Services & Technologies

Analysis	Classes Detected	Detection Limits
NMR	Amino acids, alcohols, amines, sugars, organic acids, water soluble metabolites	**Micromolar (10^{-6})**
GC-MS	Amino acids, organic acids, fatty acids, bile acids, thiols	**Nanomolar (10^{-9})**
LC-MS DI-MS	Amino acids, biogenic amines, primary amines, acylcarnitines, carbohydrates, phospholipids, sphingolipids	**Nanomolar (10^{-9})**
HPLC-UV HPLC-FD	Aromatics, secondary metabolites including polyphenols, carotenoids, vitamins (B,C,D,E,A), lipids, nucleotides and others	**Micromolar to Picomolar (10^{-6} to 10^{-12})**
ICP-MS	Up to 40 Trace Metals	**Micromolar (10^{-6})**
HPLC-ELSD	Phospholipids, TAGs, DAGs, MAGs, CEs, and free fatty acids	**Nanomolar (10^{-9})**
Tissue Imaging	Fatty acids, lipids, acylcarnitines, drug molecules and metabolites in situ	**Micromolar (10^{-6})**

We have worked with many types of samples and model organisms as shown in the table below. Please write to us if the sample type or organism you are working with is not listed below, we will try our utmost best to accommodate to your project needs.

Type of Samples:

Blood / Plasma	Leaves
Roots	Seeds
Milk	Cell Lysates
Fruits / Berries	Oils
Urine	Cerebrospinal fluid
Saliva	Growth media
Fruit Juice	Amniotic fluid
Organs & Tissues	Other biofluids

Model of Organisms:

Human	Elk / Deer
Cattle	Rabbit
Rat	Mouse
Fruit Fly	C. elegans
Bacteria	Yeast
Canola	Arabidopsis
Alfalfa	Bacterial extracts

ies, please contact us!

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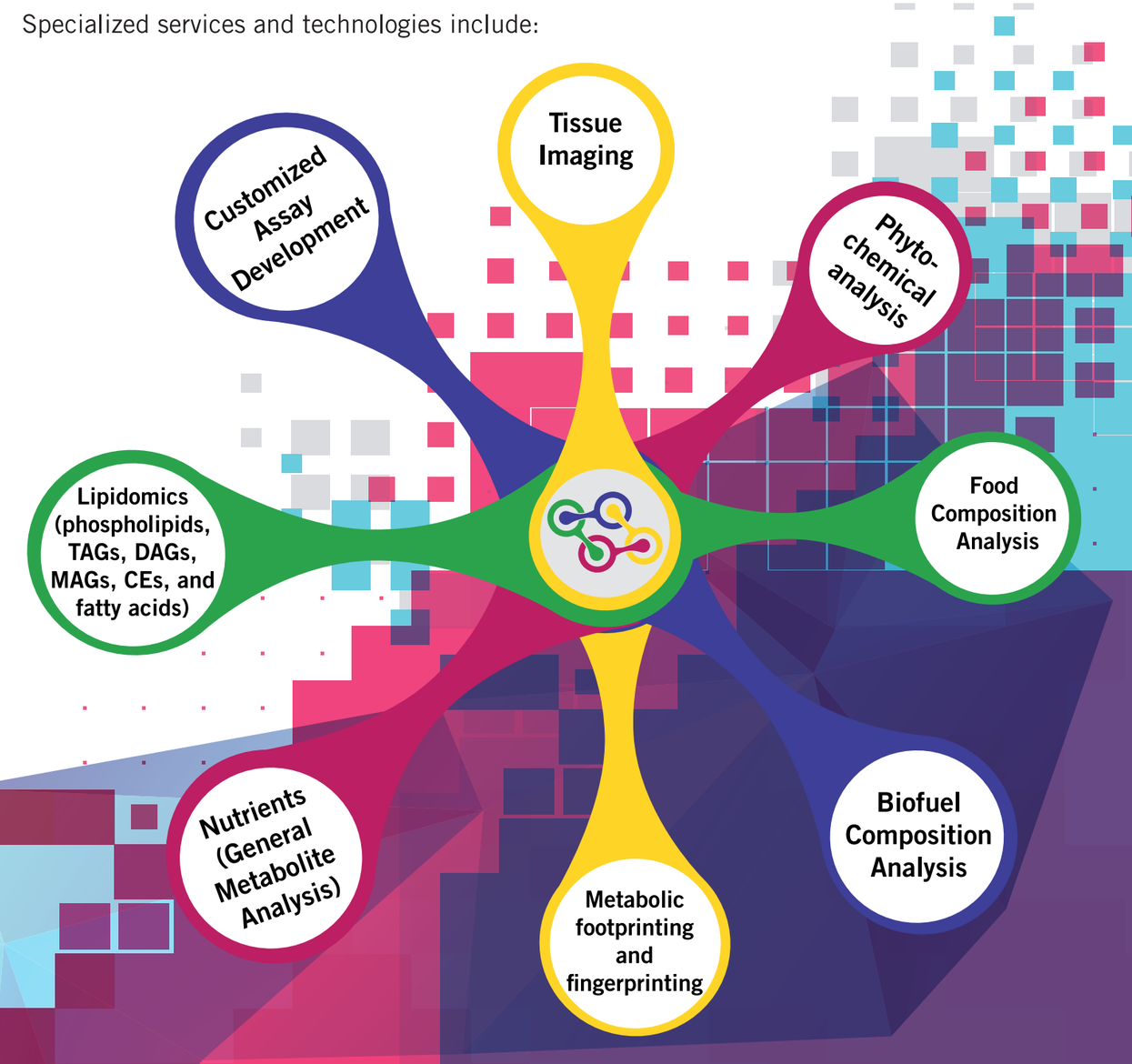
Metabolomics Services

