**TITLE**

Imbalanced Amino Acid Metabolism of Rainbow Trout Long-Term Fed a Plant-Based Diet as Revealed by 1H-NMR Metabolomics

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**Supplemental material**

**Table S1:** **Detailed composition of vitamin and mineral premix (Vit-Min premix, INRAE UPAE, Jouy en Josas, France) used in the experimental diets.** IU: vitamin activity in international unit.

|  |  |
| --- | --- |
| **Vitamins** | (IU or mg.kg-1 diet) |
| DL- tocopherol acetate (Vitamin E) | 60 IU |
| Retinil acetate (Vitamin A) | 15,000 IU |
| DL-colecalcipherol (Vitamin B3) | 3,000 IU |
| Sodium menadione bisulphate | 5 mg |
| Thiamin (Vitamin B1) | 15 mg |
| Riboflavin (Vitamin B2) | 30 mg |
| Pyridoxine (Vitamin B6) | 15 mg |
| Vitamin B12 | 0.05 mg |
| Nicotinic acid (Vitamin B3) | 175 mg |
| Folic acid (Vitamin B9) | 500 mg |
| Inositol | 1,000 mg |
| Biotin (Vitamin B7) | 2.5 mg |
| Calcium pantothenate (vitamin B5) | 50 mg |
| Choline chloride | 2,000 mg |
| **Minerals** | (g or mg.kg-1 diet) |
| Dibasic calcium phosphate (20% Ca, 18% P) | 5.00 g |
| Calcium carbonate (40% Ca) | 2.15 g |
| NaCl | 0.40 g |
| KCl | 0.90 g |
| Magnesium oxide (60% Mg) | 1.24 g |
| Ferric citrate | 0.20 g |
| Zinc sulphate (36% Zn) | 0.40 g |
| Manganese sulphate (33% Mn) | 0.30 g |
| Copper sulphate (25% Cu) | 0.30 g |
| Cobalt sulphate | 2.00 mg |
| Potassium iodide (75% I) | 0.40 mg |
| Sodium selenite (30% Se) | 3.00 mg |

**Table S2: Cumulative list of unknown resonances in the 1H-NMR spectra of hydro-alcoholic extracts of the three diet pellets** (s=singlet, d=doublet, dd=doublet of doublets. MSI status from Sumner *et al.* (2007)40: 4: unknown compound) **and their estimative contents** (µg.g-1 DM; 0=not detectable, mean (SD); n=12, ANOVA analysis significance of diet effect: \*\*\* *P* < 0.001 \*\* *P* < 0.01 \* *P* < 0.05.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Unknowns | Resonances used for quantification  (Chemical shift in ppm) and multiplicity | MSI status | Diet  (Content in µg.g-1 DM) | | | ANOVA |
|  |  |  | **Marine**  **(M)** | **Commercial (C)** | **Plant-based (P)** | **Diet Effect** |
| UnkS8.638 | 8.64 (s) | 4 | 0 | 0 | 7 (1) a | \*\*\* |
| UnkD8.59 | 8.59 (d) | 4 | 116 (10) a | 78 (8) b | 0 | \*\*\* |
| UnkS8.489 | 8.49 (s) | 4 | 0 | 0 | 12 (2) a | \*\*\* |
| UnkS8.43 | 8.43 (s) | 4 | 0 | 0 | 8 (1) a | \*\*\* |
| UnkS8.38 | 8.38 (s) | 4 | 6 (1) a | 4 (1) b | 3 (1) c | \*\*\* |
| UnkS8.35 | 8.35 (s) | 4 | 20 (1) a | 19 (1) a | 11 (1) b | \*\*\* |
| UnkS8.27 | 8.27 (s) | 4 | 50 (3) a | 46 (3) b | 0 | \*\*\* |
| UnkS8.26 | 8.26 (s) | 4 | 38 (2) a | 40 (3) a | 25 (2) b | \*\*\* |
| UnkS7.876 | 7.88 (s) | 4 | 51 (3) a | 53 (4) a | 0 | \*\*\* |
| UnkS7.86 | 7.86 (s) | 4 | 16 (2)c | 25 (3) a | 21 (2) b | \*\*\* |
| UnkM7.959 | 7.96 (m) | 4 | 0 | 0 | 28 (4)a | \*\*\* |
| UnkS7.76 | 7.76 (s) | 4 | 59 (3) a | 51 (3) b | 0 | \*\*\* |
| UnkD7.68 | 7.68 (d) | 4 | 0 | 105 (12) | 193 (9)c | \*\*\* |
| UnkD7.15 | 7.15 (d) | 4 | 0 | 49 (5) a | 42 (5) b | \*\*\* |
| UnkS6.91 | 6.91 (s) | 4 | 16 (1) a | 9 (1) b | 10 (1)b | \*\*\* |
| UnkD6.48 | 6.48 (d) | 4 | 0 | 199 (20)b | 381 (22)a | \*\*\* |
| UnkDD6.15 | 6.15 (dd) | 4 | 137 (4) a | 98 (7) b | 0 | \*\*\* |
| UnkS5.94 | 5.94 (s) | 4 | 16 (2) a | 11 (1) b | 9 (3)b | \*\*\* |
| UnkS5.93 | 5.93 (s) | 4 | 12 (2) a | 7 (2) b | 5 (2)c | \*\*\* |
| UnkS5.928 | 5.93 (s) | 4 | 15 (2)b | 19 (2) a | 14 (3) b | \*\*\* |
| UnkS5.92 | 5.92 (s) | 4 | 27 (3)b | 31 (2) a | 21 (2) c | \*\*\* |
| UnkS5.913 | 5.91 (s) | 4 | 15 (2)b | 20 (1) a | 14 (2) b | \*\*\* |
| UnkS5.906 | 5.905 (s) | 4 | 18 (3) a | 15 (2) b | 9 (2)c | \*\*\* |
| UnkS5.89 | 5.89 (s) | 4 | 14 (3)b | 19 (2) a | 14 (2) b | \*\*\* |
| UnkD5.2 | 5.2 (d) | 4 | 0 | 0 | 286 (43) a | \*\*\* |
| UnkD5.17 | 5.17 (d) | 4 | 0 | 0 | 256 (14) a | \*\*\* |
| UnkS3.23 | 3.23 (s) | 4 | 2901 (98) a | 1910 (63) b | 669 (35) c | \*\*\* |
| UnkS3.04 | 3.04 (s) | 4 | 8319 (181) a | 4887 (107) b | 0 | \*\*\* |
| UnkS2.825 | 2.82 (s) | 4 | 162 (7) a | 87 (5) b | 0 | \*\*\* |
| UnkS2.857 | 2.86 (s) | 4 | 371 (18) b | 271 (11) c | 1166 (81) a | \*\*\* |
| UnkS2.742 | 2.74 (s) | 4 | 80 (3) a | 47 (2) b | 0 | \*\*\* |

**Table S3:** **List of compounds detected in the 1H-NMR spectra of the plasma of rainbow trout.** MSI status from Sumner *et al.* (2007): 1: identified compound; 2: putatively annotated compound; 3: putatively characterized compound classes; 4: unknown compound

|  |  |  |
| --- | --- | --- |
| Compound | Chemical shift (ppm) | MSI status |
| *Amino acids* |  |  |
| alanine | 1.48; 1.49; 3.78; 3.79; 3.80 | 1 |
| glutamine | 2.11; 2.16; 2.43; 2.44; 2.45; 2.46; 2.47; 2.48; 3.76; 3.77 | 1 |
| glycine | 3.56 | 1 |
| histidine | 7.05; 7.76 | 2 |
| isoleucine | 0.94; 0.96; 1.00; 1.02 | 1 |
| leucine | 0.95; 0.97; 0.98; 1.67; 1.68; 1.73; 1.75 | 1 |
| lysine | 1.71; 1.73; 1.75; 1.77; 1.90; 1.92; 3.01; 3.03 | 1 |
| methionine | 2.11; 2.14; 2.17; 2.63; 2.65; 2.66 | 1 |
| phenylalanine | 3.17; 4.01; 7.33; 7.34; 7.38; 7.39; 7.42; 7.43; 7.45 | 1 |
| tyrosine | 6.89; 6.9; 7.19; 7.20 | 1 |
| valine | 0.99 ; 1.00 ; 1.04; 1.05; 2.25; 2.27; 2.28; 2.29; 2.30; 3.60 ; 3.62 | 1 |
|  |  |  |
| creatine | 3.04 | 2 |
| phospho-creatine | 3.05 | 2 |
| taurine | 3.17; 3.19 | 2 |
|  |  |  |
| *Carbohydrates/cyclitol* |  |  |
| α-glucose / β-glucose  inositol | 3.25; 2.37; 3.39; 3.40; 3.42; 3.43; 3.44; 3.45; 3.46; 3.47; 3.48; 3.49; 3.50; 3.51; 3.53; 3.55; 3.70; 3.71; 3.72; 3.73; 3.74; 3.76; 3.78; 3.79; 3.82; 3.84; 3.86; 3.89; 3.90; 3.91; 3.92; 4.64; 4.66; 5.23; 5.24  3.28; 3.30; 3.53; 3.53; 3.55; 3.55; 3.61; 3.63; 3.65; 4.06; 4.07; 4.07; | 1  1 |
|  |  |  |
| *Lipids* |  |  |
| unsaturated lipids + glyceryl  -C**H**=C**H**-CH2-C**H**=C**H**-  CO-CH2-C**H**(CO)-CH2-CO  unsaturated lipids  -CH=CH-C**H2**-CH=CH-  glyceryl  CO-C**H2**-CH(CO)-C**H2**-CO  lipids  C**H2**-C**H2**-CO-  lipoproteins  VLDL/LDL (C**H2**)n  VLDL/LDL -C**H3**  HDL -C**H3**  cholesterol | 5.30; 5.31; 5.32; 5.33; 5.34  2.74; 2.78; 2.83  4.32  1.52; 1.58  1.24; 1.28  0.92  0.85  0.66 | 3  3  3  3  3  3  3  3 |
| *Nucleotides/Nucleosides*  adenosine-XP like  inosine | 6.10; 6.11; 8.23; 8.34  5.91; 5.92 | 3  3 |
| *Organic acid*  lactic acid | 1.33; 1.34; 4.10; 4.11; 4.13; 4.14 | 1 |
|  |  |  |
| *Vitamins* |  |  |
| pterin | 8.55; 8.72 | 2 |
| betaine | 3. 27; 3.90 | 2 |
| choline | 3.21; 4.05; 4.08 | 2 |
|  |  |  |
| *Others*  acetyl glycoprotein  ethanol | 2.02  1.17; 1.19; 1.20; 3.66; 3.67 | 3  1 |
| DMA dimethylamine | 2.73 | 3 |
| TMAO | 3.21 | 3 |
| TMA trimethylamine | 3.26 | 3 |

Sumner LW., Amberg A., Barrett D., *et al.* (2007) Proposed minimum reporting standards for chemical analysis Chemical Analysis Working Group (CAWG) Metabolomics Standards Initiative (MSI). Metabolomics. 3:211-221.

