

List of Metabolite Assays *(Updated as of 10/27/2014; MAK)*

LC-MS/MS profiling

- Targeted Metabolomics (Biocrates Absolute IDQ p180 Kit: 180 Metabolite Panel)
 - Acylcarnitines (40)
 - Amino acids (21)
 - Monosccarides (total hexoses) (1)
 - Sphingolipids (15)
 - Glycerophospholipids (90)
 - Biogenic amines (19)
 - The full list of metabolites in Biocrates Absolute IDQ p180 Kit provided at end of this document.

- Lipid Profiling – total lipid signature including
 - Fatty acids
 - Triacylglyceride (TAG)
 - Diacylglyceride (DAG)
 - Ceramides
 - Sphingomyelins (SM)
 - Phosphatidylcholine (PC)
 - Phosphatidylethanolamine (PE)
 - phosphatidylserine (PS)
 - Phosphatidylglycerol (PG)
 - Phosphatidylinositols (PI)
 - Lyso-PC, lyso-PE

- Quinolone profiling
 - 2-akyl-4-quinolines (AQ)
 - 4-hydroxy-2-heptylquinoline N-oxide (HQNO)
 - Pseudomonas quinolone signal (PQS)
 - 2-heptyl-4-quinolone (HHQ),
 - Other quinolones also included in full profile

Targeted LC-MS/MS Assays

- Retinoic acid and metabolites
 - Retinoic acid isomers
 - All-trans retinoic acid (Tretinoin, Retin-A, Atralin, Tretin-X, Avita, Refissa)
 - 9-cis-retinoic acid (Alitretinoin, Panretin)
 - 9,13-di-cis-retinoic acid
 - 13-cis-retinoic acid (Isotretinoin, Accutane, Roaccutane, Amnesteem, Claravis, Absorcia, Isotroin, Epurius)
 - 11-cis-retinoic acid
 - 4-oxo-retinoic acid + isomers
 - Retinol
 - Retinal
 - Retinyl esters (e.g., retinyl palmitate)

- Choline and choline metabolites
 - Acetylcholine (AcCho)
 - Betaine
 - Choline (Cho)
 - Glycerophosphocholine (GPCho)
 - Phosphocholine (PCho)
 - Phosphatidylcholine (PtdCho)
 - Sphingomyelin (SM)

- Ethanol Biomarkers
 - Ethyl sulfate
 - Ethyl glucuronide
 - Fatty acid ethyl esters (9)

- Oxidative Stress biomarkers
 - GSH/GSSG (almost done)
 - Malondialdehyde (coming soon)
 - 8-OH-dG (coming soon)
 - F2-isoprostanes (coming soon)

- Radiation and Gut damage biomarker
 - Citrulline

- Drugs and Drug metabolites
 - Ibuprofen and isosorbide nitrate
 - Lamotrigine (Lamactil)
 - Acyclovir (Zovirax)
 - Prednisolone
 - Dexamethsone

- Quinolones
 - 2-alkyl-4-quinolines (AQ)
 - 4-hydroxy-2-heptylquinoline N-oxide (HQNO)
 - Pseudomonas quinolone signal (PQS)
 - 2-heptyl-4-quinolone (HHQ),
- Biliverdin (BV) isomers (Angela Wilks)
 - BVIX α
 - BVIX β
 - BVIX δ
- Metal Analysis via ICP-MS
 - Including P, S, Ca, Mn, Fe, Co, Cu, Zn
- Lysophospholipids and related compounds
 - Lysophosphatidic acid (LPA)
 - Lysophosphatidylcholine (LPC)
 - Rx100 (RxBio, Inc.) - long chain phosphate that is similar to the phospholipids
- Prostaglandins
 - 16,16-dimethyl prostaglandin E2
 - Prostaglandin E2
- Custom LC-MS/MS assays
 - Development available according to research needs
 - Quantification in plasma and/or tissue (e.g., for PK, distribution, etc.)
 - Quantification in cell models (e.g., for cellular uptake)
 - Endogenous molecules
 - Drug candidate molecules (e.g., assays have been developed for JY-3-094, SF-4-017, 3jc91-1, 3jc91-2, 3jc91-3, 3jc91-4, 3jc91-5, 3jc91-7)
 - Validation of assays according to “FDA Guidance for Bioanalytical Method Validation”
- Complimentary detectors and assay development
 - We also have a host of complimentary detection modalities that can be coupled to LC or UPLC for specialty assays
 - Ultraviolet (UV); photodiode array (PDA)
 - Evaporative light scattering detection (ELSD)
 - Electrochemical detection (ECD)
 - Fluorescence
- Additional services available upon request
- *We are open to development of new assays, workflows, and analysis strategies based upon scientific need.*

