

Table S5. Prediction chemicals of the differential content metabolites in the GCs culture media of control and ZEA-treatment groups.

| Mol_ID | Input mass | Adduct | Mass | D-ppm | Name | Formula | CAS | KEGG | MS/MS | Link |
|--------|------------|---------------------|---------|-------|---|----------------|------------|------------|-------|-----------------------------|
| 67869 | 659.28 | [M+Na] ⁺ | 636.284 | 5 | Thalimine | C38H40N2O7 | 5525-36-0 | C0966 1 | NO | metabo_info.php?molid=67869 |
| 82180 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(O-18:0/19:1(9Z)) | C40H79O7P | | | NO | metabo_info.php?molid=82180 |
| 82196 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(O-20:0/17:1(9Z)) | C40H79O7P | | | NO | metabo_info.php?molid=82196 |
| 82263 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(P-16:0/21:0) | C40H79O7P | | | NO | metabo_info.php?molid=82263 |
| 82284 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(P-18:0/19:0) | C40H79O7P | | | NO | metabo_info.php?molid=82284 |
| 82304 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(P-20:0/17:0) | C40H79O7P | | | NO | metabo_info.php?molid=82304 |
| 82180 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(O-18:0/19:1(9Z)) | C40H79O7P | | | NO | metabo_info.php?molid=82180 |
| 82196 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(O-20:0/17:1(9Z)) | C40H79O7P | | | NO | metabo_info.php?molid=82196 |
| 82263 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(P-16:0/21:0) | C40H79O7P | | | NO | metabo_info.php?molid=82263 |
| 82284 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(P-18:0/19:0) | C40H79O7P | | | NO | metabo_info.php?molid=82284 |
| 82304 | 725.55 | [M+Na] ⁺ | 702.556 | 0 | PA(P-20:0/17:0) | C40H79O7P | | | NO | metabo_info.php?molid=82304 |
| 92066 | 760.21 | [M+H] ⁺ | 759.198 | 7 | Delphinidin 3-lathyroside 5-glucoside | C32H39O21 | | | NO | metabo_info.php?molid=92066 |
| 68069 | 517.29 | [M+Na] ⁺ | 494.297 | 1 | Thiobinupharidine | C30H42N2O2S | 30343-72-7 | C0999 0 | NO | metabo_info.php?molid=68069 |
| 49167 | 468.95 | [M+Na] ⁺ | 445.961 | 4 | Luteolin 7,3'-disulfate | C15H10O12S2 | | | NO | metabo_info.php?molid=49167 |
| 50415 | 468.95 | [M+Na] ⁺ | 445.961 | 4 | Luteolin 7,3'-disulfate | C15H10O12S2 | | | NO | metabo_info.php?molid=50415 |
| 2477 | 684.19 | [M+Na] ⁺ | 661.211 | 7 | Spectinomycin adenylate | C24H36N7O13P | 27544-31-6 | C0358 0 | NO | metabo_info.php?molid=2477 |
| 3587 | 529.97 | [M+Na] ⁺ | 506.986 | 1 | 3'-Phosphoadenylyl sulfate (PAPS) | C10H15N5O13P2S | 482-67-7 | C0005 3 | YES | metabo_info.php?molid=3587 |
| 65998 | 529.97 | [M+Na] ⁺ | 506.986 | 1 | 3'-Phosphoadenylyl sulfate | C10H15N5O13P2S | | C0005 3 | NO | metabo_info.php?molid=65998 |
| 51151 | 685.2 | [M+H] ⁺ | 684.19 | 3 | 3,7,5'-trimethoxyflavone 2'-galactosyl-(1->4)-glucoside | C30H36O18 | | | NO | metabo_info.php?molid=51151 |
| 51347 | 685.2 | [M+H] ⁺ | 684.19 | 3 | Chrysofenol C 6,4'-diglucoside | C30H36O18 | | | NO | metabo_info.php?molid=51347 |
| 51384 | 685.2 | [M+H] ⁺ | 684.19 | 3 | Veronicafolin 3-glucosyl-(1->3)-galactoside | C30H36O18 | | | NO | metabo_info.php?molid=51384 |

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|----------------|-----------------|-----|-----------------------------|
| 51694 | 685.2 | [M+H] ⁺ | 684.19 | 3 | 3,3,4'-trimethoxy-7,8,4'- trimethoxyflavone 5- glucosyl-(1->2)- | C30H36O18 | | NO | metabo_info.php?molid=51694 |
| 51715 | 685.2 | [M+H] ⁺ | 684.19 | 3 | 7,4'-dimethoxy-5,6,8,8'- tetramethoxyflavone 4'- glucosyl-(1->3)- galactoside | C30H36O18 | | NO | metabo_info.php?molid=51715 |
| 51733 | 685.2 | [M+H] ⁺ | 684.19 | 3 | Limocitrol 3- neohesperidoside | C30H36O18 | | NO | metabo_info.php?molid=51733 |
| 69675 | 545.97 | [M+Na] ⁺ | 522.973 | 9 | Adenosine 5-O-(3- thiotriphosphate) | C10H16N5O12P3S | C1374 2 | NO | metabo_info.php?molid=69675 |
| 82180 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(O-18:0/19:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82180 |
| 82196 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(O-20:0/17:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82196 |
| 82263 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-16:0/21:0) | C40H79O7P | | NO | metabo_info.php?molid=82263 |
| 82284 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-18:0/19:0) | C40H79O7P | | NO | metabo_info.php?molid=82284 |
| 82304 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-20:0/17:0) | C40H79O7P | | NO | metabo_info.php?molid=82304 |
| 44057 | 487.27 | [M+H] ⁺ | 486.262 | 5 | 3α- HYDROXYDEOXODIHY DROGEDUNIN | C28H38O7 | | NO | metabo_info.php?molid=44057 |
| 44451 | 487.27 | [M+H] ⁺ | 486.262 | 5 | 1,3- DIDEACETYLD EOXYKHI VORIN | C28H38O7 | | YES | metabo_info.php?molid=44451 |
| 43758 | 487.27 | [M+H] ⁺ | 486.262 | 5 | 3beta- HYDROXYDEOXODIHY DROGEDUNIN | C28H38O7 | | NO | metabo_info.php?molid=43758 |
| 84268 | 487.27 | [M+H] ⁺ | 486.262 | 5 | 3beta- HYDROXYDEOXODIHY DROGEDUNIN | C28H38O7 | | NO | metabo_info.php?molid=84268 |
| 89072 | 487.27 | [M+H] ⁺ | 486.262 | 5 | (4beta,5beta,6beta,14bet a,15alpha,20S,22R)-5,6- Epoxy-4,14,15-trihydroxy- 1-oxowitha-2,24-dienolide | C28H38O7 | 22260 9-98-5 | NO | metabo_info.php?molid=89072 |
| 89699 | 487.27 | [M+H] ⁺ | 486.262 | 5 | Withaperuvic C | C28H38O7 | 81644 -34-0 | NO | metabo_info.php?molid=89699 |
| 89769 | 487.27 | [M+H] ⁺ | 486.262 | 5 | 4,4'-Epoxywithanolide | C28H38O7 | | NO | metabo_info.php?molid=89769 |
| 95541 | 487.27 | [M+H] ⁺ | 486.262 | 5 | Eucalyptone | C28H38O7 | 17261 7-99-1 | NO | metabo_info.php?molid=95541 |

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|-----------|-----------------|------------|--------------------------------|
| 428 | 487.27 | [M+H] ⁺ | 486.262 | 5 | Bongkrelic acid | C28H38O7 | 11076 -19-0 | NO | metabo_info.php?molid=428 |
| 73475 | 500.29 | [M+H] ⁺ | 499.278 | 8 | Aconine | C25H41NO9 | 509- 20-6 | C1999 0 | NO metabo_info.php?molid=73475 |
| 69483 | 498.3 | [M+Na] ⁺ | 475.315 | 0 | Dinoprost tromethamine | C24H45NO8 | 38562 -01-5 | C1278 6 | NO metabo_info.php?molid=69483 |
| 51968 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Okanin 3',4'-diglucoside | C27H32O16 | | | NO metabo_info.php?molid=51968 |
| 51970 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Okanin 4'-gentiobioside | C27H32O16 | | | NO metabo_info.php?molid=51970 |
| 52849 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Eriodictyol 5,3'-di-O-glucoside | C27H32O16 | | | NO metabo_info.php?molid=52849 |
| 53093 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Tetrahydroxyflavanone 6,7-diglucoside | C27H32O16 | | | NO metabo_info.php?molid=53093 |
| 87060 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Safflomin A | C27H32O16 | 78281 -02-4 | | NO metabo_info.php?molid=87060 |
| 94666 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Carunarium 6,7-diglucoside | C27H32O16 | | | NO metabo_info.php?molid=94666 |
| 95046 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Aromadendrin 3,7-diglucoside | C27H32O16 | 80212 -10-8 | | NO metabo_info.php?molid=95046 |
| 95152 | 613.17 | [M+H] ⁺ | 612.169 | 2 | Hydroxysafflor yellow A | C27H32O16 | 14608 7-19-6 | | NO metabo_info.php?molid=95152 |
| 67110 | 502.28 | [M+Na] ⁺ | 479.288 | 3 | Delcorine | C26H41NO7 | 52358 -55-1 | C0867 5 | NO metabo_info.php?molid=67110 |
| 51982 | 611.18 | [M+H] ⁺ | 610.169 | 1 | Okanin 4-methyl ether 4'-O-(6''-O-p-coumaroylglucoside) | C31H30O13 | | | NO metabo_info.php?molid=51982 |
| 53094 | 611.18 | [M+H] ⁺ | 610.169 | 1 | 4'-O-methylcarunarium 7-(2-p-coumaroylglucoside) | C31H30O13 | | | NO metabo_info.php?molid=53094 |
| 558 | 611.18 | [M+Na] ⁺ | 588.184 | 5 | Etoposide | C29H32O13 | 33419 -42-0 | C0157 6 | YES metabo_info.php?molid=558 |
| 48042 | 611.18 | [M+Na] ⁺ | 588.184 | 5 | Dalbinol O-glucoside | C29H32O13 | | | NO metabo_info.php?molid=48042 |
| 48578 | 611.18 | [M+Na] ⁺ | 588.184 | 5 | Matteuorientate C | C29H32O13 | | | NO metabo_info.php?molid=48578 |
| 704 | 611.18 | [M+Na] ⁺ | 588.184 | 5 | cis-Etoposide | C29H32O13 | 10000 7-56-5 | | NO metabo_info.php?molid=704 |

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|------------|-----------------|-----|-----------------------------|
| 45727 | 459.23 | [M+H] ⁺ | 458.228 | 3 | 17-trifluoromethylphenyl- 13,14-dihydro trinor PGF2α | C24H33F3O5 | NA | YES | metabo_info.php?molid=45727 |
| 43704 | 459.23 | [M+H] ⁺ | 458.23 | 8 | 1,3-DIDEACETYL-7- DEACETOXY-7- OXOKHIVORIN | C26H34O7 | | YES | metabo_info.php?molid=43704 |
| 43842 | 459.23 | [M+H] ⁺ | 458.23 | 8 | 1,3-DIDEACETYL-7- OXOKHIVORIN | C26H34O7 | | YES | metabo_info.php?molid=43842 |
| 53373 | 459.23 | [M+H] ⁺ | 458.23 | 8 | fumagillin | C26H34O7 | ##### | YES | metabo_info.php?molid=53373 |
| 67233 | 459.23 | [M+H] ⁺ | 458.23 | 8 | Hellebrigenin 3-acetate | C26H34O7 | ##### | NO | metabo_info.php?molid=67233 |
| 71444 | 459.23 | [M+H] ⁺ | 458.23 | 8 | Cinobufotalin | C26H34O7 | 1108- 68-5 | NO | metabo_info.php?molid=71444 |
| 90186 | 459.23 | [M+H] ⁺ | 458.23 | 8 | Hydroxystrobilurin D | C26H34O7 | 11348 9-65-9 | NO | metabo_info.php?molid=90186 |
| 49554 | 687.19 | [M+Na] ⁺ | 664.2 | 4 | Pectolarigenin 7-(4''- acetylrutinoside) | C31H36O16 | | NO | metabo_info.php?molid=49554 |
| 49563 | 687.19 | [M+Na] ⁺ | 664.2 | 4 | Scutellarein 6,4''-dimethyl ether 7-(2''- acetylrutinoside) | C31H36O16 | | NO | metabo_info.php?molid=49563 |
| 49564 | 687.19 | [M+Na] ⁺ | 664.2 | 4 | Scutellarein 6,4''-dimethyl ether 7-(3''- acetylrutinoside) | C31H36O16 | | NO | metabo_info.php?molid=49564 |
| 71033 | 516.28 | [M+Na] ⁺ | 493.29 | 5 | Syringolin A | C24H39N5O6 | | NO | metabo_info.php?molid=71033 |
| 93009 | 474.24 | [M+Na] ⁺ | 451.251 | 6 | Enterocin 900 | C31H33NO2 | 17953 0-08-6 | NO | metabo_info.php?molid=93009 |
| 82180 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(O-18:0/19:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82180 |
| 82196 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(O-20:0/17:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82196 |
| 82263 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-16:0/21:0) | C40H79O7P | | NO | metabo_info.php?molid=82263 |
| 82284 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-18:0/19:0) | C40H79O7P | | NO | metabo_info.php?molid=82284 |
| 82304 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-20:0/17:0) | C40H79O7P | | NO | metabo_info.php?molid=82304 |
| 82180 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(O-18:0/19:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82180 |
| 82196 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(O-20:0/17:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82196 |
| 82263 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-16:0/21:0) | C40H79O7P | | NO | metabo_info.php?molid=82263 |
| 82284 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-18:0/19:0) | C40H79O7P | | NO | metabo_info.php?molid=82284 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|------------|-------------|--------|----|-----------------------------|
| 82304 | 703.56 | [M+H] ⁺ | 702.556 | 1 | PA(P-20:0/17:0) | C40H79O7P | | | NO | metabo_info.php?molid=82304 |
