ARTICLE INFORMATION

**Article title**

Follow-up Validation of Urinary Metabolite Profiling to Non-Invasively Monitor the Omega-3 Index in Young Adults: Dataset

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**Keywords**

precision nutrition; metabolomics; omega-3 long-chain polyunsaturated fatty acids (n3-LCPUFA); omega-3 index; dietary biomarkers; urinary metabolites

**Abstract**

The dataset comprises metabolomic and clinical data/information collected from a double-blind, randomized controlled trial involving 120 participants (18-45 years old), who were assigned to one four groups: olive oil control (~3 g/day), low-dose EPA+DHA (~1 g/day), high-dose EPA+DHA (~3 g/day), or biweekly salmon consumption (~1.8 g EPA+DHA per serving). Data collection occurred over a 24-week period, including a 12-week intervention phase followed by a 12-week washout phase. Biological samples, as fasted blood and first-void urine were collected at baseline, during the intervention, and after the washout period.

Metabolomic analyses were performed using multisegmented injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS) and liquid chromatography-mass spectrometry (LC-MS) to generate detailed chromatograms, electropherograms, and mass spectra from the urine samples. Fatty acid profiles, including EPA and DHA concentrations in red blood cells, were measured using gas chromatography-flame ionization detection. Additional clinical data such as triglyceride levels, cholesterol profiles, blood pressure, and inflammatory markers were obtained from blood samples.

The dataset includes tabular data in .csv format for clinical variables and for processed metabolomic data. All data include a comprehensive metadata describing sample collection procedures, instrument settings for each analytical technique, quality control measures, quality assurance procedures and data preprocessing and processing workflows.

The dataset has potential reuse applications in metabolomics, cardiovascular research, and precision nutrition. It can be used for secondary analysis to explore biomarker discovery, dose-response relationships, and correlations between omega-3 intake and cardiovascular risk factors. Additionally, the data can contribute to method development for metabolomics and to statistical modelling.

# SPECIFICATIONS TABLE

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| --- | --- |
| **Subject** | Biological Sciences - Metabolomics |
| **Specific subject area** | Metabolomics data from human clinical trials examining omega-3 fatty acid intake. |
| **Type of data** | Table: .csv (clinical and metabolomic data)  Image: .mzML, .cdf (mass spectrometry data)  Chart: graphs for metabolite profiles and for statistical/chemometrics analyses for processed and pre-processed data.  Figure: .png (chromatograms, electropherograms, metabolomic spectra, figures from statistical methods applied to pre and processed data).  Data formats: Raw, processed, normalized. |
| **Data collection** | Data were collected from fasted blood and urine samples in a double-blind randomized trial with 120 participants. Metabolomic analyses were performed using MSI-CE-MS (Agilent G7100A) and LC-MS, while fatty acids were measured in RBCs via gas chromatography-flame ionization detection (Agilent 7890A). Data were pre-processed in MassHunter Quantitative Analysis Software and in Excel, normalized using log transformation and autoscaling and processed in the software Metaboanalyst. Inclusion criteria included participants aged 18-45 with an Omega-3 Index ≤4%. |
| **Data source location** | Collected: Department of Human Health and Nutritional Sciences, University of Guelph, Guelph, ON N1G 2W1, Canada  Stored*:* Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON L8S 3W3, Canada |
| **Related research article** | MacIntyre, B. C., Shanmuganathan, M., Klingel, S. L., Kroezen, Z., Helmeczi, E., Seoh, N. Y., Martinez, V., Chabowski, A., Feng, Z., Britz-McKibbin, P., & Mutch, D. M. (2023). Urinary Metabolite Profiling to Non-Invasively Monitor the Omega-3 Index: An Exploratory Secondary Analysis of a Randomized Clinical Trial in Young Adults. Metabolites, 13(10), 1071. https://doi.org/10.3390/metabo13101071 |

# VALUE OF THE DATA

* The dataset provides comprehensive metabolomic and cardiovascular health data from a double-blind randomized trial involving omega-3 supplementation, which includes various doses of EPA+DHA as well as a control group. This combination of intervention-based and metabolomic data can help researchers better understand metabolic changes associated with omega-3 intake.
* These data can be reused to explore dose-response relationships and biomarker identification in the omega-3 fatty acid metabolism, offering potential applications in nutrition, cardiovascular research, and clinical metabolomics.
* With data on both male and female participants, the dataset supports sex-based analyses, enabling researchers to investigate potential differences in metabolic responses to omega-3 supplementation across sexes.
* The dataset is structured in open formats (.csv, .mzML, .cdf), making it accessible for integration into various data analysis routes and promoting broader usage by researchers in different fields like medicina.

