

Bioanalytics, Metabolomics and Pharmacokinetics Shared Resource (BMPK)

Quantitative Targeted Metabolomics

The BMPK Shared Resource at Roswell Park is launching a new service for Targeted Metabolomics analysis to support the growing Omics research efforts in the Buffalo area. The analysis uses **Mass Spectrometry** and the **Biocrates MxP® Quant 500 kit**. Key features of the analysis include:

Broad Pathway Coverage

- Comprehensive quantification of up to 630 metabolites from 26 biochemical classes, and up to 234 metabolism indicators
- Broad coverage of metabolic pathways

Functional Microbiomics

- Includes dozens of metabolites specific for microbiome and its interaction with the host

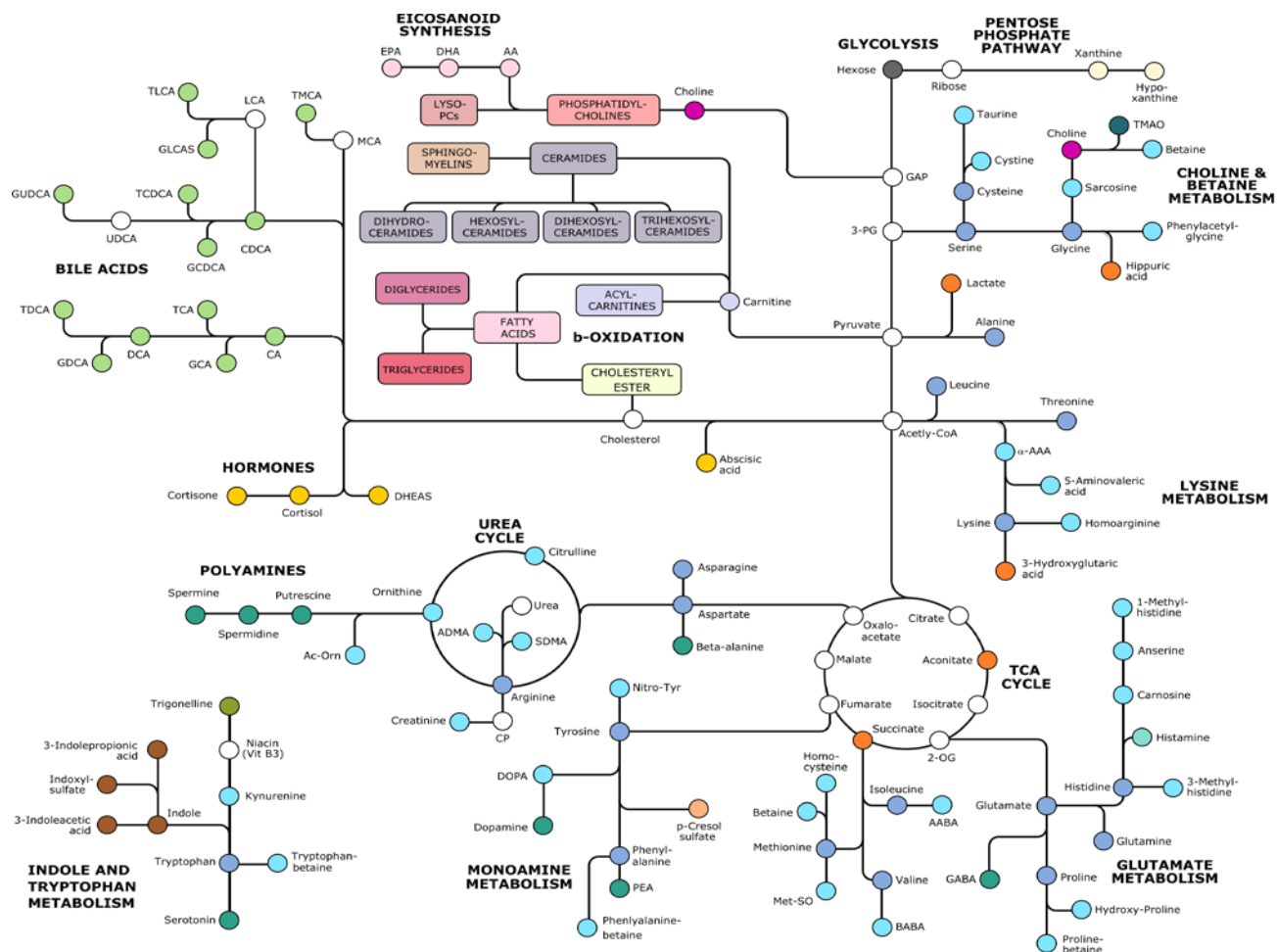
Wide Sample Applications

- Suitable for analyzing cell culture, biological fluid, tissue, and feces samples from various species
- Requires as little as 10 µL of sample

Quantitative & Reproducible

- Calibrated and quantitative readouts
- Robust with excellent accuracy and precision

