

# SMartIDQ alpha kit

List of metabolites

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## SMartIDQ alpha kit – List of metabolites

### Metabolomics in service laboratories and consumer applications

The SMartIDQ alpha is our kit for service laboratory operations making metabolomics easy and scalable at the right level of depth. Handling and throughput are attuned to higher sample numbers and turnover demands. The coverage allows for different panels to be covered adapting to changing requirements.

Analyte class (number of metabolites)		Analytical method
Small molecules (107)	Alkaloids (1)	LC-MS/MS
	Amine oxides (1)	
	Amino acids (20)	
	Amino acid related (31)	
	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)	

Alkaloids (1)			
Trigonelline	Trigonelline		

Amine oxides (1)			
TMAO	Trimethylamine N-oxide		

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 (31)**

alpha-AAA	$\alpha$ -Amino adipic acid	c4-OH-Pro	<i>cis</i> -4-Hydroxyproline
AABA	$\alpha$ -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	$\beta$ -Aminobutyric acid	Nitro-Tyr	Nitrotyrosine
Betaine	Betaine	Orn	Ornithine
C0	Carnitine	PAG	Phenylacetyl glycine
Carnosine	Carnosine	PheAlaBetaine	Phenylalanine betaine
Cit	Citrulline	ProBetaine	Proline betaine
Creatinine	Creatinine	Sarcosine	Sarcosine
Cystine	Cystine	SDMA	Symmetric dimethylarginine
DOPA	Dihydroxyphenylalanine	Taurine	Taurine
HArg	Homoarginine	TrpBetaine	Tryptophan betaine
HCys	Homocysteine		

**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	$\beta$ -Alanine	Putrescine	Putrescine
GABA	$\gamma$ -Aminobutyric acid	Serotonin	Serotonin
Dopamine	Dopamine	Spermidine	Spermidine
Histamine	Histamine	Spermine	Spermine
PEA	Phenylethylamine		

**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		
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#### 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	FA 20:4	Arachidonic acid (AA; $\omega$ 6)
FA 18:1	Octadecenoic acid	FA 20:5	Eicosapentaenoic acid (EPA; $\omega$ 3)
FA 18:2	Octadecadienoic acid	FA 22:6	Docosahexaenoic acid (DHA; $\omega$ 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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## Ordering

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