54NO10 |  |  |  | 0.1051 | 0.0178 | 2.3420 | 0.0050 | 0.1690 |
| M238T203 | 1.4500 | 238.0357 | NEG | C10H9NO6 |  |  |  | 0.0345 | 0.0650 | 1.8740 | 0.0055 | 1.8828 |
| M245T138 | 1.4500 | 245.1133 | POS | C10H13NO5 |  |  |  | 0.0943 | 0.0729 | 1.4793 | 0.0022 | 0.7735 |
| Harmine | 1.4400 | 193.0718 | NEG | C13H12N2O | HMDB0030311 | 442-51-3 | C06538 | 3.4117 | 1.9590 | 2.1817 | 0.0191 | 0.5742 |
| 2-Hydroxy-5-methylquinone | 1.4400 | 154.0511 | NEG | C7H6O3 |  |  |  | 0.0850 | 0.1494 | 1.1543 | 0.0234 | 1.7574 |
| M173T69 | 1.4400 | 173.0457 | NEG | C5H6O3 |  |  |  | 0.6389 | 0.8686 | 1.0028 | 0.0225 | 1.3596 |
| M214T99 | 1.4300 | 214.0722 | NEG | C7H9NO3 |  |  |  | 0.3766 | 0.7034 | 1.7651 | 0.0385 | 1.8675 |
| 6-O-Methylnorlaudanosoline | 1.4200 | 319.1656 | POS | C17H19NO4 |  |  |  | 0.0327 | 0.0478 | 1.3004 | 0.0319 | 1.4606 |
| M174T163 | 1.4200 | 174.0772 | NEG | C7H13NO4 |  |  |  | 0.2863 | 0.2450 | 1.4889 | 0.0479 | 0.8557 |
| N(alpha)-Acetyl-L-2,4-diaminobutyrate | 1.4100 | 161.0921 | POS | C6H12N2O3 |  |  |  | 0.0518 | 0.0391 | 2.0384 | 0.0225 | 0.7547 |
| M525T148 | 1.4100 | 525.2349 | NEG | C26H38O11 |  |  |  | 0.2051 | 0.1630 | 1.3336 | 0.0285 | 0.7947 |
| Cyclo(L-leucyl-L-phenylalanyl) | 1.3900 | 297.0982 | NEG | C15H20N2O2 |  |  |  | 0.6506 | 0.6577 | 1.2103 | 0.0430 | 1.0109 |
| M226T52\_2 | 1.3500 | 226.0722 | NEG | C10H10O5 |  |  |  | 0.6237 | 0.7090 | 1.3130 | 0.0479 | 1.1367 |
| M247T137 | 1.3200 | 246.9918 | NEG | C8H8O7S |  |  |  | 0.9391 | 0.1915 | 1.4293 | 0.0142 | 0.2039 |
| Anhalonidine | 1.3100 | 206.1176 | POS | C12H17NO3 |  |  |  | 0.0101 | 0.0209 | 1.4585 | 0.0080 | 2.0754 |
| M296T174 | 1.3000 | 296.0988 | POS | C12H15N4O3S |  |  |  | 0.0103 | 0.0188 | 1.9050 | 0.0052 | 1.8324 |
| M199T57 | 1.3000 | 199.0363 | NEG | C10H10O3 |  |  |  | 0.3405 | 0.2528 | 1.3067 | 0.0234 | 0.7426 |
| M201T119 | 1.2800 | 201.0769 | NEG | C7H10O3 |  |  |  | 0.2992 | 0.4932 | 1.3521 | 0.0142 | 1.6482 |
| M366T177\_2 | 1.2500 | 366.1087 | NEG | C13H18O11 |  |  |  | 0.2304 | 0.1676 | 1.6154 | 0.0496 | 0.7273 |
| N-Acetylbialaphos | 1.2400 | 424.1463 | NEG | C13H24N3O7P |  |  |  | 0.0904 | 0.2325 | 1.6870 | 0.0115 | 2.5716 |
| M847T132 | 1.2100 | 846.5593 | NEG | C52H78O6S |  |  |  | 0.2641 | 0.1909 | 1.4897 | 0.0446 | 0.7229 |
| M220T172 | 1.1700 | 220.0486 | NEG | C7H8O7 |  |  |  | 0.0220 | 0.0307 | 1.1084 | 0.0025 | 1.3935 |
| M291T162\_1 | 1.1400 | 291.0658 | NEG | C10H14N4O5 |  |  |  | 0.1040 | 0.1459 | 1.6151 | 0.0285 | 1.4028 |

Table 4. KEGG Enrichment data matrix before and after a 12-week BBr60 intervention