Metabolomics is an emerging field of "omics" research specializing in the near global analysis of small molecule metabolites (< 1500 Daltons) found in living organisms. Though the field of metabolomics is relatively new, its applications are already being seen in many disciplines including disease diagnostics, agriculture food and safety, and pharmaceutical research and development. These applications are leading to the discovery of many biomarkers and the development of improved screening methods. Metabolomics utilizes a number of different assays for quantitative analysis and identification of metabolites in a variety of sample types.

By working closely with international partners, 1st BASE provides real-world proven technologies with top-of-the line metabolic analysis from biofluids, tissues, bioproducts, bioprocesses, or crops. The quantitative metabolic analysis is offered by combining NMR, GC-MS, GCxGC-MS, HPLC-UV/FD, LC-MS, DI-MS, and bioinformatics.

Specialized services and technologies include:



Services Available

Platform Specific Metabolomic Assays - Absolute Quantitative Assays		
Service	**Number of Compounds**	**Volume required**
Direct Flow Injection Mass Spectrometry (DI-MS)	Up to 180	30-50 µL
Quantitative NMR Spectroscopy	50-220	500 µL
Quantitative GC-MS	30-40	100 µL
Quantitative GC-MS/MS (EI, PCI, NCI available)	30-40	100 µL
Quantitative GC/GC-MS/MS (EI, PCI, NCI available)	Depends very heavily on sample, number of targets and elution times of target(s)	Please inquire
Targeted metabolomic profiling in complex mixtures GC×GC-TOFMS (EI only)	Depends very heavily on sample, number of targets and elution times of target(s)	Please inquire
Quantitative Lipidomics	Up to 2000	Please inquire

Global (Untargeted) Metabolomic Profiling - Untargeted Assays		
Service	**Number of Compounds**	**Volume required**
Untargeted metabolomics by GC-MS (EI only)	25-80	Please inquire
Untargeted metabolomics by GC×GC-TOFMS (EI only)	>2000	Please inquire
Untargeted metabolomics by UPLC-FT-MS	>2000	75 µL
Untargeted Metabolomics by RPLC-QTOF-MS and MS/MS	>5000 features	20-200 µL or 10-50 mg lyophilized powder
Untargeted Lipidomics by RPLC-QTOF-MS and MS/MS	>4000 features	20-200 µL or 10-50 mg lyophilized powder
Untargeted metabolomics by DI-FTICR-MS	>1000	75 µL
Untargeted metabolomics by isotope labeling 1 D LC-MS	Up to 2,500 putative metabolites in urine or 1,500 in blood or 1,000 in plant extracts or 1,500 in cell extracts	20-200 µL or 10-50 mg lyophilized powder
Untargeted metabolomics by isotope labeling 2 D LC-MS	Up to 10,000 putative metabolites in urine or up to 8,000 in blood. Please contact us for other types of samples	40-200 µL or 20-100 mg lyophilized powder
Untargeted Lipidomics by 1D UPLC-MS	>800	50 µL