| 73359 | 503.26 | [M+H] ⁺ | 502.25 | 4 | Streptothricin F | C19H34N8O8 | 3808-42-2 | C19785 | NO | metabo_info.php?molid=73359 |
| 44045 | 503.26 | [M+H] ⁺ | 502.257 | 8 | 1,3'-DIDEACETYLMUNIDOPIN | C28H38O8 | | | NO | metabo_info.php?molid=44045 |
| 86914 | 503.26 | [M+H] ⁺ | 502.257 | 8 | Cavipetin B | C28H38O8 | 128530-03-0 | | NO | metabo_info.php?molid=86914 |
| 87608 | 503.26 | [M+H] ⁺ | 502.257 | 8 | 28-Hydroxywithanolide E | C28H38O8 | 188346-67-0 | | NO | metabo_info.php?molid=87608 |
| 89633 | 503.26 | [M+H] ⁺ | 502.257 | 8 | Withaperuvine G | C28H38O8 | | | NO | metabo_info.php?molid=89633 |
| 89687 | 503.26 | [M+H] ⁺ | 502.257 | 8 | 4beta-Hydroxywithanolide E | C28H38O8 | 54334-04-2 | | NO | metabo_info.php?molid=89687 |
| 89859 | 503.26 | [M+H] ⁺ | 502.257 | 8 | Ixocarpalactone B | C28H38O8 | 71801-44-0 | | NO | metabo_info.php?molid=89859 |
| 89907 | 503.26 | [M+H] ⁺ | 502.257 | 8 | Withaperuvine F | C28H38O8 | | | NO | metabo_info.php?molid=89907 |
| 42025 | 509.29 | [M+H] ⁺ | 508.278 | 9 | 26,26,26,27,27,27-hexafluoro-1αa-hydroxyvitamin D3 / 26,26,26,27,27,27-hexafluoro-1αa-hydroxycholecalciferol | C27H38F6O2 | | | NO | metabo_info.php?molid=42025 |
| 42026 | 509.29 | [M+H] ⁺ | 508.278 | 9 | 26,26,26,27,27,27-hexafluoro-25-hydroxyvitamin D3 / 26,26,26,27,27,27-hexafluoro-25-hydroxycholecalciferol | C27H38F6O2 | | | NO | metabo_info.php?molid=42026 |
| 80002 | 509.29 | [M+H] ⁺ | 508.28 | 4 | PG(18:2(9Z,12Z)/0:0) | C24H45O9P | | | NO | metabo_info.php?molid=80002 |
| 41876 | 509.29 | [M+Na] ⁺ | 486.298 | 4 | Hydrocortisone cypionate | C29H42O6 | | 6 | NO | metabo_info.php?molid=41876 |
| 48835 | 761.21 | [M+Na] ⁺ | 738.216 | 6 | Apigenin 7-rhamnosyl-(1->6)-(4''-E-p-methoxycinnamoylglucoside) | C37H38O16 | | | NO | metabo_info.php?molid=48835 |
| 57800 | 531.29 | [M+H] ⁺ | 530.288 | 5 | Proscillaridin A | C30H42O8 | | 12012 | NO | metabo_info.php?molid=57800 |

| | | | | | | | | | |
|-------|--------|--------------------|---------|---|---|------------|-----------------|-----|-----------------------------|
| 86915 | 531.29 | [M+H] ⁺ | 530.288 | 5 | Cavipetin A | C30H42O8 | 12853 0-02-9 | NO | metabo_info.php?molid=86915 |
| 88915 | 531.29 | [M+H] ⁺ | 530.288 | 5 | 7,12-Dimyoxy- 3,11,15,23- tetraoxolanost-8-en-26- oic acid | C30H42O8 | 97653 -94-6 | NO | metabo_info.php?molid=88915 |
| 89538 | 531.29 | [M+H] ⁺ | 530.288 | 5 | Physapubescin | C30H42O8 | 74747 -52-7 | NO | metabo_info.php?molid=89538 |
| 90625 | 531.29 | [M+H] ⁺ | 530.288 | 5 | Ganoderic acid N | C30H42O8 | 11024 1-19-5 | NO | metabo_info.php?molid=90625 |
| 91455 | 531.29 | [M+H] ⁺ | 530.288 | 5 | Ganoderic acid theta | C30H42O8 | 29467 4-15-0 | NO | metabo_info.php?molid=91455 |
| 41673 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Cucurbitacin I | C30H42O7 | | NO | metabo_info.php?molid=41673 |
| 53678 | 515.3 | [M+H] ⁺ | 514.293 | 2 | (-)-Euphomine A | C30H42O7 | | NO | metabo_info.php?molid=53678 |
| 69323 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Stigmatellin A | C30H42O7 | 91682 -96-1 | NO | metabo_info.php?molid=69323 |
| 90677 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganoderenic acid A | C30H42O7 | 10066 5-40-5 | NO | metabo_info.php?molid=90677 |
| 90897 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganoderic acid C1 | C30H42O7 | 95311 -97-0 | NO | metabo_info.php?molid=90897 |
| 90968 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganoderenic acid B | C30H42O7 | 10066 5-41-6 | NO | metabo_info.php?molid=90968 |
| 91453 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganoderic acid xi | C30H42O7 | 29467 4-09-2 | NO | metabo_info.php?molid=91453 |
| 91545 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganosporelactone B | C30H42O7 | 13800 8-05-6 | NO | metabo_info.php?molid=91545 |
| 94196 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganoderic acid J | C30H42O7 | 10044 0-26-4 | NO | metabo_info.php?molid=94196 |
| 94204 | 515.3 | [M+H] ⁺ | 514.293 | 2 | Ganoderic acid V1 | C30H42O7 | 15003 3-91-3 | NO | metabo_info.php?molid=94204 |
| 2098 | 515.3 | [M+H] ⁺ | 514.294 | 3 | ProbucoI spiroquinone | C31H46O2S2 | 81075 -13-0 | NO | metabo_info.php?molid=2098 |
| 43221 | 353.26 | [M+H] ⁺ | 352.251 | 7 | isopropamide | C23H32N2O | | YES | metabo_info.php?molid=43221 |
| 85059 | 353.26 | [M+H] ⁺ | 352.251 | 7 | AB005 | C23H32N2O | 89515 5-25-6 | NO | metabo_info.php?molid=85059 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|----------------|--------------|--------|-----|-----------------------------|
| 49683 | 512.98 | [M+Na] ⁺ | 489.988 | 4 | o-Hydroxyretene 6,6'-dimethyl ether 7,4'-disulfate | C17H14O13S2 | | | NO | metabo_info.php?molid=49683 |
| 51068 | 512.98 | [M+Na] ⁺ | 489.988 | 4 | Ombuin 3,3'-di-O-sulfate | C17H14O13S2 | | | NO | metabo_info.php?molid=51068 |
| 67229 | 547.29 | [M+H] ⁺ | 546.283 | 9 | Decoside | C30H42O9 | 11150-8-63-5 | C08860 | NO | metabo_info.php?molid=67229 |
| 71004 | 654.32 | [M+H] ⁺ | 653.321 | 8 | A 80987 | C37H43N5O6 | 14414-1-97-9 | C15661 | NO | metabo_info.php?molid=71004 |
| 93717 | 530.96 | [M+Na] ⁺ | 507.967 | 2 | Tartrazine calcium lake | C16H12CaN4O9S2 | | | NO | metabo_info.php?molid=93717 |
| 72537 | 527.99 | [M+H] ⁺ | 526.985 | 7 | Sulfluramid | C10H6F17NO2S | 4151-50-2 | C18766 | NO | metabo_info.php?molid=72537 |
| 5984 | 527.99 | [M+H] ⁺ | 526.986 | 8 | L-Amino-4-oxo-6-(erythro-1,2,3-trihydroxypropyl)-7,8-dihydroxypteridine triphosphate | C9H16N5O15P3 | | | NO | metabo_info.php?molid=5984 |
| 81200 | 559.32 | [M+H] ⁺ | 558.317 | 1 | PI(O-16:0/0:0) | C25H51O11P | | | NO | metabo_info.php?molid=81200 |
| 41667 | 559.32 | [M+H] ⁺ | 558.319 | 3 | Cucurbitacin B | C32H46O8 | 6199-67-3 | C08794 | YES | metabo_info.php?molid=41667 |
| 45669 | 559.32 | [M+Na] ⁺ | 536.34 | 7 | 13(S)-HODE-biotin | C28H48N4O4S | NA | | YES | metabo_info.php?molid=45669 |
| 41666 | 575.32 | [M+H] ⁺ | 574.314 | 6 | Cucurbitacin A | C32H46O9 | | C00795 | NO | metabo_info.php?molid=41666 |
| 88916 | 575.32 | [M+H] ⁺ | 574.314 | 6 | Ganoderic acid alpha | C32H46O9 | 22018-1-81-7 | | NO | metabo_info.php?molid=88916 |
| 91171 | 575.32 | [M+H] ⁺ | 574.314 | 6 | Ganoderic acid K | C32H46O9 | 10470-0-95-0 | | NO | metabo_info.php?molid=91171 |
| 6706 | 575.32 | [M+Na] ⁺ | 552.33 | 2 | Lithocholate 3-O-glucuronide | C30H48O9 | | | NO | metabo_info.php?molid=6706 |
| 68091 | 575.32 | [M+Na] ⁺ | 552.331 | 4 | Pandamine | C31H44N4O5 | 10233-81-5 | C10012 | NO | metabo_info.php?molid=68091 |
| 78873 | 673.4 | [M+Na] ⁺ | 650.416 | 2 | PG(12:0/15:1(9Z)) | C33H63O10P | | | NO | metabo_info.php?molid=78873 |
| 78895 | 673.4 | [M+Na] ⁺ | 650.416 | 2 | PG(13:0/14:1(9Z)) | C33H63O10P | | | NO | metabo_info.php?molid=78895 |
| 78935 | 673.4 | [M+Na] ⁺ | 650.416 | 2 | PG(14:1(9Z)/13:0) | C33H63O10P | | | NO | metabo_info.php?molid=78935 |
| 78986 | 673.4 | [M+Na] ⁺ | 650.416 | 2 | PG(15:1(9Z)/12:0) | C33H63O10P | | | NO | metabo_info.php?molid=78986 |
| 92150 | 523.35 | [M+H] ⁺ | 522.34 | 6 | Polysorbate 20 | C26H50O10 | 9005-64-5 | | NO | metabo_info.php?molid=92150 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|----------------|-----------------|------------|-----|-----------------------------|
| 71023 | 523.35 | [M+Na] ⁺ | 500.361 | 1 | Vicenistatin | C30H48N2O4 | 15099 9-05-6 | C1568 8 | NO | metabo_info.php?molid=71023 |
| 40316 | 542.33 | [M+H] ⁺ | 541.317 | 8 | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0) | C28H48NO7P | | | NO | metabo_info.php?molid=40316 |
| 65656 | 561.96 | [M+Na] ⁺ | 538.968 | 5 | GTP-gamma-S | C10H16N5O13P3S | | C0100 6 | NO | metabo_info.php?molid=65656 |
| 723 | 561.96 | [M+Na] ⁺ | 538.968 | 5 | 6-Thioguanosine triphosphate | C10H16N5O13P3S | 17670 -19-8 | | NO | metabo_info.php?molid=723 |
| 92968 | 465.28 | [M+Na] ⁺ | 442.293 | 5 | Ascorbyl stearate | C24H42O7 | 10605 -09-1 | | NO | metabo_info.php?molid=92968 |
| 65429 | 588.34 | [M+Na] ⁺ | 565.352 | 0 | Antillatoxin B (red color) | C33H47N3O5 | | | YES | metabo_info.php?molid=65429 |
| 6132 | 587.33 | [M+H] ⁺ | 586.319 | 3 | Presqualene diphosphate | C30H52O7P2 | | C0042 0 | NO | metabo_info.php?molid=6132 |
| 53853 | 587.33 | [M+H] ⁺ | 586.319 | 3 | all-trans-hexaprenyl diphosphate | C30H52O7P2 | | C0123 0 | NO | metabo_info.php?molid=53853 |
| 67094 | 587.33 | [M+H] ⁺ | 586.325 | 7 | Inuline | C32H46N2O8 | 22413 -78-1 | C0865 9 | NO | metabo_info.php?molid=67094 |
| 80015 | 587.33 | [M+Na] ⁺ | 564.343 | 6 | PG(22:2(13Z,16Z)/0:0) | C28H53O9P | | | NO | metabo_info.php?molid=80015 |
| 67384 | 565.31 | [M+H] ⁺ | 564.31 | 4 | Bonafousine | C35H40N4O3 | 60820 -65-7 | C0905 0 | NO | metabo_info.php?molid=67384 |
| 95773 | 609.34 | [M+H] ⁺ | 608.335 | 2 | 24-Acetyl- 25-cinnamoylvulgaroside | C36H48O8 | 17261 6-89-6 | | NO | metabo_info.php?molid=95773 |
| 81199 | 609.34 | [M+Na] ⁺ | 586.348 | 5 | PI(O-18:0/0:0) | C27H55O11P | | | NO | metabo_info.php?molid=81199 |
| 63699 | 609.34 | [M+Na] ⁺ | 586.351 | 1 | 6,8a-Seco-6,8a-deoxy-5-oxoavermectin '\2a'\ aglycone | C34H50O8 | | C1196 9 | NO | metabo_info.php?molid=63699 |
| 67637 | 659.28 | [M+Na] ⁺ | 636.284 | 8 | Calafatimine | C38H40N2O7 | 77793 -42-1 | C0936 9 | NO | metabo_info.php?molid=67637 |
| 67869 | 659.28 | [M+Na] ⁺ | 636.284 | 8 | Thalsimine | C38H40N2O7 | 5525- 36-0 | C0966 1 | NO | metabo_info.php?molid=67869 |
| 72231 | 377.04 | [M+Na] ⁺ | 354.049 | 6 | Thiodicarb | C10H18N4O4S3 | 59669 -26-0 | C1842 3 | YES | metabo_info.php?molid=72231 |
| 66420 | 377.04 | [M+Na] ⁺ | 354.054 | 6 | WIN56291 | C16H16Cl2N2O3 | | C0040 0 | NO | metabo_info.php?molid=66420 |
| 67283 | 675.38 | [M+H] ⁺ | 674.367 | 8 | Cimicifugoside | C37H54O11 | 66176 -93-0 | C0893 5 | NO | metabo_info.php?molid=67283 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---------------------------------------|-------------|------------|------------|-----|-----------------------------|
| 68083 | 675.38 | [M+H] ⁺ | 674.379 | 9 | Hymenocardine | C37H50N6O6 | 19771-56-3 | C1000 4 | NO | metabo_info.php?molid=68083 |
| 66652 | 631.35 | [M+H] ⁺ | 630.345 | 1 | Remikiren | C33H50N4O6S | 12622-34-2 | C0746 5 | NO | metabo_info.php?molid=66652 |
| 86851 | 497.34 | [M+Na] ⁺ | 474.346 | 3 | Dehydrocarpaine II | C28H46N2O4 | 72362-03-9 | | NO | metabo_info.php?molid=86851 |
| 912 | 329.18 | [M+H] ⁺ | 328.179 | 9 | Labetalol | C19H24N2O3 | 36894-69-6 | C0706 3 | YES | metabo_info.php?molid=912 |
| 66416 | 329.18 | [M+H] ⁺ | 328.179 | 9 | Compound V(S) | C19H24N2O3 | 7096-96-0 | UUUU 1 | NO | metabo_info.php?molid=66416 |
| 73469 | 329.18 | [M+H] ⁺ | 328.179 | 9 | Gelsedine | C19H24N2O3 | 7096-96-0 | C1998 2 | NO | metabo_info.php?molid=73469 |
| 64710 | 329.18 | [M+Na] ⁺ | 306.194 | 1 | W123 | C17H26N2O3 | NA | | YES | metabo_info.php?molid=64710 |
| 35919 | 329.18 | [M+Na] ⁺ | 306.196 | 7 | 9-chloro-10-hydroxy-hexadecanoic acid | C16H31ClO3 | | C1394 9 | NO | metabo_info.php?molid=35919 |
| 96785 | 329.18 | [M+Na] ⁺ | 306.196 | 7 | 9-hydroxy-10-chloro-hexadecanoic acid | C16H31ClO3 | | | NO | metabo_info.php?molid=96785 |
| 67520 | 519.32 | [M+H] ⁺ | 518.316 | 9 | Hodgkinsine | C33H38N6 | 18210-71-4 | C0921 1 | NO | metabo_info.php?molid=67520 |
