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Fast Sampling of Adherent Cell Cultures for Optimal Metabolomics Results

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Abstract

Metabolomics is a valuable tool to gain mechanistic insight into biological processes. It is frequently used to obtain complementary details to other 'omics technologies such as transcriptomics or proteomics. For knowledge generation, reproducible measurements of physiological, intact, and artifact-free metabolite levels are imperative necessitating further standardization of best practices to improve reliability of research outcomes. Here we report a novel cell sample preparation method (MxP® CellCollect) for metabolomics applications using adherent mammalian cells, which reduces the time consumption and physiological stress of conventional methods such as trypsinization or cell scraping. The most common sampling procedures to detach cells from their growth surface, trypsinization and scraping were compared to the MxP® CellCollect method investigating metabolite profiles of two breast cancer cell lines (MDA-MB-231 and MCF7). Metabolite levels as well as direction of metabolite changes differed tremendously revealing issues with trypsinization and scraping risking non-physiological or misleading results in contrast to MxP® CellCollect. Differences in metabolic profiles of cells harvested by trypsinization as compared to MxP® CellCollect or scraping can be directly attributed to prolonged, medium-free incubation time during cell detachment leading to a severely energy-depleted intracellular state. Labile metabolites or metabolites with fast intracellular turnover rates such as glycolysis and TCA cycle intermediates were strongly and significantly decreased by trypsinization. The same was true for amino acids and nucleoside triphosphates. Results obtained with scraping using methanol as solvent were multifaceted. Even mild evaporation of methanol prior metabolite extraction led to temperature- and/or light-dependent degradation of labile metabolites such as nucleoside triphosphates into di- and monophosphates liberating pyrophosphate. Furthermore, lipid metabolites, in particular cell membrane lipids, were found to have significantly lower levels than measured by trypsinization or MxP® CellCollect, indicating that lipid metabolites are insufficiently detached and/or unspecifically adsorb to the hydrophobic dish and scraping tool.

Keywords: Metabolomics; *In vitro* sampling procedures; Adherent eukaryotic cells; Scraping; Trypsinization; MxP® CellCollect

Abbreviations

ANOVA: Analysis of Variance; $CHCl_3$: Chloroform; DCM: Dichloromethane; EtOH: Ethanol; FBS: Fetal Bovine Serum; GC: Gas Chromatography; HPLC: High Performance LC; ISTD: Internal Standard; LC: Liquid Chromatography; MeOH: Methanol; MRM: Multiple Reaction Monitoring; MS: Mass Spectrometry; PBS: Phosphate Buffered Saline; PCA: Principal Component Analysis; RPMI: Roswell Park Memorial Institute; TCA: Tricarboxylic Acid Cycle; TNBC: Triple Negative Breast Cancer; s: Second(s)

Introduction

Metabolomics is a valuable tool generating biological insight from the most diverse sample types ranging from plants, to plasma, tissue or cell culture. The use of metabolomics to obtain insight into the toxicological properties and mode of action of compounds when tested in rats, has been demonstrated in the MetaMap®Tox Project [1,2] and a successful step towards using this technology for *in vitro* systems was shown by [3].With adherent cells metabolomics is now becoming an invaluable tool to study disease mechanisms and mode of action of compounds, to discover drug targets and off-target effects, to observe resistance strategies, and to investigate toxicities [4-12]. A suitable sampling method is a key feature for routine use of high quality metabolomics with adherent cells. The method must be sufficiently robust, reproducible, easily performable, and most importantly, able to capture the physiological, non-perturbed intracellular metabolism [7]. The purpose of this investigation was to compare the most commonly used sampling procedures such as trypsinization and scraping, with a newly developed method called MxP® CellCollect and to suggest better standards in metabolomics sampling practices.

Materials and Method

Cell culture and harvesting

Six technical replicates per cell line and harvest condition were cultivated. MDA-MB-231 cells were freshly obtained from ATCC (HTB-26, Lot. 59922846) using passage 8 and MCF7 house-kept cells equivalent to ATCC (HTB-22) using passage 11 for experiments. Cells harvested by trypsinization or scraping were grown in standard uncoated 8.70 cm^2 6-well polystyrene culture dishes (83.3920.300, Sarstedt AG&Co.). Cells harvested by MxP® CellCollect were grown in uncoated 6.4 cm^2 lumox® dishes 35 (94.6077.331, Sarstedt AG&Co.). Per dish $0.25 \cdot 10^6$ MDA-MB-231 and $0.3 \cdot 10^6$ MCF7 cells were seeded and grown in RPMI-1640 medium (+10% FBS+2 mM glutamine+100 µg/ml Penicillin/Streptomycin) under standard growth conditions (37°C, 5% CO_2) reaching 80% confluence after 48 h.

For trypsinization, as described in [13], cells were quickly washed once with PBS (HPLC grade) and 0.2 mL 0.05% trypsin in 0.02% EDTA (R-001-100, Gibco®) were added for 5 min at 37°C. Detached cells were gently suspended in 0.4 mL fresh medium (37°C), transferred and spun down with 900 rpm for 3 min at 4°C. To mimic cell counting an

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artificial break of 5 min was introduced. Cells were thereafter washed twice with PBS (4°C).

For scraping, as described in [12], cell monolayers were quickly washed twice with ice-cold 5% maltose solution and residual fluid was removed with vacuum. Immediately 1 mL MeOH (HPLC grade) (-20°C) was added and cells were scraped (2-Posit. Blade 25, thermoplastic elastomers, Sarstedt AG&Co).

For MxP® CellCollect (Figure 1) the lumox® membrane (with the adherent cells on) was cut out with a scalpel, falling into a dish with 37°C warm washing buffer (isotonic NaCl for MxP® Broad Profiling or 4.5 g/L glucose in isotonic NaCl for MxP® Energy) [14]. The membrane was quickly picked up with tweezers and dip-washed twice in two further dishes with fresh washing buffer. The membrane was placed on top of a 2 mL Eppendorf tube and pushed inside with a pipette tip adding 600 µL DCM/EtOH (9:11) for MxP® Broad Profiling or 900 µL (2:1) DCM/EtOH for MxP® Energy (-80°C). The procedure from cutting the membrane until freezing should not exceed 30 s for each sample to prevent metabolic changes during sampling. All harvested cells were immediately snap frozen in liquid nitrogen and stored until extraction at -80°C. Directly before extraction, the MeOH of scraped cells was removed by mild evaporation over a few minutes at 40°C and DCM/EtOH (mixtures as above) were added. Likewise, DCM/EtOH mixtures were added to trypsinized cell pellets after thawing before routine extraction and measurement (described in supplementary information).

Statistical analysis

Metabolite values were log10-transformed for all statistical analysis in order to better approximate a normal distribution. For univariate analysis a linear ANOVA model was set up in the statistical software R [15] with the categorical fixed factors METHOD and CELL_LINE (readouts: ratios, p-values, t-values, Benjamini-Hochberg corrected q-values in supplementary Table 1). For multivariate analysis, data was further centered and scaled to unit variance and multivariate statistics were performed by using Simca P+ software (version 13, Umetrics AB, Umea, Sweden).

Results and Discussion

A quick sampling is a key prerequisite in order to capture physiological intracellular metabolite levels and to avoid loss of metabolites with high turnover rates (e.g. glycolysis intermediates). Since metabolite concentrations are very sensitive to any variation in the cell environment an ideal harvest and quenching method for metabolomics analysis would immediately stop all intracellular enzymatic activities and subsequently all intracellular changes in metabolite concentrations, without first affecting the cell environment. Furthermore, such a method should be rapid, highly efficient, and reproducible to allow an unbiased measurement of cellular metabolite concentrations, and to enable direct comparison of a large number of analytical samples. At the same time all cells with all of their metabolites must be collected and contaminations from spent media have to be avoided [16]. The necessary washing must leave metabolism unperturbed and should not induce any leakage or metabolite loss. Although great advances have been achieved by introduction of direct quenching and scraping instead of trypsinization [11,16-19] still a major drawback remains, namely the need for manual scraping and collection of cells. These steps might increase the variability of biological replicates due to differences in efficiency of cell transfer from the cell culture dish or cover slight into the extraction vial. Furthermore, these steps are time-consuming and therefore, might reduce overall attractiveness of this method to be used in high throughput cell culture experiments including several hundred samples in parallel.

Figure 1: Sampling procedure. MxP® CellCollect sampling consists of cutting the membrane, dip washing the cells on the membrane, and quenching the metabolism with -80°C cold solvent. The transparent membrane was colored red for better visibility.

New sampling method – MxP® CellCollect

The cells are grown on lumox® dishes, which foremost offer excellent gas diffusion through the thin, gas-permeable, membrane-like bottom on which the cells grow. More importantly, these dishes allow cutting out the membrane and thereby to collect all cells quickly at once (Figure 1). The cells on the membrane are gently and thoroughly washed by immediate dipping into two consecutive dishes. The metabolism is then rapidly quenched by pushing the membrane into a tube with a pipette tip, immediately adding -80°C precooled solvent and further snap freezing in liquid nitrogen. The time from cells being without medium until quenching is typically around a few seconds and the whole procedure takes less than 30 s. Standard coatings such as fibronectin were well compatible and cell-free blanks incubated with medium as additional controls showed no impact on results.

Comparison of trypsinization and scraping

The two most conventional cell harvesting protocols, trypsinization [13]. and scraping in cold MeOH [12], were directly compared to the developed method for two different cell lines while all other parameters (extraction, measurement, normalization) were kept constant. Both multivariate (PCA, supplementary information Figure S1) and univariate analysis (ANOVA, Figure 2 and supplementary information Table 1) revealed obvious differences between all three methods. Differences in the metabolic profiles of cells harvested by trypsinization as compared to MxP® CellCollect or scraping can be directly attributed to the prolonged, medium-free incubation time during cell detachment leading to a severely energy-depleted intracellular state (Figure 2a). Glycolysis and TCA cycle intermediates as well as almost all amino acids and nucleoside triphosphates were strongly and statistically significantly decreased. Adenylate energy charge (AEC=ATP+0.5·ADP/(ATP+ADP+AMP)) was with a value of 0.70 (± 0.05) far below AEC levels found with scraping or MxP® CellCollect (with values of 0.82 (± 0.07) and 0.84 (± 0.03), respectively). Although trypsinization is a valuable method for cell detachment from their growth surface (e.g. for cell passaging), our results and literature data [4,20] emphasize that trypsinization is not a suitable choice for physiological metabolomics since trypsin severely alters the physiological state of cells due to its interaction with membrane proteins resulting in sustained membrane damage in combination with metabolite leakage, and decreased cell viability, all of which significantly alter metabolite levels and cellular metabolite profiles [11]. As a consequence a considerable and highly variable portion of metabolites will be released into the trypsin solution and/or washing buffer depending on the length of trypsinization and washing/centrifugation steps. Furthermore, metabolic data varies for extremely labile metabolites or for metabolites with fast turnover

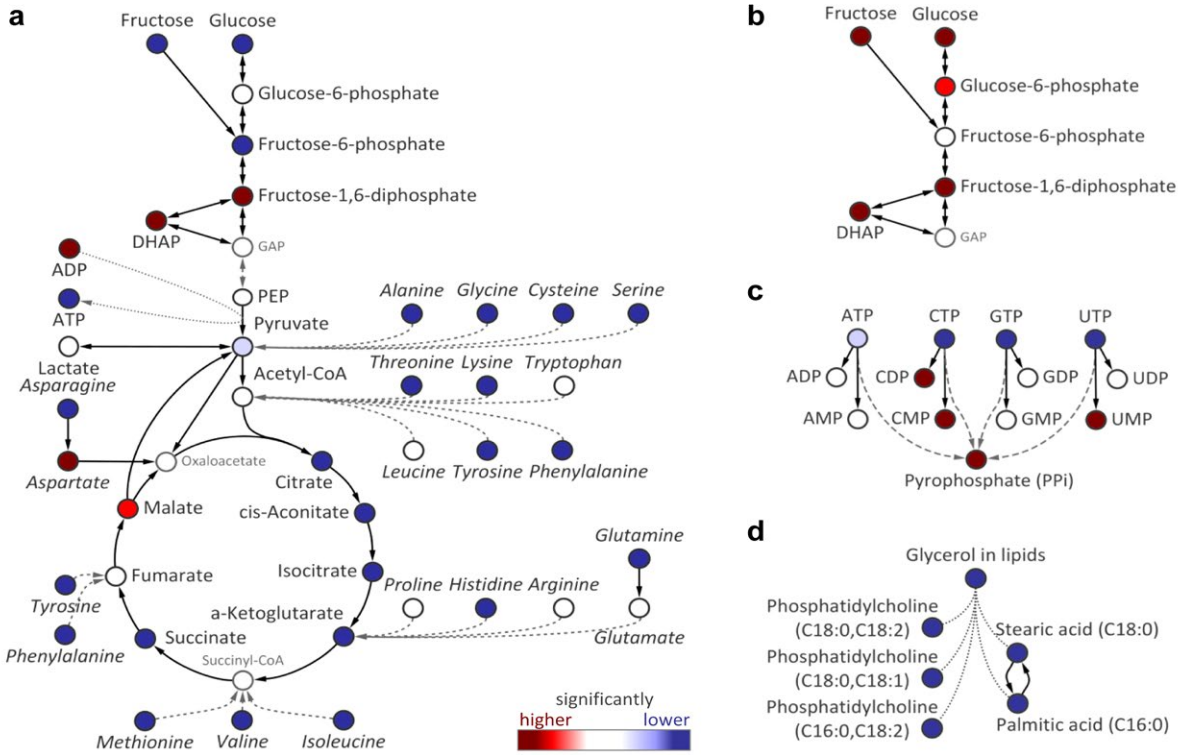

Figure 2: ANOVA comparison of different sampling methods across both cell lines. For a given comparison between two sampling methods red metabolite nodes signify higher metabolite levels while blue nodes signify lower levels with a significance of q-values <0.1 for least intensive colors to q-values <0.01 for most intensive colors. Grey metabolites were not measured and grey dashed arrows implicate several enzymatic reaction steps which were omitted for the sake of clarity. a) Comparison of trypsinization versus MxP® CellCollect reveals differences in glycolysis, TCA-cycle and proteinogenic amino acids. b), c), d) Comparison of scraping versus MxP® CellCollect with b) focusing on first steps of glycolysis, c) summarizing results for nucleoside tri-, di- and monophosphates and d showing results of selected lipid metabolites and their fatty acid precursors. The glycerol in lipids describes the sum of all glycerol moieties that is released from the lipid fraction of a biological sample after hydrolysis of complex lipids and subsequent derivatization prior to gas chromatographic analysis. Several phosphatidylcholines are shown as examples together with two saturated fatty acids which represent the sum of its occurrence both in free and in all lipid-bound forms (dotted lines indicate that fatty acids and phosphatidylcholines contribute to the total sum of conjugated glycerol in complex lipids).

rates in response to changes in cell environment and the numerous time-consuming steps (e.g. centrifugation) required before enzymatic activities are finally inhibited by cell quenching [4,11]. During this time, a considerable portion of intracellular metabolites is lost from cells due to their small molecular size, the intracellular fast turnover rates [11,21], and and the different osmotic strength of the applied solutions [22,23]. Nevertheless, trypsinization was and is still used frequently [13,24] and data obtained from trypsinized cells should be treated with utmost care, particularly if related to energy metabolism. The main reason for the use of trypsinization is the possibility to determine cell numbers for normalization purposes of the metabolic data. However, other normalization methods are available such as normalizing to cellular DNA after extraction [25]. In contrast, we have applied the median of all metabolites in a sample for normalization, which works well if the number of metabolites is sufficiently high (>50) and data per sample is sufficiently comprehensive (<30% missing values). Median normalization also saves considerable time and resources because additional measurements such as DNA or additional biological replicates for cell counting can be omitted. Additionally, harsh extraction protocols with mechanical cell disruption (e.g. bead milling) are necessary for good overall metabolite recoveries, in particular for recovery of lipid metabolites [17], but also strongly fragmented cellular DNA rendering DNA normalization impossible.

