MilliporeSigma

How reproducible is your data?

Plated metabolite libraries supplied by IROA Technologies, Inc.

IROA TECHNOLOGIES
...making metabolic profiling easy®

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the U.S. and Canada.

Sigma-Aldrich®
Lab & Production Materials

We now provide a complete offering of plated metabolite libraries from IROA Technologies, Inc. to better meet your research needs in mass spectometry.

- Confidently identify hundreds of metabolites
- Eliminate false discovery rates by identifying biological peaks and reducing noise
- QC/QA Retention Index aligns peaks, normalizes data and removes analytical variance
- Cost effectively build 400-600 internal standard metabolite libraries based on your own LC-MS system

TruQuant Workflow Kit

For Mass Spectrometry Metabolomics Applications

TruQuant IQQ is a high-quality quantitation system for making simultaneous accurate biological measurements on several hundred biochemicals in small quantities of biological samples.

This is achieved by

1. spiking a complex Internal Standard (WORKFLOW-A) into a biological sample to a) quantify all the biochemicals in the sample relative to their counterparts in the Internal Standard, b) suppression-correct each compound and c) normalize sample to sample variances; and
2. injecting the same well characterized Long-Term Reference Standard (WORKFLOW-B) to create a daily retention time (RT) library of all compounds to be found in the Internal Standard for reproducible ID, and to measure day-to-day (QA/QC) to assure reproducible instrument performance.

The system is completely automated using IROA ClusterFinder™ software.

Features and Benefits

IQQ:

Identify common and new metabolites with confidence

Quantify with accuracy: comprehensive correction of analytical and biological variability for all analytes

Quality control tools to ensure reproducible results

Employs isotopic peak patterns to remove artifacts and noise, thus eliminating false discovery
IROA patterns discriminate peaks of biological origin from artifactual peaks allowing the removal of false data.

Provides a complex internal standard (600+ compounds) for suppression correction – suppression-corrected values and normalized data significantly improve quantitation
A normalization factor is used to correct for source- and suppression-induced error. This factor can also be applied to normalize non-standardized features for sample size variation.

ClusterFinder™ builds libraries, identifies/quantitates compounds and normalizes the data generated
This software solution ensures better memory handling, faster file loading and complete automation of data.

Components

WORKFLOW contains the materials and tools for the analysis of 90 experimental samples includes:

- 3 vials of lyophilized Internal Standard (IS); U13C, 95% labeled (WORKFLOW-A)
- 3 vials of lyophilized Long-Term Reference Standard (LTRS); paired U13C, 95% and 5% labeled; mixed 1:1 (WORKFLOW-B)
- ClusterFinder™ software (including library of peaks in the Long-Term Reference Standard and their physical characteristics)

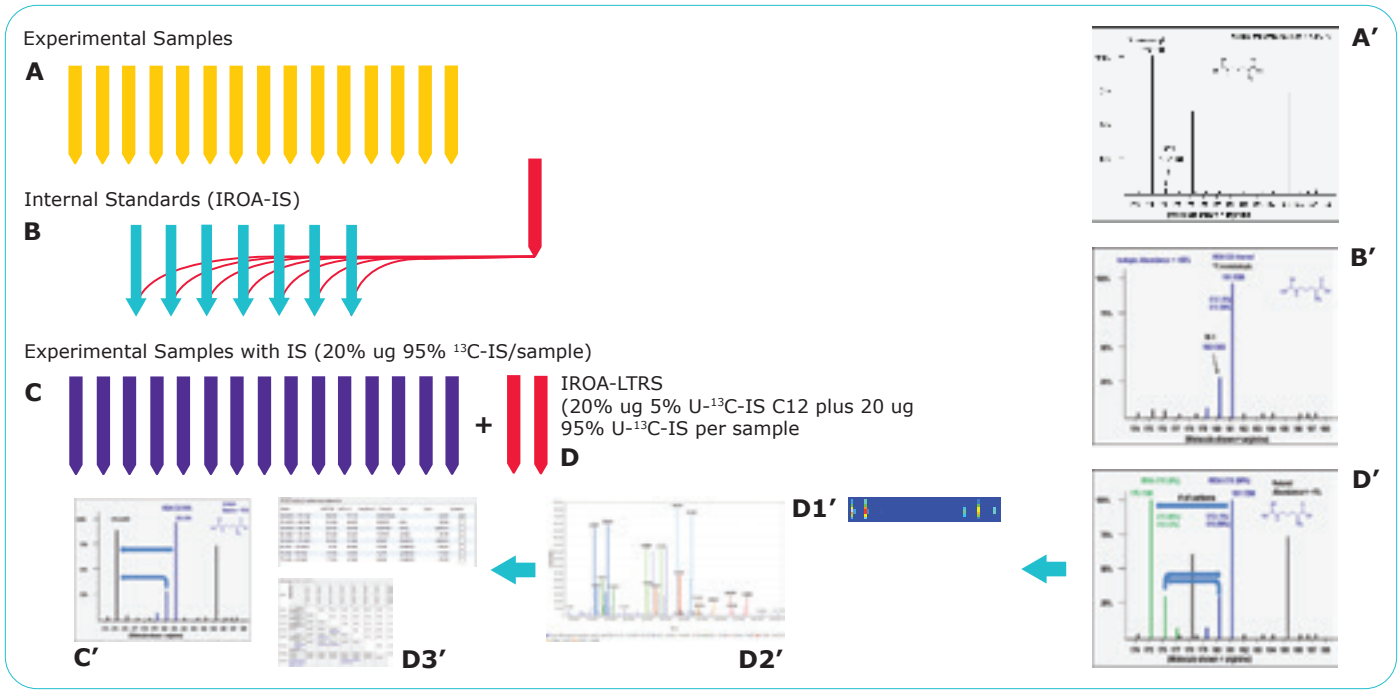
For each sample, you receive verifiable chemical identification, measurement of instrument performance, and accurate suppression-corrected data using ClusterFinder™ software.

