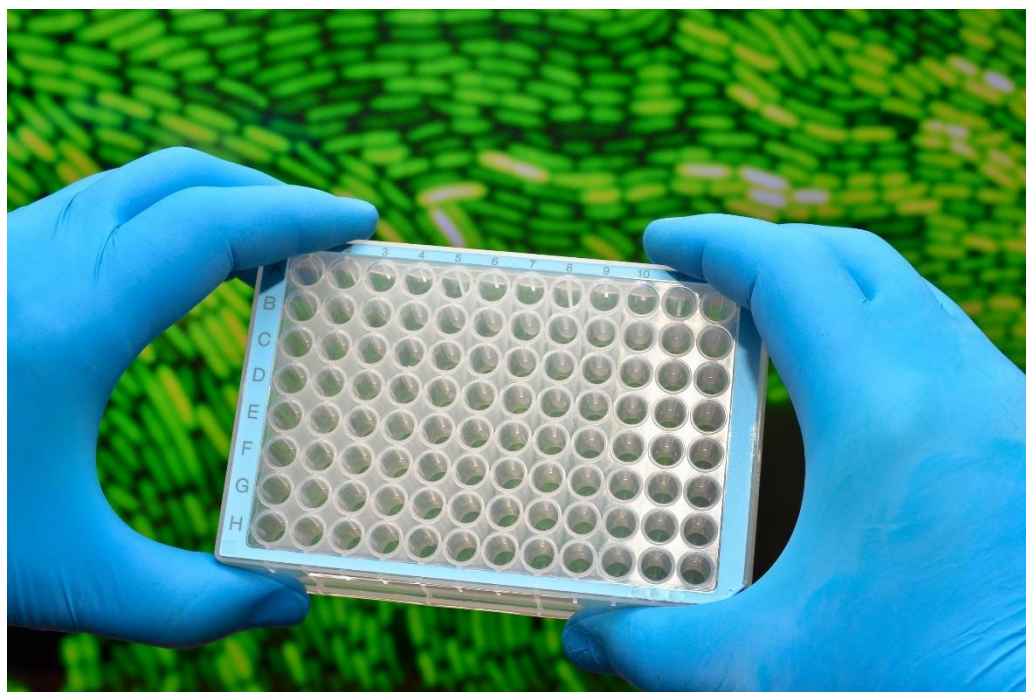


IROA MASS SPECTROMETRY METABOLITE LIBRARY STANDARDS



CONVENIENT 96-WELL FORMAT Easy storage, no glass bottles
Plated to allow row multiplexing for efficient processing

HIGH PURITY and STABLE

Supplied as 5 µg dried weight; plenty of material for multiple injections

MLSDiscovery™ SOFTWARE

Data processing, data collection and data reduction tool creates libraries in hours

Metabolite Library Standards (MLS) Available from IROA

Mass Spectrometry Metabolite Library of Standards (MSMLS) – Our “Flagship” library featuring 600 unique compounds arrayed in seven (7) 96-well plates that span a broad range of primary metabolism; 5 µg per well.

Large Scale Metabolite Library of Standards (LSMLS) - 600 unique compounds arrayed in seven (7) 96-well plates that span a broad range of primary metabolism; 1 mg per well.

Bile Acid Carnitine Sterol Metabolite Library of Standards (BACSMLS) - 96 bile acid, carnitine and sterol metabolites covering key metabolic pathways; 5 µg per well.

Fatty Acid Metabolite Library of Standards (FAMLS) - 96 unique small molecule fatty acid metabolites covering key metabolic pathways; 5 µg per well.

Organic Acid Metabolite Library of Standards (OAMLS) - 96 unique small molecule organic acid metabolites covering key metabolic pathways; 5 µg per well.

Amino Acid/Peptide Metabolite Library of Standards (AAPMLS) – 96 unique metabolites including acetylated, methylated and hydroxy amino acids and dipeptides which are building blocks of proteins in many prokaryotic and eukaryotic organisms; 5 µg per well.

Microbiome Metabolite Library of Standards (GUTMLS) – 185 unique small biochemicals that the gut microbiome produces and interacts with including bacterial, dietary and host xenobiotic metabolites; 5 µg per well.

Phytochemical Metabolite Library of Standards (PHYTOMLS) - 364 unique primary and secondary plant metabolites obtained from consuming diets containing fruits, vegetables, whole grains, legumes, nuts and plant-based beverages; 5 µg per well.

Polyphenol Metabolite Library of Standards (PPMLS) – coming soon! – 80 unique high-quality small biochemicals that have a polyphenol structure (i.e., several hydroxyl groups on aromatic rings). Polyphenols are found in many plant foods including fruits, vegetables, cereals, dry legumes, chocolate, oils, spices and some beverages, including red wine.

