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Human Plasma Metabolites Measured with Different Liquid Chromatography/Mass Spectrometry (LC/MS) Platforms

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1. Summary

Non-targeted global metabolite profiles of Standard Reference Material (SRM) 1950 Metabolites in Human Plasma were obtained on five different liquid chromatography/mass spectrometry (LC/MS) instrument combinations using identically prepared samples. Different instruments rendered significantly different metabolite profiles, however, the results were highly reproducible when working with one instrument. A full description of the measurements and data analysis have been previously published [1]. Presented here are the raw data on which Ref. [1] is based. For a further description of SRM 1950 and the general analysis of its chemical composition, see Refs. [2] and [3].

2. Data Specifications

NIST Operating Unit	Material Measurement Laboratory, Biomolecular Measurement Division, Mass Spectrometry Data Center
Format	Thermo Scientific ***.raw*** files; Agilent Technologies ***.d*** files
Instrument	Thermo Scientific Orbitrap Elite; Agilent Technologies model 6530 Q-TOF
Accessibility	All datasets submitted to *Journal of Research of NIST* are publicly available. The set discussed here can be found at: Telu_human_plasma_metabolites.zip
License	NIST Licensing Policy
Hash Value	SHA-256 Hash File

3. Methods

The liquid chromatography methods used were: conventional high-performance liquid chromatography (HPLC), ultra-high performance liquid chromatography (UHPLC), and nanoLC. The LC separations were coupled to two types of mass spectrometer: quadrupole-time of flight (QTOF), and orbitrap. The data provided includes the following combinations with replicate measurements: HPLC-orbitrap, nanoLC-orbitrap, HPLC-QTOF, UHPLC-QTOF and nanoLC-QTOF. Reference [1] and its Supporting Information give a complete description of the sample preparation methods and the experimental conditions. Reference [1] also gives in spreadsheet form the authors' analysis of the data using three different software packages: the publicly available **XCMS** produced by the Scripps Research Institute, the proprietary Agilent Mass Profiler Professional[1], and NIST's own in-house software.

4. Impact

The raw data is provided to the scientific community as a benchmark for new measurement protocol development. It also allows for additional chemical compounds to be found in human blood plasma by the application of data analysis methods not employed by NIST especially those that will undoubtedly emerge in the future.

5. References

[1] Telu KH, Yan X, Wallace WE, Stein SE, Simón-Manso Y (2016) Analysis of human plasma metabolites across different liquid chromatography/mass spectrometry platforms: Cross-platform transferable chemical signatures. *Rapid Commun Mass Spectrom* 30(5):581-593. http://dx.doi.org/10.1002/rcm.7475

[2] Phinney KW, *et al.* (2013) Development of a Standard Reference Material for metabolomics research. *Anal Chem* 85(24):11732-11738. http://dx.doi.org/10.1021/ac402689t

[3] Simón-Manso Y, *et al.* (2013) Metabolite profiling of a NIST Standard Reference Material for human plasma (SRM 1950): GC-MS, LC-MS, NMR, and clinical laboratory analyses, libraries, and web-based resources. *Anal Chem* 85(24):11725-11731. http://dx.doi.org/10.1021/ac402503m

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[1] Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.