ONCOMETABOLITE LIBRARY OF STANDARDS (ONCOMLS)

Cat No. ONCOMLS

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

IROA TECHNOLOGIES
...making metabolic profiling easy®

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ONCOMLS™ (Oncometabolite Library of Standards) is a collection of 96 high purity (>95%) compounds supplied in an economical, ready-to-use format. These standards are most commonly used to provide retention times and spectra for these key metabolic compounds, help optimize mass spectrometry analytical protocols, and qualify and quantify mass spectrometry sensitivity and limit of detection.

Oncometabolites are intracellular messengers produced by cancer cells and non-cancer cells that are involved in tumor growth or survival, playing a key role in shaping the tumor environment including the regulation of immune cells in cancer.

ONCOMLS comes with **MLSDiscovery™**, a software tool to support the extraction, manipulation, and storage of the data generated when using libraries of authentic metabolite standards produced by IROA Technologies.

Features and Benefits

Compounds

ONCOMLS contains 96 unique small molecule metabolites covering key metabolic pathways, including the following classes of compounds:

- Amines
- Amino acids, peptides, and analogues
- Bile acids, alcohols and derivatives
- Carbohydrates and carbohydrate conjugates
- Carboxylic acids and derivatives
- Fatty acids and conjugates
- Fatty Acyls and amides
- Nucleosides
- Steroids

Convenient

- High purity metabolites, pre-weighed, supplied dried, 5µg per compound
- Ideal for mass spectrometry metabolomics applications

Formatted

ONCOMLS contains 96 unique small molecule metabolites.

- Arrayed in (1) one 96-well plate
    - Greiner MASTERBLOCK® #786201 polypropylene deep-well; total volume per well = 0.5mL in combination with seals, Agilent 24214-001 PeelablePlateLoc Heatseals
- Suitable for manual and automated workflow

Software

MLSDiscovery is distributed with IROA Mass Metabolite Standards (MLS) and is tailored to help build a mass spectral library using the analytical conditions that are normally employed in the user laboratory. MLSDiscovery collects spectra, retention time, mass and relative intensity information for compounds, fragments and adducts.

The requirements of the program are that:

1) The computer should have at least 8 GB of RAM; Windows 10 or higher.
2) Data files must be able to be converted to mzXML format.

To facilitate the use of the program, the MLSDiscovery User Manual is provided to help you run through the standard workflow.

Plate Map

The library compounds are arranged in (1) one 96-well polypropylene rack with alphanumeric assigned positions. Please refer to plate map excel sheet that comes with the library for compound locations and identifiers.

Occasionally the map plate will change due to the availability of compounds. Although we try to make sure that the compounds of each row have distinct molecular weights and can be multiplexed, users should refer to the plate map before proceeding.

The excel plate map contains descriptors and represents information gathered from multiple databases and therefore may contain errors. Please report any discrepancies. A typical plate map may include the following:

Plate number - total number of plates is one (1).
Plate row letter - rows are marked A-H.
Plate column number - columns are numbered 1-12.
Primary compound name – from HMDB, KEGG or PubChem where available.

SMILES – from https://pubchem.ncbi.nlm.nih.gov/search/help_search.html#Smiles SMILES -- **S**implified **M**olecular **I**nput **L**ine **E**ntry **S**ystem, a chemical structure *line notation* (a typographical method using printable characters) for entering and representing molecules. SMILES strings can be imported or exported from many molecular editors.

Inchikey – a 27-character long identifier based on The IUPAC International Chemical Identifier (InChI™).

Molecular formula – formula of neutral form without salts or water (except in cases where compound has an innate positive charge).

KEGG ID or ChemSpider ID (CSID) – KEGG number where available, otherwise CSID provided.

CAS ID – a unique numerical identifier assigned by Chemical Abstracts Service, a division of the American Chemical Society, to every chemical substance described in the open scientific literature.

HMDB/YMDB ID – Human Metabolome Data Base or Yeast Metabolome Data Base ID number. Either the chemical name or the CAS number was used to search for the HMDB/YMDB ID entry.

Monoisotopic mass

PC CID – PubChem Compound Database ID; HMDB, KEGG or CAS number used for PC CID lookup.

PC SID – PubChem Substance Database ID; PC CID, KEGG, Vendor ID, or CAS number used for PC SID lookup.

CHEBI – Chemical Entities of Biological Interest (ChEBI); HMDB, KEGG or CAS number used for ChEBI lookup.

Class of compound

Supplier compound name

Supplier URL

Supplier Cat. No.

Preparation Instructions

Spin down the contents of each 96-well plate in a 96-well plate holder centrifuge, 3000rpm, for 2-3 minutes, to ensure any loose material is deposited at the bottom of each well.

Note: Although some of the compounds as seen in the plate wells will be colorless, many dried compounds naturally exhibit color.