**Table S4: Effect of diet (marine M, commercial C and plant-based P) and time after feeding (6h *vs* 48h) on semi-quantitative assessment of representative spectral regions or bucket of the 1H-NMR spectra of plasma in rainbow trout.** Mean +/-std MANOVA analysis \*\*\* *P* < 0.001 \*\* *P* < 0.01 \* *P* < 0.05 (6h or 48h diet effect only significant at 6 or 48h ; ↑ ↓ data significantly higher or lower at 48h than at 6h ; Int significant interaction between diet and time effect). B1\_68 means bucket centred at 1.68 ppm. unk : resonance(s) from unknown metabolite(s). See Table S2 for MSI status of resonance annotation.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | 6h post-feeding | | | | | | 48h post-feeding | | | | | | Effect | |
|  |  | Marine | | Commercial | | Plant-Based | | Marine | | Commercial | | Plant-Based | | Diet | Time |
| Bucket | Metabolite resonance annotation | mean | std | mean | std | mean | std | mean | Std | mean | std | mean | std |  |  |
| **Marine Diet > Plant Diet** | | | | | | | | | | | | |  |  |  |
| B1\_753 | unk + leucine +lysine1 | 33.9 | *5.5* | 30.1 | *3.3* | 15.5 | *3.3* | 29.6 | *5.2* | 29.1 | *4.3* | 13.9 | *3.1* | \*\*\* | \*\*\* ↓ |
| B2\_392 | unk | 1.78 | *0.45* | 1.69 | *0.57* | 0.79 | *0.26* | 0.25 | *0.08* | 0.22 | *0.07* | 0.20 | *0.06* | \*\*\* 6h | \*\*\* ↓ |
| B2\_444 | glutamine | 0.97 | *0.31* | 1.52 | *0.29* | 1.55 | *0.43* | 1.80 | *0.19* | 2.32 | *0.49* | 1.39 | *0.33* | \*\*\*48h | \*\*\* ↑ |
| B2\_452 | glutamine | 1.11 | *0.33* | 1.65 | *0.28* | 1.65 | *0.44* | 1.72 | *0.20* | 2.27 | *0.46* | 1.40 | *0.34* | \*\*\*48h | \*\*\* ↑ |
| B2\_732 | dimethylamine | 1.78 | *0.57* | 0.78 | *0.34* | 0.00 | *0.02* | 0.12 | *0.06* | 0.17 | *0.07* | 0.06 | *0.03* | \*\*\* 6h | \*\*\* ↓ |
| B2\_757 | unk | 4.19 | *1.35* | 2.43 | *0.97* | 2.06 | *0.68* | 0.25 | *0.11* | 0.31 | *0.26* | 0.31 | *0.20* | \*\*\* 6h | \*\*\* ↓ |
| B2\_903 | unk | 2.75 | *1.56* | 1.18 | *0.32* | 0.40 | *0.19* | 0.38 | *0.17* | 0.33 | *0.06* | 0.21 | *0.09* | \*\*\* | \*\*\* ↓ |
| B3\_044 | creatine + phosphocreatine | 29.65 | *6.50* | 15.72 | *2.80* | 10.71 | *1.81* | 10.97 | *2.50* | 11.13 | *1.94* | 12.42 | *2.41* | \*\*\* 6h | \*\*\* ↓ |
| B3\_119 | unk | 2.53 | *0.48* | 1.83 | *0.29* | 1.61 | *0.21* | 3.65 | *0.68* | 3.54 | *0.44* | 3.57 | *0.59* | \*\*\* 6h | \*\*\* ↑ |
| B3\_130 | unk | 2.15 | *0.65* | 1.58 | *0.35* | 1.39 | *0.33* | 1.10 | *0.24* | 1.17 | *0.12* | 1.12 | *0.17* | \*\*\* 6h | \*\*\* ↓ |
| B3\_199 | unk | 6.10 | *1.64* | 5.24 | *0.89* | 3.82 | *0.95* | 18.43 | *3.23* | 19.77 | *2.16* | 17.04 | *2.30* | \*\*\* | \*\*\* ↑ |
| B3\_270 | unk +TMAO + betaine + inositol + glucose | 270.2 | *51.7* | 138.1 | *24.8* | 95.6 | *24.2* | 168.4 | *30.6* | 113.7 | *16.8* | 81.8 | *15.0* | \*\*\* | \*\*\* ↓ |
| B3\_483 | unk | 6.91 | *1.92* | 7.67 | *1.11* | 7.54 | *1.08* | 8.27 | *0.93* | 7.38 | *0.74* | 6.99 | *0.52* | \*\*\*48h |  |
| B3\_488 | unk | 6.17 | *1.78* | 6.86 | *1.01* | 6.86 | *0.90* | 7.59 | *0.78* | 6.77 | *0.69* | 6.50 | *0.42* | \*\*\*48h |  |
| B3\_562 | unk | 29.2 | *3.6* | 27.0 | *4.7* | 21.7 | *4.2* | 32.3 | *8.6* | 31.3 | *7.2* | 29.2 | *7.0* | \*\*\* | \*\*\* ↑ |
| B3\_936 | unk | 11.95 | *3.11* | 7.27 | *1.68* | 5.45 | *1.09* | 8.80 | *1.49* | 9.47 | *1.23* | 9.77 | *1.72* | \*\*\* 6h | Int. |
| B4\_066 | unk | 6.86 | *2.16* | 4.32 | *0.86* | 3.95 | *0.75* | 2.47 | *0.34* | 3.72 | *0.76* | 4.16 | *0.72* | \*\*\* 6h | Int. |
| B5\_186 | unk | 20.7 | *4.9* | 22.1 | *3.1* | 20.4 | *2.4* | 32.7 | *3.8* | 31.1 | *3.7* | 25.4 | *2.2* | \*\*\*48h | \*\*\* ↑ |
| B5\_248 | unk | 19.9 | *6.3* | 19.9 | *2.7* | 17.6 | *2.4* | 32.7 | *3.4* | 31.1 | *3.5* | 24.7 | *2.2* | \*\*\* | \*\*\* ↑ |
| **Plant diet > Marine diet** | | | | | | | | | | | | |  |  |  |
| B0\_9765 | leucine + isoleucine + unk | 19.10 | *10.7* | 19.54 | *10.7* | 28.64 | *11.1* | 1.60 | *1.02* | 1.86 | *0.62* | 3.95 | *1.50* | \*\*\*48h | \*\*\*↓ |
| B0\_978 | leucine | 5.04 | *2.77* | 6.94 | *4.14* | 9.77 | *3.93* | 3.19 | *2.08* | 5.11 | *1.35* | 7.81 | *1.73* | \*\*\* | \*\*\*↓ |
| B0\_987 | valine | 7.62 | *2.49* | 7.09 | *1.64* | 8.29 | *2.37* | 1.21 | *0.79* | 1.85 | *0.62* | 2.91 | *0.73* | \*\*\*48h | \*\*\*↓ |
| B0\_998 | valine | 7.14 | *2.62* | 7.02 | *1.75* | 8.57 | *2.39* | 10.00 | *2.03* | 12.64 | *2.32* | 14.83 | *2.55* | \*\*\*48h | \*\*\* ↑ |
| B1\_008 | isoleucine | 3.03 | *1.45* | 3.53 | *0.93* | 4.58 | *1.24* | 8.00 | *1.95* | 10.06 | *1.95* | 12.07 | *2.28* | \*\*\* | \*\*\* ↑ |
| B1\_021 | isoleucine | 2.93 | *1.19* | 3.06 | *0.86* | 4.04 | *1.21* | 3.81 | *0.97* | 4.81 | *0.85* | 5.82 | *1.21* | \*\*\* | \*\*\* ↑ |
| B1\_036 | valine | 9.39 | *3.68* | 8.27 | *1.82* | 8.68 | *2.41* | 4.29 | *1.06* | 5.26 | *0.83* | 6.17 | *1.24* | \*\*\*48h | \*\*\* ↑ |
| B1\_051 | valine | 9.16 | *3.58* | 8.01 | *1.68* | 8.58 | *2.48* | 8.74 | *1.81* | 11.00 | *1.94* | 12.22 | *2.21* | \*\*\*48h | \*\*\* ↑ |
| B1\_061 | unk | 0.62 | *0.45* | 0.60 | *0.26* | 0.41 | *0.11* | 8.29 | *1.79* | 10.42 | *1.86* | 11.83 | *2.12* | \*\*\*48h | \*\*\* ↑ |
| B1\_447 | lysine + unk | 1.03 | *0.17* | 1.22 | *0.19* | 1.43 | *0.27* | 1.23 | *0.38* | 1.11 | *0.25* | 1.62 | *0.23* | \*\*\*6h | NS |
| B1\_459 | lysine + 13C lactic acid + unk | 0.21 | *0.10* | 0.25 | *0.11* | 0.59 | *0.15* | 0.55 | *0.17* | 0.51 | *0.15* | 0.66 | *0.14* | \*\*\*6h | \*\*\* ↑ |
| B1\_465 | unk | 0.84 | *0.26* | 1.08 | *0.24* | 1.55 | *0.22* | 1.45 | *0.25* | 1.38 | *0.19* | 1.52 | *0.20* | \*\*\*6h | Int. |
| B1\_681 | lysine + leucine | 1.17 | *0.25* | 1.88 | *0.40* | 2.98 | *0.70* | 1.28 | *0.45* | 1.48 | *0.49* | 2.26 | *0.46* | \*\*\* | \*\*\* ↑ |