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pathway** | **Description** | **Compounds.(dem)** | **Percent** | **Rich\_factor** | **p\_value** | **up\_nums** | **down\_nums** | **DA\_score** |
| hsa02010 | ABC transporters | C00208;C00407;C00079;C00065;C00140;C00245;C00330;C01083;C05512;C00123;C00064;C00526;C05402 | 20 | 0.094202899 | 5.56158E-08 | 0 | 13 | -1 |
| hsa04978 | Mineral absorption | C00407;C00079;C00065;C00078;C00123;C00064 | 9.230769231 | 0.206896552 | 2.75926E-06 | 0 | 6 | -1 |
| hsa05230 | Central carbon metabolism in cancer | C00407;C00079;C00065;C00078;C00123;C00064 | 9.230769231 | 0.162162162 | 1.23274E-05 | 0 | 6 | -1 |
| hsa01230 | Biosynthesis of amino acids | C00407;C00079;C00065;C00078;C00109;C00123;C00233;C00141;C00064;C01179 | 15.38461538 | 0.078125 | 1.24249E-05 | 0 | 10 | -1 |
| hsa00290 | Valine, leucine and isoleucine biosynthesis | C00407;C00109;C00123;C00233;C00141 | 7.692307692 | 0.217391304 | 1.54134E-05 | 0 | 5 | -1 |
| hsa01232 | Nucleotide metabolism | C00178;C00330;C00106;C05512;C00214;C00064;C00526 | 10.76923077 | 0.120689655 | 1.67553E-05 | 0 | 7 | -1 |
| hsa04974 | Protein digestion and absorption | C00407;C00079;C00065;C00078;C00123;C00064 | 9.230769231 | 0.127659574 | 5.08081E-05 | 0 | 6 | -1 |
| hsa00260 | Glycine, serine and threonine metabolism | C00065;C00078;C00109;C00546;C02737;C06231 | 9.230769231 | 0.125 | 5.74091E-05 | 2 | 4 | -0.333333333 |
| hsa00970 | Aminoacyl-tRNA biosynthesis | C00407;C00079;C00065;C00078;C00123;C00064 | 9.230769231 | 0.115384615 | 9.10031E-05 | 0 | 6 | -1 |
| hsa01210 | 2-Oxocarboxylic acid metabolism | C00407;C00079;C00078;C00109;C00123;C00233;C00141;C01179;C01180 | 13.84615385 | 0.0625 | 0.000202027 | 0 | 9 | -1 |
| hsa00591 | Linoleic acid metabolism | C14762;C01595;C14827;C00157 | 6.153846154 | 0.142857143 | 0.000645363 | 0 | 4 | -1 |
| hsa00240 | Pyrimidine metabolism | C00178;C00106;C00214;C00064;C00526 | 7.692307692 | 0.078125 | 0.002205339 | 0 | 5 | -1 |
| hsa00270 | Cysteine and methionine metabolism | C02989;C00065;C00109;C03145;C01180 | 7.692307692 | 0.074626866 | 0.002701369 | 0 | 5 | -1 |
| hsa00280 | Valine, leucine and isoleucine degradation | C00407;C00123;C00233;C00141 | 6.153846154 | 0.095238095 | 0.003028502 | 0 | 4 | -1 |
| hsa00564 | Glycerophospholipid metabolism | C00065;C04230;C00157;C02737 | 6.153846154 | 0.071428571 | 0.008536965 | 1 | 3 | -0.5 |
| hsa05231 | Choline metabolism in cancer | C04230;C00157 | 3.076923077 | 0.181818182 | 0.010555488 | 0 | 2 | -1 |
