

| Neutral mass | RT         | Name                                                                                                           | Formula  | MSI level | Kegg   | HMDB        | LipidMaps | Metlin | InChIKey                     | SMILES                             |
|--------------|------------|----------------------------------------------------------------------------------------------------------------|----------|-----------|--------|-------------|-----------|--------|------------------------------|------------------------------------|
| 90,0317      | 0,7388246  | Lactic acid                                                                                                    | C3H6O3   | 3         | C01432 | HMDB0144295 |           | 116    | JVTAAEKCZFNVCJ-UHFFFAOYSA-N  | CC(O)C(O)=O                        |
| 99,0686      | 1,4187802  | Piperidinone/Hydroxymethylbutanenitrile/Methylpyrrolidinone/Methylpyrrolidone                                  | C5H9NO   | 3         |        | HMDB0011749 |           | 62467  | XUWHAWMETYGRKB-UHFFFAOYSA-N  | O=C1CCCCN1                         |
| 103,0999     | 0,6845519  | Aminomethylbutanol<br>Valinol                                                                                  | C5H13NO  | 3         |        |             |           | 44703  | NWYYWIIJOWOLJNR-YFKPBYRVSA-N | CC(C)[C@H](CO)N                    |
| 103,0999     | 7,3616896  | Valinol                                                                                                        | C5H13NO  | 3         |        |             |           |        | NWYYWIIJOWOLJNR-RXMQYKEDSA-N | CC(C)[C@@H](CO)N                   |
| 103,0999     | 7,9646416  | Aminomethylbutanol/Valinol                                                                                     | C5H13NO  | 3         |        |             |           | 44703  | NWYYWIIJOWOLJNR-YFKPBYRVSA-N | CC(C)[C@H](CO)N                    |
| 103,0999     | 8,578954   | Valinol                                                                                                        | C5H13NO  | 3         |        |             |           |        | NWYYWIIJOWOLJNR-RXMQYKEDSA-N | CC(C)[C@@H](CO)N                   |
| 106,0417     | 1,2566688  | Benzaldehyde                                                                                                   | C7H6O    | 3         | C00193 | HMDB0006115 |           | 58358  | HUMNYLRZRPJDN-UHFFFAOYSA-N   | O=CC1=CC=CC=C1                     |
| 106,0422     | 6,5703073  | Benzaldehyde                                                                                                   | C7H6O    | 3         | C00193 | HMDB0006115 |           | 58358  | HUMNYLRZRPJDN-UHFFFAOYSA-N   | O=CC1=CC=CC=C1                     |
| 106,0638     | 5,9066973  | Trihydroxybutane/Diethylene glycol                                                                             | C4H10O3  | 3         |        | HMDB0061944 |           |        | GTTSNKDQDACYLV-UHFFFAOYSA-N  | CCCC(O)(O)O                        |
| 113,0585     | 0,7145658  | Creatinine                                                                                                     | C4H7N3O  | 3         | C00791 | HMDB0000562 |           | 8      | DDRJAANPRJIHGI-UHFFFAOYSA-N  | CN1CC(=O)NC1=N                     |
| 113,0839     | 3,0229337  | DMPO                                                                                                           | C6H11NO  | 3         |        |             |           | 64638  |                              |                                    |
| 117,0791     | 0,73305136 | Valine/Aminomethylbutyric acid/aminopentanoic acid/Norvaline/Amyl Nitrite/Urea                                 | C5H11NO2 | 3         | C06417 |             |           |        | KZSNJWFQEVHDMF-SCSAIBSYSA-N  | CC(C)[C@@H](N)C(=O)O               |
| 129,0425     | 0,7946795  | Pyrrolinehydroxycarboxylic Acid/Acryloylglycine                                                                | C5H7NO3  | 3         | C04281 | HMDB0062585 |           |        | WFOFKRKDDKGRIK-DMTCNVIQSA-N  | [H][C@@]1(O)C[C@]([H])(N=C1)C(O)=O |
| 129,0583     | 1,979581   | Methylene-indolenine                                                                                           | C9H7N    | 3         |        | HMDB0011664 |           | 62407  | BCNUXXXHEIUHJB-UHFFFAOYSA-N  | C=C1C=NC2=CC=CC=C12                |
| 129,0789     | 0,63152486 | Acetylaminobutanol/Pipecolic acid/piperidine carboxylic acid/homoproline                                       | C6H11NO2 | 3         | C05936 | HMDB0004226 |           | 58230  | DDSLGZOYEPKPSJ-UHFFFAOYSA-N  | CC(=O)NCCCC=O                      |
| 129,1514     | 5,4255986  | Octylamine/Monoctylamine                                                                                       | C8H19N   | 3         | C01740 |             |           | 65641  | IOQPZZOEVPZRBK-UHFFFAOYSA-N  | CCCCCCCCN                          |
| 131,0947     | 0,99943894 | Diethylglycine/amino-hexanoic acid/Norleucine/Aminocaproic acid/Methylvaline/Leucine/Aminomethylpentanoic acid | C6H13NO2 | 3         | C16647 |             |           | 71280  | SGDXUYKISDCAZ-UHFFFAOYSA-N   | CCN(CC)CC(=O)O                     |

|          |            |                                                                                                                                                             |           |   |        |             |                             |                                 |                                |                |
|----------|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|---|--------|-------------|-----------------------------|---------------------------------|--------------------------------|----------------|
| 134,0732 | 6,5130134  | Isochavicol/ t-Anol/Propenylphenol/Hydroxypropenylbenzene/Phenylacetone/Methylacetophenone/Indanol                                                          | C9H10O    | 3 | C20464 |             | UMFCIIBZHQXRCJ-NSCUHMNNSA-N | C/C=C/c1ccc(O)cc1               |                                |                |
| 135,0681 | 0,8531394  | Phenylacetaldehyde oxime/Phenylacetaldoxime/Phenacylamine/Phenylacetamide                                                                                   | C8H9NO    | 3 | C16075 | 63615       | CXISHLWVCSLKOJ-CLFYSBASSA-N | O/N=C\Cc1ccccc1                 |                                |                |
| 140,0451 | 0,6096473  | Trifluoromethyl-bismethyl ketone                                                                                                                            | C5H7F3O   | 3 |        | HMDB0061928 | NLCCAFQWEKMQLM-UHFFFAOYSA-N | CC(C)C(=O)C(F)(F)F              |                                |                |
| 145,0527 | 1,9850607  | Indolecarboxaldehyde                                                                                                                                        | C9H7NO    | 3 | C08493 | HMDB0029737 | 67018                       | OLNJUISKUQQNIM-UHFFFAOYSA-N     | O=CC1=CNC2=C1C=CC=C2           |                |
| 146,1054 | 0,6173267  | Lysine/Diaminohexanoic acid/diaminohexanoate/Methylornithine                                                                                                | C6H14N2O2 | 3 | C00047 | HMDB0000182 | 25                          | KDXKERNBIXSRK-YFKPBYRVSA-N      | NCCCC[C@H](N)C(O)=O            |                |
| 147,0529 | 0,743834   | lactoyl-Glycine/Glutamic acid/Glutamate/Aminopentadioic acid/Threomethylaspartate/Methylaspartate/Oxohydroxyaminovalerate/(Carboxymethyl)alanine; Strombine | C5H9NO4   | 3 |        | HMDB0062183 | CLNVOWMDSFOIPV-VKHMVHEASA-N | C[C@H](O)C(=O)NCC(O)=O          |                                |                |
| 148,0517 | 1,2564695  | hydroxyphenylpropenal/phenyloxiranecarbaldehyde                                                                                                             | C9H8O2    | 3 |        | HMDB0135274 | DCHPWNOJPJRSEADUXPYHPUSA-N  | [H]\C(C=O)=C([H])C1=CC(O)=CC=C1 |                                |                |
| 155,0351 | 0,6876102  | Aminopropanol phosphate/Aminopropanyl phosphate/Methylethanolaminium phosphate                                                                              | C3H10NO4P | 3 | C04122 |             | 63967                       | YBOLZUJJGUZUDC-GSVOUGTGSA-N     | C[C@H](CN)OP(=O)(O)O           |                |
| 157,0891 | 5,3710995  | Isoquinoline methanamine                                                                                                                                    | C11H11N   | 3 |        |             | 45036                       |                                 |                                |                |
| 159,0532 | 0,78297263 | Methyleneglutamate                                                                                                                                          | C6H9NO4   | 3 | C00651 |             | 63273                       | RCCMXKJGURLWPB-BYPYZUCNSA-N     | C=C(C[C@H](N)C(=O)O)C(=O)O     |                |
| 159,1249 | 0,7290204  | Aminooctanoic acid                                                                                                                                          | C8H17NO2  | 3 |        | HMDB0000991 | LMFA01100056                | 74884                           | AKVBCGQVQXPRLD-UHFFFAOYSA-N    | CCCCC(N)C(O)=O |
| 161,1054 | 0,7090846  | carnitine                                                                                                                                                   | C7H15NO3  | 3 | C00318 | HMDB0000062 | 52                          | PHIQHXFUZVPYIIZCFIWBFSAN        | C[N+](C)(C)C[C@H](O)CC([O-])=O |                |
| 162,1046 | 6,565699   | methylphenylbutanone/Tetrahydromethylnaphthalenone/undecadienal                                                                                             | C11H14O   | 3 |        | HMDB0133676 | YEHRRTZJTORGJLUHFFFAOYSA-N  | CC(CC1=CC=CC=C1)C(C)=O          |                                |                |
| 165,0786 | 1,2572348  | Benzyl glycinate/Norsalsolinol/Phenylalanine                                                                                                                | C9H11NO2  | 3 |        | HMDB0059934 | JXYACYYPACQCDMUHFFFAOYSA-N  | NCC(=O)OCC1=CC=CC=C1            |                                |                |
| 166,0631 | 7,3584156  | Phenyllactic acid                                                                                                                                           | C9H10O3   | 3 | C05607 | HMDB0000748 | 3291                        | VOXXWSYKYCBWHO-MRVPVSSYSA-N     | O[C@H](CC1=CC=CC=C1)C(O)=O     |                |

|          |            |                                                                                                                                                                                                                                                                               |               |   |            |                  |       |                             |                                         |
|----------|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|---|------------|------------------|-------|-----------------------------|-----------------------------------------|
| 169,0893 | 7,367191   | 5-Aminoacenaphthene/5-Acenaphthenamine/4-Aminobiphenyl                                                                                                                                                                                                                        | C12H11N       | 3 | C193<br>19 |                  | 73029 | JEUAWMJVEYFVNJ-UHFFFAOYSA-N | Nc1ccc2c3c(cccc13)CC2                   |
| 170,0948 | 5,76132    | Dendryphielllic acid B/pomeadiol                                                                                                                                                                                                                                              | C9H14O3       | 3 |            | LMFA010203<br>99 |       | KFHQKGKXRZPBOB-YFIBRCQFSA-N | C[C@@H](CCO)/C=C/C=C/C(O)=O             |
| 170,1416 | 6,0328884  | Acrylamidopropyl trimethylammonium                                                                                                                                                                                                                                            | C9H18N2O      | 3 |            |                  | 34500 |                             |                                         |
| 172,1466 | 6,834683   | Isocapric acid                                                                                                                                                                                                                                                                | C10H20O2      | 3 |            | LMFA010202<br>47 | 73686 | OA0ABCKPVCUNKO-UHFFFAOYSA-N | CC(C)CCCCC(O)=O                         |
| 174,1118 | 0,72224355 | Arginine                                                                                                                                                                                                                                                                      | C6H14N4O<br>2 | 3 | C007<br>92 | HMDB0003<br>416  | 6924  | ODKSFYDXXFIFQN-SCSAIBSYSA-N | N[C@H](CCCNC(N)=N)C(O)=O                |
| 176,0476 | 6,897944   | Epoxy-decenediynoic acid                                                                                                                                                                                                                                                      | C10H8O3       | 3 |            | LMFA010700<br>27 |       | UBMRQHZPEXIEJ-ALCCZGGFSA-N  | CC1OC1C#CC#C/C=CC(O)=O                  |
| 180,0787 | 6,319259   | (methoxyphenyl)propanoic acid/hydroxyphenylbutanoic acid                                                                                                                                                                                                                      | C10H12O3      | 3 |            | HMDB0131<br>174  |       | FIUFLISGGHNPSM-UHFFFAOYSA-N | COC1=CC=C(CCC(O)=O)C=C1                 |
| 181,0737 | 0,794167   | Tyrosine; Hydroxyphenylalanine/Threo Phenylserine/Trihydroxytetrahydroisoquinoline                                                                                                                                                                                            | C9H11NO3      | 3 | C000<br>82 | HMDB0000<br>158  | 34    | OUYCCCASQSFEME-QMMMGPBSA-N  | N[C@@H](CC1=CC=C(O)C=C1)C(O)=O          |
| 187,0633 | 1,9841279  | Indoleacrylic acid/indolacrylate/Indolylpropanoate                                                                                                                                                                                                                            | C11H9NO2      | 3 |            | HMDB0000<br>734  | 5702  | SXOUIMVOMIGLHO-AATRIKPKSA-N | OC(=O)\C=C\C1=CC2=C(N1)C=CC=C2          |
| 188,0797 | 0,8245183  | Glycyl-Hydroxyproline/Acetylglutamine                                                                                                                                                                                                                                         | C7H12N2O<br>4 | 3 |            | HMDB0011<br>173  | 62021 | ZJQXGJBINIMBOY-UHFFFAOYSA-N | NCC(=O)N1CC(O)CC1C(O)=O                 |
| 190,1361 | 7,187217   | Megastigmatrienone/dehydro-beta-Ionone/10-fluorocapric acid                                                                                                                                                                                                                   | C13H18O       | 3 |            | HMDB0059<br>906  |       | YKVWPZJHENXDAJ-VOTSOKGWSA-N | [H]\C(C=C)=C([H])C1C(C)=CC(=O)CC1(C)C   |
| 192,0275 | 0,7592171  | didehydrogluconic acid/Isocitric acid; Hydroxypropanetricarboxylate; erythro-Isocitric acid/Diketogulonate/diketogulononic acid/Citric acid /Glucarolactone/Dehydrodeoxyglucarate; Dihydroxyoxohexanedioate/Galactarolactone/Dehydrodeoxyglucarate/Carboxymethyl oxysuccinate | C6H8O7        | 3 | C027<br>80 | LMFA010504<br>71 | 65828 | RXMWXENJQAINCC-DMTCNVIQSA-N | OC(=O)C(=O)[C@@H](O)[C@H](O)C(=O)CO     |
| 194,0951 | 7,3584867  | Hydroxyphenyl-valeric acid                                                                                                                                                                                                                                                    | C11H14O3      | 3 |            | HMDB0041<br>666  | 96026 | CMLIEOOXQFWANJ-UHFFFAOYSA-N | OC(=O)CCCCC1=CC=CC(O)=C1                |
| 202,172  | 7,0167837  | Vetivenene/Curcumene/Aro                                                                                                                                                                                                                                                      | C15H22        | 3 |            | HMDB0059         |       | QSUQBKPPUWLTH               | [H][C@@]1(C)CC=CC2=CCC(C[C@@]12C)=C(C)C |