Biocrates Absolute IDQ p180 Kit: List of metabolites assayed

Absolute/DQ® p180 Kit* – 20 µL required			
Acylcarnitines (40)			
C0	Carnitine	C10:1	Decenoylcarnitine
C2	Acetylcarnitine	C10:2	Decadienoylcarnitine
C3	Propionylcarnitine	C12	Dodecanoylcarnitine
C3:1	Propenoylcarnitine	C12:1	Dodecanoylcarnitine
C3-OH	Hydroxypropionylcarnitine	C12-DC	Dodecanediacylcarnitine
C4	Butyrylcarnitine	C14	Tetradecanoylcarnitine
C4:1	Butenylcarnitine	C14:1	Tetradecanoylcarnitine
C4-OH (C3-DC)	Hydroxybutyrylcarnitine	C14:1-OH	Hydroxytetradecanoylcarnitine
C5	Valeryl carnitine	C14:2	Tetradecadienylcarnitine
C5:1	Tiglylcarnitine	C14:2-OH	Hydroxytetradecadienylcarnitine
C5:1-DC	Glutaconylcarnitine	C16	Hexadecanoylcarnitine
C5-DC (C6-OH)	Glutaryl carnitine* (β-hydroxyhexanoylcarnitine)	C16:1	Hexadecanoylcarnitine
C5-M-DC	Methylglutaryl carnitine	C16:1-OH	Hydroxyhexadecanoylcarnitine
C5-OH (C3-DC-M)	Hydroxyvaleryl carnitine (Methylmalonylcarnitine)	C16:2	Hexadecadienylcarnitine
C6 (C4:1-DC)	Hexanoylcarnitine (Fumaryl carnitine)	C16:2-OH	Hydroxyhexadecadienylcarnitine
C6:1	Hexenoylcarnitine	C16-OH	Hydroxyhexadecanoylcarnitine
C7-DC	Heptylcarnitine	C18	Octadecanoylcarnitine
C8	Octanoylcarnitine	C18:1	Octadecanoylcarnitine
C9	Nonanoylcarnitine	C18:1-OH	Hydroxyoctadecanoylcarnitine
C10	Decanoylcarnitine	C18:2	Octadecadienylcarnitine
Amino Acids and Biogenic Amines (40)			
Ala	Alanine	Ac-Om	Acetylmethine
Arg	Arginine	ADMA	Asymmetric dimethylarginine
Asn	Asparagine	SDMA	Symmetric dimethylarginine
Asp	Aspartate	total DMA	Total dimethylarginine
Cit	Citrulline	alpha-AAA	alpha-Aminoadipic acid
Gln	Glutamine	Carnosine	Carnosine
Glu	Glutamate	Creatinine	Creatinine
Gly	Glycine	Histamine	Histamine
Pro	Proline	Serotonin	Serotonin
Ser	Serine	Spermidine	Spermidine
Thr	Threonine	Spermine	Spermine
Trp	Tryptophan	Taurine	Taurine
Tyr	Tyrosine		
Val	Valine		
Monosaccharides (1)			
Sum of Hexosee (including Glucose)			
Sphingolipids (15)			
SM (OH) C14:1	SM C18:0	SM (OH) C22:1	SM (OH) C24:1
SM C16:0	SM C18:1	SM (OH) C22:2	SM C26:0
SM C16:1	SM C20:2	SM C24:0	SM C26:1
SM (OH) C16:1	SM C22:3	SM C24:1	
Glycerophospholipids (90)			
lysoPC a C14:0	PC aa C34:1	PC aa C42:0	PC ae C36:2
lysoPC a C16:0	PC aa C34:2	PC aa C42:1	PC ae C36:3
lysoPC a C16:1	PC aa C34:3	PC aa C42:2	PC ae C36:4
lysoPC a C17:0	PC aa C34:4	PC aa C42:4	PC ae C36:5
lysoPC a C18:0	PC aa C36:0	PC aa C42:5	PC ae C36:6
lysoPC a C18:1	PC aa C36:1	PC aa C42:6	PC ae C40:1
lysoPC a C18:2	PC aa C36:2	PC ae C30:0	PC ae C40:2
lysoPC a C20:3	PC aa C36:3	PC ae C30:1	PC ae C40:3
lysoPC a C20:4	PC aa C36:4	PC ae C30:2	PC aa C40:4
lysoPC a C24:0	PC aa C36:5	PC ae C32:1	PC ae C40:5
lysoPC a C26:0	PC aa C36:6	PC ae C32:2	PC ae C40:6
lysoPC a C26:1	PC aa C36:0	PC ae C34:0	PC ae C42:0
lysoPC a C26:0	PC aa C36:1	PC ae C34:1	PC ae C42:1
lysoPC a C26:1	PC aa C36:3	PC ae C34:2	PC ae C42:2
PC aa C24:0	PC aa C36:4	PC ae C34:3	PC ae C42:3
PC aa C26:0	PC aa C36:5	PC ae C36:0	PC ae C42:4
PC aa C26:1	PC aa C36:6	PC ae C36:1	PC ae C42:5
PC aa C30:0	PC aa C40:1	PC ae C36:2	PC ae C44:3
PC aa C30:2	PC aa C40:2	PC ae C36:3	PC ae C44:4
PC aa C32:0	PC aa C40:3	PC ae C36:4	PC ae C44:5
PC aa C32:1	PC aa C40:4	PC ae C36:5	PC ae C44:6
PC ae C32:2	PC aa C40:5	PC ae C36:0	
PC ae C32:3	PC aa C40:6	PC ae C36:1	