Targeted Metabolomic Profiling - Class Specific Assays		
Service	**Number of Compounds**	**Volume required**
Oxylipins Analysis	18	200 µL
Vitamin Analysis - Water soluble	9	200 µL
Vitamin Analysis - Fat soluble	3	200 µL
Endogenous vitamins and vitamin-like compounds analysis	35	200 µL
Bile acids analysis (I)	50	25 µL
Bile acids analysis (II)	66	25 µL
Bile acids analysis (III)	20	50 µL
Organic acids analysis	40-80 (sample dependent)	200 µL
Catecholamines analysis	12	200 µL
Lipidomics for cardiolipins	Identification and quantification of cardiolipin compounds by UPLC-FTMS	100 µL
Low-MW sugars analysis	14	25 µL
Acylcarnitines analysis	Up to 355 acylcarnitines	200 µL
Aldehydes analysis	12	250 µL
Oxysterols analysis	7	200 µL
Deoxynucleotide triphosphates (dNTPs) analysis	5	Please Inquire
Volatiles and semi-volatiles profiling by SPME GC×GC-TOFMS (EI only)	>2000	Please Inquire
Nucleoside/Nucleotide Analysis	9	200 µL
Polyphenol Analysis	18	200 µL
Anthocyanin/ Chlorophyll Analysis	7	Please Inquire
Thiol Analysis	7	200 µL
Carotenoid Analysis	6	200 µL
Acyl CoAs Analysis	6	200 µL
Metal Analysis (Metallomics)	40-50	200 µL
Lipidomics by MALDI-MS Tissue imaging	Up to 850 for combined (+) and (-) ion detection	Please Inquire
Meat Biomarkers	7	200 µL
High-value Disease Biomarker Profiling	30	200 µL

Targeted Metabolomic Profiling - Pathway Specific Assays		
Service	**Number of Compounds**	**Volume required**
One-carbon metabolism	10	200 µL
Central carbon metabolism	50	400 µL
Amino acid metabolism /urea cycle metabolism	>50	50 µL
Lipidomics for sphingolipid metabolism	Sample dependent – please inquire	50 µL
Fatty acid metabolism - short - to long-chain fatty acids and acyl-carnitines analysis	33 fatty acids; 21 acyl-carnitines	50 µL

Customized Assays	
Service	**Number of Compounds**
High Abundance Metabolites in Plasma/Serum	Please Inquire
Low Abundance Metabolites in Plasma/Serum	Please Inquire

Comprehensive reports including metabolite identification and concentration, experimental and quality control methods, and statistical analysis, will be provided. Take a look at what the results and report would look like below.

Metabolomics Report

Quantitation of reducing sugars, sugar phosphates and TCA cycle carboxylic acids from 10 human sera by UPLC-MRM

PI: XXX

Sample Size: 60 µL, each

Sample Type: human serum

Objective: To determine concentrations of sugars, sugar phosphates and TCA cycle carboxylic acids in 10 human sera by UPLC-MRM with internal standard calibration.

Sample preparation and analysis:

Method one: 10 uL of each serum was protein precipitated with MeOH and subjected to AEC derivatization using an optimal protocol (a manuscript for detailing the method is being prepared for publication). The assay was performed using a Dionex ultimate 3000 UPLC system coupled to a 4000 QTRAP triple-quad mass spectrometer. The MS instrument was operated in the MRM mode. A reversed phase UPLC column (2.0 x 100 mm, 1.7 um) was used, with 0.1% formic acid and ACN as the solvents for binary gradient elution.

