

Supplementary material

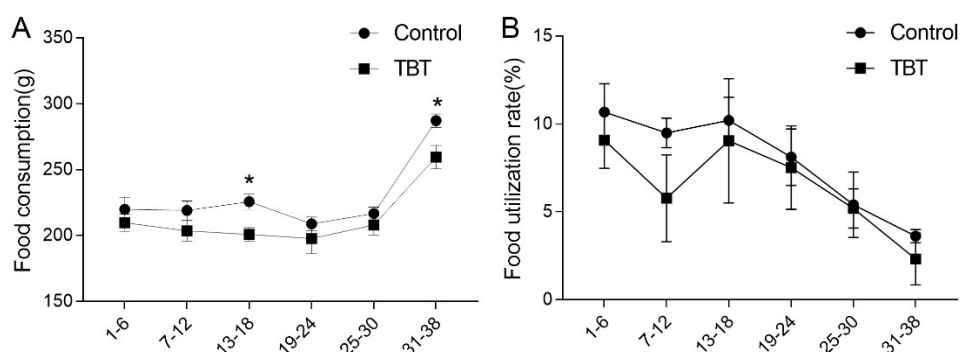


Figure S1. A. Food consumption of rats over a period. B. Food utilization rate of rats. Food utilization rate (%) = weight gain/food consumption.

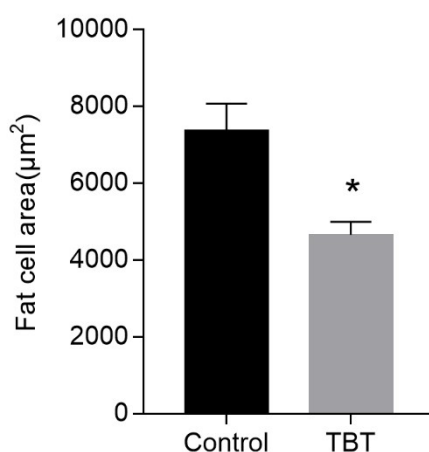


Figure S2. The calculation of adipose tissue cell area. Image J software was used to calculate the cell area of intact fat cells in the same size field of view.

Table S1. The effect of TBT on liver metabolism.

| Name | HMDB | m/z | Fold Change | q | VIP |
|---|-------------|----------|-------------|-----------|------|
| (S)-5-Diphosphomevalonic acid | HMDB0001090 | 309.0148 | 17.23 | 0.0013295 | 2.40 |
| Bovinic acid | HMDB0003797 | 279.2330 | 0.44 | 0.0016332 | 1.41 |
| 11-Dehydrocorticosterone | HMDB0004029 | 345.2036 | 1.40 | 0.0095849 | 1.30 |
| 5,6-Epoxytetraene | HMDB0061111 | 335.2216 | 0.54 | 0.0095849 | 1.45 |
| 6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine | HMDB0033249 | 188.0687 | 0.79 | 0.0095849 | 1.37 |
| FAD | HMDB0001248 | 786.1681 | 1.42 | 0.0095849 | 1.45 |
| LysoPC(15:0) | HMDB0010381 | 480.3111 | 0.61 | 0.0095849 | 1.40 |
| Elaidic acid | HMDB0000573 | 281.2486 | 0.38 | 0.0095849 | 1.53 |
| Maslinic acid | HMDB0002392 | 471.3521 | 0.29 | 0.0095849 | 1.50 |
| Urobilin | HMDB0004160 | 589.3073 | 0.64 | 0.0099701 | 1.37 |
| 9,12,13-TriHOME | HMDB0004708 | 329.2344 | 0.60 | 0.0101235 | 1.29 |
| 6-Keto-prostaglandin F1a | HMDB0002886 | 369.2287 | 0.42 | 0.0101235 | 1.43 |
| Terephthalic acid | HMDB0002428 | 165.0183 | 0.59 | 0.0102901 | 1.27 |