Results obtained with scraping were multifaceted and three major artificial influences were identified. First, the chosen protocol from Urakami et al. included a washing step with 5% maltose which led, despite the very short incubation time, to a considerable increase in early glycolysis intermediates (Figure 2b). This emphasizes the importance of choosing adequate washing solutions. Preferably non-cold, isotonic, phosphate-free solutions should be used containing the same carbon sources as the culture medium tested. These carbon sources can also be fully isotopically labeled, such as all ^{13}C, thereby slowing down ^{12}C metabolism during washing and stabilizing early glycolysis intermediates (Bordag et al. in preparation). The second observed effect was that even mild evaporation of the scraping solvent MeOH led to temperature- and/or light-dependent degradation of labile metabolites such as nucleoside triphosphates into di- and monophosphates liberating pyrophosphate (Figure 2c). For MeOH-based extractions solvent removal is not necessary. However, the MeOH poses problems for other extractions and needs to be removed which would require validation of even milder solvent removal (e.g. by lowering temperature or reducing exposure to light or evaporation time). Third, levels of lipids especially from cell membrane lipids were found to have significantly lower levels than measured by trypsinization or MxP® CellCollect (Figure 2d). These findings indicate that lipid metabolites are insufficiently detached from the dish bottom and/or lipidic metabolites unspecifically adsorb to the hydrophobic dish and scraping spatula (area offered for adsorption is very large in comparison to the low amounts of lipidic metabolites). In order to achieve complete

recovery of lipidic metabolites the use of harsher solvents for scraping is necessary which in turn might risk the dissolving of the cell culture dish polystyrene plastic. In contrast, MxP® CellCollect is compatible with many solvents and harsh mechanical cell disruption which is a prerequisite for high recovery of polar and apolar metabolites [17] from the complete sample.

Conclusion

We developed a user-friendly, fast, efficient, reproducible, and robust sampling method for adherent cells. In summary, MxP® CellCollect proves to deliver more reliable results for metabolic profiling of adherent cells than the widely used scraping and trypsinization procedures. The presented manual sampling is extremely flexible and easily adoptable. The method was developed so that it is also suitable for possible automatization and translation into 96-well format in the future. More than 150 different cell lines have been analyzed by applying MxP® CellCollect so far, indicating overall that this new method is compatible with any adherent cell type and any common extraction or measurement protocol (MS- or NMR-based), easily adoptable without the need for sophisticated equipment. Here a high-throughput, routine MS-based protocol was applied which is also commonly used for sample types such as suspension cells, plasma, blood, or urine, thereby leading to increasing comparability.

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Supplementary Information

MxP® Broad Profiling

For MxP® Broad Profiling the samples were prepared and subjected to LC-MS/MS, GC-MS analysis as described below. After addition of water the samples were extracted using a ball mill (Retsch, Germany), filtered through a centrifuge filter (Millipore, mesh size 0.2 mm) and fractionated into an aqueous, polar phase and an organic, lipophilic phase. For the transmethanolysis of the lipid extracts (lipophilic phase) a mixture of 140 µL of chloroform, 37 µL of hydrochloric acid (37% by weight HCl in water), 320 µL of methanol and 20 µL of toluene was added to the evaporated extract. The vessel was sealed tightly and heated for 2 hours at 100°C, with shaking. The solution was subsequently evaporated to dryness. The residue was dried completely. The methoximation of the carbonyl groups was carried out by reaction with methoxyamine hydrochloride (20 mg/mL in pyridine, 100 µL for 1.5 hours at 60°C) in a tightly sealed vessel. 20 µL of a solution of odd-numbered, straight-chain fatty acids (solution of each 0.3 mg/mL of fatty acids from 7 to 25 carbon atoms and each 0.6 mg/mL of fatty acids with 27, 29, and 31 carbon atoms in 3/7 (v/v) pyridine/toluene) were added as time standards. Finally, the derivatization with 100 µL of N-methyl-N-(trimethylsilyl)-2,2,2-trifluoroacetamide (MSTFA) was carried out for 30 minutes at 60°C, again in the tightly sealed vessel. The final volume before injection into the GC was 200 µL. For the dried polar phase the derivatization was performed in the following way: the methoximation of the carbonyl groups was carried out by reaction with methoxyamine hydrochloride (20 mg/mL in pyridine, 50 µL for 1.5 hours at 60°C) in a tightly sealed vessel. 10 µL of a solution of odd-numbered, straight-chain fatty acids (solution of each 0.3 mg/mL of fatty acids from 7 to 25 carbon atoms and each 0.6 mg/mL of fatty acids with 27, 29, and 31 carbon atoms in 3/7 (v/v) pyridine/toluene) were added as time standards. Finally, the derivatization with 50 µL of N-methyl-N-(trimethylsilyl)-2,2,2-trifluoroacetamide (MSTFA) was carried out for 30 minutes at 60°C, again in the tightly sealed vessel. The final volume before injection into the GC was 100 µL.

The GC-MS system consists of an Agilent 6890 GC coupled to an Agilent 5973 MSD (Agilent, Waldbronn, Germany), autosamplers were CompiPal or GCPal from CTC (CTC, Zwingen, Switzerland). In LC-MS analysis, both fractions were reconstituted in appropriate solvent mixtures. HPLC was performed by gradient elution on reversed phase separation columns. Mass spectrometric detection, which allows target and high sensitivity MRM (Multiple Reaction Monitoring) profiling in parallel to a full screen analysis, was applied as described in WO2003073464. The HPLC instruments were Agilent 1100 (Agilent, Waldbronn, Germany), the MS instruments were API4000 from SCIEX (AB SCIEX, Darmstadt, Germany). Data of 113 known and 74 unknown metabolites were normalized to the median of reference samples which were derived from a pool formed from additional biological aliquots of all sampling groups (→ polar reference material and lipid reference material) to account for inter- and intra-instrumental variation. In a second step metabolite profiling data was normalized to the sample-specific metabolite median to correct for variations in cell numbers.

MxP® Energy

For MxP® Energy UPLC-MS/MS, an Aquity (Waters) coupled to the API5500 a negative mode ESI-MS/MS-System (Applied Biosystems), were used as described in [3]. In short, samples were kept at all times at 5°C or below. For extraction 1.5 M ammonium acetate and ISTD (^{13}C-labeled yeast extract) were added to the cells in the DCM/EtOH quenching solution and the mixture was homogenized for 30 s in a bead mill FastPrep24 (MP Biomedicals) at -20°C. Phase separation was achieved by 2 min centrifugation with 14000 rpm at 4°C. Polar phases were spin-filtrated (Ultrafree®-MC 5.0 µm, Millipore) in 5 min. Samples were extracted and spin-filtrated a second time with additional 1.5 M ammonium acetate. Spin filters were finally washed with water and all three filtrates were combined and lyophilized to remove the ammonium acetate. Samples were resuspended in deionized water and the separation was performed by gradient elution at 45°C using 10 mM tributylammonium acetate (pH 6.2) in A) water and B) 50% ACN with a gradient from 5-90% on a 1.5 µm RP UPLC column (VisionHT-HL, 2.1 mm ×10 cm, Alltech-Grom). All 65 known metabolites were measured in MRM mode and each metabolite was normalized against the corresponding ^{13}C-analyte. In a second step metabolite profiling data was normalized to the median of all metabolites from one replicate dish. For production of ^{13}C-labeled, yeast extract as ISTD, a yeast culture of *Candida utilis* (DSMZ sp. 2361) was grown in shake flasks on 10 g/L [U$^{13}C_6$] D-glucose in yeast nitrogen base amino acid-free medium (Y1250 Sigma–Aldrich). Cells were cultured under aerobic conditions at 28°C at 180 rpm on an orbital shaker and harvested at an optical density of 4 (600 nm, 1 cm cuvette) by short centrifugation at 4°C. Cells were washed twice with 10 g/L [U$^{13}C_6$] D-glucose in 0.15 M ammonium acetate by centrifugation. The cell pellet was quenched with DCM/EtOH (2/1) and extracted as described for MxP® Broad Profiling. The polar phase containing the labelled metabolites was stored at -80°C until further use as ISTD.

Multivariate statistical analysis

For multivariate analysis, data was further centered and scaled to unit variance and multivariate statistics were performed by using Simca P+ software (version 13, Umetrics AB, Umea, Sweden).

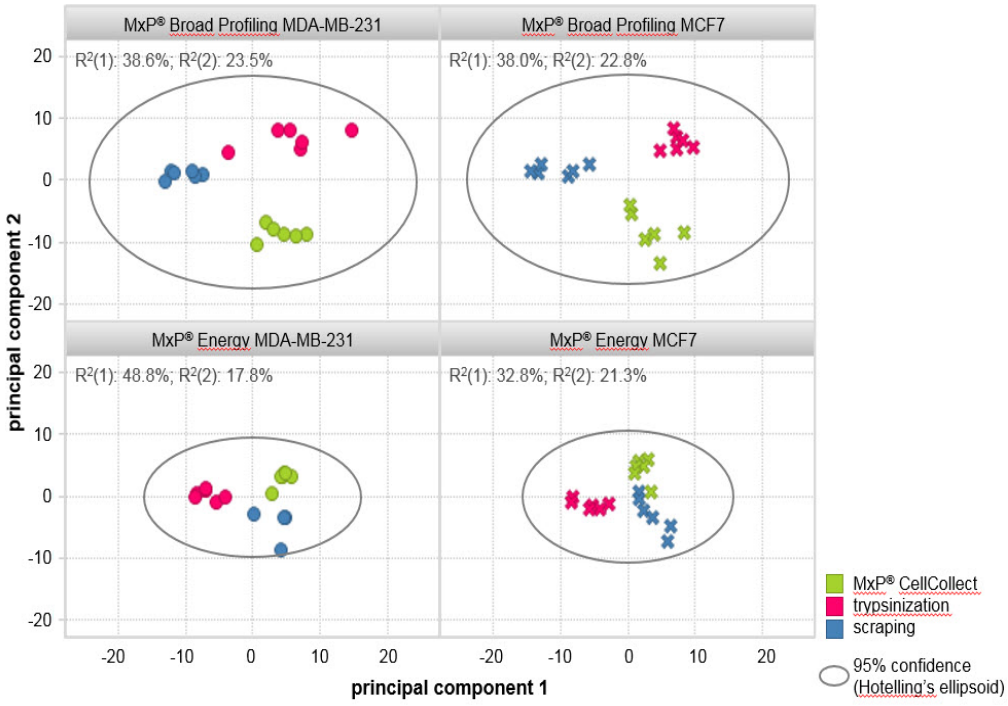

Figure S1: Principal component analysis (PCA) of cell line-specific metabolite profiles harvested either by trypsinization, scraping or MxP® CellCollect. The scores plots of all four models for the first two principal components reveal very large differences resulting from sampling within each of the two cell lines from two different measurement platforms.

