

# List of metabolites

AbsoluteIDQ<sup>®</sup> p400 HR kit

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## AbsoluteIDQ® p400 HR – List of metabolites

### Best resolution

The AbsoluteIDQ® p400 HR kit is the first ready-to-use, standardized solution for broad lipid and metabolic profiling on Q Exactive™ mass spectrometers. It provides quantification of more than 400 metabolites and lipids from 11 compound classes covering central metabolic pathways.

Analyte class (number of metabolites)		Analytical method
Small molecules (43)	Amino acids (21)	LC-MS/MS
	Biogenic amines (21)	
	Carbohydrates and related (1)	
Lipids (145)	Acylcarnitines (55)	FIA-MS/MS
	Lysophosphatidylcholines (24)	
	Phosphatidylcholines (172)	
	Sphingomyelins (31)	
	Ceramides (9)	
	Cholesteryl esters (14)	
	Diglycerides (18)	
	Triglycerides (42)	

### Amino acids (21)

Ala	Alanine	Lys	Lysine
Arg	Arginine	Met	Methionine
Asn	Asparagine	Orn	Ornithine
Asp	Aspartate	Phe	Phenylalanine
Cit	Citrulline	Pro	Proline
Glu	Glutamate	Ser	Serine
Gln	Glutamine	Thr	Threonine
Gly	Glycine	Trp	Tryptophan
His	Histidine	Tyr	Tyrosine
Ile	Isoleucine*	Val	Valine
xLeu	Leucine + Isoleucine		

\* analyzed by additional LC-MS injection in parallel reaction monitoring (PRM) mode

### Biogenic amines (21)

Ac-Orn	Acetylornithine	<b>Met-SO</b>	Methionine sulfoxide
alpha-AAA	alpha-Amino adipic acid	Nitro-Tyr	Nitrotyrosine
ADMA	Asymmetric dimethylarginine	PEA	Phenylethylamine
Carnosine	Carnosine	Putrescine	Putrescine
Creatinine	Creatinine	Sarcosine	Sarcosine
DOPA	Dihydroxyphenylalanine	Serotonin	Serotonin
Dopamine	Dopamine	Spermidine	Spermidine
Histamine	Histamine	Spermine	Spermine
c4-OH-Pro	<i>cis</i> -4-Hydroxyproline	SDMA	Symmetric dimethylarginine
<b>t4-OH-Pro</b>	<i>trans</i> -4-Hydroxyproline	Taurine	Taurine
Kynurenine	Kynurenine		

### Carbohydrates and related (1)

H1	Hexoses (including glucose)		
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### Acylcarnitines (55)

AC(0:0)	Carnitine	AC(5:0-DC)	Glutaryl carnitine
AC(2:0)	Acetylcarnitine	AC(5:0-OH)	Hydroxyvalerylcarnitine
AC(3:0)	Propionyl carnitine	AC(5:1)	Tiglylcarnitine
AC(3:0-DC)	Malonylcarnitine	AC(5:1-DC)	Glutaconyl carnitine
AC(3:0-OH)	Hydroxypropionyl carnitine	AC(6:0)	Hexanoylcarnitine
AC(3:1)	Propenoylcarnitine	AC(6:0-DC)	Adipoylcarnitine
AC(4:0)	Butyrylcarnitine	AC(6:0-OH)	Hydroxyhexanoylcarnitine
AC(4:0-DC)	Methylmalonylcarnitine	AC(6:1)	Hexenoylcarnitine
AC(4:0-OH)	Hydroxybutyrylcarnitine	AC(7:0)	Heptanoylcarnitine
AC(4:1)	Butenyl carnitine	AC(7:0-DC)	Pimeloylcarnitine
AC(4:1-DC)	Fumaryl carnitine	AC(8:0)	Octanoylcarnitine
AC(5:0)	Valerylcarnitine	AC(8:1)	Octenoylcarnitine

