Technical Bulletin

Amino Acid/Peptide Metabolite Library of Standards

Supplied by IROA Technologies

Catalog Number AAPMLS

Product Description

The **AAPMLS™** Library (Amino Acid/Peptide Metabolite Library of Standards) is a collection of high-quality small biochemicals that the gut microbiome produces and interacts with, including bacterial, dietary, and host xenobiotic metabolites. These are high purity (>95%) compounds supplied in an economical, ready-to-use format.

The library is most commonly used to provide retention times and spectra for key metabolic compounds, help optimize analytical mass spectrometry protocols, and qualify and quantify mass spectrometry sensitivity and limit of detection.

The library is intended to be used for mass spectrometry metabolomics applications and provides a broad representation of primary metabolism.

AAPMLS comes with MLSDiscovery™, a software tool to support the extraction, manipulation, and storage of the data generated when using the AAPMLS.

Components

AAPMLS contains 168 high quality peptides and amino acids and derivatives metabolites covering key metabolic pathways, including the following classes of compounds:

- Acetylated, methylated and hydroxyl amino acids
- Dipeptides

These compounds include modified amino acids and dipeptides which are building blocks of proteins in many prokaryotic and eukaryotic organisms. Proteins are digested to dipeptides and amino acids. Dipeptides have many functions including antioxidation and controlling cellular pH and their absorption takes place through a separate mechanism and occurs at a greater rate than amino acids.

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

The plate map contains descriptors and represents information gathered from multiple databases. We try to ensure the accuracy of the data, but it may contain errors. We suggest that the information provided is carefully reviewed. To help build a better database, please report any discrepancies.

AAPMLS includes:

- 2 polypropylene plates in 96-well format. The plates are polypropylene deep-well (1.2 mL, total volume per well) plates (MasterBlock®, Greiner Number 780215) in combination with seals (VIEWseal™, Greiner Number 676070)
- 5 µg (dried weight) of each metabolite
- Plate map
- Alphanumeric assigned position

- Descriptors:
    - Name
    - Parent CID
    - KEGG ID where available or ChemSpider ID
    - Molecular formula
    - Molecular mass
    - CAS Registry number
    - ChEBI
    - HMDB ID/YMDB ID
    - PubChem Compound and Substance ID
    - Metlin ID

Precautions and Disclaimer

For R&D Use Only. Not for drug, household, or other uses. Please consult the Safety Data Sheet for information regarding hazards and safe handling practices.

Storage/Stability

Store the plates at –20 °C. The product is shipped on dry ice.

Once the metabolites are dissolved, the plates should be resealed and kept at –20 °C or –80 °C for long-term storage and protected from light. Avoid repeated freeze/thaw cycles.

Preparation Instructions

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

Compounds can be solubilized using high-quality water. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.

Pool compounds for multiplexing. Be sure to check the plate map to ensure one can adequately separate the compounds using the chromatographic system prior to pooling.

Procedure

The compounds of the AAPMLS library 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. Mixing compounds by row mixtures allows multiple compounds to be analyzed per injection. Again, be sure to check the plate map to ensure one can adequately separate the compounds using the chromatographic system prior to pooling.

The following are only suggestions and depend 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 with several injections, one for each of the unique metabolites (Volumes for each well of 250 µL may be considered).
2. Simple multiplex injections – If the rows of each plate are pooled, then the entire collection may be analyzed with 8 injections of simple mixtures. Keep the total volume for each well to 100 µL or less to prevent loss due to dilution. 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.

References

1. Wishart, D.S. et al., HMDB: the Human Metabolome Database. Nucleic Acids Res., 2007, Jan; 35 (Database issue):D521-6. 17202168.
2. Wishart, D.S. et al., HMDB: a knowledge base for the human metabolome. Nucleic Acids Res., 2009, 37 (Database issue):D603-610. 18953024.
3. Wishart, D.S. 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., et al., YMDB: The Yeast Metabolome Database. Nucleic Acids Res. 2012 Jan; 40(Database Issue): D815-20 PubMed: 22064855.
5. Hastings, J. et al., The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Res., 2013.
6. CAS REGISTRY, Division of the American Chemical Society
7. Kanehisa, M., and 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. Tautenhahn, R. et al., An accelerated workflow for untargeted metabolomics using the METLIN database. Nature Biotechnology, 2012, 30: 826–828. doi:10.1038/nbt.2348.
9. Smith, C.A. et al., METLIN: a metabolite mass spectral database. The Drug Monit., 2005, 27 (6): 747–51. doi:10.1097/01.ftd.0000179845.53213.39. PMID 16404815.
10. Kim, S., et al., 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.

Notice

We provide information and advice to our customers on application technologies and regulatory matters to the best of our knowledge and ability, but without obligation or liability. Existing laws and regulations are to be observed in all cases by our customers. This also applies in respect to any rights of third parties. Our information and advice do not relieve our customers of their own responsibility for checking the suitability of our products for the envisaged purpose.

The information in this document is subject to change without notice and should not be construed as a commitment by the manufacturing or selling entity, or an affiliate. We assume no responsibility for any errors that may appear in this document.

Contact Information

For the location of the office nearest you, go to SigmaAldrich.com/offices.

Technical Service

Visit the tech service page on our web site at SigmaAldrich.com/techservice.

Standard Warranty

The applicable warranty for the products listed in this publication may be found at SigmaAldrich.com/terms.