ANOVA model, fixed categorical factors: ~ 1 | METHOD + CELL_LINE			comparison of	Trypsin	Scraping	Scraping	MCF7	Trypsin	Scraping	Scraping	MCF7	Trypsin	Scraping	Scraping	MCF7	Trypsin	Scraping	Scraping	MCF7	Trypsin	Scraping	Scraping	MCF7	Trypsin	Scraping	Scraping	MCF7	Trypsin	Scraping	Scraping	MCF7
			versus	MxP® CellCollect	MxP® CellCollect	Trypsin	MDA-MB-231	MxP® CellCollect	MxP® CellCollect	Trypsin	MDA-MB-231	MxP® CellCol	MxP® CellCol	Trypsin	MDA-MB-231	MxP® Cell	MxP® Cell	Trypsin	MDA-MB-23	MxP® Cell	MxP® Cell	Trypsin	MDA-MB-23	MxP® Cell	MxP® Cell	Trypsin	MDA-MB-23	MxP® Cell	MxP® Cell	Trypsin	MDA-MB-231
Normalization	ONTOLOGY1_NAME	ONTOLOGY2_NAME	METABOLITE_NAME	TR vs CC Ratio	SC vs CC Ratio	SC vs TR Ratio	MCF7 vs MDA-MB-	TR vs CC p.value	SC vs CC p.value	SC vs TR p.value	MCF7 vs MDA-MB-	TR vs CC q.va	SC vs CC q.va	SC vs TR q.va	MCF7 vs MD	TR vs CC t.	SC vs CC t.	SC vs TR t.	MCF7 vs M	TR vs CC Es	SC vs CC Es	SC vs TR Es	MCF7 vs M	TR vs CC St	SC vs CC St	SC vs TR St	MCF7 vs M	TR vs CC D	SC vs CC D	SC vs TR D	MCF7 vs M
pool, median	Amino acids	Amino acids, acidic	Aspartate	1.92	1.50	0.78	4.40	2.63E-10	2.28E-06	0.0007	7.99E-21	5.50E-09	1.24E-05	0.0014	9.55E-20	9.8968	6.0298	-3.8312	27.6909	0.2823	0.1760	-0.1063	0.6438	0.0285	0.0292	0.0277	0.0232	26	26	26	26
pool, median	Amino acids	Amino acids, acidic	Glutamate	1.09	0.91	0.84	0.78	0.7151	0.7251	0.4735	0.2278	0.7907	0.8018	0.5099	0.2798	0.3694	-0.3557	-0.7283	-1.2377	0.0377	-0.0393	-0.0771	-0.1077	0.1022	0.1106	0.1058	0.0870	24	24	24	24
pool, median	Amino acids	Amino acids, aromatic	Phenylalanine	0.77	0.94	1.22	2.93	0.0013	0.3943	0.0094	2.98E-16	0.0037	0.4973	0.0140	1.70E-15	-3.6153	-0.8663	2.8052	18.0909	-0.1144	-0.0280	0.0863	0.4666	0.0316	0.0324	0.0308	0.0258	26	26	26	26
pool, median	Amino acids	Amino acids, aromatic	Tryptophan	1.03	0.68	0.66	2.12	0.7199	0.0002	6.77E-05	2.40E-10	0.7926	0.0008	0.0002	7.52E-10	0.3626	-4.2915	-4.7697	10.1446	0.0143	-0.1689	-0.1832	0.3253	0.0393	0.0394	0.0384	0.0321	25	25	25	25
pool, median	Amino acids	Amino acids, aromatic	Tyrosine	0.59	0.85	1.45	2.95	2.47E-07	0.0536	3.59E-05	8.44E-16	1.94E-06	0.0886	0.0001	4.61E-15	-6.9082	-2.0215	4.9752	17.3261	-0.2298	-0.0688	0.1610	0.4698	0.0333	0.0340	0.0324	0.0271	26	26	26	26
^{13}C-ISTD, median	Amino acids	Amino acids, basic	Arginine	0.45	0.90	2.01	1.28	1.13E-05	0.5218	0.0001	0.0651	6.60E-05	0.6207	0.0004	0.0893	-5.2560	-0.6482	4.3470	1.9149	-0.3493	-0.0453	0.3039	0.1075	0.0665	0.0699	0.0699	0.0562	30	30	30	30
pool, median	Amino acids	Amino acids, basic	Asparagine	0.49	1.46	3.01	2.97	1.31E-09	9.12E-05	1.80E-13	3.70E-15	2.05E-08	0.0004	7.55E-12	1.86E-14	-9.3178	4.6548	14.1996	16.8478	-0.3143	0.1647	0.4790	0.4721	0.0337	0.0354	0.0337	0.0280	25	25	25	25
pool, median	Amino acids	Amino acids, basic	Glutamine	0.58	0.77	1.33	4.21	0.0023	0.1291	0.0798	3.53E-11	0.0062	0.1928	0.1005	1.16E-10	-3.3776	-1.5676	1.8233	10.8848	-0.2378	-0.1129	0.1249	0.6247	0.0704	0.0720	0.0685	0.0574	26	26	26	26
pool, median	Amino acids	Amino acids, basic	Histidine	0.48	1.01	2.13	2.80	3.95E-08	0.9055	1.77E-08	6.75E-13	4.13E-07	0.9353	1.44E-07	2.57E-12	-7.6602	0.1199	8.0007	13.0182	-0.3223	0.0052	0.3275	0.4465	0.0421	0.0431	0.0409	0.0343	26	26	26	26
pool, median	Amino acids	Amino acids, basic	Lysine	0.58	0.81	1.39	1.33	4.79E-05	0.0754	0.0052	0.0041	0.0002	0.1198	0.0083	0.0068	-4.8656	-1.8519	3.0539	3.1451	-0.2367	-0.0922	0.1445	0.1247	0.0486	0.0498	0.0473	0.0397	26	26	26	26
pool, median	Amino acids	Amino acids, branched chain	Isoleucine	0.51	0.93	1.83	3.10	0.0014	0.7022	0.0030	9.76E-08	0.0040	0.7904	0.0051	2.53E-07	-3.5762	-0.3866	3.2696	7.2855	-0.2960	-0.0327	0.2632	0.4915	0.0828	0.0847	0.0805	0.0675	26	26	26	26
pool, median	Amino acids	Amino acids, branched chain	Leucine	0.79	1.15	1.46	2.69	0.1206	0.3558	0.0139	1.10E-08	0.1740	0.4651	0.0201	3.03E-08	-1.6047	0.9402	2.6385	8.2044	-0.1030	0.0617	0.1647	0.4293	0.0642	0.0657	0.0624	0.0523	26	26	26	26
pool, median	Amino acids	Amino acids, branched chain	Valine	0.57	1.04	1.84	2.68	3.52E-05	0.7190	8.92E-06	6.25E-11	0.0002	0.7986	3.36E-05	2.04E-10	-4.9824	0.3637	5.5044	10.5969	-0.2467	0.0184	0.2652	0.4278	0.0495	0.0507	0.0482	0.0404	26	26	26	26
pool, median	Amino acids	Amino acids, neutral	Alanine	0.66	0.92	1.39	2.54	8.37E-05	0.3692	0.0007	8.68E-13	0.0004	0.4802	0.0015	3.25E-12	-4.6544	-0.9138	3.8235	12.8747	-0.1793	-0.0360	0.1433	0.4044	0.0385	0.0394	0.0375	0.0314	26	26	26	26
pool, median	Amino acids	Amino acids, neutral	Glycine	0.73	0.97	1.34	1.71	7.24E-08	0.5489	2.08E-07	1.47E-14	6.26E-07	0.6408	1.19E-06	6.59E-14	-7.4087	-0.6073	6.9772	15.3637	-0.1380	-0.0116	0.1264	0.2333	0.0186	0.0191	0.0181	0.0152	26	26	26	26
pool, median	Amino acids	Amino acids, neutral	Proline	0.80	0.84	1.06	1.28	0.0164	0.0661	0.5414	0.0020	0.0333	0.1063	0.5781	0.0034	-2.5650	-1.9185	0.6189	3.4344	-0.0996	-0.0762	0.0234	0.1087	0.0388	0.0397	0.0378	0.0316	26	26	26	26
pool, median	Amino acids	Amino acids, neutral	Serine	0.54	0.91	1.67	2.84	2.80E-09	0.1962	4.00E-08	1.61E-16	3.70E-08	0.2846	3.05E-07	1.01E-15	-8.8043	-1.3266	7.6553	18.5562	-0.2639	-0.0407	0.2232	0.4534	0.0300	0.0307	0.0292	0.0244	26	26	26	26
pool, median	Amino acids	Amino acids, neutral	Threonine	0.55	1.14	2.07	2.83	5.07E-08	0.1170	6.46E-10	4.37E-15	5.09E-07	0.1779	8.14E-09	2.15E-14	-7.5566	1.6215	9.4736	16.1725	-0.2593	0.0569	0.3162	0.4523	0.0343	0.0351	0.0334	0.0280	26	26	26	26
pool, median	Amino acids	Amino acids, S-containing	Cysteine (additional: Cystine)	0.42	0.89	2.13	1.09	3.68E-06	0.4602	1.88E-05	0.4646	2.43E-05	0.5663	6.25E-05	0.5114	-5.8446	-0.7496	5.2197	0.7423	-0.3768	-0.0495	0.3274	0.0390	0.0645	0.0660	0.0627	0.0526	26	26	26	26
pool, median	Amino acids	Amino acids, S-containing	Methionine	0.66	0.91	1.38	2.41	0.0003	0.3456	0.0028	3.48E-11	0.0010	0.4542	0.0048	1.16E-10	-4.1944	-0.9606	3.3014	10.8912	-0.1807	-0.0423	0.1384	0.3825	0.0431	0.0441	0.0419	0.0351	26	26	26	26
pool, median	Amino acids	Amino acids, S-containing	Taurine	0.91	3.43	3.75	3.43	0.6741	4.52E-06	6.84E-07	1.10E-07	0.7543	2.32E-05	3.45E-06	2.79E-07	-0.4253	5.7652	6.5013	7.2368	-0.0386	0.5356	0.5742	0.5356	0.0908	0.0929	0.0883	0.0740	26	26	26	26
pool, median	Amino acids related	Amino acid conjugates	N-Acetylaspartate	0.55	0.84	1.54	7.37	2.08E-07	0.0612	2.48E-05	4.75E-21	1.68E-06	0.0991	7.73E-05	6.28E-20	-6.9774	-1.9565	5.1146	28.2675	-0.2627	-0.0754	0.1873	0.8676	0.0377	0.0385	0.0366	0.0307	26	26	26	26
pool, median	Amino acids related	Amino acid metabolites	5-Oxoproline (additional: Folic acid, Glutamate,	0.85	1.21	1.42	1.11	0.0073	0.0024	6.27E-07	0.0253	0.0162	0.0056	3.29E-06	0.0371	-2.9122	3.3673	6.5356	2.3737	-0.0691	0.0818	0.1509	0.0459	0.0237	0.0243	0.0231	0.0193	26	26	26	26
pool, median	Amino acids related	Amino acid metabolites	beta-Alanine (additional: Pantothenic acid)	0.85	0.93	1.09	0.90	0.0316	0.3003	0.2321	0.0742	0.0571	0.4009	0.2646	0.1007	-2.2717	-1.0569	1.2236	-1.8599	-0.0700	-0.0333	0.0367	-0.0467	0.0308	0.0315	0.0300	0.0251	26	26	26	26
pool, median	Amino acids related	Amino acid metabolites	Hypotaurine	0.89	0.93	1.04	2.53	0.0517	0.2281	0.4322	1.86E-17	0.0860	0.3217	0.4695	1.26E-16	-2.0390	-1.2343	0.7978	20.2778	-0.0496	-0.0308	0.0189	0.4025	0.0243	0.0249	0.0237	0.0198	26	26	26	26
^{13}C-ISTD, median	Amino acids related	Amino acid metabolites	Methylmalonyl-CoA	0.82	0.47	0.57	1.45	0.1791	2.49E-05	0.0009	0.0051	0.2430	0.0001	0.0018	0.0081	-1.3757	-4.9763	-3.6689	3.0220	-0.0864	-0.3289	-0.2425	0.1605	0.0628	0.0661	0.0661	0.0531	30	30	30	30
pool, median	Amino acids related	Collagen metabolism	trans-4-Hydroxyproline	0.70	0.97	1.38	4.22	0.0011	0.7430	0.0021	2.26E-16	0.0033	0.8147	0.0037	1.35E-15	-3.6654	-0.3314	3.4194	18.3014	-0.1536	-0.0142	0.1394	0.6252	0.0419	0.0429	0.0408	0.0342	26	26	26	26
^{13}C-ISTD, median	Amino acids related	Creatine metabolism	Creatine	0.43	0.62	1.44	3.33	2.58E-09	9.23E-05	0.0018	8.48E-15	3.60E-08	0.0004	0.0033	4.10E-14	-8.3451	-4.5110	3.4200	14.1302	-0.3654	-0.2078	0.1576	0.5229	0.0438	0.0461	0.0461	0.0370	30	30	30	30
pool, median	Amino acids related	Creatine metabolism	Creatinine	0.47	0.65	1.38	1.76	3.17E-06	0.0028	0.0227	1.22E-05	2.15E-05	0.0064	0.0314	2.63E-05	-5.6306	-3.2362	2.3944	5.1690	-0.3261	-0.1875	0.1387	0.2445	0.0579	0.0579	0.0579	0.0473	32	32	32	32
^{13}C-ISTD, median	Amino acids related	Creatine metabolism	Phosphocreatine	1.23	0.83	0.68	3.60	0.0793	0.1247	0.0025	2.69E-14	0.1268	0.1874	0.0043	1.15E-13	1.8164	-1.5796	-3.3059	13.5175	0.0885	-0.0810	-0.1694	0.5564	0.0487	0.0512	0.0512	0.0412	30	30	30	30
^{13}C-ISTD, median	Amino acids related	Methyl cycle	S-Adenosylhomocysteine	1.71	1.01	0.59	0.82	0.0023	0.9743	0.0038	0.1607	0.0062	0.9782	0.0063	0.2027	3.3335	0.0325	-3.1356	-1.4382	0.2318	0.0024	-0.2294	-0.0845	0.0695	0.0732	0.0732	0.0588	30	30	30	30
^{13}C-ISTD, median	Amino acids related	Methyl cycle	S-Adenosylmethionine	0.87	1.36	1.57	1.59	0.4224	0.1105	0.0219	0.0043	0.5172	0.1696	0.0307	0.0071	-0.8134	1.6444	2.4174	3.0859	-0.0628	0.1336	0.1965	0.2014	0.0772	0.0813	0.0813	0.0653	30	30	30	30
pool, median	Amino acids related	Tyrosine metabolism	O-Phosphotyrosine	6.81	4.13	0.61	0.98	7.62E-16	2.48E-12	0.0005	0.8526	4.78E-14	6.92E-11	0.0011	0.8806	14.7739	10.9266	-3.8473	-0.1874	0.8331	0.6162	-0.2170	-0.0086	0.0564	0.0564	0.0564	0.0460	32	32	32	32
^{13}C-ISTD, median	Amino acids related	Urea cycle and related	Argininosuccinate	0.71	0.79	1.12	4.38	0.0007	0.0202	0.2569	1.71E-18	0.0021	0.0372	0.2916	1.48E-17	-3.7978	-2.4535	1.1559	19.3439	-0.1491	-0.1013	0.0477	0.6416	0.0392	0.0413	0.0413	0.0332	30	30	30	30
pool, median	Amino acids related	Urea cycle and related	Ornithine (additional: Arginine, Citrulline)	0.32	0.91	2.81	1.78	1.01E-10	0.3871	3.79E-10	6.97E-07	2.82E-09	0.4939	5.30E-09	1.60E-06	-10.3593	-0.8797	9.7238	6.4942	-0.4909	-0.0427	0.4483	0.2509	0.0474	0.0485	0.0461	0.0386	26	26	26	26
^{13}C-ISTD, median	Carbohydrates and related	Aminosugars	Glucosamine-1-phosphate	0.51	1.14	2.22	0.27	0.1328	0.7766	0.0895	0.0012	0.1905	0.8438	0.1106	0.0021	-1.5450	0.2863	1.7546	-3.5893	-0.2892	0.0564	0.3456	-0.5678	0.1872	0.1969	0.1969	0.1582	30	30	30	30
pool, median	Carbohydrates and related	Aminosugars	Mannosamine	0.43	1.18	2.72	0.76	0.0024	0.5186	0.0003	0.1837	0.0063	0.6202	0.0008	0.2294	-3.3802	0.6548	4.1498	-1.3674	-0.3634	0.0704	0.4338	-0.1189	0.1075	0.1075	0.1045	0.0870	25	25	25	25
pool, median	Carbohydrates and related	Disaccharides	iso-Maltose			1946.28				7.68E-10				8.80E-09				19.3344				3.2892				0.1701				11	
pool, median	Carbohydrates and related	Glycogen metabolism	Glucose-1-phosphate (additional: Glucose)	0.95	12.94	13.60	0.30	0.9367	0.0004	0.0002	0.0229	0.9442	0.0013	0.0005	0.0341	-0.0802	4.0447	4.3368	-2.4174	-0.0215	1.1121	1.1336	-0.5295	0.2687	0.2749	0.2614	0.2190	26	26	26	26
^{13}C-ISTD, median	Carbohydrates and related	Glycogen metabolism	UDP-Glucose	0.77	0.82	1.05	0.54	0.0034	0.0222	0.5445	3.23E-10	0.0083	0.0404	0.5790	1.00E-09	-3.1830	-2.4121	0.6130	-9.1792	-0.1111	-0.0886	0.0225	-0.2707	0.0349	0.0367	0.0367	0.0295	30	30	30	30
pool, median	Carbohydrates and related	Monosaccharides	Arabinose	0.53	5.50	10.47	0.78	4.26E-05	1.18E-12	1.97E-16	0.0281	0.0002	4.25E-11	1.24E-14	0.0408	-4.9100	12.6981	18.4039	-2.3251	-0.2797	0.7402	1.0200	-0.1080	0.0570	0.0583	0.0554	0.0464	26	26	26	26
pool, median	Carbohydrates and related	Monosaccharides	Glucose	0.18	3.21	17.74	0.68	3.57E-07	8.86E-05	9.63E-12	0.0697	2.72E-06	0.0003	1.87E-10	0.0951	-6.8438	4.6658	11.8369	-1.8950	-0.7427	0.5063	1.2491	-0.1664	0.1085	0.1085	0.1055	0.0878	25	25	25	25
pool, median	Carbohydrates and related	Polyols	Erythrol	0.95	1.38	1.45	1.02	0.5777	0.0027	0.0004	0.8288	0.6591	0.0062	0.0008	0.8704	-0.5638	3.3189	4.0706	0.2184	-0.0231	0.1391	0.1622	0.0073	0.0410	0.0419	0.0398	0.0334	26	26	26	26
pool, median	Carbohydrates and related	Polyols	myo-Inositol	0.87	1.21	1.40	0.35	0.1153	0.0447	0.0006	4.50E-14	0.1683	0.0752	0.0013	1.85E-13	-1.6293	2.1097	3.8940	-14.6457	-0.0624	0.0826	0.1450	-0.4570	0.0383	0.0392	0.0372	0.0312	26	26	26	26
pool, median	Carbohydrates and related	Polyols	scyllo-Inositol	0.91	0.44	0.48	0.56	0.4116	6.40E-08	2.02E-07	6.05E-07	0.5106	5.02E-07	1.19E-06	1.41E-06	-0.8345	-7.4596	-6.9885	-6.5500	-0.0395	-0.3612	-0.3217	-0.2526	0.0473	0.0484	0.0460	0.0386	26	26	26	26
pool, median	Carbohydrates and related	Polyols	Sorbitol	0.82	3.53	4.30	0.41	0.2449	7.16E-08	1.73E-09	5.32E-07	0.3202	5.41E-07	1.82E-08	1.25E-06	-1.1897	7.4129	9.0203	-6.6012	-0.0858	0.5472	0.6330	-0.3882	0.0721	0.0738	0.0702	0.0588	26	26	26	26
pool, median	Carbohydrates and related	Sugar acids	Erythronic acid	1.16	1.42	1.22	1.35	0.2358	0.0100	0.1058	0.0066	0.3115	0.0206	0.1282	0.0101	1.2136	2.7790	1.6756	2.9532	0.0650	0.1522	0.0872	0.1288	0.0535	0.0548	0.0521	0.0436	26	26	26	26
pool, median	Carbohydrates and related	Sugar acids	Glucuronic acid	1.05	21.53	20.60	1.03	0.8938	1.42E-10	2.00E-10	0.9168	0.9270	2.37E-09	3.14E-09	0.9316	0.1346	9.2657	9.1312	0.1053	0.0194	1.3331	1.3138	0.0124	0.1439	0.1439	0.1439	0.1175	32	32	32	32
pool, median	Complex lipids, fatty acids and	Ceramides	Ceramide (d18:1,C24:0)	1.09	0.90	0.83	0.37	0.0964	0.0551	0.0008	7.28E-22	0.1476	0.0901	0.0016	1.31E-20	1.7128	-1.9908	-3.7036	-23.7011	0.0380	-0.0442	-0.0822	-0.4293	0.0222	0.0222	0.0222	0.0181	32	32	32	32
pool, median	Complex lipids, fatty acids and	Ceramides	Ceramide (d18:1,C24:1) (additional: Ceramide (d	0.85	0.70	0.83	1.01	0.0496	0.0001	0.0242	0.8664	0.0829	0.0004	0.0331	0.8913	-2.0412	-4.4077	-2.3665	0.1696	-0.0717	-0.1548	-0.0831	0.0049	0.0351	0.0351	0.0351	0.0287	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterol and related	Cholesterol, free	0.99	0.92	0.93	1.09	0.9261	0.4153	0.4697	0.3478	0.9417	0.5187	0.5080	0.4022	-0.0935	-0.8253	-0.7317	0.9529	-0.0043	-0.0379	-0.0336	0.0357	0.0459	0.0459	0.0459	0.0375	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterol and related	Cholesterol, total	1.46	1.39	0.95	0.72	1.06E-09	1.92E-08	0.2936	2.03E-10	1.78E-08	1.66E-07	0.3288	6.44E-10	8.4884	7.4206	-1.0678	-9.1254	0.1632	0.1427	-0.0205	-0.1432	0.0192	0.0192	0.0192	0.0157	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterylesters	Cholesterylester C16:0	0.99	1.76	1.77	0.72	0.9780	0.0076	0.0070	0.0510	0.9780	0.0157	0.0110	0.0716	-0.0278	2.8516	2.8794	-2.0273	-0.0024	0.2452	0.2476	-0.1423	0.0860	0.0860	0.0860	0.0702	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterylesters	Cholesterylester C16:1	0.96	1.17	1.22	0.61	0.7797	0.2742	0.1728	0.0002	0.8399	0.3721	0.1988	0.0003	-0.2821	1.1124	1.3946	-4.2787	-0.0172	0.0679	0.0852	-0.2134	0.0611	0.0611	0.0611	0.0499	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterylesters	Cholesterylester C18:1	1.10	1.48	1.35	0.49	0.5273	0.0127	0.0541	1.43E-06	0.6128	0.0254	0.0706	3.20E-06	0.6391	2.6387	1.9997	-5.9050	0.0414	0.1711	0.1296	-0.3126	0.0648	0.0648	0.0648	0.0529	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterylesters	Cholesterylester C18:2	0.94	1.50	1.59	0.53	0.7326	0.0210	0.0092	6.54E-05	0.7995	0.0384	0.0138	0.0001	-0.3446	2.4286	2.7732	-4.5889	-0.0251	0.1771	0.2023	-0.2733	0.0729	0.0729	0.0729	0.0595	32	32	32	32
pool, median	Complex lipids, fatty acids and	Cholesterylesters	Cholesterylester C20:4	0.81	1.44	1.77	0.62	0.2301	0.0358	0.0018	0.0016	0.3056	0.0620	0.0032	0.0027	-1.2234	2.1917	3.4151	-3.4588	-0.0891	0.1597	0.2488	-0.2057	0.0729	0.0729	0.0729	0.0595	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, mono-unsaturated	Elaidic acid (C18:trans[9]1)	1.33	1.14	0.86	2.28	2.52E-05	0.0342	0.0108	6.16E-18	0.0001	0.0597	0.0159	4.55E-17	4.9182	2.2119	-2.7064	17.4878	0.1231	0.0554	-0.0677	0.3573	0.0250	0.0250	0.0250	0.0204	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, mono-unsaturated	Oleic acid (C18:cis[9]1)	1.23	1.00	0.82	1.31	6.50E-06	0.9020	9.34E-06	8.72E-10	4.08E-05	0.9353	3.46E-05	2.64E-09	5.3838	0.1242	-5.2596	8.5633	0.0899	0.0021	-0.0879	0.1168	0.0167	0.0167	0.0167	0.0136	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, mono-unsaturated	Palmitoleic acid (C16:cis[9]1)	1.07	0.88	0.82	4.42	0.5679	0.3237	0.1358	9.02E-15	0.6508	0.4276	0.1599	4.27E-14	0.5778	-1.0040	-1.5343	14.4339	0.0298	-0.0565	-0.0864	0.6457	0.0517	0.0563	0.0563	0.0447	29	29	29	29