Metabolite and Pathway Coverage



Note: Metabolites as white circles are not quantified

Small Molecules

- | | | |
|-------------------------|-------------------------------|-----------------------------|
| Alkaloids (1) | Biogenic Amines (9) | Hormones and Related (4) |
| Amine Oxides (1) | Carbohydrates and Related (1) | Indoles and Derivatives (4) |
| Amino Acids (20) | Carboxylic Acids (7) | Nucleobases and Related (2) |
| Amino Acid Related (30) | Cresols (1) | Vitamins and Cofactors (1) |
| Bile Acids (14) | Fatty Acids (12) | |

Lipids

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|-------------------------------|-------------------------|
| Acylcarnitines (40) | Ceramides (70) |
| Lysophosphatidylcholines (14) | Cholesterol Esters (22) |
| Phosphatidylcholines (76) | Diglycerides (44) |
| Sphingomyelins (15) | Triglycerides (242) |

For more information on services and other pricing, contact Joshua Prey, MS, Research Project Administrator (716) 845-3313 or Joshua.prey@roswellpark.org

MxP[®] Quant 500 kit – List of metabolites

Metabolomics in nutrition, microbiome, and disease

The MxP[®] Quant 500 is our most comprehensive kit for targeted metabolic profiling. With a coverage of up to 630 metabolites from 26 biochemical classes, we bring advanced and reproducible metabolomics technology to academic and industry researchers. The kit offers fast turnaround times and reliable quantification of a broad range of metabolites. This includes substances related to nutrition and host-microbiome interaction to ensure innovative scientific findings with sustainable impact.

Analyte class (number of metabolites)		Analytical method
Small molecules (107)	Alkaloids (1)	LC-MS/MS
	Amine oxides (1)	
	Amino acids (20)	
	Amino acid related (30)	
	Bile acids (14)	
	Biogenic amines (9)	
	Carboxylic acids (7)	
	Cresols (1)	
	Fatty acids (12)	
	Hormones and related (4)	
	Indoles and derivatives (4)	
	Nucleobases and related (2)	
	Vitamins and cofactors (1)	
	Carbohydrates and related (1)	
Lipids (523)	Acylcarnitines (40)	FIA-MS/MS
	Lysophosphatidylcholines (14)	
	Phosphatidylcholines (76)	
	Sphingomyelins (15)	
	Ceramides (28)	
	Dihydroceramides (8)	
	Hexosylceramides (19)	
	Dihexosylceramides (9)	
	Trihexosylceramides (6)	
	Cholesteryl esters (22)	
	Diglycerides (44)	
	Triglycerides (242)	

Alkaloids (1)

Trigonelline	Trigonelline		
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Amine oxides (1)

TMAO	Trimethylamine N-oxide		
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Amino acids (20)

Ala	Alanine	Leu	Leucine
Arg	Arginine	Lys	Lysine
Asn	Asparagine	Met	Methionine
Asp	Aspartate	Phe	Phenylalanine
Cys	Cysteine	Pro	Proline
Glu	Glutamate	Ser	Serine
Gln	Glutamine	Thr	Threonine
Gly	Glycine	Trp	Tryptophan
His	Histidine	Tyr	Tyrosine
Ile	Isoleucine	Val	Valine

Amino acid related (30)

alpha-AAA	α -Aminoadipic acid	c4-OH-Pro	<i>cis</i> -4-Hydroxyproline
AABA	α -Aminobutyric acid	t4-OH-Pro	<i>trans</i> -4-Hydroxyproline
Ac-Orn	Acetylornithine	Kynurenine	Kynurenine
ADMA	Asymmetric dimethylarginine	Met-SO	Methionine sulfoxide
Anserine	Anserine	1-Met-His	1-Methylhistidine
5-AVA	5-Aminovaleric acid	3-Met-His	3-Methylhistidine
BABA	β -Aminobutyric acid	Nitro-Tyr	Nitrotyrosine
Betaine	Betaine	Orn	Ornithine
Carnosine	Carnosine	PAG	Phenylacetyl glycine
Cit	Citrulline	PheAlaBetaine	Phenylalanine betaine
Creatinine	Creatinine	ProBetaine	Proline betaine
Cystine	Cystine	Sarcosine	Sarcosine
DOPA	Dihydroxyphenylalanine	SDMA	Symmetric dimethylarginine
HArg	Homoarginine	Taurine	Taurine
HCys	Homocysteine	TrpBetaine	Tryptophan betaine

Bile acids (14)

CA	Cholic acid	GLCAS	Glycolithocholic acid sulfate
CDCA	Chenodeoxycholic acid	GUDCA	Glycoursodeoxycholic acid
DCA	Deoxycholic acid	TCA	Taurocholic acid
GCA	Glycocholic acid	TCDCA	Taurochenodeoxycholic acid
GDCA	Glycodeoxycholic acid	TDCA	Taurodeoxycholic acid
GCDCA	Glycochenodeoxycholic acid	TLCA	Taurolithocholic acid
GLCA	Glycolithocholic acid	TMCA	Tauromurocholic acid

