

Supplementary Table 4 Differential metabolites between the CaOx and control group

| No. | Metabolite | Mode | Regulate | FC | <i>P</i> value | VIP value |
|-----|------------------------------------------------------------------------------------------------------------------------------------------|------|----------|--------|----------------|-----------|
| 1 | Resolvin E2 | pos | down | 0.9657 | 0.01202 | 1.1843 |
| 2 | Ketopinic acid | pos | down | 0.953 | 0.006456 | 1.4408 |
| 3 | Hexyl glucoside | pos | down | 0.8611 | 0.01012 | 2.4039 |
| 4 | 1,2-Cyclohexanedicarboxylic acid | pos | down | 0.9058 | 0.02105 | 1.7922 |
| 5 | 3,5,5-Trimethyl-1,2-cyclohexanedione | pos | down | 0.8201 | 0.004744 | 2.6467 |
| 6 | Phenylalanylhydroxyproline | pos | down | 0.7083 | 0.01246 | 2.8991 |
| 7 | 5-(delta-Carboxybutyl)homocysteine | pos | down | 0.9642 | 0.01681 | 1.1939 |
| 8 | 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(2R)-2-amino-2-(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-, (2S,5R,6R)- | pos | up | 1.2994 | 0.01732 | 2.6166 |
| 9 | Lidocaine | pos | up | 1.1431 | 0.0007363 | 2.9829 |
| 10 | Dihydrofukinolide | pos | down | 0.7619 | 0.02218 | 2.4324 |
| 11 | (5R)-5-Hydroxyhexanoylcarnitine | pos | up | 1.0587 | 0.03158 | 1.3762 |
| 12 | Pyrogallol-2-O-glucuronide | pos | down | 0.8676 | 0.02498 | 2.0153 |
| 13 | Inosine | pos | up | 1.1105 | 0.03275 | 1.654 |
| 14 | Cyclopentanol | pos | up | 1.0532 | 0.02695 | 1.3957 |
| 15 | 2-Hydroxypyridine | pos | down | 0.9413 | 0.02865 | 1.6253 |
| 16 | Creatinine | pos | down | 0.9766 | 0.002248 | 1.2081 |

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|----|--------------------------------------------------------------|-----|------|--------|-----------|--------|
| 17 | 4-Methylpyrimidine | pos | down | 0.954 | 0.01327 | 1.2046 |
| 18 | Imidazolepropionic acid | pos | down | 0.9673 | 0.01402 | 1.2485 |
| 19 | Deoxyhypusine | pos | down | 0.9228 | 0.00993 | 1.7575 |
| 20 | Urocanic acid | pos | down | 0.9696 | 0.005366 | 1.1795 |
| 21 | Alpha-amino-3-hydroxy-5-methyl-4- isoxazolepropionic acid | pos | up | 1.2005 | 0.0008183 | 2.7755 |
| 22 | 2-(4'-methylthio)butylmalate | pos | up | 1.0865 | 0.03636 | 1.4128 |
| 23 | 2,6-Diaminopurine 2',3'- dideoxyriboside | pos | down | 0.8347 | 0.04373 | 2.0873 |
| 24 | Ne,Ne dimethyllysine | pos | down | 0.9514 | 0.03195 | 1.2916 |
| 25 | Crocose | pos | up | 1.1007 | 0.02494 | 1.7727 |
| 26 | 5-Aminovaleric acid | pos | down | 0.925 | 0.0003327 | 2.0499 |
| 27 | 3-amino-1-propylpyrazin-2-one | pos | down | 0.9126 | 0.02413 | 1.7177 |
| 28 | Ethyl-4-hydroxymethyl-3(2H)- Furanone | pos | up | 1.0546 | 0.03702 | 1.32 |
| 29 | Penicilloic acid | pos | down | 0.8185 | 0.009915 | 2.7024 |
| 30 | Imidazoleacetic acid riboside | pos | down | 0.8889 | 0.04356 | 1.7872 |
| 31 | 3,7,8,15-Scirpenetretol | pos | up | 1.0566 | 0.007136 | 1.5491 |
| 32 | 2,5-Heptadien-1-ol | pos | down | 0.9157 | 0.02126 | 1.5752 |
| 33 | Isovalerylcarnitine | pos | up | 1.0622 | 0.004034 | 1.764 |
| 34 | Valganciclovir, (S)- | pos | up | 1.1339 | 0.04253 | 2.0309 |

