# Multi-Omics Approaches for Freshness Estimation and Detection of Illicit Conservation Treatments in Sea Bass (*Dicentrarchus Labrax*): Data Fusion Applications

**Alessandro Benedetto, Elisa Robotti, Masho Hilawie Belay, Arianna Ghignone, Alessia Fabbris, Eleonora Goggi, Simone Cerruti, Marcello Manfredi, Elettra Barberis, Simone Peletto, Alessandra Arillo, Nunzia Giaccio, Maria Angela Masini, Jessica Brandi, Daniela Cecconi, Emilio Marengo and Paola Brizio**

**Supplementary Material S3.**

Here are reported with more details all the discriminant molecules identified by the BE-PLS-DA models built for each matrix and for each time of treatment for global models and for single source models. For each model the name of each molecule included in the model, the corresponding label adopted in the corresponding figures (Figure 4 and 5) and the value of the regression coefficient is given. Positive coefficients correspond to molecules more present after treatment, while negative coefficients correspond to molecules decreasing after treatment.

**GLOBAL MODELS**

**Table S2.1: Muscle 3h**

| Source | Compound Name (Lipids) | Label | Coefficient |
|---|---|---|---|
| Lipidomics | CAR5:0 | L13 | -0,0096 |
| | Cer38:1;4O\|Cer14:0;3O/24:1;(2OH) | L22 | 0,011 |
| | Cer39:2;2O\|Cer21:0;2O/18:2 | L26 | 0,012 |
| | Cer45:6;2O\|Cer21:1;2O/24:5 | L37 | 0,011 |
| | Cer47:6;2O\|Cer21:1;2O/26:5 | L38 | 0,011 |
| | DG28:2 | L45 | 0,010 |
| | DG29:3 | L47 | 0,011 |
| | DG31:0 | L51 | 0,0097 |
| | DG31:3 | L53 | 0,010 |
| | DG32:3 | L56 | 0,011 |
| | DG35:5 | L68 | 0,011 |
| | DG38:2\|DG19:1_19:1 | L90 | 0,012 |
| | FA22:2;4O | L133 | -0,011 |
| | FA28:7 | L142 | -0,010 |
| | FA30:5 | L143 | -0,011 |
| | FA30:7 | L144 | -0,011 |
| | FA32:5 | L145 | -0,0097 |

| | | | |
|---|---|---|---|
| | FA34:7 | L149 | 0,011 |
| | FA36:10 | L150 | 0,011 |
| | FA36:7 | L153 | 0,012 |
| | FA44:10 | L162 | -0,010 |
| | HexCer42:2;2O\|HexCer18:1;2O/24:1 | L168 | 0,011 |
| | LPCO-18:2 | L197 | -0,011 |
| | LPE20:1 | L203 | -0,010 |
| | NAE22:3 | L232 | 0,011 |
| | NAE22:4 | L233 | 0,0096 |
| | NAE24:4 | L235 | 0,011 |
| | PE39:7;O\|PE22:6_17:1;O | L445 | 0,0084 |
| | SM32:0;3O | L557 | 0,011 |
| | TG38:3\|TG9:0_9:0_20:3 | L602 | 0,011 |
| | TG40:2\|TG9:0_9:0_22:2 | L604 | 0,010 |
| | TG40:5\|TG9:0_9:0_22:5 | L605 | 0,011 |
| | TG46:2\|TG12:0_16:0_18:2 | L622 | 0,011 |
| | TG48:5\|TG14:0_16:1_18:4 | L648 | -0,0087 |
| | TG48:9\|TG16:1_16:4_16:4 | L655 | 0,010 |
| | TG54:4\|TG16:0_18:1_20:3 | L763 | -0,0088 |
| | TG57:10\|TG17:1_18:3_22:6 | L817 | -0,0095 |
| | TG58:0\|TG16:0_17:0_25:0 | L830 | 0,0098 |
| | TG60:10\|TG20:1_18:3_22:6 | L874 | -0,010 |
| | TG61:1\|TG16:0_27:0_18:1 | L892 | -0,010 |
| | TG62:0\|TG16:0_22:0_24:0 | L896 | -0,010 |
| | TG62:1\|TG16:0_28:0_18:1 | L897 | 0,0097 |
| | TG62:13\|TG18:1_22:6_22:6 | L902 | -0,011 |
| | TG62:14\|TG18:2_22:6_22:6 | L904 | -0,0099 |
| | TG64:13\|TG20:1_22:6_22:6 | L915 | -0,010 |
| Metabolomics | 4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)- SUM 79+106 | M123 | -0,0098 |
| | 6,9,12,15-Docosatetraenoic acid, methyl ester | M141 | 0,0089 |
| | Androstane, (5á)- | M180 | 0,0090 |
| | Benzene, (1-hexyloctyl)- | M202 | 0,0096 |
| | benzoic acid, 3,5-dimethyl-, trimethylsilyl ester | M220 | 0,011 |
| | cis-7-Hexadecenoic acid SUM 292+280+236 | M250 | 0,0096 |
| | cis-9-Hexadecenoic acid, heptyl ester | M251 | 0,010 |
| | Desmethylverapamil | M275 | 0,0099 |
| | Desmethylverapamil SUM | M276 | 0,0099 |
| | Nonanal | M390 | -0,011 |
| | Octadecanoic acid, ethyl ester | M399 | 0,0098 |

| | | | |
|---|---|---|---|
| | s-Indacen-1(2H)-one, 3,5,6,7-tetrahydro-3,3,4,5,5,8-hexamethyl- | M437 | 0,0095 |
| | Squalene SUM 123+217 | M438 | 0,0088 |
| | Trimethylolpropane, 3TMS derivative | M456 | 0,0086 |
| Proteomics | Slow myosin heavy chain 2 | E6ZIC8 | 0,0099 |

**Table S2.2: Muscle 24h**

| Source | Compound Name (Lipids) | Label | Coefficient |
|---|---|---|---|
| Lipidomics | Cer41:0;4O\|Cer21:0;3O/20:0;(2OH) | L30 | 0,026 |
| | DG36:0 | L71 | 0,029 |
| | SM34:0;2O\|SM21:0;2O/13:0 | L561 | -0,025 |
| | SM34:0;3O | L562 | -0,025 |
| | TG40:0\|TG10:0_14:0_16:0 | L603 | -0,024 |
| | TG46:4\|TG14:0_16:0_16:4 | L626 | -0,026 |
| | TG49:5\|TG14:0_15:0_20:5 | L663 | -0,023 |
| | TG52:0\|TG16:0_18:0_18:0 | L707 | 0,026 |
| | TG57:6\|TG17:0_18:1_22:5 | L826 | -0,023 |
| | TG58:12\|TG18:2_18:4_22:6 | L840 | -0,025 |
| | TG59:0\|TG16:0_17:0_26:0 | L859 | 0,025 |
| Metabolomics | 1-(3-Methylbutyl)-2,3,6-trimethylbenzene | M10 | 0,023 |
| | 1-Octene, 3,7-dimethyl- | M49 | 0,029 |
| | 1-Propene-1,2,3-tricarboxylic acid, tributyl ester | M52 | 0,024 |
| | 2-Allyl-1,4-dimethoxybenzene | M81 | 0,025 |
| | 5alpha-Androstan-3alpha-ol, O-ethyl- | M138 | -0,025 |
| | 9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester | M162 | 0,023 |
| | Androstane, (5á)- | M179 | -0,024 |
| | Benzene, (1-methylundecyl)- SUM 246+105 | M206 | -0,026 |
| | Eicosanoic acid, ethyl ester | M296 | 0,024 |
| | Heptanoic acid, TMS derivative SUM 187+60 | M331 | 0,024 |
| | Hexadecanenitrile | M333 | -0,027 |
| | Hydroquinone, 2TMS derivative | M346 | 0,024 |
| | Pentadecanoic acid, butyl ester | M413 | 0,025 |
| Proteomics | Slow myosin heavy chain 2 | E6ZIC7 | -0,025 |
| | Inositol-1-monophosphatase | E6ZJ93 | -0,023 |
| | Apolipoprotein E (Fragment) | Q0GN72 | 0,024 |