Biogenic amines (9)

beta-Ala	β -Alanine	Putrescine	Putrescine
GABA	γ -Aminobutyric acid	Serotonin	Serotonin
Dopamine	Dopamine	Spermidine	Spermidine
Histamine	Histamine	Spermine	Spermine
PEA	Phenylethylamine		

Carbohydrates and related (1)

H1	Hexoses (including glucose)		
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Carboxylic acids (7)

AconAcid	Aconitic acid	OH-GlutAcid	3-Hydroxyglutaric acid
DiCA(12:0)	Dodecanedioic acid	Lac	Lactic acid
DiCA(14:0)	Tetradecanedioic acid	Suc	Succinic acid
HipAcid	Hippuric acid		

Cresols (1)

p-Cresol-SO4	p-Cresol sulfate		
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Fatty acids (12)

FA(12:0)	Lauric acid	FA(20:1)	Eicosenoic acid
FA(14:0)	Myristic acid	FA(20:2)	Eicosadienoic acid
FA(16:0)	Palmitic acid	FA(20:3)	Eicosatrienoic acid
FA(18:0)	Stearic acid	AA	Arachidonic acid (FA(20:4 ω 6))
FA(18:1)	Octadecenoic acid	EPA	Eicosapentaenoic acid (FA(20:5 ω 3))
FA(18:2)	Octadecadienoic acid	DHA	Docosahexaenoic acid (FA(22:6 ω 3))

Hormones and related (4)

AbsAcid	Abscisic acid	Cortisone	Cortisone
Cortisol	Cortisol	DHEAS	Dehydroepiandrosterone sulfate

Indoles and derivatives (4)

Indole	Indole	3-IPA	3-Indolepropionic acid
3-IAA	3-Indoleacetic acid	Ind-SO4	Indoxyl sulfate

Nucleobases and related (2)

Hypoxanthine	Hypoxanthine	Xanthine	Xanthine
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Vitamins and cofactors (1)

Choline	Choline		
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Acylcarnitines (40)

C0	Carnitine	C10:1	Decenoylcarnitine
C2	Acetylcarnitine	C10:2	Decadienoylcarnitine
C3	Propionylcarnitine	C12	Dodecanoylcarnitine
C3-DC (C4-OH)	Malonylcarnitine (Hydroxybutyrylcarnitine)	C12-DC	Dodecanedioylcarnitine
C3-OH	Hydroxypropionylcarnitine	C12:1	Dodecenoylcarnitine
C3:1	Propenoylcarnitine	C14	Tetradecanoylcarnitine
C4	Butyrylcarnitine	C14:1	Tetradecenoylcarnitine
C4:1	Butenylcarnitine	C14:1-OH	Hydroxytetradecenoylcarnitine
C5	Valerylcarnitine	C14:2	Tetradecadienoylcarnitine
C5-DC (C6-OH)	Glutaryl carnitine (Hydroxyhexanoylcarnitine)	C14:2-OH	Hydroxytetradecadienoyl- carnitine
C5-M-DC	Methylglutaryl carnitine	C16	Hexadecanoylcarnitine
C5-OH (C3-DC-M)	Hydroxyvalerylcarnitine (Methylmalonylcarnitine)	C16-OH	Hydroxyhexadecanoylcarnitine
C5:1	Tiglylcarnitine	C16:1	Hexadecenoylcarnitine
C5:1-DC	Glutaconylcarnitine	C16:1-OH	Hydroxyhexadecenoylcarnitine
C6 (C4:1-DC)	Hexanoylcarnitine (Fumaryl carnitine)	C16:2	Hexadecadienoylcarnitine
C6:1	Hexenoylcarnitine	C16:2-OH	Hydroxyhexadecadienoyl- carnitine
C7-DC	Pimeloylcarnitine	C18	Octadecanoylcarnitine
C8	Octanoylcarnitine	C18:1	Octadecenoylcarnitine
C9	Nonaylcarnitine	C18:1-OH	Hydroxyoctadecenoylcarnitine
C10	Decanoylcarnitine	C18:2	Octadecadienoylcarnitine

Lysophosphatidylcholines (14)

lysoPC a C14:0	lysoPC a C18:0	lysoPC a C20:4	lysoPC a C28:0
lysoPC a C16:0	lysoPC a C18:1	lysoPC a C24:0	lysoPC a C28:1
lysoPC a C16:1	lysoPC a C18:2	lysoPC a C26:0	
lysoPC a C17:0	lysoPC a C20:3	lysoPC a C26:1	

Phosphatidylcholines (76)