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|--------------------------------------|-------------|----------|------|-----------|------|
| Dephospho-CoA | HMDB0001373 | 688.1576 | 1.85 | 0.0107236 | 1.07 |
| 8-Oxoguanine | HMDB0041820 | 164.0206 | 0.66 | 0.010846 | 1.33 |
| cis-Aconitic acid | HMDB0000072 | 173.0086 | 3.78 | 0.011101 | 1.42 |
| Docosahexaenoic acid | HMDB0002183 | 329.2461 | 0.73 | 0.0111084 | 1.14 |
| LysoPC(18:2(9Z,12Z)) | HMDB0010386 | 520.3384 | 0.74 | 0.0113749 | 1.17 |
| Hordatine A | HMDB0030461 | 565.2878 | 0.69 | 0.0113749 | 1.30 |
| Palmitic acid | HMDB0000220 | 255.2314 | 0.68 | 0.0123522 | 1.40 |
| Crustecdysone | HMDB0030180 | 479.2992 | 0.60 | 0.0125912 | 1.39 |
| Pantetheine 4'-phosphate | HMDB0001416 | 359.1046 | 1.62 | 0.0126462 | 1.34 |
| Guanidinosuccinic acid | HMDB0003157 | 176.0661 | 0.79 | 0.0126462 | 1.22 |
| Allantoin | HMDB0000462 | 157.0358 | 0.60 | 0.0126462 | 1.24 |
| S-Adenosylhomocysteine | HMDB0000939 | 385.1293 | 1.57 | 0.0130808 | 1.10 |
| Riboflavin | HMDB0000244 | 377.1466 | 0.80 | 0.0130834 | 1.28 |
| FADH | HMDB0001197 | 788.1738 | 1.38 | 0.0130834 | 1.23 |
| Hypoxanthine | HMDB0000157 | 137.0461 | 1.74 | 0.0130834 | 1.10 |
| 5-Methyltetrahydrofolic acid | HMDB0001396 | 460.1948 | 1.75 | 0.0130834 | 1.55 |
| D-Leucine | HMDB0013773 | 132.1024 | 0.86 | 0.0130834 | 1.33 |
| Glycyrrhetic acid | HMDB0011628 | 469.3370 | 0.31 | 0.0130834 | 1.31 |
| Guanosine monophosphate | HMDB0001397 | 362.0515 | 0.73 | 0.0130834 | 1.09 |
| LysoPC(17:0) | HMDB0012108 | 508.3416 | 0.49 | 0.0130834 | 1.26 |
| Citric acid | HMDB0000094 | 193.0353 | 0.84 | 0.0131165 | 1.36 |
| Prednisone | HMDB0014773 | 359.1825 | 1.59 | 0.0131771 | 1.12 |
| Glutathione | HMDB0000125 | 308.0917 | 1.58 | 0.0131998 | 1.38 |
| Epinephrine | HMDB0000068 | 184.0974 | 1.86 | 0.0131998 | 1.28 |
| Formiminoglutamic acid | HMDB0000854 | 175.0719 | 0.40 | 0.0131998 | 1.28 |
| Buprenorphine | HMDB0015057 | 466.2953 | 0.61 | 0.0131998 | 1.24 |
| Alpha-Tocotrienol | HMDB0006327 | 423.3281 | 1.20 | 0.0139193 | 1.30 |
| Bicalutamide | HMDB0015260 | 431.0664 | 0.74 | 0.0139212 | 1.09 |
| Emedastine | HMDB0015216 | 301.2029 | 0.65 | 0.0143053 | 1.17 |
| Niacinamide | HMDB0001406 | 123.0558 | 1.25 | 0.0150447 | 1.01 |
| L-Palmitoylcarnitine | HMDB0000222 | 400.3417 | 0.48 | 0.0153032 | 1.39 |
| Calcidiol | HMDB0003550 | 401.3446 | 0.48 | 0.0153032 | 1.40 |
| Alpha-Linolenoyl ethanolamide | HMDB0013624 | 322.2727 | 0.69 | 0.0153032 | 1.19 |
| Verapamil | HMDB0001850 | 455.2945 | 0.67 | 0.0153509 | 1.29 |
| Biflorin | HMDB0002336 | 353.0897 | 0.68 | 0.0153746 | 1.24 |
| Punicic acid | HMDB0030963 | 277.2176 | 0.59 | 0.0161111 | 1.18 |
| 9,10-DHOME | HMDB0004704 | 313.2391 | 0.73 | 0.0163247 | 1.15 |
| 5a-Cholesta-7,24-dien-3b-ol | HMDB0006842 | 385.3499 | 1.25 | 0.0170143 | 1.25 |
| LysoPC(16:1(9Z)/0:0) | HMDB0010383 | 492.3109 | 0.54 | 0.018128 | 1.29 |
| Linoleic acid | HMDB0000673 | 281.2463 | 0.68 | 0.0183177 | 1.22 |
| Hexadecanedioic acid | HMDB0000672 | 285.2079 | 0.65 | 0.018513 | 1.14 |
| LysoPC(18:3(6Z,9Z,12Z)) | HMDB0010387 | 518.3236 | 0.63 | 0.0187985 | 1.16 |
| Drostanolone | HMDB0014996 | 303.2334 | 0.74 | 0.0190267 | 1.07 |
| Glutaric acid | HMDB0000661 | 131.0339 | 0.64 | 0.0190267 | 1.57 |
| D-1-Piperidine-2-carboxylic acid | HMDB0001084 | 128.0711 | 0.68 | 0.0196576 | 1.60 |
| (2S,4R,5S)-Muscarine | HMDB0029936 | 174.1493 | 0.66 | 0.0197939 | 1.19 |
| Mupirocin | HMDB0014554 | 501.3078 | 2.04 | 0.0199235 | 1.88 |
| Adipic acid | HMDB0000448 | 145.0499 | 0.27 | 0.0199235 | 1.23 |
| PC(22:5(4Z,7Z,10Z,13Z,16Z)/14:1(9Z)) | HMDB0008657 | 778.5357 | 0.81 | 0.0204899 | 1.11 |