# BACKGROUND

The motivation for compiling this dataset comes from the need to find non-invasive biomarkers for omega-3 fatty acid levels, which are important for monitoring cardiovascular disease (CVD) risk factors. Given the limitations of current methods, like blood sampling, the dataset focuses on urinary metabolites as a possible alternative. The use of a double-blind randomized clinical trial design ensures that the dataset can accurately show the effects of different doses of EPA and DHA on both metabolomic profiles and CVD risk factors. Including both male and female participants allows for exploring sex-specific differences in metabolic responses to omega-3 supplementation. This dataset adds value by offering a detailed view of the metabolome in relation to omega-3 status and can be reused in future research related to nutrition, metabolomics, and cardiovascular health.

# DATA DESCRIPTION

1. Clinical Data: Contains .csv files with demographic information, cardiovascular health markers (e.g., triglyceride levels, cholesterol profiles), and omega-3 intake data from each participant at baseline and after supplementation.
2. Metabolomic Data: Includes .mzML and .cdf files representing raw and processed metabolomic data obtained from MSI-CE-MS and LC-MS analyses of urine samples. These files are organized by participant ID and collection time point (e.g., baseline, post-supplementation).
3. Metadata: Comprehensive metadata in .txt format describes each dataset, including sample collection protocols, instrument settings, and normalization methods (log transformation and autoscaling).

# EXPERIMENTAL DESIGN, MATERIALS AND METHODS

The data were acquired through a double-blind randomized controlled trial involving 120 participants who consumed either olive oil (control), low-dose EPA+DHA, high-dose EPA+DHA, or salmon (twice weekly) for 12 weeks, followed by a 12-week washout period. Biological samples, including fasted blood and first-void urine, were collected at multiple time points (baseline, during supplementation, post-washout).

Instruments: Urine samples were analyzed using MSI-CE-MS (Agilent G7100A) and LC-MS, while blood samples were used to measure EPA and DHA levels in red blood cells via gas chromatography-flame ionization detection (Agilent 7890A).

Software: Mass spectrometry data were processed using Mass Hunter and analyzed with MetaboAnalyst 5.0. Clinical data were organized and analyzed using standard statistical software (e.g., R or Python).

Normalization: Data were normalized using log transformation and autoscaling to minimize variability across samples.

All data, including raw and processed formats, are made available for reuse, and detailed metadata accompanies each dataset.

# LIMITATIONS

The dataset is limited to a specific population group (participants aged 18-45) and may not fully represent other age groups or populations with different dietary habits or health conditions.

While the sample size (n=120) is sufficient for exploring dose-response relationships, larger datasets may be required for identifying rare metabolites or performing more complex subgroup analyses.

The trial focuses on omega-3 fatty acids, specifically EPA and DHA, and may not capture broader dietary or lifestyle influences that could affect metabolomic profiles.

# ETHICS STATEMENT

This research was carried out in accordance with the Declaration of Helsinki and received approval from the institutional Research Ethics Board (REB). Informed consent was obtained from all participants prior to their inclusion in the study.

# CRediT AUTHOR STATEMENT

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| *David M. Mutch* | *Conceptualization,*  *Methodology.* |
| *Mariana Buitrago* | *Validation,*  *Formal analysis,*  *Investigation.* |
| *Zachary Kroezen* | *Resources.* |
| *Philip Britz-McKibbin* | *Supervision,*  *Project administration,*  *Funding acquisition.* |

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# DECLARATION OF COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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