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

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Description of this data

Those datasets are characteristics of urine samples separated by UHPLC - QTOF MS. The mzML format has been developed by the Human Proteome Organisation (HUPO) and allows 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 Urine dataset - centroid scan mode.mzml 48 MB

MZML Urine dataset - profile scan mode.mzml

Latest version

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2.7 GB

Steps to reproduce

UHPLC-Q/TOF analysis was carried out using a 1290 system (Agilent) coupled to a quadrupole-time-of-flight (Q/TOF) 6540 (Agilent) equipped with an orthogonal electrospray ionisation (ESI) source (Agilent Jet Stream, AJS). The separation was performed on a Zorbax Eclipse Plus C8 (2.1 x 100 mm, 1.8 µm) column using phase A (water with 0.1% (v/v) formic acid) and phase B (acetonitrile with 0.1% (v/v) formic acid) and following gradient program: the run was started at 0% B and maintained for 2 min. From 2-6 min phase, B increased linearly till reached 30%. From 6-8 min phase B was increased to 100% and maintained for 2 min (from 8-10). Before each run, the column was re-equilibrated for 3 min using the initial solvent composition. TOF-MS operation parameters were the following: capillary voltage, -4000 V; nebuliser pressure, 25 psi; drying gas flow rate, 7 L/min; gas temperature, 300 °C; skimmer voltage, 45 V; fragmentor voltage was 125 V; 50-1000 m/z mass scan in positive ionisation mode. External calibration of the TOF MS was carried out using a commercial mixture from Agilent with next m/z values: 118.0863, 322.0481, 622.0290, 1221.9906, 1521.9715, 1821.9523, 2121.9331, 2421.9139 and 2721.8948. The numerical threshold was set to 200.

Related links

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Institutions

University of Porto Faculty of Engineering

Categories

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