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Separation Workflow

Overall study design

Title of the study			
Humans resilient to coronary artery disease share a common lipidomic signature with chimpanzees, influenced by genetic factors			
Document creation date	05/27/2025	Corresponding Email	peter.meikle@baker.edu.au
Principal investigator	Peter Meikle	Is the workflow targeted or untargeted?	Targeted
Institution	Baker Heart and Diabetes Institute	Clinical	Yes

Lipid extraction

Extraction method	1-phase system	Were internal standards used?	Yes
pH adjustment	None	Deposition method	standards reconstituted in BUME and added to sample with positive displacement pipette
1-phase system	Butanol/Methanol (1/1)	Internal standards used	AcylCarnitine 16:0 d3, CE 18:0-d6, Cer(d18:1-d7/18:0), Cholic Acid d4, COH-d7, DE(18:1) ester d6, DG(15:0 18:1) d7, dhCer 8:0, FA(18:1) d9, FA(20:4) d11, FA(22:6) d5, Hex2Cer(d18:1/15:0) d7, Hex3Cer(d18:1/17:0), HexCer(d18:1/15:0) d7, LPC(18:1) d7, LPE(18:1) d7, LPI 13:0, MG(18:1) d7, PA(15:0_18:1) d7, PC(15:0_18:1) d7, PC(P-18:0/18:1) d9, PE(15:0_18:1) d7, PE(P-18:0/18:1) d9, PG(15:0_18:1) d7, PI(15:0_18:1) d7, PS(15:0_18:1) d7, S1P(d18:1) d7, SM(d18:1/15:0) d9, Sph(d17:1), SHexCer(d18:1/12:0), TG(48:1) [NL-18:1] d7

Analytical platform

Ionization additives	Ammonium formate	Mass resolution for detected ion at MS ¹	Low resolution
Number of separation dimensions	One dimension	Resolution at MS ¹	Low
Separation type 1	LC	Recording mode of raw data at MS ¹	Centroid mode
Separation mode 1 (liquid)	RP	Mass window for precursor ion isolation (in Da total isolation window)	0.7
Detector	Mass spectrometer	Mass resolution for detected ion at MS ²	Low resolution
MS type	QQQ	Resolution at MS ²	Low
MS vendor	Agilent	Recording mode of raw data at MS ²	Centroid mode
Ion source	ESI	Was/Were additional dimension/techniques used	No
MS Level	MS ¹ , MS ²		

Quality control

Blanks	Yes	Quality control	Yes
Type of Blanks	Extraction blank, Internal standard blank	Type of QC sample	Commercial sample

Method qualification and validation

Method validation	No
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Reporting

Are reported raw data uploaded into repository?	Available on request	Raw data upload	Available on request
Are metadata available?	No		

Sample Descriptions

Chimpanzee / chimpanzee / Plasma

Storage and collection conditions	Available	Storage temperature	-80 °C
Temperature handling original sample	Room temperature	Additives	EDTA
Instant sample preparation	No		

BioHeart / Human / Plasma

Storage and collection conditions	Available	Storage temperature	-80 °C
Temperature handling original sample	Room temperature	Additives	BHT
Instant sample preparation	No		

Lipid Class Descriptions

1) CAR / Lipid identification

Lipid class	CAR	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
PI, m/z 85.1			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	No	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

1) CAR / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
AC(16:0) d3	PI, m/z 85.1	all CAR and CAR-OH	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

2) CE[M+NH4]⁺ / Lipid identification

Lipid class	CE	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interference confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
COH - water (369)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

2) CE[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
CE 18:0 d6	COH - water (369)	all CE	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	Response model	Batch correction	Normalization by reference material/QC

3) Cer / Lipid identification

Lipid class	Cer	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
LCB(-HO)			
LCB(-H3O2)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

3) Cer / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
18:1-D7;O2/18:0 Cer	LCB(-H3O2)	all other Ceramides	
Cer 18:0;O2/8:0	LCB(-HO)	all Cer 18:0;O2/XX:X	
18:1-D7;O2/18:0 Cer	LCB(-HO)	all Cer 18:X;O/XX:X	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

4) FC[M+H]⁺-[H₂O]⁺ / Lipid identification

Lipid class	FC	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+H] ⁺ -[H ₂ O] ⁺	Separation of isobaric/isomeric interference confirmed	Yes
Fragments for identification	Model for separation prediction	No	
Fragment name			
PI m/z 161.2			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	No	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

4) FC[M+H]⁺-[H₂O]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²	Normalization to reference	Yes	
Internal standard	Fragment(s)	Endogenous subclass	
COH d7	PI m/z 161.2	COH	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

5) DG[M+NH4]⁺ / Lipid identification

Lipid class	DG	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interference confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name -FA1(-H)-(H2O+NH3)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

5) DG[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard Fragment(s) Endogenous subclass DG(15:0_18:1-d7) -FA1(-H)-(H2O+NH3) all DGs			
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

6) FA[M-H]⁻ / Lipid identification

Lipid class	FA	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ¹	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ¹ adduct	[M-H] ⁻	Separation of isobaric/isomeric interference confirmed	Yes
Isotope correction at MS ¹	No	Model for separation prediction	No
MS ¹ verified by standard	Yes	Lipid Identification Software	Homemade
Background check at MS ¹	No	Data manipulation	Smoothing
Did you presume assumptions for identification?	No	Nomenclature for intact lipid molecule	Yes

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

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ¹	Limit of quantification	No
Internal lipid standard(s) MS ¹		Normalization to reference	Yes
Internal standard	Endogenous subclass		
FFA 18:1 d9	all FAs		
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