| hsa00400 | Phenylalanine, tyrosine and tryptophan biosynthesis | C00079;C00078;C01179 | 4.615384615 | 0.085714286 | 0.013846445 | 0 | 3 | -1 |
| hsa05131 | Shigellosis | C00407;C00123 | 3.076923077 | 0.142857143 | 0.016980892 | 0 | 2 | -1 |
| hsa00470 | D-Amino acid metabolism | C00079;C00065;C00064;C01180 | 6.153846154 | 0.057971014 | 0.01746161 | 0 | 4 | -1 |
| hsa04071 | Sphingolipid signaling pathway | C00065;C00319 | 3.076923077 | 0.133333333 | 0.019411164 | 0 | 2 | -1 |
| hsa00120 | Primary bile acid biosynthesis | C00695;C00245;C01921 | 4.615384615 | 0.063829787 | 0.030331059 | 0 | 3 | -1 |
| hsa04148 | Efferocytosis | C04230;C02737 | 3.076923077 | 0.095238095 | 0.036714093 | 1 | 1 | 0 |
| hsa05322 | Systemic lupus erythematosus | C02737 | 1.538461538 | 0.333333333 | 0.043068836 | 1 | 0 | 1 |
| hsa00430 | Taurine and hypotaurine metabolism | C00245;C14179 | 3.076923077 | 0.083333333 | 0.046930803 | 1 | 1 | 0 |
| hsa00053 | Ascorbate and aldarate metabolism | C01620;C01114;C03033 | 4.615384615 | 0.052631579 | 0.049431996 | 1 | 2 | -0.333333333 |
| hsa04976 | Bile secretion | C00695;C01921;C07210;C03033 | 6.153846154 | 0.041237113 | 0.051847637 | 1 | 3 | -0.5 |
| hsa04150 | mTOR signaling pathway | C00123 | 1.538461538 | 0.25 | 0.057015142 | 0 | 1 | -1 |
| hsa04210 | Apoptosis | C00319 | 1.538461538 | 0.25 | 0.057015142 | 0 | 1 | -1 |
| hsa04973 | Carbohydrate digestion and absorption | C00208;C12285 | 3.076923077 | 0.074074074 | 0.058053944 | 1 | 1 | 0 |
| hsa00770 | Pantothenate and CoA biosynthesis | C00106;C00141 | 3.076923077 | 0.066666667 | 0.069989068 | 0 | 2 | -1 |
| hsa03320 | PPAR signaling pathway | C14762 | 1.538461538 | 0.2 | 0.070761277 | 0 | 1 | -1 |
| hsa05140 | Leishmaniasis | C02737 | 1.538461538 | 0.166666667 | 0.08431007 | 1 | 0 | 1 |
| hsa00920 | Sulfur metabolism | C00065;C00245 | 3.076923077 | 0.058823529 | 0.087014051 | 0 | 2 | -1 |
| hsa00600 | Sphingolipid metabolism | C00065;C00319 | 3.076923077 | 0.057142857 | 0.091448452 | 0 | 2 | -1 |
| hsa01100 | Metabolic pathways | C00695;C00208;C02989;C00407;C00079;C00178;C00065;C00140;C00245;C00078;C00330;C01595;C01083;C01620;C01921;C00106;C12115;C01216;C05512;C00109;C00319;C00123;C00233;C00645;C00214;C01114;C00141;C00064;C01909;C03150;C00954;C00526;C05402;C00884;C01494;C00844;C01179;C01542;C01744;C00546;C05582;C00643;C06730;C14827;C01180;C06202;C00157;C03033;C02737;C06231 | 76.92307692 | 0.016265452 | 0.098699196 | 8 | 42 | -0.68 |
| hsa00500 | Starch and sucrose metabolism | C00208;C01083 | 3.076923077 | 0.054054054 | 0.100510907 | 0 | 2 | -1 |