| B1\_694 | lysine + leucine | 0.27 | *0.27* | 0.79 | *0.24* | 1.57 | *0.35* | 0.66 | *0.31* | 0.75 | *0.25* | 1.25 | *0.29* | \*\*\* | \*\*\* ↑ |
| B1\_702 | lysine + leucine | 0.95 | *0.66* | 1.97 | *0.38* | 3.35 | *0.79* | 1.22 | *0.50* | 1.47 | *0.43* | 2.25 | *0.49* | \*\*\* | \*\*\* ↑ |
| B1\_694 | lysine + leucine | 2.47 | *1.18* | 3.78 | *0.60* | 5.78 | *1.35* | 2.76 | *1.04* | 3.24 | *0.86* | 4.65 | *1.19* | \*\*\* | \*\*\* ↑ |
| B1\_914 | lysine | 0.72 | *0.23* | 0.53 | *0.16* | 0.78 | *0.23* | 0.42 | *0.21* | 0.44 | *0.14* | 0.73 | *0.20* | \*\*\*48h | NS |
| B2\_358 | unk | 1.48 | *0.34* | 1.48 | *0.38* | 1.53 | *0.26* | 2.43 | *0.66* | 2.75 | *0.69* | 3.46 | *0.73* | \*\*\*48h | \*\*\* ↑ |
| B2\_375 | unk | 2.15 | *0.41* | 2.61 | *0.41* | 3.02 | *0.49* | 1.93 | *0.87* | 1.98 | *0.51* | 2.87 | *0.52* | \*\*\* | Int. |
| B2\_436 | glutamine | 0.97 | *0.31* | 1.52 | *0.29* | 1.55 | *0.43* | 1.80 | *0.19* | 2.32 | *0.49* | 1.39 | *0.33* | \*\*\*6h | Int. |
| B2\_444 | glutamine | 1.11 | *0.33* | 1.65 | *0.28* | 1.65 | *0.44* | 1.72 | *0.20* | 2.27 | *0.46* | 1.40 | *0.34* | \*\*\*6h | Int. |
| B2\_421 | glutamine | 1.84 | *0.57* | 2.88 | *0.51* | 2.80 | *0.75* | 2.41 | *0.34* | 3.33 | *0.68* | 1.99 | *0.53* | \*\*\*6h | Int. |
| B2\_460 | glutamine | 2.06 | *0.61* | 3.09 | *0.53* | 2.97 | *0.78* | 2.54 | *0.35* | 3.48 | *0.75* | 2.13 | *0.57* | \*\*\*6h | Int. |
| B2\_468 | glutamine | 0.73 | *0.22* | 1.23 | *0.23* | 1.20 | *0.27* | 1.11 | *0.19* | 1.54 | *0.31* | 0.97 | *0.26* | \*\*\*6h | Int. |
| B2\_479 | glutamine | 1.00 | *0.25* | 1.61 | *0.29* | 1.79 | *0.38* | 1.47 | *0.26* | 1.98 | *0.37* | 1.39 | *0.36* | \*\*\*6h | Int. |
| B2\_549 | unk | 0.79 | *0.18* | 0.96 | *0.21* | 1.11 | *0.37* | 1.02 | *0.15* | 1.36 | *0.29* | 1.49 | *0.25* | \*\*\* | \*\*\* ↑ |
| B3\_011 | unk | 4.51 | *1.03* | 4.21 | *0.53* | 4.52 | *0.71* | 3.49 | *0.84* | 3.94 | *0.49* | 4.81 | *0.71* | \*\*\*48h | Int. |
| B3\_028 | unk | 5.62 | *1.35* | 4.54 | *0.49* | 5.11 | *0.83* | 3.70 | *1.10* | 4.10 | *0.63* | 5.46 | *1.09* | \*\*\*48h | Int. |
| B3\_060 | unk | 2.91 | *0.61* | 2.79 | *0.40* | 2.74 | *0.46* | 2.17 | *0.48* | 2.40 | *0.34* | 2.90 | *0.46* | \*\*\*48h | Int. |
| B3\_286 | inositol | 7.85 | *2.45* | 10.00 | *1.81* | 10.44 | *1.60* | 6.47 | *0.96* | 8.38 | *1.67* | 7.52 | *1.13* | \*\*\* | \*\*\*↓ |
| B3\_307 | inositol | 6.63 | *2.36* | 8.21 | *1.42* | 8.53 | *1.21* | 5.23 | *0.87* | 6.46 | *1.46* | 5.87 | *0.80* | \*\* | \*\*\*↓ |
| B3\_534 | glucose | 12.42 | *2.95* | 14.92 | *1.82* | 16.40 | *1.41* | 13.84 | *1.16* | 13.92 | *1.24* | 14.23 | *1.06* | \*\*\*6h | Int |
| B3\_598 | unk | 2.83 | *0.55* | 4.79 | *0.59* | 4.02 | *0.63* | 2.66 | *0.49* | 5.08 | *0.95* | 3.86 | *0.55* | \*\*\* | NS |
| B3\_607 | valine + inositol | 8.51 | *1.69* | 10.80 | *1.62* | 13.38 | *2.27* | 6.06 | *0.93* | 9.40 | *1.63* | 10.60 | *1.76* | \*\*\* | \*\*\*↓ |
| B3\_618 | unk | 5.93 | *0.55* | 6.66 | *0.70* | 6.80 | *1.12* | 4.88 | *0.64* | 6.47 | *0.96* | 6.52 | *0.99* | \*\*\* | \*\*\*↓ |
| B3\_628 | inositol | 6.96 | *1.09* | 10.90 | *2.15* | 14.51 | *2.64* | 5.30 | *0.85* | 9.09 | *1.93* | 10.48 | *2.21* | \*\*\* | \*\*\*↓ |
| B3\_652 | ethanol + inositol | 39.8 | *10.3* | 51.6 | *7.1* | 48.1 | *8.4* | 36.8 | *8.3* | 43.2 | *8.4* | 42.6 | *9.5* | \*\*\*6h | \*\*\*↓ |
| B3\_676 | ethanol | 8.62 | *0.91* | 9.69 | *0.96* | 8.95 | *1.23* | 7.15 | *0.56* | 8.94 | *1.04* | 8.17 | *0.76* | \*6h | \*↓ |
| B3\_763 | glucose + alanine + glutamine | 9.94 | *1.68* | 12.21 | *1.57* | 12.20 | *1.26* | 16.77 | *1.09* | 18.28 | *1.32* | 17.35 | *1.13* | \*\*\*6h | \*\*\*↑ |
| B3\_796 | alanine | 3.41 | *0.43* | 3.35 | *0.39* | 3.42 | *0.33* | 6.19 | *0.37* | 6.76 | *0.58* | 6.92 | *0.34* | \*\*\*48h | \*\*\*↑ |
| B3\_808 | alanine | 0.30 | *0.14* | 0.32 | *0.06* | 0.26 | *0.07* | 1.46 | *0.10* | 1.89 | *0.20* | 1.81 | *0.14* | \*\*\*48h | \*\*\*↑ |
| B4\_034 | unk | 0.24 | *0.10* | 0.80 | *0.24* | 0.58 | *0.14* | 1.48 | *0.25* | 3.06 | *0.56* | 2.27 | *0.50* | \*\*\* | \*\*\* ↑ |
| B4\_028 | unk | 0.14 | *0.11* | 0.65 | *0.22* | 0.50 | *0.13* | 0.90 | *0.18* | 1.82 | *0.39* | 1.56 | *0.37* | \*\*\* | \*\*\* ↑ |
| B4\_060 | inositol | 6.86 | *2.16* | 4.32 | *0.86* | 3.95 | *0.75* | 2.47 | *0.34* | 3.72 | *0.76* | 4.16 | *0.72* | \*\*\*48h | Int. |
| B4\_068 | inositol | 2.92 | *0.96* | 4.24 | *1.08* | 5.97 | *1.25* | 2.42 | *0.40* | 4.24 | *1.03* | 5.01 | *1.02* | \*\*\* | NS |
| B4\_076 | inositol | 1.72 | *0.67* | 2.51 | *0.61* | 3.29 | *0.65* | 1.84 | *0.29* | 3.03 | *0.69* | 3.34 | *0.61* | \*\*\* | NS |
| B4\_147 | lactic acid | 5.37 | *1.77* | 6.22 | *1.00* | 6.94 | *0.73* | 4.50 | *0.85* | 5.41 | *1.02* | 5.16 | *1.27* | \*\*\*6h | \*\*\*↓ |
| B6\_906 | tyrosine | 2.45 | *0.60* | 3.68 | *0.70* | 4.11 | *0.82* | 0.96 | *0.34* | 1.33 | *0.27* | 1.43 | *0.37* | \*\*\* | \*\*\*↓ |
| B6\_888 | tyrosine | 2.12 | *0.62* | 2.78 | *0.66* | 3.33 | *0.78* | 0.97 | *0.32* | 1.22 | *0.38* | 1.27 | *0.31* | \*\*\* | \*\*\*↓ |
| B7\_207 | tyrosine | 2.00 | *0.63* | 2.58 | *0.58* | 3.11 | *0.74* | 1.41 | *0.43* | 1.63 | *0.52* | 1.86 | *0.41* | \*\*\* | \*\*\*↓ |
| B7\_766 | unk | 1.93 | *0.51* | 2.34 | *0.38* | 2.71 | *0.34* | 1.81 | *0.65* | 1.99 | *0.56* | 2.37 | *0.70* | \*\*\*6h | NS |
| B8\_549 | pterin | 0.16 | *0.13* | 0.07 | *0.12* | 0.53 | *0.15* | 0.00 | *0.00* | 0.00 | *0.00* | 0.16 | *0.13* | \*\*\* | \*\*\*↓ |
| B8\_721 | pterin | 0.08 | *0.15* | 0.11 | *0.19* | 0.60 | *0.14* | 0.02 | *0.07* | 0.01 | *0.04* | 0.22 | *0.15* | \*\*\* | \*\*\*↓ |