|          |            |                                                                                                                                                   |            |   |        |             |              |       |                              |                                       |
|----------|------------|---------------------------------------------------------------------------------------------------------------------------------------------------|------------|---|--------|-------------|--------------|-------|------------------------------|---------------------------------------|
|          |            | madendradiene/Calamenene                                                                                                                          |            |   | 857    |             |              |       | -DOMZBBRYSA-N                |                                       |
| 203,1158 | 0,74607474 | Acetylcarnitine/Lactoyl-Leucine                                                                                                                   | C9H17NO4   | 3 |        | HMDB0000201 | LMFA07070050 | 956   | RDHQFKQIGNGIED-MRVPVSSYSA-N  | CC(=O)O[C@@H](CC([O-])=O)C[N+](C)(C)C |
| 204,0789 | 8,416487   | Levulinic Acid, 3-Benzylidenyl-/3-Butylidene-7-hydroxyphthalide                                                                                   | C12H12O3   | 3 |        |             |              | 44382 |                              |                                       |
| 204,0895 | 1,9823583  | D-Tryptophan                                                                                                                                      | C11H12N2O2 | 3 | C00525 | HMDB0013609 |              | 65364 | QIVBCDIJAIJPQS-SECBINFHSA-N  | N[C@H](CC1=CNC2=C1C=CC=C2)C(O)=O      |
| 204,0899 | 1,9823583  | Hydroxymethylantipyrine/Tryptophan                                                                                                                | C11H12N2O2 | 3 |        | HMDB0013840 |              | 85279 | JBKAGOWIZGVTR-UHFFFAOYSA-N   | CN1N(C(=O)C=C1CO)C1=CC=CC=C1          |
| 208,0848 | 1,2005575  | Kynurenine/Anthraniloylalanine/Formylhydroxykynurenamine                                                                                          | C10H12N2O3 | 3 | C00328 | HMDB0000684 |              |       | YGPSJZOEDVAXAB-QMMMGMPOBSA-N | N[C@@H](CC(=O)C1=CC=CC=C1N)C(O)=O     |
| 208,1104 | 6,7832627  | oxo-dodecatricenoic acid/(tert-Butyl-phenoxy)-acetic acid/Cyclohexene-acrylic acid-trimethyloxo/(tert-Butyl-phenoxy)-acetic acid/Coronafacic acid | C12H16O3   | 3 |        |             | LMFA01060095 | 74733 | ZRIOISYGDYRQIK-JDNZBGOLSA-N  | OC(=O)CCC/C=C/C=C/C=C\C=C=O           |
| 213,2454 | 6,48777    | Tetradecylamine                                                                                                                                   | C14H31N    | 3 |        |             |              | 3313  |                              |                                       |
| 217,1314 | 0,8019142  | Propionylcarnitine                                                                                                                                | C10H19NO4  | 3 | C03017 | HMDB0000824 | LMFA07070105 | 36668 | UFAHZIUFPNSHSL-UHFFFAOYSA-N  | CCC(=O)OC(CC([O-])=O)C[N+](C)(C)C     |
| 218,0197 | 0,68900734 | dihydroxyfurochromenone                                                                                                                           | C11H6O5    | 3 |        | HMDB0135848 |              |       | FQNXUBCEYKWIGF-UHFFFAOYSA-N  | OC1=CC2=C(O1)C=CC1=C2OC(=O)C=C1O      |
| 218,167  | 6,0282784  | Octyl phenyl ketone/benzyl octanal/(phenylmethylidene)octanol                                                                                     | C15H22O    | 3 |        | HMDB0094674 |              |       | PFUPABFCHVRLLY-UHFFFAOYSA-N  | CCCCCCCC(=O)C1=CC=CC=C1               |
| 218,1672 | 6,244601   | N-Octyl phenyl ketone/2-benzyl octanal/(phenylmethylidene)octanol                                                                                 | C15H22O    | 3 |        | HMDB0094674 |              |       | PFUPABFCHVRLLY-UHFFFAOYSA-N  | CCCCCCCC(=O)C1=CC=CC=C1               |
| 221,178  | 5,8445644  | Tapentadol                                                                                                                                        | C14H23NO   | 3 |        |             |              | 96332 |                              |                                       |
| 222,0567 | 6,6430306  | Triethyl-trithiane/(Methylthio)propyl malate                                                                                                      | C9H18S3    | 3 |        | HMDB0040262 |              | 94791 | PHQSYHLEPPMJSU-UHFFFAOYSA-N  | CCC1SC(CC)SC(CC)S1                    |
| 224,1888 | 6,694408   | Anaferine/Anapheline/Dicyclohexylurea                                                                                                             | C13H24N2O  | 3 | C06183 |             |              | 64435 | JFMCQBGUJUOAB-RYUDHWBXSA-N   | O=C(C[C@@H]1CCCCN1)C[C@@H]1CCCCN1     |
| 225,9452 |            | Dichlorooxohexenedioate                                                                                                                           | C6H4Cl2O5  | 3 | C12835 | HMDB0060363 | LMFA01090152 | 69492 | PLPVRWUZGSFJJB-OWOJBTEDSA-N  | OC(=O)/C(/Cl)=CC(=O)C(Cl)C(O)=O       |
| 228,1475 | 0,76670134 | Leucylproline/Isoleucylproline                                                                                                                    | C11H20N2O3 | 3 |        | HMDB0011175 |              |       | VTJUNIYRYIAIHF-UHFFFAOYSA-N  | CC(C)CC(N)C(=O)N1CCCC1C(O)=O          |
| 228,2088 | 9,566135   | Myristic acid                                                                                                                                     | C14H28O2   | 3 | C06424 | HMDB0000806 | LMFA01010014 | 196   | TUNFSRHWOTWDN-C-UHFFFAOYSA-N | CCCCCCCCCCCC(O)=O                     |
| 229,1686 | 5,679458   | Decanoylglycine                                                                                                                                   | C12H23NO   | 3 |        | HMDB0013    |              |       | WRRYZYASRAUROW               | CCCCCCCCC(=O)NCC(O)=O                 |

|                 |            |                                                                                                                                                                                                                                                                   |                |   |            |                  |       |                                 |                                                     |
|-----------------|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|---|------------|------------------|-------|---------------------------------|-----------------------------------------------------|
|                 |            |                                                                                                                                                                                                                                                                   | 3              |   | 267        |                  |       | -UHFFFAOYSA-N                   |                                                     |
| <b>229,2405</b> | 6,25078    | Xestoaminol C                                                                                                                                                                                                                                                     | C14H31NO       | 3 |            | LMSP010800<br>33 | 53933 | WMUMHAZHWIUBP<br>N-UONOGXRCSA-N | C[C@@H](N)[C@@H](O)CCCCCCCCC                        |
| <b>234,0853</b> | 0,8481127  | Ethylenediaminetriacetic acid/Ethylenediaminetriacetate ED3A/Aspartyl-Threonine/Glutamylserine/Asparaginylglutamate                                                                                                                                               | C8H14N2O<br>6  | 3 | C213<br>96 |                  |       | OUDFSQBUEBFS-<br>UHFFFAOYSA-N   | O=C(O)CNCCN(CC(=O)O)CC(=O)O                         |
| <b>234,1621</b> | 7,9165196  | Valerenic acid                                                                                                                                                                                                                                                    | C15H22O2       | 3 | C097<br>43 |                  |       | FEBNTWHYQKGEIQ-<br>SUKRRCSA-N   | CC1=C2[C@H](/C=C\C(C)=O)O)CC[C@@H](C)[C@H]2CC1      |
| <b>238,0845</b> | 5,700519   | Trimethoxycinnamic acid/Trimethoxycinnamate/dimethoxybenzodioxolpropenol/hydroxytrimethoxyphenylpropenal/dimethoxybenzodioxolpropanal/trimethoxyphenylpropenoic acid/Propanoic acid, hydroxy(propenyloxy)phenoxy                                                  | C12H14O5       | 3 |            | HMDB0002<br>511  | 6705  | YTFVRYKNXDADBI-<br>SNAWJCMRSA-N | COC1=CC(\C=C\C(O)=O)=CC(OC)=C1OC                    |
| <b>240,0996</b> | 6,319      | trimethoxyphenylpropanoic acid                                                                                                                                                                                                                                    | C12H16O5       | 3 |            | HMDB0142<br>074  |       | QOPNYPCVRBRZOP-<br>UHFFFAOYSA-N | COC1=C(OC)C(OC)=C(CCC(O)=O)C=C1                     |
| <b>240,1001</b> | 6,319      | (hydroxymethyl)methoxymethylhydrobenzopyrandiol/(hydroxypropenyl)trimethoxyphenol/(trimethoxyphenyl)propanoic acid/methoxydimethyldihydrobenzopyrantriol/hydroxyhydroxymethoxyphenylpentanoic acid/dimethoxybenzodioxolpropanol/(hydroxytrimethoxyphenyl)propanal | C12H16O5       | 3 |            | HMDB0125<br>804  |       | WPDUHZUOYGPEOT-<br>UHFFFAOYSA-N | COC1=CC(O)=C2C(O)CC(C)(CO)OC2=C1                    |
| <b>240,1471</b> | 0,76480293 | Pirbuterol                                                                                                                                                                                                                                                        | C12H20N2<br>O3 | 3 | C078<br>07 | HMDB0015<br>407  | 66744 | VQDBNKDJNJQRDG-<br>UHFFFAOYSA-N | CC(C)(C)NCC(O)C1=NC(CO)=C(O)C=C1                    |
| <b>243,1836</b> | 5,770232   | N-Undecanoylglycine                                                                                                                                                                                                                                               | C13H25NO<br>3  | 3 |            | HMDB0013<br>286  |       | HEUQYIQQCNOXOG-<br>UHFFFAOYSA-N | CCCCCCCCC(=O)NCC(O)=O                               |
| <b>246,0854</b> | 0,78740627 | Aspartylhydroxyproline/Dihydrodouridine                                                                                                                                                                                                                           | C9H14N2O<br>6  | 3 |            | HMDB0011<br>160  | 62009 | WJDWENBTQEKDZ-<br>UHFFFAOYSA-N  | NC(CC(O)=O)C(=O)N1CC(O)CC1C(O)=O                    |
| <b>246,1215</b> | 1,1686447  | Bis(acetamido)trideoxyaltropyranose/Aspartyl-Leucine/Glutamylvaline/Diacetamidotrideoxymannopyran                                                                                                                                                                 | C10H18N2<br>O5 | 3 | C199<br>72 |                  | 73461 | NRXWTRNYICXMBF-<br>SGZWNVLDSA-N | CC(=O)N[C@H]1[C@H](C)O[C@H](O)[C@H](NC(C)=O)[C@H]1O |



|          |            |                                                                                   |                |   |            |                 |                  |       |                                  |                                                                   |
|----------|------------|-----------------------------------------------------------------------------------|----------------|---|------------|-----------------|------------------|-------|----------------------------------|-------------------------------------------------------------------|
| 275,1383 | 0,90102667 | Glutaryl carnitine                                                                | C12H21NO<br>6  | 3 |            | HMDB0013<br>130 |                  |       | NXJAXUYOQLTISD-<br>SECBINFHSA-N  | C[N+](C)(C)C[C@@H](CC([O-])=O)OC(=O)CCCC(O)=O                     |
| 278,0866 | 6,5708075  | (2-Chlorophenyl)diphenylmethane/Triphenylphosphine oxide/11-bromo-dodecanoic acid | C19H15Cl       | 3 |            |                 | 1898             |       |                                  |                                                                   |
| 278,1521 | 8,4037     | dimethyloxiranylmethylpent enyllbenzenetriol                                      | C16H22O4       | 3 |            | HMDB0133<br>086 |                  |       | JYHLZRSNMLULIG-<br>UHFFFAOYSA-N  | CC(CCC1OC1(C)C)=CCC1=C(O)C=C(O)C=C1O                              |
| 278,2247 | 7,7563353  | Linolenic acid                                                                    | C18H30O2       | 3 | C064<br>27 | HMDB0001<br>388 | LMFA010301<br>52 | 192   | DTOSIQBPPRVQHS-<br>PDBXOOCHSA-N  | CC/C=C\C/C=C\C/C=C\C\CCCCCCC(O)=O                                 |
| 278,2247 | 9,395291   | Linolenic acid                                                                    | C18H30O2       | 3 | C064<br>27 | HMDB0001<br>388 | LMFA010301<br>52 | 192   | DTOSIQBPPRVQHS-<br>PDBXOOCHSA-N  | CC/C=C\C/C=C\C/C=C\C\CCCCCCC(O)=O                                 |
| 279,0867 | 0,6778833  | Ser Ala Cys/Gly Thr Cys                                                           | C9H17N3O<br>55 | 3 |            |                 |                  | 15654 |                                  |                                                                   |
| 279,2566 | 9,135976   | Linoleamide                                                                       | C18H33NO       | 3 |            | HMDB0062<br>656 | LMFA080100<br>08 | 43435 | SFIHQZFZMWZOJV-<br>HZJYTTRNSA-N  | CCCCC/C=C\C/C=C\C\CCCCCCC(N)=O                                    |
| 280,2403 | 10,150115  | Linoleic acid                                                                     | C18H32O2       | 3 | C015<br>95 | HMDB0000<br>673 | LMFA010301<br>20 | 191   | OYHQOLUKZRVURQ-<br>HZJYTTRNSA-N  | CCCCC/C=C\C/C=C\C\CCCCCCC(O)=O                                    |
| 281,2722 | 10,082904  | Oleamide                                                                          | C18H35NO       | 3 | C196<br>70 | HMDB0002<br>117 | LMFA080100<br>04 | 4115  | FATBGEAMMYZAF-<br>KTKRTIGZSA-N   | CCCCCCCC/C=C\C\CCCCCCC(N)=O                                       |
| 282,1676 | 5,360094   | Hexaethylene glycol                                                               | C12H26O7       | 3 |            | HMDB0061<br>822 |                  |       | IIRDTKBZINWQAW-<br>UHFFFAOYSA-N  | OCCOCCOCCOCCOCCOCCO                                               |
| 282,256  | 10,967361  | vaccenic acid/octadecenoic acid/oleic acid/elaidic acid                           | C18H34O2       | 3 | C083<br>67 | HMDB0003<br>231 | LMFA010300<br>77 | 3407  | UWHZIFQPPBDJPM-<br>BQYQJAHWSA-N  | CCCCC/C=C/C\CCCCCCCC(O)=O                                         |
| 283,2883 | 11,3391    | Stearamide                                                                        | C18H37NO       | 3 | C138<br>46 | HMDB0034<br>146 | LMFA080100<br>03 | 34494 | LYRFLYHAGKPMFH-<br>UHFFFAOYSA-N  | CCCCCCCCCCCCCCCC(N)=O                                             |
| 284,2143 | 9,365747   | Dimethyl-norandrostadienone                                                       | C20H28O        | 3 | C146<br>55 |                 |                  | 70237 | SPKAUGWCKWXQF-<br>M-QSFXBCCZSA-N | CC1(C)CCC2=C1CC[C@H]1[C@H]2CCC2=CC(=O)CC[C@H]121C                 |
| 285,1366 | 6,883469   | Cherylline                                                                        | C17H19NO<br>3  | 3 | C121<br>67 |                 |                  | 69337 | VXXVFIKKBBVGIR-<br>HNNXBMYFSA-N  | COc1cc2c(cc1O)CN(C)C[C@H]2c1ccc(O)cc1                             |
| 285,194  | 5,708251   | Octenoyl carnitine                                                                | C15H27NO<br>4  | 3 |            | HMDB0013<br>324 |                  |       | YMIVWYONPRZBEJ-<br>LXKVQUBZSA-N  | CCCCC\C=C\C(=O)O[C@@H](CCC([O-])=O)[N+](C)(C)C                    |
| 287,1957 | 5,3906727  | Arginyl-Leucine                                                                   | C12H25N5<br>O3 | 3 |            | HMDB0028<br>713 |                  | 85628 | WYBVBIHNJWOLCJ-<br>UHFFFAOYSA-N  | CC(C)CC(NC(=O)C(N)CCCNC(N)=N)C(O)=O                               |
| 287,2095 | 5,834523   | Octanoyl carnitine                                                                | C15H29NO<br>4  | 3 |            |                 |                  | 85173 |                                  |                                                                   |
| 287,2826 | 6,359945   | C17 Sphinganine                                                                   | C17H37NO<br>2  | 3 |            |                 | LMSP010400<br>03 | 41558 | KFQUQCQFDMSIJF-<br>DLBZAZTESA-N  | CCCCCCCCCCCC[C@H](O)[C@H](N)CO                                    |
| 290,1881 | 7,6473913  | oxooctadecatetraenoic acid                                                        | C18H26O3       | 3 |            |                 | LMFA020002<br>70 | 74765 | ZYOSGENSARGRME-<br>BEGPLMEHSA-N  | CC/C=C/C=C/C=C\C/C=C/C\CCCC(=O)CCC(O)=O                           |
| 292,2404 | 9,074539   | Dihydroxyandrostane                                                               | C19H32O2       | 3 |            |                 | LMST020200<br>93 |       | CBMYJHIOYJESB-<br>ULTMTAQRSA-N   | C[C@@]12CC[C@H]3[C@H](CC[C@H]4C[C@H](O)CC[C@H]43C)[C@H]1CC[C@H]2O |