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|----|-------------------------------------------------------------------------------------|-----|------|--------|-----------|--------|
| 35 | 3-Methoxybenzenepropanoic acid | pos | down | 0.8847 | 0.01465 | 2.0298 |
| 36 | N1-(alpha-D-ribose)-5,6-dimethyl-benzimidazole | pos | down | 0.8682 | 0.03471 | 1.8999 |
| 37 | 2-Dicyclohexylphosphino-2',6'-dimethoxybiphenyl | pos | down | 0.8793 | 0.01196 | 2.2909 |
| 38 | 6-Ethyl-3-hydroxy-2-methyl-4-pyrone | pos | down | 0.8953 | 0.01558 | 1.8895 |
| 39 | Coixinden B | pos | down | 0.9229 | 0.0269 | 1.668 |
| 40 | D-Kynurenine | pos | down | 0.8343 | 0.04011 | 1.9333 |
| 41 | Isoferulic acid | pos | down | 0.9329 | 0.04224 | 1.4417 |
| 42 | Biotin | pos | down | 0.8686 | 0.02878 | 1.9322 |
| 43 | Glycylprolylarginine | pos | up | 1.0817 | 0.0009314 | 1.9787 |
| 44 | 1-Carboxycyclohexaneacetic acid | pos | down | 0.9438 | 0.03314 | 1.3279 |
| 45 | 1,2-Dihydronaphthalene-1,2-diol | pos | down | 0.9018 | 0.04007 | 1.6729 |
| 46 | 7-[(1R,2R,3R)-3-Hydroxy-2-[(3S)-3-hydroxyoctyl]-5-oxocyclopentyl]heptanoylcarnitine | pos | up | 1.2213 | 0.01566 | 2.6161 |
| 47 | Gibberellin A14 | pos | down | 0.9364 | 0.03208 | 1.3395 |
| 48 | (15Z)-tetracosenoate | pos | up | 1.0415 | 0.007201 | 1.3642 |
| 49 | (2S)-2-Hydroxyhexadecanoylcarnitine | pos | up | 1.1692 | 0.0453 | 2.0498 |
| 50 | Diphenhydramine N-glucuronide | pos | up | 1.1377 | 0.00211 | 2.2505 |
| 51 | Xi-5-Isopropyl-2(5H)-furanone | pos | up | 1.0584 | 0.001545 | 1.5861 |

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|----|-------------------------------------------------------------------------------------------------------------------|-----|------|--------|-----------|--------|
| 52 | Polyoxyethylene 40 monostearate | pos | down | 0.8631 | 0.005168 | 2.3809 |
| 53 | 3,4-Dihydroxy-2-methoxy-4-methyl-3-[2-methyl-3-(3-methyl-but-2-enyl)-oxiranyl]-cyclohexanone | pos | down | 0.9577 | 0.04359 | 1.1774 |
| 54 | 2,3-Dipalmitoyl-S-glycerylcysteine | pos | up | 1.0685 | 0.0271 | 1.4261 |
| 55 | P-Menthane-3,8-diol | pos | down | 0.7827 | 0.001473 | 2.6463 |
| 56 | Dimethyl-3-hydroxypyrid-4-one | pos | down | 0.9577 | 0.004419 | 1.2463 |
| 57 | PE(16:0/18:0) | pos | up | 1.0824 | 0.03309 | 1.5343 |
| 58 | Gibberellin A53 | pos | down | 0.9215 | 0.003815 | 1.7722 |
| 59 | 2-[2-[2-[2-[2-[2-[(Z)-2-[2-[2-(2-Octadecoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol | pos | down | 0.7336 | 0.0001761 | 3.0566 |
| 60 | 2,3-Dihydroxypropyl dodecanoate | pos | down | 0.8972 | 0.02411 | 1.7236 |
| 61 | Solutol HS 15 | pos | up | 1.0841 | 0.007103 | 1.8565 |
| 62 | Ile-Glu-Thr-Asp-fluoromethyl ketone | pos | up | 1.1191 | 0.0146 | 1.9195 |
| 63 | 7-Epi-12-hydroxyjasmonic acid | pos | down | 0.9054 | 0.007579 | 1.9629 |
| 64 | Tsangane L 3-glucoside | pos | up | 1.2738 | 0.01807 | 2.6225 |
| 65 | 6-Hydroxydodeca-8,10-dienoylcarnitine | pos | down | 0.9613 | 0.01191 | 1.3092 |
| 66 | 3,3-Bis(carboxymethyl)hexadecanedioic acid | pos | down | 0.8724 | 0.01582 | 2.1669 |
| 67 | 3,4-Methylenesebacic acid | pos | down | 0.9454 | 0.01552 | 1.4612 |