**Table S2.3: Skin 3h**

| Source | Compound Name (Lipids) | Label | Coefficient |
|---|---|---|---|
| Lipidomics | CAR16/0 | L9 | 0,013 |
| | CAR19/0 | L12 | -0,012 |
| | CAR19/3 | L13 | -0,012 |
| | DG34/7 | L67 | 0,014 |
| | DG37/1 | L77 | 0,014 |
| | DG42/11\|DG20/5_22/6 | L101 | -0,013 |
| | NAE22/4 | L167 | -0,011 |
| | PC28/1 | L174 | -0,012 |
| | PC40/7 | L247 | 0,012 |
| | PCO-36/3 | L275 | 0,012 |
| | PE38/5\|PE16/0_22/5 | L300 | 0,012 |
| | PG47/5 | L330 | -0,012 |
| | SM35/1/2O\|SM19/1/2O/16/0 | L349 | 0,011 |
| | SM39/2/2O\|SM24/2/2O/15/0 | L354 | -0,013 |
| | SM40/2/2O\|SM18/1/2O/22/1 | L358 | 0,011 |
| | SM42/2/2O\|SM18/1/2O/24/1 | L363 | 0,013 |
| | FA16/0 | L609 | 0,011 |
| | FA34/9 | L639 | 0,013 |
| | FA36/7 | L643 | 0,013 |
| | FA42/5 | L653 | 0,013 |
| | FA44/5 | L658 | 0,013 |
| | PC34/2/3O\|PC16/0_18/2/3O | L723 | -0,012 |
| | PCO-34/2\|PCO-16/0_18/2 | L798 | -0,013 |
| | PCO-36/2\|PCO-18/0_18/2 | L806 | -0,012 |
| | PCO-40/6\|PCO-18/0_22/6 | L826 | -0,013 |
| | SM42/3/2O\|SM17/2/2O/25/1 | L939 | -0,011 |
| Metabolomics | 1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E,Z,E,E)]- SUM 229+190 | M14 | -0,011 |
| | 11-Tricosene | M28 | -0,012 |
| | 1-Dodecanamine, N,N-dimethyl- | M41 | 0,015 |
| | 1-Dodecanol, TMS derivative | M43 | 0,011 |
| | 1-Methyl-N,N-bis(trimethylsilyl)-4-[(trimethylsilyl)oxy]-1H-imidazol-2-amine | M46 | 0,012 |
| | 2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (, (R*,R*)-) SUM 292 | M67 | 0,013 |
| | 2-Aminomalonic acid, N,O,O,-TMS | M84 | 0,011 |
| | 2-Butenedioic acid, (E)-, 2TMS derivative | M86 | 0,014 |
| | 2-Heptanamine, N-(phenylmethylene)- | M89 | 0,014 |

| | | | |
|---|---|---|---|
| | 3,5-di-tert-Butyl-4-hydroxycinnamic acid | M104 | -0,012 |
| | 3-Phenyl-2-trimethylsiloxypropene | M111 | -0,011 |
| | 6H-Dibenzo[b,d]-pyran | M131 | -0,012 |
| | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | M132 | -0,014 |
| | 7-Methoxy-3-(2-methoxyphenyl)-2-methylchromen-4-one | M134 | -0,011 |
| | Benzaldehyde, 2,4-dimethyl- SUM 63+134 | M168 | -0,012 |
| | Benzoic Acid, TMS derivative | M188 | -0,011 |
| | D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2) SUM 217 | M216 | 0,012 |
| | D-Arabinopyranose, 4TMS derivative (isomer 2) | M218 | 0,012 |
| | D-Fructose, 5TMS derivative | M220 | 0,011 |
| | Glycol salicylate, TBDMS derivative | M263 | 0,014 |
| | Heptanoic acid, TMS derivative SUM 187+60 | M269 | 0,012 |
| | Nonanoic acid, TMS derivative | M316 | 0,013 |
| | Octadecanoic acid, ethenyl ester | M319 | -0,012 |
| | Octanoic acid, TMS derivative SUM 201+116 | M322 | 0,011 |
| | Pregna-1,4,6-triene-3,20-dione, 17-(acetyloxy)-6,16-dimethyl-, (16$\alpha$)- | M343 | -0,013 |
| | Triacetin | M367 | 0,013 |
| Proteomics | Apolipoprotein B-100 | Q9I8I1 | -0,012 |

**Table S2.4: Skin 24h**

| Source | Compound Name (Lipids) | Label | Coefficient |
|---|---|---|---|
| Lipidomics | CAR12/2 | L5 | 0,0046 |
| | CAR19/0 | L12 | 0,0053 |
| | CAR21/0 | L15 | -0,0046 |
| | Cer32/1/2O\|Cer18/1/2O/14/0 | L24 | 0,0044 |
| | DG32/7 | L61 | 0,0046 |
| | DG36/1 | L71 | 0,0054 |
| | DG40/6 | L93 | -0,0049 |
| | DG40/6\|DG16/0_24/6 | L94 | -0,0047 |
| | DGO-30/1\|DGO-16/0_14/1 | L104 | -0,0042 |
| | DGO-32/1\|DGO-16/0_16/1 | L105 | -0,0041 |
| | DGO-34/1\|DGO-18/0_16/1 | L106 | -0,0056 |
| | LPC20/5 | L132 | 0,0048 |
| | LPCO-14/0 | L137 | 0,0040 |
| | LPCO-14/1 | L138 | 0,0042 |
| | NAE22/5 | L168 | -0,0046 |

| | | | |
|---|---|---|---|
| | PC30/1 | L177 | 0,0040 |
| | PC32/0 | L181 | 0,0041 |
| | PC37/7 | L225 | 0,0058 |
| | PCO-43/8 | L292 | 0,0044 |
| | PG41/5 | L325 | 0,0044 |
| | SM36/2/2O\|SM23/2/2O/13/0 | L351 | 0,0041 |
| | TG43/1\|TG13/0_14/0_16/1 | L381 | 0,0057 |
| | TG44/3\|TG14/0_14/0_16/3 | L386 | 0,0054 |
| | TG50/7\|TG14/0_16/2_20/5 | L426 | 0,0042 |
| | TG50/9\|TG14/0_16/4_20/5 | L428 | 0,0042 |
| | TG51/4\|TG16/1_17/1_18/2 | L434 | 0,0051 |
| | TG52/0\|TG14/0_18/0_20/0 | L439 | -0,0061 |
| | TG53/0\|TG14/0_15/0_24/0 | L461 | -0,0063 |
| | TG53/1\|TG16/0_19/0_18/1 | L462 | 0,0053 |
| | TG53/1\|TG17/0_17/0_19/1 | L463 | -0,0045 |
| | TG54/0\|TG16/0_18/0_20/0 | L472 | -0,0061 |
| | TG54/8\|TG14/0_18/2_22/6 | L485 | 0,0041 |
| | TG55/0\|TG15/0_16/0_24/0 | L490 | -0,0051 |
| | TG55/1\|TG15/0_24/0_16/1 | L491 | -0,0042 |
| | TG58/12\|TG16/1_20/5_22/6 | L540 | 0,0062 |
| | TG59/1\|TG16/0_25/0_18/1 | L554 | -0,0047 |
| | TG59/12\|TG17/1_20/5_22/6 | L556 | 0,0040 |
| | TG61/1\|TG16/0_27/0_18/1 | L579 | 0,0055 |
| | TG62/2\|TG28/0_16/1_18/1 | L594 | 0,0045 |
| | TG62/9\|TG22/1_18/2_22/6 | L599 | 0,0055 |
| | FA16/4 | L611 | 0,0048 |
| | FA22/5 | L621 | 0,0060 |
| | FA24/5 | L627 | 0,0055 |
| | FA26/6 | L628 | 0,0042 |
| | FA26/7 | L629 | 0,0067 |
| | FA28/7 | L630 | 0,0057 |
| | FA30/5 | L631 | 0,0048 |
| | FA30/7 | L632 | 0,0055 |
| | FA32/6 | L634 | -0,0047 |
| | FA32/7 | L635 | 0,0051 |
| | FA34/9 | L639 | 0,0046 |
| | FA36/5 | L641 | -0,0045 |
| | FA36/6 | L642 | -0,0043 |
| | FA38/5 | L645 | -0,0041 |