pool, median	Complex lipids, fatty acids and	Fatty acids, poly-unsaturated	Arachidonic acid (C20:cis[5,8,11,14]4)	1.22	0.99	0.82	0.63	0.0092	0.9317	0.0063	5.54E-09	0.0203	0.9506	0.0100	1.56E-08	2.7832	-0.0864	-2.9351	-8.0476	0.0850	-0.0026	-0.0876	-0.1977	0.0305	0.0298	0.0298	0.0246	30	30	30	30
pool, median	Complex lipids, fatty acids and	Fatty acids, poly-unsaturated	Docosahexaenoic acid (C22:cis[4,7,10,13,16,19]6	1.24	1.02	0.82	0.52	0.0109	0.8485	0.0172	1.24E-11	0.0233	0.9063	0.0245	4.25E-11	2.7051	0.1926	-2.5126	-10.2497	0.0920	0.0066	-0.0855	-0.2847	0.0340	0.0340	0.0340	0.0278	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, poly-unsaturated	Docosapentaenoic acid (C22:cis[7,10,13,16,19]5)	1.68	1.30	0.77	0.32	4.35E-06	0.0071	0.0067	1.30E-15	2.80E-05	0.0148	0.0106	6.79E-15	5.6353	2.8973	-2.9203	-15.5606	0.2250	0.1136	-0.1114	-0.4982	0.0399	0.0392	0.0381	0.0320	29	29	29	29
pool, median	Complex lipids, fatty acids and	Fatty acids, poly-unsaturated	Eicosapentaenoic acid (C20:cis[5,8,11,14,17]5)	1.27	0.91	0.72	0.76	0.0340	0.3845	0.0036	0.0030	0.0605	0.4939	0.0060	0.0052	2.2217	-0.8825	-3.1564	-3.2252	0.1041	-0.0404	-0.1445	-0.1215	0.0468	0.0458	0.0458	0.0377	30	30	30	30
pool, median	Complex lipids, fatty acids and	Fatty acids, poly-unsaturated	Linoleic acid (C18:cis[9,12]2)	1.20	0.92	0.77	0.70	0.0002	0.0553	4.87E-07	9.86E-12	0.0006	0.0901	2.67E-06	3.44E-11	4.2884	-1.9891	-6.2775	-10.3433	0.0787	-0.0365	-0.1152	-0.1549	0.0183	0.0183	0.0183	0.0150	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, saturated	Lignoceric acid (C24:0)	1.28	1.01	0.79	0.18	0.0002	0.9261	0.0002	7.67E-28	0.0006	0.9488	0.0005	3.21E-26	4.2951	0.0935	-4.2016	-37.0144	0.1064	0.0023	-0.1041	-0.7488	0.0248	0.0248	0.0248	0.0202	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, saturated	Myristic acid (C14:0)	0.82	0.73	0.88	2.23	0.1349	0.0183	0.3480	1.07E-08	0.1913	0.0343	0.3846	2.98E-08	-1.5339	-2.4864	-0.9525	7.6332	-0.0858	-0.1390	-0.0533	0.3485	0.0559	0.0559	0.0559	0.0457	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, saturated	Palmitic acid (C16:0)	0.86	0.76	0.88	1.33	0.0307	0.0002	0.0590	5.49E-06	0.0559	0.0007	0.0766	1.20E-05	-2.2607	-4.2187	-1.9580	5.4419	-0.0631	-0.1178	-0.0547	0.1241	0.0279	0.0279	0.0279	0.0228	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty acids, saturated	Stearic acid (C18:0)	0.96	0.83	0.87	0.55	0.3383	0.0002	0.0032	7.56E-17	0.4311	0.0008	0.0053	5.00E-16	-0.9721	-4.1641	-3.1920	-16.0301	-0.0191	-0.0817	-0.0626	-0.2568	0.0196	0.0196	0.0196	0.0160	32	32	32	32
pool, median	Complex lipids, fatty acids and	Fatty alcohols	Glycerol, lipid fraction	1.12	0.78	0.70	1.10	0.0444	4.69E-05	1.11E-07	0.0421	0.0748	0.0002	7.50E-07	0.0600	2.0929	-4.7035	-6.7964	2.1176	0.0479	-0.1077	-0.1556	0.0396	0.0229	0.0229	0.0229	0.0187	32	32	32	32
pool, median	Complex lipids, fatty acids and	Glycolipids	Galactose, lipid fraction	1.24	1.01	0.81	0.51	5.93E-05	0.7872	0.0001	5.39E-18	0.0003	0.8516	0.0003	4.18E-17	4.6226	0.2723	-4.3504	-17.5679	0.0946	0.0056	-0.0890	-0.2935	0.0205	0.0205	0.0205	0.0167	32	32	32	32
pool, median	Complex lipids, fatty acids and	Glycolipids	Glucose, lipid fraction	1.02	2.19	2.15	1.12	0.9175	3.94E-05	3.89E-05	0.3823	0.9399	0.0002	0.0001	0.4381	0.1045	4.7884	4.7925	0.8863	0.0074	0.3395	0.3321	0.0509	0.0709	0.0709	0.0693	0.0575	31	31	31	31
pool, median	Complex lipids, fatty acids and	Glycolipids	myo-Inositol, lipid fraction	1.21	1.03	0.85	1.06	0.0018	0.6483	0.0058	0.2044	0.0049	0.7430	0.0094	0.2527	3.4144	0.4604	-2.9540	1.2955	0.0826	0.0111	-0.0715	0.0256	0.0242	0.0242	0.0242	0.0197	32	32	32	32
pool, median	Complex lipids, fatty acids and	Lipid hydroperoxides	Phosphatidylcholine hydroperoxide (C18:0,C18:2	1.05	1.09	1.04	1.25	0.6762	0.4903	0.7840	0.0368	0.7543	0.5974	0.7967	0.0527	0.4215	0.6979	0.2764	2.1795	0.0228	0.0377	0.0150	0.0963	0.0541	0.0541	0.0541	0.0442	32	32	32	32
^{13}C-ISTD, median	Complex lipids, fatty acids and	Lipid precursors	Choline phosphate	0.86	0.77	0.90	0.54	0.1059	0.0114	0.2758	4.82E-09	0.1573	0.0233	0.3103	1.38E-08	-1.6670	-2.6943	-1.1100	-8.1012	-0.0656	-0.1115	-0.0460	-0.2694	0.0393	0.0414	0.0414	0.0332	30	30	30	30
^{13}C-ISTD, median	Complex lipids, fatty acids and	Lipid precursors	Glycerol-3-phosphate, polar fraction	0.09	0.42	4.49	0.94	3.93E-17	1.37E-06	1.81E-11	0.5813	3.29E-15	8.17E-06	3.25E-10	0.6371	-17.2671	-6.0071	10.4033	-0.5576	-1.0285	-0.3765	0.6520	-0.0281	0.0596	0.0627	0.0627	0.0503	30	30	30	30
pool, median	Complex lipids, fatty acids and	Lipid precursors	O-Phosphoethanolamine	1.56	1.28	0.82	6.04	0.1383	0.3900	0.4835	4.72E-07	0.1951	0.4944	0.5185	1.12E-06	1.5438	0.8787	-0.7140	7.2932	0.1943	0.1087	-0.0856	0.7811	0.1259	0.1237	0.1199	0.1071	20	20	20	20
pool, median	Complex lipids, fatty acids and	Lysophosphatidylcholines	Lysophosphatidylcholine (C16:0)	0.94	1.38	1.46	0.73	0.4701	0.0003	3.28E-05	3.11E-05	0.5618	0.0009	9.97E-05	6.51E-05	-0.7311	4.0960	4.8271	-4.8454	-0.0247	0.1385	0.1632	-0.1338	0.0338	0.0338	0.0338	0.0276	32	32	32	32
pool, median	Complex lipids, fatty acids and	Lysophosphatidylcholines	Lysophosphatidylcholine (C18:0)	1.08	1.46	1.35	0.26	0.4456	0.0005	0.0038	1.13E-17	0.5429	0.0014	0.0063	7.86E-17	0.7724	3.8903	3.1180	-17.1275	0.0326	0.1641	0.1315	-0.5900	0.0422	0.0422	0.0422	0.0344	32	32	32	32
pool, median	Complex lipids, fatty acids and	Lysophosphatidylcholines	Lysophosphatidylcholine (C20:4)	0.79	0.64	0.81	1.01	0.0146	3.44E-05	0.0330	0.8930	0.0305	0.0002	0.0440	0.9118	-2.5824	-4.8107	-2.2283	0.1356	-0.1042	-0.1942	-0.0900	0.0045	0.0404	0.0404	0.0404	0.0330	32	32	32	32
pool, median	Complex lipids, fatty acids and	Lysophosphatidylethanolamines	Lysophosphatidylethanolamine (C18:0)	1.32	1.01	0.77	0.79	0.0307	0.9453	0.0358	0.0235	0.0559	0.9606	0.0475	0.0347	2.2611	0.0692	-2.1919	-2.3787	0.1189	0.0036	-0.1153	-0.1021	0.0526	0.0526	0.0526	0.0429	32	32	32	32
pool, median	Complex lipids, fatty acids and	Lysophosphatidylethanolamines	Lysophosphatidylethanolamine (C18:1)	0.88	1.37	1.56	1.57	0.1141	0.0003	2.91E-06	4.57E-08	0.1675	0.0010	1.22E-05	1.22E-07	-1.6244	4.0361	5.6604	7.1095	-0.0550	0.1367	0.1917	0.1966	0.0339	0.0339	0.0339	0.0277	32	32	32	32
^{13}C-ISTD, median	Complex lipids, fatty acids and	Mevalonate pathway	3-Hydroxy-3-methylglutaryl-CoA	1.47	1.07	0.73	1.15	0.0244	0.6916	0.0739	0.3144	0.0464	0.7820	0.0945	0.3654	2.3703	0.4005	-1.8521	1.0231	0.1685	0.0300	-0.1386	0.0615	0.0711	0.0748	0.0748	0.0601	30	30	30	30
pool, median	Complex lipids, fatty acids and	Mevalonate pathway	Isopentenyl pyrophosphate (IPP)	14.38	2.21	0.15	0.64	1.80E-19	1.10E-06	1.92E-15	0.0002	2.26E-17	6.74E-06	9.70E-14	0.0004	20.3112	6.0380	-14.6039	-4.1890	1.1578	0.3442	-0.8136	-0.1935	0.0570	0.0570	0.0557	0.0462	31	31	31	31
pool, median	Complex lipids, fatty acids and	Mevalonate pathway	Mevalonate	1.37	6.65	4.86	1.10	0.0361	2.75E-14	2.65E-12	0.4121	0.0625	1.38E-12	6.07E-11	0.4618	2.1945	13.5070	11.2669	0.8318	0.1365	0.8231	0.6866	0.0417	0.0622	0.0609	0.0609	0.0502	30	30	30	30
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C16:0,C18:2)	0.87	0.73	0.84	1.04	0.0009	3.97E-09	0.0001	0.2344	0.0028	4.75E-08	0.0003	0.2842	-3.6580	-7.9956	-4.3376	1.2121	-0.0624	-0.1365	-0.0741	0.0169	0.0171	0.0171	0.0171	0.0139	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C16:0,C20:4) (additional: P	0.90	0.73	0.81	0.90	0.0165	1.11E-08	1.54E-05	0.0036	0.0333	1.03E-07	5.24E-05	0.0061	-2.5316	-7.6193	-5.0878	-3.1379	-0.0445	-0.1339	-0.0894	-0.0450	0.0176	0.0176	0.0176	0.0143	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C16:0,C22:6) (additional: P	1.00	0.86	0.86	0.87	0.9170	0.0009	0.0007	0.0002	0.9399	0.0025	0.0014	0.0004	0.1051	-3.6585	-3.7636	-4.2404	0.0019	-0.0660	-0.0679	-0.0624	0.0180	0.0180	0.0180	0.0147	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C16:1,C18:2)	1.14	0.92	0.81	1.28	0.0063	0.0797	4.27E-05	1.02E-07	0.0144	0.1250	0.0001	2.60E-07	2.9265	-1.8102	-4.7366	6.8262	0.0558	-0.0345	-0.0904	0.1064	0.0191	0.0191	0.0191	0.0156	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C18:0,C18:1)	0.87	0.74	0.85	0.80	0.0027	3.45E-08	0.0004	1.99E-07	0.0070	2.79E-07	0.0008	4.76E-07	-3.2516	-7.2104	-3.9588	-6.5898	-0.0594	-0.1318	-0.0724	-0.0984	0.0183	0.0183	0.0183	0.0149	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C18:0,C18:2)	0.90	0.76	0.85	1.01	0.0149	4.31E-07	0.0007	0.7695	0.0308	2.84E-06	0.0014	0.8185	-2.5747	-6.3205	-3.7458	0.2955	-0.0477	-0.1172	-0.0694	0.0045	0.0185	0.0185	0.0185	0.0151	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C18:0,C20:4)	0.87	0.74	0.85	0.48	0.0010	7.08E-09	0.0002	1.38E-21	0.0032	7.92E-08	0.0005	2.31E-20	-3.6076	-7.7830	-4.1753	-23.2055	-0.0605	-0.1305	-0.0700	-0.3177	0.0168	0.0168	0.0168	0.0137	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine (C18:0,C22:6)	0.93	0.81	0.88	0.53	0.0686	1.42E-05	0.0029	5.52E-19	0.1117	6.88E-05	0.0049	5.13E-18	-1.8849	-5.1144	-3.2295	-18.9905	-0.0334	-0.0906	-0.0572	-0.2746	0.0177	0.0177	0.0177	0.0145	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phosphatidylcholines	Phosphatidylcholine No 02	0.88	0.79	0.89	0.76	0.0042	1.55E-06	0.0088	2.34E-09	0.0101	9.03E-06	0.0132	6.84E-09	-3.0858	-5.8776	-2.7917	-8.1915	-0.0550	-0.1048	-0.0498	-0.1192	0.0178	0.0178	0.0178	0.0146	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phospholipid metabolites	Glycerol phosphate, lipid fraction	1.76	1.45	0.82	1.35	2.53E-05	0.0030	0.0984	0.0030	0.0001	0.0067	0.1204	0.0052	4.9169	3.2149	-1.7020	3.2074	0.2465	0.1612	-0.0853	0.1313	0.0501	0.0501	0.0501	0.0409	32	32	32	32
pool, median	Complex lipids, fatty acids and	Phospholipid metabolites	Phosphate, lipid fraction	1.24	0.95	0.76	1.07	0.0015	0.3736	0.0001	0.1863	0.0044	0.4833	0.0003	0.2314	3.4613	-0.9024	-4.3638	1.3507	0.0941	-0.0245	-0.1186	0.0300	0.0272	0.0272	0.0272	0.0222	32	32	32	32
pool, median	Complex lipids, fatty acids and	Sphingolipids	erythro-Sphingosine (d18:1) (additional: Sphingo	1.67	1.78	1.07	0.39	0.0055	0.0016	0.7025	1.83E-07	0.0129	0.0041	0.7255	4.45E-07	3.0029	3.4818	0.3858	-6.7991	0.2220	0.2512	0.0291	-0.4093	0.0739	0.0721	0.0755	0.0602	29	29	29	29
pool, median	Complex lipids, fatty acids and	Sphingolipids	threo-Sphingosine (d18:1) (additional: Sphingoli	1.45	1.75	1.20	0.24	0.0356	0.0024	0.2665	8.27E-11	0.0621	0.0057	0.3011	2.66E-10	2.2162	3.3569	1.1356	-10.4586	0.1628	0.2421	0.0793	-0.6254	0.0735	0.0721	0.0698	0.0598	26	26	26	26
pool, median	Complex lipids, fatty acids and	Sphingomyelins	Sphingomyelin (d18:1,C16:0)	0.89	0.74	0.83	0.94	0.0229	5.35E-07	0.0005	0.1249	0.0449	3.44E-06	0.0011	0.1626	-2.3903	-6.2453	-3.8550	-1.5760	-0.0496	-0.1297	-0.0801	-0.0267	0.0208	0.0208	0.0208	0.0170	32	32	32	32
pool, median	Complex lipids, fatty acids and	Sphingomyelins	Sphingomyelin (d18:1,C18:0) (additional: Sphing	0.97	0.84	0.86	1.60	0.3206	2.75E-06	5.16E-05	1.88E-18	0.4105	1.47E-05	0.0001	1.57E-17	-1.0089	-5.6798	-4.6709	18.2155	-0.0139	-0.0783	-0.0644	0.2049	0.0138	0.0138	0.0138	0.0112	32	32	32	32
pool, median	Complex lipids, fatty acids and	Sphingomyelins	Sphingomyelin (d18:1,C23:0)	0.97	0.85	0.87	0.59	0.5223	0.0003	0.0021	1.87E-16	0.6098	0.0011	0.0037	1.15E-15	-0.6469	-4.0008	-3.3540	-15.5283	-0.0118	-0.0727	-0.0610	-0.2305	0.0182	0.0182	0.0182	0.0148	32	32	32	32
pool, median	Complex lipids, fatty acids and	Sphingomyelins	Sphingomyelin (d18:1,C24:0)	0.95	0.81	0.85	0.64	0.1187	1.09E-07	1.12E-05	8.08E-18	0.1722	7.85E-07	3.98E-05	5.79E-17	-1.6034	-6.8002	-5.1968	-17.3252	-0.0217	-0.0919	-0.0703	-0.1912	0.0135	0.0135	0.0135	0.0110	32	32	32	32
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	alpha-Ketoglutarate	0.45	0.92	2.05	1.05	0.0002	0.6812	0.0011	0.7519	0.0007	0.7737	0.0021	0.8065	-4.2294	-0.4148	3.6047	0.3191	-0.3465	-0.0358	0.3108	0.0221	0.0819	0.0862	0.0862	0.0692	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	cis-Aconitate	0.39	1.13	2.90	0.70	2.54E-09	0.3047	5.25E-10	0.0007	3.60E-08	0.4046	6.96E-09	0.0012	-8.3514	1.0443	8.9813	-3.7852	-0.4084	0.0537	0.4621	-0.1564	0.0489	0.0515	0.0515	0.0413	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	Citrate	0.51	1.04	2.05	0.73	7.23E-08	0.7058	6.67E-08	0.0005	6.26E-07	0.7908	4.80E-07	0.0010	-7.0754	0.3812	7.1055	-3.8769	-0.2944	0.0167	0.3111	-0.1363	0.0416	0.0438	0.0438	0.0352	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	Fumarate	0.74	1.79	2.42	1.48	0.3523	0.0927	0.0132	0.1553	0.4467	0.1444	0.0192	0.1979	-0.9447	1.7370	2.6348	1.4578	-0.1308	0.2531	0.3839	0.1706	0.1385	0.1457	0.1457	0.1170	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	Isocitrate	0.47	1.19	2.56	0.68	1.62E-05	0.2701	1.40E-06	0.0051	9.03E-05	0.3684	6.80E-06	0.0081	-5.1287	1.1237	5.9979	-3.0182	-0.3316	0.0764	0.4080	-0.1649	0.0647	0.0680	0.0680	0.0546	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	Malate	1.20	1.24	1.03	1.48	0.0350	0.0190	0.7064	4.83E-06	0.0614	0.0353	0.7266	1.06E-05	2.2090	2.4796	0.3803	5.5571	0.0796	0.0941	0.0144	0.1693	0.0361	0.0379	0.0379	0.0305	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Citrate cycle	Succinate	0.57	1.03	1.80	1.47	0.0011	0.8581	0.0011	0.0062	0.0033	0.9126	0.0021	0.0096	-3.6040	0.1804	3.6055	2.9469	-0.2435	0.0128	0.2563	0.1683	0.0676	0.0711	0.0711	0.0571	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Energy metabolism, miscellaneo	Ribulose-1,5-diphosphate	0.64	1.94	3.02	1.08	0.0873	0.0173	0.0002	0.7159	0.1361	0.0328	0.0005	0.7746	-1.7675	2.5201	4.1999	0.3673	-0.1918	0.2878	0.4796	0.0337	0.1085	0.1142	0.1142	0.0917	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Fatty acid oxidation/synthesis	Acetyl-CoA	1.02	0.92	0.90	1.15	0.8526	0.5126	0.4071	0.1520	0.8992	0.6185	0.4441	0.1946	0.1874	-0.6627	-0.8408	1.4699	0.0094	-0.0350	-0.0444	0.0624	0.0502	0.0529	0.0529	0.0425	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Glycolysis/Gluconeogenesis	2-Phosphoglycerate (2-PGA)	1.56	0.94	0.61	1.02	0.4168	0.9183	0.3827	0.9572	0.5128	0.9447	0.4211	0.9610	0.8234	-0.1034	-0.8859	0.0541	0.1926	-0.0255	-0.2181	0.0107	0.2339	0.2462	0.2462	0.1977	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Glycolysis/Gluconeogenesis	3-Phosphoglycerate (3-PGA)	2.48	0.77	0.31	1.28	1.58E-10	0.0129	1.17E-12	0.0045	3.97E-09	0.0255	3.68E-11	0.0073	9.4753	-2.6436	-11.6487	3.0720	0.3939	-0.1156	-0.5095	0.1079	0.0416	0.0437	0.0437	0.0351	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and related	Glycolysis/Gluconeogenesis	Dihydroxyacetone phosphate	1.49	2.32	1.56	0.42	9.27E-05	3.85E-10	3.85E-05	1.30E-12	0.0004	6.04E-09	0.0001	4.81E-12	4.5095	9.1075	4.8218	-11.5974	0.1722	0.3659	0.1937	-0.3743	0.0382	0.0402	0.0402	0.0323	30	30	30	30
pool, median	Energy metabolism and related	Glycolysis/Gluconeogenesis	Fructose	0.26	1.77	6.77	0.67	9.41E-09	0.0021	3.49E-12	0.0050	1.07E-07	0.0051	7.32E-11	0.0080	-8.2714	3.4197	12.0998	-3.0691	-0.5834	0.2468	0.8303	-0.1765	0.0705	0.0722	0.0686	0.0575	26	26	26	26
^{13}C-ISTD, median	Energy metabolism and related	Glycolysis/Gluconeogenesis	Fructose-1,6-diphosphate	5.54	3.26	0.59	0.20	1.02E-20	1.21E-15	1.37E-07	4.56E-22	2.56E-18	7.59E-14	8.83E-07	8.81E-21	23.2026	15.2105	-6.8409	-25.8631	0.7434	0.5128	-0.2306	-0.7004	0.0320	0.0337	0.0337	0.0271	30	30	30	30