PC aa C24:0	PC aa C36:3	PC aa C42:0	PC ae C36:1
PC aa C26:0	PC aa C36:4	PC aa C42:1	PC ae C36:2
PC aa C28:1	PC aa C36:5	PC aa C42:2	PC ae C36:3
PC aa C30:0	PC aa C36:6	PC aa C42:4	PC ae C36:4
PC aa C30:2 ¹	PC aa C38:0	PC aa C42:5	PC ae C36:5
PC aa C32:0	PC aa C38:1	PC aa C42:6	PC ae C38:0
PC aa C32:1	PC aa C38:3	PC ae C30:0	PC ae C38:1
PC aa C32:2	PC aa C38:4	PC ae C30:1	PC ae C38:2
PC aa C32:3	PC aa C38:5	PC ae C30:2	PC ae C38:3
PC aa C34:1	PC aa C38:6	PC ae C32:1	PC ae C38:4
PC aa C34:2	PC aa C40:1	PC ae C32:2	PC ae C38:5
PC aa C34:3	PC aa C40:2	PC ae C34:0	PC ae C38:6
PC aa C34:4	PC aa C40:3	PC ae C34:1	PC ae C40:1
PC aa C36:0	PC aa C40:4	PC ae C34:2	PC ae C40:2
PC aa C36:1	PC aa C40:5	PC ae C34:3	PC ae C40:3
PC aa C36:2	PC aa C40:6	PC ae C36:0	PC ae C40:4
PC ae C40:5	PC ae C42:1	PC ae C42:4	PC ae C44:4
PC ae C40:6	PC ae C42:2	PC ae C42:5	PC ae C44:5
PC ae C42:0	PC ae C42:3	PC ae C44:3	PC ae C44:6

Sphingomyelins (15)

SM (OH) C14:1	SM C18:0	SM (OH) C22:2	SM (OH) C24:1
SM C16:0	SM C18:1	SM C22:3 ¹	SM C26:0
SM C16:1	SM C20:2	SM C24:0	SM C26:1
SM (OH) C16:1	SM (OH) C22:1	SM C24:1	

¹ SCIEX only

Ceramides (28)			
Cer(d16:1/18:0)	Cer(d18:1/18:0(OH))	Cer(d18:1/24:1)	Cer(d18:2/20:0)
Cer(d16:1/20:0)	Cer(d18:1/18:0)	Cer(d18:1/25:0)	Cer(d18:2/22:0)
Cer(d16:1/22:0)	Cer(d18:1/18:1)	Cer(d18:1/26:0)	Cer(d18:2/23:0)
Cer(d16:1/23:0)	Cer(d18:1/20:0(OH))	Cer(d18:1/26:1) ³	Cer(d18:2/24:0)
Cer(d16:1/24:0)	Cer(d18:1/20:0)	Cer(d18:2/14:0)	Cer(d18:2/24:1)
Cer(d18:0/16:0) ²	Cer(d18:1/22:0)	Cer(d18:2/16:0)	
Cer(d18:1/14:0)	Cer(d18:1/23:0)	Cer(d18:2/18:0)	
Cer(d18:1/16:0)	Cer(d18:1/24:0)	Cer(d18:2/18:1)	

Dihydroceramides (8)			
Cer(d18:0/18:0(OH))	Cer(d18:0/20:0)	Cer(d18:0/24:0)	Cer(d18:0/26:1(OH))
Cer(d18:0/18:0)	Cer(d18:0/22:0)	Cer(d18:0/24:1)	Cer(d18:0/26:1)

Hexosylceramides (19)			
HexCer(d16:1/20:0) ⁴	HexCer(d18:1/18:0)	HexCer(d18:1/24:0)	HexCer(d18:2/18:0)
HexCer(d16:1/22:0)	HexCer(d18:1/18:1)	HexCer(d18:1/24:1)	HexCer(d18:2/20:0)
HexCer(d16:1/24:0)	HexCer(d18:1/20:0)	HexCer(d18:1/26:0)	HexCer(d18:2/22:0)
HexCer(d18:1/14:0)	HexCer(d18:1/22:0)	HexCer(d18:1/26:1)	HexCer(d18:2/23:0)
HexCer(d18:1/16:0)	HexCer(d18:1/23:0)	HexCer(d18:2/16:0)	HexCer(d18:2/24:0)

Dihexosylceramides (9)			
Hex2Cer(d18:1/14:0)	Hex2Cer(d18:1/20:0)	Hex2Cer(d18:1/24:1)	
Hex2Cer(d18:1/16:0)	Hex2Cer(d18:1/22:0)	Hex2Cer(d18:1/26:0)	
Hex2Cer(d18:1/18:0)	Hex2Cer(d18:1/24:0)	Hex2Cer(d18:1/26:1)	

Trihexosylceramides (6)			
Hex3Cer(d18:1/16:0)	Hex3Cer(d18:1/20:0)	Hex3Cer(d18:1/24:1)	
Hex3Cer(d18:1/18:0)	Hex3Cer(d18:1/22:0)	Hex3Cer(d18:1/26:1)	

Cholesteryl esters (22)			
CE(14:0)	CE(17:0)	CE(20:0)	CE(22:1)
CE(14:1)	CE(17:1)	CE(20:1)	CE(22:2)
CE(15:0)	CE(18:0)	CE(20:3)	CE(22:5)
CE(15:1)	CE(18:1)	CE(20:4)	CE(22:6)
CE(16:0)	CE(18:2)	CE(20:5)	
CE(16:1)	CE(18:3)	CE(22:0)	