|          |           |                                                                                                                                                                          |            |   |        |             |              |       |                             |                                                      |
|----------|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|---|--------|-------------|--------------|-------|-----------------------------|------------------------------------------------------|
| 294,2192 | 7,147893  | hydroxyoctadecatrienoic acid                                                                                                                                             | C18H30O3   | 3 |        | HMDB0010203 | LMFA02000029 | 36032 | KLLGGGQNRVTBSU-JDTPQGGVSA-N | CC/C=C\CC(O)/C=C/C=C\CCCCCCCC(O)=O                   |
| 294,2196 | 7,8034964 | hydroxy-linolenic acid                                                                                                                                                   | C18H30O3   | 3 |        |             |              | 45842 |                             |                                                      |
| 294,2196 | 8,048426  | hydroxy-linolenic acid                                                                                                                                                   | C18H30O3   | 3 |        |             |              | 45842 |                             |                                                      |
| 295,0595 | 0,6855486 | Aminoimidazole ribonucleotide                                                                                                                                            | C8H14N3O7P | 3 | C03373 | HMDB0001235 |              | 6097  | PDACUKOKVHBVHJ-XVFCMESISA-N | NC1=CN=CN1[C@@H]1O[C@H](COP(O)(O)=O)[C@@H](O)[C@H]1O |
| 296,2351 | 7,7652965 | Epoxyoctadecenoic acid/Hydroxyoctadecadienoic acid                                                                                                                       | C18H32O3   | 3 | C08368 |             |              |       | CCPPLLJZDQAOHD-BEBBCNLGSA-N | CCCC[C@@H]1O[C@@H]1C/C=C\CCCCCCCC(=O)O               |
| 298,1934 | 6,751142  | All-TransDidehydro-Retinoic acid/Hydroxy-norpregnatrienone/Eremolactone/Methoxy secocycloandrostatrienone/Dimethylhexestrol/Norethynodrel/Methoxyhomoestrateraenabeta-ol | C20H26O2   | 3 |        | HMDB0060092 | LMPR01090020 | 41514 | SYESMXTWAOQFET-YNINQYBTSAN  | CC1C=CCC(C)(C)C=1/C=C/C(/C)=C/C=C/C(/C)=C/C(O)=O     |
| 299,2825 | 9,26306   | ketosphinganine/Sphingosine                                                                                                                                              | C18H37NO2  | 3 | C02934 | HMDB0001480 | LMSP01020002 | 3428  | KBUNOSOGGAARKZ-KRWDZBQOSA-N | CCCCCCCCCCCCCCCC(=O)[C@@H](N)CO                      |
| 300,2092 | 7,411182  | Retinoic Acid                                                                                                                                                            | C20H28O2   | 3 | C00777 | HMDB0001852 | LMPR01090019 | 2277  | SHGAZHPJCJPHSC-YNINQYBTSAN  | CC1CCCC(C)(C)C=1/C=C/C(/C)=C/C=C/C(/C)=C/C(O)=O      |
| 301,2249 | 5,893207  | dimethylheptanoyl carnitine/Nonanoylcarnitine                                                                                                                            | C16H31NO4  | 3 |        | HMDB0006320 | LMFA07070029 | 58391 | QBYXBONNCVATNQ-UHFFFAOYSA-N | CC(C)CCCC(C)(=O)OC(C[N+](C)(C)C)[O-])=O              |
| 302,2247 | 8,156109  | eicosapentaenoic acid                                                                                                                                                    | C20H30O2   | 3 |        |             | LMFA01030396 | 74063 | IFPCWRDOHFTYMB-BWKGZPQXSA-N | CCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C/C(O)=O              |
| 302,2247 | 9,263333  | eicosapentaenoic acid                                                                                                                                                    | C20H30O2   | 3 |        |             | LMFA01030396 | 74063 | IFPCWRDOHFTYMB-BWKGZPQXSA-N | CCCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C/C(O)=O              |
| 302,2248 | 8,017053  | EPA                                                                                                                                                                      | C20H30O2   | 3 | C06428 | HMDB0001999 | LMFA01030759 | 6423  | JAZBEHYOTPTENJ-JLNKQSITSA-N | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C\CCCC(O)=O           |
| 302,2455 | 8,689119  | MG(14:0)/3,4-dihydroxy-4-methylhexadecanoic acid                                                                                                                         | C17H34O4   | 3 |        | HMDB0011561 |              | 62344 | DCBSHORRWZKAKO-INIZCTEOSA-N | [H][C@](O)(CO)COC(=O)CCCCCCCCCCCC                    |
| 302,2459 | 8,885422  | MG(14:0)/3,4-dihydroxy-4-methylhexadecanoic acid                                                                                                                         | C17H34O4   | 3 |        | HMDB0011530 |              | 62314 | TVIMZSOUQXNWHO-UHFFFAOYSA-N | [H]C(CO)(CO)OC(=O)CCCCCCCCCCCC                       |
| 303,205  | 5,5893235 | hydroxyoctanoyl carnitine                                                                                                                                                | C15H29NO5  | 3 |        | HMDB0061634 |              |       | LUBMSOHGUAXA-M-UHFFFAOYSA-N | CCCCC(O)CC(=O)OC(CC([O-])=O)C[N+](C)(C)C             |
| 303,2927 | 6,741168  | 1-hexadecylpyridinium/Cetylpyridinium                                                                                                                                    | C21H37N    | 3 |        |             |              | 34547 |                             |                                                      |
| 304,2388 | 8,170919  | Arachidonic acid                                                                                                                                                         | C20H32O2   | 3 | C00219 | HMDB0001043 | LMFA01030001 | 193   | YZXBAPSDXZRGB-DOFZRALJSA-N  | CCCC/C=C\C/C=C\C/C=C\C/C=C\C\CCCC(O)=O               |
| 304,2401 | 9,9404125 | Arachidonic acid                                                                                                                                                         | C20H32O2   | 3 | C00219 | HMDB0001043 | LMFA01030001 | 193   | YZXBAPSDXZRGB-DOFZRALJSA-N  | CCCC/C=C\C/C=C\C/C=C\C/C=C\C\CCCC(O)=O               |
| 308,1973 | 9,14654   | Trifluorotetradecenyl acetate                                                                                                                                            | C16H27F3O2 | 3 |        |             | LMFA07010327 | 46326 | QVAHKGHMXZIUOO-PKNBQFBNSA-N | CC(=O)OCCCCCCCCC/C=C/CC(F)(F)F                       |

|          |           |                                                                                                                                 |            |   |        |             |              |       |                              |                                                                                      |
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| 308,235  | 9,36398   | methylepoxyoctadecadienoate                                                                                                     | C19H32O3   | 3 |        |             | LMFA01070012 | 74809 | WJRQEOOGBUSIOJ-OCJIRGAFA-N   | COC(=O)CCCCCCCC1OC1C/C=C/C/C=CC                                                      |
| 308,2351 | 9,459208  | Methylpropylfuranundecanoic acid/methyl epoxyoctadecadienoate/Hexyldimethylfuranheptanoic acid/Dimethylpentylfuranoctanoic acid | C19H32O3   | 3 |        | HMDB0061646 |              |       | XZOBJEOEOJXQBF-UHFFFAOYSA-N  | [H]C1=C(CCC)OC(CCCCCCCCC(O)=O)=C1C                                                   |
| 308,271  | 10,554331 | Dihomolinoleic acid/eicosadienoic acid/linoleic acid/keteleeronic acid/Dimethyloctadienyl decanoate/Octadecadienyl acetate      | C20H36O2   | 3 | C16525 | HMDB0005060 | LMFA01031043 | 62964 | XSXIVVZCUAHUJO-HZIYTTRNSA-N  | CCCCC/C=CC/C=CCCCCCCC(O)=O                                                           |
| 310,1172 | 1,2156205 | Leu-Ala-OH/Abu-Val-OH/Glutamyltyrosine/Cl-Amidine                                                                               | C14H18N2O6 | 3 |        |             |              | 64986 |                              |                                                                                      |
| 313,2252 | 5,9851847 | 9-Decenoylcarnitine                                                                                                             | C17H31NO4  | 3 |        | HMDB0013205 | LMFA07070048 |       | GOOOCIIXFLVRAG-UHFFFAOYSA-N  | C[N+](C)(C)CC(CC([O-])=O)OC(=O)CCCCCCCC=C                                            |
| 315,2411 | 6,0916    | Decanoylcarnitine                                                                                                               | C17H33NO4  | 3 |        | HMDB0000651 | LMFA07070059 |       | LZOSYCMHQXPBFU-UHFFFAOYSA-N  | CCCCCCCCC(=O)OC(CC([O-])=O)C[N+](C)(C)C                                              |
| 316,2038 | 6,6744666 | deoxy-PGJ2/Hydroxy-methylandrostenedione                                                                                        | C20H28O3   | 3 | C14717 | HMDB0005079 | LMFA03010021 | 36099 | VHRUMKCAEVRUBK-GODQJPCRSA-N  | CCCCC/C=C/C=C1\[C@@H](C/C=C\CCCC(O)=O)C=C C\1=O                                      |
| 316,2039 | 7,177156  | Epoxy-hydroxymethylandrostenone                                                                                                 | C20H28O3   | 3 | C15192 |             |              | 70681 | BJYNFFDYDZKDTE-NPBKEMFKSA-N  | C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@@]4(C)[C@@]34O[C@H]4C[C@@]21C                |
| 316,2402 | 9,371267  | Pregnenolone                                                                                                                    | C21H32O2   | 3 |        | HMDB0000253 |              | 24078 | ORNBQBCIOKFOEO-STZXPNGSSA-N  | [H][C@@]12CC[C@H](C(C)=O)[C@@]1(C)CC[C@@]1([H])C2CC=C2C[C@H](O)CC[C@]12C             |
| 318,2172 | 7,8977923 | HEPE                                                                                                                            | C20H30O3   | 3 |        | HMDB0012611 | LMFA03070054 |       | LRWYBGFSVUBWM-O-NQZHIPPKSA-N | CC[C@@H](O)/C=C/C=CC/C=C/C/C=CC/C=CCCC(O)=O                                          |
| 318,2191 | 7,3433642 | HEPE/EpETE                                                                                                                      | C20H30O3   | 3 |        | HMDB0010209 | LMFA03070053 | 61547 | UDXLGBLAJBYSZ-XBCQTNLFSA-N   | CC/C=CC(O)C/C=C/C=CC/C=CC/C=CCCC(O)=O                                                |
| 318,2192 | 8,442302  | 15-HEPE/oxoETE                                                                                                                  | C20H30O3   | 3 |        | HMDB0010209 | LMFA03070053 | 61547 | UDXLGBLAJBYSZ-XBCQTNLFSA-N   | CC/C=CC(O)C/C=C/C=CC/C=CC/C=CCCC(O)=O                                                |
| 318,2193 | 6,8250985 | HEPE/Oxo-ETE                                                                                                                    | C20H30O3   | 3 |        | HMDB0012611 | LMFA03070054 |       | LRWYBGFSVUBWM-O-NQZHIPPKSA-N | CC[C@@H](O)/C=C/C=CC/C=C/C/C=CC/C=CCCC(O)=O                                          |
| 318,2196 | 7,0328355 | 5-Oxo-ETE/5S-HEPE                                                                                                               | C20H30O3   | 3 | C14732 | HMDB0010217 | LMFA03060011 | 3844  | MEASLHGILYBXFO-XTDASVJISA-N  | CCCCC/C=C\C/C=C\C/C=C\C=C\CCCC(O)=O                                                  |
| 320,2351 | 8,165472  | Epoxyeicosatrienoic acid/HETE                                                                                                   | C20H32O3   | 3 |        | HMDB0004673 | LMFA03090011 |       | DXOYQVHGIODESM-ATELOPIESA-N  | CCCCC/C=C/CC1OC1C/C=C/C/C=C/CCCC(O)=O                                                |
| 323,2099 | 8,402247  | oxo-tetradecenoyl-L-Homoserine lactone                                                                                          | C18H29NO4  | 3 |        |             |              | 45495 |                              |                                                                                      |
| 324,209  | 7,9583597 | Etonogestrel/Docosatetranoic acid/Fluoro-B-                                                                                     | C22H28O2   | 3 |        | HMDB0014439 |              | 1954  | GCKFYUQCUCGESZ-BPIQYHPVSA-N  | [H][C@@]12CC[C@@](O)(C#C)[C@@]1(CC)CC(=C)[C@@]1([H])[C@@]3([H])CCC(=O)C=C3CC[C@@]21H |