ONCOMLS compounds are conveniently provided at 5 µg per well, enough for multiple injections. The compounds can either be used as standards and injected individually or mixed in such a way that the entire library may be examined with reasonable efficiency. The compounds in each row *may* all have unique masses; mixing compounds by row *may* allow multiple compounds to be analyzed per injection*.

The following are suggestions and dependent on user chromatography and instrumentation.

1) Individual injections. As standards, each well represents a single compound; the entire library may be examined in great detail in 96 injections for each of the unique compounds. (Volumes of 250 µL may be considered).
2) Simple multiplex injections. If each row is pooled, then the entire collection may be analyzed in 8 injections of simple mixtures. Keep the well volume to 100 µl or less to prevent loss due to dilution and take 5-10 µl of each well for the pooled sample, then inject 2, 4, or 6 µl of the pooled material as needed.
   *Note: Be sure to check the individual masses across plate rows to ensure these compounds can be separated with the chromatographic system employed.

Solubilization and compound preparation procedure

The following are suggestions and dependent on user chromatography and instrumentation.

1) Use high-quality solvents. Compounds in Plate 1 Rows A-D can be solubilized using Ethanol; compounds in Rows E-H are Water soluble. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.
2) Pool compounds as desired for multiplexing. Again, be sure to check the compound masses you wish to multiplex on the plate map to ensure you can adequately separate the compounds using your chromatographic system prior to pooling.

Precautions and Disclaimer

The ONCOMLS product is for laboratory research use only. Wear safety glasses and handle with gloves. Avoid contact with skin and eyes. Please consult the Safety Data Sheet for safe handling practices and hazards information.

Storage/Stability

Store plate at -20° C. Once diluted the plate should be resealed and kept at -20° C or -80° C for long-term storage and protected from moisture and light. Avoid repeated freeze/thaw cycles.

Metabolite Libraries Available from IROA

MS Metabolite Library of Standards (MSMLS) - Over 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) - Over 500 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.

Oncometabolite Library of Standards (ONCOMLS) – 96 unique small oncometabolites produced by cancer cells and non-cancer cells that are involved in tumor growth or survival; 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 (ONCOMLS) – 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.

Legal Information

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MasterBlock is a trademark of Greiner Bio-One GmbH.

Acknowledgements

We gratefully acknowledge usage of the following websites and databases for their publicly accessible information.

Database	Website
The Human Metabolome Database (HMDB), v 2.5 [1-3]	http://www.hmdb.ca/
The Yeast Metabolome Database [4]	http://www.ymdb.ca/
Chemical Entities of Biological Interest (ChEBI) [5]	https://www.ebi.ac.uk/chebi/
Chemical Abstracts Service (CAS) REGISTRY Database [6]	https://www.cas.org/
Kyoto Encyclopedia of Genes and Genomes (KEGG) [7]	http://www.genome.jp/kegg/
The PubChem Compound and Substance Database [8]	https://pubchem.ncbi.nlm.nih.gov/

References

[1] Wishart DS, Tzur D, Knox C, et al., HMDB: the Human Metabolome Database. Nucleic Acids Res. 2007 Jan;35 (Database issue):D521-6. 17202168.

[2] Wishart DS, Knox C, Guo AC, et al., HMDB: a knowledgebase for the human metabolome. Nucleic Acids Res. 2009 37(Database issue):D603-610. 18953024.

[3] Wishart DS, Jewison T, Guo AC, Wilson M, Knox C, et al., HMDB 3.0 — The Human Metabolome Database in 2013. Nucleic Acids Res. 2013. Jan 1;41(D1):D801-7. 23161693.

[4] Jewison T, Neveu V, Lee J, Knox C, Liu P, Mandal R, Murthy RK, Sinelnikov I, Guo AC, Wilson M, Djoumbou Y and Wishart DS. YMDB: The Yeast Metabolome Database. Nucleic Acids Res. 2012 Jan; 40(Database Issue): D815-20 PubMed: 22064855.

[5] Hastings J, de Matos P, Dekker A, Ennis M, Harsha B, Kale N, Muthukrishnan V, Owen G, Turner S, Williams M, Steinbeck C. The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Res. 2013. Jan;41(Database issue):D456-63. doi: 10.1093/nar/gks1146. Epub 2012 Nov 24.

[6] CAS REGISTRY, Division of the American Chemical Society

[7] Kanehisa M, Goto S. "KEGG: Kyoto Encyclopedia of Genes and Genomes". Nucleic Acids Res. 2000 28 (1): 27–30. doi:10.1093/nar/28.1.27. PMC 102409.PMID 10592173.

[8] Kim S, Thiessen PA, Bolton EE, Chen J, Fu G, Gindulyte A, Han L, He J, He S, Shoemaker BA, Wang J, Yu B, Zhang J, Bryant SH. PubChem Substance and Compound databases. Nucleic Acids Res. 2016 Jan 4; 44(D1):D1202-13. Epub 2015 Sep 22 [PubMed PMID: 26400175] doi: 10.1093/nar/gkv951 [Free Full Text at Oxford Journals]

Selected IROA MLS Referenced Peer-Reviewed Papers

Zarth AT, Magallanes López AM. A New UHPLC-UV-MS Method for Detection and Identification of Bioactive Compounds. J AOAC Int. 2025 Apr 18:qsaf039. doi: 10.1093/jaoacint/qsaf039. Epub ahead of print. PMID: 40249097.