Ordering Information

Description	Cat. No.
IROA TruQuant IQQ Workflow Kit	**WORKFLOW-1EA**

For more information:
SigmaAldrich.com/Workflow-Kit

Example of TruQuant Workflow



The IROA TruQuant IQQ workflow is based on a well-characterized, long-term reference standard (D = LTRS) and a carefully matched internal standard (B = IS) to provide instrument and process QA/QC, as well as validated compound identification and quantitation.

Experimental samples (A), such as plasma, urine, or cells, are mixed with a complex internal standard (IS) of more than 600 compounds (B), which is fully labeled with 95% U-13C (B', arginine shown here). Experimental/IS samples are analyzed using LC-MS, injecting the LTRS (D) intermittently, approximately after every 10 samples. The LTRS has the same concentration as the IS, and is chemically identical, but contains a 1:1 mixture of fully labeled 5% and 95% U-13C metabolites, producing a U-shaped pattern of carbon envelopes (D').

Over 1000 peaks can be detected in the IROA-LTRS

The relative height of M+1, the relative height of M-1, and the distance between the monoisotopic peaks all provide confirmation of the number of carbons in each molecule, resulting in a triply redundant quality control check point.

The IROA peaks represent actual compounds, fragments and adducts, which are readily discriminated from unsigned artifacts and noise, and removed from the data, thereby eliminating false discoveries. As a composite sample, analytical and sample-to-sample variance is removed, identical compounds (labeled with either 5% or 95% U-13C) experience the same ionization efficiency and suppression during MS analysis.

Following analysis, the resulting IROA-LTRS dictionary of compounds is used to identify compounds in the IROA-IS, thus saving time, effort and related costs. The IROA-IS and ClusterFinder™ software are used to co-locate, identify, and quantitate 400 to 600 biochemicals in experimental samples, depending upon the chromatographic mode(s) employed. The characteristics of each compound in the IROA-IS allow the calculation of a suppression-corrected area for each compound.

Unambiguous ID and quantitation (MS2) in a single injection

Complete identification of compounds is achieved with the addition of IM or SWATH. The IROA IM peaks retain their patterns perfectly because all IROA isotopomers share the same CCS (D'). In IROA MSMS fragmentation, such as SWATH, the IROA peaks retain their patterns (D2') because wide windows are used. Since all fragments retain their IROA character, their formula and the relationships between them (D3') are determinable.

Mass Spectrometry Metabolite Library of Standards

MSMLS™ (Mass Spectrometry Metabolite Library of Standards) and LSMLS™ (Large Scale Metabolite Library of Standards) collections of high-quality small biochemical are most commonly used to provide retention times and spectra for key metabolic compounds, help optimize mass spectrometry analytical protocols, qualify and quantify mass spectrometry sensitivity, and perform NMR, functional cellular assays, phenotypic screening and limit of detection. These are high purity (>95%) compounds supplied in an economical, ready-to-use format. Suitable for manual and automated workflows.

Features and Benefits

Compounds

Unique small molecule metabolites are organized in a 96-well format according to solubility. A broad metabolite spectrum of key primary metabolites and intermediates covers key metabolic pathways, including the following classes of compounds:

- Carboxylic acids and amino acids
- Biogenic amines and polyamines
- Nucleotides, coenzymes, and vitamins
- Mono- and disaccharides
- Fatty acids, lipids, steroids, and hormones

MSMLS™ library features 619 unique metabolites as 5 µg dried weight

LSMLS™ library features 504 unique metabolites as 1 mg dried weight

Convenient

- High-purity metabolites; pre-weighed solubilized in either water, 40% aqueous methanol, or 100% ethanol; and supplied dried

MLSDiscovery™ software tool is provided to support the extraction, manipulation, and storage of the data generated when using the MSMLS™ and LSMLS™ libraries.

