Separation Workflow

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Overall study design

Title of the study	Workflow for biomarker discovery using soil lipidome		
Document creation date	11/26/2023	Corresponding Email	rahul.samrat@univie.ac.at
Principle investigator	Univ. Prof. Dr. Wolfgang Wanek	Is the workflow targeted or untargeted?	-
Institution	University of vienna	Clinical	No

Lipid extraction

Extraction method	2-phase system	2-phase system	Bligh&Dyer
pH adjustment	None	Were internal standards added prior extraction?	Yes

Analytical platform

Number of separation dimensions	One dimension	Ion source	ESI
Separation Type 1	LC	MS Level	MS1, MS2
Separation Mode 1	RP	Mass resolution for detected ion at MS1	High resolution
Separation window (1) for lipid analyte selection (±) in minutes	1	Resolution at m/z 200 at MS1	70000
RT verified by standard	Yes	Mass accuracy in ppm at MS1	5
CCS verified by standard	Yes	Mass window for precursor ion isolation (in Da total isolation window)	10
Separation of isobaric/isomeric interferece confirmed	No	Mass resolution for detected ion at MS2	Low resolution
Model for separation prediction	Yes	Resolution in Da at MS2	17000
MS type	Orbitrap	Was/Were additional dimension/techniques used	No
MS vendor	Thermo		

Quality control

Blanks	Yes	Quality control	Yes
Type of Blanks	Extraction blank, Injection blank	Type of QC sample	Commercial sample, Sample pool

Method qualification and validation

Method validation	Yes	Precison	Yes
Lipid recovery	Yes	Accuracy	Yes
Dynamic quantification range	Yes	Guidelines followed	None
Limit of quantitation (LOQ)/Limit of detection (LOD)	Yes		

Reporting

Are reported raw data uploaded into repository?	Available on request	Additional comments	-
Raw data upload	Available on request		

Sample Descriptions

Bacterial IPLs / Bacteria / Cells

Provided information	Storage time (month), Freeze-thaw cycles	Freeze-thaw cycles	3
Temperature handling original sample	4-8 °C	Additives	None
Instant sample preparation	No	Were samples stored under inert gas?	No
Storage temperature	-20 °C	Additional preservation methods	No
Storage time (month)	14	Biobank samples	No