² Waters Xevo® TQ-S only

³ SCIEX and Waters Xevo® TQ-XS only

⁴ Waters Xevo® TQ-XS only



Diglycerides (44)			
DG(14:0_14:0)	DG(16:0_20:4)	DG(18:1_18:4)	DG(18:2_20:4)
DG(14:0_18:1)	DG(16:1_18:0)	DG(18:1_20:0)	DG(18:3_18:3)
DG(14:0_18:2)	DG(16:1_18:1)	DG(18:1_20:1)	DG(18:3_20:2)
DG(14:0_20:0)	DG(16:1_18:2)	DG(18:1_20:2)	DG(21:0_22:6)
DG(14:1_18:1)	DG(16:1_20:0)	DG(18:1_20:3)	DG(22:1_22:2)
DG(14:1_20:2)	DG(17:0_17:1)	DG(18:1_20:4)	DG-O(14:0_18:2)
DG(16:0_16:0)	DG(17:0_18:1)	DG(18:1_22:5)	DG-O(16:0_18:1) ³
DG(16:0_16:1)	DG(18:0_20:0)	DG(18:1_22:6)	DG-O(16:0_20:4) ⁵
DG(16:0_18:1)	DG(18:0_20:4)	DG(18:2_18:2)	DG-O(18:2_18:2) ⁶
DG(16:0_18:2)	DG(18:1_18:1)	DG(18:2_18:3)	
DG(16:0_20:0)	DG(18:1_18:2)	DG(18:2_18:4)	
DG(16:0_20:3)	DG(18:1_18:3)	DG(18:2_20:0)	

Triglycerides (242)			
TG(14:0_32:2)	TG(16:0_34:1)	TG(16:1_32:0)	TG(17:1_34:3)
TG(14:0_34:0)	TG(16:0_34:2)	TG(16:1_32:1)	TG(17:1_36:3)
TG(14:0_34:1)	TG(16:0_34:3)	TG(16:1_32:2)	TG(17:1_36:4)
TG(14:0_34:2)	TG(16:0_34:4)	TG(16:1_33:1)	TG(17:1_36:5)
TG(14:0_34:3)	TG(16:0_35:1)	TG(16:1_34:0)	TG(17:1_38:5)
TG(14:0_35:1)	TG(16:0_35:2)	TG(16:1_34:1)	TG(17:1_38:6)
TG(14:0_35:2)	TG(16:0_35:3)	TG(16:1_34:2)	TG(17:1_38:7)
TG(14:0_36:1)	TG(16:0_36:2)	TG(16:1_34:3)	TG(17:2_34:2)
TG(14:0_36:2)	TG(16:0_36:3)	TG(16:1_36:1)	TG(17:2_34:3)
TG(14:0_36:3)	TG(16:0_36:4)	TG(16:1_36:2)	TG(17:2_36:2)
TG(14:0_36:4)	TG(16:0_36:5)	TG(16:1_36:3)	TG(17:2_36:3)
TG(14:0_38:4)	TG(16:0_36:6)	TG(16:1_36:4)	TG(17:2_36:4)
TG(14:0_38:5)	TG(16:0_37:3)	TG(16:1_36:5)	TG(17:2_38:5)
TG(14:0_39:3) ¹	TG(16:0_38:1)	TG(16:1_38:3)	TG(17:2_38:6)
TG(14:0_40:5) ⁶	TG(16:0_38:2)	TG(16:1_38:4)	TG(17:2_38:7)
TG(16:0_28:1)	TG(16:0_38:3)	TG(16:1_38:5)	TG(18:0_30:0)
TG(16:0_28:2)	TG(16:0_38:4)	TG(17:0_32:1)	TG(18:0_30:1)
TG(16:0_30:2)	TG(16:0_38:5)	TG(17:0_34:1)	TG(18:0_32:0)
TG(16:0_32:0)	TG(16:0_38:6)	TG(17:0_34:2)	TG(18:0_32:1)
TG(16:0_32:1)	TG(16:0_38:7)	TG(17:0_34:3)	TG(18:0_32:2)
TG(16:0_32:2)	TG(16:0_40:6)	TG(17:0_36:3)	TG(18:0_34:2)
TG(16:0_32:3)	TG(16:0_40:7)	TG(17:0_36:4)	TG(18:0_34:3)
TG(16:0_33:1)	TG(16:0_40:8)	TG(17:1_32:1)	TG(18:0_36:1)
TG(16:0_33:2)	TG(16:1_28:0)	TG(17:1_34:1)	TG(18:0_36:2)
TG(16:0_34:0)	TG(16:1_30:1)	TG(17:1_34:2)	TG(18:0_36:3)

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⁵ SCIEX and Waters Xevo® TQ-S only