Ordering Information

Description	Cat. No.
Mass Spectrometry Metabolite Library	**MSMLS-1EA**
Large Scale Metabolite Library	**LSMLS-1EA**
Large Scale Metabolite Library (International)	**LSMLSINT-1EA**

For more information, visit
SigmaAldrich.com/MSMLS
SigmaAldrich.com/LSMLS

Individual Plated Libraries

Features and Benefits

Individual MSMLS and LSMLS plate compounds can also be ordered separately to better fulfill your research needs. These compounds are conveniently provided at 5 µg per well, enough for multiple injections. Compounds can either be used as standards and injected individually or a strategy may be employed to pool compounds by row to allow multiple mixtures to be analyzed per injection. For more information, please refer to the product information sheet.

The complete plate map with name, Parent CID, molecular formula, molecular weight, CAS, ChEBI, HMBD ID, PubChem Compound, and Substance ID are provided with the software download.

To view a complete list of compounds in the library, visit **SigmaAldrich.com/MSMLS-Online-Plate-Map**

MLSDiscovery™ software package, a user manual and video instructions are provided.

To download the software package, visit **SigmaAldrich.com/mlsdiscovery**.

To view the MLSDiscovery™ Video visit: **MLSDiscovery™ Tutorial Video**.

Ordering Information

Description	Cat. No.
MSMLS Plate 1 (Water Soluble)	**MSMLS01-1EA**
LSMLS Plate 1 (Water Soluble)	**LSMLS01-1EA**
MSMLS Plate 2 (Water Soluble)	**MSMLS02-1EA**
LSMLS Plate 2 (Water Soluble)	**LSMLS02-1EA**
MSMLS Plate 3 (Water Soluble)	**MSMLS03-1EA**
LSMLS Plate 3 (Water Soluble)	**LSMLS03-1EA**
MSMLS Plate 4 (Water Soluble)	**MSMLS04-1EA**
LSMLS Plate 4 (Water Soluble)	**LSMLS04-1EA**
MSMLS Plate 5 (Water Soluble)	**MSMLS05-1EA**
LSMLS Plate 5 (Water Soluble)	**LSMLS05-1EA**
MSMLS Plate 6 (Lipophilic)	**MSMLS06-1EA**
LSMLS Plate 6 (Lipophilic)	**LSMLS06-1EA**
MSMLS Plate 7 (Lipophilic)	**MSMLS07-1EA**
LSMLS Plate 7 (Lipophilic)	**LSMLS07-1EA**

Libraries for Mass Spectrometry

Features and Benefits

Compounds are pre-weighed and provided at 5 µg per well, enough for multiple injections, arranged in a 96-well polypropylene plate with alphanumerically assigned positions, suitable for manual and automated workflows.

Compounds can either be used as standards and injected individually or a strategy may be employed to pool compounds to allow multiple mixtures to be analyzed per injection.

MLSDiscovery™ software tool is provided to support the extraction, manipulation, and storage of the data generated when using authentic libraries of metabolite standards supplied by IROA Technologies. The software includes a User Manual and training videos.

To download the software package, visit SigmaAldrich.com/MLSDiscovery.

Components

- 1 polypropylene plate in 96 well format
- 5 µg (dried weight) of each metabolite
- Polypropylene deepwell (1.2 mL, total volume per well) plates (MasterBlock®, Greiner #780215) in combination with seals (VIEWseal™, Greiner #676070)
- Plate map
- Alphanumeric assigned position
- Descriptors: Name, Parent CID, KEGG ID where available or ChemSpider ID, molecular formula, molecular weight, CAS, ChEBI, HMDB ID/YMDB ID, PubChem Compound and Substance ID, Metlin ID

BACS Metabolite Library of Standards

- Bile acids
- Carnitines
- Sterols

Fatty Acid Metabolite Library of Standards

- Short chain
- Medium chain
- Long chain
- Very long chain
- Saturated and unsaturated
- Branched

Organic Acid Metabolite Library of Standards

- Carboxylic acids
- Benzoic acids
- Keto acids
- Hydroxy acids

Ordering Information

Description	Cat. No.
Bile Acid/Carnitine/Sterol Metabolite Library	**BACSMLS-1EA**
Fatty Acid Metabolite Library	**FAMLS-1EA**
Organic Acid Metabolite Library	**OAMLS-1EA**

For more information, visit
SigmaAldrich.com/BACSMLS
SigmaAldrich.com/FAMLS
SigmaAldrich.com/OAMLS

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Lab & Production Materials

MilliporeSigma
400 Summit Drive
Burlington, MA 01803

SigmaAldrich.com

Find all IROA Technologies Libraries for Metabolic Profiling here: **SigmaAldrich.com/IROA**

To place an order or receive technical assistance in the U.S. and Canada, call toll-free 1-800-645-5476
For other countries across Europe and the world, please visit: **SigmaAldrich.com/offices**
For Technical Service, please visit: **SigmaAldrich.com/techservice**

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