

# **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**

Yamil Simón-Manso,<sup>1</sup> Mark S. Lowenthal,<sup>1</sup> Lisa E. Kilpatrick,<sup>1</sup> Maureen L. Sampson,<sup>2</sup> Kelly H. Telu,<sup>3</sup> Paul A. Rudnick,<sup>1</sup> W. Gary Mallard,<sup>1</sup> Daniel W. Bearden,<sup>4</sup> Tracey B. Schock,<sup>4</sup> Dmitrii V. Tchekhovskoi,<sup>1</sup> Niksa Blonder,<sup>1</sup> Xinjian Yan,<sup>1</sup> Yuxue Liang<sup>1</sup>, Yufang Zheng<sup>1</sup>, William E. Wallace,<sup>3</sup> Pedatsur Neta,<sup>1</sup> Karen W. Phinney,<sup>1</sup> Alan T. Remaley,<sup>2</sup> and Stephen E. Stein<sup>1</sup>

1. Biomolecular Measurement Division, National Institute of Standards and Technology, Gaithersburg, Maryland, USA
2. Department of Laboratory Medicine, National Institutes of Health, Bethesda, Maryland, USA
3. Chemical Sciences Division, National Institute of Standards and Technology, Gaithersburg, MD, USA
4. Hollings Marine Laboratory, Chemical Sciences Division, National Institute of Standards and Technology, Charleston, SC, USA

Supporting Information available:

- Table S.1 contains all metabolites identified in SRM 1950 using GC-MS (MSExcel file, Table\_S1.xlsx).
- Table S.2 contains all metabolites identified in SRM 1950 using LC-MS/MS (MSExcel file, Table\_S2.xlsx).
- Table\_I\_S2 is an extended version of Table I from manuscript.
- Table S.3 contains all metabolites identified in SRM 1950 using NMR (MSWord file, Table\_S3.docx).
- Table S.4 shows the clinical analysis results (MSExcel file, Table\_S4.xls).
- The MSWord document, NIST\_SRMD\_website.docx, shows an example of the user interaction with the SRMD webpage.
- TOC , For\_TOC\_only.tif