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|---|-------------|----------|------|-----------|------|
| 2-Arachidonylglycerol | HMDB0004666 | 379.2831 | 0.63 | 0.020517 | 1.19 |
| PE(14:0/22:5(4Z,7Z,10Z,13Z,16Z)) | HMDB0008845 | 736.4931 | 0.48 | 0.020517 | 1.43 |
| Sarmentosin | HMDB0030697 | 276.1077 | 2.36 | 0.0207399 | 1.19 |
| 14,15-DiHETrE | HMDB0002265 | 337.2395 | 0.58 | 0.0210631 | 1.16 |
| Piroxicam | HMDB0014694 | 330.0547 | 1.44 | 0.0222314 | 1.15 |
| Mollicellin C | HMDB0033341 | 411.1083 | 0.78 | 0.0223736 | 1.21 |
| L-Methionine | HMDB0000696 | 148.0430 | 0.81 | 0.0225028 | 1.09 |
| Bisoprolol | HMDB0014750 | 324.2185 | 0.64 | 0.0226401 | 1.11 |
| Equol | HMDB0002209 | 241.0867 | 4.39 | 0.0226401 | 1.42 |
| dCDP | HMDB0001245 | 386.0185 | 1.57 | 0.0226401 | 1.16 |
| Itaconic acid | HMDB0002092 | 129.0183 | 0.71 | 0.0232486 | 1.13 |
| Tartaric acid | HMDB0000956 | 149.0095 | 0.68 | 0.0232598 | 1.36 |
| Adenosine monophosphate | HMDB0000045 | 348.0715 | 1.36 | 0.0237814 | 1.38 |
| 9,10,13-TriHOME | HMDB0004710 | 329.2344 | 0.61 | 0.0241238 | 1.11 |
| Phosphorylcholine | HMDB0001565 | 184.0722 | 0.81 | 0.0241717 | 1.05 |
| LysoPC(16:0) | HMDB0010382 | 496.3394 | 0.86 | 0.0244155 | 1.03 |
| Aesculin | HMDB0030820 | 339.0749 | 0.43 | 0.0246582 | 1.28 |
| Pyridoxamine 5'-phosphate | HMDB0001555 | 249.0617 | 0.83 | 0.0247835 | 1.22 |
| dIDP | HMDB0003536 | 411.0095 | 1.82 | 0.0250509 | 1.01 |
| Imidazoleacetic acid riboside | HMDB0002331 | 259.0932 | 1.39 | 0.0276693 | 1.07 |
| Casimiroin | HMDB0033349 | 232.0593 | 0.70 | 0.0280125 | 1.04 |
| Gibberellin A3 | HMDB0003559 | 345.1323 | 1.26 | 0.0287937 | 1.04 |
| Phosphatidyl-N-methylethanolamine | HMDB0061372 | 675.4811 | 1.63 | 0.0292234 | 1.04 |
| Metoprolol | HMDB0001932 | 268.1883 | 1.14 | 0.029489 | 1.15 |
| Cholesteryl acetate | HMDB0003822 | 429.3728 | 0.79 | 0.0295944 | 1.11 |
| Beta-Glycerophosphoric acid | HMDB0002520 | 171.0058 | 2.46 | 0.0302563 | 1.25 |
| N-alpha-Acetyl-L-lysine | HMDB0000446 | 189.1238 | 0.54 | 0.0303723 | 1.26 |
| Myricitrin | HMDB0034360 | 465.1006 | 0.79 | 0.030436 | 1.07 |
| Lithocholate 3-O-glucuronide | HMDB0002513 | 553.3400 | 0.51 | 0.0310855 | 1.35 |
| LysoPC(22:4(7Z,10Z,13Z,16Z)) | HMDB0010401 | 572.3698 | 0.80 | 0.0314235 | 1.03 |
| L-Octanoylcarnitine | HMDB0000791 | 288.2170 | 0.63 | 0.0321906 | 1.21 |
| Hetacillin | HMDB0014877 | 390.1516 | 2.27 | 0.0323967 | 1.01 |
| N2-gamma-Glutamylglutamine | HMDB0011738 | 274.1068 | 0.88 | 0.0323967 | 1.13 |
| Risperidone | HMDB0005020 | 411.2228 | 2.03 | 0.0324895 | 1.44 |
| (N-acetylneuraminosyl(a2-6)lactosamine) | HMDB0001081 | 673.2340 | 0.78 | 0.032989 | 1.34 |
| Phosphoribosyl pyrophosphate | HMDB0000280 | 388.9431 | 1.92 | 0.0333061 | 1.42 |
| PE(22:2(13Z,16Z)/16:1(9Z)) | HMDB0009551 | 770.5695 | 1.42 | 0.0339867 | 1.13 |
| Hexobarbital | HMDB0015444 | 237.1239 | 0.66 | 0.0346269 | 1.01 |
| 12-Keto-tetrahydro-leukotriene B4 | HMDB0002995 | 337.2391 | 0.66 | 0.0346269 | 1.13 |
| Maclurin | HMDB0032644 | 261.0420 | 0.81 | 0.0346775 | 1.08 |
| Stearidonic acid | HMDB0006547 | 277.2155 | 0.63 | 0.0350954 | 1.02 |
| Soyasapogenol D | HMDB0034507 | 473.3990 | 0.76 | 0.0362153 | 1.35 |
| LysoPC(20:5(5Z,8Z,11Z,14Z,17Z)) | HMDB0010397 | 542.3243 | 0.63 | 0.0363982 | 1.03 |
| Sphingosine 1-phosphate | HMDB0000277 | 380.2533 | 1.16 | 0.0367963 | 1.09 |
| LysoPC(18:4(6Z,9Z,12Z,15Z)) | HMDB0010389 | 516.3099 | 2.26 | 0.0396298 | 1.21 |
| Repaglinide | HMDB0015048 | 451.2634 | 0.70 | 0.0403849 | 1.30 |
| Practolol | HMDB0015411 | 267.1714 | 1.25 | 0.0408583 | 1.09 |
| Capsaicin | HMDB0002227 | 306.2051 | 1.26 | 0.0417407 | 1.98 |