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|----|--------------------------------------------|-----|------|--------|-----------|--------|
| 68 | Ovalicin | pos | down | 0.9569 | 0.04379 | 1.1444 |
| 69 | 11-Hydroxyyohimbine | pos | up | 1.0788 | 0.004541 | 1.8137 |
| 70 | 5(6)-Epoxy Prostaglandin E1 | pos | up | 1.0386 | 0.02821 | 1.2009 |
| 71 | 8-Hydroxydodecanoylcarnitine | pos | up | 1.0477 | 0.01838 | 1.4147 |
| 72 | Arctiopicrin | pos | up | 1.0834 | 0.03869 | 1.5942 |
| 73 | Cinnassiol A 19-glucoside | pos | up | 1.2721 | 0.003093 | 2.8859 |
| 74 | Latrunculin B | pos | up | 1.0643 | 0.03095 | 1.4327 |
| 75 | 4-Pyridoxic acid | pos | down | 0.9308 | 0.01561 | 1.5758 |
| 76 | Pantolactone | pos | up | 1.1108 | 0.02997 | 1.8865 |
| 77 | Laurenoniolide | pos | up | 1.1242 | 0.0002927 | 2.5493 |
| 78 | 4-Hydroxydodecanedioylcarnitine | pos | down | 0.943 | 0.01673 | 1.5636 |
| 79 | D-Cathine | pos | down | 0.9222 | 0.03646 | 1.4366 |
| 80 | Baicalin | pos | down | 0.6308 | 0.01029 | 3.2735 |
| 81 | 10,11-dihydro-20-trihydroxy-leukotriene B4 | pos | up | 1.1258 | 0.03484 | 1.8366 |
| 82 | 17-Hydroxymethylethisterone | pos | up | 1.204 | 0.03723 | 2.1068 |
| 83 | Midodrine | pos | down | 0.8872 | 0.02993 | 1.6939 |
| 84 | Polygonal | pos | down | 0.836 | 0.03432 | 2.1057 |
| 85 | (5E)-3-Hydroxyhept-5-enoylcarnitine | pos | up | 1.0529 | 0.005986 | 1.5319 |
| 86 | seneciophylline | pos | up | 1.0941 | 0.04324 | 1.5653 |

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| 87 | 2-Quinolincarboxylic acid | pos | down | 0.9281 | 0.02138 | 1.6785 |
| 88 | (4E)-3-Hydroxyhex-4-enoylcarnitine | pos | up | 1.2443 | 0.00181 | 2.9718 |
| 89 | 4-Hydroxy-6-Methyl-2-Pyrone | pos | down | 0.9013 | 0.01162 | 1.861 |
| 90 | FAPy-adenine | pos | down | 0.9508 | 0.009006 | 1.409 |
| 91 | B-Octylglucoside | pos | up | 1.0978 | 0.04143 | 1.4736 |
| 92 | 5-Hydroxycarvone | pos | down | 0.9174 | 0.03039 | 1.5035 |
| 93 | Naloxone | pos | up | 1.178 | 0.03244 | 2.0837 |
| 94 | Captopril-cysteine disulfide | pos | up | 1.1467 | 0.04439 | 2.0682 |
| 95 | Octanedioylcarnitine | pos | down | 0.9675 | 0.02916 | 1.1503 |
| 96 | S-(2-Hydroxyethyl)glutathione | pos | down | 0.9586 | 0.01295 | 1.2274 |
| 97 | Guanine | pos | down | 0.957 | 0.01711 | 1.2089 |
| 98 | Lindleyin | pos | down | 0.9268 | 0.02603 | 1.3985 |
| 99 | Alanylalanine | pos | down | 0.8707 | 0.008408 | 2.0739 |
| 100 | 4(1H)-Pyridinone, 3-hydroxy-1-(3-hydroxypropyl)-2-methyl- | pos | down | 0.9273 | 0.006054 | 1.617 |
| 101 | 2-Amino-4-[carbamimidoyl(methyl)amino]butanoic acid | pos | up | 1.0946 | 0.01419 | 1.5681 |
| 102 | (-)-Bornesitol | pos | up | 1.2104 | 0.001041 | 2.4936 |
| 103 | Delta-Valerolactone | pos | up | 1.0751 | 0.004143 | 1.945 |
| 104 | N-iminoethyl-l-ornithine | pos | down | 0.9459 | 0.001023 | 1.8557 |