|          |           |                                                                                                                                         |           |    |        |              |                             |                                                                              |                                                                                   |
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|          |           | /Hydroxyketopregnanolone                                                                                                                |           | 98 |        |              | YOBHSELKSA-N                | 4C[C@H](O)CC[C@]4(C)[C@H]3C(=O)C[C@@]21C                                     |                                                                                   |
| 348,2283 | 8,156172  | Trihydroxypregnenone                                                                                                                    | C21H32O4  | 3  |        | 84296        |                             |                                                                              |                                                                                   |
| 350,2091 | 6,102922  | Prostaglandin E3/oxo-leukotriene B4/Oxo-lipoxin A4/oxodihydroxyeicosatetraenoic acid                                                    | C20H30O5  | 3  |        | 45612        |                             |                                                                              |                                                                                   |
| 350,2091 | 6,309252  | Epoxyhydroxyoxoprostadienoate/HEPE/Prostaglandin E3                                                                                     | C20H30O5  | 3  | C04835 |              | YCLHGWBUYYKBPM-NBFHXWWSA-N  | CCCCC(=O)/C=C/[C@H]1[C@H](O)C[C@@H]2O/C(=C/CCCC(=O)O)C[C@@H]21               |                                                                                   |
| 352,2228 | 6,224995  | hydroperoxy-HETE/hydroxy LTB4/keto-PGF2                                                                                                 | C20H32O5  | 3  |        | HMDB0062798  | AZHSPOPMNJPF-DHRRBLAHS-A-N  | [H]\C(C\C([H])=C([H])C([H])=C([H])C(CCCC(O)=O)O)=C/[H])C([H])=C([H])C(O)CCCC |                                                                                   |
| 354,2749 | 8,647746  | MG(18:2)/Linoleoyl Glycerol/PGF2 methyl ether/Ceriporic acid B                                                                          | C21H38O4  | 3  |        | HMDB0011568  | WECGLUPZRHLCT-GSNKCQISSA-N  | [H][C@](O)(CO)COC(=O)CCCCCCC\C=C/C\C=C/CCC                                   |                                                                                   |
| 354,2772 | 9,474519  | MG(18:2)/PGF2 methyl ether/Ceriporic acid B/Linoleoyl Glycerol                                                                          | C21H38O4  | 3  |        | LMFA03010073 | 36144                       | VWEVSUSNDAHANL-GPPFPWBLSA-N                                                  | CCCC[C@@H](O)/C=C/[C@H]1[C@H](C/C=C\CCCOC)[C@H](O)C[C@@H]1O                       |
| 356,1969 | 6,5716314 | Estradiol diacetate/Dioxopregnadienol c acid methyl ester/Nitenin                                                                       | C22H28O4  | 3  |        |              |                             | 43494                                                                        |                                                                                   |
| 356,197  | 6,8928103 | Estradiol diacetate/Dioxopregnadienol c acid methyl ester                                                                               | C22H28O4  | 3  |        |              |                             | 43494                                                                        |                                                                                   |
| 356,2335 | 9,368629  | Arachidonyltrifluoromethane /AACOCF3/Estradiol valerate/14-HDoHE/16-Dehydropregnenolone acetate/3beta-Acetyloxy-pregna-5,16-dien-20-one | C21H31F3O | 3  | C01397 | 63007        | PLWROONZUDKYKG-DOFZRALISA-N | CCCCC/C=C\C/C=C\C/C=C\C/C=C\C\CCCC(=O)C(F)(F)F                               |                                                                                   |
| 356,2717 | 7,200472  | Tetracosahexaenoic acid/Docosahexaenoic Acid ethyl ester                                                                                | C24H36O2  | 3  |        |              |                             | 6430                                                                         |                                                                                   |
| 357,2878 | 6,4788375 | palmitoyl threonine                                                                                                                     | C20H39NO4 | 3  |        | LMFA08020107 | 75489                       | JOIXCEREMHWULC-MJGOQNOKSA-N                                                  | C[C@@H](O)[C@H](NC(=O)CCCCCCCCCCCCCCC)C(O)=O                                      |
| 358,2123 | 7,3337665 | Piperoic acid                                                                                                                           | C22H30O4  | 3  |        | HMDB0040619  | 95097                       | VWHKYMBXCXSEZ-KKYJLSSQSA-N                                                   | CC(C)=CCC\C(C)=C/CC\C(C)=C\CC1=CC(=CC(O)=C1)C(O)=O                                |
| 358,2135 | 6,817359  | Canrenoate                                                                                                                              | C22H30O4  | 3  |        |              |                             | 1469                                                                         |                                                                                   |
| 358,3082 | 11,087643 | MG(0:0/18:0/0:0)                                                                                                                        | C21H42O4  | 3  |        | HMDB0011535  | 62319                       | YQEMORVAKMFKLG-UHFFFAOYSA-N                                                  | [H]C(CO)(CO)OC(=O)CCCCCCCCCCCCCCCC                                                |
| 358,3089 | 11,316808 | MG(0:0/18:0/0:0)                                                                                                                        | C21H42O4  | 3  |        | HMDB0011535  | 62319                       | YQEMORVAKMFKLG-UHFFFAOYSA-N                                                  | [H]C(CO)(CO)OC(=O)CCCCCCCCCCCCCCCC                                                |
| 362,2091 | 6,028     | Hydroxycorticosterone/Trihydroxypregnenedione/cortisol                                                                                  | C21H30O5  | 3  | C15034 |              | 70528                       | WPZNCXVXQMWZQ-E-FDNLDMUSA-N                                                  | C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1C[C@@H](O)[C@@H]2C(=O)C |

|          |           |                                                                                                            |           |   |             |              |       |                             |                                                                                    |
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|          |           | /trihydroxyoxohexanorvitamin D3 / trihydroxyoxohexanorcholecalciferol                                      |           |   |             |              |       |                             | O)CO                                                                               |
| 364,1289 | 8,133217  | Dimethoxydimethylphenylbenzodipyrone/Carpachromene dimethyl ether                                          | C22H20O5  | 3 |             | LMPK12111650 | 50067 | IMHUWBJRQHCKTE-UHFFFAOYSA-N | COC1C(=O)c2c(OC(=1c1ccccc1)c1C=CC(C)(C)Oc1cc2OC                                    |
| 364,2016 | 7,820534  | (Dimethylpropenyl)(methylbutenyl)xanthyletin/Fluorodihydroxypregnenedione                                  | C24H28O3  | 3 | HMDB0030730 |              | 87156 | PIOKBHKPGZHPHS-UHFFFAOYSA-N | CC(C)=CCC1=C2OC(=O)C(=CC2=CC2=C1OC(C)(C)=C2)C(C)(C)C=C                             |
| 364,2016 | 7,9646416 | Fluorodihydroxypregnenedione/Fluorodihydroxyprogesterone/Dimethylpropenyl(methylbutenyl)xanthyletin        | C21H29FO4 | 3 | C15172      |              | 70662 | AIFBIDNFKTLIRSBWHNKUSA-N    | CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C[C@H](F)C4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C |
| 366,2044 | 6,08435   | ox-LGD2/carboxy-LTB4                                                                                       | C20H30O6  | 3 |             | LMFA03100037 | 96929 | RAQOIYLDXSAKSS-DPLATEDBSA-N | CCCC[C@@H](O)/C=C/C1=C(C/C=C\CCCC(O)=O)C(=O)OC1(C)O                                |
| 367,2719 | 6,359678  | Tetradecadienecarnitine                                                                                    | C21H37NO4 | 3 | HMDB0013331 |              |       | HXOGMKPCIDSSKJ-NKBLVAAJSA-N | CCCCCCCC\C=C\C=C\CC(=O)O[C@H]([N+](C)(C)C)CC([O-])=O                               |
| 368,1662 | 6,476347  | Testosterone sulfate/Dehydroepiandrosterone sulfate/Hydroxyandrostenedione sulfate/Epitestosterone sulfate | C19H28O5S | 3 | HMDB0002833 | LMST05020032 | 3558  | WAQBISPOEAOCOG-DYKIIFRCSA-N | C[C@@]12CC[C@H]3[C@H](CCC4=CC(=O)CC[C@]43C)[C@H]1CC[C@H]2OS(O)(=O)=O               |
| 368,2331 | 10,123493 | Oxocholatrienoic Acid                                                                                      | C24H32O3  | 3 |             | LMST04010429 | 84733 | GFECBJJQSLNADTIHMUCKAYSA-N  | C[C@@H](CCC(O)=O)[C@@H]1CC[C@@H]2[C@H]3C=CC4=CC(=O)C=C[C@@]4(C)[C@@H]3CC[C@]21C    |
| 368,3442 | 11,223261 | Deoxyvitamin D3                                                                                            | C27H44    | 3 |             | LMST03020618 | 42544 | FXKMDILIEQILCAVDVRBEGSSA-N  | CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2/C/CCC[C@@]21C)=C/C=C1/CCCC/1=C                     |
| 369,288  | 6,5254145 | OleoylSerine/Tetradecenoylcarnitine                                                                        | C21H39NO4 | 3 |             |              | 45444 |                             |                                                                                    |
| 370,1815 | 6,697586  | 5a-Dihydrotestosterone sulfate/Epiandrosterone sulfate                                                     | C19H30O5S | 3 |             | LMST05020023 | 57975 | KYVPWJSGFKNNLD-UXMGNZLBSA-N | C[C@@]12CC[C@H]3[C@H](CC[C@@H]4CC(=O)CC[C@]43C)[C@H]1CCC2OS(O)(=O)=O               |
| 370,2123 | 7,401573  | phenyl trinordihydro Prostaglandin A2                                                                      | C23H30O4  | 3 |             |              | 45409 |                             |                                                                                    |
| 371,3033 | 6,7111597 | (±)-Myristoylcarnitine/O-tetradecanoylcarnitine/N-stearoylserine/Tetradecanoylcarnitine                    | C21H41NO4 | 3 |             |              | 85175 |                             |                                                                                    |
| 372,192  | 6,029889  | Methylprednisone/clavulolactone/phenyl-tetranor-PGE2                                                       | C22H28O5  | 3 |             |              | 1236  |                             |                                                                                    |
| 372,2276 | 7,563183  | Hydroxyprogesterone                                                                                        | C23H32O4  | 3 |             |              | 1093  |                             |                                                                                    |

|          |            |                                                                                                                                                                   |              |   |        |             |              |       |                              |                                                                                            |
|----------|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|---|--------|-------------|--------------|-------|------------------------------|--------------------------------------------------------------------------------------------|
| acetate  |            |                                                                                                                                                                   |              |   |        |             |              |       |                              |                                                                                            |
| 372,2283 | 8,083069   | Epoxyoxopregnenyl acetate/Hydroxyprogesterone acetate/AcetoxypregnEnDione/Deoxycorticosterone acetate/Hydroxypregnenedioneacetate/Carboxy-tocotrienol             | C23H32O4     | 3 | C14635 |             |              | 70223 | YRLVTBXOGJMNZC-QHKUYLHMSA-N  | CC(=O)O[C@H]1CC[C@@]2(C)C(=CC[C@H]3[C@@H]4C[C@H]5O[C@@]5(C(C)=O)[C@@]4(C)CC[C@@H]32)C1     |
| 374,2429 | 8,717892   | Androstenediol diacetate/Diacetoxyandrostene/Calcitroic acid /hydroxytetranorvitamin D3 carboxylic acid                                                           | C23H34O4     | 3 | C15423 |             |              | 70892 | FKDRTPPOFBKQAT-KVWWBZGASA-N  | CC(=O)O[C@H]1CC[C@H]2[C@@H]3CCC4=C[C@H](OC(C)=O)CC[C@]4(C)[C@H]3CC[C@]12C                  |
| 375,3113 | 10,080096  | Adrenoyl-EA                                                                                                                                                       | C24H41NO2    | 3 | C13829 | HMDB0013626 | LMFA08040047 | 3725  | FMVHVRYFQIXOAF-DOFZRALJSA-N  | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC(=O)NCCO                                                  |
| 378,2748 | 10,213872  | Norursodeoxycholic acid                                                                                                                                           | C23H38O4     | 3 |        |             | LMST04060021 |       | QYYDXDSPYPOWRO-JHMCBHKWSA-N  | C[C@@H](CC(O)=O)[C@@H]1CC[C@@H]2[C@@H]3[C@@H](CC[C@]21C)[C@]1(C)CC[C@H](O)C[C@@H]1C[C@H]3O |
| 379,2486 | 6,9456434  | Sphingosine phosphate/palmitoyl-phosphoethanolamine/                                                                                                              | C18H38NO5P   | 3 | C06124 | HMDB0000277 | LMSP01050001 | 3891  | DUYSYHSSBDVJSM-KRWOKUGFSA-N  | CCCCCCCCCCCCC/C=C/[C@@H](O)[C@@H](N)COP(O)(O)=O                                            |
| 380,019  | 0,68728715 | Thioxanthine-monophosphate/Thioxanthylic acid                                                                                                                     | C10H13N4O8PS | 3 | C16618 | HMDB0060418 |              | 71265 | WMRIQGFRLQENF-UUOKFMHZSA-N   | O[C@@H]1[C@@H](COP(O)(O)=O)O[C@H]([C@@H]1O)N1C=NC2=C1N=C(O)N=C2S                           |
| 380,1966 | 6,7421584  | PA(14:1)/Fludrocortisone                                                                                                                                          | C17H33O7P    | 3 |        | HMDB0062311 | LMGP10050038 | 82357 | IQSHJASKBUVXAG-OGZRUICASA-N  | CCCC/C=C\CCCCCCCC(=O)OC[C@@H](O)COP(O)(O)=O                                                |
| 381,2643 | 7,071735   | Sphinganine-phosphate                                                                                                                                             | C18H40NO5P   | 3 | C01120 | HMDB0001383 | LMSP01050002 | 3512  | YHEDRJPUIRMZMP-ZWKOTPCBSA-N  | CCCCCCCCCCCCC[C@@H](O)[C@@H](N)COP(O)(O)=O                                                 |
| 382,1088 | 0,70761234 | Deoxyaklanonic acid                                                                                                                                               | C21H18O7     | 3 | C12420 |             |              | 63798 | GOOWFUBMXUJYPR-UHFFFAOYSA-N  | CCC(=O)CC(=O)c1c(CC(=O)O)cc2c(c1O)C(=O)c1c(O)ccc1C2                                        |
| 382,2127 | 7,3865623  | LPA(14:0)/Dioxocholatrienoic Acid                                                                                                                                 | C17H35O7P    | 3 |        | HMDB0114765 |              |       | QWRVNPWTRIUQK D-UHFFFAOYSA-N | CC(C)CCCCCCCCC(=O)OCC(O)COP(O)(O)=O                                                        |
| 387,2464 | 5,478015   | Lys Gln Leu/linoleoyl taurine                                                                                                                                     | C17H33N5O5   | 3 |        |             |              | 19534 |                              |                                                                                            |
| 388,1871 | 6,0318613  | dihydroxyhydroxypropylmethylbutenylmethylbutanoylchomenone/phenoxy tetranor Prostaglandin E2/ethyl(pentanyl)trihydroxy (hydroxymethyl)tetrahydropyranylpurimidine | C22H28O6     | 3 |        | HMDB0132234 |              |       | LVYGPLHUPURZDF-UHFFFAOYSA-N  | CCC(C)C(=O)C1=C(O)C(CC=C(C)C)=C(O)C2=C1OC(=O)C=C2C(O)CC                                    |
| 388,2231 | 7,2913384  | phenyl trinor PGF2a                                                                                                                                               | C23H32O5     | 3 |        |             |              | 45710 |                              |                                                                                            |