| 68035 | 525.3 | [M+Na] ⁺ | 502.308 | 8 | Kolanone | C33H42O4 | 81827-55-6 | C0994 8 | NO | metabo_info.php?molid=68035 |
| 65437 | 520.33 | [M+Na] ⁺ | 497.335 | 3 | Tumonoic Acid I | C27H47NO7 | | | YES | metabo_info.php?molid=65437 |
| 81188 | 653.37 | [M+H] ⁺ | 652.359 | 0 | PI(22:2(13Z,16Z)/0:0) | C31H57O12P | | | NO | metabo_info.php?molid=81188 |
| 89978 | 653.37 | [M+Na] ⁺ | 630.377 | 1 | 2,3,23-Triacetylsericic acid | C36H54O9 | 58096-15-4 | | NO | metabo_info.php?molid=89978 |
| 90636 | 653.37 | [M+Na] ⁺ | 630.377 | 1 | Ganoderic acid Mb | C36H54O9 | | | NO | metabo_info.php?molid=90636 |
| 90981 | 653.37 | [M+Na] ⁺ | 630.377 | 1 | Ganoderic acid Mc | C36H54O9 | | | NO | metabo_info.php?molid=90981 |
| 65447 | 608.38 | [M+H] ⁺ | 607.372 | 2 | Malyngamide J | C33H53NO9 | | | YES | metabo_info.php?molid=65447 |
| 92842 | 391.28 | [M+Na] ⁺ | 368.293 | 5 | Octadecyl fumarate | C22H40O4 | 1741-93-1 | | NO | metabo_info.php?molid=92842 |
| 92150 | 523.35 | [M+H] ⁺ | 522.34 | 7 | Polysorbate 20 | C26H50O10 | 9005-64-5 | | NO | metabo_info.php?molid=92150 |
| 71023 | 523.35 | [M+Na] ⁺ | 500.361 | 2 | Vicenistatin | C30H48N2O4 | 15099-05-6 | C1568 8 | NO | metabo_info.php?molid=71023 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|------------------------------|----------------|-----------------|------------|-----|-----------------------------|
| 68077 | 666.37 | [M+H] ⁺ | 665.358 | 0 | Amphibine B | C39H47N5O5 | 38541 -74-1 | C0999 8 | NO | metabo_info.php?molid=68077 |
| 92249 | 666.37 | [M+H] ⁺ | 665.358 | 0 | Jubanine C | C39H47N5O5 | 15922 6-00-3 | | NO | metabo_info.php?molid=92249 |
| 65656 | 539.98 | [M+H] ⁺ | 538.968 | 5 | GTP-gamma-S | C10H16N5O13P3S | | C0100 8 | NO | metabo_info.php?molid=65656 |
| 723 | 539.98 | [M+H] ⁺ | 538.968 | 5 | 6-Thioguanosine triphosphate | C10H16N5O13P3S | 17670 -19-8 | | NO | metabo_info.php?molid=723 |
| 92150 | 545.33 | [M+Na] ⁺ | 522.34 | 6 | Polysorbate 20 | C26H50O10 | 9005- 64-5 | | NO | metabo_info.php?molid=92150 |
| 85482 | 540.31 | [M+Na] ⁺ | 517.323 | 0 | Retapamulin | C30H47NO4S | 22445 2-66-8 | | NO | metabo_info.php?molid=85482 |
| 77743 | 738.44 | [M+Na] ⁺ | 715.442 | 9 | PS(13:0/18:3(6Z,9Z,12Z)) | C37H66NO10P | | | NO | metabo_info.php?molid=77743 |
| 77744 | 738.44 | [M+Na] ⁺ | 715.442 | 9 | PS(13:0/10:0(9Z,12Z,15Z)) | C37H66NO10P | | | NO | metabo_info.php?molid=77744 |
| 77782 | 738.44 | [M+Na] ⁺ | 715.442 | 9 | PS(14:1(9Z))//17:2(9Z,12Z) | C37H66NO10P | | | NO | metabo_info.php?molid=77782 |
| 77945 | 738.44 | [M+Na] ⁺ | 715.442 | 9 | PS(17:2(9Z,11Z))//14:1(9Z) | C37H66NO10P | | | NO | metabo_info.php?molid=77945 |
| 78031 | 738.44 | [M+Na] ⁺ | 715.442 | 9 | PS(18:3(6Z,9Z,12Z))/13:0 | C37H66NO10P | | | NO | metabo_info.php?molid=78031 |
| 78062 | 738.44 | [M+Na] ⁺ | 715.442 | 9 | PS(10:0(9Z,12Z,15Z))//13:0 | C37H66NO10P | | | NO | metabo_info.php?molid=78062 |
| 72057 | 738.44 | [M+Na] ⁺ | 715.447 | 3 | Heptabromodiphenyl | C12H3Br7O | | C1813 9 | NO | metabo_info.php?molid=72057 |
| 72058 | 738.44 | [M+Na] ⁺ | 715.447 | 3 | Heptabromodiphenyl ether | C12H3Br7O | 20712 2-16-5 | C1814 0 | NO | metabo_info.php?molid=72058 |
| 65956 | 373.21 | [M+H] ⁺ | 372.201 | 0 | (Ac)2-L-Lys-D-Ala-D-Ala | C16H28N4O6 | | C0332 8 | NO | metabo_info.php?molid=65956 |
| 1799 | 373.21 | [M+Na] ⁺ | 350.221 | 3 | Perindopril lactam | C19H30N2O4 | 12997 0-98-5 | | NO | metabo_info.php?molid=1799 |
| 85136 | 406.21 | [M+Na] ⁺ | 383.225 | 5 | JWH011 | C27H29NO | 15547 1-13-9 | | YES | metabo_info.php?molid=85136 |
| 85148 | 406.21 | [M+Na] ⁺ | 383.225 | 5 | JWH182 | C27H29NO | 82496 0-02-3 | | YES | metabo_info.php?molid=85148 |
| 85150 | 406.21 | [M+Na] ⁺ | 383.225 | 5 | JWH213 | C27H29NO | 82495 9-83-3 | | YES | metabo_info.php?molid=85150 |
| 78851 | 600.33 | [M+Na] ⁺ | 577.338 | 1 | PS(22:2(13Z,16Z))/0:0 | C28H52NO9P | | | NO | metabo_info.php?molid=78851 |
| 90958 | 719.4 | [M+Na] ⁺ | 696.408 | 9 | Momordicoside E | C37H60O12 | 78887 -74-8 | | NO | metabo_info.php?molid=90958 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|-------------|--------------|------------|-----|------------------------------|
| 92882 | 719.4 | [M+Na] ⁺ | 696.408 | 9 | Glucosyl passiflorate | C37H60O12 | 1392-82-1 | | NO | metabo_info.php?molid=92882 |
| 58223 | 589.3 | [M+H] ⁺ | 588.295 | 4 | D-Urobilin | C33H40N4O6 | 3947-38-4 | C0579 5 | NO | metabo_info.php?molid=58223 |
| 73308 | 589.3 | [M+H] ⁺ | 588.295 | 4 | Dinoflagellate luciferin | C33H40N4O6 | | C1183 4 | NO | metabo_info.php?molid=73308 |
| 36732 | 194.08 | [M+Na] ⁺ | 171.09 | 0 | N-butanoyl-l-homoserine lactone | C8H13NO3 | 67605-85-0 | C1183 7 | YES | metabo_info.php?molid=36732 |
| 68218 | 194.08 | [M+Na] ⁺ | 171.09 | 0 | Crotanecine | C8H13NO3 | 5096-50-4 | C1028 4 | NO | metabo_info.php?molid=68218 |
| 6386 | 194.08 | [M+Na] ⁺ | 171.09 | 0 | (3-Methylcrotonyl)glycine methyl ester | C8H13NO3 | | | NO | metabo_info.php?molid=6386 |
| 1E+05 | 804.54 | [M+Na] ⁺ | 781.547 | 1 | PI-Cer(d18:0/16:0) | C40H80NO11P | | | NO | metabo_info.php?molid=103135 |
| 64483 | 727.2 | [M+H] ⁺ | 726.191 | 0 | Lampranthin II | C34H34N2O16 | 32074-65-0 | C0855 2 | NO | metabo_info.php?molid=64483 |
| 67055 | 727.2 | [M+H] ⁺ | 726.191 | 0 | Gomphrenin-V | C34H34N2O16 | 16955-52-5 | C0854 7 | NO | metabo_info.php?molid=67055 |
| 52735 | 727.2 | [M+H] ⁺ | 726.195 | 5 | Prunin 3''',6'''-di-p-coumarate | C39H34O14 | | | NO | metabo_info.php?molid=52735 |
| 46739 | 805.54 | [M+H] ⁺ | 804.531 | 2 | 1-(8-[3]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanoyl)-sn-glycero-3-phospho-(1''-sn-glycerol) | C46H77O9P | | | NO | metabo_info.php?molid=46739 |
| 79896 | 805.54 | [M+Na] ⁺ | 782.546 | 5 | PG(O-18:0/20:5(5Z,8Z,11Z,14Z,17Z)) | C44H79O9P | | | NO | metabo_info.php?molid=79896 |
| 79931 | 805.54 | [M+Na] ⁺ | 782.546 | 5 | PG(O-16:0/22:4(7Z,10Z,13Z,16Z)) | C44H79O9P | | | NO | metabo_info.php?molid=79931 |
| 79976 | 805.54 | [M+Na] ⁺ | 782.546 | 5 | PG(O-20:0/18:4(6Z,9Z,12Z,15Z)) | C44H79O9P | | | NO | metabo_info.php?molid=79976 |
| 79994 | 805.54 | [M+Na] ⁺ | 782.546 | 5 | PG(O-18:0/20:4(5Z,8Z,11Z,14Z)) | C44H79O9P | | | NO | metabo_info.php?molid=79994 |
| 71005 | 567.29 | [M+H] ⁺ | 566.278 | 9 | Dmp 323 | C35H38N2O5 | 15186-7-81-1 | C1566 2 | NO | metabo_info.php?molid=71005 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---------------------------------------|----------------|-----------------|------------|-----|-----------------------------|
| 6655 | 567.29 | [M+H] ⁺ | 566.289 | 9 | Mesoporphyrin IX | C34H38N4O4 | | | NO | metabo_info.php?molid=6655 |
| 69112 | 611.32 | [M+H] ⁺ | 610.311 | 1 | BQ 123 | C31H42N6O7 | 13655 3-81-6 | C1158 7 | NO | metabo_info.php?molid=69112 |
| 63688 | 611.32 | [M+Na] ⁺ | 588.33 | 1 | Avermectin B2b aglycone | C33H48O9 | | C1150 5 | NO | metabo_info.php?molid=63688 |
| 40874 | 485.28 | [M+H] ⁺ | 484.28 | 8 | PG(16:0/0:0)[U] | C22H45O9P | | | YES | metabo_info.php?molid=40874 |
| 46733 | 485.28 | [M+H] ⁺ | 484.28 | 8 | PG(16:0/0:0) | C22H45O9P | | | NO | metabo_info.php?molid=46733 |
| 57617 | 485.28 | [M+Na] ⁺ | 462.298 | 8 | 3-dehydroecdysone | C27H42O6 | | C0831 5 | NO | metabo_info.php?molid=57617 |
| 57625 | 485.28 | [M+Na] ⁺ | 462.298 | 8 | 2-dehydroecdysone | C27H42O6 | | | NO | metabo_info.php?molid=57625 |
| 57638 | 485.28 | [M+Na] ⁺ | 462.298 | 8 | shidasterone | C27H42O6 | | | NO | metabo_info.php?molid=57638 |
| 67216 | 485.28 | [M+Na] ⁺ | 462.298 | 8 | Podecdysone B | C27H42O6 | 22612 -27-7 | C0883 2 | NO | metabo_info.php?molid=67216 |
| 91159 | 485.28 | [M+Na] ⁺ | 462.298 | 8 | Lucidenic acid M | C27H42O6 | 11024 1-33-3 | | NO | metabo_info.php?molid=91159 |
| 69492 | 226.95 | [M+H] ⁺ | 225.944 | 9 | 2,5-Dichloro-4-oxohex-2-enedioate | C6H4Cl2O5 | | C1283 5 | NO | metabo_info.php?molid=69492 |
| 92458 | 356.06 | [M+H] ⁺ | 355.051 | 9 | Quinoline yellow | C18H13NO5S | 8004- 92-0 | | NO | metabo_info.php?molid=92458 |
| 72505 | 356.06 | [M+H] ⁺ | 355.055 | 0 | Fluchloralin | C12H13ClF3N3O4 | 33245 -39-5 | C1873 0 | NO | metabo_info.php?molid=72505 |
| 3939 | 356.06 | [M+Na] ⁺ | 333.073 | 0 | bromodiphenhydramine | C17H20BrNO | | | NO | metabo_info.php?molid=3939 |
| 58054 | 731.09 | [M+Na] ⁺ | 708.105 | 3 | Diguanosine diphosphate | C20H26N10O15P2 | 34692 -44-9 | | NO | metabo_info.php?molid=58054 |
| 72013 | 731.09 | [M+Na] ⁺ | 708.105 | 3 | 5'-Phosphoguananylyl(3'->5')guanosine | C20H26N10O15P2 | | C1807 6 | NO | metabo_info.php?molid=72013 |
| 92919 | 167.09 | [M+H] ⁺ | 166.082 | 8 | 3-(4-Methyl-3-pentenyl)thiophene | C10H14S | 62469 -65-2 | | NO | metabo_info.php?molid=92919 |
| 67863 | 697.35 | [M+H] ⁺ | 696.341 | 6 | Thalicarpine | C41H48N2O8 | 5373- 42-2 | C0965 5 | NO | metabo_info.php?molid=67863 |
| 67283 | 697.35 | [M+Na] ⁺ | 674.367 | 4 | Cimicifugoside | C37H54O11 | 66176 -93-0 | C0893 5 | NO | metabo_info.php?molid=67283 |
| 85819 | 263.14 | [M+H] ⁺ | 262.135 | 1 | Isoleucyl-Methionine | C11H22N2O3S | | | NO | metabo_info.php?molid=85819 |
| 85838 | 263.14 | [M+H] ⁺ | 262.135 | 1 | Leucyl-Methionine | C11H22N2O3S | | | NO | metabo_info.php?molid=85838 |
| 85878 | 263.14 | [M+H] ⁺ | 262.135 | 1 | Methionyl-Isoleucine | C11H22N2O3S | | | NO | metabo_info.php?molid=85878 |
| 85879 | 263.14 | [M+H] ⁺ | 262.135 | 1 | Methionyl-Leucine | C11H22N2O3S | | | NO | metabo_info.php?molid=85879 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|----------------|-----------------|--|-----|-----------------------------|
| 87844 | 263.14 | [M+H] ⁺ | 262.136 | 0 | Alnustone | C19H18O | 33457 -62-4 | | NO | metabo_info.php?molid=87844 |
| 66981 | 263.14 | [M+Na] ⁺ | 240.151 | 8 | Dehydrofalcarinone | C17H20O | ##### | C ₁₅ O ₄ ⁺ | NO | metabo_info.php?molid=66981 |
| 7089 | 166.08 | [M+Na] ⁺ | 143.095 | 3 | Proline betaine | C7H13NO2 | | C ₁₅ O ₁₁ ⁺ | NO | metabo_info.php?molid=7089 |
| 66118 | 166.08 | [M+Na] ⁺ | 143.095 | 3 | (Trimethylammonio)but- 2-enoate | C7H13NO2 | | C ₀₄ H ₁₁ ⁺ | NO | metabo_info.php?molid=66118 |
| 86954 | 166.08 | [M+Na] ⁺ | 143.095 | 3 | L-2-Amino-3- methylenehexanoic acid | C7H13NO2 | 29784 -96-1 | | NO | metabo_info.php?molid=86954 |
| 93560 | 166.08 | [M+Na] ⁺ | 143.095 | 3 | 3beta,6beta- Dihydroxynortropane | C7H13NO2 | | | NO | metabo_info.php?molid=93560 |
| 6589 | 166.08 | [M+Na] ⁺ | 143.095 | 3 | Aminocyclohexanecarbox- ylic acid | C7H13NO2 | | | YES | metabo_info.php?molid=6589 |
| 84924 | 657.36 | [M+Na] ⁺ | 634.372 | 3 | Pandaroside B | C35H54O10 | | | NO | metabo_info.php?molid=84924 |
| 2038 | 657.36 | [M+Na] ⁺ | 634.372 | 3 | Digitoxigenin bisdigitoxoside | C35H54O10 | 16479 -50-8 | | NO | metabo_info.php?molid=2038 |
| 68633 | 308.15 | [M+H] ⁺ | 307.142 | 4 | Convuloline | C16H21NO5 | 89783 -61-9 | C ₁₀ H ₅ ⁺ | NO | metabo_info.php?molid=68633 |
| 93249 | 308.15 | [M+H] ⁺ | 307.142 | 4 | 5-Amino-2,3-dihydro-6- (3-hydroxy-4-methoxy-1- oxobutyl)-2,2-dimethyl- 4H-1-benzopyran-4-one | C16H21NO5 | 13076 7-47-4 | | NO | metabo_info.php?molid=93249 |
| 3186 | 308.15 | [M+H] ⁺ | 307.145 | 6 | Desethylhydroxychloroqui- n | C16H22ClN3O | 4298- 15-1 | | NO | metabo_info.php?molid=3186 |
