# ARTICLE INFORMATION

**Article title**

*Dataset for quantification of urinary metabolites from patients who develop delirium post-hip-fracture surgery*

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**Keywords**

*Delirium, metabolomics, mass spectrometry, capillary electrophoresis, hip-fracture surgery*

**Abstract**

*The urinary metabolome of patients pre- and post-surgery was determined from urine samples of patients. Each urine sample was prepared and run using multisegment injection-capillary electrophoresis-mass spectrometry (MSI-CE-MS), a method that was optimized in the Britz-McKibbin lab. The data was then pre-processed, and the quality of the data was checked. The data provided in this dataset contains the raw electropherograms as well as pre-processed data. This data can be used to determine patterns in metabolites seen in patients who develop delirium.*

# SPECIFICATIONS TABLE

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| **Subject** | *Omics: metabolomics* |
| **Specific subject area** | *Urinary metabolome and analytical chemistry* |
| **Type of data** | Raw tables, analyzed figures. |
| **Data collection** | *The data was collected after separation using capillary electrophoresis (Agilent Technologies, 7100 CE System), ionization using electrospray ionization (Agilent Technologies, G1948B), then detection by mass spectrometry (Agilent Technologies, 6230 Time of Flight (TOF) MS).* |
| **Data source location** | *The data was collected at McMaster University, Arthur N. Bourns Building, 43°15'38.0"N 79°55'21.2"W. The data is stored at McMaster University, at the same coordinates as where the data was collected.* |
| **Data accessibility** | Repository name: TBD  Data identification number: *TBD*  Direct URL to data: **TBD** |
| **Related research article** | *None* |

# VALUE OF THE DATA

* These data are valuable because it encompasses the urinary metabolome of patients who develop delirium compared to those who do not develop delirium
* They can be reused by other reseachers to identify new patterns that are seen in the urinary metabolome
* This dataset can also be used as a training dataset for a machine learning model to later test other samples against this model

# BACKGROUND

The original motivation for compiling this dataset was to determine biomarkers that can be used to diagnose delirium in its early stages. A delirium diagnosis currently relies on subjective measures, and therefore is often missed, especially in a critical care setting where clinicians are extremely busy. A biomarker for delirium can provide an objective measure for diagnosing delirium, enabling clinicians to reliably diagnose delirium.

# DATA DESCRIPTION

The data currently is in [NAME OF REPOSITORY] and contains 2 folders. The first folder, called “raw\_data”, contains the raw data that was obtained from the mass spectrometry, while the second folder, called “pre-processed\_data”, contains the pre-processed data.

Within the “raw\_data” folder, there are two more folders: “positive\_mode” and “negative\_mode”. The folder “positive\_mode” contains the .d files for the runs that took place in positive mode, while the “negative\_mode” contains the .d files for the runs that took place in negative mode. Within each of these two folders, each file is named with the following naming convention: “YYYYMMDD\_##”, where “YYYYMMDD” represents the year (YYYY), month (MM), and day (DD) the sample was run, and “##” represents the chronological order of the run for this date.

Within the “pre-processed\_data” folder, there is an Excel sheet containing the pre-processed data. Within this Excel sheet, the first sheet contains the pre-processed data, while the second, third, and fourth sheets contain quality checks to ensure the pre-processed data is accurate.

# EXPERIMENTAL DESIGN, MATERIALS AND METHODS

*Urine samples were collected before surgery, as well as after surgery at as many timepoints as possible, up to 9 timepoints. Once the sample has been collected, the specimen cup was immediately sealed and stored at 4ºC. Urine was fractionated into 10x10 mL aliquots by laboratory staff before being transferred to an -80°C freezer within 24 hours.*

*At the time of analysis, 1 of 10 urine aliquots were thawed, and 1mL aliquot of urine was placed in a sterile 2mL Eppendorf tube, with the remaining raw urine being immediately refrozen at -80°C until required for further study. The tube was then centrifuged, and 900 μL of urine was removed from the supernatant and transferred to a sterile 2mL eppendorff tube, where internal standards were added to each sample. The sample was then refrigerated until it was ready to be analyzed using MSI-CE-MS.*

*The MSI-CE-MS method that was used to collect the data in this dataset can be found in the following paper: MacIntyre et al., 2023.*

# LIMITATIONS

*The number of samples in this dataset is a bit limited, as there were only 9 patients who could provide urine samples.*

# ETHICS STATEMENT

*The relevant informed consent was obtained by the subjects who provided a urine sample and was approved by the ethics board (protocol #: ########). The research was carried out in accordance with the Declaration of Helsinki.*

# CRediT AUTHOR STATEMENT

*Zaineb Hamoodi – Methodology, validation, formal analysis, investigation, writing – original draft, visualization.*

*Philip Britz-McKibbin – Conceptualization, methodology, resources, writing – review and editing, supervision, project administration, funding acquisition.*

# ACKNOWLEDGEMENTS

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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.*

# REFERENCES

*MacIntyre BC, Shanmuganathan M, Klingel SL, Kroezen Z, Helmeczi E, Seoh NY, Martinez V, Chabowski A, Feng Z, Britz-McKibbin P, Mutch DM. Urinary Metabolite Profiling to Non-Invasively Monitor the Omega-3 Index: An Exploratory Secondary Analysis of a Randomized Clinical Trial in Young Adults. Metabolites. 2023 Oct 12;13(10):1071. doi: 10.3390/metabo13101071.*