

# AbsoluteIDQ<sup>®</sup> p400 HR kit

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List of metabolites

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## AbsoluteIDQ® p400 HR – List of metabolites

### Broad quantitative metabolic profiling with Thermo Orbitrap mass spectrometers

Powered by biocrates’ standardized, quality-controlled, and reproducible metabolomics technology, the AbsoluteIDQ® p400 HR kit offers a high-resolution workflow for clinical and epidemiological research. It provides quantification of more than 400 lipids and small molecules 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 (365)	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	Met-SO	Methionine sulfoxide
alpha-AAA	alpha-Aminoadipic 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
t4-OH-Pro	<i>trans</i> -4-Hydroxyproline	Taurine	Taurine
Kynurenine	Kynurenine		

Carbohydrates and related (1)			
Hexose	Hexoses (including glucose)		

Acylcarnitines (55)			
AC(0:0)	Carnitine	AC(4:0-OH)	Hydroxybutyrylcarnitine
AC(2:0)	Acetylcarnitine	AC(4:1)	Butenylcarnitine
AC(3:0)	Propionylcarnitine	AC(4:1-DC)	Fumarylacarnitine
AC(3:0-DC)	Malonylcarnitine	AC(5:0)	Valerylcarnitine
AC(3:0-OH)	Hydroxypropionylcarnitine	AC(5:0-DC)	Glutarylacarnitine
AC(3:1)	Propenoylcarnitine	AC(5:0-OH)	Hydroxyvalerylcarnitine
AC(4:0)	Butyrylcarnitine	AC(5:1)	Tiglylcarnitine
AC(4:0-DC)	Methylmalonylcarnitine	AC(5:1-DC)	Glutaconylcarnitine

Acylcarnitines (continued)			
AC(6:0)	Hexanoylcarnitine	AC(14:0-OH)	Hydroxymyristoylcarnitine
AC(6:0-DC)	Adipoylcarnitine	AC(14:1)	Tetradecenoylcarnitine
AC(6:0-OH)	Hydroxyhexanoylcarnitine	AC(14:1-DC)	Carboxytridecenoylcarnitine
AC(6:1)	Hexenoylcarnitine	AC(14:1-OH)	Hydroxytetradecenoylcarnitine
AC(7:0)	Heptanoylcarnitine	AC(14:2)	Tetradecadienoylcarnitine
AC(7:0-DC)	Pimeloylcarnitine	AC(14:2-OH)	Hydroxytetradecadienoylcarnitine
AC(8:0)	Octanoylcarnitine	AC(15:0)	Pentadecanoylcarnitine
AC(8:1)	Octenoylcarnitine	AC(16:0)	Hexadecanoylcarnitine
AC(8:1-OH)	Hydroxyoctenoylcarnitine	AC(16:0-OH)	Hydroxyhexadecanoylcarnitine
AC(9:0)	Nonanoylcarnitine	AC(16:1)	Hexadecenoylcarnitine
AC(10:0)	Decanoylcarnitine	AC(16:1-OH)	Hydroxyhexadecenoylcarnitine
AC(10:1)	Decenoylcarnitine	AC(16:2)	Hexadecadienoylcarnitine
AC(10:2)	Decadienoylcarnitine	AC(16:2-OH)	Hydroxyhexadecadienoylcarnitine
AC(10:3)	Decatrienoylcarnitine	AC(17:0)	Heptadecanoylcarnitine
AC(11:0)	Dimethylnonanoylcarnitine	AC(18:0)	Octadecanoylcarnitine
AC(12:0)	Dodecanoylcarnitine	AC(18:1)	Octadecenoylcarnitine
AC(12:0-DC)	Dodecanedioylcarnitine	AC(18:1-OH)	Hydroxyoctadecenoylcarnitine
AC(12:1)	Dodecenoylcarnitine	AC(18:2)	Octadecadienylcarnitine
AC(13:0)	Tridecanoylcarnitine	AC(19:0)	Nonadecanoylcarnitine
AC(14:0)	Tetradecanoylcarnitine		

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(30:1)	PC(32:3)	PC(34:0)
PC(25:0)	PC(30:2)	PC(32:4)	PC(34:1)
PC(26:0)	PC(30:3)	PC(32:5)	PC(34:2)
PC(27:0)	PC(31:0)	PC(32:6)	PC(34:3)
PC(27:1)	PC(31:1)	PC(33:0)	PC(34:4)
PC(28:1)	PC(31:2)	PC(33:1)	PC(34:5)
PC(29:0)	PC(31:3)	PC(33:2)	PC(35:0)
PC(29:1)	PC(32:0)	PC(33:3)	PC(35:1)
PC(29:2)	PC(32:1)	PC(33:4)	PC(35:2)
PC(30:0)	PC(32:2)	PC(33:5)	PC(35:3)



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

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