Acylcarnitines (continued)			
AC(8:1-OH)	Hydroxyoctenoylcarnitine	AC(14:2)	Tetradecadienoylcarnitine
AC(9:0)	Nonacylcarnitine	AC(14:2-OH)	Hydroxytetradecadienoylcarnitine
AC(10:0)	Decanoylcarnitine	AC(15:0)	Pentadecanoylcarnitine
AC(10:1)	Decenoylcarnitine	AC(16:0)	Hexadecanoylcarnitine
AC(10:2)	Decadienoylcarnitine	AC(16:0-OH)	Hydroxyhexadecanoylcarnitine
AC(10:3)	Decatrienoylcarnitine	AC(16:1)	Hexadecenoylcarnitine
AC(11:0)	Dimethylnonanoylcarnitine	AC(16:1-OH)	Hydroxyhexadecenoylcarnitine
AC(12:0)	Dodecanoylcarnitine	AC(16:2)	Hexadecadienoylcarnitine
AC(12:0-DC)	Dodecanedioylcarnitine	AC(16:2-OH)	Hydroxyhexadecadienoylcarnitine
AC(12:1)	Dodecenoylcarnitine	AC(17:0)	Heptadecanoylcarnitine
AC(13:0)	Tridecanoylcarnitine	AC(18:0)	Octadecanoylcarnitine
AC(14:0)	Tetradecanoylcarnitine	AC(18:1)	Octadecenoylcarnitine
AC(14:0-OH)	Hydroxymyristoylcarnitine	AC(18:1-OH)	Hydroxyoctadecenoylcarnitine
AC(14:1)	Tetradecenoylcarnitine	AC(18:2)	Octadecadienylcarnitine
AC(14:1-DC)	Carboxytridecenoylcarnitine	AC(19:0)	Nonadecanoylcarnitine
AC(14:1-OH)	Hydroxytetradecenoylcarnitine		

Lysophosphatidylcholines (24)			
LPC(12:0)	LPC(17:1)	LPC(20:2)	LPC(24:1)
LPC(14:0)	LPC(18:0)	LPC(20:3)	LPC-O(16:1)
LPC(15:0)	LPC(18:1)	LPC(20:4)	LPC-O(17:1)
LPC(16:0)	LPC(18:2)	LPC(22:5)	LPC-O(18:0)
LPC(16:1)	LPC(20:0)	LPC(22:6)	LPC-O(18:1)
LPC(17:0)	LPC(20:1)	LPC(24:0)	LPC-O(18:2)

Phosphatidylcholines (172)			
PC(24:0)	PC(32:1)	PC(35:0)	PC(37:5)
PC(25:0)	PC(32:2)	PC(35:1)	PC(37:6)
PC(26:0)	PC(32:3)	PC(35:2)	PC(37:7)
PC(27:0)	PC(32:4)	PC(35:3)	PC(38:0)
PC(27:1)	PC(32:5)	PC(35:4)	PC(38:1)
PC(28:1)	PC(32:6)	PC(35:5)	PC(38:2)
PC(29:0)	PC(33:0)	PC(36:0)	PC(38:3)
PC(29:1)	PC(33:1)	PC(36:1)	PC(38:4)
PC(29:2)	PC(33:2)	PC(36:2)	PC(38:5)
PC(30:0)	PC(33:3)	PC(36:3)	PC(38:6)
PC(30:1)	PC(33:4)	PC(36:4)	PC(38:7)
PC(30:2)	PC(33:5)	PC(36:5)	PC(39:0)
PC(30:3)	PC(34:0)	PC(36:6)	PC(39:1)
PC(31:0)	PC(34:1)	PC(37:0)	PC(39:2)
PC(31:1)	PC(34:2)	PC(37:1)	PC(39:3)
PC(31:2)	PC(34:3)	PC(37:2)	PC(39:4)
PC(31:3)	PC(34:4)	PC(37:3)	PC(39:5)
PC(32:0)	PC(34:5)	PC(37:4)	PC(39:6)



