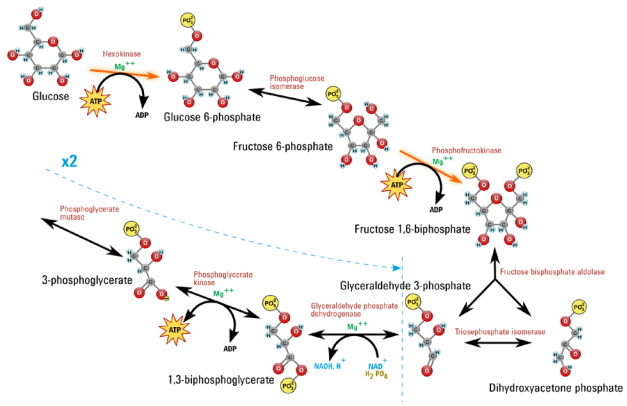
TARGETED METABOLOMICS ANALYSIS AT YOUR FINGERTIPS

Agilent Metabolomics dMRM Database and Method

Routine analysis of central carbon pathway metabolites

Targeted metabolomics experiments based on Triple Quadrupole LC/MS can be used to identify altered reactions and disrupted pathways within a defined group of metabolites in a cell, tissue or organism. Depending on the size of the target metabolite group, method development can be very time consuming and requires availability of a wide range of standards to optimize MRM transitions and retention times.

The metabolomics dynamic MRM database and method for >215 metabolites in the central carbon pathway enables straightforward implementation of a targeted metabolomic method in your research lab. Relying on Agilent's 1290 Infinity II Series LC and 6400 series LC/MS systems, the ion-pairing LC/MS method enables effective separation of key compounds with stable retention times. The compound database with MRM transitions was developed and curated together with the Rosebrock lab, a leading lab in the metabolomics field, for generating highest quality results.



Glycolysis Pathway

The Metabolomics dMRM Database and Method includes:

- Curated database with >215 compounds from central carbon metabolism pathways
- Optimized MRM transitions for all compounds in the database
- Retention times for all compounds in the database
- Quick-start guide with example data and familiarization exercises
- Method setup guide with a recommended LC/MS acquisition method
- Technical note with typical results

Learn more
www.agilent.com/chem/dmrm

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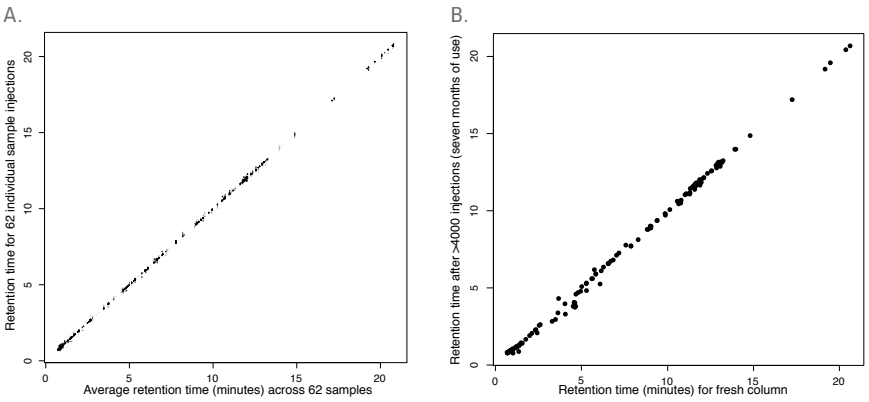
Straightforward method implementation

- Curated database eliminates the need to develop MRM transitions for a large numbers of compounds.
- Method guidance enables quick implementation of a dMRM screening method for all compounds in the database.
- Robust ion-pairing method provides superior separation and stable retention times.



Retention times (RTs) are very stable with this method. A. RT versus average RT for 62 different yeast extracts analyzed over 3 days B. RTs in yeast extract analyzed before and after 4000 injections of biological samples.

Extensive pathway coverage using targeted analysis

The dMRM database and method are part of Agilent's comprehensive metabolomics workflows and results are supported in Agilent's leading software workflow including Mass Profiler Professional and Pathway Architect. Compounds in the database include a wide range of compound classes from central carbon metabolism, including organic acids, sugars, sugar phosphates, and nucleotides.

Database curation produces high quality results

Each curated database entry includes:

- Compound common name
- MRM transitions (precursor and product *m/z*)
- Fragmentor voltage
- Collision energy
- Retention time and retention time window
- Unit mass of neutral molecule
- Molecular formula
- CAS number of the native compound

Complete workflow solutions from Agilent

Agilent MassHunter data acquisition and analysis software lets you quickly implement targeted screening methods, which you can modify to meet your future needs.

The Agilent 1290 Infinity II LC system and Agilent 6400 Series Triple Quadrupole LC/MS systems are proven choices for quantitative applications, giving you unmatched separation performance, superior sensitivity, renowned reliability, and overall system robustness.

Best-in-class application consulting and a large portfolio of sample preparation products, LC column phases, and other consumables round off Agilent's complete workflow solution.

Ordering information

Product Description	Part Number
Agilent Metabolomics dMRM Database and Method • Database with >215 compounds from the central carbon pathway • Optimized MRM transitions for >215 compounds • Retention times for >215 compounds • Screening methods for analysis of all compounds in database • Quick Start Guide • Method Setup Guide • Analysis guide with sample preparation information • Database content list • Related application and technical notes	G6412AA

Recommended Instrument Configuration and Consumables

Product Description	Part Number
1290 Infinity II Flexible Pump	G7104A
1290 Infinity II Multisampler	G7167B
Agilent Infinity Sample Cooler	G7167B #100
1290 Infinity II Multicolumn Thermostat	G7116B
Valve drive for 1290MCT	G7116B #058
2 pos/6 port ultra high pressure (1200 bar) valve head	5067-4117
ZORBAX RRHD Extend-C18, 2.1 x 150 mm, 1.8 µm	759700-902
UHPLC Grd, Extend-C18,2.1 mm, 1.8 µm, 3pk	821725-907

The following are required but not included with the database:

- Agilent 1290 Infinity II LC system – see Table for configuration listing major compounds
- Agilent 6460/6470 Series Triple Quadrupole LC/MS system
- Agilent MassHunter acquisition software B.06 or higher and Windows 7 64-bit
- Agilent MassHunter quantitative analysis software B.07 or higher

To learn more about Agilent metabolomics tools, call 800-227-9770 (in the United States or Canada) or visit
www.agilent.com/chem/dmrm

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