| 72295 | 308.15 | [M+H] ⁺ | 307.145 | 6 | Tebuconazole | C16H22ClN3O | 10753 4-96-3 | C ₁₈ H ₉ ⁺ | YES | metabo_info.php?molid=72295 |
| 72231 | 377.04 | [M+Na] ⁺ | 354.049 | 6 | Thiodicarb | C10H18N4O4S3 | 59669 -26-0 | C ₁₈ H ₃ ⁺ | YES | metabo_info.php?molid=72231 |
| 66420 | 377.04 | [M+Na] ⁺ | 354.054 | 6 | WIN56291 | C16H16Cl2N2O3 | | C ₁₅ O ₄ ⁺ | NO | metabo_info.php?molid=66420 |
| 92458 | 378.04 | [M+Na] ⁺ | 355.051 | 8 | Quinoline yellow | C18H13NO5S | 8004- 92-0 | | NO | metabo_info.php?molid=92458 |
| 72505 | 378.04 | [M+Na] ⁺ | 355.055 | 0 | Fluchloralin | C12H13ClF3N3O4 | 33245 -39-5 | C ₁₈ H ₇ ⁺ | NO | metabo_info.php?molid=72505 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|-----------|------------|--------|-----------------------------|-----------------------------|
| 693 | 188.07 | [M+H] ⁺ | 187.059 | 9 | 1-(2-Hydroxyethyl)-2-hydroxymethyl-5-nitroimidazole | C6H9N3O4 | NA | NO | metabo_info.php?molid=693 | |
| 66434 | 188.07 | [M+H] ⁺ | 187.062 | 7 | Deethylatrazine | C6H10CIN5 | 6190-65-4 | C06559 | NO | metabo_info.php?molid=66434 |
| 28 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | L-Phenylalanine | C9H11NO2 | 55-51-1 | YES | metabo_info.php?molid=28 | |
| 3934 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | benzocaine | C9H11NO2 | ##### | NO | metabo_info.php?molid=3934 | |
| 63528 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | D-Phenylalanine | C9H11NO2 | 673-06-3 | C02265 | NO | metabo_info.php?molid=63528 |
| 65707 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | DL-Phenylalanine | C9H11NO2 | 150-30-1 | C02057 | YES | metabo_info.php?molid=65707 |
| 72021 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | Tricaine | C9H11NO2 | 582-33-2 | C18090 | NO | metabo_info.php?molid=72021 |
| 72521 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | Metolcarb | C9H11NO2 | 1129-41-5 | C18747 | NO | metabo_info.php?molid=72521 |
| 73234 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | 4-Hydroxy-1-(3-pyridinyl)-1-butanone | C9H11NO2 | 59578-62-0 | C19565 | NO | metabo_info.php?molid=73234 |
| 73241 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | 5-(3-Pyridyl)-2-hydroxytetrahydrofuran | C9H11NO2 | 53798-73-5 | C19578 | NO | metabo_info.php?molid=73241 |
| 89305 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | Gentiatibetine | C9H11NO2 | 26005-36-7 | NO | metabo_info.php?molid=89305 | |
| 89395 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | Ethyl 2-aminobenzoate | C9H11NO2 | 91-23-0 | NO | metabo_info.php?molid=89395 | |
| 89753 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | methylnicotinate | C9H11NO2 | 55-23-1 | NO | metabo_info.php?molid=89753 | |
| 855 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | Hydroxyphenyl)propanamide | C9H11NO2 | 1693-37-4 | NO | metabo_info.php?molid=855 | |
| 2018 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | 2-amino-4'-hydroxy-Propiophenone | C9H11NO2 | 18259-42-2 | NO | metabo_info.php?molid=2018 | |
| 2183 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | 2-Propylisonicotinic acid | C9H11NO2 | 57663-82-8 | NO | metabo_info.php?molid=2183 | |
| 5937 | 188.07 | [M+Na] ⁺ | 165.079 | 0 | 4-(3-pyridyl)-butanoic acid | C9H11NO2 | | NO | metabo_info.php?molid=5937 | |
| 48047 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Neobanone | C21H18O7 | | NO | metabo_info.php?molid=48047 | |
| 48201 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Hildecarpidin | C21H18O7 | | NO | metabo_info.php?molid=48201 | |
| 49036 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Velloquercetin 4'-methyl ether | C21H18O7 | | NO | metabo_info.php?molid=49036 | |

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|----------|----------------|----|-----------------------------|
| 49943 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Artonin K | C21H18O7 | | NO | metabo_info.php?molid=49943 |
| 49958 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Artoindonesianin T | C21H18O7 | | NO | metabo_info.php?molid=49958 |
| 51130 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Velloquercetin 3-methyl ether | C21H18O7 | | NO | metabo_info.php?molid=51130 |
| 51141 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Sarothranol | C21H18O7 | | NO | metabo_info.php?molid=51141 |
| 51489 | 383.11 | [M+H] ⁺ | 382.105 | 3 | 8-Hydroxygalangin 3-methyl ether 8-angelate | C21H18O7 | | NO | metabo_info.php?molid=51489 |
| 51490 | 383.11 | [M+H] ⁺ | 382.105 | 3 | 5,7,8-Trihydroxy-3-methoxyflavone 3-angelate | C21H18O7 | | NO | metabo_info.php?molid=51490 |
| 51493 | 383.11 | [M+H] ⁺ | 382.105 | 3 | 5,7,8-Trihydroxy-3-methoxyflavone 8-((E)-2-methylbut-2-enoate) | C21H18O7 | | NO | metabo_info.php?molid=51493 |
| 53182 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Lisetin | C21H18O7 | | NO | metabo_info.php?molid=53182 |
| 63798 | 383.11 | [M+H] ⁺ | 382.105 | 3 | 12-Deoxyaklanonic acid | C21H18O7 | | NO | metabo_info.php?molid=63798 |
| 68373 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Austrobailignan 1 | C21H18O7 | 55955 -07-2 | NO | metabo_info.php?molid=68373 |
| 89187 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Mollicellin A | C21H18O7 | 68455 -06-1 | NO | metabo_info.php?molid=89187 |
| 89188 | 383.11 | [M+H] ⁺ | 382.105 | 3 | Mollicellin B | C21H18O7 | 68455 -07-2 | NO | metabo_info.php?molid=89188 |
| 41192 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Elephantopin | C19H20O7 | 55955 -07-2 | NO | metabo_info.php?molid=41192 |
| 47303 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 9,10-Dihydro-8-hydroxy-10-methyl-8H-pyrano[2,3-h]epicatechin | C19H20O7 | | NO | metabo_info.php?molid=47303 |
| 47304 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Pyranochromene | C19H20O7 | | NO | metabo_info.php?molid=47304 |
| 47369 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Elaeocyanidin | C19H20O7 | | NO | metabo_info.php?molid=47369 |
| 48176 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 8-Hydroxy-3,4,9,10-tetramethoxypterocarpan | C19H20O7 | | NO | metabo_info.php?molid=48176 |
| 48299 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Abuquinone A | C19H20O7 | | NO | metabo_info.php?molid=48299 |
| 52167 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 4,3',4'',6''-tetramethoxy-2',5''-dihydroxy- | C19H20O7 | | NO | metabo_info.php?molid=52167 |
| 52168 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 2',4',5',6''-methoxy- | C19H20O7 | | NO | metabo_info.php?molid=52168 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|------------|-----------------|------------|-----------------------------|-----------------------------|
| 52940 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 5,7,3'-Trihydroxy-4',5'-dimethoxy-6,8-di-C-methylflavanone | C19H20O7 | | NO | metabo_info.php?molid=52940 | |
| 53016 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Heteroflavanone A | C19H20O7 | | NO | metabo_info.php?molid=53016 | |
| 53069 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 5-Hydroxy-7,3',4',5'-tetramethoxyflavanone | C19H20O7 | | NO | metabo_info.php?molid=53069 | |
| 53105 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Agestricin C | C19H20O7 | | NO | metabo_info.php?molid=53105 | |
| 53108 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 5-Hydroxy-6,7,3',4'-tetramethoxyflavanone | C19H20O7 | | NO | metabo_info.php?molid=53108 | |
| 53109 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Agecorynin E | C19H20O7 | | NO | metabo_info.php?molid=53109 | |
| 53162 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 5-Hydroxy-6,7,8,4'-tetramethoxyflavanone | C19H20O7 | | NO | metabo_info.php?molid=53162 | |
| 67724 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Goyazensolide | C19H20O7 | 60066 -35-5 | C0946 7 | NO | metabo_info.php?molid=67724 |
| 67818 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Vernodaline | C19H20O7 | 21871 -10-3 | C0957 6 | NO | metabo_info.php?molid=67818 |
| 70442 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | 2,3-Dihydro-2-(4-hydroxyphenyl)-5,6,7,8-tetramethoxy-4H-1-benzopyran-4-one | C19H20O7 | 70460 -59-2 | C1494 0 | NO | metabo_info.php?molid=70442 |
| 90406 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Gibberellin A59 | C19H20O7 | 78333 -20-7 | | NO | metabo_info.php?molid=90406 |
| 95618 | 383.11 | [M+Na] ⁺ | 360.121 | 2 | Edulisin IV | C19H20O7 | 15844 6-38-9 | | NO | metabo_info.php?molid=95618 |
| 909 | 310.13 | [M+H] ⁺ | 309.119 | 0 | Ketotifen | C19H19NOS | 34580 -13-7 | | YES | metabo_info.php?molid=909 |
| 2897 | 310.13 | [M+H] ⁺ | 309.121 | 7 | Tranlycypromine glucuronide | C15H19NO6 | | | NO | metabo_info.php?molid=2897 |
| 2261 | 600.28 | [M+H] ⁺ | 599.274 | 9 | Hydroxydihydroergotamin | C33H37N5O6 | 90650 -44-5 | | NO | metabo_info.php?molid=2261 |
| 40326 | 312.12 | [M+H] ⁺ | 311.113 | 6 | PC(3:1(2E)/0:0)[U] | C11H22NO7P | | | NO | metabo_info.php?molid=40326 |
| 40354 | 312.12 | [M+H] ⁺ | 311.113 | 6 | PC(0:0/3:1(2E)) | C11H22NO7P | | | NO | metabo_info.php?molid=40354 |
| 67600 | 312.12 | [M+H] ⁺ | 311.116 | 0 | Actinodaphnine | C18H17NO4 | 517- 69-1 | C0932 2 | NO | metabo_info.php?molid=67600 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|------------------------------------|-------------|--------------|--------|-----|-----------------------------|
| 67661 | 312.12 | [M+H] ⁺ | 311.116 | 0 | Cularicine | C18H17NO4 | ##### | 00000 | NO | metabo_info.php?molid=67661 |
| 68444 | 312.12 | [M+H] ⁺ | 311.116 | 0 | Acronidine | C18H17NO4 | 518-68-3 | C10629 | NO | metabo_info.php?molid=68444 |
| 86806 | 312.12 | [M+H] ⁺ | 311.116 | 0 | Launobine | C18H17NO4 | 20497-21-6 | | NO | metabo_info.php?molid=86806 |
| 89205 | 312.12 | [M+H] ⁺ | 311.116 | 0 | Norisodomesticine | C18H17NO4 | 80151-84-4 | | NO | metabo_info.php?molid=89205 |
| 89206 | 312.12 | [M+H] ⁺ | 311.116 | 0 | (S)-Nandigerine | C18H17NO4 | 31520-97-5 | | NO | metabo_info.php?molid=89206 |
| 89969 | 312.12 | [M+H] ⁺ | 311.116 | 0 | (S)-Nandigerine | C18H17NO4 | | | NO | metabo_info.php?molid=89969 |
| 91512 | 312.12 | [M+H] ⁺ | 311.116 | 0 | Annocherine B | C18H17NO4 | | | NO | metabo_info.php?molid=91512 |
| 1904 | 312.12 | [M+Na] ⁺ | 289.131 | 6 | Benzoylecgonine | C16H19NO4 | 519-09-5 | C10847 | NO | metabo_info.php?molid=1904 |
| 68462 | 312.12 | [M+Na] ⁺ | 289.131 | 6 | Balfouridine | C16H19NO4 | 484-61-7 | C10647 | NO | metabo_info.php?molid=68462 |
| 69340 | 312.12 | [M+Na] ⁺ | 289.131 | 6 | Zephyranthine | C16H19NO4 | 2030-55-9 | C12170 | NO | metabo_info.php?molid=69340 |
| 69354 | 312.12 | [M+Na] ⁺ | 289.131 | 6 | Pseudolycorine | C16H19NO4 | 29429-03-6 | C12187 | NO | metabo_info.php?molid=69354 |
| 1401 | 312.12 | [M+Na] ⁺ | 289.131 | 6 | 7,8-Dihydro-14-hydroxynormorphine | C16H19NO4 | 58477-92-2 | | NO | metabo_info.php?molid=1401 |
| 1905 | 312.12 | [M+Na] ⁺ | 289.131 | 6 | Norcocaine | C16H19NO4 | 18717-72-1 | | NO | metabo_info.php?molid=1905 |
| 85586 | 312.12 | [M+Na] ⁺ | 289.135 | 3 | Chloropyramine | C16H20CIN3 | 13355-0-35-3 | | NO | metabo_info.php?molid=85586 |
| 45230 | 281.09 | [M+H] ⁺ | 280.085 | 0 | AG-494 | C16H12N2O3 | 18110-87-7 | C16996 | YES | metabo_info.php?molid=45230 |