⁶ Waters only

Triglycerides (continued)			
TG(18:0_36:4)	TG(18:2_30:1)	TG(18:3_36:3)	TG(20:4_30:0)
TG(18:0_36:5)	TG(18:2_31:0)	TG(18:3_36:4)	TG(20:4_32:0)
TG(18:0_38:6)	TG(18:2_32:0)	TG(18:3_38:5)	TG(20:4_32:1)
TG(18:0_38:7)	TG(18:2_32:1)	TG(18:3_38:6)	TG(20:4_32:2)
TG(18:1_26:0)	TG(18:2_32:2)	TG(20:0_32:3)	TG(20:4_33:2)
TG(18:1_28:1)	TG(18:2_33:0)	TG(20:0_32:4)	TG(20:4_34:0)
TG(18:1_30:0)	TG(18:2_33:1)	TG(20:0_34:1)	TG(20:4_34:1)
TG(18:1_30:1)	TG(18:2_33:2)	TG(20:1_24:3)	TG(20:4_34:2)
TG(18:1_30:2)	TG(18:2_34:0)	TG(20:1_26:1)	TG(20:4_34:3)
TG(18:1_31:0)	TG(18:2_34:1)	TG(20:1_30:1)	TG(20:4_35:3)
TG(18:1_32:0)	TG(18:2_34:2)	TG(20:1_31:0) ¹	TG(20:4_36:2)
TG(18:1_32:1)	TG(18:2_34:3)	TG(20:1_32:0) ⁶	TG(20:4_36:3)
TG(18:1_32:2)	TG(18:2_34:4)	TG(20:1_32:1)	TG(20:4_36:4)
TG(18:1_32:3)	TG(18:2_35:1)	TG(20:1_32:2)	TG(20:4_36:5)
TG(18:1_33:0)	TG(18:2_35:2)	TG(20:1_32:3)	TG(20:5_34:0)
TG(18:1_33:1)	TG(18:2_35:3)	TG(20:1_34:0)	TG(20:5_34:1)
TG(18:1_33:2)	TG(18:2_36:0)	TG(20:1_34:1)	TG(20:5_34:2)
TG(18:1_33:3)	TG(18:2_36:1)	TG(20:1_34:2)	TG(20:5_36:2)
TG(18:1_34:1)	TG(18:2_36:2)	TG(20:1_34:3)	TG(20:5_36:3)
TG(18:1_34:2)	TG(18:2_36:3)	TG(20:2_32:0)	TG(22:0_32:4)
TG(18:1_34:3)	TG(18:2_36:4)	TG(20:2_32:1)	TG(22:1_32:5)
TG(18:1_34:4)	TG(18:2_36:5)	TG(20:2_34:1)	TG(22:2_32:4)
TG(18:1_35:2)	TG(18:2_38:4)	TG(20:2_34:2)	TG(22:3_30:2)
TG(18:1_35:3)	TG(18:2_38:5)	TG(20:2_34:3)	TG(22:4_32:0)
TG(18:1_36:0)	TG(18:2_38:6)	TG(20:2_34:4)	TG(22:4_32:2)
TG(18:1_36:1)	TG(18:3_30:0)	TG(20:2_36:5)	TG(22:4_34:2)
TG(18:1_36:2)	TG(18:3_32:0)	TG(20:3_32:0)	TG(22:5_32:0)
TG(18:1_36:3)	TG(18:3_32:1)	TG(20:3_32:1)	TG(22:5_32:1)
TG(18:1_36:4)	TG(18:3_33:2)	TG(20:3_32:2)	TG(22:5_34:1)
TG(18:1_36:5)	TG(18:3_34:0)	TG(20:3_34:0)	TG(22:5_34:2)
TG(18:1_36:6)	TG(18:3_34:1)	TG(20:3_34:1)	TG(22:5_34:3)
TG(18:1_38:5)	TG(18:3_34:2)	TG(20:3_34:2)	TG(22:6_32:0)
TG(18:1_38:6)	TG(18:3_34:3)	TG(20:3_34:3)	TG(22:6_32:1)
TG(18:1_38:7)	TG(18:3_35:2)	TG(20:3_36:3)	TG(22:6_34:1)
TG(18:2_28:0)	TG(18:3_36:1)	TG(20:3_36:4)	TG(22:6_34:2)
TG(18:2_30:0)	TG(18:3_36:2)	TG(20:3_36:5)	TG(22:6_34:3)

¹ SCIEX only
⁶ Waters only

MetaboINDICATOR™ – MxP® Quant 500 kit

List of metabolite sums and ratios

Calculating and understanding metabolite sums and ratios makes your biological data interpretation easier and more comprehensive. That is why we created MetaboINDICATOR™ as an add-on tool to MetIDQ™. Give your data a meaningful impact. Find out how metabolite sums and ratios are associated with related biological functions.

All 234 sums and ratios, or metabolism indicators, are part of the MetIDQ™ MetaboINDICATOR™ module and are designed specifically for MxP® Quant 500 kit data. Please note that the listed sums and ratios may indicate specific enzyme activities and diseases, but changes in metabolite levels could be also due to other reasons.