1 Unk + leucine + lysine in C and M diets; leucine + lysine in P diet

**Table S5: List of compounds detected in the 1H-NMR spectra of the liver or/and muscle of rainbow trout.** MSI status from Sumner *et al.* (2007): 1: identified compound; 2: putatively annotated compound; 3: putatively characterized compound classes; 4: unknown compound

|  |  |  |
| --- | --- | --- |
| Compound | Chemical shift (ppm) | MSI status |
| *Amino acids* |  |  |
| alanine | 1.48; 1.50; 3.79; 3.80; 3.82 | 1 |
| asparagine | 2.86; 2.88; 2.89; 2.91; 2.95; 2.98; 2.99; 4.05 | 1 |
| aspartic acid | 2.79; 2.80; 2.83; 2.84 | 2 |
| beta-alanine | 2.56; 2.57; 2.58; 3.18; 3.19; 3.20 | 1 |
| glutamic acid | 2.04; 2.05; 2.07; 2.08; 2.10; 2.11; 2.12; 2.13; 2.32; 2.34; 2.34; 2.35; 2.36; 2.37; 2.37; 2.39 | 1 |
| glutamine | 2.13; 2.16; 2.17; 2.18; 2.44; 2.46; 2.47; 2.47; 2.48; 2.49 | 1 |
| glycine | 3.57 | 2 |
| histidine | 3.14; 3.15; 3.17; 3.18; 3.99; 4.00; 4.01; 4.02; 7.11; 7.9 | 1 |
| isoleucine | 0.93; 0.94; 0.96; 1.00; 1.02 | 1 |
| leucine | 0.96; 0.97; 0.98; 1.67; 1.69; 1.77; 2.25; 2.27; 2.27; 2.28; 2.29; 2.29; 2.30 | 1 |
| lysine | 1.71; 1.72; 1.74; 1.75; 1.77; 1.89; 1.90; 1.91; 1.94; 1.95; 3.01; 3.02 | 1 |
| methionine | 2.15; 2.64; 2.66; 2.67 | 1 |
| phenylalanine | 7.33; 7.34; 7.37; 7.38; 7.39; 7.40; 7.42; 7.43; 7.44; 7.45; 7.46 | 1 |
| threonine | 1.33; 1.35; | 2 |
| tryptophan | 7.28; 7.29; 7.33; 7.73; 7.75 | 2 |
| tyrosine | 6.90; 6.92; 7.20; 7.21 | 1 |
| valine | 0.99; 1.00 ; 1.04; 1.06; 2.25; 2.30 | 1 |
|  |  |  |
| anserine | 2.65; 2.66; 2.68; 2.68; 2.70; 2.70; 2.71; 2.72; 2.73; 2.75; 2.76; 3.03; 3.07; 3.08; 3.22; 3.23; 3.24; 3.25; 3.26; 3.79; 4.48; 4.49; 4.50; 4.50; 7.10; 8.25 | 1 |
| taurine | 3.26; 3.29; 3.43; 3.44; 3.45 | 1 |
| creatine | 3.05; 3.94 | 2 |
|  |  |  |
| *Carbohydrates* |  |  |
| α-glucose / β-glucose | 3.25; 3.26; 3.26; 3.28; 3.40; 3.41; 3.42; 3.43; 3.44; 3.47; 3.48; 3.49; 3.49; 3.50; 3.51; 3.51; 3.52; 3.53; 3.54; 3.55; 3.56; 3.57; 3.70; 3.71; 3.73; 3.74; 3.75; 3.76; 3.78; 3.79; 3.83; 3.83; 3.84; 3.85; 3.85; 3.86; 3.87; 3.89; 3.90; 3.91; 3.92; 4.65; 4.67; 5.25; 5.26 | 1 |
| mannose | 3.66; 3.67; 3.69; 3.88; 3.95; 3.95; 3.96; 4.93; 4.93; 5.20; 5.20 | 1 |
|  |  |  |
| *Nucleotides/Nucleosides*  inosine  uracile  uridine | 4.28; 4.28; 4.29; 4.29; 4.29; 4.30; 4.40; 4.45; 4.45; 4.46; 4.77; 4.78; 4.79; 6.10; 6.11; 8.25; 8.36  5.81; 5.83; 7.55; 7.57  4.17; 4.24; 4.25; 4.26; 4.37; 4.38; 4.39; 5.92; 5.93; 5.93; 5.94; 7.87; 7.88 | 2  2  2 |
| *Organic acids*  acetic acid  formic acid | 1.92  8.46 | 3  2 |
| lactic acid | 1.33; 1.34; 4.10; 4.12; 4.13; 4.14 | 1 |
|  |  |  |
| *Vitamin precursors* |  |  |
| betaine | 3. 28; 3.91 | 1 |
| choline | 3.22; 4.06; 4.07; 4.07; 4.08; 4.09;4.09 | 1 |
| niacinamide | 7.60; 7.60; 7.61; 7.62; 7.62; 7.63; 7.63; 8.72; 8.72; 8.73; 8.73; 8.95; 8.95 | 1 |
| *Others*  ethanol  putrescine | 1.17; 1.19; 1.20;  1.76; 1.77; 1.78; 1.79; 1.80; 3.06; 3.07; 3.08 | 2  2 |

