

Overall study design

Title of the study	Single Cell lipidomics		
Document creation date	03/21/2023	Corresponding Email	dominik.kopczynski@univie.ac.at
Principle investigator	Dominik Kopczynski	Is the workflow targeted or untargeted?	Targeted
Institution	University of Vienna	Clinical	No

Lipid extraction

Extraction method	1-phase system	1-phase system	Acetonitrile
pH adjustment	Hydrochloric acid	Were internal standards added prior extraction?	Yes

Analytical platform

MS type	Q	MS Level	MS1
MS vendor	Bruker	Mass resolution for detected ion at MS1	Low resolution
Ion source	ESI	Resolution in Da at MS1	200000
Direct type	Syringe	Was/Were additional dimension/techniques used	Yes

Quality control

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

Method qualification and validation

Method validation	Yes	Precision	Yes
Lipid recovery	Yes	Accuracy	No
Dynamic quantification range	No	Guidelines followed	EMA
Limit of quantitation (LOQ)/Limit of detection (LOD)	No		

Reporting

Are reported raw data uploaded into repository?	Yes	Raw data upload	Available on request
Are metadata available?	No	Additional comments	-
Summary data	Quantification and identification data		

Sample Descriptions

MM201 / Mouse / Plasma

Provided information	Storage time (month)	Additives	None
Temperature handling original sample	4-8 °C	Were samples stored under inert gas?	No
Instant sample preparation	No	Additional preservation methods	Yes
Storage temperature	Room temperature	Type of preservation method	Deep freezer
Storage time (month)	3	Biobank samples	No

Lipid Class Descriptions

1) TG[M-H]- / Lipid identification

Lipid class	TG	Check isomer overlap	No
MS Level for identification	MS1	Additional dimension/techniques	IMS
Identification level	Molecular species level	How was/were the additional dimension(s) used?	For separation of isobaric/isomeric interferece
Polarity mode	Negative	Was a model used to predict lipid molecule separation?	Yes
Type of negative (precursor)ion	[M-H]-	Lipid Identification Software	Homemade
Isotope correction at MS1	No	Data manipulation	Centroiding
MS1 verified by standard	No	Nomenclature for intact lipid molecule	No
Background check at MS1	No		

1) TG[M-H]- / For additional separation methods/analytical dimension

Quantitative	No	Batch correction	No
Normalization to reference	No		

2) CL[M-2H]2- / Lipid identification

Lipid class	CL	Check isomer overlap	No
MS Level for identification	MS1	Additional dimension/techniques	IMS
Identification level	Molecular species level	How was/were the additional dimension(s) used?	For separation of isobaric/isomeric interferece
Polarity mode	Negative	Was a model used to predict lipid molecule separation?	Yes
Type of negative (precursor)ion	[M-2H]2-	Lipid Identification Software	Homemade
Isotope correction at MS1	No	Data manipulation	Centroiding
MS1 verified by standard	No	Nomenclature for intact lipid molecule	No
Background check at MS1	No		

2) CL[M-2H]2- / For additional separation methods/analytical dimension

Quantitative	No	Batch correction	No
Normalization to reference	No		

3) Cer[M+H]+ / Lipid identification

Lipid class	Cer	Check isomer overlap	No
MS Level for identification	MS1	Additional dimension/techniques	IMS
Identification level	Molecular species level	How was/were the additional dimension(s) used?	For separation of isobaric/isomeric interferece
Polarity mode	Positive	Was a model used to predict lipid molecule separation?	Yes
Type of positive (precursor)ion	[M+H]+	Lipid Identification Software	Homemade
Isotope correction at MS1	Type 2	Data manipulation	Smoothing, Centroiding
MS1 verified by standard	Yes	Nomenclature for intact lipid molecule	No
Background check at MS1	Yes		

3) Cer[M+H]+ / For additional separation methods/analytical dimension

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS2	Limit of quantification	No
Internal lipid standard(s) for MS2		Normalization to reference	No
Internal standard	Fragment(s)	Endogenous class	
Cer 18:1;O2/12:0	LCB-H2O3	Cer 18:1;O2/XX:X	
Type of quantification	Internal standard amount	Lipid Quantification Software	LipidXplorer
Response correction	No	Batch correction	No