| 71489 | 281.09 | [M+H] ⁺ | 280.085 | 0 | Methyl nigakinone | C16H12N2O3 | 10432-8-21-4 | | NO | metabo_info.php?molid=71489 |
| 2834 | 281.09 | [M+Na] ⁺ | 258.104 | 3 | Hydroxythiopental | C11H18N2O3S | | | NO | metabo_info.php?molid=2834 |
| 38963 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 13(10Z,13Z,16Z)/22:3(10Z,13Z,16Z)) | C69H122O6 | | | NO | metabo_info.php?molid=38963 |
| 39010 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 13(13Z,16Z)/22:2(13Z,16Z)) | C69H122O6 | | | NO | metabo_info.php?molid=39010 |

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|-------------|-----------------|-----|------------------------------|
| 39014 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 13(22:0/22:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6 | C69H122O6 | | NO | metabo_info.php?molid=39014 |
| 39019 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 13(22:0/22:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6 | C69H122O6 | | NO | metabo_info.php?molid=39019 |
| 39026 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | TG(22:0/22:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso3] | C69H122O6 | | NO | metabo_info.php?molid=39026 |
| 39030 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 2:4(7Z,10Z,13Z,16Z))[iso6] | C69H122O6 | | NO | metabo_info.php?molid=39030 |
| 39057 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | TG(22:2(13Z,16Z)/22:2(13Z,16Z)/22:2(13Z,16Z))[iso3] | C69H122O6 | | NO | metabo_info.php?molid=39057 |
| 99024 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 22:4(7Z,10Z,13Z,16Z))[iso6] | C69H122O6 | | NO | metabo_info.php?molid=99024 |
| 1E+05 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 22:4(7Z,10Z,13Z,16Z,19Z))[iso6] | C69H122O6 | | NO | metabo_info.php?molid=102714 |
| 1E+05 | 1069.9 | [M+Na] ⁺ | 1046.92 | 4 | 6Z)/22:3(10Z,13Z,16Z))[iso6] | C69H122O6 | | NO | metabo_info.php?molid=102717 |
| 82180 | 703.57 | [M+H] ⁺ | 702.556 | 5 | PA(O-18:0/19:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82180 |
| 82196 | 703.57 | [M+H] ⁺ | 702.556 | 5 | PA(O-20:0/17:1(9Z)) | C40H79O7P | | NO | metabo_info.php?molid=82196 |
| 82263 | 703.57 | [M+H] ⁺ | 702.556 | 5 | PA(P-16:0/21:0) | C40H79O7P | | NO | metabo_info.php?molid=82263 |
| 82284 | 703.57 | [M+H] ⁺ | 702.556 | 5 | PA(P-18:0/19:0) | C40H79O7P | | NO | metabo_info.php?molid=82284 |
| 82304 | 703.57 | [M+H] ⁺ | 702.556 | 5 | PA(P-20:0/17:0) | C40H79O7P | | NO | metabo_info.php?molid=82304 |
| 69711 | 460.26 | [M+Na] ⁺ | 437.27 | 8 | ORG 20599 | C25H40CINO3 | 12997 0-98-5 | NO | metabo_info.php?molid=69711 |
| 1799 | 351.22 | [M+H] ⁺ | 350.221 | 9 | Perindopril lactam | C19H30N2O4 | | NO | metabo_info.php?molid=1799 |
| 34827 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 5,8,11-eicosatrienoic acid | C20H34O2 | | NO | metabo_info.php?molid=34827 |
| 34829 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 11,14,17-eicosatrienoic acid | C20H34O2 | | NO | metabo_info.php?molid=34829 |
| 34830 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Podocarpic acid | C20H34O2 | | NO | metabo_info.php?molid=34830 |
| 35043 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 2E,4E,8Z-eicosatrienoic acid | C20H34O2 | | NO | metabo_info.php?molid=35043 |
| 35044 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 5(Z),11(Z),14(Z)-Eicosatrienoic acid | C20H34O2 | 7019-85-4 | YES | metabo_info.php?molid=35044 |
| 35045 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 5(Z),8(Z),11(Z)-Eicosatrienoic Acid | C20H34O2 | 20590-32-3 | YES | metabo_info.php?molid=35045 |
| 35046 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7,10,13-Eicosatrienoic acid | C20H34O2 | | NO | metabo_info.php?molid=35046 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|----------|--------------|------------|-----|-----------------------------|
| 35047 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7,11,14-Eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=35047 |
| 35048 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7Z,10Z,13Z-eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=35048 |
| 35049 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7Z,11Z,14E-eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=35049 |
| 35050 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7Z,11Z,14Z-eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=35050 |
| 35051 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 8Z,12E,14Z-eicosatrienoic acid | C20H34O2 | NA | | NO | metabo_info.php?molid=35051 |
| 259 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Eicosatrienoic acid | C20H34O2 | 27070-56-0 | | NO | metabo_info.php?molid=259 |
| 43737 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | LARIXOL | C20H34O2 | | | NO | metabo_info.php?molid=43737 |
| 45006 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Linolenic Acid ethyl ester | C20H34O2 | 1191-41-9 | | YES | metabo_info.php?molid=45006 |
| 45018 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 9(Z),11(E),13(E)-Octadecatrienoic Acid ethyl ester | C20H34O2 | 42021-86-3 | | YES | metabo_info.php?molid=45018 |
| 34828 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Dihomo-γ-Linolenic Acid | C20H34O2 | 1783-84-2 | C0324 2 | YES | metabo_info.php?molid=34828 |
| 35042 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 11(Z),14(Z),17(Z)-Eicosatrienoic Acid | C20H34O2 | 17046-59-2 | C1652 2 | YES | metabo_info.php?molid=35042 |
| 45143 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Pinolenic Acid ethyl ester | C20H34O2 | 49301-5-74-0 | | YES | metabo_info.php?molid=45143 |
| 45191 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 5(Z),8(Z),14(Z)-Eicosatrienoic Acid | C20H34O2 | 90105-02-5 | | YES | metabo_info.php?molid=45191 |
| 45776 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | (5Z,9E,14Z)-icosa-5,9,14-trienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=45776 |
| 45901 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Oncobic acid | C20H34O2 | | | NO | metabo_info.php?molid=45901 |
| 46394 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 3Z,6Z,9Z-Octadecatrienyl acetate | C20H34O2 | | | NO | metabo_info.php?molid=46394 |
| 46395 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 9Z,12Z,15Z-Octadecatrienyl acetate | C20H34O2 | | | NO | metabo_info.php?molid=46395 |
| 53579 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | plaunotol | C20H34O2 | | C1521 5 | NO | metabo_info.php?molid=53579 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|----------|----------------|------------|----|-----------------------------|
| 67404 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 2,7,11-Cembratrien-4,6-diol | C20H34O2 | 57605 -80-8 | C0907 2 | NO | metabo_info.php?molid=67404 |
| 70385 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 2alpha-Methyl-5alpha-androstane-3alpha,17beta-diol | C20H34O2 | | C1488 2 | NO | metabo_info.php?molid=70385 |
| 70552 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 2alpha-Methyl-5alpha-androstane-3beta,17beta-diol | C20H34O2 | | C1505 8 | NO | metabo_info.php?molid=70552 |
| 70847 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 17alpha-Methyl-5alpha-androstane-3alpha,17beta-diol | C20H34O2 | | C1537 6 | NO | metabo_info.php?molid=70847 |
| 70868 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 17-Methyl-5alpha-androstane-11beta,17beta-diol | C20H34O2 | | C1539 9 | NO | metabo_info.php?molid=70868 |
| 73667 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 18-methyl-8Z,11Z,14Z-nonadecatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=73667 |
| 73853 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 5, 8, 11-icosatrienoic acid; C20:3n-9,12,15 | C20H34O2 | | | NO | metabo_info.php?molid=73853 |
| 73854 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 11, 14, 17-icosatrienoic acid; C20:3n-3,6,9 | C20H34O2 | | | NO | metabo_info.php?molid=73854 |
| 74048 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | C20:3n-12,16,18 | C20H34O2 | | | NO | metabo_info.php?molid=74048 |
| 74049 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Sciadonic acid | C20H34O2 | | | NO | metabo_info.php?molid=74049 |
| 74050 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7, 10, 13-Eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=74050 |
| 74051 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7, 11, 14-Eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=74051 |
| 74052 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7Z,10Z,13Z-eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=74052 |
| 74053 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7Z,11Z,14E-eicosatrienoic acid | C20H34O2 | 81861 -75-8 | | NO | metabo_info.php?molid=74053 |
| 74054 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 7Z,11Z,14Z-eicosatrienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=74054 |
| 74055 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | C20:3n-6,8,12 | C20H34O2 | | | NO | metabo_info.php?molid=74055 |
| 74347 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | eicosa-5Z,8Z,14Z-trienoic acid | C20H34O2 | | | NO | metabo_info.php?molid=74347 |
| 74399 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | 20:3(5Z,13Z,16Z) | C20H34O2 | | | NO | metabo_info.php?molid=74399 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|-----------|-----------------|------------|------------------------------|-----------------------------|
| 91848 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Sagittariol | C20H34O2 | 56497 -92-8 | NO | metabo_info.php?molid=91848 | |
| 96550 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | γ-Linolenic Acid ethyl ester | C20H34O2 | 31450 -14-3 | YES | metabo_info.php?molid=96550 | |
| 97248 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | (E,E)-3,7,11-Trimethyl-2,6,10-dodecatrienyl 3-methylbutanoate | C20H34O2 | | NO | metabo_info.php?molid=97248 | |
| 97250 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | (E,E)-3,7,11-Trimethyl-2,6,10-dodecatrienyl pentanoate | C20H34O2 | | NO | metabo_info.php?molid=97250 | |
| 3E+05 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Isoincensole | C20H34O2 | | YES | metabo_info.php?molid=265077 | |
| 3E+05 | 329.24 | [M+Na] ⁺ | 306.256 | 6 | Incensole | C20H34O2 | | YES | metabo_info.php?molid=265078 | |
| 89303 | 178.08 | [M+H] ⁺ | 177.079 | 9 | Plantagonine | C10H11NO2 | 21857 -97-6 | NO | metabo_info.php?molid=89303 | |
| 92517 | 178.08 | [M+H] ⁺ | 177.079 | 9 | 2-Propenyl 2-aminobenzoate | C10H11NO2 | 7493- 63-2 | NO | metabo_info.php?molid=92517 | |
| 94586 | 178.08 | [M+H] ⁺ | 177.079 | 9 | 5-[2H-Pyrrol-4-(3H)-ylidenemethyl]-2-furanmethanol | C10H11NO2 | | NO | metabo_info.php?molid=94586 | |
| 96729 | 178.08 | [M+H] ⁺ | 177.079 | 9 | MDAI | C10H11NO2 | 15534 4-90-4 | YES | metabo_info.php?molid=96729 | |
| 44702 | 178.08 | [M+Na] ⁺ | 155.095 | 4 | z-AMINO-z-Norbornanecarboxylic acid | C8H13NO2 | 20448 -79-7 | NO | metabo_info.php?molid=44702 | |
| 43570 | 178.08 | [M+Na] ⁺ | 155.095 | 4 | ARECOLINE | C8H13NO2 | 300- 08-3 | C1012 9 | YES | metabo_info.php?molid=43570 |