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| 105 | Monopropionylcadaverine | pos | down | 0.7779 | 0.00116 | 2.9317 |
| 106 | N-Acetylhistamine | pos | down | 0.8823 | 0.02925 | 1.8905 |
| 107 | Niacinamide | pos | down | 0.9669 | 0.0338 | 1.1271 |
| 108 | 4-Hydroxymethylpyrazole | pos | down | 0.8911 | 0.005545 | 2.0141 |
| 109 | N,N-Dimethylarginine | pos | down | 0.9642 | 0.0001882 | 1.5117 |
| 110 | Trigonelline | pos | down | 0.7263 | 8.82E-05 | 3.5187 |
| 111 | L-Carnitine | pos | up | 1.044 | 0.008266 | 1.4958 |
| 112 | 6Z-8-Hydroxygeraniol 8-O-glucoside | pos | up | 1.0677 | 0.03921 | 1.3276 |
| 113 | Glycerolphosphorylcholine | pos | up | 1.1934 | 0.0267 | 2.0738 |
| 114 | Pyridin-3-yl sulfate | pos | down | 0.8675 | 0.01979 | 1.9802 |
| 115 | 1,2-Diethyl-3-hydroxypyridin-4-one | pos | up | 1.0553 | 0.00685 | 1.3704 |
| 116 | Loliolide | pos | down | 0.9518 | 0.03178 | 1.2199 |
| 117 | Perindoprilat glucuronide | pos | up | 1.3759 | 0.003033 | 3.1183 |
| 118 | Humulinic acid A | pos | up | 1.0756 | 0.004048 | 1.8969 |
| 119 | Chlorhexidine | pos | up | 1.3812 | 0.0003071 | 3.5722 |
| 120 | Trimazosin | pos | up | 1.1275 | 0.02856 | 1.7849 |
| 121 | (+)-Nicotine | pos | down | 0.7112 | 0.0002583 | 3.397 |
| 122 | Acetylcysteine | pos | up | 1.0678 | 0.04066 | 1.5144 |
| 123 | Artecanin | pos | down | 0.7843 | 0.03283 | 1.9862 |

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|-----|-----------------------------------------------------------|-----|------|--------|-----------|--------|
| 124 | Kynurenine | pos | down | 0.836 | 0.03497 | 1.9714 |
| 125 | P-Aminobenzoic acid | pos | down | 0.9448 | 0.03499 | 1.4328 |
| 126 | 13,14-dihydro-15-keto-tetranor Prostaglandin D2 | neg | down | 0.9607 | 0.004633 | 1.3685 |
| 127 | (R)-8-Acetoxyarvotanacetone | neg | down | 0.9505 | 0.009835 | 1.4133 |
| 128 | 1-Deoxy-D-xylulose-5-phosphate | neg | up | 1.0878 | 0.03765 | 1.5692 |
| 129 | Guanidoacetic acid | neg | down | 0.9035 | 0.04586 | 1.4933 |
| 130 | Shikimic acid | neg | down | 0.9692 | 0.02771 | 1.0541 |
| 131 | 4-Hydroxyphenytoin glucuronide | neg | up | 1.1073 | 0.03953 | 1.7028 |
| 132 | Norepinephrine sulfate | neg | down | 0.8688 | 0.0386 | 1.8982 |
| 133 | D-Sorbitol | neg | down | 0.9641 | 0.01635 | 1.1784 |
| 134 | 5-Methyl-2-furancarboxylic acid | neg | down | 0.8783 | 0.03592 | 1.9397 |
| 135 | Citrazinic acid | neg | down | 0.8257 | 0.01072 | 2.2668 |
| 136 | 4-Hydroxy-5-(dihydroxyphenyl)- valeric acid-O-sulphate | neg | down | 0.834 | 0.0001188 | 2.8982 |
| 137 | 3-Indole carboxylic acid glucuronide | neg | down | 0.9646 | 0.00992 | 1.1358 |
| 138 | Abscisic alcohol 11-glucoside | neg | down | 0.929 | 0.0182 | 1.6564 |
| 139 | 3,6-Dihydroxycyclohepta-2,4,6-trien- 1-one | neg | down | 0.8281 | 0.0102 | 2.5662 |
| 140 | 1-(2-Furyl)butan-3-one | neg | down | 0.9467 | 0.01603 | 1.3213 |
| 141 | Senkyunolide N | neg | down | 0.863 | 0.03297 | 1.8797 |