Overview of 234 predefined metabolite sums and ratios

Metabolite class	Number of metabolism indicators
Amine oxides	2
Amino acids	22
Amino acid related	35
Bile acids	32
Biogenic amines	11
Carboxylic acids	3
Cresols	1
Fatty acids	11
Hormones and related	2
Indoles and derivatives	5
Nucleobases and related	2
Vitamins and cofactors	1
Acylcarnitines	39
Lysophosphatidylcholines	12
Phosphatidylcholines	13
Sphingomyelins	8
Ceramides, dihydroceramides, hexosylceramides, dihexosylceramides, trihexosylceramides	20
Cholesteryl esters	6
Diglycerides	5
Triglycerides	4


Please contact BMPK Shared Resource for more information related to metabolite sums and ratios.

MetaboINDICATOR™ – Examples

- Make data coherent – Why quantitation matters?

Fischer ratio

↓ ratio
↑ severity of **liver failure**




$$\frac{\text{BCAA (Val + Leu + Ile)}}{\text{AAA (Phe + Tyr + Trp)}}$$

Fischer et al., Am J Surg 1974;127:40.

IDO activity

↑ ratio
↑ **cancer** invasiveness and progression




$$\frac{\text{Kynurenine (Kyn)}}{\text{Tryptophan (Trp)}}$$

Hornýák et al. 2018, Front Immunol 2018; 9:151.

Phospholipase A2 activity

↑ ratio
↑ **inflammation** and CVD




$$\frac{\text{Lysophosphatidylcholines (LPCs)}}{\text{Phosphatidylcholines (PCs)}}$$

Paapstel et al. Nutr Metab Cardiovasc Dis 2018; 28(1):44–52.

Gut bacterial profile

↑ ratio
↑ **cytotoxicity** → NAFLD, AD, cancer



$$\frac{\text{Secondary bile acids}}{\text{Primary bile acids}}$$

Nho et al. Alzheimers Dement 2019; 15(2):232–44.

AAA: aromatic amino acids, BCAA: branched-chain amino acids, IDO: indoleamine 2,3-dioxygenase.
CVD: cardiovascular disease, NAFLD: non-alcoholic fatty liver disease, AD: Alzheimer's disease.

- Additional Cancer-specific Sums and Ratios

Asn Synthesis

↑ ratio
↑ asparagine synthetase (**ovarian cancer** biomarker; downregulation induces cell cycle arrest & inhibits cell proliferation of **breast cancer**).

$$\frac{\text{Asparagine (Asn)}}{\text{Aspartate (Asp)}}$$

Lomelino et al. 2017, DOI: 10.1074/jbc.R117.819060

Glutaminase activity

↑ ratio
↑ hydrolysis of glutamine to glutamate in **cancer**

$$\frac{\text{Glutamate (Glu)}}{\text{Glutamine (Gln)}}$$

Scalise et al. 2017, DOI: 10.3389/fonc.2017.00306

Gly synthesis

↑ ratio
potential diagnostic marker for **glioma** and **breast cancer**

$$\frac{\text{Glycine (Gly)}}{\text{Serine (Ser)}}$$

Wang et al. 2017, DOI: 10.1016/j.clineuro.2017.01.005;

Glutaminolysis rate

↑ ratio
cancer diagnostic marker

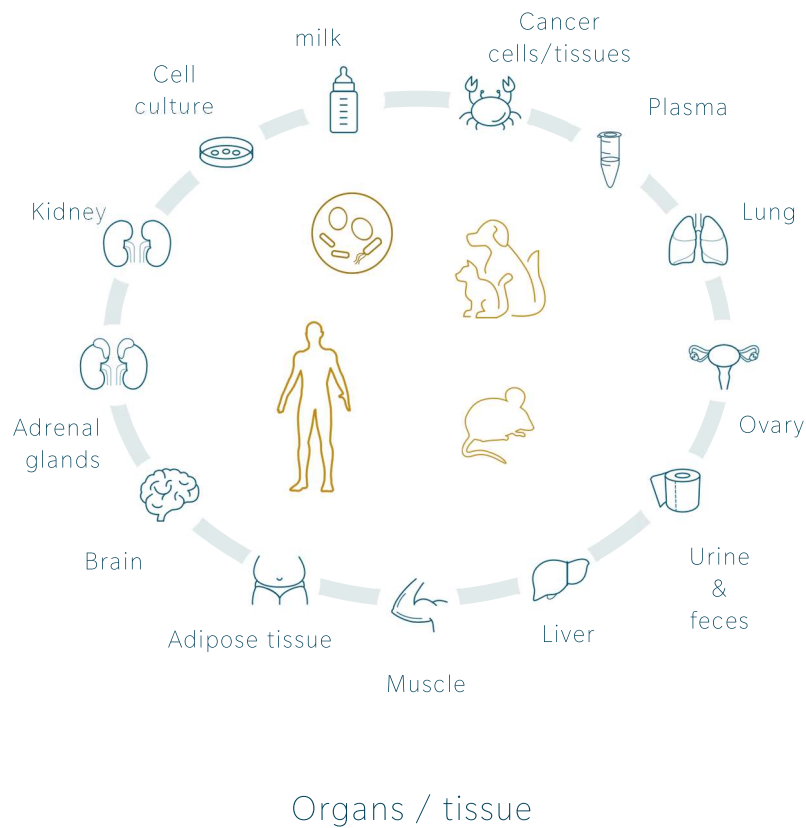
$$\frac{\text{Ala + Asp + Glu + Lac + Suc}}{\text{Gln}}$$

