Quartet Metabolite Reference Materials

Human Metabolite for Quality Control and Performance Assessment of Metabolomic Profiling
(Chinese Quartet Family of Monozygotic Twin Daughters, Father, and Mother: **D5**, **D6**, **F7**, and **M8**)

The Quartet Metabolite Reference Materials suite (RM) was prepared as part of "***The Quartet Project: Quality Control and Data Integration of Multi-omics Profiling***" in which matched reference materials of DNA, RNA, proteins, and metabolites were simultaneously manufactured from the same batch of cultured cells. A unit of the Quartet Metabolite Reference Materials consists of four vials containing metabolites extracted from the immortalized B-lymphoblastoid cell line of a specific family member of a Chinese Quartet family from Fudan Taizhou Cohort, including father (F7), mother (M8), and two monozygotic twin daughters (D5 and D6). Each vial contains dried cell extracts from approximately 10^6 cells using methanol:water (6:1) solution. Eleven external controls are spiked in at known amounts.

SPECIFICATIONS

Name of Metabolite Reference Material	Color	Amount	Description	External Controls (pmol)
FDU_Quartet_Metabolite_D5_20171028		Extracts from 10^6 cells	Dried cell extracts from 10^6 cells using methanol:water (6:1) solution	1. Cholic acid (25) 2. Deoxycholic acid (50) 3. Glycocholic acid (5) 4. Glycodeoxycholic acid (0.5) 5. Glycoursodeoxycholic acid (1) 6. Indoleacetic acid (25) 7. Sulfadimethoxine (5) 8. Taurocholic acid (1) 9. Taurodeoxycholic acid (7.5) 10. Tauroursodeoxycholic acid (2.5) 11. Ursodeoxycholic acid (25)
FDU_Quartet_Metabolite_D6_20171028				
FDU_Quartet_Metabolite_F7_20171028				
FDU_Quartet_Metabolite_M8_20171028				

Quartet Metabolite Reference Materials suite is stored at -80 ºC and shipped with dry ice. External controls are spiked in the cell extracts at known amounts.

INTENDED USES

The Quartet Metabolite Reference Materials suite is intended for quality control and performance assessment of quantitative metabolomic profiling. It can measure and mitigate technical variation, enabling more accurate data integration in large cohort studies. The Quartet performance metrics for metabolomic profiling are: 1) Quartet multi-sample based signal-to-noise ratio (SNR); and 2) Reference datasets based correlation coefficient. This metabolite RM suite should be profiled in the same way as study samples in each batch within a lab. Because the RM is cell extracts, it is not suitable for assessing the pre-analytical steps such as cell extraction, and it aims to evaluate the performances of following metabolomics profiling steps. It is for research purpose only.

REFERENCE DATASETS

The Quartet Metabolite Reference Datasets are provided as the relative expression values of six sample pairs (D5/D6, D5/F7, D5/M8, D6/F7, D6/M8, and F7/M8), using methods described in the Quartet metabolite manuscript. The v1.0 of metabolite reference datasets covers approximately 40-50 metabolites. As metabolomics profiling technologies and data analysis methods improve, the reference datasets will be updated periodically. All the reference datasets and the quality assessment tools can be accessed through the Quartet Data Portal (http://chinese-quartet.org/).

NOTICE AND WARRANTIES TO USERS

The Quartet Metabolite Reference Materials are being provided on an "AS IS" basis. The provider hereby warrants that the Quartet Metabolite Reference Materials have been obtained or created a) in full compliance with all applicable local, governmental and international laws, regulations and guidelines, b) after obtaining and in full compliance with all necessary approvals from the relevant research ethics committees, and c) after obtaining and in full compliance with all necessary, properly signed informed consents and acknowledgement forms from any human subjects, or their legal guardians. The provider makes no representation or warranty, whether expressed or implied, with respect to the Quartet Metabolite Reference Materials, including any representation or warranty as to the durability, storage, disposal, merchantability or fitness for a particular purpose or to the non-infringement of the Quartet Metabolite Reference Materials on the proprietary rights of a third party. The recipient shall use the Quartet Metabolite Reference Materials obtained or created as described above at its sole risk and liability.

The Quartet Metabolite reference materials and raw datasets are publicly available and accessible. Researchers are encouraged to access and analyze the datasets. The recipients of the Reference Materials are highly encouraged to share their data with Fudan University through the Quartet Data Portal in order for us to improve the reference datasets and to better serve the community.

For other questions, please feel free to contact the Quartet Project team (quartet@fudan.edu.cn and http://chinese-quartet.org/), and/or Drs. Yuanting Zheng (zhengyuanting@fudan.edu.cn) and Leming Shi (lemingshi@fudan.edu.cn).