Quantitation was calculated using linear regression with internal standard (fucose-13C) calibration.

Method two: 25 µL of each serum was protein precipitated with MeOH and subjected to NPH derivatization using an optimal protocol (a manuscript for detailing the method is being prepared for publication) developed in house. The assay was performed using a Dionex ultimate 3000 UPLC system coupled to a 4000 QTRAP triple-quad mass spectrometer. The MS instrument was operated in the MRM mode. A reversed phase UPLC column (2.0 x 100 mm, 1.7 um) was used, with 0.01% formic acid and ACN as the solvents for binary gradient elution.

Quantitation was calculated using linearity curves for 8 of 9 targeted carboxylic acids with deuterium-labeled standard substances as the internal standards for individual carboxylic acids. External standard calibration was applied for isocitric acid because no isotope-labeled standard substance is commercially available.

QA/QC Data:

Table 1. On-column LODs and LOQs.

Compound	Glc 6-P	Man-6-P	Rib 5-P	Ery 4-P	Gly 3-P	Maltose	Glucose	Ribose	Fucose	Glyceraldehyde
LOD [pmol]	0.4	0.2	0.8	1.4	0.2	0.2	0.1	0.1	0.1	0.1
LOQ [pmol]	1.3	0.7	2.5	4.1	0.7	0.5	0.2	0.3	0.3	0.3

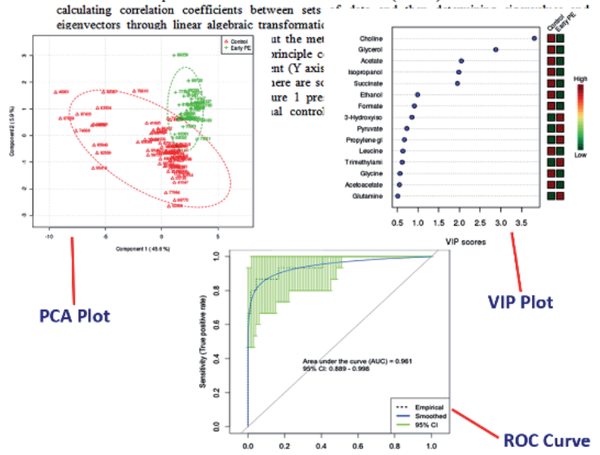
Method

QA/QC

Statistical Analysis

Data normalization – Data normalization is critical to creating a normal or Gaussian distribution of metabolite values. This allows conventional statistical tests to be performed and it simplifies data interpretation. There are many different normalization options available – here we used pareto scaling normalization (mean-centered and divided by the square root of standard deviation of each variable)

PCA analysis – PCA is also known as principle component analysis. It is an unsupervised classification technique that allows one to detect whether two (or more) sets of data. PCA involves calculating correlation coefficients between sets of data and then determining eigenvectors through linear algebraic transformati