^{13}C-ISTD, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Fructose-2,6-diphosphate	0.71	3.19	4.50	1.14	0.4812	0.0305	0.0061	0.7438	0.5697	0.0538	0.0098	0.8013	-0.7132	2.2714	2.9493	0.3299	-0.1502	0.5033	0.6535	0.0587	0.2106	0.2216	0.2216	0.1780	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Fructose-6-phosphate	0.18	1.34	7.48	1.71	7.17E-06	0.3877	1.30E-06	0.0547	4.39E-05	0.4939	6.42E-06	0.0758	-5.4175	0.8766	6.0253	1.9997	-0.7468	0.1272	0.8740	0.2330	0.1379	0.1451	0.1451	0.1165	30	30	30	30
pool, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Glucose-6-phosphate	1.14	1.69	1.48	0.67	0.5150	0.0151	0.0433	0.0190	0.6066	0.0293	0.0571	0.0284	0.6605	2.6100	2.1290	-2.5085	0.0566	0.2280	0.1714	-0.1718	0.0856	0.0874	0.0805	0.0685	25	25	25	25
^{13}C-ISTD, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Glycerate	0.75	1.86	2.48	0.97	0.1090	0.0019	2.43E-05	0.8353	0.1610	0.0046	7.67E-05	0.8735	-1.6517	3.4147	4.9844	-0.2098	-0.1242	0.2702	0.3944	-0.0133	0.0752	0.0791	0.0791	0.0636	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Lactate	0.52	1.20	2.29	0.69	9.03E-05	0.2341	5.78E-06	0.0041	0.0004	0.3264	2.31E-05	0.0067	-4.5425	1.2152	5.5323	-3.1208	-0.2828	0.0778	0.3606	-0.1631	0.0623	0.0640	0.0652	0.0523	29	29	29	29
^{13}C-ISTD, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Phosphoenolpyruvate (PEP)	5.08	1.68	0.33	2.45	0.0001	0.1903	0.0081	0.0074	0.0005	0.2778	0.0124	0.0113	4.3945	1.3399	-2.8365	2.8728	0.7055	0.2263	-0.4791	0.3898	0.1605	0.1689	0.1689	0.1357	30	30	30	30
pool, median	Energy metabolism and relate	Glycolysis/Gluconeogenesis	Pyruvate (additional: Phosphoenolpyruvate (PEP	0.43	0.77	1.79	2.30	0.0193	0.4509	0.0903	0.0058	0.0384	0.5575	0.1110	0.0091	-2.4945	-0.7655	1.7591	3.0069	-0.3682	-0.1156	0.2526	0.3618	0.1476	0.1510	0.1436	0.1203	26	26	26	26
pool, median	Energy metabolism and relate	Ketone bodies	3-Hydroxybutyrate (additional: 2-Hydroxy-3-oxo	1.38	1.65	1.20	0.96	2.39E-05	7.71E-09	0.0083	0.4098	0.0001	8.07E-08	0.0126	0.4612	4.9366	7.7516	2.8150	-0.8352	0.1389	0.2181	0.0792	-0.0192	0.0281	0.0281	0.0281	0.0230	32	32	32	32
^{13}C-ISTD, median	Energy metabolism and relate	Pentose phosphate pathway	6-Phosphogluconic acid	0.40	0.65	1.62	0.92	1.89E-10	0.0002	4.59E-05	0.3027	4.32E-09	0.0008	0.0001	0.3567	-9.4002	-4.1738	4.7599	-1.0488	-0.3943	-0.1842	0.2101	-0.0372	0.0419	0.0441	0.0441	0.0355	30	30	30	30
pool, median	Energy metabolism and relate	Pentose phosphate pathway	Ribose-5-phosphate	1.32	2.50	1.90	1.33	0.0031	7.29E-11	3.46E-08	0.0004	0.0080	1.41E-09	2.72E-07	0.0007	3.2588	10.5207	7.7162	4.1027	0.1206	0.3985	0.2779	0.1238	0.0370	0.0379	0.0360	0.0302	26	26	26	26
^{13}C-ISTD, median	Energy metabolism and relate	Pentose phosphate pathway	Ribulose-5-phosphate (additional: Xylulose-5-ph	1.07	1.03	0.96	1.16	0.5413	0.7934	0.7489	0.1250	0.6261	0.8545	0.7641	0.1626	0.6180	0.2643	-0.3230	1.5782	0.0291	0.0131	-0.0160	0.0629	0.0472	0.0496	0.0496	0.0399	30	30	30	30
^{13}C-ISTD, median	Energy metabolism and relate	Pentose phosphate pathway	Sedoheptulose-7-phosphate	0.72	0.32	0.44	0.76	0.4559	0.0174	0.0818	0.4510	0.5529	0.0328	0.1021	0.4987	-0.7553	-2.5184	-1.8006	-0.7637	-0.1411	-0.4951	-0.3540	-0.1206	0.1869	0.1966	0.1966	0.1579	30	30	30	30
^{13}C-ISTD, median	Hormones, signal substances a	Other hormones, signal substanc	Adenosine monophosphate, cyclic (cAMP)	0.86	2.55	2.97	0.58	0.6571	0.0120	0.0042	0.0634	0.7396	0.0242	0.0069	0.0874	-0.4483	2.6733	3.0994	-1.9277	-0.0649	0.4072	0.4721	-0.2358	0.1448	0.1523	0.1523	0.1223	30	30	30	30
pool, median	Hormones, signal substances a	Other hormones, signal substanc	gamma-Aminobutyrate (GABA)	0.65	0.75	1.17	0.88	1.47E-05	0.0023	0.0666	0.0781	8.39E-05	0.0056	0.0860	0.1055	-5.3139	-3.3729	1.9148	-1.8339	-0.1893	-0.1229	0.0663	-0.0532	0.0356	0.0364	0.0346	0.0290	26	26	26	26
pool, median	Miscellaneous	Miscellaneous	Pyrophosphate (PPi) (additional: Phosphate (ino	1.51	2.47	1.63	1.43	0.0007	1.02E-08	7.72E-05	0.0004	0.0021	9.84E-08	0.0002	0.0007	3.8705	8.2367	4.6850	4.0907	0.1800	0.3918	0.2119	0.1550	0.0465	0.0476	0.0452	0.0379	26	26	26	26
pool, median	Miscellaneous	Miscellaneous	Serine, lipid fraction	1.25	1.05	0.84	0.84	0.0052	0.5281	0.0243	0.0063	0.0124	0.6251	0.0331	0.0097	3.0021	0.6379	-2.3642	-2.9267	0.0976	0.0207	-0.0769	-0.0777	0.0325	0.0325	0.0325	0.0265	32	32	32	32
pool, median	Miscellaneous	Polyamines	Putrescine (additional: Agmatine)	1.19	0.88	0.74	1.36	0.0070	0.0488	2.07E-05	9.53E-07	0.0159	0.0816	6.79E-05	2.16E-06	2.9265	-2.0674	-5.1830	6.3704	0.0746	-0.0539	-0.1286	0.1324	0.0255	0.0261	0.0248	0.0208	26	26	26	26
pool, median	Miscellaneous	Polyamines	Spermidine	1.13	0.80	0.71	2.12	0.0292	0.0003	3.70E-07	5.39E-16	0.0543	0.0010	2.07E-06	3.01E-15	2.3085	-4.1571	-6.7457	17.6520	0.0525	-0.0968	-0.1493	0.3273	0.0227	0.0233	0.0221	0.0185	26	26	26	26
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Adenosine diphosphate (ADP)	2.91	0.79	0.27	0.72	5.52E-08	0.1454	2.79E-09	0.0130	5.33E-07	0.2134	2.60E-08	0.0199	7.1760	-1.4950	-8.3149	-2.6393	0.4644	-0.1018	-0.5662	-0.1443	0.0647	0.0681	0.0681	0.0547	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Adenosine monophosphate (AMP)	0.82	1.00	1.21	0.98	0.1403	0.9723	0.1704	0.8438	0.1957	0.9782	0.1970	0.8788	-1.5147	-0.0350	1.4046	-0.1987	-0.0840	-0.0020	0.0819	-0.0093	0.0554	0.0583	0.0583	0.0469	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Adenosine triphosphate (ATP)	0.63	0.81	1.28	0.75	3.38E-05	0.0426	0.0177	0.0011	0.0002	0.0727	0.0250	0.0020	-4.8684	-2.1179	2.5089	-3.6097	-0.2001	-0.0916	0.1085	-0.1254	0.0411	0.0432	0.0432	0.0347	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Cytidine diphosphate (CDP)	3.35	1.67	0.50	0.66	2.83E-08	0.0056	0.0003	0.0049	3.09E-07	0.0121	0.0007	0.0079	7.4250	2.9824	-4.0742	-3.0365	0.5251	0.2219	-0.3032	-0.1815	0.0707	0.0744	0.0744	0.0598	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Cytidine monophosphate (CMP)	0.69	2.13	3.09	0.58	0.0771	0.0013	1.01E-05	0.0034	0.1240	0.0034	3.70E-05	0.0058	-1.8309	3.5549	5.2950	-3.1780	-0.1609	0.3288	0.4897	-0.2361	0.0879	0.0925	0.0925	0.0743	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Cytidine triphosphate (CTP)	0.86	0.73	0.85	0.71	0.1028	0.0026	0.1022	0.0001	0.1535	0.0060	0.1244	0.0002	-1.6829	-3.2854	-1.6860	-4.4235	-0.0671	-0.1378	-0.0707	-0.1490	0.0398	0.0419	0.0419	0.0337	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Deoxyadenosine diphosphate (dADP)	0.95	1.85	1.94	0.78	0.7836	0.0020	0.0010	0.1062	0.8406	0.0050	0.0019	0.1407	-0.2771	3.3812	3.6445	-1.6655	-0.0209	0.2679	0.2887	-0.1060	0.0753	0.0792	0.0792	0.0636	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Deoxyadenosine monophosphate (dAMP)	0.84	1.71	2.04	0.82	0.3918	0.0174	0.0022	0.2537	0.4892	0.0328	0.0039	0.3033	-0.8690	2.5179	3.3437	-1.1637	-0.0765	0.2332	0.3097	-0.0866	0.0880	0.0926	0.0926	0.0744	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Deoxycytidine triphosphate (dCTP)	0.62	1.36	2.18	1.05	0.0894	0.2930	0.0103	0.8268	0.1385	0.3933	0.0152	0.8704	-1.7554	1.0703	2.7385	0.2207	-0.2062	0.1323	0.3384	0.0219	0.1174	0.1236	0.1236	0.0993	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Deoxythymidine diphosphate (dTDP)	2.70	1.54	0.57	0.66	0.0057	0.2294	0.1195	0.1493	0.0134	0.3217	0.1440	0.1922	2.9771	1.2268	-1.6025	-1.4801	0.4312	0.1870	-0.2442	-0.1812	0.1449	0.1524	0.1524	0.1224	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Deoxythymidine triphosphate (dTTP)	0.80	0.77	0.97	1.01	0.1479	0.1192	0.8487	0.9549	0.2050	0.1802	0.8590	0.9610	-1.4855	-1.6042	-0.1924	0.0570	-0.0995	-0.1131	-0.0136	0.0032	0.0670	0.0705	0.0705	0.0566	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Deoxyuridine triphosphate (dUTP)	0.66	1.38	2.09	1.05	0.3019	0.4436	0.0861	0.8937	0.3886	0.5512	0.1069	0.9118	-1.0504	0.7764	1.7748	0.1348	-0.1806	0.1405	0.3211	0.0196	0.1720	0.1809	0.1809	0.1453	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Guanosine diphosphate (GDP)	4.63	1.25	0.27	0.74	9.24E-05	0.5404	0.0009	0.2951	0.0004	0.6338	0.0018	0.3494	4.5106	0.6193	-3.6675	-1.0655	0.6654	0.0961	-0.5693	-0.1328	0.1475	0.1552	0.1552	0.1247	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Guanosine monophosphate (GMP)	0.80	1.20	1.50	1.07	0.4130	0.5305	0.1649	0.7801	0.5106	0.6251	0.1915	0.8262	-0.8302	0.6346	1.4236	0.2817	-0.0984	0.0791	0.1775	0.0282	0.1185	0.1247	0.1247	0.1002	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Guanosine triphosphate (GTP)	0.71	0.72	1.01	0.86	0.0024	0.0051	0.9007	0.1065	0.0063	0.0110	0.9079	0.1407	-3.3154	-3.0250	0.1259	-1.6640	-0.1493	-0.1434	0.0060	-0.0633	0.0450	0.0474	0.0474	0.0381	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Inosine monophosphate (IMP)	0.68	0.51	0.75	1.40	0.0345	0.0009	0.1215	0.0322	0.0609	0.0025	0.1452	0.0464	-2.2156	-3.6991	-1.5935	2.2467	-0.1689	-0.2967	-0.1278	0.1447	0.0762	0.0802	0.0802	0.0644	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Uridine diphosphate (UDP)	3.82	1.28	0.33	0.67	6.06E-10	0.1338	1.05E-07	0.0035	1.17E-08	0.1987	7.32E-07	0.0058	8.9233	1.5410	-6.9395	-3.1713	0.5820	0.1058	-0.4762	-0.1748	0.0652	0.0686	0.0686	0.0551	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Uridine monophosphate (UMP)	0.68	3.06	4.49	1.25	0.0325	7.50E-07	2.53E-09	0.1339	0.0582	4.70E-06	2.45E-08	0.1732	-2.2425	6.2226	8.3539	1.5407	-0.1664	0.4859	0.6524	0.0966	0.0742	0.0781	0.0781	0.0627	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Nucleotides	Uridine triphosphate (UTP)	0.71	0.69	0.96	0.71	0.0006	0.0003	0.6896	6.39E-05	0.0020	0.0011	0.7173	0.0001	-3.8180	-4.0318	-0.4032	-4.6421	-0.1469	-0.1633	-0.0163	-0.1510	0.0385	0.0405	0.0405	0.0325	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Purine metabolism	5-Aminoimidazole-4-carboxamide-1-beta-ribofu	0.50	0.89	1.78	0.16	0.0023	0.6062	0.0131	1.76E-11	0.0063	0.6979	0.0192	5.96E-11	-3.3238	-0.5210	2.6379	-10.4156	-0.2985	-0.0492	0.2493	-0.7906	0.0898	0.0945	0.0945	0.0759	30	30	30	30
pool, median	Nucleobases and related	Purine metabolism	Adenine	1.04	0.69	0.66	1.30	0.4682	7.33E-08	5.04E-09	8.14E-07	0.5618	5.41E-07	4.38E-08	1.86E-06	0.7362	-7.4033	-8.5439	6.4326	0.0160	-0.1643	-0.1803	0.1137	0.0217	0.0222	0.0211	0.0177	26	26	26	26
^{13}C-ISTD, median	Nucleobases and related	Purine metabolism	Adenosine	1.05	1.42	1.35	0.85	0.8247	0.1436	0.2071	0.3848	0.8771	0.2120	0.2372	0.4391	0.2235	1.5019	1.2895	-0.8819	0.0215	0.1521	0.1306	-0.0717	0.0963	0.1013	0.1013	0.0813	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Purine metabolism	Adenylosuccinic acid	0.97	0.77	0.79	0.99	0.9353	0.5189	0.5614	0.9812	0.9442	0.6202	0.5944	0.9812	-0.0819	-0.6533	-0.5877	-0.0238	-0.0133	-0.1140	-0.1007	-0.0033	0.1621	0.1744	0.1713	0.1376	28	28	28	28
pool, median	Nucleobases and related	Purine metabolism	Guanine	1.33	0.86	0.65	0.96	0.0305	0.2436	0.0013	0.7011	0.0559	0.3359	0.0024	0.7618	2.2881	-1.1932	-3.6072	-0.3881	0.1232	-0.0657	-0.1889	-0.0170	0.0538	0.0551	0.0524	0.0439	26	26	26	26
^{13}C-ISTD, median	Nucleobases and related	Purine metabolism	Guanosine	0.93	2.69	2.89	0.51	0.7242	3.92E-05	1.51E-05	0.0003	0.7937	0.0002	5.21E-05	0.0006	-0.3562	4.8151	5.1537	-4.0645	-0.0303	0.4303	0.4606	-0.2918	0.0849	0.0894	0.0894	0.0718	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Purine metabolism	Phosphoribosyl pyrophosphate (PRPP)	0.69	0.77	1.12	0.71	0.0013	0.0241	0.3302	0.0005	0.0038	0.0436	0.3665	0.0010	-3.5405	-2.3749	0.9899	-3.8761	-0.1639	-0.1157	0.0482	-0.1517	0.0463	0.0487	0.0487	0.0391	30	30	30	30
^{13}C-ISTD, median	Nucleobases and related	Pyrimidine metabolism	Carbamoylaspartate	0.23	1.02	4.47	0.41	8.87E-13	0.8905	2.30E-12	2.34E-09	4.45E-11	0.9291	5.79E-11	6.84E-09	-11.7786	0.1389	11.3331	-8.3846	-0.6427	0.0080	0.6507	-0.3867	0.0546	0.0574	0.0574	0.0461	30	30	30	30
pool, median	Nucleobases and related	Pyrimidine metabolism	Uridine	7.97	11.25	1.41	0.10	9.86E-11	2.23E-12	0.1277	2.39E-14	2.82E-09	6.92E-11	0.1518	1.03E-13	9.4085	10.9722	1.5636	-13.0386	0.9012	1.0510	0.1498	-1.0198	0.0958	0.0958	0.0958	0.0782	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (29971286)	1.54	1.19	0.77	0.06	9.53E-05	0.0782	0.0079	3.39E-22	0.0004	0.1234	0.0122	7.24E-21	4.6734	1.8400	-2.8952	-35.2897	0.1888	0.0767	-0.1120	-1.2106	0.0404	0.0417	0.0387	0.0343	24	24	24	24
pool, median	Unknown	Unknown lipid	Unknown lipid (29971443)	0.91	0.79	0.86	0.95	0.1529	0.0006	0.0271	0.3090	0.2097	0.0019	0.0366	0.3624	-1.4642	-3.7799	-2.3157	-1.0338	-0.0404	-0.1043	-0.0639	-0.0233	0.0276	0.0276	0.0276	0.0225	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (29971883)	0.97	0.83	0.85	0.54	0.6522	0.0058	0.0178	3.97E-13	0.7374	0.0124	0.0250	1.56E-12	-0.4550	-2.9543	-2.4993	-11.7321	-0.0126	-0.0817	-0.0691	-0.2650	0.0277	0.0277	0.0277	0.0226	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970017)	1.01	0.82	0.82	0.90	0.8927	9.74E-06	6.55E-06	0.0018	0.9270	4.89E-05	2.54E-05	0.0032	0.1359	-5.2452	-5.3811	-3.3949	0.0022	-0.0863	-0.0886	-0.0456	0.0165	0.0165	0.0165	0.0134	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970020)	1.11	0.88	0.79	0.19	0.0105	0.0016	6.50E-07	9.63E-33	0.0228	0.0040	3.34E-06	1.21E-30	2.7174	-3.4602	-6.1776	-52.9674	0.0451	-0.0574	-0.1024	-0.7171	0.0166	0.0166	0.0166	0.0135	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970121)	0.79	0.82	1.04	0.58	0.0038	0.0140	0.6036	5.70E-10	0.0092	0.0274	0.6312	1.75E-09	-3.1248	-2.6004	0.5244	-8.7253	-0.1050	-0.0874	0.0176	-0.2394	0.0336	0.0336	0.0336	0.0274	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970127)	0.65	0.48	0.74	2.91	0.0002	3.05E-08	0.0049	3.10E-14	0.0007	2.55E-07	0.0080	1.30E-13	-4.2347	-7.2539	-3.0192	12.9124	-0.1863	-0.3192	-0.1328	0.4639	0.0440	0.0440	0.0440	0.0359	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970150)	1.09	0.92	0.85	0.48	0.0592	0.0495	0.0004	1.47E-20	0.0977	0.0823	0.0008	1.67E-19	1.9567	-2.0416	-3.9983	-21.4555	0.0357	-0.0372	-0.0729	-0.3193	0.0182	0.0182	0.0182	0.0149	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970151)	1.13	0.90	0.80	1.20	0.0012	0.0029	1.13E-07	1.53E-07	0.0034	0.0066	7.50E-07	3.76E-07	3.5659	-3.2228	-6.7887	6.6828	0.0517	-0.0468	-0.0985	0.0792	0.0145	0.0145	0.0145	0.0118	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970153)	1.20	1.01	0.85	0.95	0.0001	0.7433	0.0003	0.1685	0.0005	0.8147	0.0007	0.2115	4.3928	0.3304	-4.0624	-1.4090	0.0784	0.0059	-0.0725	-0.0205	0.0178	0.0178	0.0178	0.0146	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970154)	1.09	0.91	0.84	0.77	0.0259	0.0265	5.30E-05	1.33E-09	0.0489	0.0476	0.0001	3.98E-09	2.3364	-2.3255	-4.6618	-8.4034	0.0391	