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# List of metabolites

AbsoluteIDQ® 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) | FIA-MS/MS |
| Lipids (145) | Acylcarnitines (55) | |
| | 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 | *cis*-4-Hydroxyproline | SDMA | Symmetric dimethylarginine |
| t4-OH-Pro | *trans*-4-Hydroxyproline | Taurine | Taurine |
| Kynurenine | Kynurenine | | |

| Carbohydrates and related (1) | | | |
|---|---|---|---|
| H1 | Hexoses (including glucose) | | |

| Acylcarnitines (55) | | | |
|---|---|---|---|
| AC(0:0) | Carnitine | AC(5:0-DC) | Glutarylcarnitine |
| AC(2:0) | Acetylcarnitine | AC(5:0-OH) | Hydroxyvalerylcarnitine |
| AC(3:0) | Propionylcarnitine | AC(5:1) | Tiglylcarnitine |
| AC(3:0-DC) | Malonylcarnitine | AC(5:1-DC) | Glutaconylcarnitine |
| AC(3:0-OH) | Hydroxypropionylcarnitine | 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) | Butenylcarnitine | AC(7:0-DC) | Pimeloylcarnitine |
| AC(4:1-DC) | Fumarylcarnitine | 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) | Nonaylcarnitine | 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) | |

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