Phosphatidylcholines (continued)			
PC(39:7)	PC(43:2)	PC-O(32:3)	PC-O(38:2)
PC(40:1)	PC(43:6)	PC-O(33:0)	PC-O(38:3)
PC(40:2)	PC(44:1)	PC-O(33:1)	PC-O(38:4)
PC(40:3)	PC(44:3)	PC-O(33:2)	PC-O(38:5)
PC(40:4)	PC(44:5)	PC-O(33:3)	PC-O(38:6)
PC(40:5)	PC(44:6)	PC-O(33:4)	PC-O(40:0)
PC(40:6)	PC(44:7)	PC-O(33:6)	PC-O(40:1)
PC(40:7)	PC(44:10)	PC-O(34:0)	PC-O(40:2)
PC(40:8)	PC(44:12)	PC-O(34:1)	PC-O(40:3)
PC(40:9)	PC(46:1)	PC-O(34:2)	PC-O(40:4)
PC(41:1)	PC(46:2)	PC-O(34:3)	PC-O(40:5)
PC(41:2)	PC-O(26:0)	PC-O(34:4)	PC-O(40:6)
PC(41:3)	PC-O(26:1)	PC-O(35:3)	PC-O(40:7)
PC(41:4)	PC-O(28:0)	PC-O(35:4)	PC-O(40:8)
PC(41:5)	PC-O(28:1)	PC-O(36:0)	PC-O(42:0)
PC(41:8)	PC-O(29:0)	PC-O(36:1)	PC-O(42:1)
PC(42:0)	PC-O(30:0)	PC-O(36:2)	PC-O(42:2)
PC(42:1)	PC-O(30:1)	PC-O(36:3)	PC-O(42:3)
PC(42:2)	PC-O(30:2)	PC-O(36:4)	PC-O(42:4)
PC(42:3)	PC-O(31:0)	PC-O(36:5)	PC-O(42:5)
PC(42:4)	PC-O(31:1)	PC-O(36:6)	PC-O(42:6)
PC(42:5)	PC-O(31:3)	PC-O(37:6)	PC-O(44:3)
PC(42:6)	PC-O(32:0)	PC-O(37:7)	PC-O(44:4)
PC(42:7)	PC-O(32:1)	PC-O(38:0)	PC-O(44:5)
PC(42:10)	PC-O(32:2)	PC-O(38:1)	PC-O(44:6)

Sphingomyelins (31)			
SM(30:1)	SM(34:2)	SM(38:3)	SM(42:1)
SM(31:0)	SM(35:1)	SM(39:1)	SM(42:2)
SM(31:1)	SM(36:0)	SM(39:2)	SM(42:3)
SM(32:1)	SM(36:1)	SM(40:1)	SM(43:1)
SM(32:2)	SM(36:2)	SM(40:2)	SM(43:2)
SM(33:1)	SM(37:1)	SM(40:4)	SM(44:1)
SM(33:2)	SM(38:1)	SM(41:1)	SM(44:2)
SM(34:1)	SM(38:2)	SM(41:2)	

Ceramides (9)			
Cer(34:0)	Cer(40:1)	Cer(42:2)	
Cer(34:1)	Cer(41:1)	Cer(43:1)	
Cer(38:1)	Cer(42:1)	Cer(44:0)	

#### Cholesteryl esters (14)

CE(16:0)	CE(17:2)	CE(19:2)	CE(22:5)
CE(16:1)	CE(18:1)	CE(19:3)	CE(22:6)
CE(17:0)	CE(18:2)	CE(20:4)	
CE(17:1)	CE(18:3)	CE(20:5)	

#### Diglycerides (18)

DG(32:1)	DG(36:3)	DG(41:1)	DG-O(32:2)
DG(32:2)	DG(36:4)	DG(42:0)	DG-O(34:1)
DG(34:1)	DG(38:0)	DG(42:1)	DG-O(36:4)
DG(34:3)	DG(38:5)	DG(42:2)	
DG(36:2)	DG(39:0)	DG(44:3)	

#### Triglycerides (42)

TG(44:1)	TG(50:3)	TG(52:6)	TG(54:7)
TG(44:2)	TG(50:4)	TG(52:7)	TG(55:6)
TG(44:4)	TG(51:1)	TG(53:3)	TG(55:7)
TG(46:2)	TG(51:2)	TG(53:4)	TG(55:8)
TG(48:1)	TG(51:3)	TG(53:5)	TG(55:9)
TG(48:2)	TG(51:4)	TG(53:6)	TG(56:6)
TG(48:3)	TG(51:5)	TG(54:2)	TG(56:7)
TG(49:1)	TG(52:2)	TG(54:3)	TG(56:8)
TG(49:2)	TG(52:3)	TG(54:4)	TG(56:9)
TG(50:1)	TG(52:4)	TG(54:5)	
TG(50:2)	TG(52:5)	TG(54:6)	

## Ordering

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