Jin et al. 2016, DOI: 10.1038/onc.2015.447;

Matrices and species

Connecting biological systems

biocrates kits & services



Matrices

- Plasma, serum (only 10 μ L)
- Dried blood spots
- Cell culture medium
- Tissue
- Tumor tissue:
- Lung lavage (BALF)
- Skin samples
- Blister liquid / skins
- Feces
- Follicular fluid
- Milk
- Urine
- CSF
- Saliva
- Cells
- Cell culture supplements

Species

- Human
- Mouse
- Rat
- Monkey
- Cow
- Sheep
- Pig
- Dog
- Chicken
- Horse
- Rabbit
- Zebrafish
- Chinese hamster
- *C. elegans*
- Soy
- Yeast:
Pichia pastoris
- *E. coli*

Scientific impact

> 1,400 publications; > 50,000 citations; h-index 103



2021	Nature Genetics	Betto et al.	Epidemiology
2021	Nature Genetics	Lotta et al.	Epidemiology
2021	Cell Metabolism	Palma et al.	Infectiology
2020	Gut	Abot et al.	Gastroenterology
2020	Acta Neuropathologica	Demarest et al.	Neuroscience
2020	Science Translational Medicine	Riba et al.	Infectiology
2020	Hepatology	Frissen et al.	Hepatology
2020	Nature Communications	Brami-Cherrier et al.	Pharmacology

Impact factor
> 12.000



2020	Nature Communications	Arnold et al.	Neuroscience
2020	Nature Communications	Keipert et al	Nutrition
2020	Nucleic Acids Research	Tadaka et al,	Epidemiology
2020	PLoS Medicine	Atabaki-Pasdar et al.	Hepatology
2020	Genome Medicine	Reustle et al.	Oncology
2020	Microbiome	Haange et al.	Microbiomics
2020	Redox Biology	Aquilano et al.	Nutrition

Impact factor
> 9.500



2021	PNAS	Foley et al.	Microbiomics
2021	Journal of Cell Biology	Audano et al.	Development
2021	Cell Reports	Rosario et al.	Neuroscience
2021	Diabetes	Sharif et al.	Diabetology
2021	Gut microbes	Vijay et al.	Microbiomics
2021	Diabetologia	Gar et al.	Diabetology

Impact factor
> 7.000

- Higher plasma levels of lysophosphatidylcholine 18:0 are related to a lower risk of common cancers in a prospective metabolomics study. Kühn et al., *BMC Med.* 2016 Jan 28;14:13.
- Prospective analysis of circulating metabolites and breast cancer in EPIC. His et al., *BMC Med.* 2019 Sep 24;17(1):178.
- Gut microbiome influences efficacy of PD-1-based immunotherapy against epithelial tumors. Routy et al., *Science* 2018 Jan 5;359(6371):91-97.
- Serum very long-chain fatty acid-containing lipids predict response to immune checkpoint inhibitors in urological cancers. Mock et al., *Cancer Immunol Immunother.* 2019 Dec;68(12):2005-2014.
- Pharmacometabolomics study identifies circulating spermidine and tryptophan as potential biomarkers associated with the complete pathological response to trastuzumab-paclitaxel neoadjuvant therapy in HER-2 positive breast cancer. Miolo et al. *Oncotarget* 2016; 7(26):39809–22.
- Plasma Metabolomic Changes following PI3K Inhibition as Pharmacodynamic Biomarkers: Preclinical Discovery to Phase I Trial Evaluation. Ang et al., *Mol Cancer Ther* 2016; 15(6):1412–24.
- Modulation of plasma metabolite biomarkers of MAPK pathway with the MEK inhibitor RO4987655: pharmacodynamic and predictive potential in metastatic melanoma. Ang et al., *Mol Can Ther* 2017; 16(10):2315–23.
- Comparing Metabolomics Profiles in Various Types of Liquid Biopsies among Screening Participants with and without Advanced Colorectal Neoplasms. Erben et al., *Diagnostics* 2021; 11(3):561.
- Perioperative changes in the plasma metabolome of patients receiving general anesthesia for pancreatic cancer surgery. Mock-Ohnesorge et al., *Oncotarget* 2021; 12(10):996–1010.
- Targeted Metabolomics Identifies Plasma Biomarkers in Mice with Metabolically Heterogeneous Melanoma Xenografts. Weber et al., *Cancers* 2021; 13(3):434.
- Circulating metabolites as a concept beyond tumor biology determining disease recurrence after resection of colorectal liver metastasis. Jonas et al., *HBP* 2021; Jun 24; S1365-182X(21) 00586-4. doi: 10.1016/j.hpb.2021.06.415.