| 43998 | 178.08 | [M+Na] ⁺ | 155.095 | 4 | SCOPOLINE | C8H13NO2 | 487- 27-4 | C1086 6 | YES | metabo_info.php?molid=43998 |
| 64442 | 178.08 | [M+Na] ⁺ | 155.095 | 4 | Retronecine | C8H13NO2 | 480- 85-3 | C0617 7 | NO | metabo_info.php?molid=64442 |
| 43431 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | Eicosa-5Z,8Z-dienoic acid (20:2, n-12) | C20H36O2 | | YES | metabo_info.php?molid=43431 | |
| 35037 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 11Z,13Z-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=35037 | |
| 35038 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 5,11-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=35038 | |
| 35039 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 7,13-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=35039 | |

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|--------------------------------------|----------|-------------|-----|-----------------------------|
| 35040 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 8,11-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=35040 |
| 35041 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 8,11-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=35041 |
| 45005 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | Linoleic Acid ethyl ester | C20H36O2 | 544-35-4 | YES | metabo_info.php?molid=45005 |
| 24088 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 11,14-trans-Eicosadienoic acid | C20H36O2 | | YES | metabo_info.php?molid=24088 |
| 46383 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 3E,13E-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46383 |
| 46384 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 2E,13Z-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46384 |
| 46385 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 3E,13Z-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46385 |
| 46389 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 2Z,13E-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46389 |
| 46390 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 3Z,13E-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46390 |
| 46391 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 2Z,13Z-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46391 |
| 46392 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 3Z,13Z-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46392 |
| 46393 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 9Z,12Z-Octadecadienyl acetate | C20H36O2 | | NO | metabo_info.php?molid=46393 |
| 53595 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | sclareol | C20H36O2 | 2091-39-6 | YES | metabo_info.php?molid=53595 |
| 62964 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 11(Z),14(Z)-Eicosadienoic Acid | C20H36O2 | C16525 | YES | metabo_info.php?molid=62964 |
| 64791 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 8(Z),14(Z)-Eicosadienoic Acid | C20H36O2 | 135498-07-6 | YES | metabo_info.php?molid=64791 |
| 73840 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 11, 14-icosadienoic acid; C20:2n-6,9 | C20H36O2 | | NO | metabo_info.php?molid=73840 |
| 74043 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | C20:2n-5,9 | C20H36O2 | | NO | metabo_info.php?molid=74043 |
| 74044 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | C20:2n-9,15 | C20H36O2 | | NO | metabo_info.php?molid=74044 |
| 74045 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | C20:2n-7,13 | C20H36O2 | | NO | metabo_info.php?molid=74045 |
| 74046 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 8,11-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=74046 |
| 74047 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 8,11-Eicosadienoic acid | C20H36O2 | | NO | metabo_info.php?molid=74047 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|------------|----------|------------|-----|-----------------------------|
| 74395 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 20:2(7Z,14Z) | C20H36O2 | | | NO | metabo_info.php?molid=74395 |
| 74396 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 20:2(5Z,13Z) | C20H36O2 | | | NO | metabo_info.php?molid=74396 |
| 74401 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 20:2(5Z,11Z) | C20H36O2 | | | NO | metabo_info.php?molid=74401 |
| 74403 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 20:2(5Z,15Z) | C20H36O2 | | | NO | metabo_info.php?molid=74403 |
| 74433 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 20:2(6,11) | C20H36O2 | | | NO | metabo_info.php?molid=74433 |
| 74435 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 20:2(5Z,9Z) | C20H36O2 | | | NO | metabo_info.php?molid=74435 |
| 96465 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | 5(Z),14(Z)-Eicosadienoic Acid | C20H36O2 | 12205 | | YES | metabo_info.php?molid=96465 |
| | | | | | | | 5-58-7 | | | |
| 97305 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | (E)-3,7-Dimethyl-2,6-octadienyl decanoate | C20H36O2 | | | NO | metabo_info.php?molid=97305 |
| 97317 | 331.26 | [M+Na] ⁺ | 308.272 | 6 | (Z)-3,7-Dimethyl-2,6-octadienyl decanoate | C20H36O2 | | | NO | metabo_info.php?molid=97317 |
| 72401 | 327.22 | [M+Na] ⁺ | 304.238 | 6 | Sodium oleate | C18H33NaO2 | 143-19-1 | C1860 1 | NO | metabo_info.php?molid=72401 |
| 72401 | 305.24 | [M+H] ⁺ | 304.238 | 6 | Sodium oleate | C18H33NaO2 | 143-19-1 | C1860 1 | NO | metabo_info.php?molid=72401 |
| 34748 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 2Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34748 |
| 34749 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-2-oleic acid | C18H34O2 | | | NO | metabo_info.php?molid=34749 |
| 34750 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 3-octadecylenic acid | C18H34O2 | | | NO | metabo_info.php?molid=34750 |
| 34751 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 4-octadecylenic acid | C18H34O2 | | | NO | metabo_info.php?molid=34751 |
| 34752 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 5-octadecylenic acid | C18H34O2 | | | NO | metabo_info.php?molid=34752 |
| 34753 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Petroselaidic acid | C18H34O2 | | | NO | metabo_info.php?molid=34753 |
| 34754 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 7Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34754 |
| 34755 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 7E-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34755 |
| 34756 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | cis-8-oleic acid | C18H34O2 | | | NO | metabo_info.php?molid=34756 |
| 34757 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-8-elaidic acid | C18H34O2 | | | NO | metabo_info.php?molid=34757 |
| 34758 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | cis-10-oleic acid | C18H34O2 | | | NO | metabo_info.php?molid=34758 |
| 34759 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 10E-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34759 |
| 34760 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | cis-12-oleic acid | C18H34O2 | | | NO | metabo_info.php?molid=34760 |
| 34761 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-12-elaidic acid | C18H34O2 | | | NO | metabo_info.php?molid=34761 |
| 34762 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 15E-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34762 |
| 34763 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 16E-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34763 |
| 34954 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 13Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34954 |
| 34955 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 15Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34955 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--------------------------------|----------|------------|--------|-----|-----------------------------|
| 34956 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 16Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34956 |
| 34957 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 17-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34957 |
| 34958 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 3Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34958 |
| 34959 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 4Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34959 |
| 34960 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 5Z-octadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=34960 |
| 45010 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Palmitoleic Acid ethyl ester | C18H34O2 | 56219-10-4 | | YES | metabo_info.php?molid=45010 |
| 190 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Oleic Acid | C18H34O2 | 112-80-1 | C00712 | YES | metabo_info.php?molid=190 |
| 3406 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Elaidic Acid | C18H34O2 | 112-79-8 | C01712 | YES | metabo_info.php?molid=3406 |
| 3407 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Vaccenic acid | C18H34O2 | 693-72-1 | C08367 | YES | metabo_info.php?molid=3407 |
| 3552 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | cis-vaccenic acid | C18H34O2 | 506-17-2 | C08367 | YES | metabo_info.php?molid=3552 |
| 3553 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Petroselinic acid | C18H34O2 | 593-39-5 | C08363 | YES | metabo_info.php?molid=3553 |
| 45890 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Cycloheptylundecanoic acid | C18H34O2 | | C12103 | NO | metabo_info.php?molid=45890 |
| 46342 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 11E-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46342 |
| 46343 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 5E-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46343 |
| 46344 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 6E-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46344 |
| 46345 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 8E-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46345 |
| 46346 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 9E-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46346 |
| 46360 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 10Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46360 |
| 46361 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 11Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46361 |
| 46362 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 12Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46362 |
| 46364 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 3Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46364 |
| 46365 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 5Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46365 |
| 46366 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 7Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46366 |
| 46367 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 9Z-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46367 |
| 46377 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 7-Hexadecenyl acetate | C18H34O2 | | | NO | metabo_info.php?molid=46377 |