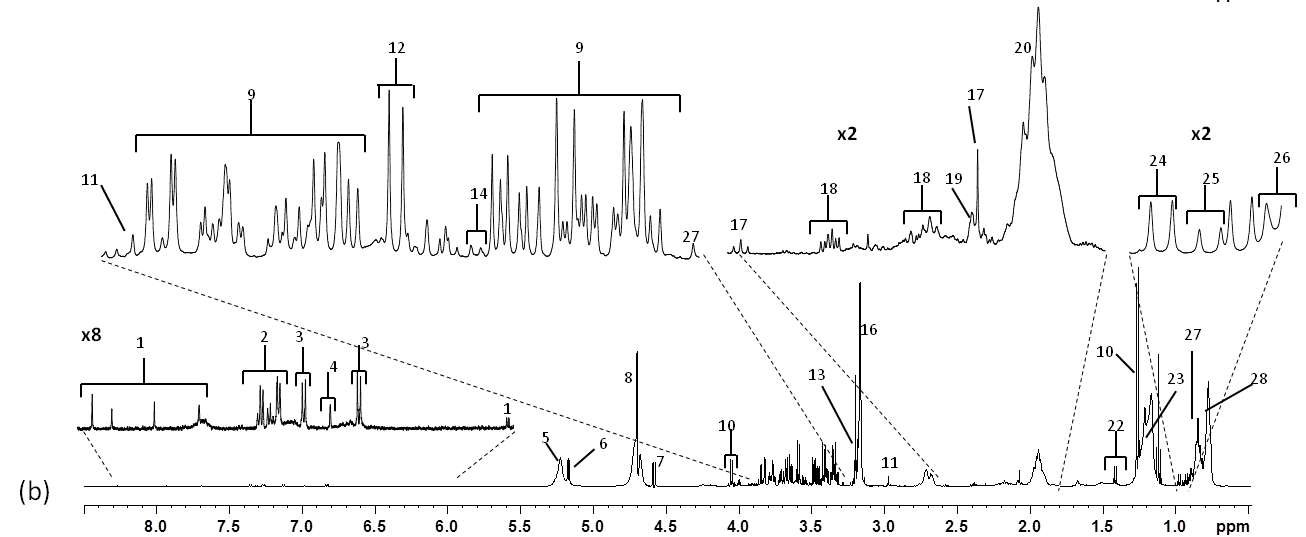
**Table S6: Effect of diet (marine M, commercial C and plant-based P) on semi-quantitative assessment of representative spectral regions or bucket of the 1H-NMR spectra of hydro-alcoholic extract of liver in rainbow trout.** Mean +/-std ANOVA analysis \*\*\* P< 0.001 \*\* P < 0.01 \* P<0.05. B8\_27 means bucket centred at 8.27 ppm. unk : resonance(s) from unknown metabolite(s). See Table S4 for MSI status of resonance annotation. unkS: singlet resonance of unknown metabolite; unkD: doublet of resonances of unknown metabolite; unkT: triplet of resonances of unknown metabolite; b: broad signal.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Bucket | Metabolite resonance annotation | Plant-Based diet | | Commercial diet | | Marine diet | | Diet Effect . |
|  |  | mean | std | mean | std | mean | std |  |
| **Marine Diet > Plant Diet** | |  |  |  |  |  |  |  |
| B8\_267 | niacinamide | 0.050 | 0.029 | 0.068 | 0.010 | 0.092 | 0.022 | \*\* |
| B8\_223 | unkD8.22 | 0.013 | 0.013 | 0.043 | 0.012 | 0.032 | 0.008 | \*\*\* |
| B8\_212 | unkS8.21 | 0.006 | 0.006 | 0.011 | 0.003 | 0.017 | 0.007 | \*\*\* |
| B8\_202 | unkD8.22 | 0.011 | 0.012 | 0.040 | 0.011 | 0.031 | 0.009 | \*\*\* |
| B6\_158 | unkD6.16 | 0.000 | 0.000 | 0.002 | 0.006 | 0.014 | 0.011 | \*\*\* |
| B6\_093 | unk | 0.028 | 0.003 | 0.024 | 0.009 | 0.038 | 0.008 | \*\*\* |
| B6\_080 | unkD6.088 | 0.020 | 0.005 | 0.017 | 0.009 | 0.034 | 0.009 | \*\*\* |
| B4\_312 | Unk + Uridine | 0.031 | 0.009 | 0.040 | 0.009 | 0.058 | 0.018 | \*\*\* |
| B3\_911 | unk | 1.100 | 0.111 | 1.365 | 0.081 | 1.300 | 0.122 | \* |
| B3\_844 | unk | 0.293 | 0.030 | 0.435 | 0.039 | 0.375 | 0.061 | \*\*\* |
| B3\_787 | unk | 1.495 | 0.143 | 1.823 | 0.105 | 1.779 | 0.256 | \*\* |
| B3\_774 | glucose +mannose | 0.642 | 0.060 | 0.910 | 0.088 | 0.965 | 0.094 | \*\*\* |
| B3\_587 | unk + mannose + threonine | 0.075 | 0.070 | 0.289 | 0.123 | 0.312 | 0.081 | \*\*\* |
| B3\_432 | unk | 1.355 | 0.097 | 1.763 | 0.082 | 1.528 | 0.125 | \*\* |
| B2\_952 | unkS2.95 | 0.001 | 0.002 | 0.003 | 0.002 | 0.007 | 0.002 | \*\*\* |
| B2\_912 | unkS2.91 | 0.013 | 0.006 | 0.057 | 0.020 | 0.135 | 0.079 | \*\*\* |
| B2\_750 | unkS2.75 | 0.016 | 0.003 | 0.022 | 0.011 | 0.057 | 0.024 | \*\*\* |
| B2\_737 | unkS2.73 | 0.023 | 0.012 | 0.092 | 0.035 | 0.202 | 0.114 | \*\*\* |
| B2\_487 | glutamine | 0.055 | 0.018 | 0.099 | 0.021 | 0.088 | 0.027 | \*\*\* |
| B2\_478 | glutamine | 0.036 | 0.012 | 0.068 | 0.014 | 0.058 | 0.017 | \*\*\* |
| B2\_461 | unk | 0.090 | 0.031 | 0.174 | 0.038 | 0.151 | 0.045 | \*\*\* |
| B2\_453 | unk | 0.052 | 0.017 | 0.100 | 0.020 | 0.083 | 0.025 | \*\*\* |
| B2\_445 | glutamine | 0.055 | 0.018 | 0.111 | 0.022 | 0.097 | 0.027 | \*\*\* |
| B1\_322 | unk | 1.248 | 0.292 | 1.142 | 0.289 | 1.700 | 0.378 | \*\* |
| **Plant diet > Marine diet** | |  |  |  |  |  |  |  |
| B8\_940 | niacinamide | 0.07 | 0.01 | 0.07 | 0.01 | 0.06 | 0.01 | \*\* |
| B8\_46 | formic acid | 0.10 | 0.01 | 0.05 | 0.01 | 0.04 | 0.01 | \*\*\* |
| B8\_392 | unkS8.39 | 0.01 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | \*\*\* |
| B8\_361 | inosine | 0.71 | 0.10 | 0.64 | 0.08 | 0.52 | 0.11 | \*\*\* |
| B7\_791 | unkD7.79 | 0.03 | 0.01 | 0.02 | 0.00 | 0.01 | 0.00 | \*\* |
| B7\_772 | unkD7.79 | 0.03 | 0.01 | 0.02 | 0.00 | 0.01 | 0.00 | \*\*\* |
| B7\_563 | uracile | 0.03 | 0.01 | 0.03 | 0.01 | 0.02 | 0.01 | \*\*\* |
| B7\_548 | uracile | 0.03 | 0.01 | 0.03 | 0.01 | 0.02 | 0.01 | \*\*\* |
| B7\_310 | unk + tryptophan | 0.03 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | \*\*\* |
| B6\_124 | inosine | 0.33 | 0.05 | 0.31 | 0.04 | 0.23 | 0.05 | \*\*\* |
| B6\_105 | inosine | 0.35 | 0.05 | 0.32 | 0.04 | 0.23 | 0.05 | \*\*\* |
| B5\_824 | uracile | 0.03 | 0.01 | 0.03 | 0.01 | 0.02 | 0.01 | \*\*\* |
| B5\_804 | uracile | 0.03 | 0.01 | 0.03 | 0.01 | 0.02 | 0.01 | \*\*\* |
| B5\_579 | unkbS5.58 | 0.02 | 0.01 | 0.02 | 0.01 | 0.01 | 0.01 | \*\*\* |
| B4\_924 | mannose | 0.14 | 0.02 | 0.18 | 0.02 | 0.12 | 0.02 | \*\*\* |
| B4\_798 | inosine | 0.18 | 0.04 | 0.16 | 0.04 | 0.11 | 0.06 | \*\* |
| B4\_787 | inosine | 0.38 | 0.05 | 0.31 | 0.09 | 0.20 | 0.11 | \*\*\* |
| B4\_776 | inosine | 0.19 | 0.04 | 0.12 | 0.03 | 0.09 | 0.06 | \*\*\* |
| B4\_462 | inosine | 0.16 | 0.02 | 0.15 | 0.02 | 0.11 | 0.03 | \*\*\* |
| B4\_453 | inosine | 0.17 | 0.02 | 0.15 | 0.02 | 0.12 | 0.02 | \*\*\* |
| B4\_448 | inosine | 0.19 | 0.03 | 0.17 | 0.02 | 0.14 | 0.03 | \*\*\* |
| B4\_438 | inosine | 0.21 | 0.03 | 0.18 | 0.02 | 0.15 | 0.03 | \*\*\* |
| B4\_303 | inosine | 0.09 | 0.01 | 0.07 | 0.01 | 0.07 | 0.02 | \*\*\* |
| B4\_294 | inosine | 0.29 | 0.04 | 0.27 | 0.03 | 0.21 | 0.05 | \*\*\* |
| B4\_285 | inosine | 0.27 | 0.04 | 0.25 | 0.03 | 0.17 | 0.04 | \*\*\* |
| B4\_073 | unk + choline | 0.83 | 0.17 | 0.61 | 0.16 | 0.53 | 0.11 | \*\*\* |
| B3\_920 | glucose | 0.89 | 0.12 | 0.92 | 0.11 | 0.70 | 0.13 | \*\*\* |
| B3\_566 | glucose | 0.80 | 0.09 | 0.89 | 0.07 | 0.67 | 0.10 | \*\*\* |
| B3\_557 | glucose | 0.72 | 0.10 | 0.76 | 0.10 | 0.56 | 0.11 | \*\*\* |
| B3\_547 | unk | 0.75 | 0.08 | 0.78 | 0.09 | 0.63 | 0.08 | \*\*\* |
| B3\_537 | unk | 0.87 | 0.13 | 0.89 | 0.09 | 0.70 | 0.09 | \*\*\* |
| B3\_486 | unk | 0.66 | 0.09 | 0.72 | 0.09 | 0.56 | 0.06 | \*\*\* |
| B3\_424 | unk | 4.44 | 0.20 | 4.20 | 0.25 | 3.88 | 0.36 | \* |
| B3\_390 | glucose | 0.72 | 0.08 | 0.82 | 0.07 | 0.61 | 0.09 | \*\*\* |
| B3\_267 | unk | 2.70 | 0.73 | 1.86 | 0.21 | 1.84 | 0.28 | \*\*\* |
| B3\_255 | glucose | 1.00 | 0.09 | 1.17 | 0.16 | 0.76 | 0.22 | \*\*\* |
| B3\_080 | unkT3.09 | 0.06 | 0.02 | 0.06 | 0.03 | 0.03 | 0.02 | \*\*\* |
| B2\_775 | unkS2.78 | 0.02 | 0.01 | 0.01 | 0.00 | 0.01 | 0.00 | \*\*\* |
| B2\_391 | unkS2.39 + glutamic acid | 0.08 | 0.01 | 0.04 | 0.01 | 0.04 | 0.01 | \*\*\* |
| B1\_802 | putrescine | 0.04 | 0.02 | 0.04 | 0.01 | 0.03 | 0.01 | \* |
| B1\_350 | threonine + lactic acid | 0.36 | 0.06 | 0.25 | 0.07 | 0.19 | 0.05 | \*\*\* |
| B1\_216 | ethanol | 0.02 | 0.01 | 0.02 | 0.00 | 0.01 | 0.01 | \*\* |
| B1\_072 | unkS1.07 | 0.02 | 0.00 | 0.01 | 0.00 | 0.02 | 0.00 | \*\*\* |
| B0\_928 | isoleucine | 0.04 | 0.01 | 0.04 | 0.01 | 0.03 | 0.01 | \* |