-0.0389	-0.0779	-0.1147	0.0167	0.0167	0.0167	0.0136	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970507)	0.73	1.39	1.90	0.59	0.0228	0.0160	2.40E-05	2.68E-05	0.0449	0.0309	7.67E-05	5.70E-05	-2.3914	2.5431	4.9345	-4.8973	-0.1352	0.1438	0.2790	-0.2261	0.0565	0.0565	0.0565	0.0462	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970512)	0.87	0.92	1.06	0.77	0.3546	0.5935	0.6917	0.0435	0.4473	0.6897	0.7173	0.0613	-0.9393	-0.5391	0.4002	-2.1026	-0.0614	-0.0353	0.0262	-0.1123	0.0654	0.0654	0.0654	0.0534	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970534)	1.81	0.67	0.37	0.29	9.28E-06	0.0010	3.74E-10	1.10E-14	5.54E-05	0.0027	5.30E-09	5.09E-14	5.2618	-3.6256	-8.8875	-13.4171	0.2569	-0.1770	-0.4339	-0.5348	0.0488	0.0488	0.0488	0.0399	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970538)	0.90	0.74	0.82	1.01	0.4668	0.0372	0.1602	0.9473	0.5618	0.0639	0.1877	0.9588	-0.7365	-2.1745	-1.4379	0.0666	-0.0448	-0.1323	-0.0875	0.0033	0.0609	0.0609	0.0609	0.0497	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970546)	1.38	1.03	0.75	1.95	0.0002	0.6672	0.0007	4.86E-12	0.0007	0.7612	0.0014	1.77E-11	4.2045	0.4340	-3.7705	10.6405	0.1408	0.0145	-0.1262	0.2909	0.0335	0.0335	0.0335	0.0273	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970547)	1.21	0.96	0.79	1.42	0.0033	0.4656	0.0004	3.43E-08	0.0082	0.5700	0.0009	9.36E-08	3.1777	-0.7386	-3.9163	7.2121	0.0823	-0.0191	-0.1014	0.1525	0.0259	0.0259	0.0259	0.0211	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970550)	0.26	0.23	0.90	1.11	4.16E-05	1.48E-05	0.7246	0.6602	0.0002	7.03E-05	0.7422	0.7205	-4.7451	-5.1005	-0.3555	0.4438	-0.5886	-0.6326	-0.0441	0.0449	0.1240	0.1240	0.1240	0.1013	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970553)	1.09	0.81	0.74	3.37	0.0989	0.0004	2.73E-06	2.01E-24	0.1496	0.0011	1.19E-05	6.31E-23	1.6994	-3.9821	-5.6815	28.7330	0.0382	-0.0896	-0.1279	0.5280	0.0225	0.0225	0.0225	0.0184	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970558)	1.21	0.88	0.73	2.58	0.0004	0.0116	1.76E-07	3.46E-22	0.0013	0.0234	1.11E-06	7.24E-21	3.9538	-2.6787	-6.6325	24.2891	0.0821	-0.0556	-0.1377	0.4118	0.0208	0.0208	0.0208	0.0170	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970574)	1.12	0.93	0.83	1.44	0.0070	0.0687	3.94E-05	5.23E-13	0.0159	0.1098	0.0001	2.02E-12	2.8801	-1.8841	-4.7642	11.6087	0.0478	-0.0313	-0.0790	0.1573	0.0166	0.0166	0.0166	0.0135	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970597)	0.84	1.10	1.32	0.76	0.0432	0.2605	0.0027	0.0004	0.0742	0.3573	0.0047	0.0008	-2.1056	1.1455	3.2511	-3.9111	-0.0782	0.0425	0.1207	-0.1186	0.0371	0.0371	0.0371	0.0303	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970610)	0.90	0.77	0.85	1.05	0.2275	0.0039	0.0689	0.4412	0.3037	0.0085	0.0885	0.4901	-1.2305	-3.1132	-1.8827	0.7798	-0.0446	-0.1128	-0.0682	0.0231	0.0362	0.0362	0.0362	0.0296	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970611)	1.01	0.87	0.86	0.39	0.9080	0.0342	0.0264	5.50E-18	0.9379	0.0597	0.0357	4.18E-17	0.1164	-2.2121	-2.3286	-17.5565	0.0033	-0.0626	-0.0659	-0.4055	0.0283	0.0283	0.0283	0.0231	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970615)	1.09	0.96	0.88	1.90	0.0999	0.4086	0.0165	1.21E-16	0.1502	0.5127	0.0236	7.80E-16	1.6942	-0.8374	-2.5316	15.7673	0.0367	-0.0181	-0.0548	0.2788	0.0217	0.0217	0.0217	0.0177	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970619)	0.74	0.63	0.86	2.81	9.71E-05	1.38E-07	0.0302	9.46E-19	0.0004	9.60E-07	0.0405	8.48E-18	-4.4514	-6.7191	-2.2677	18.6457	-0.1312	-0.1980	-0.0668	0.4486	0.0295	0.0295	0.0295	0.0241	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970620)	0.91	0.74	0.81	1.85	0.0244	7.26E-09	6.00E-06	2.06E-19	0.0464	7.92E-08	2.36E-05	2.07E-18	-2.3624	-7.7739	-5.4114	19.6339	-0.0392	-0.1291	-0.0899	0.2663	0.0166	0.0166	0.0166	0.0136	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970621)	1.22	0.93	0.76	1.42	0.0033	0.2354	0.0001	7.20E-08	0.0083	0.3264	0.0003	1.88E-07	3.1703	-1.2094	-4.3797	6.9480	0.0850	-0.0324	-0.1175	0.1521	0.0268	0.0268	0.0268	0.0219	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970623)	0.92	0.77	0.84	1.22	0.0172	1.58E-08	2.11E-05	3.80E-08	0.0346	1.41E-07	6.82E-05	1.03E-07	-2.5125	-7.4918	-4.9794	7.1755	-0.0372	-0.1111	-0.0738	0.0869	0.0148	0.0148	0.0148	0.0121	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970625)	0.88	0.69	0.79	1.52	0.0032	5.30E-10	3.85E-06	9.18E-14	0.0081	7.83E-09	1.57E-05	3.72E-13	-3.1898	-8.7534	-5.5636	12.4006	-0.0577	-0.1584	-0.1007	0.1832	0.0181	0.0181	0.0181	0.0148	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970626)	0.90	0.72	0.80	1.52	0.0060	7.15E-11	1.98E-07	8.63E-16	0.0139	1.41E-09	1.19E-06	4.61E-15	-2.9439	-9.5363	-6.5923	14.7080	-0.0443	-0.1434	-0.0991	0.1806	0.0150	0.0150	0.0150	0.0123	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970627)	0.93	0.74	0.80	0.87	0.1349	1.94E-07	1.64E-05	0.0005	0.1913	1.31E-06	5.52E-05	0.0009	-1.5339	-6.5995	-5.0656	-3.8821	-0.0299	-0.1286	-0.0987	-0.0618	0.0195	0.0195	0.0195	0.0159	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970629)	1.01	0.83	0.82	0.55	0.7114	4.29E-06	1.45E-06	1.61E-20	0.7901	2.24E-05	6.90E-06	1.75E-19	0.3733	-5.5265	-5.8999	-21.3895	0.0055	-0.0816	-0.0871	-0.2579	0.0148	0.0148	0.0148	0.0121	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970631)	1.01	0.87	0.87	0.85	0.8383	0.0020	0.0012	1.85E-05	0.8878	0.0050	0.0022	3.98E-05	0.2057	-3.3594	-3.5652	-5.0237	0.0036	-0.0582	-0.0617	-0.0710	0.0173	0.0173	0.0173	0.0141	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970632)	0.89	0.74	0.83	1.27	0.0004	6.25E-12	2.03E-07	9.45E-12	0.0013	1.57E-10	1.19E-06	3.34E-11	-3.9513	-10.5339	-6.5826	10.3611	-0.0489	-0.1304	-0.0815	0.1047	0.0124	0.0124	0.0124	0.0101	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970633)	0.99	0.87	0.88	0.55	0.7506	0.0001	0.0004	7.52E-21	0.8121	0.0005	0.0008	9.44E-20	-0.3206	-4.3035	-3.9829	-21.9372	-0.0046	-0.0616	-0.0570	-0.2565	0.0143	0.0143	0.0143	0.0117	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970636)	1.41	1.40	0.99	0.61	0.0006	0.0009	0.9044	1.88E-07	0.0020	0.0025	0.9080	4.54E-07	3.7938	3.6728	-0.1210	-6.6096	0.1502	0.1454	-0.0048	-0.2137	0.0396	0.0396	0.0396	0.0323	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970638)	1.30	1.30	1.00	0.50	0.0002	0.0002	0.9725	1.12E-14	0.0007	0.0008	0.9725	5.12E-14	4.1843	4.1496	-0.0348	-13.4052	0.1152	0.1143	-0.0010	-0.3014	0.0275	0.0275	0.0275	0.0225	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970639)	1.20	0.99	0.83	0.77	8.78E-05	0.7468	3.43E-05	2.68E-09	0.0004	0.8149	0.0001	7.72E-09	4.4865	-0.3257	-4.8122	-8.1422	0.0777	-0.0056	-0.0834	-0.1152	0.0173	0.0173	0.0173	0.0141	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970641)	0.92	0.82	0.89	0.50	0.0616	7.84E-05	0.0144	4.53E-19	0.1010	0.0003	0.0207	4.37E-18	-1.9375	-4.5260	-2.5885	-19.1185	-0.0378	-0.0883	-0.0505	-0.3045	0.0195	0.0195	0.0195	0.0159	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970642)	1.01	0.85	0.85	0.80	0.8812	0.0006	0.0004	1.44E-07	0.9225	0.0017	0.0008	3.59E-07	0.1507	-3.8274	-3.9781	-6.7028	0.0027	-0.0689	-0.0716	-0.0985	0.0180	0.0180	0.0180	0.0147	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970658)	0.74	0.56	0.76	0.40	9.39E-07	3.96E-13	2.73E-06	1.56E-21	6.74E-06	1.66E-11	1.19E-05	2.40E-20	-6.0499	-11.7326	-5.6827	-23.1124	-0.1281	-0.2485	-0.1203	-0.3996	0.0212	0.0212	0.0212	0.0173	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970801)	1.13	0.86	0.76	2.82	0.0858	0.0442	0.0005	3.61E-18	0.1355	0.0750	0.0011	2.92E-17	1.7725	-2.0944	-3.8669	17.8117	0.0549	-0.0649	-0.1198	0.4507	0.0310	0.0310	0.0310	0.0253	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970802)	0.98	0.75	0.77	1.05	0.5621	9.65E-09	4.91E-08	0.1202	0.6472	9.69E-08	3.64E-07	0.1580	-0.5858	-7.6700	-7.0842	1.5965	-0.0095	-0.1237	-0.1143	0.0210	0.0161	0.0161	0.0161	0.0132	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970803)	1.03	0.85	0.82	0.36	0.5997	0.0014	0.0003	3.10E-23	0.6812	0.0037	0.0007	7.78E-22	0.5300	-3.5054	-4.0355	-26.2876	0.0110	-0.0729	-0.0839	-0.4463	0.0208	0.0208	0.0208	0.0170	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970806)	1.04	0.90	0.86	2.68	0.2151	0.0015	4.38E-05	2.22E-28	0.2903	0.0040	0.0001	1.39E-26	1.2647	-3.4632	-4.7278	38.5088	0.0172	-0.0471	-0.0643	0.4278	0.0136	0.0136	0.0136	0.0111	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970813)	0.83	0.67	0.80	0.34	0.0002	9.90E-11	1.28E-05	3.80E-25	0.0006	1.77E-09	4.48E-05	1.36E-23	-4.2560	-9.4071	-5.1511	-30.3264	-0.0795	-0.1758	-0.0963	-0.4628	0.0187	0.0187	0.0187	0.0153	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970814)	0.87	0.77	0.88	0.76	0.0984	0.0024	0.1200	0.0003	0.1496	0.0056	0.1440	0.0005	-1.7025	-3.3000	-1.5975	-4.0736	-0.0598	-0.1159	-0.0561	-0.1168	0.0351	0.0351	0.0351	0.0287	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970815)	0.99	0.81	0.82	0.91	0.8118	0.0005	0.0009	0.0429	0.8671	0.0014	0.0018	0.0608	-0.2401	-3.8861	-3.6460	-2.1090	-0.0057	-0.0928	-0.0871	-0.0411	0.0239	0.0239	0.0239	0.0195	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970816)	0.93	0.78	0.84	0.99	0.2244	0.0003	0.0074	0.8476	0.3012	0.0009	0.0115	0.8791	-1.2389	-4.1009	-2.8620	-0.1937	-0.0328	-0.1085	-0.0758	-0.0042	0.0265	0.0265	0.0265	0.0216	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970817)	0.82	0.71	0.86	2.60	5.97E-05	3.40E-09	0.0017	9.57E-24	0.0003	4.27E-08	0.0030	2.67E-22	-4.6204	-8.0532	-3.4329	27.3135	-0.0859	-0.1497	-0.0638	0.4145	0.0186	0.0186	0.0186	0.0152	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970818)	0.85	0.68	0.79	0.04	0.0005	6.48E-11	2.73E-06	3.12E-41	0.0016	1.41E-09	1.19E-05	7.82E-39	-3.8938	-9.5753	-5.6815	-97.9519	-0.0693	-0.1704	-0.1011	-1.4235	0.0178	0.0178	0.0178	0.0145	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970819)	0.96	0.82	0.85	0.36	0.2817	2.03E-06	4.89E-05	4.62E-28	0.3664	1.13E-05	0.0001	2.32E-26	-1.0949	-5.7845	-4.6896	-37.6177	-0.0160	-0.0844	-0.0684	-0.4479	0.0146	0.0146	0.0146	0.0119	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970820)	1.17	0.99	0.85	0.03	0.1493	0.9547	0.1347	7.23E-29	0.2059	0.9663	0.1593	6.05E-27	1.4776	-0.0572	-1.5348	-39.9105	0.0682	-0.0026	-0.0708	-1.5031	0.0461	0.0461	0.0461	0.0377	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970823)	1.00	0.81	0.81	1.04	0.9531	2.00E-06	1.68E-06	0.1575	0.9570	1.13E-05	7.71E-06	0.1997	0.0592	-5.7894	-5.8486	1.4474	0.0009	-0.0925	-0.0934	0.0189	0.0160	0.0160	0.0160	0.0130	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970824)	0.92	0.79	0.85	1.34	0.0071	5.68E-10	1.68E-06	2.34E-14	0.0159	7.93E-09	7.71E-06	1.03E-13	-2.8770	-8.7266	-5.8496	13.0474	-0.0344	-0.1042	-0.0699	0.1273	0.0119	0.0119	0.0119	0.0098	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970825)	1.16	1.01	0.87	1.79	0.0164	0.8832	0.0232	1.20E-13	0.0333	0.9275	0.0319	4.78E-13	2.5328	0.1482	-2.3847	12.2765	0.0639	0.0037	-0.0601	0.2527	0.0252	0.0252	0.0252	0.0206	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970831)	1.08	0.93	0.87	0.46	0.0866	0.1083	0.0017	1.72E-21	0.1359	0.1677	0.0031	2.40E-20	1.7679	-1.6523	-3.4202	-23.0363	0.0321	-0.0300	-0.0620	-0.3412	0.0181	0.0181	0.0181	0.0148	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970832)	1.00	0.85	0.85	0.89	0.9267	5.25E-05	6.86E-05	0.0002	0.9417	0.0002	0.0002	0.0005	-0.0928	-4.6649	-4.5721	-4.1410	-0.0014	-0.0716	-0.0702	-0.0519	0.0154	0.0154	0.0154	0.0125	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970841)	0.99	0.83	0.83	0.60	0.8821	5.86E-05	9.02E-05	2.52E-16	0.9225	0.0002	0.0002	1.47E-15	-0.1495	-4.6266	-4.4771	-15.3663	-0.0027	-0.0829	-0.0802	-0.2248	0.0179	0.0179	0.0179	0.0146	32	32	32	32
pool, median	Unknown	Unknown lipid	Unknown lipid (69970843)	1.14	0.85	0.75	2.77	0.0240	0.0060	7.94E-06	1.68E-21	0.0464	0.0126	3.03E-05	2.40E-20	2.3700	-2.9452	-5.3152	23.0541	0.0556	-0.0691	-0.1247	0.4417	0.0235	0.0235	0.0235	0.0192	32	32	32	32
pool, median	Unknown	Unknown polar	Unknown polar (39970147)	0.69	31.73	46.19	0.85	0.0440	8.50E-17	1.96E-18	0.2573	0.0748	7.11E-15	1.64E-16	0.3061	-2.1172	19.0530	22.2172	-1.1583	-0.1631	1.5015	1.6646	-0.0727	0.0770	0.0788	0.0749	0.0628	26	26	26	26
pool, median	Unknown	Unknown polar	Unknown polar (39970148)	0.82	48.87	59.70	0.90	0.1556	1.47E-20	2.39E-21	0.3536	0.2122	2.27E-18	3.01E-19	0.4071	-1.4644	28.4334	30.6407	-0.9452	-0.0870	1.6890	1.7760	-0.0457	0.0594	0.0594	0.0580	0.0484	25	25	25	25
pool, median	Unknown	Unknown polar	Unknown polar (39970175)	0.64	314.39	493.30	0.67	0.0283	1.81E-20	7.72E-22	0.0155	0.0530	2.27E-18	1.95E-19	0.0233	-2.3340	29.7953	34.0782	-2.6070	-0.1956	2.4975	2.6931	-0.1741	0.0838	0.0838	0.0790	0.0668	24	24	24	24
pool, median	Unknown	Unknown polar	Unknown polar (39970411)	1.08	0.92	0.85	0.95	0.2841	0.2241	0.0221	0.3944	0.3676	0.3209	0.0308	0.4479	1.0937	-1.2454	-2.4343	-0.8660	0.0325	-0.0379	-0.0704	-0.0210	0.0297	0.0304	0.0289	0.0242	26	26	26	26
pool, median	Unknown	Unknown polar	Unknown polar (39970992)	0.76	1.02	1.35	2.50	0.0743	0.8921	0.0500	6.97E-08	0.1203	0.9291	0.0656	1.84E-07	-1.8595	0.1370	2.0556	7.4244	-0.1220	0.0092	0.1312	0.3972	0.0656	0.0672	0.0638	0.0535	26	26	26	26
pool, median	Unknown	Unknown polar	Unknown polar (39971140)	1.18	2.06	1.75	1.21	0.2438	2.52E-05	0.0003	0.1025	0.3202	0.0001	0.0007	0.1368	1.1927	5.1091	4.1480	1.6927	0.0715	0.3133	0.2418	0.0827	0.0599	0.0613	0.0583	0.0489	26	26	26	26
pool, median	Unknown	Unknown polar	Unknown polar (39971995)	0.88	1.02	1.17	1.09	0.1399	0.7966	0.0773	0.2426	0.1957	0.8545	0.0979	0.2928	-1.5229	0.2604	1.8394	1.1956	-0.0566	0.0099	0.0665	0.0362	0.0372	0.0380	0.0361	0.0303	26	26	26	26
pool, median	Unknown	Unknown polar	Unknown polar (39972117)	0.59	6.97	11.76	1.23	0.0242	3.02E-09	3.96E-11	0.2339	0.0464	3.99E-08	6.65E-10	0.2842	-2.4201	9.5044	12.0027	1.2239	-0.2274	0.8430	1.0703	0.0906	0.0939	0.0887	0.0892	0.0741	22	22	22	22
pool, median	Unknown	Unknown polar	Unknown polar (39972124)	1.79	3.19	1.78	1.08	0.0823	0.0014	0.0808	0.7653	0.1308	0.0038	0.1012	0.8174	1.8101	3.5853	1.8200	0.3018	0.2539	0.5032	0.2492	0.0345	0.1403	0.1403	0.1369	0.1143	25	25	25	25
pool, median	Unknown	Unknown polar	Unknown polar (39972135)	2.06	1.83	0.89	1.72	1.66E-05	0.0003	0.3861	6.40E-05	9.07E-05	0.0009	0.4231	0.0001	5.3128	4.2246	-0.8821	4.7913	0.3142	0.2620	-0.0522	0.2354	0.0591	0.0620	0.0591	0.0491	25	25	25	25
pool, median	Unknown	Unknown polar	Unknown polar (59970914)	0.74	0.87	1.17	0.91	0.0102	0.2041	0.1612	0.3135	0.0223	0.2945	0.1881	0.3654	-2.7305	-1.2963	1.4342	-1.0240	-0.1307	-0.0620	0.0686	-0.0400	0.0479	0.0479	0.0479	0.0391	32	32	32	32