| hsa04724 | Glutamatergic synapse | C00064 | 1.538461538 | 0.125 | 0.110826746 | 0 | 1 | -1 |
| hsa05143 | African trypanosomiasis | C00078 | 1.538461538 | 0.125 | 0.110826746 | 0 | 1 | -1 |
| hsa00640 | Propanoate metabolism | C00109;C00546 | 3.076923077 | 0.048780488 | 0.119334958 | 0 | 2 | -1 |
| hsa00380 | Tryptophan metabolism | C00078;C00954;C00643 | 4.615384615 | 0.036144578 | 0.119494562 | 1 | 2 | -0.333333333 |
| hsa04727 | GABAergic synapse | C00064 | 1.538461538 | 0.111111111 | 0.123800093 | 0 | 1 | -1 |
| hsa04726 | Serotonergic synapse | C00078;C00643 | 3.076923077 | 0.047619048 | 0.124171629 | 0 | 2 | -1 |
| hsa00785 | Lipoic acid metabolism | C00233;C00141 | 3.076923077 | 0.045454545 | 0.133984712 | 0 | 2 | -1 |
| hsa04217 | Necroptosis | C00319 | 1.538461538 | 0.1 | 0.136587025 | 0 | 1 | -1 |
| hsa04979 | Cholesterol metabolism | C01921 | 1.538461538 | 0.1 | 0.136587025 | 0 | 1 | -1 |
| hsa00052 | Galactose metabolism | C01216;C05402 | 3.076923077 | 0.043478261 | 0.143968744 | 0 | 2 | -1 |
| hsa05215 | Prostate cancer | C07653 | 1.538461538 | 0.090909091 | 0.149190179 | 0 | 1 | -1 |
| hsa04728 | Dopaminergic synapse | C05582 | 1.538461538 | 0.083333333 | 0.161612155 | 0 | 1 | -1 |
| hsa05146 | Amoebiasis | C02737 | 1.538461538 | 0.076923077 | 0.173855518 | 1 | 0 | 1 |
| hsa04080 | Neuroactive ligand-receptor interaction | C00245;C16512 | 3.076923077 | 0.037735849 | 0.180011454 | 0 | 2 | -1 |
| hsa00230 | Purine metabolism | C00330;C05512;C00064 | 4.615384615 | 0.02970297 | 0.181358166 | 0 | 3 | -1 |
| hsa01240 | Biosynthesis of cofactors | C00065;C00078;C00141;C00064;C01909;C01179;C03033 | 10.76923077 | 0.021341463 | 0.197980862 | 1 | 6 | -0.714285714 |
| hsa04964 | Proximal tubule bicarbonate reclamation | C00064 | 1.538461538 | 0.058823529 | 0.221092889 | 0 | 1 | -1 |
| hsa00630 | Glyoxylate and dicarboxylate metabolism | C00065;C00064 | 3.076923077 | 0.03125 | 0.238867034 | 0 | 2 | -1 |
| hsa04723 | Retrograde endocannabinoid signaling | C00157 | 1.538461538 | 0.052631579 | 0.243703991 | 0 | 1 | -1 |
| hsa00910 | Nitrogen metabolism | C00064 | 1.538461538 | 0.05 | 0.254765926 | 0 | 1 | -1 |
| hsa00220 | Arginine biosynthesis | C00064 | 1.538461538 | 0.043478261 | 0.287004679 | 0 | 1 | -1 |
| hsa01040 | Biosynthesis of unsaturated fatty acids | C01595;C16513 | 3.076923077 | 0.027027027 | 0.293208343 | 0 | 2 | -1 |
| hsa00350 | Tyrosine metabolism | C01179;C05582 | 3.076923077 | 0.025641026 | 0.314877805 | 0 | 2 | -1 |
| hsa00590 | Arachidonic acid metabolism | C05960;C00157 | 3.076923077 | 0.025316456 | 0.320276322 | 1 | 1 | 0 |