PCA Plot

VIP Plot

ROC Curve

Metabolomics Results

Metabolomic Analysis of Urine Samples

HMDB ID

Concentration [µM]								
Sample Identification					1028	1165	3908	400
Metabolites	Metabolites (Full Name)	Class	HMDB ID#	LOD, [µM]				
C0	Carnitine	acylcarnitines	HMDB00062	4.00	51.1	31	95.7	78.3
C10	Decanoylcarnitine	acylcarnitines	HMDB00651	0.160	0.166	0.313	0.426	0.178
C10:1	Decenoylcarnitine	acylcarnitines	HMDB13205	0.120	0.829	1.63	0.954	0.573
C10:2	Decadienylcarnitine	acylcarnitines	HMDB13325	0.040	0.565	2.02	0.76	0.43
C12	Dodecanoylcarnitine	acylcarnitines	HMDB02250	0.057	0.126	0.299	0.217	0.087
C12:1	Dodecenoylcarnitine	acylcarnitines	HMDB13326	0.200	<LOD	0.239	<LOD	<LOD
C14	Tetradecanoylcarnitine	acylcarnitines	HMDB05066	0.030	0.049	0.075	0.064	0.033
C14:1	Tetradecenoylcarnitine	acylcarnitines	HMDB02014	0.015	0.02	0.051	0.031	<LOD
C14:1-OH	Hydroxytetradecenoylcarnitine	acylcarnitines	HMDB13330	0.015	0.02	0.042	0.019	<LOD
C14:2	Tetradecadienylcarnitine	acylcarnitines	HMDB13331	0.012	0.017	0.046	0.023	<LOD
C14:2-OH	Hydroxytetradecadienylcarnitine	acylcarnitines	HMDB13332	0.015	0.016	0.028	0.021	<LOD
C16	Hexadecanoylcarnitine	acylcarnitines	HMDB00222	0.018	0.03	0.029	0.02	<LOD
C16-OH	Hydroxyhexadecanoylcarnitine	acylcarnitines	HMDB13336,HMDB13337	0.015	0.037	0.019	0.018	<LOD
C16:1-OH	Hydroxyhexadecenoylcarnitine	acylcarnitines	HMDB13333	0.020	<LOD	<LOD	<LOD	<LOD
C16:2	Hexadecadienylcarnitine	acylcarnitines	HMDB13334	0.008	<LOD	0.016	0.012	<LOD
C2	Acetylcarnitine	acylcarnitines	HMDB00201	0.150	16.5	6.37	32.6	35
C3	Propionylcarnitine	acylcarnitines	HMDB00824	0.080	1.3	0.578	1.75	2.86
C3-DC (C4-OH)	Hydroxybutyrylcarnitine	acylcarnitines	HMDB13127	0.090	0.187	0.201	0.521	0.238
C3-OH	Hydroxypropionylcarnitine	acylcarnitines	HMDB13125	0.050	<LOD	<LOD	<LOD	<LOD
C4	Butyrylcarnitine	acylcarnitines	HMDB02013	0.030	5.37	5.03	4.3	6.91
C4:1	Butenylcarnitine	acylcarnitines	HMDB13126	0.030	0.092	0.208	0.17	0.1
C5	Valerylcarnitine	acylcarnitines	HMDB00378,HMDB00688	0.040	1.46	0.975	1.87	2.93
C5-DC (C6-OH)	Glutarylcarnitine(Hydroxyhexanoylcarnitine	acylcarnitines	HMDB13130, 13131	0.035	0.455	0.661	1.04	0.323
C5-M-DC	Methylglutarylcarnitine	acylcarnitines	HMDB00552	0.060	0.306	0.269	0.158	0.211
C5-OH (C3-DC-M)	drosyvalerylcarnitine(Methylmalonylcarnit	acylcarnitines	HMDB13132, 13133	0.100	0.955	1.08	1.02	0.631
C5:1	Tiglylcarnitine	acylcarnitines	HMDB02366	0.040	0.635	1.17	1.8	0.65
C5:1-DC	Glutaconylcarnitine	acylcarnitines	HMDB13129	0.015	0.175	0.217	0.226	0.159
C6 (C4:1-DC)	Hexanoylcarnitine(Fumarylcarnitine)	acylcarnitines	IMDB00705, 00756, 1313	0.080	0.439	0.429	0.338	0.325
C6:1	Hexenoylcarnitine	acylcarnitines	HMDB13135	0.035	0.17	0.573	0.45	0.171
C7-DC	Pimelylcarnitine	acylcarnitines	HMDB13328	0.035	0.222	0.352	0.461	0.227
C8	Octanoylcarnitine	acylcarnitines	HMDB00791	0.170	0.324	0.822	0.693	0.381
C8:1	Octenoylcarnitine	acylcarnitines	HMDB13324	0.025	2.24	7.24	7.71	2.5
C9	Nonanoylcarnitine	acylcarnitines	HMDB13288	0.040	0.569	1.26	0.787	0.944
Arg	Arginine	aminoacids	HMDB00517,HMDB03416	4.00	22.7	19.2	49.3	36.4
Gln	Glutamine	aminoacids	HMDB00641,HMDB03423	3.00	377	391	310	249

Metabolite Full Names

LODs

Absolute Concentrations