| | | | |
|---|---|---|---|
| | FA40/11 | L648 | 0,0053 |
| | FA44/11 | L657 | 0,0043 |
| | FA44/7 | L660 | 0,0043 |
| | FAHFA40/5/O\|FAHFA20/3/20/2/O | L662 | 0,0043 |
| | NAE21/2 | L705 | 0,0058 |
| | PC36/5\|PC16/1_20/4 | L744 | 0,0049 |
| | PEO-34/2\|PEO-18/1_16/1 | L868 | -0,0055 |
| | SL38/0/O | L913 | 0,0056 |
| | SL40/0/2O | L915 | 0,0055 |
| | ST27/1/O/S | L944 | 0,0053 |
| Metabolomics | (E)-9-Octadecenoic acid ethyl ester | M4 | -0,0044 |
| | 1,3-Propanediol, TMS derivative | M15 | 0,0046 |
| | 10-Heptadecenoic acid, (Z)-, TMS derivative SUM 325+327 | M23 | 0,0053 |
| | 11-Octadecenoic acid, (E)-, TMS derivative | M27 | 0,0057 |
| | 1-Dodecanamine, N,N-dimethyl- | M41 | -0,0047 |
| | 1-Monopalmitin, 2TMS derivative | M49 | 0,0055 |
| | 2(3H)-Furanone, 5-dodecyldihydro- | M60 | 0,0058 |
| | 2(3H)-Furanone, dihydro-5-tetradecyl- | M61 | 0,0044 |
| | 2-(Decanoyloxy)propane-1,3-diyl dioctanoate | M62 | 0,0049 |
| | 2,3-Dihydroxypropyl icosanoate, 2TMS derivative | M68 | 0,0042 |
| | 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)- | M73 | -0,0061 |
| | 2,5-Dihydroxyacetophenone, 2TBDMS derivative | M74 | -0,0052 |
| | 2,5-Di-tert-butyl-4-((trimethylsilyl)oxy)phenol | M79 | 0,0053 |
| | 2-Heptanamine, N-(phenylmethylene)- | M89 | 0,0043 |
| | 2H-Pyran-2-one, tetrahydro-6-undecyl- | M90 | 0,0057 |
| | 2-Oleoylglycerol, 2TMS derivative | M96 | 0,0047 |
| | 4-Pyrimidinamine, N-(trimethylsilyl)-2-[(trimethylsilyl)oxy]- | M122 | -0,0048 |
| | 7-Methyl-Z,Z-8,10-hexadecadien-1-ol acetate | M135 | 0,0053 |
| | 9,12-Octadecadien-1-ol, (Z,Z)- | M138 | 0,0050 |
| | 9,12-Octadecadienoic acid, methyl ester, (E,E)- | M142 | 0,0055 |
| | 9-Hexadecenoic acid | M145 | 0,0050 |
| | 9-Nonadecene SUM 266+97 | M149 | -0,0043 |
| | 9-Octadecenamide, (Z)- SUM 72+59 | M151 | 0,0049 |
| | 9-Octadecenenitrile, (Z)- | M152 | 0,0048 |
| | 9-Octadecynenitrile | M154 | 0,0048 |
| | 9-Tricosene, (Z)- | M156 | -0,0046 |
| | Acetamide, N-ethyl- | M159 | -0,0041 |
| | Adrenaline, 4TMS derivative | M163 | 0,0040 |
| | Arachidic acid, TMS derivative | M165 | 0,0066 |

| | | | |
|---|---|---|---|
| | Benzaldehyde, 2,5-dimethoxy- SUM 166 | M169 | 0,0053 |
| | Benzyl alcohol, TMS derivative SUM 165+180 | M191 | 0,0053 |
| | Bicyclo[2.2.2]oct-5-en-2-yldimethylamine | M192 | 0,0062 |
| | Bisphenol A monomethyl ether, TMS derivativeSUM 299+314 | M194 | -0,0040 |
| | Cholest-3,5-diene | M200 | 0,0050 |
| | D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 2) SUM 337+217 | M214 | 0,0047 |
| | Decanoic acid, TMS derivative | M219 | 0,0048 |
| | Diphenyl ether | M227 | 0,0051 |
| | Docosanoic acid, ethyl ester | M230 | -0,0049 |
| | Dodecanamide | M232 | 0,0061 |
| | E,E,Z-1,3,12-Nonadecatriene-5,14-diol | M239 | 0,0055 |
| | Ethyl 9-hexadecenoate | M249 | 0,0045 |
| | Ethyl iso-allocholate | M250 | 0,0050 |
| | Gallacetophenone-4'-methylether, bis(trimethylsilyl) ether | M253 | -0,0058 |
| | Glycerol monostearate, 2TMS derivative | M258 | 0,0042 |
| | Glycidyl (Z)-9-Heptadecenoate | M260 | -0,0053 |
| | Glycidyl palmitoleate SUM 116 | M262 | -0,0054 |
| | Heptanoic acid, TMS derivative SUM 187+60 | M269 | 0,0044 |
| | Hexadecanoic acid, methyl ester | M272 | 0,0059 |
| | Hexanoic acid, TMS derivative | M278 | 0,0044 |
| | Hydracrylic acid, 2TMS derivative | M280 | 0,0052 |
| | Lignoceric acid, TMS derivative | M291 | -0,0047 |
| | Methyl (3,4-dimethoxyphenyl)(hydroxy)acetate, TMS derivative SUM 239+298 | M296 | -0,0058 |
| | Methyl stearate | M299 | 0,0053 |
| | Monocaprin, 2TMS derivative | M303 | 0,0040 |
| | Monolaurin, 2TMS derivative | M304 | 0,0064 |
| | Niacin, TMS derivative | M313 | 0,0056 |
| | Octadecanamide | M318 | 0,0048 |
| | Octadecanoic acid, ethyl ester | M320 | -0,0042 |
| | Oleic Acid SUM 280+264 | M323 | 0,0044 |
| | Oleic Acid, (Z)-, TMS derivative SUM 339+117 | M324 | -0,0041 |
| | Palmitic Acid, TMS derivative SUM 286+72+311+313+145+129+327+185+287 | M331 | -0,0050 |
| | Phloroglucinol, O,O'-bis(trimethylsilyl)- | M339 | 0,0041 |
| | Silicic acid, diethyl bis(trimethylsilyl) ester | M355 | -0,0042 |
| | ß-Eudesmol, TMS derivative | M358 | 0,0047 |
| | Tridecanoic acid SUM 70+98+84 | M369 | -0,0041 |
| | Tyrosine, 2TMS derivative | M376 | 0,0052 |

| | | | |
|---|---|---|---|
| | Undecanoic acid, TMS derivative | M378 | 0,0049 |
| | Urea, 2TMS derivative | M379 | 0,0052 |
| | Z-14-Octadecen-1-ol acetate | M380 | 0,0042 |
| Proteomics | Myosin heavy chain | Q2PMW9 | 0,0048 |
| | Fructose-bisphosphate aldolase | E6ZH34 | 0,0041 |
| | Glyceraldehyde-3-phosphate dehydrogenase | Q5I1Z5 | 0,0051 |
| | Keratin, type I cytoskeletal 18 | E6ZFH0 | 0,0047 |
| | Complement component c3-1 | F8R8R0 | 0,0041 |
| | MN-Alpha1 | A0A1L6V014 | 0,0046 |
| | Lipocalin | E6ZIH5 | 0,0045 |
| | Myosin light chain | E6ZH67 | 0,0052 |
| | Serine/arginine-rich splicing factor 2 | E6ZHT0 | 0,0044 |
| | Tubulin alpha chain (Fragment) | Q7T1F9 | -0,0051 |
| | Ribosomal protein L5 | Q0GN71 | 0,0048 |
| | Tubulin beta chain | E6ZF69 | -0,0040 |
| | Cardiac muscle myosin heavy chain 6 alpha (Fragment) | D5JZI9 | 0,0061 |
| | Carbonic anhydrase | E6ZJA5 | 0,0052 |