**Table S6: Effect of diet (marine M, commercial C and plant-based P) on semi-quantitative assessment of representative spectral regions or bucket of the 1H-NMR spectra of hydro-alcoholic extract of muscle in rainbow trout.** Mean +/-std ANOVA analysis \*\*\* *P* < 0.001 \*\* *P* < 0.01 \* *P* < 0 .05. B8\_27 means bucket centred at 8.27 ppm. unk : resonance(s) from unknown metabolite(s). See Table S4 for MSI status of resonance annotation. unkS: singlet resonance of unknown metabolite; unkD: doublet of resonances of unknown metabolite; unkT: triplet of resonances of unknown metabolite; b: broad.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Bucket | Metabolite resonance annotation | Plant Based diet | | Commercial diet | | Marine diet | | Diet effect |
|  |  | mean | std | mean | std | mean | std |  |
| **Marine > Plant Based-diet** | | | | | | | |  |
| B9\_332 | unk | nd | 0.001 | 0.001 | 0.001 | 0.004 | 0.002 | \*\*\* |
| B9\_139 | unk | nd |  | nd |  | 0.005 | 0.002 | \*\*\* |
| B8\_953 | niacinamide | 0.012 | 0.001 | 0.022 | 0.003 | 0.023 | 0.004 | \*\*\* |
| B8\_942 | niacinamide | 0.010 | 0.001 | 0.020 | 0.002 | 0.020 | 0.003 | \*\*\* |
| B8\_861 | unk | nd |  | nd |  | 0.002 | 0.001 | \*\*\* |
| B8\_843 | unk | 0.000 | 0.001 | 0.000 | 0.001 | 0.002 | 0.001 | \*\*\* |
| B8\_732 | niacinamide | 0.006 | 0.001 | 0.011 | 0.001 | 0.012 | 0.002 | \*\*\* |
| B8\_725 | niacinamide | 0.005 | 0.001 | 0.010 | 0.001 | 0.010 | 0.002 | \*\*\* |
| B8\_720 | niacinamide | 0.006 | 0.001 | 0.011 | 0.001 | 0.011 | 0.002 | \*\*\* |
| B8\_714 | niacinamide | 0.005 | 0.001 | 0.009 | 0.001 | 0.009 | 0.001 | \*\*\* |
| B7\_624 | niacinamide | 0.007 | 0.001 | 0.013 | 0.002 | 0.013 | 0.002 | \*\*\* |
| B7\_612 | niacinamide | 0.006 | 0.001 | 0.012 | 0.001 | 0.012 | 0.002 | \*\*\* |
| B7\_604 | niacinamide | 0.006 | 0.001 | 0.011 | 0.001 | 0.011 | 0.002 | \*\*\* |
| B7\_590 | niacinamide | 0.007 | 0.001 | 0.012 | 0.002 | 0.012 | 0.002 | \*\*\* |
| B6\_034 | unk | 0.001 | 0.000 | 0.001 | 0.000 | 0.002 | 0.001 | \*\*\* |
| B5\_917 | uridine | 0.000 | 0.001 | nd |  | 0.002 | 0.001 | \*\*\* |
| B5\_619 | unk | 0.003 | 0.001 | 0.005 | 0.001 | 0.006 | 0.001 | \*\*\* |
| B5\_602 | unk | 0.001 | 0.001 | 0.004 | 0.002 | 0.004 | 0.002 | \*\* |
| B5\_451 | unk | nd |  | 0.001 | 0.001 | 0.001 | 0.001 | \* |
| B5\_377 | unk | 0.024 | 0.017 | 0.053 | 0.034 | 0.050 | 0.017 | \*\* |
| B5\_239 | unk | 0.000 | 0.000 | 0.024 | 0.023 | 0.045 | 0.005 | \*\*\* |
| B5\_030 | unk | 0.006 | 0.003 | 0.019 | 0.012 | 0.013 | 0.006 | \*\*\* |
| B4\_836 | unk | 0.003 | 0.002 | 0.219 | 0.193 | 0.076 | 0.055 | \*\*\* |
| B4\_348 | unk | 0.032 | 0.017 | 0.052 | 0.014 | 0.062 | 0.025 | \*\* |
| B4\_074 | choline + 13C creatine | 0.053 | 0.007 | 0.046 | 0.004 | 0.063 | 0.012 | \*\*\* |
| B4\_063 | choline | 0.020 | 0.006 | 0.019 | 0.003 | 0.026 | 0.006 | \*\*\* |
| B3\_547 | choline | 0.089 | 0.014 | 0.091 | 0.006 | 0.121 | 0.026 | \*\*\* |
| B3\_536 | choline | 0.051 | 0.008 | 0.048 | 0.005 | 0.068 | 0.012 | \*\*\* |
| B3\_413 | unk | 0.087 | 0.013 | 0.090 | 0.017 | 0.117 | 0.012 | \*\*\* |
| B3\_225 | choline + anserine + taurine + betaine + histidine + unk | 10.693 | 1.076 | 15.847 | 1.654 | 18.542 | 1.900 | \*\*\* |
| B2\_592 | unk | 0.003 | 0.001 | 0.011 | 0.007 | 0.008 | 0.003 | \*\*\* |
| B2\_425 | unk | 0.002 | 0.002 | 0.011 | 0.003 | 0.007 | 0.003 | \*\*\* |
| B2\_420 | unk | 0.001 | 0.001 | 0.003 | 0.001 | 0.003 | 0.001 | \*\*\* |
| B2\_294 | unk + leucine | 0.005 | 0.001 | 0.007 | 0.002 | 0.008 | 0.002 | \*\* |
| B2\_287 | unk + leucine | 0.010 | 0.005 | 0.013 | 0.009 | 0.019 | 0.005 | \*\* |
| B2\_263 | unk + leucine | 0.006 | 0.002 | 0.007 | 0.005 | 0.011 | 0.003 | \*\* |
| B2\_242 | unk | 0.000 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | \*\*\* |
| B2\_162 | unk | 0.039 | 0.007 | 0.059 | 0.006 | 0.052 | 0.008 | \*\*\* |
| B1\_946 | unkS1.94 | 0.009 | 0.004 | 0.010 | 0.002 | 0.016 | 0.002 | \*\*\* |
| B1\_126 | unk | 0.001 | 0.000 | 0.002 | 0.001 | 0.004 | 0.001 | \*\*\* |
| B0\_936 | unkS0.94 | 0.009 | 0.002 | 0.015 | 0.002 | 0.014 | 0.003 | \*\*\* |
| B0\_910 | unkbS0.91 | 0.016 | 0.003 | 0.021 | 0.003 | 0.021 | 0.004 | \*\*\* |
| P**lant-Based diet > Marine diet** | | | | | | | |  |
| B8\_123 | anserine + histidine | 2.840 | 0.221 | 2.301 | 0.122 | 2.150 | 0.214 | \*\*\* |
| B7\_146 | anserine + histidine | 2.414 | 0.117 | 1.927 | 0.126 | 1.738 | 0.191 | \*\*\* |
| B6\_903 | tyrosine | 0.012 | 0.002 | 0.010 | 0.003 | 0.008 | 0.003 | \* |
| B6\_915 | tyrosine | 0.003 | 0.001 | 0.002 | 0.001 | 0.002 | 0.001 | \*\* |
| B4\_460 | inosine | 0.030 | 0.010 | 0.027 | 0.007 | 0.017 | 0.009 | \*\* |
| B4\_449 | inosine | 0.070 | 0.022 | 0.061 | 0.013 | 0.037 | 0.021 | \*\* |
| B4\_437 | inosine | 0.043 | 0.014 | 0.035 | 0.007 | 0.022 | 0.012 | \*\* |
| B4\_285 | inosine + unk | 0.072 | 0.023 | 0.090 | 0.028 | 0.041 | 0.016 | \*\*\* |
| B4\_277 | inosine + unk | 0.022 | 0.007 | 0.017 | 0.008 | 0.012 | 0.005 | \*\* |
| B4\_269 | unk | 0.030 | 0.006 | 0.035 | 0.006 | 0.024 | 0.007 | \*\* |
| B4\_263 | unk | 0.024 | 0.006 | 0.044 | 0.011 | 0.016 | 0.003 | \*\*\* |
| B4\_167 | unk | 0.031 | 0.012 | 0.012 | 0.004 | 0.011 | 0.005 | \*\*\* |
| B4\_146 | lactic acid | 1.022 | 0.112 | 0.914 | 0.059 | 0.899 | 0.061 | \* |
| B4\_127 | lactic acid | 2.901 | 0.273 | 2.669 | 0.202 | 2.643 | 0.201 | \* |
| B4\_112 | lactic acid | 2.870 | 0.271 | 2.665 | 0.208 | 2.623 | 0.208 | \* |
| B4\_098 | lactic acid | 0.936 | 0.093 | 0.878 | 0.073 | 0.850 | 0.075 | \* |
| B4\_021 | unk | 0.177 | 0.043 | 0.096 | 0.013 | 0.126 | 0.023 | \*\*\* |
| B4\_012 | histidine | 0.136 | 0.027 | 0.050 | 0.013 | 0.083 | 0.019 | \*\*\* |
| B4\_005 | histidine | 0.101 | 0.035 | 0.038 | 0.007 | 0.060 | 0.025 | \*\*\* |
| B3\_997 | histidine | 0.147 | 0.031 | 0.046 | 0.012 | 0.075 | 0.022 | \*\*\* |
| B3\_997 | histidine + unk | 0.043 | 0.016 | 0.020 | 0.012 | 0.027 | 0.013 | \*\* |
| B3\_876 | unk | 0.140 | 0.037 | 0.077 | 0.014 | 0.102 | 0.027 | \*\*\* |
| B3\_854 | unk + glucose | 0.116 | 0.030 | 0.074 | 0.013 | 0.075 | 0.019 | \*\*\* |
| B3\_785 | unkS3.79 + unk | 6.338 | 0.621 | 5.667 | 0.442 | 5.114 | 0.396 | \*\*\* |
| B3\_613 | unk +valine | 0.064 | 0.015 | 0.061 | 0.018 | 0.044 | 0.011 | \* |
| B3\_563 | glucose | 0.040 | 0.007 | 0.032 | 0.007 | 0.030 | 0.005 | \*\* |
| B3\_454 | taurine | 0.294 | 0.049 | 0.223 | 0.080 | 0.211 | 0.048 | \*\* |
| B3\_440 | taurine | 0.759 | 0.118 | 0.566 | 0.191 | 0.552 | 0.121 | \*\* |
| B3\_431 | glucose | 0.059 | 0.008 | 0.039 | 0.014 | 0.048 | 0.006 | \*\*\* |
| B3\_424 | taurine | 0.488 | 0.064 | 0.348 | 0.113 | 0.347 | 0.067 | \*\*\* |
| B3\_057 | creatine | 17.307 | 1.959 | 13.927 | 0.915 | 15.494 | 1.020 | \* |
| B2\_580 | unkT2.56 | 0.026 | 0.012 | 0.016 | 0.004 | 0.014 | 0.003 | \*\* |
| B2\_566 | unkT2.56 | 0.047 | 0.024 | 0.029 | 0.009 | 0.022 | 0.006 | \*\* |
| B2\_553 | unkT2.56 | 0.021 | 0.011 | 0.015 | 0.005 | 0.010 | 0.003 | \*\* |
| B2\_407 | unkS2.39 + glutamic acid | 0.003 | 0.003 | 0.001 | 0.001 | 0.000 | 0.000 | \*\* |
| B2\_391 | unk | 0.011 | 0.004 | 0.006 | 0.001 | 0.007 | 0.002 | \*\*\* |
| B2\_371 | glutamic acid + unk | 0.039 | 0.018 | 0.025 | 0.006 | 0.020 | 0.005 | \*\* |
| B2\_356 | glutamic acid + unk | 0.077 | 0.025 | 0.050 | 0.012 | 0.042 | 0.013 | \*\*\* |
| B2\_339 | glutamic acid + unk | 0.047 | 0.016 | 0.019 | 0.016 | 0.002 | 0.007 | \*\*\* |
| B2\_326 | glutamic acid + unk | 0.006 | 0.004 | 0.003 | 0.001 | 0.001 | 0.001 | \*\*\* |
| B2\_309 | valine | 0.001 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | \* |
| B2\_232 | unk | 0.002 | 0.000 | 0.001 | 0.000 | 0.001 | 0.000 | \*\*\* |
| B2\_110 | glutamic acid + unk | 0.006 | 0.003 | 0.003 | 0.001 | 0.004 | 0.001 | \*\*\* |
| B2\_099 | glutamic acid + unk | 0.022 | 0.011 | 0.010 | 0.003 | 0.007 | 0.002 | \*\*\* |
| B2\_085 | glutamic acid + unk | 0.035 | 0.016 | 0.017 | 0.005 | 0.012 | 0.003 | \*\*\* |
| B2\_071 | glutamic acid + unk | 0.039 | 0.016 | 0.019 | 0.005 | 0.016 | 0.004 | \*\*\* |
| B2\_062 | glutamic acid + unk | 0.007 | 0.006 | 0.002 | 0.001 | 0.002 | 0.000 | \*\* |
| B2\_056 | glutamic acid + unk | 0.024 | 0.007 | 0.011 | 0.003 | 0.009 | 0.002 | \*\*\* |
| B2\_049 | glutamic acid + unk | 0.012 | 0.009 | 0.004 | 0.002 | 0.004 | 0.001 | \*\* |
| B2\_039 | unk | 0.037 | 0.017 | 0.013 | 0.005 | 0.010 | 0.002 | \*\*\* |
| B2\_024 | unk | 0.054 | 0.032 | 0.018 | 0.007 | 0.013 | 0.003 | \*\*\* |
| B2\_009 | unk | 0.049 | 0.034 | 0.015 | 0.008 | 0.009 | 0.003 | \*\*\* |
| B1\_991 | unk | 0.074 | 0.026 | 0.039 | 0.014 | 0.038 | 0.014 | \*\*\* |
| B1\_979 | unk | 0.004 | 0.002 | 0.001 | 0.000 | 0.001 | 0.000 | \*\*\* |
| B1\_966 | unk | 0.005 | 0.002 | 0.002 | 0.000 | 0.002 | 0.001 | \*\*\* |
| B1\_924 | acetic acid | 0.152 | 0.036 | 0.114 | 0.020 | 0.091 | 0.042 | \*\*\* |
| B1\_889 | lysine + unk | 0.010 | 0.003 | 0.004 | 0.001 | 0.007 | 0.002 | \*\*\* |
| B1\_873 | lysine + unk | 0.011 | 0.002 | 0.004 | 0.001 | 0.005 | 0.001 | \*\*\* |
| B1\_711 | leucine + lysine | 0.020 | 0.007 | 0.010 | 0.003 | 0.012 | 0.005 | \*\*\* |
| B1\_694 | leucine + unk | 0.011 | 0.004 | 0.005 | 0.003 | 0.006 | 0.002 | \*\*\* |
| B1\_466 | 13C lactic acid | 0.066 | 0.004 | 0.063 | 0.004 | 0.056 | 0.004 |  |
| B1\_451 | 13C lactic acid | 0.066 | 0.006 | 0.061 | 0.003 | 0.056 | 0.006 |  |
| B1\_440 | unk | 0.008 | 0.002 | 0.002 | 0.001 | 0.003 | 0.001 | \*\*\* |
| B1\_354 | lactic acid | 12.422 | 1.213 | 11.546 | 0.721 | 11.033 | 0.903 | \* |
| B1\_312 | lactic acid | 12.180 | 1.238 | 11.470 | 0.756 | 10.861 | 0.872 | \* |
| B1\_155 | unk | 0.002 | 0.001 | 0.001 | 0.000 | 0.001 | 0.000 | \*\* |
| B1\_059 | unk | 0.075 | 0.020 | 0.051 | 0.011 | 0.044 | 0.020 | \*\* |
| B1\_041 | valine | 0.066 | 0.019 | 0.045 | 0.011 | 0.042 | 0.013 | \*\* |
|  |  |  |  |  |  |  |  |  |
| B1\_012 | isoleucine | 0.030 | 0.010 | 0.018 | 0.006 | 0.018 | 0.008 | \*\* |
| B1\_003 | isoleucine | 0.063 | 0.017 | 0.044 | 0.010 | 0.042 | 0.012 | \*\* |
| B0\_993 | valine | 0.061 | 0.016 | 0.042 | 0.009 | 0.040 | 0.012 | \*\* |
| B0\_986 | valine | 0.014 | 0.002 | 0.011 | 0.002 | 0.011 | 0.002 | \*\*\* |
| B0\_979 | leucine | 0.041 | 0.011 | 0.022 | 0.007 | 0.022 | 0.009 | \*\*\* |
| B0\_960 | isoleucine | 0.101 | 0.031 | 0.052 | 0.018 | 0.057 | 0.023 | \*\*\* |
| B0\_953 | leucine | 0.028 | 0.010 | 0.015 | 0.005 | 0.016 | 0.007 | \*\*\* |
| B0\_944 | isoleucine | 0.022 | 0.009 | 0.010 | 0.004 | 0.013 | 0.005 | \*\*\* |
| B0\_936 | unkS0.93 | 0.028 | 0.011 | 0.017 | 0.005 | 0.017 | 0.007 | \*\* |
| B0\_927 | isoleucine | 0.013 | 0.005 | 0.008 | 0.003 | 0.009 | 0.004 | \*\* |

