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Data Article

Raw *N*-glycan mass spectrometry imaging data on formalin-fixed mouse kidney

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ABSTRACT

Provided is the annotated raw data for *N*-glycan mass spectrometry imaging (MSI) annotations in thin cross-sections of formalin-fixed and paraffin-embedded murine kidney. Relevant meta-data have been provided in this brief and the raw MSI data can be accessed using ProteomeXchange with the PRoteomics IDentifications (PRIDE) identifier PXD009808. This brief is the first in a set of submissions from our group which will make raw data publicly accessible for existing and future MSI studies.

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Specifications table

Subject area	Chemistry
More specific subject area	Analytical chemistry (mass spectrometry)
Type of data	*.imzML (imaging)
How data was acquired	Mass spectrometry (Bruker Daltonics ultrafleXtreme MALDI-ToF/ToF)
Data format	Raw data (*.imzML)
Experimental factors	Antigen retrieval, PNGaseF digestion and MALDI matrix deposition
Experimental features	Tissue-specific mapping of N-glycan distribution in mouse kidney
Data source location	Data was collected at the Adelaide Proteomics Centre (APC) located within the University of Adelaide (South Australia)
Data accessibility	Raw data (*.imzML) is available on PRIDE (PXD009808)

Value of the data

- The data supported method development for profiling and MSI of N-glycans on FFPE tissue sections.
- The data is linked to orthogonal methods for derivatization and LC-MS/MS identification of N-glycan composition.
- Other MSI researchers are now able to view, process and further analyze this N-glycan data.

1. Data

Prior to this data-brief the N-glycan MSI data [1] was made partially available as an upload to SciLS Cloud. This provided a tool for online visualization of the spatial distribution for a selection of ions detected from the FFPE murine kidney sections used in these experiments – and limited figure or ion map downloads. The selectable ions included both a set of 18 N-glycan candidates and a filtered set of 203 m/z intervals (Signal to Noise Ratio (SNR) > 3 and m/z > 933), all of which can be visualized using multiple signal normalization approaches, including Root Mean Square (RMS), Total Ion Count (TIC) or median. The SciLS Cloud availability of the MSI data was a step in the right direction. To complete the transparent dissemination of this data it was uploaded to ProteomeXchange Consortium [2] via the PRIDE partner repository [3] in the community standard *.imzML format as a partial submission: the data is available at the following link (<https://www.ebi.ac.uk/pride/archive/projects/PXD009808>) with the dataset identifier PXD009808.

2. Experimental design, materials and methods

The materials used, as well as the supplier, are provided in the tables below. For clarity these are split between chemicals (Table 1), mass standards (Table 2) and equipment/consumables (Table 3). The experimental design and methods are described below. The data acquisition was split by the experimental design into two aspects: profiling MS and MSI (see Fig. 1).

1. Profiling of specific kidney tissue regions using high volume (750 nL) printed PNGase F deposited at a centre to centre spacing of 1300 μm . This also incorporated control 25 mM Ammonium Bicarbonate (NH_4HCO_3) buffer-only spots (see Fig. 1).

Number of sections	4
PNGase F replicate spots (total)	2/tissue region ($N = 4$)
Control replicate spots	4 replicate spots in kidney cortex

2. MSI using 30 nL printed PNGase F deposited in an array of spots with a centre to centre spacing of 250 μm .

<i>Number of sections</i>	3
PNGase F regions (total)	1 per kidney, complete section ($N = 2$)
Control regions	1 (half kidney section)

For both the profiling and MSI modes, the PNGase F was deposited using a Chemical InkJet Printer 1000 (ChIP-1000) instrument. Following incubation to allow the enzyme to cleave *N*-glycans from the fixed tissue the sections were overlaid with 2,5-dihydroxybenzoic acid (DHB) in 1 mM sodium chloride (NaCl) and 0.1% trifluoroacetic acid (TFA) using a capillary nebulized spray delivered via a TM-sprayer instrument.

Table 1

List of chemicals and suppliers.

<i>Item</i>	<i>Details (supplier)</i>
Glycerol-free PNGase F	P0705L, 75000 NEB units (New England BioLabs, Ipswich, MA, USA)
Formalin	Sigma-Aldrich
Trifluoroacetic acid (TFA)	Merck (Darmstadt, Germany)
Ethanol (EtOH)	Merck (Darmstadt, Germany)
Sodium chloride (NaCl)	Merck (Darmstadt, Germany)
2,5-dihydroxybenzoic acid (DHB)	Sigma-Aldrich/Bruker Daltonics (Bremen, Germany)
Xylene	Chem-Supply (Gillman, South Australia)

Table 2

Mass standards used to externally calibrate mass spectrometry data.

<i>Item</i>	<i>Supplier</i>	<i>m/z</i>
Man5GlcNAc2	Prozyme (CA, USA)	[M+Na] ⁺ : 1257.4225
Man3GlcNAc5	Prozyme (CA, USA)	[M+Na] ⁺ : 1542.5551
Man3Gal4GlcNAc6	Prozyme (CA, USA)	[M+Na] ⁺ : 2393.8457

Table 3

Consumables and equipment, including suppliers.

<i>Item</i>	<i>Supplier</i>
Indium tin oxide (ITO) slides	Bruker Daltonics (Bremen, Germany)
Poly Ethylene Naphthalate (PEN) slides	MicroDissect (Herborn, Germany)
0.025 μm VWSP nitrocellulose membranes	Millipore (Cork, Ireland)
TP 1020 processors	Leica Biosystems (North Ryde, Australia)
EG 1140H embedder	Leica Biosystems
Microm HM 325 microtome	Zeiss (Gottingen, Germany)
TM-sprayer	HTX Instruments (NC, USA)
UltrafleXtreme MALDI-ToF/ToF	Bruker Daltonics
Chemical Inkjet Printer (ChIP)-1000	Shimadzu (Japan)

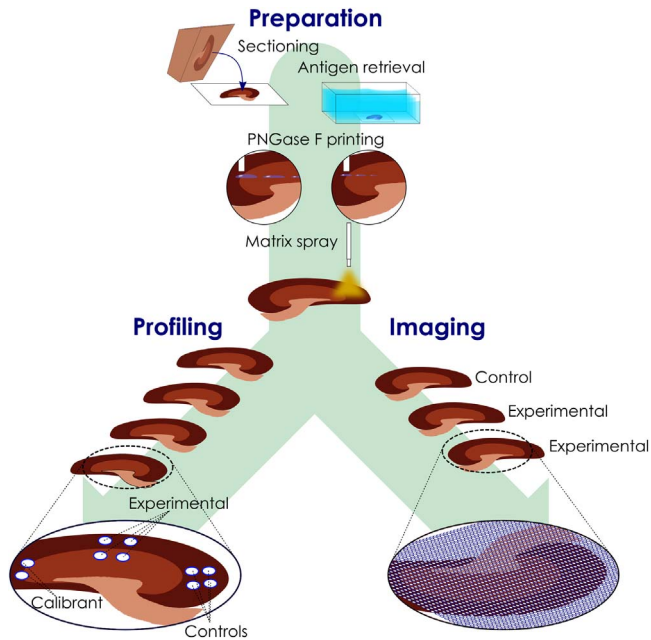


Fig. 1. N-glycan profiling MS and MSI workflow.

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Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2018.08.186>.

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