pool, median	Unknown	Unknown polar	Unknown polar (59970918)	0.26	0.98	3.70	0.89	1.51E-12	0.8686	2.21E-12	0.2285	6.30E-11	0.9199	5.79E-11	0.2798	-11.1428	-0.1668	10.9759	-1.2277	-0.5774	-0.0086	0.5687	-0.0519	0.0518	0.0518	0.0518	0.0423	32	32	32	32	
pool, median	Unknown	Unknown polar	Unknown polar (59970919)	0.40	0.86	2.14	0.83	1.48E-07	0.2882	3.34E-06	0.0990	1.24E-06	0.3889	1.38E-05	0.1329	-6.6929	-1.0801	5.6129	-1.6990	-0.3939	-0.0636	0.3303	-0.0816	0.0588	0.0588	0.0588	0.0480	32	32	32	32	
^{13}C-ISTD, median	Vitamins, cofactors and related	Acyl-carriers and related	Coenzyme A	0.88	1.87	2.12	1.34	0.3567	0.0001	1.04E-05	0.0155	0.4477	0.0005	3.76E-05	0.0233	-0.9360	4.3946	5.2842	2.5661	-0.0548	0.2709	0.3258	0.1271	0.0586	0.0616	0.0616	0.0495	30	30	30	30	
^{13}C-ISTD, median	Vitamins, cofactors and related	Acyl-carriers and related	Pantothenic acid	0.59	0.79	1.32	0.73	4.47E-09	0.0012	0.0003	2.50E-06	5.35E-08	0.0033	0.0006	5.56E-06	-8.1306	-3.5801	4.1471	-5.7913	-0.2267	-0.1051	0.1217	-0.1365	0.0279	0.0293	0.0293	0.0236	30	30	30	30	
pool, median	Vitamins, cofactors and related	Amino-carriers and related	Pyridoxine	0.33	1.22	3.67	1.12	5.86E-08	0.2250	1.96E-09	0.4028	5.44E-07	0.3209	1.97E-08	0.4555	-7.0213	1.2372	8.2585	0.8478	-0.4800	0.0846	0.5645	0.0473	0.0684	0.0684	0.0684	0.0558	32	32	32	32	
pool, median	Vitamins, cofactors and related	C1-carriers and related	Biotin	0.50	1.44	2.91	1.95	1.39E-06	0.0033	1.05E-09	1.35E-07	9.68E-06	0.0073	1.15E-08	3.40E-07	-6.1028	3.2143	8.9516	6.9845	-0.3034	0.1598	0.4632	0.2894	0.0497	0.0497	0.0518	0.0414	28	28	28	28	
pool, median	Vitamins, cofactors and related	C1-carriers and related	Folic acid	0.23	0.99	4.29	0.68	5.34E-07	0.9793	5.76E-07	0.0533	3.94E-06	0.9793	3.09E-06	0.0743	-6.2458	-0.0262	6.2197	-2.0065	-0.6350	-0.0027	0.6323	-0.1666	0.1017	0.1017	0.1017	0.0830	32	32	32	32	
pool, median	Vitamins, cofactors and related	Carotenoids	beta-Carotene	1.26	0.77	0.61	0.37	0.0118	0.0051	2.78E-06	1.90E-15	0.0248	0.0111	1.19E-05	9.75E-15	2.6721	-3.0038	-5.6759	-14.2972	0.1000	-0.1124	-0.2124	-0.4369	0.0374	0.0374	0.0374	0.0306	32	32	32	32	
pool, median	Vitamins, cofactors and related	Redox-carrier and related	Coenzyme Q10	1.21	0.76	0.63	2.52	0.0022	3.90E-05	3.05E-09	1.27E-19	0.0061	0.0002	2.75E-08	1.32E-18	3.3258	-4.7675	-8.0934	19.9595	0.0820	-0.1176	-0.1997	0.4020	0.0247	0.0247	0.0247	0.0201	32	32	32	32	
pool, median	Vitamins, cofactors and related	Redox-carrier and related	Flavine adenine dinucleotide (FAD)	1.74	0.95	0.55	1.83	4.28E-09	0.5118	7.29E-10	5.88E-12	5.35E-08	0.6185	8.75E-09	2.11E-11	7.9681	-0.6635	-8.6316	10.5600	0.2416	-0.0201	-0.2617	0.2614	0.0303	0.0303	0.0303	0.0248	32	32	32	32	
pool, median	Vitamins, cofactors and related	Redox-carrier and related	Glutathione (GSH)	1.85	1.45	0.79	2.48	0.0110	0.1108	0.2967	2.74E-05	0.0233	0.1696	0.3308	5.78E-05	2.7007	1.6398	-1.0609	4.8895	0.2674	0.1624	-0.1050	0.3953	0.0990	0.0990	0.0990	0.0808	32	32	32	32	
^{13}C-ISTD, median	Vitamins, cofactors and related	Redox-carrier and related	Glutathione disulfide (GSSG)	1.17	1.32	1.13	2.03	0.4781	0.2275	0.5870	0.0005	0.5687	0.3217	0.6163	0.0010	0.7184	1.2319	0.5492	3.8726	0.0675	0.1217	0.0543	0.3074	0.0939	0.0988	0.0988	0.0794	30	30	30	30	
pool, median	Vitamins, cofactors and related	Redox-carrier and related	Nicotinamide	3.65	0.94	0.26	1.25	3.04E-12	0.6004	8.99E-13	0.0270	1.09E-10	0.6944	3.24E-11	0.0395	10.8394	-0.5291	-11.3685	2.3174	0.5621	-0.0274	-0.5896	0.0981	0.0519	0.0519	0.0519	0.0423	32	32	32	32	
pool, median	Vitamins, cofactors and related	Redox-carrier and related	Nicotinamide adenine dinucleotide (NAD)	1.02	1.36	1.34	1.19	0.7505	1.14E-05	2.88E-05	0.0010	0.8121	5.59E-05	8.86E-05	0.0017	0.3208	5.1925	4.8718	3.6374	0.0083	0.1348	0.1264	0.0771	0.0260	0.0260	0.0260	0.0212	32	32	32	32	
^{13}C-ISTD, median	Vitamins, cofactors and related	Redox-carrier and related	Nicotinamide adenine dinucleotide phosphate (	2.44	1.04	0.43	0.93	7.30E-10	0.7150	5.64E-09	0.4221	1.31E-08	0.7976	4.74E-08	0.4709	8.8481	0.3686	-8.0405	-0.8139	0.3870	0.0170	-0.3700	-0.0301	0.0437	0.0460	0.0460	0.0370	30	30	30	30	
^{13}C-ISTD, median	Vitamins, cofactors and related	Redox-carrier and related	Nicotinamide adenine dinucleotide phosphate, (	0.95	0.73	0.78	0.73	0.5172	0.0016	0.0078	0.0001	0.6066	0.0041	0.0121	0.0003	-0.6555	-3.4741	-2.8512	-4.3913	-0.0241	-0.1346	-0.1105	-0.1367	0.0368	0.0388	0.0388	0.0311	30	30	30	30	
^{13}C-ISTD, median	Vitamins, cofactors and related	Redox-carrier and related	Nicotinamide adenine dinucleotide, reduced (NA	1.66	1.04	0.63	0.49	0.0442	0.8815	0.0748	0.0015	0.0748	0.9275	0.0952	0.0026	2.1004	0.1504	-1.8458	-3.4919	0.2203	0.0166	-0.2037	-0.3096	0.1049	0.1104	0.1104	0.0886	30	30	30	30	
pool, median	Vitamins, cofactors and related	Tocopherols and related	alpha-Tocopherol	1.24	1.33	1.07	1.13	0.0926	0.0275	0.5684	0.2498	0.1426	0.0489	0.5993	0.3000	1.7338	2.3102	0.5764	1.1722	0.0941	0.1254	0.0313	0.0519	0.0543	0.0543	0.0543	0.0443	32	32	32	32	

