Direct Infusion Workflow

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Overall study design

Title of the study	Glycerophospholipid remodeling is critical for orthoflavivirus infection		
Document creation date	01/11/2024	Corresponding Email	dschwudke@fz-borstel.de
Principle investigator	Dominik Schwudke	Is the workflow targeted or untargeted?	Untargeted
Institution	Research Center Borstel	Clinical	No

Lipid extraction

Extraction method	2-phase system	2-phase system	MTBE
pH adjustment	acetic acid addition	Were internal standards added prior extraction?	Yes

Analytical platform

Which solvent was used	IPA:Methanol:Chloroform(4:2:1) + Amonium acetate	Resolution at m/z 200 at MS1	288000
Detector	Mass spectrometer	Mass accuracy in ppm at MS1	4
MS type	Q Exactive	Mass window for precursor ion isolation (in Da total isolation window)	1
MS vendor	Thermo	Mass resolution for detected ion at MS2	High resolution
Direct type	Chip	Resolution at m/z 200 at MS2	70000
MS Level	MS1, MS2	Mass accuracy in ppm at MS2	4
Mass resolution for detected ion at MS1	High resolution	Was/Were additional dimension/techniques used	No

Quality control

Blanks	Yes	Quality control	No
Type of Blanks	Extraction blank		

Method qualification and validation

Method validation	No

Reporting

Are reported raw data uploaded into repository?	No	Raw data upload	No
Are metadata available?	Yes	Additional comments	Further information are available at https://lifs-tools.org/

Sample Descriptions

Huh7 cells with/without viral infection / Cell line Huh7 / Cells

Provided information	-	Additives	BHT
Temperature handling original sample	Room temperature	Were samples stored under inert gas?	No
Instant sample preparation	No	Additional preservation methods	No
Storage temperature	-80 °C	Biobank samples	No

Lipid Class Descriptions

1) CE[M+NH4]+ / Lipid identification

Lipid class	CE	Background check at MS1	Yes
MS Level for identification	MS1, MS2	Background check at MS2	Yes
Identification level	Species level	Did you presume assumptions for identification?	No
Polarity mode	Positive	Check isomer overlap	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
-FA1(+HO)-Cholesterol(35)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-

1) CE[M+NH4]+ / Lipid quantification

Quantitative	Yes	Type I isotope correction	Yes
MS Level for quantification	MS1, MS2	Limit of quantification	No
Internal lipid standard(s) MS1		Normalization to reference	Yes

Internal standard	Endogenous subclass
18:1(d7) Chol Ester	

Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
18:1(d7) Chol Ester	-FA1(+HO)-Cholesterol(35)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-

2) Cer[M+CH3COO]- / Lipid identification

Lipid class	Cer	Did you presume assumptions for identification?	Yes
MS Level for identification	MS1	Which assumptions were presumed?	Even numbered fatty acids, Even numbered sphingosine,
Identification level	Species level	Check isomer overlap	Yes
Polarity mode	Negative	Additional dimension/techniques	-
Type of negative (precursor)ion	[M+CH3COO]-	Lipid Identification Software	LipidXplorer
Isotope correction at MS1	Type 2	Data manipulation	-
MS1 verified by standard	Yes	Nomenclature for intact lipid molecule	No
Background check at MS1	Yes	Further identification remarks	-

2) Cer[M+CH3COO]- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS1	Normalization to reference	Yes
Internal lipid standard(s) MS1		Lipid Quantification Software	LipidXplorer
Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

Internal standard	Endogenous subclass
C15 Ceramide-d7 (d18:1-d7/15:0)	

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

Lipid class	CL	Did you presume assumptions for identification?	Yes
MS Level for identification	MS1	Which assumptions were presumed?	even numbered fatty acids
Identification level	Species level	Check isomer overlap	Yes
Polarity mode	Negative	Additional dimension/techniques	-
Type of negative (precursor)ion	[M-2H]2-	Lipid Identification Software	LipidXplorer
Isotope correction at MS1	No	Data manipulation	-
MS1 verified by standard	Yes	Nomenclature for intact lipid molecule	No
Background check at MS1	Yes	Further identification remarks	-

3) CL[M-2H]2- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS1	Normalization to reference	Yes
Internal lipid standard(s) MS1		Lipid Quantification Software	LipidXplorer

Internal standard	Endogenous subclass
18:2 CARDIOLIPIN-D5	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	No		

4) DG[M+NH4]+ / Lipid identification

Lipid class	DG	Background check at MS1	Yes
MS Level for identification	MS1, MS2	Background check at MS2	No
Identification level	Species level	Did you presume assumptions for identification?	No
Polarity mode	Positive	Check isomer overlap	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
-FA1(-H)-(H2O+NH3)
-FA2(-H)-(H2O+NH3)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	No	Nomenclature for intact lipid molecule	No
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	No	Further identification remarks	-

4) DG[M+NH4]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) DG	-FA 15:0(-H)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

5) LPC[M+H]+ / Lipid identification

Lipid class	LPC	Background check at MS1	Yes
MS Level for identification	MS1, MS2	Background check at MS2	Yes
Identification level	Species level	Did you presume assumptions for identification?	No
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
HG(PC,184)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-

5) LPC[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
18:1(d7) LPC	HG(PC,184)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

6) LPE[M-H]- / Lipid identification

Lipid class	LPE	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FA
Polarity mode	Negative	Check isomer overlap	Yes
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
FA1(+O)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

6) LPE[M-H]- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
18:1(d7) LPE	FA1(+O)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

7) LPI[M-H]- / Lipid identification

Lipid class	LPI	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FAs
Polarity mode	Negative	Check isomer overlap	Yes
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
FA1(+O)
HG(PI,241)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