**Table S2.5: Gills 3h**

| Source | Compound Name (Metabolites) | Label | Coefficient |
|---|---|---|---|
| Metabolomics | 1,3-Dihydroxyacetone dimer, 4TMS derivative | M9 | 0,011 |
| | 13-Octadecenoic acid, (Z)-, TMS derivative | M24 | 0,0098 |
| | 1-Monopalmitin, 2TMS derivative | M43 | -0,011 |
| | 1-Tetradecanol, TMS derivative | M51 | -0,0095 |
| | 2,3-Dihydroxypropyl icosanoate, 2TMS derivative | M58 | -0,0088 |
| | 2,4,7,9-Tetramethyl-5-decyne-4,7-diol, 2TMS derivative | M59 | 0,010 |
| | 2,5-Dimethoxybenzhydrazide | M64 | -0,012 |
| | 2,6-Dihydroxyacetophenone, 2TMS derivative | M70 | 0,012 |
| | 2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one | M71 | -0,0088 |
| | 2-Monolinolenoylglycerol 1,3-bis(trimethylsilyl) ether SUM 103 | M82 | -0,011 |
| | 3-(2-Hydroxyethyl)imidazole-2-thione | M89 | 0,0092 |
| | 3,5-di-tert-Butyl-4-hydroxyacetophenone | M91 | 0,0099 |
| | 3-Methylcyclopentanol, trimethylsilyl ether | M98 | 0,0096 |
| | 3-Octenoic acid, TMS derivative | M100 | 0,010 |
| | 4-tert-Butylphenol, TMS derivative | M110 | 0,0091 |
| | 9(E),11(E)-Conjugated linoleic acid SUM 280 | M118 | -0,010 |

| | | | |
|---|---|---|---|
| | 9,12-Octadecadienoic acid (Z,Z)-, TMS derivative SUM 337+309+338 | M120 | -0,0098 |
| | 9-Hexadecenoic acid, (Z)-, TBDMS derivative | M122 | 0,014 |
| | 9-Octadecenenitrile, (Z)- | M129 | -0,012 |
| | 9-Tetradecenal, (Z)- | M134 | 0,013 |
| | 9-Tetradecenoic acid, (E)-, TMS derivative | M135 | 0,010 |
| | Acetophenone | M137 | 0,013 |
| | Anthranilic acid, 2TMS derivative | M142 | 0,011 |
| | Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)- | M145 | -0,011 |
| | Arachidic acid, TMS derivative | M147 | 0,012 |
| | Arachidonic acid, TMS derivative SUM 188+286 | M148 | -0,0099 |
| | Benzaldehyde, 2,5-dimethyl- | M157 | -0,0091 |
| | Benzene, (1-ethylnonyl)- | M160 | -0,012 |
| | Benzene, 1,3-bis(1,1-dimethylethyl)- | M169 | 0,0097 |
| | Calealactone E | M181 | -0,0092 |
| | Carbonic acid, allyl pentadecyl ester | M183 | -0,011 |
| | cis-Vaccenic acid SUM 264+94 | M197 | -0,011 |
| | Cyclohexanemethanol, TMS derivative | M200 | 0,010 |
| | D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 2) SUM 217+292 | M202 | -0,0099 |
| | D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1) SUM 204+333 | M205 | 0,011 |
| | D-Fructose, 5TMS derivative SUM 306 | M213 | 0,0096 |
| | Diethylene glycol, 2TMS derivative SUM 73+117 | M216 | 0,014 |
| | Diethylene glycol, isobutyl ether, trimethylsilyl ether | M217 | 0,0089 |
| | Doconexent, TMS derivative SUM 103+129+299+108+319+331+106 | M223 | 0,010 |
| | Eicosapentaenoic Acid, TMS derivative SUM 291+374+217+129+305 | M230 | -0,0096 |
| | Erucic acid SUM 292+181 | M231 | -0,012 |
| | Ethanamine, 2TMS derivative | M235 | 0,0092 |
| | Glucose, 5TMS derivative | M246 | 0,010 |
| | Glycerol monostearate, 2TMS derivative SUM 331+402 | M248 | -0,0093 |
| | Heptanoic acid, 4-octyl ester | M257 | 0,0092 |
| | Hexadecanoic acid, hexadecyl ester | M263 | -0,0096 |
| | Hexanoic acid, 2-ethyl-, oxybis(2,1-ethanediyloxy-2,1-ethanediyl) ester | M269 | 0,012 |
| | Isonicotinic Acid, TBDMS derivative | M274 | 0,012 |
| | L-Leucine, TMS derivative | M288 | -0,014 |

| | | | |
|---|---|---|---|
| | L-Serine, 2TMS derivative SUM 116+149 | M290 | 0,013 |
| | N-Acetyl-dl-alanine methylamide | M307 | 0,0089 |
| | Oleic Acid SUM 284+264+222 | M320 | -0,0090 |
| | Palmitelaidic acid, TMS derivative SUM 311 | M327 | 0,011 |
| | p-Dicyclohexylbenzene | M333 | -0,013 |
| | Pentadecanoic acid, TMS derivative SUM 299 | M335 | 0,013 |
| | phenoxyethanol, TMS derivative | M340 | 0,0094 |
| | Triacontane, 1-iodo- SUM 113+69 | M366 | 0,014 |
| | Triethylene glycol, 2TMS derivative | M372 | 0,0093 |
| | Tyrosine, 2TMS derivative | M377 | 0,010 |
| Proteomics | 40S ribosomal protein | E6ZEX1 | -0,011 |
| | Inter-alpha-trypsin inhibitor heavy chain H3 | E6ZFW4 | 0,0098 |
| | Glutaredoxin-1 | E6ZG15 | -0,014 |
| | Small nuclear ribonucleoprotein E | E6ZG90 | 0,010 |
| | 40S ribosomal protein S23 | E6ZGE0 | -0,012 |
| | Fructose-bisphosphate aldolase | E6ZH34 | 0,0088 |
| | Ribosomal protein L19 | E6ZHE6 | 0,015 |
| | TANK-binding kinase 1-binding protein | E6ZI15 | 0,010 |
| | Cystatin-B | E6ZIU0 | 0,011 |
| | 40S ribosomal protein SA | K7DWA9 | -0,017 |
| | Calreticulin | M9QRZ6 | -0,010 |
| | Na-K-2Cl cotransporter | Q0P6K3 | 0,0090 |
| | 60S ribosomal protein L23 | Q9YHX0 | -0,0095 |

**Table S2.6: Gills 24h**

| Source | Compound Name (Metabolites) | Label | Coefficient |
|---|---|---|---|
| Metabolomics | 1-Tetradecanol, TMS derivative | M51 | -0,083 |
| | 2-Monolinolenoylglycerol 1,3-bis(trimethylsilyl) ether SUM 103 | M82 | -0,082 |
| | Calealactone E | M181 | 0,073 |
| | Glycerol, 3TMS derivative SUM 71+205 | M250 | -0,080 |
| | Oxazole, 2-(3Z,6Z,9Z,12Z,15Z,18Z)-3,6,9,12,15,18-heneicosahexaen-1-yl-4,5-dihydro- | M325 | -0,077 |
| | p-Dicyclohexylbenzene | M333 | -0,077 |
| | Syringaldehyde, TMS derivative | M361 | -0,070 |
| Proteomics | Type II keratin E3 | E6ZFH2 | 0,087 |