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| 142 | L-Kynurenine | neg | down | 0.9282 | 0.04553 | 1.5149 |
| 143 | 2-Phenylethanol glucuronide | neg | down | 0.9487 | 0.04597 | 1.3351 |
| 144 | PA(8:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)) | neg | down | 0.9419 | 0.0383 | 1.3637 |
| 145 | 2-Hydroxyethyl methacrylate | neg | down | 0.8874 | 0.0001849 | 2.3245 |
| 146 | (Z)-2-Methyl-2-butene-1,4-diol 4-O-beta-D-Glucopyranoside | neg | up | 1.0672 | 0.04604 | 1.3375 |
| 147 | Dihydroconiferyl alcohol | neg | down | 0.9312 | 0.02717 | 1.5105 |
| 148 | 2-Hydroxycampholonic acid | neg | down | 0.9392 | 0.04136 | 1.3149 |
| 149 | 4-(4-Fluorophenyl)-3-(4-hydroxy-3-methoxyphenoxyethyl)piperidine | neg | down | 0.9331 | 0.001671 | 1.756 |
| 150 | Tazobactam | neg | down | 0.7952 | 0.02689 | 2.7087 |
| 151 | Dehydronootkatone | neg | down | 0.88 | 0.0358 | 1.6542 |
| 152 | Hesperetin 3'-O-sulfate | neg | down | 0.8422 | 0.02038 | 2.3033 |
| 153 | 2-(4-Methoxyphenyl)ethyl hydrogen sulfate | neg | down | 0.9004 | 0.04333 | 1.6393 |
| 154 | 5-Methylhexanoic acid | neg | down | 0.9317 | 0.008646 | 1.6404 |
| 155 | LysoPA(22:5(4Z,7Z,10Z,13Z,16Z)/0:0) | neg | up | 1.1497 | 0.008843 | 2.096 |
| 156 | Anthra(1,9-cd)pyrazol-6(2H)-one, 2-(2-((2-hydroxyethyl)amino)ethyl)-5-((2-((2-hydroxyethyl)amino)ethyl)amino)- | neg | up | 1.2336 | 0.03404 | 2.1157 |
| 157 | 2-n-Propyl-4-oxopentanoic acid | neg | down | 0.8568 | 8.19E-05 | 2.7076 |

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|-----|---------------------------------------------|-----|------|--------|-----------|--------|
| 158 | Ibuprofen glucuronide | neg | up | 1.0485 | 0.03227 | 1.1727 |
| 159 | 8-Methylnonenoate | neg | down | 0.9565 | 0.02849 | 1.1387 |
| 160 | 2-tert-Butyl-4-methoxyphenol | neg | down | 0.9575 | 0.02804 | 1.2698 |
| 161 | Traumatins | neg | down | 0.9584 | 0.03928 | 1.3373 |
| 162 | Nonate | neg | down | 0.9281 | 0.002729 | 1.6331 |
| 163 | 16-alpha-Hydroxyandrosterone | neg | down | 0.9319 | 0.01075 | 1.5522 |
| 164 | Neocnidolide | neg | down | 0.9576 | 0.02675 | 1.2289 |
| 165 | 12S-HHT | neg | down | 0.9475 | 0.01855 | 1.3593 |
| 166 | Ginsenoside A | neg | down | 0.7776 | 0.007977 | 2.7622 |
| 167 | 4-Tert-Amylphenol | neg | down | 0.9046 | 0.002682 | 2.0659 |
| 168 | (+)-Dehydrovomifoliol | neg | down | 0.9071 | 0.004761 | 1.9566 |
| 169 | 3-Methylbut-2-enoylcarnitine | neg | up | 1.1065 | 0.009499 | 1.8853 |
| 170 | Glyoxal | neg | up | 1.0888 | 0.03677 | 1.783 |
| 171 | Oryzalide B | neg | down | 0.9022 | 0.009346 | 2.0244 |
| 172 | Furanogerminone | neg | down | 0.9035 | 0.002236 | 2.1379 |
| 173 | 4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one | neg | down | 0.9446 | 0.03328 | 1.339 |
| 174 | 3,5,5-Trimethyl-2-cyclohexen-1-one | neg | down | 0.9233 | 0.0007123 | 1.9351 |
| 175 | Sugeonol | neg | down | 0.9407 | 0.003321 | 1.6219 |
| 176 | Isopiperitenone | neg | down | 0.9305 | 0.00522 | 1.6574 |

