TMIC
The Metabolomics Innovation Centre

www.metabolomicscentre.ca

NMR Metabolomic Analysis Kit
for Plasma, Serum and CSF

Fast, High-throughput, Fully Quantitative

TMIC NMR Metabolomics Analysis Kit for Plasma, Serum and cerebrospinal fluid (CSF) provides all the reagents, standards and methods to process samples, acquire the NMR spectra and automatically profile the metabolites in three simple steps. Each kit can be used for metabolomic profiling of up to 40 samples.

Sample processing is simple and takes less than 15 minutes to complete. After Processing, the sample is transferred to a 3 mm or 5 mm tube for NMR acquisition. The kit provides acquisition methods for maximum compatibility with Varian/Agilent or Bruker instruments. Typical acquisition time is 20 minutes. Spectra can be collected on 500 MHz, 600 MHz and 700 MHz spectrometers.

The Bayesil software application provided with the kit, is a web-based tool developed by TMIC for deconvolution of complex NMR spectra and automatic profiling from a variety of aqueous samples (e.g., serum, plasma, CSF). The results are fully quantitative enabling the identification of up to 47 metabolites in the test samples. The library is regularly updated by TMIC scientific team.

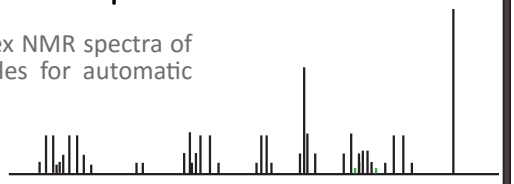
Two application modes are available depending on the level of accuracy required. In fast processing mode Bayesil can interpret the spectra in only two minutes. More accurate processing can be obtained by extending the sample processing time to seven minutes. The metabolomics analysis results are reported in a table which includes the identification and the quantification of the metabolites. The results can then be saved on the Bayesil server for future access

1. Sample processing — 15 min

Use the TMIC NMR kit to rapidly process serum, plasma or CSF samples for NMR acquisition

2. NMR acquisition — 20 min

Acquire complex NMR spectra of aqueous samples for automatic profiling



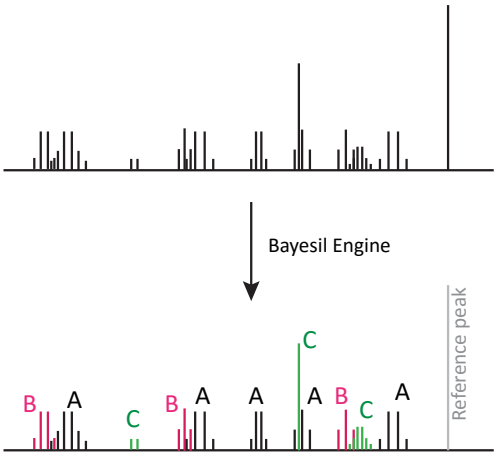
3. Automatic profiling — 7 min

Automatically analyse the metabolomic profile of the samples using the Bayesil web application

BAYESIL

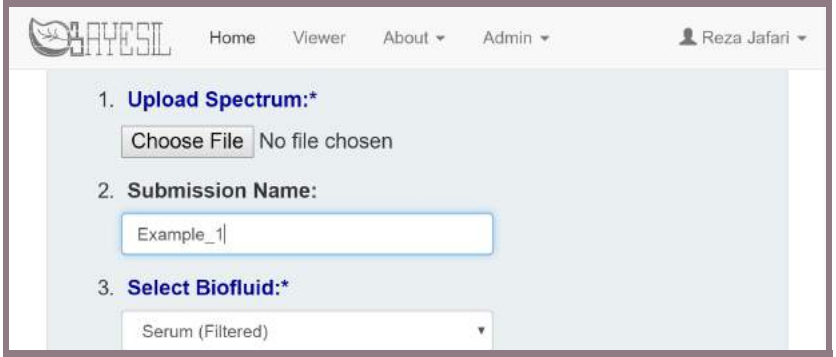
TMIC is Canada's national metabolomics facility, supporting a wide range of state-of-the-art metabolomics analysis for clinical trials research, biomedical studies, bio-products studies, nutrient profiling, and environmental testing.

Bayesil is a web-based system that automatically identifies and quantifies metabolites using 1D 1H NMR spectra of ultra-filtered plasma, serum or cerebrospinal fluid. The NMR spectra must be collected in a standardized fashion for Bayesil to perform optimally. Each kit contains an access code to process 50 NMR samples

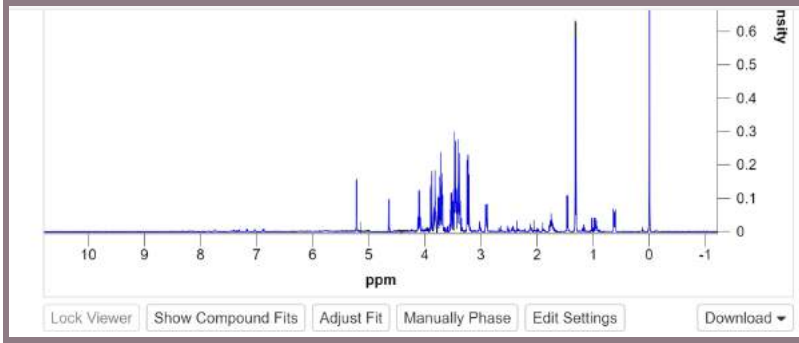


TMIC offers metabolomic profiling services by NMR performed on state-of-the-art instruments by highly quality scientists. Our clients include Canadian and international academics, industries and government agencies. For more information, please see **www.metabolomicscentre.ca**

Bayesil Automatic Profiling Workflow



1. Upload the *.fid* file on www.tmic.bayesil.com



2. Bayesil processes the spectra to find the best fit for the metabolomic profile.

HMDB ID	Compound Name	Concentration (μM)	Confidence Score
-	DSS	800.0	
HMDB00001	1-Methylhistidine	58.6	5
HMDB00008	2-Hydroxybutyrate	19.8	9
HMDB00042	Acetic acid	43.1	10
HMDB00043	Betaine	21.6	10
HMDB00060	*Acetoacetate*	*0.0*	*8*
HMDB00062	L-Carnitine	25.4	9
HMDB00064	Creatine	23.8	7

3. Results are reported in a table along with the quantification of metabolites' concentration

A list of metabolites that can be determined by the TMIC NMR Kit

1-Methylhistidine
2-Hydroxybutyric acid
3-Hydroxybutyric acid
Acetic acid
Acetoacetic acid
Acetone
Betaine
Choline
Citric acid
Creatine
Creatinine
D-Glucose
Dimethyl sulfone
Ethanol
Formic acid
Glycerol
Glycine
Hypoxanthine
Isobutyric acid
Isopropyl alcohol
L-Alanine
L-Arginine
L-Asparagine
L-Aspartic acid
L-Carnitine
L-Glutamic acid
L-Glutamine
L-Histidine
L-Isoleucine
L-Lactic acid
L-Leucine
L-Lysine
L-Methionine
L-Phenylalanine
L-Proline
L-Serine
L-Threonine
L-Tryptophan
L-Tyrosine
L-Valine
Malonic acid
Methanol
Ornithine
Propylene glycol
Pyruvic acid
Succinic acid
Urea

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