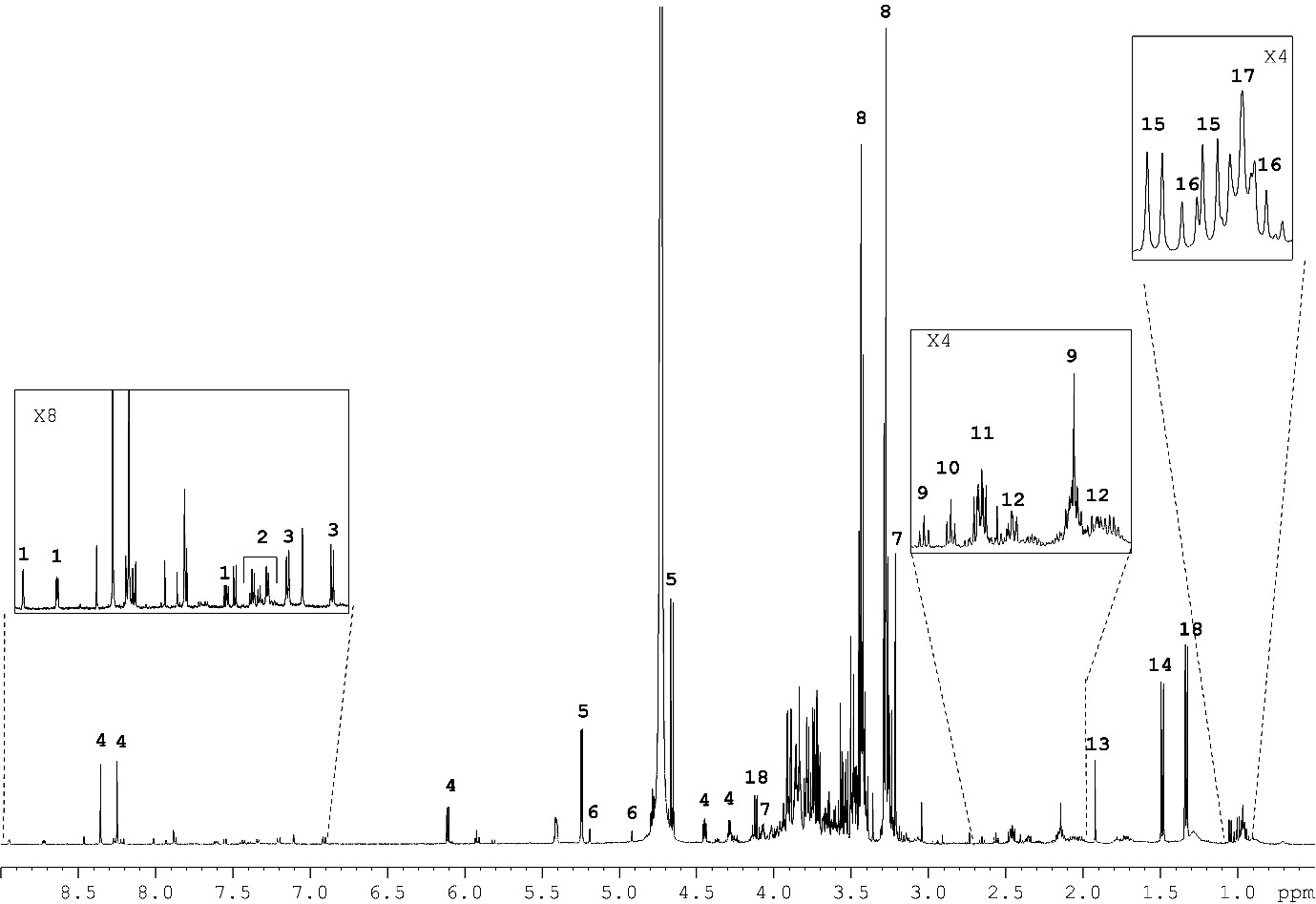
**Figure S1** Representative 500 MHz 1H-NMR spectra of rainbow trout plasma fed a commercial diet, 6 h after the last meal. Spectra was acquired with a (a) *zgpr* and (b) *cpmg* sequence. Legend: 1 (adenosine-XP like) ; 2 (PHE); 3 (TYR) ; 4 (HIS\*); 5 (-CH=CH-, unsaturated lipids); 6 (α-glucose); 7 (β-glucose) ; 8 (HOD) ; 9 (-CH2-, glucose); 10 (lactate); 11 (creatine); 12 (ethanol); 13 (choline); 14 (THR); 15 (LYS); 16 (-CH3, lipoprotein, VLDL); 17 (MET); 18 (GLN); 19 (-CH2-C=O, lipids); 20 (acetyl glycoprotein\*); 21 (-CH2-CH2-C=O, lipids); 22 (ALA); 23 (-(CH2) n—, lipoprotein, HDL); 24 (VAL); 25 (ILE); 26 (LEU); 27 (betaine).