**Single source models**

**Table S2.7: Muscle 3h Lipidomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Cer 38:1;4O\|Cer 14:0;3O/24:1;(2OH) | L22 | 0,037 |
| Cer 39:2;2O\|Cer 21:0;2O/18:2 | L26 | 0,038 |
| Cer 45:6;2O\|Cer 21:1;2O/24:5 | L37 | 0,036 |
| DG28:2 | L45 | 0,032 |
| DG29:3 | L47 | 0,035 |
| DG32:3 | L56 | 0,035 |
| DG 38:2\|DG 19:1_19:1 | L90 | 0,038 |
| FA22:2;4O | L133 | -0,036 |
| FA30:7 | L144 | -0,037 |
| FA36:7 | L153 | 0,038 |
| NAE22:3 | L232 | 0,037 |
| NAE24:4 | L235 | 0,036 |
| TG38:3\|TG9:0_9:0_20:3 | L602 | 0,035 |
| TG46:2\|TG12:0_16:0_18:2 | L622 | 0,034 |
| TG54:4\|TG16:0_18:1_20:3 | L763 | -0,028 |
| TG57:10\|TG17:0_20:5_20:5 | L816 | -0,030 |
| TG58:0\|TG16:0_17:0_25:0 | L830 | 0,031 |
| TG62:1\|TG16:0_28:0_18:1 | L897 | 0,031 |

**Table S2.8: Muscle 24h Lipidomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Cer41:0;4O\|Cer21:0;3O/20:0;(2OH) | L30 | 0,029 |
| DG36:0 | L71 | 0,032 |
| NAE20:1 | L230 | -0,024 |
| PC40:2\|PC16:1_24:1 | L327 | 0,020 |
| PCO-32:1 | L371 | 0,025 |
| SM 34:0;2O\|SM 21:0;2O/13:0 | L561 | -0,028 |
| SM 34:0;3O | L562 | -0,029 |
| SM36:1;2O\|SM18:1;2O/18:0 | L565 | 0,022 |
| ST24:2;O4 | L598 | 0,023 |
| TG40:0\|TG10:0_14:0_16:0 | L603 | -0,027 |
| TG42:1\|TG12:0_14:0_16:1 | L609 | -0,023 |
| TG44:3\|TG14:0_14:0_16:3 | L616 | -0,027 |

| | | |
|---|---|---|
| TG46:4\|TG14:0_16:0_16:4 | L628 | -0,030 |
| TG50:1\|TG16:0_18:0_16:1 | L670 | 0,020 |
| TG50:7\|TG14:0_16:2_20:5 | L684 | -0,027 |
| TG51:0\|TG16:0_17:0_18:0 | L691 | 0,025 |
| TG52:0\|TG16:0_18:0_18:0 | L707 | 0,029 |
| TG52:11\|TG16:2_16:4_20:5 | L712 | -0,027 |
| TG53:0\|TG14:0_15:0_24:0 | L733 | 0,026 |
| TG55:1\|TG15:0_24:0_16:1 | L775 | 0,030 |
| TG56:13\|TG16:3_18:4_22:6 | L800 | -0,029 |
| TG57:6\|TG17:0_18:1_22:5 | L826 | -0,026 |
| TG58:12\|TG18:2_18:4_22:6 | L840 | -0,028 |
| TG58:13\|TG16:2_20:5_22:6 | L841 | -0,028 |
| TG59:0\|TG16:0_17:0_26:0 | L859 | 0,028 |
| TG61:11\|TG17:0_22:5_22:6 | L893 | -0,027 |
| TG62:0\|TG16:0_22:0_24:0 | L896 | 0,022 |

**Table S2.9: Skin 3h Lipidomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| CAR16:0 | L9 | 0,035 |
| CAR19:3 | L13 | -0,032 |
| DG34:7 | L67 | 0,038 |
| DG37:1 | L77 | 0,038 |
| DG42:11\|DG20:5_22:6 | L101 | -0,035 |
| PC28:1 | L174 | -0,034 |
| PG47:5 | L330 | -0,034 |
| SM39:2;2O\|SM24:2;2O/15:0 | L354 | -0,036 |
| TG59:12\|TG17:1_20:5_22:6 | L556 | -0,034 |
| FA34:9 | L639 | 0,037 |
| FA36:7 | L643 | 0,035 |
| FA42:5 | L653 | 0,035 |
| FA44:5 | L658 | 0,036 |
| PC34:2;3O\|PC16:0_18:2;3O | L723 | -0,034 |
| PCO-34:2\|PCO-16:0_18:2 | L798 | -0,035 |
| PCO-36:2\|PCO-18:0_18:2 | L806 | -0,032 |
| PCO-36:3\|PCO-18:1_18:2 | L808 | -0,035 |
| PCO-40:6\|PCO-18:0_22:6 | L826 | -0,037 |

**Table S2.10: Skin 24h Lipidomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| CAR19:0 | L12 | 0,047 |
| DG36:1 | L71 | 0,049 |
| DGO-34:1\|DGO-18:0_16:1 | L106 | -0,050 |
| PC37:7 | L225 | 0,052 |
| TG52:0\|TG14:0_18:0_20:0 | L439 | -0,054 |
| TG53:0\|TG14:0_15:0_24:0 | L461 | -0,056 |
| TG53:1\|TG16:0_19:0_18:1 | L462 | 0,047 |
| TG54:0\|TG16:0_18:0_20:0 | L472 | -0,054 |
| TG58:12\|TG16:1_20:5_22:6 | L540 | 0,055 |
| TG61:1\|TG16:0_27:0_18:1 | L579 | 0,050 |
| FA26:7 | L629 | 0,059 |
| PEO-34:2\|PEO-18:1_16:1 | L868 | -0,049 |

**Table S2.11: Muscle 3h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1-Deoxypentitol, 4TMS derivative SUM 307 | M35 | 0,046 |
| 1-Methyl-N,N-bis(trimethylsilyl)-4-[(trimethylsilyl)oxy]-1H-imidazol-2-amine | M41 | 0,046 |
| 4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)- SUM 79+106 | M123 | -0,049 |
| 4-Methylcinnamic acid, trimethylsilyl ester | M132 | 0,048 |
| Benzene, 1,3,5-triethenyl-2,4,6-triethyl- | M213 | 0,044 |
| Benzoic acid, 3,5-dimethyl-, trimethylsilyl ester | M220 | 0,053 |
| Caprolactam | M233 | 0,045 |
| Cis-9-Hexadecenoic acid, heptyl ester | M251 | 0,051 |
| Desmethylverapamil | M275 | 0,049 |
| Desmethylverapamil SUM | M276 | 0,049 |
| Glycidyl palmitate SUM 116 | M321 | -0,043 |
| Nonanal | M390 | -0,056 |
| Octadecanoic acid, ethyl ester | M399 | 0,049 |
| Urea, 2TMS derivative | M462 | 0,043 |

**Table S2.12: Muscle 24h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1-(3-Methylbutyl)-2,3,6-trimethylbenzene | M10 | 0,043 |
| 11,14-Eicosadienoic acid, (Z)-, TMS derivative SUM 365 | M25 | 0,041 |
| 1-Octene, 3,7-dimethyl- | M49 | 0,054 |

| | | |
|---|---|---|
| 1-Propene-1,2,3-tricarboxylic acid, tributyl ester | M52 | 0,044 |
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | M60 | 0,047 |
| 2-Allyl-1,4-dimethoxybenzene | M81 | 0,047 |
| 4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)- SUM 79+106 | M123 | -0,046 |
| 9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester | M162 | 0,042 |
| Benzene, (1-methylundecyl)- SUM 246+105 | M206 | -0,048 |
| Benzophenone | M222 | -0,041 |
| D-Fructose, 5TMS derivative | M278 | 0,045 |
| Eicosanoic acid, ethyl ester | M296 | 0,045 |
| Hexadecanenitrile | M333 | -0,051 |
| Nonanoic acid, TMS derivative | M391 | 0,043 |
| Sulfurous acid, pentyl tridecyl ester | M441 | -0,046 |