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|-----------------------------|-------------|----------|------|-----------|------|
| Sphingosine | HMDB0000252 | 300.2894 | 0.92 | 0.0437102 | 1.40 |
| Bilirubin | HMDB0000054 | 585.2689 | 0.60 | 0.0437711 | 1.13 |
| Zanamivir | HMDB0014698 | 331.1285 | 0.70 | 0.0451272 | 1.03 |
| Fosinopril | HMDB0014635 | 564.3044 | 0.64 | 0.0452769 | 1.01 |
| Urocanic acid | HMDB0000301 | 137.0346 | 0.79 | 0.0464 | 1.11 |
| 5-Phosphoribosylamine | HMDB0001128 | 228.0277 | 1.72 | 0.0470486 | 1.36 |
| 9,10-Epoxyoctadecenoic acid | HMDB0004701 | 297.2419 | 0.86 | 0.0474906 | 1.73 |
| Tangeritin | HMDB0030539 | 371.1108 | 1.89 | 0.0485393 | 1.28 |
| Beta-Cortolone | HMDB0013221 | 365.2341 | 1.32 | 0.0494565 | 1.62 |
| LysoPC(20:3(5Z,8Z,11Z)) | HMDB0010393 | 546.3538 | 0.74 | 0.0496171 | 1.12 |
| 2,2-dichloro-1,1-ethanediol | HMDB0062193 | 130.9668 | 1.17 | 0.0498405 | 1.01 |