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| 177 | 15-Acetyl-4-deoxynivalenol | neg | down | 0.8759 | 0.01962 | 2.2116 |
| 178 | Desacetyl-laurenobiolide | neg | down | 0.9415 | 0.0006943 | 1.7627 |
| 179 | Blumenol C glucoside | neg | up | 1.0539 | 0.04145 | 1.3238 |
| 180 | Isoforskolin | neg | up | 1.1548 | 0.02105 | 2.1814 |
| 181 | (2E,4E)-2,4-Octadien-1-ol | neg | down | 0.9345 | 0.003125 | 1.6168 |
| 182 | Phomalone | neg | down | 0.9296 | 0.003451 | 1.9774 |
| 183 | Tetranorprostanedioic acid | neg | down | 0.9507 | 0.033 | 1.2593 |
| 184 | 3b-Hydroxy-6b-methoxy-7(11)- eremophilen-12,8a-olide | neg | down | 0.9042 | 0.001264 | 2.1399 |
| 185 | Isobutyl 4-hydroxybenzoate | neg | down | 0.9641 | 0.04619 | 1.1553 |
| 186 | Trans-4,5-epoxy-2(E)-Decenal | neg | down | 0.9565 | 0.005364 | 1.2905 |
| 187 | Phosphocreatine | neg | down | 0.8111 | 0.01582 | 2.4961 |
| 188 | Caprylic acid | neg | down | 0.9404 | 0.0424 | 1.2835 |
| 189 | 2-(1-Ethoxyethoxy)propanoic acid | neg | down | 0.9619 | 0.03369 | 1.1127 |
| 190 | 11-Dehydro-2,3-dinor-txb2 | neg | down | 0.9178 | 0.009378 | 1.7204 |
| 191 | Ethyladipic acid | neg | down | 0.95 | 0.008172 | 1.2908 |
| 192 | 3-Quinolinecarboxylic acid, 7-((3R)- 3-(1-aminocyclopropyl)-1- pyrrolidinyl)-1-((1R,2S)-2- fluorocyclopropyl)-1,4-dihydro-8- methoxy-4-oxo- | neg | down | 0.7876 | 0.00987 | 2.8861 |
| 193 | 5beta-1,3,7(11)-Eudesmatrien-8-one | neg | down | 0.8657 | 0.04497 | 1.7133 |

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| 194 | Octanoylglucuronide | neg | down | 0.9358 | 0.00848 | 1.5997 |
| 195 | Indole-3-acetaldehyde | neg | down | 0.9415 | 0.03293 | 1.3181 |
| 196 | 3-(3,5-dihydroxyphenyl)-1-propanoic acid sulphate | neg | down | 0.9547 | 0.003018 | 1.6623 |
| 197 | 7,8-Dihydroxycoumarin | neg | down | 0.8476 | 0.04075 | 1.9035 |
| 198 | Alpha-CEHC glucuronide | neg | down | 0.9164 | 0.04908 | 1.7771 |
| 199 | Hydroxyethyl methacrylic acid | neg | down | 0.9052 | 0.0004115 | 2.1449 |
| 200 | Phenylpyruvic Acid | neg | down | 0.9094 | 0.04589 | 1.417 |
| 201 | Geniposide | neg | down | 0.924 | 0.04956 | 1.4225 |
| 202 | Bruceine D | neg | down | 0.8916 | 0.03537 | 1.9741 |
| 203 | Ptaquiloside | neg | down | 0.9394 | 0.03595 | 1.5188 |
| 204 | D-Linalool 3-(6"-malonylglucoside) | neg | down | 0.9341 | 0.03069 | 1.5665 |
| 205 | 1,2-Cyclohexanedicarboxylic acid, 4-methyl- | neg | down | 0.8807 | 0.02104 | 1.7498 |
| 206 | (2R,3S,9R)-5-Acetyl-8,8-dimethyl-7,16-diazapentacyclo[9.6.1.02,9.03,7.015,18]octadeca-1(17),11(18),12,14-tetraene-4,6-dione | neg | down | 0.7143 | 0.03264 | 2.8729 |
| 207 | 1-(3-Methylbutanoyl)-6-apiosylglucose | neg | down | 0.9446 | 0.00326 | 1.6479 |
| 208 | Phthalate | neg | down | 0.9456 | 0.03599 | 1.2354 |
| 209 | 1,2-Cyclohexanediol | neg | down | 0.9154 | 0.002422 | 1.8018 |