Statistical quantities	Explanation
Ratio	ANOVA estimate of effect on ratio scale (transformed Estimate: 10^Est.log)
p.value	p-value of ANOVA t-statistics
t.value	ANOVA t-statistics
Est.log	ANOVA contrast estimate (on log10-scale)
Std.Err	Standard error of ANOVA contrast estimate (on log10-scale)
DF	Degrees of freedom for contrast estimate
q.value	Benjamini-Hochberg multiple comparisons q-value (= False-discovery rate/FDR)

Coloring of ratios:
ratio > 1 & p-value < 0.01
ratio > 1 & 0.01 ≤ p-value < 0.05
ratio > 1 & 0.05 ≤ p-value < 0.10
ratio < 1 & 0.05 ≤ p-value < 0.10
ratio < 1 & 0.01 ≤ p-value < 0.05
ratio < 1 & p-value < 0.01

Font style of ratios:
bold: (ratio < 0.5) or (ratio > 2)
normal: (ratio > 0.5) or (ratio < 2)

Coloring of p-values:
0.05 ≤ p < 0.10
0.01 ≤ p < 0.05
p < 0.01

METABOLITE_NAME contains an "Additional ": Quantitation can be disturbed by metabolites exhibiting identical analytical characteristics with respect to quantitation method. Literature data and/or comparison with alternative methods (e.g. LC-MS/MS, GC-MS) suggest that disturbing metabolite is present at minor levels only.