|          |            |                                                                                                      |            |   |        |              |              |       |                              |                                                                                        |
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| 390,2018 | 6,110873   | phenoxy tetranor PGF2a                                                                               | C22H30O6   | 3 |        |              |              | 45692 |                              |                                                                                        |
| 390,202  | 6,110873   | trifluoro-LTB4/Leu Arg Cys/phenoxy tetranor PGF2a                                                    | C20H29F3O4 | 3 |        | LMFA03020019 |              | 36250 | YKIRCSCMMMEEDI-QAASZIRWSA-N  | OC(=O)CCC[C@@H](O)/C=C\C=C\C=C\C[C@@H](O)C/C=C\CCCC(F)(F)F                             |
| 392,2175 | 6,1693935  | Phe Ala Arg/dodecatetraenyldioxolanylhydroperoxyheptenoic acid                                       | C18H28N6O4 | 3 |        |              |              | 17594 |                              |                                                                                        |
| 394,2146 | 10,832013  | dimethyloctadientrihydroxyphenylphenylpropanone/Dihydrodexamethasone                                 | C25H30O4   | 3 |        | HMDB0133093  |              |       | XZHQFEUSMBHNND-UHFFFAOYSA-N  | CC(C)=CCCC(C)=CCC1=C(O)C(C(=O)CCC2=CC=CC=C2)=C(O)C=C1O                                 |
| 394,2696 | 8,254971   | Prostaglandin E2 isopropyl ester                                                                     | C23H38O5   | 3 |        |              |              | 44811 |                              |                                                                                        |
| 396,2282 | 7,6592965  | PA(15:0)/hydroxy-(phosphonoxy)octadecanoic acid/CG 4305/CG 4305                                      | C18H37O7P  | 3 |        | HMDB0062324  | LMGP10050037 | 82356 | RZDCKQARKXMIQI-QGZVFWFLSA-N  | CCCCCCCCCCCCC(=O)OC[C@@H](O)COP(O)(O)=O                                                |
| 396,2291 | 7,487876   | PA(15:0)                                                                                             | C25H32O4   | 3 | C14642 |              |              | 43240 | UDKABVSQKJNBH-DWNQPYOZSA-N   | C=C1C[C@H]2[C@@H]3C=C(C)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@@]1(OC(C)=O)C(C)=O       |
| 398,2069 | 6,756163   | Trioxocholadienoic Acid                                                                              | C24H30O5   | 3 |        |              | LMST04010365 | 84672 | OWMHJRCOYHXTBV-UJRNQWHJSA-N  | C[C@@H](CCC(O)=O)[C@@H]1CC[C@@H]2[C@@H]3[C@@H](CC(=O)[C@]21C)[C@]1(C)C=CC(=O)C=C1CC3=O |
| 398,2081 | 6,162063   | Beraprost/Taprostene/Trioxocholadienoic Acid                                                         | C24H30O5   | 3 |        |              |              | 45629 |                              |                                                                                        |
| 398,2127 | 6,5254145  | Pregnanalone sulfate (Allopregnanolone sulfate)/Trioxocholadienoic Acid                              | C21H34O5S  | 3 |        |              |              | 3560  |                              |                                                                                        |
| 399,335  | 7,092093   | Palmitoylcarnitine                                                                                   | C23H45NO4  | 3 | C02990 | HMDB0000222  | LMFA07070004 | 36667 | XOMRRQXKHMYSO-C-OAQYLSRUSA-N | CCCCCCCCCCCCC(=O)O[C@@H](CC([O-])=O)[C@H](C)C                                          |
| 404,2171 | 6,5185633  | Cortisol acetate/adonitoxigenin/phenoxy tetranor PGF2a methyl ester/phenoxy trinor Prostaglandin F2a | C23H32O6   | 3 | C02821 |              | LMST02030093 | 41869 | ALEXXDVDISNDU-JZYPGELDSA-N   | CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@]12C       |
| 408,2123 | 5,9047856  | Tyr Ala Arg/Arg Ser Phe                                                                              | C18H28N6O5 | 3 |        |              |              | 16793 |                              |                                                                                        |
| 414,2044 | 7,0528126  | Estratrienetriol triacetate/His Met Lys                                                              | C24H30O6   | 3 | C15382 |              |              | 70852 | LMXGPAGGDXXVARU-ULHSUKCYSA-N | CC(=O)Oc1ccc2c(c1)[C@@H](OC(C)=O)C[C@@H]1[C@@H]2CC[C@]2(C)[C@@H](OC(C)=O)CC[C@@H]12    |
| 416,2151 | 10,154117  | Gln Arg Asn                                                                                          | C15H28N8O6 | 3 |        |              |              | 19732 |                              |                                                                                        |
| 420,2465 | 10,122856  | Arg Phe Val                                                                                          | C20H32N6O4 | 3 |        |              |              | 16471 |                              |                                                                                        |
| 421,3184 | 11,3297205 | linolenyl carnitine                                                                                  | C25H43NO4  | 3 |        | HMDB0006319  |              | 58390 | DFVGGGHKDAHYIU-UHMZJXMFSA-N  | CC\C=C/C\C=C/C\C=C/C/CCCCC(=O)O[C@H]([N+](C)(C)C)CCC([O-])=O                           |

|          |            |                                                                                                                                                                              |                |   |                 |                  |       |                                 |                                                                                |
|----------|------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|---|-----------------|------------------|-------|---------------------------------|--------------------------------------------------------------------------------|
| 422,2276 | 6,194133   | Phe Arg Thr                                                                                                                                                                  | C19H30N6<br>O5 | 3 |                 |                  | 15663 |                                 |                                                                                |
| 423,3346 | 6,9261303  | Hexadecadienylcarnitine/Lin<br>oleaidyl carnitine/O-<br>linoleoylcarnitine                                                                                                   | C25H45NO<br>4  | 3 | HMDB0006<br>469 | LMFA070700<br>09 | 58418 | MJLXQSQYKZWZCB-<br>DQFWFXSYSA-N | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O[C@@H](CC([O-])=O)C[N+](C)(C)C                    |
| 425,3503 | 7,183352   | 11Z-<br>Octadecenylcarnitine/Oleoyl<br>carnitine/Elaidic<br>carnitine/Vaccenyl carnitine/                                                                                    | C25H47NO<br>4  | 3 | HMDB0013<br>338 |                  |       | HITOYGLMAFIRNI-<br>JCKUYFFHSA-N | CCCCC\C=C/CCCCCCCC(=O)O[C@H]([N+](C)(C)C)CCC([O-])=O                           |
| 426,2952 | 9,472426   | Leupeptin                                                                                                                                                                    | C20H38N6<br>O4 | 3 |                 |                  | 44689 |                                 |                                                                                |
| 427,3671 | 7,5383897  | Stearoylcarnitine/Acylcarniti<br>ne C18:0                                                                                                                                    | C25H49NO<br>4  | 3 | HMDB0000<br>848 | LMFA070700<br>08 | 46553 | FNPHNLNTJNMAEE-<br>HSZRJFAPSA-N | CCCCCCCCCCCCCCCC(=O)O[C@@H](CC([O-])=O)C[N+](C)(C)C                            |
| 430,3071 | 7,6004715  | Dioxo-cholestanoic acid                                                                                                                                                      | C27H42O4       | 3 |                 |                  | 43135 |                                 |                                                                                |
| 430,3767 | 10,410296  | toxisterol3<br>B1/ethoxydihydrovitamin D3<br>/<br>ethoxydihydrocholecalciferol<br>/Dimethylcholestendiol/Hydr<br>oxymethylmethylcholestenol<br>/hydroxysterol/tocopher<br>ol | C29H50O2       | 3 |                 | LMST030204<br>41 | 42370 | XLEDFPGAWKXGKL-<br>HADSMPNGSA-N | CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2/C/CCC[C@@]21C=C/C=C1\C[C@@H](O)CC[C@@]1(C)OCC  |
| 437,2906 | 7,856079   | PE(16:0)                                                                                                                                                                     | C21H44NO<br>6P | 3 | HMDB0011<br>152 | LMGP020700<br>01 | 46719 | QYTPGOLNLFESQC-<br>NUTQULCTSA-N | CCCCCCCCCCCCC/C=C\OC[C@@H](O)COP(O)(=O)OCCN                                    |
| 440,29   | 0,86470366 | trifluorohydroxynorvitamin<br>/trifluorohydroxynorcholecal<br>ciferol/Suillin/Acetoxysterany<br>lgeranyldihydroxybenzene/C<br>arboxytocotrienol                              | C26H39F3O<br>2 | 3 |                 | LMST030200<br>24 | 41965 | QZGLVEKNRHZOIB-<br>PXKDVQFDSA-N | C[C@@]12CCC/C(=C\C=C3\C[C@H](O)CCC\3=C)/[C@H]1CC[C@H]2[C@@H](C)CCCC(O)C(F)(F)F |
| 440,2902 | 10,597854  | trifluorohydroxynorvitamin<br>D3 /<br>trifluorohydroxynorcholecalc<br>iferol/Carboxytocotrienol                                                                              | C26H39F3O<br>2 | 3 |                 | LMST030200<br>24 | 41965 | QZGLVEKNRHZOIB-<br>PXKDVQFDSA-N | C[C@@]12CCC/C(=C\C=C3\C[C@H](O)CCC\3=C)/[C@H]1CC[C@H]2[C@@H](C)CCCC(O)C(F)(F)F |
| 440,2903 | 10,007158  | trifluorohydroxynorvitamin<br>D3<br>/trifluorohydroxynorcholecal<br>ciferol/Carboxy-tocotrienol                                                                              | C26H39F3O<br>2 | 3 |                 | LMST030200<br>24 | 41965 | QZGLVEKNRHZOIB-<br>PXKDVQFDSA-N | C[C@@]12CCC/C(=C\C=C3\C[C@H](O)CCC\3=C)/[C@H]1CC[C@H]2[C@@H](C)CCCC(O)C(F)(F)F |
| 440,2906 | 10,936895  | trifluorohydroxynorvitamin<br>D3 /<br>trifluorohydroxynorcholecalc<br>iferol/Carboxytocotrienol                                                                              | C26H39F3O<br>2 | 3 |                 | LMST030200<br>24 | 41965 | QZGLVEKNRHZOIB-<br>PXKDVQFDSA-N | C[C@@]12CCC/C(=C\C=C3\C[C@H](O)CCC\3=C)/[C@H]1CC[C@H]2[C@@H](C)CCCC(O)C(F)(F)F |
| 446,1922 | 5,7208805  | Tyr His Gln/Asn Gln<br>Trp/Estrone glucuronide                                                                                                                               | C20H26N6<br>O6 | 3 |                 |                  | 15736 |                                 |                                                                                |
| 451,2706 | 7,1423097  | PC(O-                                                                                                                                                                        | C21H42NO       | 3 |                 | LMGP010201       | 40007 | BDCLOBVQLDSEOA-                 | CC(=O)O[C@@H](COCCCCCCCCC=C)COP([O-                                            |