| 73652 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 2-methyl-16-heptadecenoic acid | C18H34O2 | | | NO | metabo_info.php?molid=73652 |

| | | | | | | | | |
|-------|--------|---------------------|---------|---|---|-------------|----|------------------------------|
| 73782 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 17:1(4)(16Me) | C18H34O2 | NO | metabo_info.php?molid=73782 |
| 73783 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 17:1(6)(9Me) | C18H34O2 | NO | metabo_info.php?molid=73783 |
| 73784 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 17:1(12)(7Me) | C18H34O2 | NO | metabo_info.php?molid=73784 |
| 73804 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | cis-2-octadecenoic acid; C18:1n-16 | C18H34O2 | NO | metabo_info.php?molid=73804 |
| 73805 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | cis-7-octadecenoic acid; C18:1n-11 | C18H34O2 | NO | metabo_info.php?molid=73805 |
| 73806 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-7-octadecenoic acid; C18:1n-11 | C18H34O2 | NO | metabo_info.php?molid=73806 |
| 73807 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-10-octadecenoic acid; C18:1n-8 | C18H34O2 | NO | metabo_info.php?molid=73807 |
| 73808 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-15-octadecenoic acid; C18:1n-3 | C18H34O2 | NO | metabo_info.php?molid=73808 |
| 73809 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | trans-16-octadecenoic acid; C18:1n-2 | C18H34O2 | NO | metabo_info.php?molid=73809 |
| 73963 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-5 | C18H34O2 | NO | metabo_info.php?molid=73963 |
| 73964 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-3 | C18H34O2 | NO | metabo_info.php?molid=73964 |
| 73965 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-2 | C18H34O2 | NO | metabo_info.php?molid=73965 |
| 73966 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-1 | C18H34O2 | NO | metabo_info.php?molid=73966 |
| 73967 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-15 | C18H34O2 | NO | metabo_info.php?molid=73967 |
| 73968 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-14 | C18H34O2 | NO | metabo_info.php?molid=73968 |
| 73969 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | C18:1n-13 | C18H34O2 | NO | metabo_info.php?molid=73969 |
| 74416 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 18:1(13E) | C18H34O2 | NO | metabo_info.php?molid=74416 |
| 74417 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 18:1(14E) | C18H34O2 | NO | metabo_info.php?molid=74417 |
| 74418 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 18:1(14Z) | C18H34O2 | NO | metabo_info.php?molid=74418 |
| 74431 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 17:1(4)(15Me) | C18H34O2 | NO | metabo_info.php?molid=74431 |
| 97217 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | ethyl 7Z-hexadecenoate | C18H34O2 | NO | metabo_info.php?molid=97217 |
| 97218 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | formyl 14-methyl-8E- hexadecenoate | C18H34O2 | NO | metabo_info.php?molid=97218 |
| 97220 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | formyl 14-methyl-8Z- hexadecenoate | C18H34O2 | NO | metabo_info.php?molid=97220 |
| 97323 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | Ethyl 9-hexadecenoate | C18H34O2 | NO | metabo_info.php?molid=97323 |
| 97409 | 305.24 | [M+Na] ⁺ | 282.256 | 6 | 18-Octadecanolide | C18H34O2 | NO | metabo_info.php?molid=97409 |
| 1E+05 | 782.56 | [M+H] ⁺ | 781.547 | 6 | PI-Cer(d18:0/16:0) | C40H80NO11P | NO | metabo_info.php?molid=103135 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---|-------------|-------------|--------|-----|------------------------------|
| 1E+05 | 782.56 | [M+H] ⁺ | 781.547 | 5 | PI-Cer(d18:0/16:0) | C40H80NO11P | | | NO | metabo_info.php?molid=103135 |
| 1E+05 | 782.56 | [M+H] ⁺ | 781.547 | 5 | PI-Cer(d18:0/16:0) | C40H80NO11P | | | NO | metabo_info.php?molid=103135 |
| 44825 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | α-CEHC | C16H22O4 | NA | | YES | metabo_info.php?molid=44825 |
| 53414 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | Emmotin A | C16H22O4 | | | NO | metabo_info.php?molid=53414 |
| 53844 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | tocopheronic acid | C16H22O4 | | | NO | metabo_info.php?molid=53844 |
| 44802 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | Phthalic acid Mono-2-ethylhexyl Ester | C16H22O4 | 4376-20-9 | C03343 | NO | metabo_info.php?molid=44802 |
| 58055 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | Alpha-CEHC | C16H22O4 | 4072-32-6 | | NO | metabo_info.php?molid=58055 |
| 69881 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | Dibutyl phthalate | C16H22O4 | 04-14-04 | C1421 | NO | metabo_info.php?molid=69881 |
| 70692 | 301.14 | [M+Na] ⁺ | 278.152 | 3 | Diisobutyl phthalate | C16H22O4 | 04-20-05 | C1320 | NO | metabo_info.php?molid=70692 |
| 2764 | 424.16 | [M+Na] ⁺ | 401.169 | 7 | Terbutaline-1-glucuronide | C18H27NO9 | | | NO | metabo_info.php?molid=2764 |
| 43893 | 424.16 | [M+Na] ⁺ | 401.175 | 7 | MOXIFLOXACIN | C21H24FN3O4 | 354812-41-2 | | YES | metabo_info.php?molid=43893 |
| 66708 | 424.16 | [M+Na] ⁺ | 401.175 | 7 | Moxifloxacin | C21H24FN3O4 | 151096-09-2 | C07663 | NO | metabo_info.php?molid=66708 |
| 53843 | 319.15 | [M+Na] ⁺ | 296.162 | 8 | alpha-tocopheronic acid | C16H24O5 | | | NO | metabo_info.php?molid=53843 |
| 67878 | 319.15 | [M+Na] ⁺ | 296.162 | 8 | Graphinone | C16H24O5 | 19683-98-8 | C09674 | NO | metabo_info.php?molid=67878 |
| 93953 | 319.15 | [M+Na] ⁺ | 296.162 | 8 | Methyl dihydrophaseate | C16H24O5 | | | NO | metabo_info.php?molid=93953 |
| 95934 | 319.15 | [M+Na] ⁺ | 296.162 | 8 | 3,8-Dihydroxy-6-methoxy-7(11)-eremophilene-12,8-olide | C16H24O5 | | | NO | metabo_info.php?molid=95934 |
| 2295 | 319.15 | [M+Na] ⁺ | 296.162 | 8 | Lactone of PGF-MUM | C16H24O5 | | | NO | metabo_info.php?molid=2295 |
| 39317 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(11E)) | C42H82NO8P | | | NO | metabo_info.php?molid=39317 |
| 39319 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(11Z))[U] | C42H82NO8P | | | NO | metabo_info.php?molid=39319 |
| 39320 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(6E)) | C42H82NO8P | | | NO | metabo_info.php?molid=39320 |
| 39321 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(6Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=39321 |
| 39322 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(6Z))[U] | C42H82NO8P | | | NO | metabo_info.php?molid=39322 |
| 39323 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9E)) | C42H82NO8P | | | NO | metabo_info.php?molid=39323 |
| 39324 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9E))[U] | C42H82NO8P | | | NO | metabo_info.php?molid=39324 |
| 39325 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9Z))[S] | C42H82NO8P | | C1301 | NO | metabo_info.php?molid=39325 |
| 39326 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9Z))[U] | C42H82NO8P | | | NO | metabo_info.php?molid=39326 |
| 39420 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:1(7Z)/18:0)[U] | C42H82NO8P | | | NO | metabo_info.php?molid=39420 |

| | | | | | | | | |
|-------|--------|--------------------|---------|---|----------------------|------------|----|-----------------------------|
| 39427 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:1(9Z)/18:0)[U] | C42H82NO8P | NO | metabo_info.php?molid=39427 |
| 39615 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(9E)/16:0)[U] | C42H82NO8P | NO | metabo_info.php?molid=39615 |
| 39626 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(9Z)/16:0)[U] | C42H82NO8P | NO | metabo_info.php?molid=39626 |
| 59329 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(14:0/20:1(11Z)) | C42H82NO8P | NO | metabo_info.php?molid=59329 |
| 59361 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(14:1(9Z)/20:0) | C42H82NO8P | NO | metabo_info.php?molid=59361 |
| 59420 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(11Z)) | C42H82NO8P | NO | metabo_info.php?molid=59420 |
| 59421 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=59421 |
| 59451 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:1(9Z)/18:0) | C42H82NO8P | NO | metabo_info.php?molid=59451 |
| 59483 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:0/16:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=59483 |
| 59514 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(11Z)/16:0) | C42H82NO8P | NO | metabo_info.php?molid=59514 |
| 59547 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(9Z)/16:0) | C42H82NO8P | NO | metabo_info.php?molid=59547 |
| 59709 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(20:0/14:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=59709 |
| 59741 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(20:1(11Z)/14:0) | C42H82NO8P | NO | metabo_info.php?molid=59741 |
| 60351 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(15:0/22:1(13Z)) | C42H82NO8P | NO | metabo_info.php?molid=60351 |
| 60905 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(22:1(13Z)/15:0) | C42H82NO8P | NO | metabo_info.php?molid=60905 |
| 75615 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(12:0/22:1(11Z)) | C42H82NO8P | NO | metabo_info.php?molid=75615 |
| 75699 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(15:0/19:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=75699 |
| 75728 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(15:1(9Z)/19:0) | C42H82NO8P | NO | metabo_info.php?molid=75728 |
| 75783 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(17:0/17:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=75783 |
| 75809 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(17:1(9Z)/17:0) | C42H82NO8P | NO | metabo_info.php?molid=75809 |
| 76012 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(19:0/15:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=76012 |
| 76040 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(19:1(9Z)/15:0) | C42H82NO8P | NO | metabo_info.php?molid=76040 |
| 76284 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(22:1(11Z)/12:0) | C42H82NO8P | NO | metabo_info.php?molid=76284 |
| 76705 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(15:0/22:1(11Z)) | C42H82NO8P | NO | metabo_info.php?molid=76705 |
| 76735 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(15:1(9Z)/22:0) | C42H82NO8P | NO | metabo_info.php?molid=76735 |
| 76769 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(16:1(9Z)/21:0) | C42H82NO8P | NO | metabo_info.php?molid=76769 |
| 76787 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(17:0/20:1(11Z)) | C42H82NO8P | NO | metabo_info.php?molid=76787 |
| 76814 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(17:1(9Z)/20:0) | C42H82NO8P | NO | metabo_info.php?molid=76814 |
| 76866 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(18:0/19:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=76866 |
| 76880 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(18:1(9Z)/19:0) | C42H82NO8P | NO | metabo_info.php?molid=76880 |