| hsa00250 | Alanine, aspartate and glutamate metabolism | C00064 | 1.538461538 | 0.035714286 | 0.337710951 | 0 | 1 | -1 |
| hsa00750 | Vitamin B6 metabolism | C00064 | 1.538461538 | 0.034482759 | 0.347417555 | 0 | 1 | -1 |
| hsa00780 | Biotin metabolism | C01909 | 1.538461538 | 0.034482759 | 0.347417555 | 0 | 1 | -1 |
| hsa00982 | Drug metabolism - cytochrome P450 | C16561;C11785 | 3.076923077 | 0.022988506 | 0.363058137 | 2 | 0 | 1 |
| hsa05200 | Pathways in cancer | C07653 | 1.538461538 | 0.032258065 | 0.366412441 | 0 | 1 | -1 |
| hsa00620 | Pyruvate metabolism | C00546 | 1.538461538 | 0.03125 | 0.375704677 | 0 | 1 | -1 |
| hsa00410 | beta-Alanine metabolism | C00106 | 1.538461538 | 0.03125 | 0.375704677 | 0 | 1 | -1 |
| hsa04742 | Taste transduction | C00208 | 1.538461538 | 0.03125 | 0.375704677 | 0 | 1 | -1 |
| hsa05415 | Diabetic cardiomyopathy | C00546 | 1.538461538 | 0.025641026 | 0.43709737 | 0 | 1 | -1 |
| hsa00592 | alpha-Linolenic acid metabolism | C00157 | 1.538461538 | 0.022727273 | 0.477270051 | 0 | 1 | -1 |
| hsa00360 | Phenylalanine metabolism | C00079 | 1.538461538 | 0.020408163 | 0.514616715 | 0 | 1 | -1 |
| hsa00520 | Amino sugar and nucleotide sugar metabolism | C00140;C00645 | 3.076923077 | 0.016949153 | 0.517056851 | 0 | 2 | -1 |
| hsa00071 | Fatty acid degradation | C02990 | 1.538461538 | 0.02 | 0.521764407 | 0 | 1 | -1 |
| hsa00760 | Nicotinate and nicotinamide metabolism | C03150 | 1.538461538 | 0.018181818 | 0.555977259 | 1 | 0 | 1 |
| hsa00040 | Pentose and glucuronate interconversions | C03033 | 1.538461538 | 0.016949153 | 0.581602255 | 1 | 0 | 1 |
| hsa00330 | Arginine and proline metabolism | C00884 | 1.538461538 | 0.014492754 | 0.639466056 | 1 | 0 | 1 |
| hsa00130 | Ubiquinone and other terpenoid-quinone biosynthesis | C01179 | 1.538461538 | 0.014084507 | 0.650055041 | 0 | 1 | -1 |
| hsa05204 | Chemical carcinogenesis - DNA adducts | C19255 | 1.538461538 | 0.012820513 | 0.684760621 | 1 | 0 | 1 |
| hsa00140 | Steroid hormone biosynthesis | C05490 | 1.538461538 | 0.00990099 | 0.776597737 | 1 | 0 | 1 |
| hsa01250 | Biosynthesis of nucleotide sugars | C00140;C00645 | 3.076923077 | 0.01 | 0.796522812 | 0 | 2 | -1 |
| hsa01200 | Carbon metabolism | C00065 | 1.538461538 | 0.008928571 | 0.810643065 | 0 | 1 | -1 |
| hsa01212 | Fatty acid metabolism | C02990 | 1.538461538 | 0.008196721 | 0.837128974 | 0 | 1 | -1 |

DA score, Differential Abundance Score

Table 5. Composition of intestinal microbiota in the Bbr60-after and Bbr60-before groups at phylum level.