**Table S2.13: Skin 3h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 11-Tricosene | M28 | -0,028 |
| 1-Dodecanamine, N,N-dimethyl- | M41 | 0,034 |
| 1-Methyl-N,N-bis(trimethylsilyl)-4-[(trimethylsilyl)oxy]-1H-imidazol-2-amine | M46 | 0,027 |
| 2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (, (R*,R*)-) SUM 292 | M67 | 0,029 |
| 2-Butenedioic acid, (E)-, 2TMS derivative | M86 | 0,031 |
| 2-Heptanamine, N-(phenylmethylene)- | M89 | 0,032 |
| 6H-Dibenzo[b,d]-pyran | M131 | -0,027 |
| 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | M132 | -0,031 |
| 7-Methoxy-3-(2-methoxyphenyl)-2-methylchromen-4-one | M134 | -0,025 |
| 9-Tricosene, (Z)- | M156 | -0,024 |
| Benzaldehyde, 2,4-dimethyl- SUM 63+134 | M168 | -0,027 |
| Benzoic Acid, TMS derivative | M188 | -0,026 |
| D-(-)-Tagatofuranose, pentakis(trimethylsilyl) ether (isomer 2) SUM 217 | M216 | 0,027 |
| D-Arabinopyranose, 4TMS derivative (isomer 2) | M218 | 0,026 |
| D-Glucose, 5TMS derivative | M221 | 0,024 |
| Glycol salicylate, TBDMS derivative | M263 | 0,031 |
| Heptanoic acid, TMS derivative SUM 187+60 | M269 | 0,027 |
| N,N-Diethyl(trimethylsilyl)carbamate | M307 | 0,021 |
| Nonanoic acid, TMS derivative | M316 | 0,030 |
| Octanoic acid, TMS derivative SUM 201+116 | M322 | 0,026 |

| | | |
|---|---|---|
| Pregna-1,4,6-triene-3,20-dione, 17-(acetyloxy)-6,16-dimethyl-, (16$\alpha$)- | M343 | -0,029 |
| Sorbic acid, TBDMS derivative | M357 | 0,024 |
| Triacetin | M367 | 0,030 |
| Z-5-Nonadecene | M381 | -0,022 |

**Table S2.14: Skin 24h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1,3-Propanediol, TMS derivative | M15 | 0,017 |
| 10-Heptadecenoic acid, (Z)-, TMS derivative SUM 325+327 | M23 | 0,020 |
| 11-Octadecenoic acid, (E)-, TMS derivative | M27 | 0,021 |
| 1-Dodecanamine, N,N-dimethyl- | M41 | -0,017 |
| 2-(Decanoyloxy)propane-1,3-diyl dioctanoate | M62 | 0,018 |
| 2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)- | M73 | -0,022 |
| 2,5-Dihydroxyacetophenone, 2TBDMS derivative | M74 | -0,019 |
| 2,5-Di-tert-butyl-4-((trimethylsilyl)oxy)phenol | M79 | 0,020 |
| 2H-Pyran-2-one, tetrahydro-6-undecyl- | M90 | 0,021 |
| 2-Oleoylglycerol, 2TMS derivative | M96 | 0,017 |
| 7-Methyl-Z,Z-8,10-hexadecadien-1-ol acetate | M135 | 0,020 |
| 9,12-Octadecadien-1-ol, (Z,Z)- | M138 | 0,018 |
| 9-Hexadecenoic acid | M145 | 0,018 |
| Arachidic acid, TMS derivative | M165 | 0,024 |
| Benzaldehyde, 2,5-dimethoxy- SUM 166 | M169 | 0,020 |
| Benzyl alcohol, TMS derivative SUM 165+180 | M191 | 0,020 |
| Bicyclo[2.2.2]oct-5-en-2-yldimethylamine | M192 | 0,023 |
| Cholest-3,5-diene | M200 | 0,018 |
| Decanoic acid, TMS derivative | M219 | 0,018 |
| Diphenyl ether | M227 | 0,019 |
| Docosanoic acid, ethyl ester | M230 | -0,018 |
| Dodecanamide | M232 | 0,023 |
| E,E,Z-1,3,12-Nonadecatriene-5,14-diol | M239 | 0,020 |
| Ethyl iso-allocholate | M250 | 0,019 |
| Gallacetophenone-4'-methylether, bis(trimethylsilyl) ether | M253 | -0,022 |
| Glycidyl (Z)-9-Heptadecenoate | M260 | -0,020 |
| Glycidyl palmitoleate SUM 116 | M262 | -0,020 |
| Hexadecanoic acid, methyl ester | M272 | 0,022 |
| Lignoceric acid, TMS derivative | M291 | -0,017 |

| | | |
|---|---|---|
| Monolaurin, 2TMS derivative | M304 | 0,024 |
| Niacin, TMS derivative | M313 | 0,021 |
| Palmitic Acid, TMS derivative SUM 286+72+311+313+145+129+327+185+287 | M331 | -0,019 |
| Undecanoic acid, TMS derivative | M378 | 0,018 |
| Urea, 2TMS derivative | M379 | 0,019 |

**Table S2.15: Gills 3h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1,3-Dihydroxyacetone dimer, 4TMS derivative | M9 | 0,013 |
| 1-Monopalmitin, 2TMS derivative | M43 | -0,014 |
| 1-Tetradecanol, TMS derivative | M51 | -0,011 |
| 2,3,3-Trimethyl-5-amino-3H-indole | M56 | 0,010 |
| 2,3-Dihydroxypropyl icosanoate, 2TMS derivative | M58 | -0,011 |
| 2,4,7,9-Tetramethyl-5-decyne-4,7-diol, 2TMS derivative | M59 | 0,012 |
| 2,5-Dimethoxybenzhydrazide | M64 | -0,015 |
| 2,6-Dihydroxyacetophenone, 2TMS derivative | M70 | 0,014 |
| 2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one | M71 | -0,011 |
| 2'-Hydroxy-4'-methoxyacetophenone, TMS derivative | M79 | -0,010 |
| 2-Monolinolenoylglycerol 1,3-bis(trimethylsilyl) ether SUM 103 | M82 | -0,014 |
| 3-(2-Hydroxyethyl)imidazole-2-thione | M89 | 0,011 |
| 3,4-Dimethylbenzoic acid, TMS derivative | M90 | 0,010 |
| 3,5-di-tert-Butyl-4-hydroxyacetophenone | M91 | 0,012 |
| 3-Methylcyclopentanol, trimethylsilyl ether | M98 | 0,012 |
| 4-tert-Butylphenol, TMS derivative | M110 | 0,011 |
| 5-hydroxy-7-methoxyflavanone, tert.-butyldimethylsilyl ether | M114 | -0,010 |
| 9(E),11(E)-Conjugated linoleic acid SUM 280 | M118 | -0,012 |
| 9-Hexadecenoic acid, (Z)-, TBDMS derivative | M122 | 0,016 |
| 9-Octadecenenitrile, (Z)- | M129 | -0,014 |
| 9-Tetradecenal, (Z)- | M134 | 0,015 |
| 9-Tetradecenoic acid, (E)-, TMS derivative | M135 | 0,012 |
| Acetophenone | M137 | 0,016 |
| Anthranilic acid, 2TMS derivative | M142 | 0,013 |
| Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)- | M145 | -0,013 |
| Arachidic acid, TMS derivative | M147 | 0,014 |
| Arachidonic acid, TMS derivative SUM 188+286 | M148 | -0,012 |