|          |           |                                                                                              |                |   |                  |                  |                                           |                                                                                                                  |
|----------|-----------|----------------------------------------------------------------------------------------------|----------------|---|------------------|------------------|-------------------------------------------|------------------------------------------------------------------------------------------------------------------|
|          |           | 13:1)/PE(16:1)/LysoPE(16:1)/<br>Terpendole G                                                 | 7P             |   | 46               |                  | OAQYLSRUSA-N                              | ]](=O)OCC[N+](C)(C)C                                                                                             |
| 451,3058 | 8,302436  | PC(O-14:1)/PC(P-14:0)                                                                        | C22H46NO<br>6P | 3 | LMGP010700<br>01 | 40397            | AAFONNYQRYRPOU<br>-WTYVIMSDSA-N           | CCCCCCCCCCC/C=C/OC[C@@H](O)COP([O-<br>])(=O)OCC[N+](C)(C)C                                                       |
| 451,3066 | 8,163846  | PC(O-14:1)/PC(P-14:0)                                                                        | C22H46NO<br>6P | 3 | LMGP010700<br>01 | 40397            | AAFONNYQRYRPOU<br>-WTYVIMSDSA-N           | CCCCCCCCCCC/C=C/OC[C@@H](O)COP([O-<br>])(=O)OCC[N+](C)(C)C                                                       |
| 453,2854 | 7,6167297 | LysoPC(13:0)/LysoPE(16:0)                                                                    | C21H44NO<br>7P | 3 |                  | 40277            |                                           |                                                                                                                  |
| 453,2861 | 7,484446  | LPC(13:0)/LysoPE(16:0)                                                                       | C21H44NO<br>7P | 3 |                  | 45334            |                                           |                                                                                                                  |
| 454,3262 | 10,718492 | Norcholestanehexol                                                                           | C26H46O6       | 3 | HMDB0002<br>157  | LMST040200<br>29 | 57911<br>PYLPANOYZCSFOX-<br>UCIVWCSPSA-N  | C[C@@H](CCC(O)C(O)CO)[C@@H]1CC[C@@H]2[C<br>@@H]3[C@@H](C[C@@H](O)[C@]21C)[C@]1(C)C<br>C[C@H](O)C[C@@H]1C[C@@H]3O |
| 456,2644 | 0,6178456 | bromopentacosadienoic<br>acid/bromomethyltetracosa<br>dienoic acid                           | C25H45BrO<br>2 | 3 |                  | LMFA010901<br>03 | 96830<br>VRACWEMNOVUYQ<br>J-YIRKJRPSPA-N  | CCCCCCCCCCCCC/C=C\CC/C(/Br)=C\CCCC(O)=O                                                                          |
| 465,3217 | 8,848652  | PC(P-15:0)/PE(P-18:0)/PE(O-<br>18:1)/TetraHCA                                                | C23H48NO<br>6P | 3 |                  | LMGP010700<br>03 | 40399<br>CORCYSWIDKFRAW-<br>HIVNOOBXSA-N  | CCCCCCCCCCCCC/C=C\OC[C@@H](O)COP([O-<br>])(=O)OCC[N+](C)(C)C                                                     |
| 467,3009 | 6,8983583 | PC(14:0)/PE(17:0)/N-<br>Arachidonoyl tyrosine                                                | C22H46NO<br>7P | 3 | HMDB0010<br>379  | LMGP010500<br>12 | 40278<br>VXUOFDJKYGDUJI-<br>OAQYLSRUSA-N  | CCCCCCCCCCCCC(=O)OC[C@@H](O)COP([O-<br>])(=O)OCC[N+](C)(C)C                                                      |
| 467,3012 | 7,0025916 | PC(O-<br>12:0/2:0)/PC(0:0/14:0)/PC(1<br>4:0/0:0)/PE(17:0/0:0)/Arachi<br>donoyl tyrosine      | C22H46NO<br>7P | 3 |                  | LMGP010200<br>09 | 40038<br>WNCMKZYTILBIUSK-<br>JOCHJYFZSA-N | CCCCCCCCCCCCOC[C@@H](COP([O-<br>])(=O)OCC[N+](C)(C)C)OC(C)=O                                                     |
| 467,3364 | 7,4883213 | LPC(15:0)/LPE(18:0)                                                                          | C23H50NO<br>6P | 3 |                  | LMGP010600<br>09 | 40383<br>PPXKEQMZYFQYCI-<br>HSZRJFAPSA-N  | CCCCCCCCCCCCCCCCOC[C@@H](O)COP([O-<br>])(=O)OCC[N+](C)(C)C                                                       |
| 475,2731 | 7,031012  | PE(18:3)/LysoPE(18:3)                                                                        | C23H42NO<br>7P | 3 | HMDB0011<br>508  | LMGP020500<br>17 | 62293<br>QULMFYWLWOKODU<br>-CSLWLMPESA-N  | CCCCC/C=C\C/C=C\C/C=C\CCCC(=O)OC[C@@H](<br>O)COP(O)(=O)OCCN                                                      |
| 476,0961 | 0,996174  | trihydroxy-hydroxy-<br>hydroxyphenyl)-methoxy-<br>oxo-chromenyl]oxyoxane-<br>carboxylic acid | C22H20O1<br>2  | 3 | HMDB0133<br>833  |                  | FZMPWQPHUKBBS<br>-UHFFFAOYSA-N            | COC1=CC2=C(C(OC3OC(C(O)C3O)C(O)=O)=C1)<br>C(O)C(O)=C(O2)C1=CC(O)=CC=C1                                           |
| 477,2857 | 7,3418517 | LysoPE(18:2)                                                                                 | C23H44NO<br>7P | 3 | HMDB0011<br>477  | LMGP020500<br>41 | 62265<br>SVRBKLJIDJHADS-<br>USWSLJGRSA-N  | CCCCC/C=CC/C=CCCCCCCC(=O)O[C@@H](COP(O)<br>(=O)OCCN)CO                                                           |
| 477,286  | 7,330837  | LysoPE(18:2)                                                                                 | C23H44NO<br>7P | 3 | HMDB0011<br>507  | LMGP020500<br>11 | 62292<br>DBHKHNGBGVWQJE<br>-USWSLJGRSA-N  | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@@H](O)C<br>OP(O)(=O)OCCN                                                        |
| 477,2863 | 7,240903  | PE(18:2)/LysoPE(18:2)                                                                        | C23H44NO<br>7P | 3 | HMDB0011<br>507  | LMGP020500<br>11 | 62292<br>DBHKHNGBGVWQJE<br>-USWSLJGRSA-N  | CCCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@@H](O)C<br>OP(O)(=O)OCCN                                                        |
| 477,3214 | 7,510645  | LPE(19:1)/LPC(16:2)                                                                          | C24H48NO<br>6P | 3 |                  | LMGP020700<br>03 | 46721<br>QKXTUVCVRMVDML<br>-IPCSYXIDSA-N  | CCCCC/C=C\CCCCCCCCC/C=C\OC[C@@H](O)COP(<br>O)(=O)OCCN                                                            |
| 477,3216 | 7,6578    | PC(O-16:2)/PE(P-19:1)/PE(P-<br>19:1)                                                         | C24H48NO<br>6P | 3 |                  |                  | 40371                                     |                                                                                                                  |
| 479,3011 | 7,814056  | LysoPE(18:1)/LysoPC(15:1)                                                                    | C23H46NO<br>7P | 3 | HMDB0011<br>505  | LMGP020500<br>64 | 62291<br>WAYKKNOEMJFLDI-<br>KOIKXXGWSA-N  | CCCCC/C=CCCCCCCCC(=O)OC[C@@H](O)COP(<br>O)(=O)OCCN                                                               |

|          |           |                                                                                                                                                                     |                  |   |            |                 |                  |       |                                                                                                                              |
|----------|-----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|---|------------|-----------------|------------------|-------|------------------------------------------------------------------------------------------------------------------------------|
| 479,302  | 7,7994123 | LysoPE(18:1)/LysoPC(15:1)                                                                                                                                           | C23H46NO<br>7P   | 3 |            |                 | 45335            |       |                                                                                                                              |
| 479,3372 | 7,885849  | PC(P-16:0)/PC(O-16:1)                                                                                                                                               | C24H50NO<br>6P   | 3 |            | HMDB0010<br>407 | LMGP010700<br>06 | 40402 | HTZINLFNXLXRB-<br>CQLBIITFSA-N<br>CCCCCCCCCCCCC/C=C\OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                   |
| 481,3164 | 7,6690063 | PC(15:0)/LysoPE(18:0)/PE(18:0)                                                                                                                                      | C23H48NO<br>7P   | 3 |            | HMDB0010<br>381 | LMGP010500<br>16 | 40282 | RJZVWDTYEWCUAR-<br>JOCHJYFZSA-N<br>CCCCCCCCCCCCC(=O)OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                   |
| 481,3165 | 8,521498  | LysoPC(15:0)/LysoPE(18:0)                                                                                                                                           | C23H48NO<br>7P   | 3 |            | HMDB0010<br>381 | LMGP010500<br>16 | 40282 | RJZVWDTYEWCUAR-<br>JOCHJYFZSA-N<br>CCCCCCCCCCCCC(=O)OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                   |
| 481,3167 | 7,1401525 | PC(15:0)/LysoPE(18:0)/PE(18:0)                                                                                                                                      | C23H48NO<br>7P   | 3 |            | HMDB0010<br>381 | LMGP010500<br>16 | 40282 | RJZVWDTYEWCUAR-<br>JOCHJYFZSA-N<br>CCCCCCCCCCCCC(=O)OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                   |
| 481,3167 | 7,302617  | PC(15:0)/LysoPE(18:0)                                                                                                                                               | C23H48NO<br>7P   | 3 |            |                 |                  | 40379 |                                                                                                                              |
| 481,317  | 8,492235  | LysoPC(15:0)/LysoPE(18:0)                                                                                                                                           | C23H48NO<br>7P   | 3 |            |                 |                  | 40283 |                                                                                                                              |
| 481,3173 | 8,016298  | PC(15:0)/LysoPE(18:0)/PE(18:0)                                                                                                                                      | C23H48NO<br>7P   | 3 |            | HMDB0010<br>381 | LMGP010500<br>16 | 40282 | RJZVWDTYEWCUAR-<br>JOCHJYFZSA-N<br>CCCCCCCCCCCCC(=O)OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                   |
| 481,3173 | 10,053656 | LysoPC(15:0)/LysoPE(18:0)                                                                                                                                           | C23H48NO<br>7P   | 3 | C214<br>84 | HMDB0011<br>130 | LMGP020500<br>01 | 40775 | BBYWOYAFBUOUFP-<br>JOCHJYFZSA-N<br>CCCCCCCCCCCCCCCCC(=O)OC[C@@H](O)COP(O)(=O)OCCN                                            |
| 481,3531 | 7,8826065 | PC(O-16:0)/Lyso-PAF C-16/Hexadecyllysoglycerophosphocholine/Hexadecyllysoglycerophosphocholine                                                                      | C24H52NO<br>6P   | 3 | C139<br>03 |                 |                  | 40386 | VLBPWIYTPAXCFJ-<br>UHFFFAOYSA-N<br>CCCCCCCCCCCCC(O)COP(=O)([O-])OCC[N+](C)(C)C                                               |
| 484,1057 | 9,395986  | Tyr-Phe4Cl-OH                                                                                                                                                       | C24H21ClN<br>2O7 | 3 |            |                 |                  | 64977 |                                                                                                                              |
| 484,2826 | 8,861693  | PG(16:0)/Biotin-XX hydrazide                                                                                                                                        | C22H45O9<br>P    | 3 |            |                 | LMGP040500<br>08 | 46733 | BVJSKAUUFXBDOB-<br>LEWJYISDSA-N<br>CCCCCCCCCCCCC(=O)OC[C@@H](O)COP(O)(=O)OC[C@@H](O)CO                                       |
| 484,3532 | 10,349505 | Hydroxyvitamin D3 diacetate/Hydroxyprevitamin D3 diacetate/dihydroxymethoxydimethyltetrahydrohomovitamin D3 / dihydroxymethoxydimethyltetrahydrohomocholecalciferol | C31H48O4         | 3 |            |                 | LMST030206<br>56 | 42582 | JRQYVHHHASBIEU-<br>NQTFQPGQSA-N<br>CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2/C/CCC[C@@H]21C=C/C=C1/C[C@H](C[C@H](OC(C)=O)C/1=C)OC(C)=O |
| 493,3167 | 7,1728024 | PC(16:1)/PE(19:1)                                                                                                                                                   | C24H48NO<br>7P   | 3 |            |                 | LMGP010500<br>21 | 40287 | LFUDDCMNKWEOR-<br>N-BREAQWACSA-N<br>CCCCC/C=C/CCCCCCCC(=O)OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                             |
| 493,3531 | 8,112179  | LysoPC(P-17:0)                                                                                                                                                      | C25H52NO<br>6P   | 3 |            |                 | LMGP010700<br>07 | 40403 | JJALPXFJIIZPRV-<br>HFQDTZRISA-N<br>CCCCCCCCCCCCC/C=C\OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                  |
| 493,3531 | 8,321449  | PC(P-17:0)/PE(P-20:0)                                                                                                                                               | C25H52NO<br>6P   | 3 |            |                 | LMGP010700<br>07 | 40403 | JJALPXFJIIZPRV-<br>HFQDTZRISA-N<br>CCCCCCCCCCCCC/C=C\OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                  |
| 493,3542 | 10,067764 | PC(P-17:0)/PE(P-20:0)                                                                                                                                               | C25H52NO<br>6P   | 3 |            |                 | LMGP010700<br>07 | 40403 | JJALPXFJIIZPRV-<br>HFQDTZRISA-N<br>CCCCCCCCCCCCC/C=C\OC[C@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                  |
| 495,3329 | 7,657617  | LPC(16:0)                                                                                                                                                           | C24H50N          | 2 |            |                 | LMGP01020        | 40048 | HEALIQQDEGDS<br>CCCCCCCCCCCCCOC[C@@H](COP([O-                                                                                |