Table S2. The effect of TBT on serum metabolism.

| Name | HMDB | m/z | Fold Change | q | VIP |
|---|-------------|----------|-------------|-----------|------|
| (+)-Calycanthine | HMDB0029561 | 345.2080 | 2.02 | 0.0087588 | 2.12 |
| Oxalosuccinic acid | HMDB0003974 | 189.0022 | 2.23 | 0.0105079 | 2.18 |
| 2-Amino-4-oxo-6-(1',2',3'-trihydroxypropyl)-diquinoid-7,8-dihydroxypterin | HMDB0012144 | 288.0925 | 1.52 | 0.016308 | 1.64 |
| Glucarubin | HMDB0035626 | 497.2405 | 3.31 | 0.0192926 | 1.15 |
| 2-Oxo-4-methylthiobutanoic acid | HMDB0001553 | 147.0129 | 1.49 | 0.0195282 | 1.24 |
| Imazamethabenz-methyl | HMDB0034913 | 289.1572 | 0.79 | 0.0197308 | 1.59 |
| 7-Dehydrodesmosterol | HMDB0003896 | 383.3304 | 0.71 | 0.0201422 | 1.38 |
| 4-Hydroxy-D4-neuroprostane | HMDB0012777 | 377.2292 | 0.57 | 0.0208393 | 1.37 |
| Vaccenic acid | HMDB0003231 | 283.2637 | 1.64 | 0.0224288 | 1.26 |
| LysoPC(P-16:0) | HMDB0010407 | 480.3446 | 0.84 | 0.0245634 | 1.24 |
| Capsidiol | HMDB0002352 | 237.1845 | 0.52 | 0.0253301 | 1.27 |
| Tartaric acid | HMDB0000956 | 149.0092 | 1.61 | 0.0258524 | 1.40 |
| Fexofenadine | HMDB0005030 | 502.2908 | 0.37 | 0.0260677 | 1.23 |
| Nitroprusside | HMDB0014470 | 218.9698 | 2.24 | 0.026904 | 1.49 |
| 17alpha,21-Dihydroxypregnenolone | HMDB0006762 | 347.2232 | 1.40 | 0.027858 | 1.85 |
| Niacinamide | HMDB0001406 | 123.0558 | 0.71 | 0.0291717 | 1.17 |
| Calcidiol | HMDB0003550 | 401.3449 | 0.82 | 0.0330207 | 1.51 |
| Crustecdysone | HMDB0030180 | 479.2990 | 0.47 | 0.0330207 | 1.39 |
| Carmustine | HMDB0014407 | 212.0020 | 1.96 | 0.0331094 | 1.06 |
| Dihydrocortisol | HMDB0003259 | 363.2187 | 1.82 | 0.0354489 | 1.94 |
| L-Ribulose | HMDB0003371 | 149.0447 | 1.22 | 0.0356176 | 1.44 |
| Eicosapentaenoic acid | HMDB0001999 | 303.2310 | 0.59 | 0.0375477 | 1.25 |
| N1-Acetylspermidine | HMDB0001276 | 188.1758 | 1.80 | 0.03912 | 1.41 |
| Metocurine | HMDB0015429 | 649.3270 | 0.79 | 0.0395799 | 1.28 |
| Drostanolone | HMDB0014996 | 305.2465 | 0.75 | 0.0399769 | 1.08 |
| L-Palmitoylcarnitine | HMDB0000222 | 400.3418 | 0.82 | 0.0399769 | 1.50 |
| Pravastatin | HMDB0005022 | 425.2510 | 0.63 | 0.0411741 | 1.24 |