| | | |
|---|---|---|
| Benzaldehyde, 2,5-dimethyl- | M157 | -0,011 |
| Benzene, (1-ethyldecyl)- | M159 | -0,010 |
| Benzene, (1-ethylnonyl)- | M160 | -0,014 |
| Benzene, (1-propylnonyl)- | M167 | -0,010 |
| Benzene, 1,3-bis(1,1-dimethylethyl)- | M169 | 0,012 |
| Bis(2-ethylhexyl) methylenesuccinate | M177 | 0,010 |
| Calealactone E | M181 | -0,011 |
| Carbonic acid, allyl pentadecyl ester | M183 | -0,014 |
| cis-Vaccenic acid SUM 264+94 | M197 | -0,013 |
| Cyclohexanemethanol, TMS derivative | M200 | 0,012 |
| D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1) SUM 204+333 | M205 | 0,013 |
| D-Fructose, 5TMS derivative SUM 306 | M213 | 0,012 |
| Diethylene glycol, 2TMS derivative SUM 73+117 | M216 | 0,017 |
| Diethylene glycol, isobutyl ether, trimethylsilyl ether | M217 | 0,011 |
| Di-trimethylsilyl peroxide | M220 | -0,010 |
| Doconexent, TMS derivative SUM 103+129+299+108+319+331+106 | M223 | 0,012 |
| Eicosapentaenoic Acid, TMS derivative SUM 291+374+217+129+305 | M230 | -0,012 |
| Erucic acid SUM 292+181 | M231 | -0,015 |
| Ethanamine, 2TMS derivative | M235 | 0,011 |
| Glucose, 5TMS derivative | M246 | 0,012 |
| Glutaric acid, di(2-ethylhexyl) ester | M247 | 0,010 |
| Glycerol monostearate, 2TMS derivative SUM 331+402 | M248 | -0,011 |
| Heptacosan-9-ol | M254 | 0,011 |
| Heptanoic acid, 4-octyl ester | M257 | 0,011 |
| Hexadecanoic acid, hexadecyl ester | M263 | -0,012 |
| Hexanoic acid | M268 | 0,010 |
| Hexanoic acid, 2-ethyl-, oxybis(2,1-ethanediyloxy-2,1-ethanediyl) ester | M269 | 0,015 |
| Isoimperatorin SUM 91+225 | M273 | 0,010 |
| Isonicotinic Acid, TBDMS derivative | M274 | 0,015 |
| L-Leucine, TMS derivative | M288 | -0,016 |
| L-Serine, 2TMS derivative SUM 116+149 | M290 | 0,016 |
| Methylsuccinic acid, 2TMS derivative | M302 | 0,010 |
| N-Acetyl-dl-alanine methylamide | M307 | 0,011 |
| Oleic Acid SUM 284+264+222 | M320 | -0,011 |
| Palmitelaidic acid, TMS derivative SUM 311 | M327 | 0,013 |
| p-Dicyclohexylbenzene | M333 | -0,016 |

| | | |
|---|---|---|
| Pentadecanoic acid, TMS derivative SUM 299 | M335 | 0,016 |
| Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl- | M352 | 0,010 |
| Triacontane, 1-iodo- SUM 113+69 | M366 | 0,017 |
| Triethylene glycol, 2TMS derivative | M372 | 0,011 |
| Tripropylene glycol monomethyl ether, TMS derivative | M375 | -0,010 |
| Tyrosine, 2TMS derivative | M377 | 0,013 |

**Table S2.16: Gills 24h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1-Tetradecanol, TMS derivative | M51 | -0,056 |
| 2,5-Dimethoxybenzonitrile | M65 | -0,052 |
| 2-Monolinolenoylglycerol 1,3-bis(trimethylsilyl) ether SUM 103 | M82 | -0,055 |
| 5-Nonanol, TMS derivative | M115 | 0,045 |
| Arachidonoyl dimethylaminoethanol | M149 | -0,053 |
| Benzene, (1-methyldodecyl)- | M163 | 0,044 |
| Calealactone E | M181 | 0,049 |
| Carbonic acid, heptadecyl isobutyl ester | M184 | -0,044 |
| D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1) SUM 217 | M201 | -0,044 |
| D-(-)-Fructopyranose, 5TMS derivative (isomer 2) SUM 204 | M203 | -0,044 |
| L-Lactic acid | M287 | 0,045 |
| Oxazole, 2-(3Z,6Z,9Z,12Z,15Z,18Z)-3,6,9,12,15,18-heneicosahexaen-1-yl-4,5-dihydro- | M325 | -0,052 |
| p-Dicyclohexylbenzene | M333 | -0,052 |
| Syringaldehyde, TMS derivative | M361 | -0,048 |

**Table S2.17: Eye 3h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1,3-Dihydroxyacetone dimer, 4TMS derivative | M9 | 0,013 |
| 1-Monopalmitin, 2TMS derivative | M43 | -0,014 |
| 1-Tetradecanol, TMS derivative | M51 | -0,011 |
| 2,3,3-Trimethyl-5-amino-3H-indole | M56 | 0,010 |
| 2,3-Dihydroxypropyl icosanoate, 2TMS derivative | M58 | -0,011 |
| 2,4,7,9-Tetramethyl-5-decyne-4,7-diol, 2TMS derivative | M59 | 0,012 |

| | | |
|---|---|---|
| 2,5-Dimethoxybenzhydrazide | M64 | -0,015 |
| 2,6-Dihydroxyacetophenone, 2TMS derivative | M70 | 0,014 |
| 2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one | M71 | -0,011 |
| 2'-Hydroxy-4'-methoxyacetophenone, TMS derivative | M79 | -0,010 |
| 2-Monolinolenoylglycerol 1,3-bis(trimethylsilyl) ether SUM 103 | M82 | -0,014 |
| 3-(2-Hydroxyethyl)imidazole-2-thione | M89 | 0,011 |
| 3,4-Dimethylbenzoic acid, TMS derivative | M90 | 0,010 |
| 3,5-di-tert-Butyl-4-hydroxyacetophenone | M91 | 0,012 |
| 3-Methylcyclopentanol, trimethylsilyl ether | M98 | 0,012 |
| 4-tert-Butylphenol, TMS derivative | M110 | 0,011 |
| 5-hydroxy-7-methoxyflavanone, tert.-butyldimethylsilyl ether | M114 | -0,010 |
| 9(E),11(E)-Conjugated linoleic acid SUM 280 | M118 | -0,012 |
| 9-Hexadecenoic acid, (Z)-, TBDMS derivative | M122 | 0,016 |
| 9-Octadecenenitrile, (Z)- | M129 | -0,014 |
| 9-Tetradecenal, (Z)- | M134 | 0,015 |
| 9-Tetradecenoic acid, (E)-, TMS derivative | M135 | 0,012 |
| Acetophenone | M137 | 0,016 |
| Anthranilic acid, 2TMS derivative | M142 | 0,013 |
| Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)- | M145 | -0,013 |
| Arachidic acid, TMS derivative | M147 | 0,014 |
| Arachidonic acid, TMS derivative SUM 188+286 | M148 | -0,012 |
| Benzaldehyde, 2,5-dimethyl- | M157 | -0,011 |
| Benzene, (1-ethyldecyl)- | M159 | -0,010 |
| Benzene, (1-ethylnonyl)- | M160 | -0,014 |
| Benzene, (1-propylnonyl)- | M167 | -0,010 |
| Benzene, 1,3-bis(1,1-dimethylethyl)- | M169 | 0,012 |
| Bis(2-ethylhexyl) methylenesuccinate | M177 | 0,010 |
| Calealactone E | M181 | -0,011 |
| Carbonic acid, allyl pentadecyl ester | M183 | -0,014 |
| cis-Vaccenic acid SUM 264+94 | M197 | -0,013 |
| Cyclohexanemethanol, TMS derivative | M200 | 0,012 |
| D-(-)-Ribofuranose, tetrakis(trimethylsilyl) ether (isomer 1) SUM 204+333 | M205 | 0,013 |
| D-Fructose, 5TMS derivative SUM 306 | M213 | 0,012 |
| Diethylene glycol, 2TMS derivative SUM 73+117 | M216 | 0,017 |
| Diethylene glycol, isobutyl ether, trimethylsilyl ether | M217 | 0,011 |