|          |           |                                                                                                                                                                          |                |   |                  |                  |                                 |                                                           |                                                                                            |
|----------|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|---|------------------|------------------|---------------------------------|-----------------------------------------------------------|--------------------------------------------------------------------------------------------|
|          |           | A                                                                                                                                                                        | 8P             |   | 02               |                  | -PKTZIBPZSA-N                   | OC[C@H](N)C(O)=O                                          |                                                                                            |
| 511,3273 | 7,1057754 | PS(O-18:0)/Scyphostatin A                                                                                                                                                | C24H50NO<br>8P | 3 | LMGP030600<br>02 | 78862            | LLZPQHOZAQNDCM<br>-PKTZIBPZSA-N | CCCCCCCCCCCCCCCCCOC[C@H](O)COP(O)(=O)<br>OC[C@H](N)C(O)=O |                                                                                            |
| 517,3164 | 6,313918  | PC(18:3)                                                                                                                                                                 | C26H48NO<br>7P | 3 |                  | 40303            |                                 |                                                           |                                                                                            |
| 517,3166 | 7,0514975 | PC(18:3)                                                                                                                                                                 | C26H48NO<br>7P | 3 | HMDB0010<br>387  | LMGP010501<br>28 | 61697                           | MRTUWVDDQVMU<br>CR-ACHCNROVSA-N                           | CCCC/C=C\C/C=C\C/C=C\C\CCCC(=O)OC[C@H](<br>O)COP([O-])(=O)OCC[N+](C)(C)C                   |
| 517,3167 | 6,4401526 | PC(18:3)                                                                                                                                                                 | C26H48NO<br>7P | 3 |                  | 40303            |                                 |                                                           |                                                                                            |
| 519,3327 | 7,1977835 | PC(18:2)/linoleoylglycerop<br>hosphocholine                                                                                                                              | C26H50N<br>O7P | 2 | HMDB001<br>0386  | LMGP01050<br>035 | 40301                           | SPJFYYJXNPEZD<br>W-FTJOPAKQSA-<br>N                       | CCCC/C=C\C/C=C\C\CCCCCCCC(=O)OC[C<br>@H](O)COP([O-])(=O)OCC[N+](C)(C)C                     |
| 519,3336 | 7,362615  | LPC(18:2)                                                                                                                                                                | C26H50NO<br>7P | 3 | HMDB0062<br>711  |                  |                                 | LSUXCWJOIAWGOU-<br>FZVXUVPBSA-N                           | [H]C(CCCCC)=C([H])C\C([H])=C([H])CCCCCCCC(=O)<br>O[C@]([H])(CO)COP([O-])(=O)OCC[N+](C)(C)C |
| 521,3484 | 7,700527  | PC(O-<br>18:1)/LysoPC(18:1)/PC(P-<br>18:0)/PC(18:1)                                                                                                                      | C26H52NO<br>7P | 3 |                  | LMGP010201<br>47 | 40008                           | ZOFBAJKPGIIQFN-<br>RASRKNKNSA-N                           | CCCC/C=C\CCCCCCCCCOC[C@H](COP([O-<br>])(=O)OCC[N+](C)(C)C)OC(C)=O                          |
| 521,3489 | 7,8368483 | LysoPC(18:1)                                                                                                                                                             | C26H52N<br>O7P | 2 |                  | LMGP01030<br>009 | 40174                           | MULVVBYNDZRK<br>PA-<br>XCZWIQLXSA-N                       | CCCCCCCCCCCCCCCC/C=C\OC[C@H](COP<br>([O-])(=O)OCC[N+](C)(C)C)OC(C)=O                       |
| 523,3642 | 8,344322  | PE(21:0)/PC(18:0)/enantio-<br>PAF C-16/PAF C-16                                                                                                                          | C26H54NO<br>7P | 3 |                  | LMGP020500<br>26 | 77692                           | JPTRRYQAYCFMLQ-<br>RUZDIDTESA-N                           | CCCCCCCCCCCCCCCCCCCC(=O)OC[C@H](O)COP<br>(O)(=O)OCCN                                       |
| 523,3646 | 8,5379    | LysoPC(18:0)                                                                                                                                                             | C26H54N<br>O7P | 2 |                  | LMGP02050<br>026 | 77692                           | JPTRRYQAYCFM<br>LQ-RUZDIDTESA-<br>N                       | CCCCCCCCCCCCCCCCCCCCCCCC(=O)OC[C@<br>@H](O)COP(O)(=O)OCCN                                  |
| 525,2856 | 7,2928596 | LysoPE(22:6)                                                                                                                                                             | C27H44NO<br>7P | 3 | HMDB0011<br>526  | LMGP020500<br>13 | 62310                           | XEVRBOQZSXWGO<br>-PAUXPOVSA-N                             | CC/C=C\C/C=C\C\C/C=C\C\C/C=C\C\C/C=C\CCC(=<br>O)OC[C@H](O)COP(O)(=O)OCCN                   |
| 527,3014 | 7,466227  | LysoPE(22:5)                                                                                                                                                             | C27H46NO<br>7P | 3 | HMDB0011<br>525  | LMGP020500<br>70 | 62309                           | OSRWIBSJTWIKA-<br>SCFYABBUSA-N                            | CC/C=CC/C=CC/C=CC/C=CC/C=CCCCCCC(=O)OC[C<br>@H](O)COP(O)(=O)OCCN                           |
| 528,2007 | 7,541605  | Physalin                                                                                                                                                                 | C28H32O1<br>0  | 3 | HMDB0039<br>081  |                  | 93687                           | QFAOFAWTSOFSQA-<br>UHFFFAOYSA-N                           | CC1C(=O)OC2CC1(C)C1C(=O)C3(O)OC11C2(C)OC(=<br>O)C1(O)CCC1C3C(O)C=C2CC=CC(=O)C12C           |
| 535,3272 | 6,4479384 | PC(18:1)                                                                                                                                                                 | C26H50NO<br>8P | 3 |                  | LMGP010106<br>93 | 39434                           | QALLXIUHRUVULB-<br>OKFWSBNLSA-N                           | CC(=O)O[C@H](COP([O-<br>])(=O)OCC[N+](C)(C)C)COC(=O)CCCCCCC/C=C\CCCC<br>CC                 |
| 535,3645 | 8,235748  | PC(O-<br>19:1)/LysoPE(22:1)/PE(22:1)/<br>PC(19:1)                                                                                                                        | C27H54NO<br>7P | 3 |                  | LMGP010200<br>70 | 40097                           | FZTHXYOLVRRAMJ-<br>AREMUKBSSA-N                           | CCCCCCCCCCCCCCCCCOC[C@H](COP([O-<br>])(=O)OCC[N+](C)(C)C)OC(=O)C=C                         |
| 535,3998 | 9,048944  | PC(O-20:0)/11alpha-(4-<br>dimethylaminophenyl)-<br>1alpha,25-dihydroxyvitamin<br>D3 / 11alpha-(4-<br>dimethylaminophenyl)-<br>1alpha,25-<br>dihydroxycholecalciferol/dl- | C28H58NO<br>6P | 3 |                  |                  | 40228                           |                                                           |                                                                                            |

|                              |           |                                                     |                |   |                 |                  |       |                                  |                                                                                                    |
|------------------------------|-----------|-----------------------------------------------------|----------------|---|-----------------|------------------|-------|----------------------------------|----------------------------------------------------------------------------------------------------|
| alpha-Tocopherol nicotinate; |           |                                                     |                |   |                 |                  |       |                                  |                                                                                                    |
| 537,3427                     | 6,621509  | PC(18:0)/PS(P-20:0)                                 | C26H52NO<br>8P | 3 |                 | LMGP010109<br>89 | 40025 | KDXVSDQFHRZPKV-<br>RUZDIDTESA-N  | CC(=O)OC[C@@H](COP([O-])<br>(=O)OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCC                                 |
| 537,3788                     | 8,903561  | LysoPE(22:0)                                        | C27H56NO<br>7P | 3 | HMDB0011<br>490 | LMGP020500<br>54 | 62278 | NVLXNEISHNIEBO-<br>AREMUKBSSA-N  | CCCCCCCCCCCCCCCCCCCC(=O)O[C@@H](COP(O<br>(=O)OCCN)CO                                               |
| 537,3796                     | 9,109756  | PC(O-19:0)/LysoPE(22:0)/PE(22:0)                    | C27H56NO<br>7P | 3 |                 | LMGP010200<br>68 | 40095 | IMFQQPWSHMFNRT<br>-AREMUKBSSA-N  | CCC(=O)O[C@@H](CCCCCCCCCCCCCCCC)COP([O-])<br>(=O)OCC[N+](C)(C)C                                    |
| 537,4147                     | 10,150806 | PC(O-20:0)                                          | C28H60NO<br>6P | 3 |                 |                  | 40181 |                                  |                                                                                                    |
| 539,3226                     | 7,16983   | LPS(19:0)                                           | C25H50NO<br>9P | 3 |                 | LMGP030500<br>28 | 78855 | QZTQWDNDCFZUCX<br>-PKTZIBPZSA-N  | CCCCCCCCCCCCCCCC(=O)OC[C@@H](O)COP(O<br>(=O)OC[C@H](N)C(O)=O                                       |
| 541,3168                     | 7,0437965 | PC(20:5)                                            | C28H48NO<br>7P | 3 | HMDB0010<br>397 | LMGP010500<br>50 | 40316 | PDIGSOAOQOXRDU-<br>WJPZTBRDSA-N  | CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OC[C@@H](O)COP([O-])<br>(=O)OCC[N+](C)(C)C                  |
| 541,3396                     | 7,5290046 | dihydroxycholestanoyl<br>taurine                    | C29H51NO<br>6S | 3 |                 | LMST050400<br>08 | 57994 | JPTLXYYSWLLUOV-<br>NZSCTMKGSA-N  | C[C@@]12CCC3C(C1CCC2[C@@H](C)CCC[C@H](C)<br>C(=O)NCCS(O)(=O)=O)[C@@H](O)C[C@H]1C[C@@H](O)CC[C@]13C |
| 541,3404                     | 7,667154  | dihydroxycholestanoyl<br>taurine                    | C29H51NO<br>6S | 3 |                 | LMST050400<br>08 | 57994 | JPTLXYYSWLLUOV-<br>NZSCTMKGSA-N  | C[C@@]12CCC3C(C1CCC2[C@@H](C)CCC[C@H](C)<br>C(=O)NCCS(O)(=O)=O)[C@@H](O)C[C@H]1C[C@@H](O)CC[C@]13C |
| 543,3321                     | 7,177292  | PC(20:4)/LysoPC(20:4)                               | C28H50NO<br>7P | 3 |                 | LMGP010501<br>21 | 46690 | IGJKYDBBINVMLH-<br>JXRLJXCWSA-N  | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)O[C@@H](CO)COP([O-])<br>(=O)OCC[N+](C)(C)C                     |
| 543,3325                     | 7,348899  | PC(20:4)/LysoPC(20:4)                               | C28H50NO<br>7P | 3 |                 |                  | 40315 |                                  |                                                                                                    |
| 545,3479                     | 7,495645  | LysoPC(20:3)                                        | C28H52NO<br>7P | 3 | HMDB0010<br>394 | LMGP010501<br>33 | 61704 | BBNHCUQBQEQJHIG-<br>FZZJNMCHSA-N | CCCCC/C=C\C/C=C\C/C=C\CCCCCCC(=O)OC[C@@H](O)COP([O-])<br>(=O)OCC[N+](C)(C)C                        |
| 545,3481                     | 7,6089    | LysoPC(20:3)                                        | C28H52NO<br>7P | 3 | HMDB0010<br>394 | LMGP010501<br>33 | 61704 | BBNHCUQBQEQJHIG-<br>FZZJNMCHSA-N | CCCCC/C=C\C/C=C\C/C=C\CCCCCCC(=O)OC[C@@H](O)COP([O-])<br>(=O)OCC[N+](C)(C)C                        |
| 547,3633                     | 7,902995  | PC(O-20:2)                                          | C28H54NO<br>7P | 3 |                 | LMGP010201<br>58 | 40019 | ICPPVEDRGDADTQ-<br>IZZMTCJOSA-N  | CCCCC/C=C\C/C=C\CCCCCCCCOC[C@@H](COP([O-])<br>(=O)OCC[N+](C)(C)C)OC(C)=O                           |
| 547,3633                     | 8,040506  | LysoPC(O-20:2)                                      | C28H54NO<br>7P | 3 |                 | LMGP010201<br>58 | 40019 | ICPPVEDRGDADTQ-<br>IZZMTCJOSA-N  | CCCCC/C=C\C/C=C\CCCCCCCCOC[C@@H](COP([O-])<br>(=O)OCC[N+](C)(C)C)OC(C)=O                           |
| 549,3774                     | 8,516408  | Pyrrolidino PAF C-16/PC(P-20:0)/PC(20:1)/PC(O-20:1) | C28H56NO<br>7P | 3 |                 |                  | 62930 |                                  |                                                                                                    |
| 549,3791                     | 8,702327  | PC(20:1)/PC(P-20:0)/Pyrrolidino PAF C-16            | C28H56NO<br>7P | 3 |                 | LMGP010500<br>47 | 40313 | GJTDRNFWIDPARY-<br>GTPZACKGSA-N  | CCCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](O)COP([O-])<br>(=O)OCC[N+](C)(C)C                               |
| 551,322                      | 6,1284285 | PS(20:1/0:0)                                        | C26H50NO<br>9P | 3 |                 | LMGP030500<br>20 | 78847 | WQWSUENXYNSINA<br>-KCVNTPOGSA-N  | CCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](O)COP(O)<br>(=O)OC[C@H](N)C(O)=O                                 |
| 551,322                      | 6,5090704 | PS(20:1)                                            | C26H50NO<br>9P | 3 |                 | LMGP030500<br>20 | 78847 | WQWSUENXYNSINA<br>-KCVNTPOGSA-N  | CCCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](O)COP(O)<br>(=O)OC[C@H](N)C(O)=O                                |
| 551,3934                     | 8,822981  | PC(20:0)/PAF C-18                                   | C28H58NO<br>7P | 3 |                 |                  | 40164 |                                  |                                                                                                    |
| 551,3949                     | 9,710144  | LysoPC(20:0)                                        | C28H58NO<br>7P | 3 | HMDB0010<br>390 | LMGP010500<br>45 | 40311 | UATOAILWGVRQS-<br>HHHXNRCGSA-N   | CCCCCCCCCCCCCCCC(=O)OC[C@@H](O)COP([O-])<br>(=O)OCC[N+](C)(C)C                                     |

|          |           |                                                                                                |                 |   |                 |                  |        |                                                                                                                                                                  |
|----------|-----------|------------------------------------------------------------------------------------------------|-----------------|---|-----------------|------------------|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 557,3102 | 6,192817  | PC(20:4)                                                                                       | C28H48NO<br>8P  | 3 |                 | 39147            |        |                                                                                                                                                                  |
| 562,4201 | 10,640892 | Campesteryl glucoside                                                                          | C34H58O6        | 3 |                 | LMST010311<br>26 | 103408 | FWNZEKQVBDXWKA<br>-ZCWREFTMSA-N<br>CC(C)[C@@H](C)CC[C@H](C)[C@@H]1CC[C@@H]<br>2[C@H]3CC=C4C[C@@H](CC[C@@H]4(C)[C@@H]3<br>CC[C@H]21C)O[C@H]1OC(CO)[C@H](O)C(O)C1O |
| 567,3173 | 6,245624  | PS(10:0/10:0)/Glucuronosylh<br>yodeoxycholate                                                  | C26H50NO<br>10P | 3 |                 | LMGP030100<br>22 | 40807  | LRIPXDCMGANCAE-<br>PKTZIBPZSA-N<br>CCCCCCCCC(=O)OC[C@H](COP(O)(=O)OC[C@H]<br>(N)C(O)=O)OC(=O)CCCCCCCCC                                                           |
| 567,3322 | 7,3212414 | PC(22:6)                                                                                       | C30H50NO<br>7P  | 3 |                 |                  | 40321  |                                                                                                                                                                  |
| 567,3542 | 7,7095814 | PS(21:0)                                                                                       | C27H54NO<br>9P  | 3 |                 | LMGP030500<br>26 | 78853  | IFZCAKDVWKLKEK-<br>RPBOFIJWSA-N<br>CCCCCCCCCCCCCCCCC(=O)OC[C@@H](O)COP<br>(O)(=O)OC[C@H](N)C(O)=O                                                                |
| 567,3554 | 7,8525476 | PS(21:0)                                                                                       | C27H54NO<br>9P  | 3 |                 | LMGP030500<br>26 | 78853  | IFZCAKDVWKLKEK-<br>RPBOFIJWSA-N<br>CCCCCCCCCCCCCCCCC(=O)OC[C@@H](O)COP<br>(O)(=O)OC[C@H](N)C(O)=O                                                                |
| 569,346  | 7,4238377 | LysoPC(22:5)                                                                                   | C30H52NO<br>7P  | 3 | HMDB0010<br>403 | LMGP010501<br>43 | 61712  | BIEOSECQPGGZMF-<br>NAIWXXGBSA-N<br>CC/C=CC/C=CC/C=CC/C=CC/C=CCCCC(=O)OC[C<br>@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                                  |
| 569,3475 | 7,680326  | LysoPC(22:5)                                                                                   | C30H52NO<br>7P  | 3 | HMDB0010<br>403 | LMGP010501<br>43 | 61712  | BIEOSECQPGGZMF-<br>NAIWXXGBSA-N<br>CC/C=CC/C=CC/C=CC/C=CC/C=CCCCC(=O)OC[C<br>@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                                  |
| 571,3617 | 7,899891  | PC(22:4)/Diprenylpaxilline                                                                     | C30H54NO<br>7P  | 3 | HMDB0010<br>401 | LMGP010501<br>24 | 61710  | ZOJBSSVHFSBHMP-<br>JJJSWPRASA-N<br>CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC(=O)OC[C<br>@@H](O)COP([O-])(=O)OCC[N+](C)(C)C                                               |
| 577,3736 | 8,338145  | PC(42:1)                                                                                       | C29H56NO<br>8P  | 3 |                 | LMGP010106<br>73 | 39414  | SOZUKXUDKQAUF-<br>HHHXNRCGSA-N<br>CCCCCCCCCCCCCCC(=O)OC[C@@H](COP([O-]<br>])(=O)OCC[N+](C)(C)C)OC(=O)CCC=C                                                       |
| 579,3528 | 8,013977  | PC(20:0(CHO))/1-palmitoyl-<br>4-oxobutanoyl-sn-glycero-3-<br>phosphocholine/OB-<br>PC/PS(22:1) | C44H81NO<br>8P  | 3 |                 |                  |        |                                                                                                                                                                  |
| 579,389  | 8,415118  | PC(21:0)/PE(24:0)                                                                              | C29H58NO<br>8P  | 3 |                 | LMGP010108<br>29 | 39570  | BTUFMQGOQOCKK<br>M-HHHXNRCGSA-N<br>CCC(=O)O[C@@H](COP([O-]<br>])(=O)OCC[N+](C)(C)C)COC(=O)CCCCCCCCCCCC<br>CC                                                     |
| 593,3689 | 8,116122  | PC(16:0/5:0(CHO))/palmitoyl<br>(oxovaleroyl)glycerophospho<br>choline/POV-PC/OV-PC             | C29H56NO<br>9P  | 3 |                 |                  |        |                                                                                                                                                                  |
| 605,4047 | 8,590739  | PE(26:0)                                                                                       | C31H60NO<br>8P  | 3 |                 | LMGP020103<br>59 | 76594  | YKTMHVWVXDZXEQ<br>-HQGHLRICSA-N<br>CCCCCCCCCCC(=O)OC[C@@H](COP(O)(=O)OCCN)<br>OC(=O)CCCCCCC/C=C\CCCC                                                             |
| 609,3643 | 7,812722  | LysoPC(21:0)                                                                                   | C28H54NO<br>10P | 3 |                 |                  |        |                                                                                                                                                                  |
| 618,2778 | 8,923297  | PI(20:5)                                                                                       | C29H47O1<br>2P  | 3 |                 | LMGP060500<br>26 | 81191  | NAVULVNLGJVPQU-<br>DFBNLFNOSA-N<br>CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OC[C<br>@H](O)COP(O)(=O)O[C@@H]1C(O)[C@H](O)C<br>(O)C(O)C1O                            |
| 620,2958 | 8,775469  | PI(20:4)/arachidonoylglycero<br>phosphomyoinositol                                             | C29H49O1<br>2P  | 3 |                 | LMGP060500<br>06 | 46748  | LXUGKKVCTSYZFK-<br>MUOQEERCISA-N<br>CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)OC[C@<br>H](O)COP(O)(=O)O[C@@H]1C(O)[C@H](O)C(O)C<br>(O)C1O                              |
| 649,3969 | 7,903001  | PC(17:1(CHO-<br>OH))/PS(26:1)/palmitoyl(hyd<br>roxoxooctenoyl)glyceropho                       | C32H60NO<br>10P | 3 |                 |                  |        |                                                                                                                                                                  |