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|---------------------------------------|-------------|----------|------|-----------|------|
| Phosphoroselenoic acid | HMDB0003840 | 160.8916 | 1.22 | 0.0413963 | 1.26 |
| Oxoglutaric acid | HMDB0000208 | 145.0134 | 0.41 | 0.041471 | 1.41 |
| Glutathione | HMDB0000125 | 308.0916 | 0.53 | 0.0435869 | 1.35 |
| Prostaglandin E1 | HMDB0001442 | 353.2343 | 0.72 | 0.0442039 | 1.27 |
| Eplerenone | HMDB0014838 | 415.2113 | 0.90 | 0.0452968 | 1.07 |
| L-2-Amino adipate adenylate | HMDB0006941 | 489.1109 | 1.51 | 0.0460326 | 1.13 |
| Cadmium | HMDB0003638 | 112.8961 | 0.58 | 0.0463813 | 1.29 |
| Nalidixic Acid | HMDB0014917 | 231.0780 | 1.66 | 0.0473197 | 1.07 |
| (R)-Methysticin | HMDB0033590 | 273.0760 | 1.26 | 0.0475848 | 1.19 |
| Midazolam | HMDB0014821 | 324.0709 | 1.28 | 0.0475848 | 1.07 |
| Lipoxin B4 | HMDB0005082 | 351.2181 | 0.59 | 0.0475848 | 1.22 |
| Punicic acid | HMDB0030963 | 279.2312 | 0.61 | 0.0493853 | 1.19 |
| Ginkgoic acid | HMDB0033897 | 345.2443 | 0.54 | 0.0493853 | 1.33 |
| Lincomycin | HMDB0015564 | 405.2098 | 0.61 | 0.0493853 | 1.25 |
| all-trans-Retinoic acid | HMDB0001852 | 301.2155 | 0.60 | 0.0497424 | 1.33 |
| Prostaglandin A2 | HMDB0002752 | 335.2198 | 0.61 | 0.0497424 | 1.10 |
| Medrysone | HMDB0014398 | 343.2283 | 0.59 | 0.0497424 | 1.33 |
| Deoxyuridine | HMDB0000012 | 227.0673 | 1.50 | 0.0497424 | 1.16 |
| 5,6-Epoxy-8,11,14-eicosatrienoic acid | HMDB0002190 | 319.2285 | 0.64 | 0.049811 | 1.25 |

Table S3. The effect of TBT on fecal metabolism.