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|-----|-------------------------------------------|-----|------|--------|----------|--------|
| 210 | Aesculin | neg | down | 0.5272 | 0.007879 | 3.5234 |
| 211 | Osmundalactone | neg | down | 0.9297 | 0.02685 | 1.5729 |
| 212 | Dihydrocaffeic acid 3-O-glucuronide | neg | down | 0.8026 | 0.02209 | 2.3072 |
| 213 | 2-Methoxy-4-vinylphenol | neg | down | 0.9051 | 0.02781 | 1.7724 |
| 214 | Carbamazepine-O-quinone | neg | down | 0.8971 | 0.03991 | 1.8304 |
| 215 | N-Biotinyl-4-aminobenzoic acid | neg | down | 0.9304 | 0.007001 | 1.6246 |
| 216 | Mecoprop | neg | down | 0.8974 | 0.01006 | 2.1128 |
| 217 | Isoferuloyl C1-glucuronide | neg | down | 0.7657 | 0.004341 | 2.9805 |
| 218 | Ethyl 2-furanacrylate | neg | down | 0.9127 | 0.01865 | 1.7224 |
| 219 | Protocatechuic acid 3-O-sulfate | neg | down | 0.9417 | 0.01536 | 1.5657 |
| 220 | 6-Thiourate | neg | down | 0.9182 | 0.001547 | 2.1228 |
| 221 | Zidovudine glucuronide | neg | up | 1.4047 | 0.01702 | 2.907 |
| 222 | 5-Carboxy-2'-deoxyuridine | neg | down | 0.9125 | 0.009533 | 1.6837 |
| 223 | 5-Megastigmen-7-yne-3,9-diol | neg | down | 0.9595 | 0.004774 | 1.4028 |
| 224 | L-prolinamide | neg | down | 0.8767 | 0.01463 | 1.869 |
| 225 | 2,8-Dihydroxyquinoline-beta-D-glucuronide | neg | down | 0.9711 | 0.007901 | 1.078 |
| 226 | 3-Methylguanidine | neg | down | 0.9386 | 0.005368 | 1.5025 |
| 227 | Maleic Acid | neg | up | 1.066 | 0.006469 | 1.6398 |
| 228 | Hydroxypropyl-Histidine | neg | down | 0.9295 | 0.04701 | 1.3109 |

| | | | | | | |
|-----|-----------------------------------------------------------------|-----|------|--------|-----------|--------|
| 229 | Raffinose | neg | down | 0.7848 | 0.0009919 | 3.0595 |
| 230 | 2-amino-5-(amino-dimethylamino-methylidene)amino-pentanoic acid | neg | down | 0.9 | 0.001287 | 2.0299 |
| 231 | Tryptophyl-Glutamine | neg | down | 0.9081 | 0.02555 | 1.7028 |
| 232 | Oleoside | neg | down | 0.9175 | 0.003857 | 1.9813 |
| 233 | O-Cresol | neg | down | 0.8948 | 0.003386 | 2.1137 |
| 234 | (6E,8S,10Z)-8-hydroxy-3-oxohexadecadienoic acid | neg | down | 0.9512 | 0.01876 | 1.3645 |
| 235 | NeuNGc | neg | down | 0.8677 | 0.0442 | 1.9272 |
| 236 | 2,6-Dimethoxy-4-propylphenol | neg | down | 0.9667 | 0.001139 | 1.2997 |
| 237 | Valeric acid | neg | down | 0.9369 | 0.00684 | 1.5303 |
| 238 | Polyethylene, oxidized | neg | down | 0.957 | 0.007196 | 1.4107 |
| 239 | 4-Hydroxyphenylacetic acid | neg | down | 0.9652 | 0.0184 | 1.1007 |
| 240 | Phenyllactic acid | neg | down | 0.9597 | 0.008116 | 1.3075 |
| 241 | Pyrocatechol | neg | down | 0.9161 | 0.0113 | 1.7452 |