| | | |
|---|---|---|
| Di-trimethylsilyl peroxide | M220 | -0,010 |
| Doconexent, TMS derivative SUM 103+129+299+108+319+331+106 | M223 | 0,012 |
| Eicosapentaenoic Acid, TMS derivative SUM 291+374+217+129+305 | M230 | -0,012 |
| Erucic acid SUM 292+181 | M231 | -0,015 |
| Ethanamine, 2TMS derivative | M235 | 0,011 |
| Glucose, 5TMS derivative | M246 | 0,012 |
| Glutaric acid, di(2-ethylhexyl) ester | M247 | 0,010 |
| Glycerol monostearate, 2TMS derivative SUM 331+402 | M248 | -0,011 |
| Heptacosan-9-ol | M254 | 0,011 |
| Heptanoic acid, 4-octyl ester | M257 | 0,011 |
| Hexadecanoic acid, hexadecyl ester | M263 | -0,012 |
| Hexanoic acid | M268 | 0,010 |
| Hexanoic acid, 2-ethyl-, oxybis(2,1-ethanediyloxy-2,1-ethanediyl) ester | M269 | 0,015 |
| Isoimperatorin SUM 91+225 | M273 | 0,010 |
| Isonicotinic Acid, TBDMS derivative | M274 | 0,015 |
| L-Leucine, TMS derivative | M288 | -0,016 |
| L-Serine, 2TMS derivative SUM 116+149 | M290 | 0,016 |
| Methylsuccinic acid, 2TMS derivative | M302 | 0,010 |
| N-Acetyl-dl-alanine methylamide | M307 | 0,011 |
| Oleic Acid SUM 284+264+222 | M320 | -0,011 |
| Palmitelaidic acid, TMS derivative SUM 311 | M327 | 0,013 |
| p-Dicyclohexylbenzene | M333 | -0,016 |
| Pentadecanoic acid, TMS derivative SUM 299 | M335 | 0,016 |
| Silanamine, N,N'-methanetetraylbis[1,1,1-trimethyl- | M352 | 0,010 |
| Triacontane, 1-iodo- SUM 113+69 | M366 | 0,017 |
| Triethylene glycol, 2TMS derivative | M372 | 0,011 |
| Tripropylene glycol monomethyl ether, TMS derivative | M375 | -0,010 |
| Tyrosine, 2TMS derivative | M377 | 0,013 |

**Table S2.18: Eye 24h Metabolomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 1-Monolinolein, 2TMS derivative | M40 | -0,033 |
| 1-Tetradecanol, TMS derivative | M51 | -0,037 |
| 2,5-Dimethoxybenzonitrile | M65 | -0,035 |
| 2,6-Dihydroxyacetophenone, 2TMS derivative | M70 | 0,029 |

| | | |
|---|---|---|
| 2-Monolinolenoylglycerol 1,3-bis(trimethylsilyl) ether SUM 103 | M82 | -0,037 |
| 5-Nonanol, TMS derivative | M115 | 0,030 |
| Acrylic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester | M138 | -0,031 |
| Arabinofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)- | M145 | -0,031 |
| Arachidonoyl dimethylaminoethanol | M149 | -0,035 |
| Benzene, (1-methyldodecyl)- | M163 | 0,029 |
| Calealactone E | M181 | 0,033 |
| Carbonic acid, heptadecyl isobutyl ester | M184 | -0,029 |
| D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 1) SUM 217 | M201 | -0,029 |
| D-(-)-Fructopyranose, 5TMS derivative (isomer 2) SUM 204 | M203 | -0,029 |
| Glycerol, 3TMS derivative SUM 71+205 | M250 | -0,036 |
| Hexadecanoic acid, methyl ester | M264 | -0,033 |
| L-Lactic acid | M287 | 0,030 |
| Methyl stearate | M299 | -0,030 |
| Oxazole, 2-(3Z,6Z,9Z,12Z,15Z,18Z)-3,6,9,12,15,18-heneicosahexaen-1-yl-4,5-dihydro- | M325 | -0,035 |
| p-Dicyclohexylbenzene | M333 | -0,035 |
| Syringaldehyde, TMS derivative | M361 | -0,032 |

**Table S2.19: Muscle 3h Proteomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Myosin heavy chain | Q2PMW9 | 0,12 |
| Glyceraldehyde-3-phosphate dehydrogenase | Q5I1Z5 | -0,12 |
| Slow myosin heavy chain 2 | E6ZIC8 | 0,12 |
| Myomesin-1 | E6ZJ46 | 0,097 |
| Annexin | E6ZHH6 | -0,099 |
| Proteasome subunit beta | A0A455ZB90 | 0,12 |

**Table S2.20: Muscle 24h Proteomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Slow myosin heavy chain 2 | E6ZIC7 | -0,15 |
| Inositol-1-monophosphatase | E6ZJ93 | -0,13 |
| Myosin heavy chain 1 | E6ZIC5 | 0,11 |
| Annexin | E6ZHH6 | 0,13 |
| Attractin-like protein 1 | E6ZHA4 | -0,11 |

| | | |
|---|---|---|
| 40S ribosomal protein S10 | E6ZEX1 | -0,12 |

**Table S2.21: Skin 3h Proteomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Type II keratin E3 | E6ZFH2 | -0,070 |
| HSP-90 | Q6TL18 | 0,060 |
| Histone H2B | G5CUP6 | 0,072 |
| Lipocalin | E6ZIH5 | -0,081 |
| Hemoglobin-beta | G5CUP5 | 0,073 |
| Proteasome activator complex | E6ZJF1 | 0,065 |
| 40S ribosomal protein S10 | E6ZEX1 | 0,072 |
| Myosin regulatory light chain 2, smooth muscle isoform | E6ZJ48 | -0,059 |
| Keratin, type II cytoskeletal 8 | E6ZFH1 | -0,073 |
| Apolipoprotein B-100 | Q9I8I1 | -0,098 |
| Complement component c3-2 | F8R8R1 | -0,083 |
| Protein disulfide-isomerase A4 | E6ZII6 | 0,086 |

**Table S2.22: Skin 24h Proteomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Myosin light chain 2 | E6ZH67 | 0,17 |
| Tubulin alpha chain | Q7T1F9 | -0,17 |
| Cardiac muscle myosin heavy chain 6 alpha | D5JZI9 | 0,21 |
| BHMT | A0A6G9HCT5 | 0,12 |

**Table S2.23: Gills 3h Proteomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| 40S ribosomal protein | E6ZEX1 | -0,057 |
| Inter-alpha-trypsin inhibitor heavy chain H3 | E6ZFW4 | 0,051 |
| Glutaredoxin-1 | E6ZG15 | -0,071 |
| Small nuclear ribonucleoprotein E | E6ZG90 | 0,053 |
| 40S ribosomal protein S23 | E6ZGE0 | -0,062 |
| Ribosomal protein L19 | E6ZHE6 | 0,077 |
| TANK-binding kinase 1-binding protein | E6ZI15 | 0,052 |
| Cystatin-B | E6ZIU0 | 0,059 |
| 40S ribosomal protein SA | K7DWA9 | -0,087 |
| Calreticulin | M9QRZ6 | -0,053 |
| Na-K-2Cl cotransporter | Q0P6K3 | 0,047 |

| | | |
|---|---|---|
| 60S ribosomal protein L23 | Q9YHX0 | -0,049 |

**Table S2.24: Gills 24h Proteomics**

| Compound Name | Label | Coefficient |
|---|---|---|
| Interleukin 4/13-2 | A0A076YF48 | 0,046 |
| Phosphotransferase | A0A0A0N292 | -0,053 |
| Sodium/potassium-transporting ATPase subunit alpha | A0A0H4U807 | 0,060 |
| Eukaryotic translation initiation factor 4B | E6ZFG9 | -0,046 |
| Keratin, type I cytoskeletal 18 | E6ZFH0 | -0,058 |
| Type II keratin E3 | E6ZFH2 | 0,072 |
| WD repeat-containing protein 1 | E6ZG03 | -0,046 |
| Ribonucloprotein | E6ZGP5 | -0,054 |
| Histone H1.0 | E6ZGX2 | -0,048 |
| Serine/arginine-rich splicing factor 2 | E6ZHT0 | -0,046 |
| 40S ribosomal protein S20 | E6ZI93 | 0,050 |
| Inositol-1-monophosphatase | E6ZJ93 | -0,050 |
| 40S ribosomal protein SA | K7DWA9 | 0,054 |
| 60S ribosomal protein L23 | Q9YHX0 | 0,063 |