| Name | HMDB | m/z | Fold Change | q | VIP |
|---|-------------|-----------|-------------|-----------|---------|
| 1,4-beta-D-Glucan | HMDB0006944 | 537.16681 | 0.206090169 | 0.0116967 | 2.12561 |
| Kuwanon Z | HMDB0033297 | 595.15952 | 0.194293406 | 0.0116967 | 2.04862 |
| N-Undecanoylglycine | HMDB0013286 | 244.19053 | 1.319622524 | 0.0220329 | 1.72503 |
| Beta-Citryl-L-glutamic acid | HMDB0013220 | 322.07738 | 0.536010852 | 0.0331825 | 1.81804 |
| (R)-3,4-Dihydro-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-2H-1-benzopyran-6-ol | HMDB0036013 | 369.28235 | 0.700349392 | 0.0356921 | 1.1245 |
| 6,7-Dihydro-4-(hydroxymethyl)-2-(p-hydroxyphenethyl)-7-methyl-5H-2-pyridinium | HMDB0033483 | 284.16252 | 1.26666828 | 0.0391903 | 1.13647 |
| 17-Hydroxylinolenic acid | HMDB0011108 | 295.22686 | 0.737444915 | 0.0411782 | 1.1612 |
| 3-Methyldioxyindole | HMDB0004186 | 164.07072 | 1.801557833 | 0.0461546 | 1.83312 |
| Asparaginy-Proline | HMDB0028739 | 230.11456 | 1.874775732 | 0.0461546 | 1.7073 |
| 7(14)-Bisabolene-2,3,10,11-tetrol | HMDB0035918 | 273.20566 | 1.305420833 | 0.0461546 | 1.22439 |
| Phosphohydroxypyruvic acid | HMDB0001024 | 184.98591 | 1.127993484 | 0.0470272 | 1.14358 |
| Hydroxy-alpha-sanshool | HMDB0029567 | 264.19318 | 1.272107864 | 0.0470272 | 1.31989 |
| Hexylcaine | HMDB0014616 | 262.17762 | 1.191833625 | 0.0470272 | 1.29731 |

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|---|-------------|-----------|-------------|-----------|---------|
| Undecanoylcholine | HMDB0013322 | 272.25832 | 3.066368407 | 0.0470272 | 1.53924 |
| Ginsenoynes L | HMDB0035524 | 463.35514 | 1.299058152 | 0.0470272 | 1.18983 |
| Thiamine aldehyde | HMDB0155991 | 263.09648 | 1.340264837 | 0.0474873 | 1.19584 |
| N-(2-Hydroxyisobutyl)- 2,4,8,10,12- tetradecapentaenamide | HMDB0031183 | 290.2093 | 1.257149337 | 0.0474873 | 1.29772 |
| 5-Hydroxy-N- formylkynurenine | HMDB0004086 | 253.07985 | 1.469117167 | 0.048114 | 1.27354 |
| Coagulin R 3-glucoside | HMDB0033207 | 633.32717 | 0.645174543 | 0.048114 | 1.05551 |
| Methohexital | HMDB0014617 | 263.13758 | 2.157218867 | 0.048114 | 1.2059 |
| Benzothiazole | HMDB0032930 | 136.02186 | 1.62284154 | 0.0488217 | 1.3144 |
| (S)-a-Amino-2,5- dihydro-5-oxo-4- isoxazolepropanoic acid N2-glucoside | HMDB0029404 | 335.10648 | 1.158692416 | 0.0498483 | 1.45615 |
| Cholesterol sulfate | HMDB0000653 | 467.31588 | 1.295901089 | 0.0498483 | 1.47586 |
| Alizapride | HMDB0015494 | 316.17617 | 1.314408654 | 0.0498483 | 1.27882 |
| Melleolide M | HMDB0035068 | 453.16719 | 1.577260267 | 0.0498483 | 1.1284 |
| Quinolinic acid | HMDB0000232 | 166.01382 | 0.320179061 | 0.0240044 | 1.77679 |
| 10-Hydroxymyristic acid methyl ester | HMDB0031061 | 257.21293 | 1.509980338 | 0.0361776 | 1.1394 |
| (S,E)-Zearalenone | HMDB0031752 | 317.14048 | 2.773220745 | 0.0428275 | 1.7556 |
| Ascorbic acid | HMDB0014273 | 175.02446 | 1.462427793 | 0.048114 | 1.16115 |
| Norrubrofusarin 6-beta- gentiobioside | HMDB0034570 | 581.15159 | 2.180286285 | 0.0498483 | 2.56754 |
| D-glycero-L-galacto- Octulose | HMDB0029954 | 239.07788 | 0.770600014 | 0.0498483 | 1.12401 |
| 5,10-Methylene-THF | HMDB0001533 | 456.16171 | 1.425083572 | 0.0498483 | 1.47441 |