

List of metabolites

MxP® Quant 500 kit
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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 – Free/non-covalently bound (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	GDCA	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)		

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)			
<i>p</i> -Cresol-SO4	<i>p</i> -Cresol sulfate		

Fatty acids – Free/non-covalently bound (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	Abcsic 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

Vitamins and cofactors (1)			
Choline	Choline		

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	Valeryl carnitine	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)	Hydroxyvaleryl carnitine (Methylmalonylcarnitine)	C16-OH	Hydroxyhexadecanoylcarnitine
C5:1	Tiglylcarnitine	C16:1	Hexadecenoylcarnitine
C5:1-DC	Glutaconyl carnitine	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	Nonanoylcarnitine	C18:1-OH	Hydroxyoctadecenoylcarnitine
C10	Decanoylcarnitine	C18:2	Octadecadienylcarnitine

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	

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)	

¹ SCIEX and Agilent only

² Waters Xevo® TQ-S only

³ SCIEX, Agilent, and Waters Xevo® TQ-XS only

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)	

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)	

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⁴ Waters Xevo® TQ-XS only

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Triglycerides (242)			
TG(14:0_32:2)	TG(16:0_40:6)	TG(18:0_30:0)	TG(18:2_30:0)
TG(14:0_34:0)	TG(16:0_40:7)	TG(18:0_30:1)	TG(18:2_30:1)
TG(14:0_34:1)	TG(16:0_40:8)	TG(18:0_32:0)	TG(18:2_31:0)
TG(14:0_34:2)	TG(16:1_28:0)	TG(18:0_32:1)	TG(18:2_32:0)
TG(14:0_34:3)	TG(16:1_30:1)	TG(18:0_32:2)	TG(18:2_32:1)
TG(14:0_35:1)	TG(16:1_32:0)	TG(18:0_34:2)	TG(18:2_32:2)
TG(14:0_35:2)	TG(16:1_32:1)	TG(18:0_34:3)	TG(18:2_33:0)
TG(14:0_36:1)	TG(16:1_32:2)	TG(18:0_36:1)	TG(18:2_33:1)
TG(14:0_36:2)	TG(16:1_33:1)	TG(18:0_36:2)	TG(18:2_33:2)
TG(14:0_36:3)	TG(16:1_34:0)	TG(18:0_36:3)	TG(18:2_34:0)
TG(14:0_36:4)	TG(16:1_34:1)	TG(18:0_36:4)	TG(18:2_34:1)
TG(14:0_38:4)	TG(16:1_34:2)	TG(18:0_36:5)	TG(18:2_34:2)
TG(14:0_38:5)	TG(16:1_34:3)	TG(18:0_38:6)	TG(18:2_34:3)
TG(14:0_39:3) ¹	TG(16:1_36:1)	TG(18:0_38:7)	TG(18:2_34:4)
TG(14:0_40:5) ⁶	TG(16:1_36:2)	TG(18:1_26:0)	TG(18:2_35:1)
TG(16:0_28:1)	TG(16:1_36:3)	TG(18:1_28:1)	TG(18:2_35:2)
TG(16:0_28:2)	TG(16:1_36:4)	TG(18:1_30:0)	TG(18:2_35:3)
TG(16:0_30:2)	TG(16:1_36:5)	TG(18:1_30:1)	TG(18:2_36:0)
TG(16:0_32:0)	TG(16:1_38:3)	TG(18:1_30:2)	TG(18:2_36:1)
TG(16:0_32:1)	TG(16:1_38:4)	TG(18:1_31:0)	TG(18:2_36:2)
TG(16:0_32:2)	TG(16:1_38:5)	TG(18:1_32:0)	TG(18:2_36:3)
TG(16:0_32:3)	TG(17:0_32:1)	TG(18:1_32:1)	TG(18:2_36:4)
TG(16:0_33:1)	TG(17:0_34:1)	TG(18:1_32:2)	TG(18:2_36:5)
TG(16:0_33:2)	TG(17:0_34:2)	TG(18:1_32:3)	TG(18:2_38:4)
TG(16:0_34:0)	TG(17:0_34:3)	TG(18:1_33:0)	TG(18:2_38:5)
TG(16:0_34:1)	TG(17:0_36:3)	TG(18:1_33:1)	TG(18:2_38:6)
TG(16:0_34:2)	TG(17:0_36:4)	TG(18:1_33:2)	TG(18:3_30:0)
TG(16:0_34:3)	TG(17:1_32:1)	TG(18:1_33:3)	TG(18:3_32:0)
TG(16:0_34:4)	TG(17:1_34:1)	TG(18:1_34:1)	TG(18:3_32:1)
TG(16:0_35:1)	TG(17:1_34:2)	TG(18:1_34:2)	TG(18:3_33:2)
TG(16:0_35:2)	TG(17:1_34:3)	TG(18:1_34:3)	TG(18:3_34:0)
TG(16:0_35:3)	TG(17:1_36:3)	TG(18:1_34:4)	TG(18:3_34:1)
TG(16:0_36:2)	TG(17:1_36:4)	TG(18:1_35:2)	TG(18:3_34:2)
TG(16:0_36:3)	TG(17:1_36:5)	TG(18:1_35:3)	TG(18:3_34:3)
TG(16:0_36:4)	TG(17:1_38:5)	TG(18:1_36:0)	TG(18:3_35:2)
TG(16:0_36:5)	TG(17:1_38:6)	TG(18:1_36:1)	TG(18:3_36:1)
TG(16:0_36:6)	TG(17:1_38:7)	TG(18:1_36:2)	TG(18:3_36:2)
TG(16:0_37:3)	TG(17:2_34:2)	TG(18:1_36:3)	TG(18:3_36:3)
TG(16:0_38:1)	TG(17:2_34:3)	TG(18:1_36:4)	TG(18:3_36:4)
TG(16:0_38:2)	TG(17:2_36:2)	TG(18:1_36:5)	TG(18:3_38:5)
TG(16:0_38:3)	TG(17:2_36:3)	TG(18:1_36:6)	TG(18:3_38:6)
TG(16:0_38:4)	TG(17:2_36:4)	TG(18:1_38:5)	TG(20:0_32:3)
TG(16:0_38:5)	TG(17:2_38:5)	TG(18:1_38:6)	TG(20:0_32:4)
TG(16:0_38:6)	TG(17:2_38:6)	TG(18:1_38:7)	TG(20:0_34:1)
TG(16:0_38:7)	TG(17:2_38:7)	TG(18:2_28:0)	TG(20:1_24:3)

¹ SCIEX and Agilent only

⁶ Waters only

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

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