Monteiro J, Ple K, Lefèvre A, Marzag H, Blondeau B, Dupuy C, Oury A, Routier S, Nadal-Desbarats L, Emond P. Evaluation of a New Chemical Label *BASA*: A Comparison with Gold Standards. Anal Chem. 2025 Jul 22;97(28):14956-14963. doi: 10.1021/acs.analchem.5c00096. Epub 2025 Jul 13. PMID: 40653635.

Xue, B., Bi, X., Dong, Z. *et al.* Deep spectral component filtering as a foundation model for spectral analysis demonstrated in metabolic profiling. Nat Mach Intell. 2025; (7):743–757. doi:10.1038/s42256-025-01027-5

Takeda H, Matsuzawa Y, Takeuchi M, Takahashi M, Nishida K, Harayama T, Todoroki Y, Shimizu K, Sakamoto N, Oka T, Maekawa M, Chung MH, Kurizaki Y, Kiuchi S, Tokiyoshi K, Buyantogtokh B, Kurata M, Kvasnička A, Takeda U, Uchino H, Hasegawa M, Miyamoto J, Tanabe K, Takeda S, Mori T, Kumakubo R, Tanaka T, Yoshino T, Okamoto M, Takahashi H, Arita M, Tsugawa H. MS-DIAL 5 multimodal mass spectrometry data mining unveils lipidome complexities. Nat Commun. 2024 Nov 28;15(1):9903. doi: 10.1038/s41467-024-54137-w. PMID: 39609386; PMCID: PMC11605090.

Nemkov T, Stauffer E, Cendali F, Stephenson D, Nader E, Robert M, Skinner S, Dzieciatkowska M, Hansen KC, Robach P, Millet GY, Connes P, D'Alessandro A. Long-Distance Trail Running Induces Inflammatory-Associated Protein, Lipid, and Purine Oxidation in Red Blood Cells. bioRxiv [Preprint]. 2025 May 19:2025.04.09.648006. doi: 10.1101/2025.04.09.648006. PMID: 40291720; PMCID: PMC12027326.

Diamantidou D, Sampsonidis I, Liapikos T, Gika H, Theodoridis G. Liquid chromatography-mass spectrometry metabolite library for metabolomics: Evaluating column suitability using a scoring approach, *J. Chromatogr. A.* 2023 Feb 8;1690:463779. doi: 10.1016/j.chroma.2023.463779. Epub 2023 Jan 11. PMID: 36681007

Yap TA, Daver N, Mahendra M, Zhang J, Kamiya-Matsuoka C, Meric-Bernstam F, Kantarjian HM, Ravandi F, Collins ME, Francesco MED, Dumbrava EE, Fu S, Gao S, Gay JP, Gera S, Han J, Hong DS, Jabbour EJ, Ju Z, Karp DD, Lodi A, Molina JR, Baran N, Naing A, Ohanian M, Pant S, Pemmaraju N, Bose P, Piha-Paul SA, Rodon J, Salguero C, Sasaki K, Singh AK, Subbiah V, Tsimberidou AM, Xu QA, Yilmaz M, Zhang Q, Li Y, Bristow CA, Bhattacharjee MB, Tiziani S, Heffernan TP, Vellano CP, Jones P, Heijnen CJ, Kavelaars A, Marszalek JR, Konopleva M. Complex I inhibitor of oxidative phosphorylation in advanced solid tumors and acute myeloid leukemia: phase I trials. Nat Med. 2023 Jan;29(1):115-126. doi: 10.1038/s41591-022-02103-8. Epub 2023 Jan 19. PMID: 36658425; PMCID: PMC11975418.

Patrick M, Gu Z, Zhang G, Wynn RM, Kaphle P, Cao H, Vu H, Cai F, Gao X, Zhang Y, Chen M, Ni M, Chuang DT, DeBerardinis RJ, Xu J. Metabolon formation regulates branched-chain amino acid oxidation and

homeostasis. Nat Metab. 2022 Dec;4(12):1775-1791. doi: 10.1038/s42255-022-00689-4. Epub 2022 Nov 28. PMID: 36443523; PMCID: PMC11977170.

Fraisier-Vannier O, Chervin J, Cabanac G, et al. MS-CleanR: A Feature-Filtering Workflow for Untargeted LC-MS Based Metabolomics. *Anal Chem*. 2020;92(14):9971-9981. doi:10.1021/acs.analchem.0c01594. PMID: 32589017

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

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

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

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

Pezzatti J, González-Ruiz V, Codesido S, Gagnebin Y, Joshi A, Guillarme 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

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