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CE-TOFMS data from a urine sample - mzML files with scans in profile or centroid spectrum format

Published: 3 Jan 2017 | **Version 2** | **DOI:** 10.17632/cb4hv9cp2c.2 Viewed 90 Downloaded 21

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Description of this data

Those datasets are characteristics of urine samples separated by capillary electrophoresis hyphenated with high-resolution mass spectrometry (HRMS). The mzML format has been developed by the Human Proteome Organisation (HUPO) and allow to convert proprietary instrument files to an open format that can be used with the various numerical computing environment. Those datasets have been used in the development of the Finnee Matlab toolbox.

The original Bruker file that was used to create the mzML files has been graciously donated by Alejandro Cifuentes from the Laboratory of Foodomics (CIAL, CSIC, Madrid, Spain).

Experiment data files

Download all files (2)

MZML ACID-198-rep1.mzml

638 MB

'profile spectrum' format

Latest version

Version 2 2017-01-03

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MZML ACID-198-rep1_ctr.mzml

33 MB

'centroid spectrum' format

Steps to reproduce

Chemicals and samples: All reagents employed in the preparation of the CE buffer and sheath liquid (isopropanol, formic acid and ammonium hydroxide, all of MS grade) were from Sigma–Aldrich (St. Louis, MO, USA). The urine was filtered through 0.2 m polyethersulfone filter before CE-MS analysis.

CE-TOF MS analysis: The capillary electrophoresis (CE) apparatus used was a P/ACE 5010 from Beckman (Fullerton, CA, USA). The CE instrument was controlled by a PC running System GOLD software from Beckman. The CE equipment was coupled to a time-of-flight (TOF)instrument “microTOF” from Bruker Daltonik. CE-TOF coupling was carried out via an ESI interface model G1607A from Agilent Technologies. Electrical contact at the electrospray needle tip was established via a flow of sheath liquid composed of 2-propanol-water (50:50, v/v) delivered by a 74900-00-05 Cole Palmer syringe pump (Vernon Hills, IL, USA) at a flow rate of 4 L/min. Bare fused-silica capillary with 50 m i.d. and 85 cm of total length was from Composite Metal Services (Worcester, England). The inner capillary wall was coated with a cationic TEDETAMA-co-HPMA copolymer. CE separation was performed at −20 kV in an acidic BGE (1 M formic acid adjusted to pH 2.4 with ammonium hydroxide). Nebulizer pressure was 0.4 bar, drying gas flow rate was 4 L/min, and ESI chamber temperature was set at 200 ◦C. TOF MS was operated in the negative ion mode (capillary voltage was 4 kV), and spectra were acquired in the range of 50–700 m/z.

Conversion to mzML: The proprietary file was converted to mzML using CompassXport the freeware from Bruker. This file has been converted to 'profile spectrum' format.

Related links

Previous versions

Version 1 2016-11-10

Compare to version

Version 2

Institutions

University of Porto Faculty of Engineering

Categories

High Resolution Spectroscopy, Metabolite, Chemometrics, Hyphenated Separation Technique, Capillary Electrophoresis Mass Spectrometry

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doi:10.1016/j.chemolab.2016.04.013

glerny/Finnee2016

software is source of this dataset

Contribute to Finnee2016 development by creating an account on GitHub.

https://github.com

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mzML 1.1.0 Specification | HUPO Proteomics Standards Initiative

dataset is source of this dataset

http://psidev.info

Mass Spectrometry Resource

dataset is derived from this dataset

A mass spectrometry resource web site, featured are mass spectrometry tutorials.

http://www.ionsource.com

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dataset is related to this dataset

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