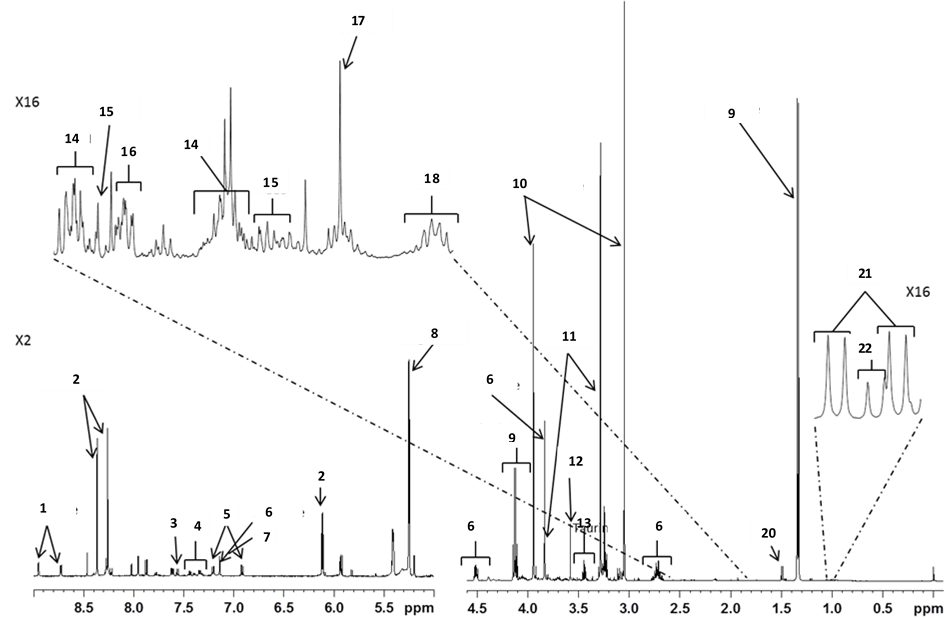
**Figure S2:** Multidimensional PCA analysis of 1H-NMR spectra (*CPMG* sequence) of plasma segmented into 212 variable-size spectral regions. A) representation on the first and third PC axes of the scores of plasma of individuals fish fed a marine M diet (triangle), a plant-based P diet (circle) and a commercial C diet (diamond) either 6h post feeding (straight line) or 48h post feeding (dotted line) and (B) representation of the main significant spectral regions involved in the PC3 axis differences related to time after feeding

|  |  |
| --- | --- |
| **A** |  |

**Figure S3** Representative 500 MHz 1H-NMR spectra of liver hydro-alcoolic polar extracts in rainbow trout fed a commercial diet. Legend: 1: niacinamide; 2: phenylalanine; 3: tyrosine; 4: inosine; 5: glucose; 6: mannose; 7: choline; 8: taurine; 9: methionine; 10: beta-alanine; 11: glutamine; 12: glutamate; 13: acetate; 14: alanine; 15: valine; 17: leucine; 16: isoleucine; 18: lactate



**Figure S4** Representative 500 MHz 1H-NMR spectrum of muscle tissue hydro-alcoolic extracts in rainbow trout fed a commercial C diet. Legend: GLU (Glutamate), GLN (Glutamine), TYR (Tyrosine), PHE (Phenylalanine), TRP (Tryptophan), HIS (Histidine), ALA (Alanine), LYS (Lysine), ILE (Isoleucine), VAL (Valine), ADP/ATP (Adenosine Di and/or Triphosphate).



*Methodological consideration for successful development of 1H-NMR methodologies on diet, plasma and tissues*

*Diet*

The alcoholic extracts of diet contained a rich mixture of soluble compounds representative of the free soluble compounds already present originally in the marine products (fish meal) or in the plant products but contained also probably the end-products of the degradation process occurring during process and storage. The profiles of these compounds were found to be stable during storage of the diet. The quantification of these compounds was possible as the 1H-NMR spectra of diet comprised at least one or several resonances for each compound with few overlapping between resonance patterns.

*Plasma*

A direct analysis of plasma without extraction was implemented. The raw 1H-NMR profile was however complex due to the presence of macromolecules namely lipoproteins - sometimes at high concentration as it is for chylomicrons after feeding - and other circulating plasmatic protein such as glyco-protein. A serum preparation with blood clotting is currently practiced in mammals to eliminate a large part of the circulating protein ([[1]](#endnote-1)). Clotting is however not easy to manage in fish as blood contained erythrocytes nucleated cells to ensure oxygen transport rather than enucleated one in mammals. Furthermore, fish such as salmonids live at lower temperature than mammals and the kinetic of clotting is slowed. For these reason, plasma is usually preferred in these species ([[2]](#endnote-2), [[3]](#endnote-3)).

The 1H-NMR spectra of plasma after CPGM revealed a relatively comprehensive set of 40 compounds amongst the main expected circulating metabolites: amino acids, sugars, organic acids, nucleic acids and even cholesterol and lipid-soluble compounds. The relative changes with time after feeding (6 h and 48 h) was in concordance with the known changes after feeding of circulating metabolites *i.e.* peak of amino acids at 6 h after feeding ([[4]](#endnote-4)) and accumulation of glucose and other related compounds at 48 h after feeding ([[5]](#endnote-5),[[6]](#endnote-6)).

The plasmatic content of some compounds such as glucose and lactate detected by 1H-NMR was compared to that measured by classical biochemical method. Only semi-quantitative assessment of compounds in plasma was possible with the CPMG sequence of acquisition which does not saturated the signal of proton in molecules analysed. The comparison was clear enough for glucose which was measured by the two methods at relatively stable concentration at 6 h and 48 h after feeding except a higher concentration in marine diet at 48h compared to the two other diets. For lactate the comparison of the two measurements showed discrepancies as lactate measured by 1H-NMR was found to be higher in plant-based diet compared to marine diet, a difference that was not observed by classical method. Specific signals of lactate were identified at 1.33 and 4.13 ppm, thus 1H-NMR analysis could be considered as feasible for this compounds although not quantitative. The interesting differences observed with 1H-NMR has however to be investigated further as it could not only accounts for changes in fish metabolism but also in microbiota metabolism.

For the preparation of tissues, different methods have been tested in mammals [[7]](#endnote-7)and even in fish ([[8]](#endnote-8)) for metabolomic studies. The solvent extraction in two steps seems to extract the maximum number of metabolites and it is current practice in fish (ii, iii, [[9]](#endnote-9), [[10]](#endnote-10), [[11]](#endnote-11)). Other methods based on protein precipitation with either acetonitrile, PCA or TCA are still used even in fish ([[12]](#endnote-12)[[13]](#endnote-13)) but are less applicable for NMR analysis as it requires adjustment of pH and ionic strength.

The 1H-NMR spectra of liver and muscle revealed the main expected compounds *i.e.* amino acids, carbohydrates, organic acids, nucleotides and derivatives. The few number of compounds identified - 18 in liver and 16 in muscle - were however quite similar to that found by previous works in fish for liver: 9 to 19 compounds ([[14]](#endnote-14)) and for muscle : from 10-13 compounds (X, XIII, XIV,[[15]](#endnote-15)) to 28-39 compounds (IX, XII). The other compounds not identified were glycogen in liver extractand TMA/TMAO and hypoxanthine in muscle. Glycogen is not soluble in a hydroalcoholic extract thus it could not be detected in our study. TMA and TMAO are mainly the results of alteration of fish flesh by micro-organisms thus they are not present at high concentration in live fresh fish. Furthermore, these last compounds were not also detected in the marine and commercial diets demonstrating the high quality of fish meals used in our experimental diets.

Different segmentation of the 1H-NMR profile were implemented to increase the specificity and the number of signals. The final semi-automatic segmentation process with NMRProcFlow raised almost but 300 spectral regions in liver and muscle compared to 80 to 100 spectral regions with the initial manual segmentation. Further annotation of these signals will thus largely improved the number of metabolites that could be detected and analysed in fish.

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