Technical Bulletin

Phytochemical Metabolite Library of Standards

Supplied by IROA Technologies

Catalog Number PHYTOMLS

Product Description

The **PHYTOMLS™** Library (Phytochemical Metabolite Library of Standards) is a collection of high-quality phytochemicals produced by many edible plants. 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.

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

Components

PHYTOMLS contains 364 unique primary and secondary plant metabolites, covering Key metabolic pathways, including the following classes of compounds:

- Terpenes
- Phytosterols
- Flavonoids
- Phenolic acids
- Tannins
- Stilbenes
- Lignans
- Carotenoids

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 weights 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.

PHYTOMLS includes:

- 4 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 weight
    - 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.

Preparation Instructions

The following are suggestions and dependent on user chromatography and instrumentation

Use high-quality solvents. Compounds in Plates 1 and 2 can be solubilized using Ethanol. Compounds in Plate 3 (all compounds) and Plate 4 Rows A-D are soluble in Water. Compounds in Plate 4 Rows E-H are soluble in Methanol. Pipet liquid up and down in the well 2-3 times to facilitate solubilization.

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.

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.

Procedure

The compounds of the PHYTOMLS 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 may allow multiple compounds to be analyzed per injection. Be sure to check the plate map to ensure you can adequately separate the compounds using your chromatographic system prior to pooling.

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 364 injections for each of the unique compounds. (Volumes of approximately 250 µL may be considered).
2. Simple multiplex injections: If the rows of each plate are pooled, then the entire collection may be analyzed in 31 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.

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.

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