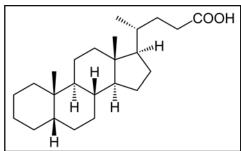
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Assay Sheet: Biocrates Bile Acids Kit

Description:

This targeted metabolomics approach is based on reversed phase liquid chromatography-electrospray ionization tandem mass spectrometry measurements (LC-ESI-MS/MS) by Bile Acids Kit (biocrates life sciences ag).

The assay allows simultaneous quantification of 20 bile acids out of 10 μ L plasma or similar volumes of other



biological material or extracts, and includes cholic acid, chenodeoxycholic acid, deoxycholic acid, glycocholic acid, glycochenodeoxycholic acid, glycodeoxycholic acid, glycolithocholic acid, glycoursodeoxycholic acid, hyodeoxycholic acid, lithocholic acid, alpha-muricholic acid, beta-muricholic acid, omega-murichoclic acid, taurocholic acid, taurochenodeoxycholic acid, taurodeoxycholic acid, taurolithocholic acid, tauromuricholic acid (sum of alpha and beta), tauroursodeoxycholic acid, ursodeoxycholic acid. Compound identification and quantification are based on scheduled multiple reaction monitoring measurements (sMRM).

Sample handling is performed by a Hamilton Microlab STARTM robot, beside standard laboratory equipment. Mass spectrometric analyses are done on a SCIEX API 4000 triple quadrupole system equipped with an Agilent 1260 Series HPLC and a CTC HTC-xc PAL auto sampler. Quantitative data evaluation and quality assessment are performed with the SCIEX software MultiQuant and the BIOCRATES MetIDQTM software package. Metabolite concentrations are calculated using internal standards and reported in μ M.

Each measurement batch additionally includes five aliquots of a pooled reference plasma as well as three aliquots of a spiked quality control sample. The results of these reference plasma and quality control samples can be used for calculation of potential batch effects and data normalization of different measurements.

Matrices:

- Plasma (min. 50 μl)
- Serum (min. 50 μl)
- Tissue (25-50 mg)
- Feces (25-50 mg)

Tissue types:

- Liver
- White Adipose Tissue

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Species

- Human
- Mouse
- Rat
- Hamster
- Sheep
- Bovine
- Porcine

Selected References

McCreight LJ, Stage TB, Connelly P, Lonergan M, Nielsen F, Prehn C, Adamski J, Brosen K, Pearson ER (2018) Pharmacokinetics of metformin in patients with gastrointestinal intolerance. Diabetes Obes Metab 20: 1593-1601

Pham HT, Arnhard K, Asad YJ, Deng L, Felder TK, St. John-Williams L, Kaever V, Leadley M, Mitro N, Muccio S, Prehn C, Rauh M, Rolle-Kampczyk U, Thompson JW, Uhl O, Ulaszewska M, Vogeser M, Wishart DS, Koal T (2016) Inter-Laboratory Robustness of Next-Generation Bile Acid Study in Mice and Humans: International Ring Trial Involving 12 Laboratories. The Journal of Applied Laboratory Medicine: An AACC Publication: 129-142

Metabolite Overview:

Metabolite Class	Acronym	Number of Metabolites
Bile Acids	BA	20

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Detailed List of Metabolites:

Abbrev.	Name	Metabolite Class	Formula	ChEBI
CA	Cholic acid	Bile Acid	C24H40O5	CHEBI:16359
CDCA	Chenodeoxycholic acid	Bile Acid	C24H40O4	CHEBI:16755
DCA	Deoxycholic acid	Bile Acid	C24H40O4	CHEBI:28834
GCA	Glycocholic acid	Bile Acid	C26H43NO6	CHEBI:17687
GCDCA	Glycochenodeoxycholic acid	Bile Acid	C26H43NO5	CHEBI:36274
GDCA	Glycodeoxycholic acid	Bile Acid	C26H43NO5	CHEBI:27471
GLCA	Glycolithocholic acid	Bile Acid	C26H43NO4	CHEBI:37998
GUDCA	Glycoursodeoxycholic acid	Bile Acid	C26H43NO5	CHEBI:89929
HDCA	Hyodeoxycholic acid	Bile Acid	C24H40O4	CHEBI:52023
LCA	Lithocholic acid	Bile Acid	C24H40O3	CHEBI:16325
MCA(a)	Alpha-Muricholic acid	Bile Acid	C24H40O5	CHEBI:81243
MCA(b)	Beta-Muricholic acid	Bile Acid	C24H40O5	CHEBI:81298
MCA(o)	Omega-Muricholic acid	Bile Acid	C24H40O5	CHEBI:81299
TCA	Taurocholic acid	Bile Acid	C26H45NO7S	CHEBI:28865
TCDCA	Taurochenodeoxycholic acid	Bile Acid	C26H45NO6S	CHEBI:16525
TDCA	Taurodeoxycholic acid	Bile Acid	C26H45NO6S	CHEBI:9410
TLCA	Taurolithocholic acid	Bile Acid	C26H45NO5S	CHEBI:36259
TMCA (a+b)	Tauromuricholic acid (sum of alpha and beta)	Bile Acid	C26H45NO7S	alpha: CHEBI:139136 beta: CHEBI:133057
TUDCA	Tauroursodeoxycholic acid	Bile Acid	C26H45NO6S	CHEBI:80774
UDCA	Ursodeoxycholic acid	Bile Acid	C24H40O4	CHEBI:9907