| 77010 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(19:0/18:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=77010 |
| 77039 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(19:1(9Z)/18:0) | C42H82NO8P | NO | metabo_info.php?molid=77039 |
| 77064 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(20:0/17:1(9Z)) | C42H82NO8P | NO | metabo_info.php?molid=77064 |
| 77084 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(20:1(11Z)/17:0) | C42H82NO8P | NO | metabo_info.php?molid=77084 |

39427
 39615
 39626
 59329
 59361
 59420
 59421
 59451
 59483
 59514
 59547
 59709
 59741
 60351
 60905
 75615
 75699
 75728
 75783
 75809
 76012
 76040
 76284
 76705
 76735
 76769
 76787
 76814
 76866
 76880
 77010
 77039
 77064
 77084

| | | | | | | | | | |
|-------|--------|---------------------|---------|---|-----------------------|-------------|----------------|------------|--------------------------------|
| 77230 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(21:0/16:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=77230 |
| 77253 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(22:0/15:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=77253 |
| 77279 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(22:1(11Z)/15:0) | C42H82NO8P | | NO | metabo_info.php?molid=77279 |
| 71650 | 512.21 | [M+Na] ⁺ | 489.214 | 6 | OA-6129 E | C21H35N3O8S | 85414 -26-2 | C1737 6 | NO metabo_info.php?molid=71650 |
| 39317 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(11E)) | C42H82NO8P | | NO | metabo_info.php?molid=39317 |
| 39319 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(11Z))[U] | C42H82NO8P | | NO | metabo_info.php?molid=39319 |
| 39320 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(6E)) | C42H82NO8P | | NO | metabo_info.php?molid=39320 |
| 39321 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(6Z)) | C42H82NO8P | | NO | metabo_info.php?molid=39321 |
| 39322 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(6Z))[U] | C42H82NO8P | | NO | metabo_info.php?molid=39322 |
| 39323 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9E)) | C42H82NO8P | | NO | metabo_info.php?molid=39323 |
| 39324 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9E))[U] | C42H82NO8P | | NO | metabo_info.php?molid=39324 |
| 39325 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9Z))[S] | C42H82NO8P | | NO | metabo_info.php?molid=39325 |
| 39326 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9Z))[U] | C42H82NO8P | | NO | metabo_info.php?molid=39326 |
| 39420 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:1(7Z)/18:0)[U] | C42H82NO8P | | NO | metabo_info.php?molid=39420 |
| 39427 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:1(9Z)/18:0)[U] | C42H82NO8P | | NO | metabo_info.php?molid=39427 |
| 39615 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(9E)/16:0)[U] | C42H82NO8P | | NO | metabo_info.php?molid=39615 |
| 39626 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(9Z)/16:0)[U] | C42H82NO8P | | NO | metabo_info.php?molid=39626 |
| 59329 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(14:0/20:1(11Z)) | C42H82NO8P | | NO | metabo_info.php?molid=59329 |
| 59361 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(14:1(9Z)/20:0) | C42H82NO8P | | NO | metabo_info.php?molid=59361 |
| 59420 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(11Z)) | C42H82NO8P | | NO | metabo_info.php?molid=59420 |
| 59421 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:0/18:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=59421 |
| 59451 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(16:1(9Z)/18:0) | C42H82NO8P | | NO | metabo_info.php?molid=59451 |
| 59483 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:0/16:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=59483 |
| 59514 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(11Z)/16:0) | C42H82NO8P | | NO | metabo_info.php?molid=59514 |
| 59547 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(18:1(9Z)/16:0) | C42H82NO8P | | NO | metabo_info.php?molid=59547 |
| 59709 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(20:0/14:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=59709 |
| 59741 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(20:1(11Z)/14:0) | C42H82NO8P | | NO | metabo_info.php?molid=59741 |
| 60351 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(15:0/22:1(13Z)) | C42H82NO8P | | NO | metabo_info.php?molid=60351 |
| 60905 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(22:1(13Z)/15:0) | C42H82NO8P | | NO | metabo_info.php?molid=60905 |
| 75615 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(12:0/22:1(11Z)) | C42H82NO8P | | NO | metabo_info.php?molid=75615 |
| 75699 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(15:0/19:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=75699 |
| 75728 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(15:1(9Z)/19:0) | C42H82NO8P | | NO | metabo_info.php?molid=75728 |
| 75783 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(17:0/17:1(9Z)) | C42H82NO8P | | NO | metabo_info.php?molid=75783 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|---------------------------------------|------------|------------|--------|-----|-----------------------------|
| 75809 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(17:1(9Z)/17:0) | C42H82NO8P | | | NO | metabo_info.php?molid=75809 |
| 76012 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(19:0/15:1(9Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=76012 |
| 76040 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(19:1(9Z)/15:0) | C42H82NO8P | | | NO | metabo_info.php?molid=76040 |
| 76284 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PC(22:1(11Z)/12:0) | C42H82NO8P | | | NO | metabo_info.php?molid=76284 |
| 76705 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(15:0/22:1(11Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=76705 |
| 76735 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(15:1(9Z)/22:0) | C42H82NO8P | | | NO | metabo_info.php?molid=76735 |
| 76769 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(16:1(9Z)/21:0) | C42H82NO8P | | | NO | metabo_info.php?molid=76769 |
| 76787 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(17:0/20:1(11Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=76787 |
| 76814 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(17:1(9Z)/20:0) | C42H82NO8P | | | NO | metabo_info.php?molid=76814 |
| 76866 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(18:0/19:1(9Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=76866 |
| 76880 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(18:1(9Z)/19:0) | C42H82NO8P | | | NO | metabo_info.php?molid=76880 |
| 77010 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(19:0/18:1(9Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=77010 |
| 77039 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(19:1(9Z)/18:0) | C42H82NO8P | | | NO | metabo_info.php?molid=77039 |
| 77064 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(20:0/17:1(9Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=77064 |
| 77084 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(20:1(11Z)/17:0) | C42H82NO8P | | | NO | metabo_info.php?molid=77084 |
| 77230 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(21:0/16:1(9Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=77230 |
| 77253 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(22:0/15:1(9Z)) | C42H82NO8P | | | NO | metabo_info.php?molid=77253 |
| 77279 | 760.58 | [M+H] ⁺ | 759.578 | 9 | PE(22:1(11Z)/15:0) | C42H82NO8P | | | NO | metabo_info.php?molid=77279 |
| 44825 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | α-CEHC | C16H22O4 | NA | | YES | metabo_info.php?molid=44825 |
| 53414 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | Emmotin A | C16H22O4 | | | NO | metabo_info.php?molid=53414 |
| 53844 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | Phthalic acid Mono-2-ethylhexyl Ester | C16H22O4 | | | NO | metabo_info.php?molid=53844 |
| 44802 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | Phthalic acid Mono-2-ethylhexyl Ester | C16H22O4 | 4376-20-9 | C03343 | NO | metabo_info.php?molid=44802 |
| 58055 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | Alpha-CEHC | C16H22O4 | 4072-32-6 | | NO | metabo_info.php?molid=58055 |
| 69881 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | Dibutyl phthalate | C16H22O4 | 04-71-4 | C1421 | NO | metabo_info.php?molid=69881 |
| 70692 | 301.14 | [M+Na] ⁺ | 278.152 | 2 | Diisobutyl phthalate | C16H22O4 | 04-70-5 | C1420 | NO | metabo_info.php?molid=70692 |
| 65100 | 517.16 | [M+Na] ⁺ | 494.169 | 8 | TyrMe-TyrMe-OH | C26H26N2O8 | | | YES | metabo_info.php?molid=65100 |
| 67647 | 342.14 | [M+H] ⁺ | 341.126 | 4 | Cassythine | C19H19NO5 | 4030-51-7 | C09380 | NO | metabo_info.php?molid=67647 |
| 86190 | 342.14 | [M+H] ⁺ | 341.126 | 4 | Gravacridonediol | C19H19NO5 | 37551-75-0 | | NO | metabo_info.php?molid=86190 |
| 89210 | 342.14 | [M+H] ⁺ | 341.126 | 4 | 4-Hydroxynornantenine | C19H19NO5 | 69128-21-8 | | NO | metabo_info.php?molid=89210 |

| | | | | | | | | | | |
|-------|--------|---------------------|---------|---|--|-------------|-----------------|------------|-----|-----------------------------|
| 72282 | 342.14 | [M+Na] ⁺ | 319.145 | 2 | Metconazole | C17H22ClN3O | 12511 6-23-6 | C1847 6 | YES | metabo_info.php?molid=72282 |
| 44812 | 342.14 | [M+Na] ⁺ | 319.145 | 1 | 4-hydroxy Nonenal Mercapturic Acid | C14H25NO5S | 14676 4-24-1 | | YES | metabo_info.php?molid=44812 |
| 65132 | 341.13 | [M+H] ⁺ | 340.127 | 9 | Thr-Val-OH | C15H20N2O7 | | | YES | metabo_info.php?molid=65132 |
| 65106 | 341.13 | [M+H] ⁺ | 340.127 | 9 | Leu-Thr-OH | C15H20N2O7 | | | YES | metabo_info.php?molid=65106 |
| 65114 | 341.13 | [M+H] ⁺ | 340.127 | 9 | Ile-Thr-OH | C15H20N2O7 | | | YES | metabo_info.php?molid=65114 |
| 65223 | 341.13 | [M+H] ⁺ | 340.127 | 9 | Ser-Leu-OH | C15H20N2O7 | | | YES | metabo_info.php?molid=65223 |
| 65243 | 341.13 | [M+H] ⁺ | 340.127 | 9 | Ser-Ile-OH | C15H20N2O7 | | | YES | metabo_info.php?molid=65243 |
| 72282 | 320.15 | [M+H] ⁺ | 319.145 | 3 | Metconazole | C17H22ClN3O | 12511 6-23-6 | C1847 6 | YES | metabo_info.php?molid=72282 |
| 44812 | 320.15 | [M+H] ⁺ | 319.145 | 3 | 4-hydroxy Nonenal Mercapturic Acid | C14H25NO5S | 14676 4-24-1 | | YES | metabo_info.php?molid=44812 |
| 53843 | 319.15 | [M+Na] ⁺ | 296.162 | 4 | alpha-tocopheronic acid | C16H24O5 | | | NO | metabo_info.php?molid=53843 |
| 67878 | 319.15 | [M+Na] ⁺ | 296.162 | 4 | Graphinone | C16H24O5 | 19683 -98-8 | C0967 4 | NO | metabo_info.php?molid=67878 |
| 93953 | 319.15 | [M+Na] ⁺ | 296.162 | 4 | Methyl dihydrophaseate 3,8-Dihydroxy-6-methoxy- 7(11)-eremophilen-12,8- olide | C16H24O5 | | | NO | metabo_info.php?molid=93953 |
| 95934 | 319.15 | [M+Na] ⁺ | 296.162 | 4 | Lactone of PGF-MUM | C16H24O5 | | | NO | metabo_info.php?molid=95934 |
| 2295 | 319.15 | [M+Na] ⁺ | 296.162 | 4 | Lactone of PGF-MUM | C16H24O5 | | | NO | metabo_info.php?molid=2295 |
| 67637 | 659.28 | [M+Na] ⁺ | 636.284 | 5 | Calafatimine | C38H40N2O7 | 77793 -42-1 | C0936 9 | NO | metabo_info.php?molid=67637 |