7) LPI[M-H]- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS1	Normalization to reference	Yes
Internal lipid standard(s) MS1		Lipid Quantification Software	LipidXplorer

Internal standard	Endogenous subclass
15:0-18:1(d7) PI	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

8) PA[M-H]- / Lipid identification

Lipid class	PA	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FA
Polarity mode	Negative	Check isomer overlap	Yes
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
-FA2(+HO)
-FA1(+HO)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	Yes
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

8) PA[M-H]- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PA	-FA2(+HO)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

9) PC[M+H]+ / Lipid identification

Lipid class	PC	Did you presume assumptions for identification?	Yes
MS Level for identification	MS1	Which assumptions were presumed?	even numbered FAs, max num,ber of DBs
Identification level	Species level	Check isomer overlap	Yes
Polarity mode	Positive	Additional dimension/techniques	-
Type of positive (precursor)ion	[M+H]+	Lipid Identification Software	LipidXplorer
Isotope correction at MS1	Type 2	Data manipulation	-
MS1 verified by standard	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS1	Yes	Further identification remarks	-

9) PC[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PC	HG (PC) 184	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

10) PC O[M+H]+ / Lipid identification

Lipid class	PC O	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FAs, max number of DBs
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
HG(PC,184)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

10) PC O[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PC	HG(PC,184)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

11) PE[M+H]+ / Lipid identification

Lipid class	PE	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FAs, max number DBs
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer
Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	Yes
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

Fragment name
-HG(PE,141)

11) PE[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer
Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PE	-HG(PE,141)	

12) PG[M-H]- / Lipid identification

Lipid class	PG	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FAs
Polarity mode	Negative	Check isomer overlap	Yes
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer
Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

Fragment name
FA1(+O)
FA2(+O)

12) PG[M-H]- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PG(Na-Salt)	FA2(+O)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

13) PI[M-H]- / Lipid identification

Lipid class	PI	Background check at MS1	Yes
MS Level for identification	MS1, MS2	Background check at MS2	Yes
Identification level	Species level	Did you presume assumptions for identification?	No
Polarity mode	Negative	Check isomer overlap	Yes
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
FA1(+O)
FA2(+O)
HG(PI,241)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-

13) PI[M-H]- / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PI	FA2(+O)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

14) PS[M+H]+ / Lipid identification

Lipid class	PS	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered FA
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
-HG(PS,185)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	Yes
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

14) PS[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
15:0-18:1(d7) PS	-HG(PS,185)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

15) SM[M+H]+ / Lipid identification

Lipid class	SM	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	Even numbered LCB and FA
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
HG(PC,184)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	No
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

15) SM[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS1	Normalization to reference	Yes
Internal lipid standard(s) MS1		Lipid Quantification Software	LipidXplorer

Internal standard	Endogenous subclass
18:1(d9) SM	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

16) TG[M+NH4]+ / Lipid identification

Lipid class	TG	Did you presume assumptions for identification?	No
MS Level for identification	MS1	Check isomer overlap	Yes
Identification level	Species level	Additional dimension/techniques	-
Polarity mode	Positive	Lipid Identification Software	LipidXplorer
Type of positive (precursor)ion	[M+NH4]+	Data manipulation	-
Isotope correction at MS1	Type 2	Nomenclature for intact lipid molecule	No
MS1 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

16) TG[M+NH4]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS1	Normalization to reference	Yes
Internal lipid standard(s) MS1		Lipid Quantification Software	LipidXplorer

Internal standard	Endogenous subclass
15:0-18:1(d7)-18:1 TG	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

17) ST[M+NH4]+ / Lipid identification

Lipid class	ST	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	targeted on cholesterol
Polarity mode	Positive	Check isomer overlap	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
-Cholesterol(35)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	No
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	acquisition after acetylation
Background check at MS1	Yes		

17) ST[M+NH4]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
Cholesterol(d7)	-Cholesterol(35)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	acetylation was performed
Type I isotope correction	Yes		

18) HexCer[M+H]+ / Lipid identification

Lipid class	HexCer	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	even numbered LCB and FA, Hydroxylation only on FA
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
LCB(-CH3O2)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	No
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

18) HexCer[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
C15 GLUCOSYL(BETA) CERAMIDE-D7 (D18:1-D7)	LCB(-CH3O2)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		

19) PE P[M+H]+ / Lipid identification

Lipid class	PE P	Background check at MS2	Yes
MS Level for identification	MS1, MS2	Did you presume assumptions for identification?	Yes
Identification level	Species level	Which assumptions were presumed?	Even numbered aliphatic chains
Polarity mode	Positive	Check isomer overlap	Yes
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	-
Fragments for identification		Lipid Identification Software	LipidXplorer

Fragment name
-FA2+(C3H5O2)
-FA1(-H)

Isotope correction at MS1	Type 2	Data manipulation	-
Isotope correction at MS2	Type 2	Nomenclature for intact lipid molecule	No
MS1 verified by standard	Yes	Nomenclature for fragment ions	N/A
MS2 verified by standard	Yes	Further identification remarks	-
Background check at MS1	Yes		

19) PE P[M+H]+ / Lipid quantification

Quantitative	Yes	Limit of quantification	No
MS Level for quantification	MS2	Normalization to reference	Yes
Internal lipid standard(s) MS2		Lipid Quantification Software	LipidXplorer

Internal standard	Fragment(s)	Endogenous subclass
C18(PLASM)-18:1(D9) PE	-FA2+(C3H5O2)	
C18(PLASM)-18:1(D9) PE	-FA1(-H)	

Type of quantification	Internal standard amount	Batch correction	No
Response correction	No	Further quantification remarks	-
Type I isotope correction	Yes		