“中华家系” 1 号人源细胞系代谢物参考物质

LC-MS/MS 代谢组检测质量评价用人源细胞系代谢物

（中国同卵双胞胎家庭，两个女儿、父亲和母亲：**D5**, **D6**, **F7** 和 **M8**)

“中华家系” 1 号代谢物参考物质来源于“**Quartet 中华家系 1 号项目：多组学质量控制和数据整合**”，该项目研制了同批次细胞来源的 DNA、RNA、蛋白质、代谢物的多组学参考物质。“中华家系” 1 号代谢物参考物质一套内含 4 管人源永生化 B 淋巴母细胞系的细胞提取物，细胞系建立自复旦泰州队列的中国同卵双胞胎家庭，包括父亲(F7)、母亲(M8)和两个同卵双胞胎女儿 (D5 和 D6)。每管代谢物参考物质包含 10^6 细胞的甲醇:水(6:1)溶液提取物；按照已知摩尔量加入 10 个菌群代谢物和磺胺二甲氧嘧啶作为外加质控品。代谢物参考物质以冻干粉的形式保存。

规格参数

代谢物参考物质的名称	颜色	总量	特征描述	外加质控品 (pmol)
FDU_Quartet_Metabolite_D5_20171028	蓝	相当于 10^6 细胞所含有的代谢物	10^6 细胞的甲醇:水(6:1)提取物冻干粉	1. Cholic acid (25) 2. Deoxycholic acid (50) 3. Glycocholic acid (5) 4. Glycodeoxycholic acid (0.5) 5. Glycoursodeoxycholic acid (1) 6. Indoleacetic acid (25) 7. Sulfadimethoxine (5) 8. Taurocholic acid (1) 9. Taurodeoxycholic acid (7.5) 10. Tauroursodeoxycholic acid (2.5) 11. Ursodeoxycholic acid (25)
FDU_Quartet_Metabolite_D6_20171028	绿			
FDU_Quartet_Metabolite_F7_20171028	黄			
FDU_Quartet_Metabolite_M8_20171028	红			

“中华家系” 1 号代谢物参考物质在-80 ℃条件下长期保存，采用干冰运输。外加质控按照表格中的摩尔量添加到细胞提取物中。

预期用途

“中华家系”1 号代谢物参考物质的预期用途是对代谢组检测进行质量控制和性能评价，也可用于评估和消除多批次检测中的技术噪音，为多中心、长期大队列研究的数据整合提供质量保证。采用“中华家系” 1 号代谢物参考物质进行高通量代谢组表达谱性能评价的指标包括：1)基于“中华家系” 1 号多样本的信噪比；2)基于参考数据集的相关性系数。代谢物参考物质需要和研究样本平行检测，才能保证对每个实验室、每批次数据的质量进行有效的评价。本代谢物参考物质是细胞提取物，适用于评价代谢组的上机检测及后续生物信息学分析过程。不适用于评价代谢物提取等样本前处理过程。本代谢物参考物质仅适用于科学研究。

参考数据集

“中华家系” 1 号代谢物参考数据集是样本对的相对表达值(D5/D6, D5/F7, D5/M8, D6/F7, D6/M8, F7/M8)，具体整合构建方法参考“中华家系” 1 号代谢组文章。v1.0 版本参考数据集覆盖 40-50 个差异表达代谢物。随着高通量代谢组检测技术和分析算法的进步，将定期发布参考数据集的升级版。“中华家系” 1 号代谢组参考数据集、原始数据以及质量评价工具可以通过 Quartet Data Portal 获取使用(http://chinese-quartet.org/)。

用户使用条款

“中华家系” 1 号代谢物参考物质按照“原样”提供。研究者保证本参考物质的研制：a) 完全符地区、政府和国际相关法律、法规和指导原则；b) 获得伦理委员会审批并遵守相关条款；c) 志愿者或其法定监护人已知情并签署知情同意书。研究者对“中华家系” 1 号代谢物参考物质不作任何明示或暗示的陈述或保证，包括其耐用性、储存、处置、特定用途的适用性或适销性，或不侵犯“中华家系” 1 号代谢物参考物质的第三方的所有权。物质接收者使用本参考物质涉及上述条款的，应自行承担相关风险和责任。

“中华家系” 1 号代谢物参考物质和参考数据提供开放获取和非商业使用。鼓励任何团队基于“中华家系” 1 号开放数据进行数据质量相关研究，研究不能涉及志愿者隐私和疾病风险预测。获取参考物质者需要通过 Quartet Data Portal 与复旦大学项目团队共享数据，以促进参考数据集的更新，更好地为领域服务。

如有其它问题，请联系“中华家系”1 号项目团队(quartet@fudan.edu.cn 或 http://chinese-quartet.org/)，或者项目负责人郑媛婷博士(zhengyuanting@fudan.edu.cn) 和石乐明博士(lemingshi@fudan.edu.cn)。