|  |  |  |
| --- | --- | --- |
| **Phylum** | **Bbr60-after (%)** | **Bbr60-before (%)** |
| p\_\_Firmicutes | 59.32 | 62.44 |
| p\_\_Actinobacteriota | 22.18 | 29.11 |
| p\_\_Proteobacteria | 12.49 | 3.99 |
| p\_\_Bacteroidota | 5.23 | 4.00 |
| p\_\_Desulfobacterota | 0.51 | 0.12 |
| p\_\_Fusobacteriota | 0.08 | 0.20 |
| p\_\_Verrucomicrobiota | 0.09 | 0.02 |
| p\_\_Cyanobacteria | 0.03 | 0.06 |
| p\_\_Patescibacteria | 0.04 | 0.04 |
| p\_\_Campylobacterota | 0.01 | 0.01 |
| p\_\_Synergistota | 0.02 | 0.00 |
| p\_\_Planctomycetota | 0.00 | 0.01 |
| p\_\_Gemmatimonadota | 0.00 | 0.00 |
| p\_\_Spirochaetota | 0.00 | 0.00 |
| p\_\_Deinococcota | 0.00 | 0.00 |
| p\_\_Acidobacteriota | 0.00 | 0.00 |
| p\_\_Chloroflexi | 0.00 | 0.00 |
| p\_\_Fibrobacterota | 0.00 | 0.00 |
| p\_\_Methylomirabilota | 0.00 | 0.00 |
| p\_\_Myxococcota | 0.00 | 0.00 |
| p\_\_Armatimonadota | 0.00 | 0.00 |
| p\_\_Candidatus\_Saccharibacteria | 0.00 | 0.00 |
| p\_\_Hydrogenedentes | 0.00 | 0.00 |
| p\_\_Deferribacterota | 0.00 | 0.00 |
| p\_\_Nitrospirota | 0.00 | 0.00 |
| p\_\_MBNT15 | 0.00 | 0.00 |
| Others | 0.00 | 0.00 |

Table 6. Composition of intestinal microbiota in the Bbr60-after and Bbr60-before groups at genus level.

|  |  |  |
| --- | --- | --- |
| **Genus** | **Bbr60-after**  **(%)** | **Bbr60-before (%)** |
| *g\_\_Bifidobacterium* | 18.86 | 24.45 |
| *g\_\_Streptococcus* | 4.71 | 8.96 |
| *g\_\_Agathobacter* | 6.09 | 5.60 |
| *g\_\_Escherichia-Shigella* | 8.63 | 1.79 |
| *g\_\_Faecalibacterium* | 5.31 | 4.28 |
| *g\_\_Megamonas* | 3.47 | 4.10 |
| *g\_\_Erysipelotrichaceae\_UCG-003* | 1.01 | 4.71 |
| *g\_\_Dialister* | 4.33 | 1.27 |
| *g\_\_Romboutsia* | 1.24 | 3.86 |
| *g\_\_Collinsella* | 2.04 | 2.84 |
| *g\_\_Bacteroides* | 2.74 | 1.62 |
| *g\_\_Clostridium\_sensu\_stricto\_1* | 2.87 | 1.39 |
| *g\_\_Fusicatenibacter* | 1.84 | 2.01 |
| *g\_\_Subdoligranulum* | 1.50 | 1.90 |
| *g\_\_Ruminococcus]\_gnavus\_group* | 0.96 | 2.39 |
| *g\_\_Phascolarctobacterium* | 2.58 | 0.48 |
| *g\_\_Ruminococcus]\_torques\_group* | 1.13 | 1.78 |
| *g\_\_Dorea* | 0.97 | 1.80 |
| *g\_\_Catenibacterium* | 0.98 | 1.68 |
| *g\_\_Lachnoclostridium* | 2.17 | 0.36 |
| *g\_\_Blautia* | 0.97 | 1.47 |
| *g\_\_Klebsiella* | 1.96 | 0.40 |
| *g\_\_Prevotella\_9* | 0.85 | 1.42 |
| *g\_\_Monoglobus* | 1.41 | 0.83 |
| *g\_\_Megasphaera* | 1.20 | 0.85 |
| *g\_\_Ruminococcus* | 0.73 | 0.88 |
| *g\_\_Veillonella* | 1.15 | 0.44 |
| *g\_\_UCG-002* | 0.88 | 0.58 |
| *g\_\_Roseburia* | 0.71 | 0.62 |
| *g\_\_Coprococcus* | 0.69 | 0.57 |
| *Others* | 16.04 | 14.66 |