IROA MLS Referenced Peer-Reviewed Publications

1. Misra BB, Olivier M. High Resolution GC-Orbitrap-MS Metabolomics Using Both Electron Ionization and Chemical Ionization for Analysis of Human Plasma [published online ahead of print, 2020 Feb 10]. *J Proteome Res.* 2020;10. doi:10.1021/acs.jproteome.9b00774. PMID: 31978300
2. Vargas F, Weldon KC, Sikora N, et al. Protocol for Community-created Public MS/MS Reference Spectra Within the Global Natural Products Social Molecular Networking Infrastructure [published online ahead of print, 2020 Jan 13]. *Rapid Commun Mass Spectrom.* 2020; e8725. doi:10.1002/rcm.8725. PMID: 31930757
3. Nye LC, Williams JP, Munjoma NC, et al. A comparison of collision cross section values obtained via travelling wave ion mobility-mass spectrometry and ultra high-performance liquid chromatography-ion mobility-mass spectrometry: Application to the characterisation of metabolites in rat urine. *J Chromatogr A.* 2019 Sept ;1602:386–396. doi:10.1016/j.chroma.2019.06.056. PMID: 31285057
4. Dueñas ME, Larson EA and LEee YJ. Toward Mass Spectrometry Imaging in the Metabolomics Scale: Increasing Metabolic Coverage Through Multiple On-Tissue Chemical Modifications. *Front. Plant Sci.* 2019 July 10;860. Doi 10.3389/fpls.2019.00860. PMID: 31354754
5. Pezzatti J, González-Ruiz V, Codesido S, Gagnebin Y, Joshi A, Guillaume D, Schappler J, Picard D, Boccard J, Rudaz S. A scoring approach for multi-platform acquisition in metabolomics. *J Chromatogr A.* 2019 May 10;1592:47-54. doi: 10.1016/j.chroma.2019.01.023. Epub 2019 Jan 10. PMID: 30685186
6. González-Ruiz V, Schvartz D, Sandström J, Pezzatti J, Jeanneret F, Tonoli D, Boccard J, Monnet-Tschudi F, Sanchez JC, Rudaz S. An Integrative Multi-Omics Workflow to Address Multifactorial Toxicology Experiments. *Metabolites.* 2019 Apr 24;9(4). pii: E79. doi: 10.3390/metabo9040079. PMID: 31022902
7. Nichols CM, Dodds JN, Rose BS, et al. Untargeted Molecular Discovery in Primary Metabolism: Collision Cross Section as a Molecular Descriptor in Ion Mobility-Mass Spectrometry. *Analytical Chemistry.* 2018 Dec;90(24):14484-14492. DOI: 10.1021/acs.analchem.8b04322. PMID: 30449086
8. Pimentel G, Burton KJ, von Ah U, Bütikofer U, Pralong FP, Vionnet N, Portmann R, Vergères G. Metabolic Footprinting of Fermented Milk Consumption in Serum of Healthy Men. *J Nutr.* 2018 Jun 1;148(6):851–860. doi: 10.1093/jn/nxy053. PMID: 29788433
9. Thomason K, Babar MA, Erickson JE, Mulvaney M, Beecher C, MacDonald G. Comparative physiological and metabolomics analysis of wheat (*Triticum aestivum* L.) following post-anthesis heat stress. *PLoS ONE* 2018 June13(6): e0197919. <https://doi.org/10.1371/journal.pone.0197919>.
10. Nemkov T, Hansen KC, D'Alessandro A. A three-minute method for high throughput quantitative metabolomics and quantitative tracing experiments of central carbon and nitrogen pathways. *Rapid Commun Mass Spectrom.* 2017 Apr 30;31(8):663-673. doi: 10.1002/rcm.7834. PMID: 28195377
11. Depke T, Franke R, Brönstrup M. Clustering of MS² spectra using unsupervised methods to aid the identification of secondary metabolites from *Pseudomonas aeruginosa*. *J Chromatogr B Analyt Technol Biomed Life Sci.* 2017 Dec 15;1071:19-28. doi: 10.1016/j.jchromb.2017.06.002. Epub 2017 Jun 4. PMID: 28642031
12. González-Ruiz V, Pezzatti J, Roux A, Stoppini L, Boccard J, Rudaz S. Unravelling the effects of multiple experimental factors in metabolomics, analysis of human neural cells with hydrophilic interaction

- liquid chromatography hyphenated to high resolution mass spectrometry. J Chromatogr A. 2017 Dec 8;1527:53-60. doi: 10.1016/j.chroma.2017.10.055. Epub 2017 Oct 25. [PMID: 29106965](#)
13. Lu, X., Solmonson, A., Lodi, A. et al. The early metabolomic response of adipose tissue during acute cold exposure in mice. Sci Rep 2017 June 7; 3455. doi.org/10.1038/s41598-017-03108-x. [PMID: 27399036](#)
14. Korte AR, Stopka SA, Morris N, Razunguzwa T, Vertes A. Large-Scale Metabolite Analysis of Standards and Human Serum by Laser Desorption Ionization Mass Spectrometry from Silicon Nanopost Arrays. Anal Chem. 2016 Sep 20;88(18):8989-96. doi: 10.1021/acs.analchem.6b01186. Epub 2016 Jul 22. [PMID: 27399036](#)