|                    |           |                                                                                               |                 |   |                 |                  |       |                                 |                                                                                                                                                                                       |
|--------------------|-----------|-----------------------------------------------------------------------------------------------|-----------------|---|-----------------|------------------|-------|---------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| sphocholineHOOA-PC |           |                                                                                               |                 |   |                 |                  |       |                                 |                                                                                                                                                                                       |
| 649,4316           | 8,972283  | PC(25:0 CHO)                                                                                  | C33H64NO<br>9P  | 3 |                 | LMGP200100<br>08 | 82381 | PPTNNIINSQWCE-<br>WJOKGBTCSA-N  | CCCCCCCCCCCCCCCC(=O)OC[C@@H](COP([O-])<br>(=O)OCC[N+](C)(C)C)OC(=O)CCCCCCC=O                                                                                                          |
| 649,432            | 9,514757  | PC(16:0/9:0)/palmitoyloxono<br>nanoyl)-sn-<br>glycerophosphocholine                           | C33H64NO<br>9P  | 3 |                 |                  |       |                                 |                                                                                                                                                                                       |
| 663,4475           | 9,803808  | PC(26:0(COH))/palmitoyl(oxo<br>decanoyl)-sn-glycero-3-<br>phosphocholine/OD-<br>PC/PS(P-28:0) | C34H66NO<br>9P  | 3 |                 |                  |       |                                 |                                                                                                                                                                                       |
| 665,427            | 8,336828  | PC(25:0(COOH))/palmitoylaz<br>elaoylglycerophosphocholine<br>/AZ-PC/PS(27:0)/PAz-PC           | C33H64NO<br>10P | 3 |                 |                  |       |                                 |                                                                                                                                                                                       |
| 677,4635           | 10,12566  | PC(16:0/11:0)/palmitoyl(oxo<br>undecanoyl)-sn-<br>glycerophosphocholine/OU-<br>PC/PS(P-29:0)  | C35H68NO<br>9P  | 3 |                 |                  |       |                                 |                                                                                                                                                                                       |
| 689,4282           | 9,229844  | PS(29:2)                                                                                      | C35H64NO<br>10P | 3 |                 | LMGP030102<br>78 | 77942 | YZWDXSZQZCNQND<br>-JKHFDAINSA-N | CCCC/C=C\C/C=C\CCCCCCCC(=O)OC[C@@H](COP(O)<br>(=O)OC[C@@H](N)C(O)=O)OC(=O)CCCCCCCCC<br>C                                                                                              |
| 691,4412           | 8,511854  | PS(29:1)                                                                                      | C35H66NO<br>10P | 3 |                 | LMGP030102<br>48 | 77912 | ODAOIIMAACFDKX-<br>UKODLXMQSA-N | CCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](COP(O)(<br>=O)OC[C@@H](N)C(O)=O)OC(=O)CCCCCCCCC                                                                                                      |
| 691,4433           | 8,947102  | PS(29:1)                                                                                      | C35H66NO<br>10P | 3 |                 | LMGP030100<br>51 | 77715 | AZRMVTACVQNFOG<br>-UKODLXMQSA-N | CCCCCCCCCCCC(=O)OC[C@@H](COP(O)(=O)OC[C<br>@@H](N)C(O)=O)OC(=O)CCCCCCC/C=C\CCCCCCC                                                                                                    |
| 693,4582           | 9,350933  | PS(29:0)                                                                                      | C35H68NO<br>10P | 3 | HMDB0112<br>273 | LMGP030109<br>30 | 78594 | RDGOWVQONPEGM<br>L-ZWXJPIIXSA-N | CCCCCCCCCCCCCCCC(=O)OC[C@@H](COP(O)(=O)OC<br>C@@H](N)C(O)=O)OC(=O)CCCCCCCCCCCCC                                                                                                       |
| 714,4812           | 5,7083187 | Deoxymyxol fucoside                                                                           | C46H66O6        | 3 | C159<br>40      |                  | 64118 | LQRQZOJVMFJJLX-<br>LISSMLHSA-N  | CC1=C/C=C/C(C)=C/C=C/C(C)=C/C=C/C(C)/C=C/<br>C=C(C)/C=C/C=C(C)/C=C/[C@H](O)[C@@H]2O[C@<br>@H](C)[C@@H](O)[C@@H](O)[C@@H]2O)C(C)(C)<br>O)C(C)(C)CCC1                                   |
| 716,4579           | 5,698094  | PG(32:3)                                                                                      | C38H69O1<br>0P  | 3 |                 | LMGP040103<br>68 | 79193 | PZHKWBXQKJOTIF-<br>GIJSEMSA-N   | CCCCCCCCCCCCCCCC(=O)O[C@@H](COP(O)(=O)OC[C<br>@@H](O)CO)COC(=O)CCCC/C=C\C/C=C\C/C=C\C<br>CCC                                                                                          |
| 732,4243           | 5,704729  | Kurilensoside J                                                                               | C37H64O1<br>4   | 3 |                 | LMST050500<br>20 | 84940 | KHUZIKFEVDFTLS-<br>ISWDZEJHSA-N | CC(C)[C@@H](CC[C@H](C)[C@@H]1C[C@@H](O)[<br>C@@H]2[C@@@]3(O)C[C@H](O)[C@@H]4[C@H](O<br>)[C@@H](CC[C@@]4(C)[C@@H]3CC[C@@]12C)O[<br>C@H]1OC[C@H](O)C(O)C1OC)O[C@H]1O[C@H](O)<br>C(O)C1O |
| 749,3086           | 8,553471  | Debenzoyltaxol/Phenylisoser<br>inoyl baccatin III                                             | C40H47NO<br>13  | 3 | C165<br>24      |                  | 64037 | DLACRDONFBNRSP-<br>UHTFTNQHSA-N | CC(=O)O[C@H]1C(=O)[C@@]2(C)C([C@H](OC(=O)c<br>3cccc3)[C@]3(O)C[C@H](OC(=O)[C@H](O)[C@<br>H](N)c4cccc4)C(C)=C1C3(C)C)[C@]1(OC(C)=O)CO[<br>C@@H]1C[C@@H]2O                              |
| 755,5472           | 11,690027 | PC(34:3)                                                                                      | C42H78NO<br>8P  | 3 | HMDB0008<br>199 | LMGP010116<br>77 | 59645 | RAPKGPDUGWBPHR<br>-QWFQJEORSA-N | CCCCCCCCCCCCCCCC(=O)O[C@@H](COP([O-]<br>])(=O)OCC[N+](C)(C)C)COC(=O)CCCCCCC/C=C\C/C=                                                                                                  |

|           |           |                                                                                                                           |                     |   |            |                  |       |                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-----------|-----------|---------------------------------------------------------------------------------------------------------------------------|---------------------|---|------------|------------------|-------|-----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|           |           |                                                                                                                           |                     |   |            |                  |       |                                   | C\C/C=C\CC                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 792,4981  | 5,709619  | PG(38:7)                                                                                                                  | C44H73O1<br>OP      | 3 |            | LMGP040106<br>60 | 79485 | YEAIPFFGULDBAZ-<br>SEVDQDBBSA-N   | CCCCC/C=C\C/C=C\C\CCCCCCC(=O)O[C@@H](COP(<br>O)(=O)OC[C@H](O)CO)COC(=O)CCC/C=C\C/C=C\<br>C/C=C\C/C/C=C\C/C/C=C\C\CC                                                                                                                                                                                                                                                                                                                           |
| 922,6826  | 5,5540676 | PI(O-41:0)                                                                                                                | C50H99O1<br>2P      | 3 |            | LMGP060200<br>66 | 81050 | DAJWPQITDOHFGF-<br>ULZUSFMRSA-N   | CCCCCCCCCCCCCCCCCCCCCOC[C@H](COP(O)(=O)<br>O[C@H]1C(O)[C@H](O)C(O)C(O)C1O)OC(=O)CCC<br>CCCCCCCCCCCCCCCCCC                                                                                                                                                                                                                                                                                                                                     |
| 942,6242  | 5,759816  | PI(42:4)                                                                                                                  | C51H91O1<br>3P      | 3 |            | LMGP060106<br>88 | 80710 | OILYSISDPYNFGDU-<br>JSQJEHOFSAN   | CCCCCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(<br>O)(=O)O[C@H]1C(O)[C@H](O)C(O)C(O)C1O)OC(<br>=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C\CCCC                                                                                                                                                                                                                                                                                                                      |
| 950,6785  | 5,7493453 | PI(42:0)/PC(DiMe(13,5)/DiM<br>e(11,5))/PC(MonoMe(13,5)/<br>MonoMe(13,5))/PC(DiMe(11<br>,5)/DiMe(13,5))                    | C51H99O1<br>3P      | 3 |            | LMGP060106<br>85 | 80707 | AMGJMFGIJRCTHV-<br>OFJFGGNTSANA   | CCCCCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(<br>O)(=O)O[C@H]1C(O)[C@H](O)C(O)C(O)C1O)OC(<br>=O)CCCCCCCCCCCCCCCCCC                                                                                                                                                                                                                                                                                                                                    |
| 1059,5627 | 5,40907   | Bradykinin                                                                                                                | C50H73N15<br>O11    | 3 | C003<br>06 | HMDB0004<br>246  | 58231 | QXZGBUJJYSLZLT-<br>FDISYFBBSA-N   | N[C@@H](CCCNC(N)=N)C(=O)N1CCC[C@H]1C(=O)<br>N1CCC[C@H]1C(=O)NCC(=O)N[C@@H](CC1=CC=C<br>C=C1)C(=O)N[C@@H](CO)C(=O)N1CCC[C@H]1C(<br>=O)N[C@@H](CC1=CC=CC=C1)C(=O)N[C@@H](CCC<br>NC(N)=N)C(O)=O                                                                                                                                                                                                                                                  |
| 2161,2676 | 7,658147  | (Mannosyl)3-(N-<br>acetylglucosaminy l)2-<br>diphosphodolichol                                                            | C114H190N<br>2O32P2 | 3 |            | HMDB0012<br>119  | 62794 | BKUXVZCTYBVOAV-<br>JLQUOVFM SAN   | OC[C@H]1O[C@H](OC[C@H]2O[C@@H](O[C@H]3<br>[C@H](O)[C@@H](NC(C)=O)[C@@H](O[C@@H]3C<br>O)O[C@H]3[C@H](O)[C@@H](NC(C)=O)[C@@H]<br>O[C@@H]3CO)OP(=O)(O)OP(=O)(O)OCCC(C)CC=C<br>C(/C)CC\C=C(/C)CC\C=C(/C)CC\C=C(/C)CC\C=C(/C)C<br>C\C=C(/C)CC\C=C(/C)CC\C=C(/C)CC\C=C(/C)CC\C=C<br>(/C)CC\C=C(/C)CC\C=C(/C)CC\C=C(/C)CC\C=C(/C)CC<br>C=C(C)C[C@@H](O)[C@@H](O[C@H]3O[C@H](C<br>O)[C@@H](O)[C@H](O)[C@@H]3O)[C@@H]2O)[C<br>@@H](O)[C@@H](O)[C@@H]1O |
| 2174,0803 | 5,981447  | NeuAalpha2-<br>8NeuAalpha2-3Galbeta1-<br>4GlcNAc beta1-3Galbeta1-<br>4GlcNAc beta1-3Galbeta1-<br>4Glcbeta-Cer(d18:1/16:0) | C96H167N5<br>O49    | 3 |            | LMSP0601GB<br>01 | 57382 | BEOTWPTXP HLJB M-<br>ZDBWLZBKSA-N |                                                                                                                                                                                                                                                                                                                                                                                                                                               |