7) GM3 / Lipid identification

Lipid class	GM3	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
LCB(-H3O2)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

7) GM3 / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
Hex3Cer 18:1;O2/17:0	LCB(-H3O2)	all GM3	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

8) GM1[M+2H]²⁺ / Lipid identification

Lipid class	GM1	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	sn Position	RT verified by standard	Yes
MS ² adduct	[M+2H] ²⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification	Model for separation prediction	No	
Fragment name			
LCB(-H3O2)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

8) GM1[M+2H]²⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²	Normalization to reference	Yes	
Internal standard	Fragment(s)	Endogenous subclass	
Hex3Cer 18:1;O2/17:0	LCB(-H3O2)	all GM1	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

9) HexCer / Lipid identification

Lipid class	HexCer	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
LCB(-HO)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

9) HexCer / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
18:1-D7;O2/15:0 GlucCer	LCB(-HO)	HexCer	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

10) Hex2Cer / Lipid identification

Lipid class	Hex2Cer	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
LCB(-HO)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

10) Hex2Cer / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
Hex2Cer 18:1;O2-d7/15:0	LCB(-HO)	Hex2Cer	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

11) Hex3Cer / Lipid identification

Lipid class	Hex3Cer	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
LCB(-HO)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

11) Hex3Cer / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
Hex3Cer 18:1;O2/17:0	LCB(-HO)	Hex3Cer	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

12) LPC / Lipid identification

Lipid class	LPC	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
HG(PC,184)			
(C5H13NO,104)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

12) LPC / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
18:1-D7 LPC	HG(PC,184)	LPC	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

13) LPC O / Lipid identification

Lipid class	LPC O	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name (C5H13NO,104)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

13) LPC O / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
18:1-D7 LPC	HG(184)	LPC(O)	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

14) LPC P / Lipid identification

Lipid class	LPC P	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name (C5H13NO,104)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

14) LPC P / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
18:1-D7 LPC	HG(184)	LPC(P)	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

15) LPE / Lipid identification

Lipid class	LPE	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
-HG(PE,141)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

15) LPE / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
		Endogenous subclass	
LPE 18:1 d7	-HG(PE,141)	LPE	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

16) LPE P / Lipid identification

Lipid class	LPE P	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
NL 171.9			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

16) LPE P / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
		Endogenous subclass	
LPE 18:1 d7	-HG(PE,141)	LPE(P)	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

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

Lipid class	LPI	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	sn Position	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
NL 277.0 Da			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

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

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
LPI 13:0	NL 277.0 Da	Endogenous subclass	LPI
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

18) PA[M+NH4]⁺ / Lipid identification

Lipid class	PA	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
NL 115 Da			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

18) PA[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
PA 15:0_18:1-d7	NL 115 Da	Endogenous subclass	PA
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

19) PC / Lipid identification

Lipid class	PC	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
HG(PC,184)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation	Further identification remarks	Annotated from additional fragmentation studies on pooled sample. Annotations aligned using rts. Some PCs reported as species level, some at molecular species level

19) PC / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
15:0/18:1-D7 PC	HG(PC,184)	Endogenous subclass	PC
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

20) PC O / Lipid identification

Lipid class	PC O	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
HG(PC,184)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation	Further identification remarks	Annotated from additional fragmentation studies on pooled sample. Annotations aligned using rts. Some reported as species level, some at molecular species level

20) PC O / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
15:0/18:1-D7 PC	HG(PC,184)	Endogenous subclass	PC(O)s
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

21) PC P / Lipid identification

Lipid class	PC P	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
HG(PC,184)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation	Further identification remarks	Annotated from additional fragmentation studies on pooled sample. Annotations aligned using rts. Some reported as species level, some at molecular species level

21) PC P / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
PC P-18:0/18:1 d9	HG(PC,184)	Endogenous subclass	PC(P)s
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

22) PE / Lipid identification

Lipid class	PE	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
-HG(PE,141)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation	Further identification remarks	Annotated from additional fragmentation studies on pooled sample. Annotations aligned using rts. Some species reported at species level, some at molecular species level.

22) PE / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
15:0/18:1-D7 PE	-HG(PE,141)	Endogenous subclass	all PEs
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

23) PE O / Lipid identification

Lipid class	PE O	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
-HG(PE,141)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation	Further identification remarks	Annotated from additional fragmentation studies on pooled sample. Annotations aligned using rts. Some reported as species level, some at molecular species level

23) PE O / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
15:0/18:1-D7 PE	-HG(PE,141)	Endogenous subclass	all PE(O)s
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

24) PE P / Lipid identification

Lipid class	PE P	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
acyl chain specific			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

24) PE P / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
		Endogenous subclass	
PE P-18:0/18:1-d9	PI, 348.3 Da	all PE(P)s	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

25) PG[M+NH4]⁺ / Lipid identification

Lipid class	PG	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	sn Position	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification	Model for separation prediction	No	
Fragment name -HG(PG,172+NH4)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

25) PG[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²	Normalization to reference	Yes	
Internal standard Fragment(s) Endogenous subclass PG 15:0_18:1-d7 -HG(PG,172+NH4) all PGs			
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

26) PI[M+NH4]⁺ / Lipid identification

Lipid class	PI	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name -HG(PI,260+NH4)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

26) PI[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard Fragment(s) Endogenous subclass PI 15:0/18:1-D7 -HG(PI,260+NH4) all PIs			
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

27) PS / Lipid identification

Lipid class	PS	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
-HG(PS,185)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

27) PS / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
		Endogenous subclass	
PS 15:0_18:1-d7	-HG(PS,185)	all PS	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

28) SHexCer / Lipid identification

Lipid class	SHexCer	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
LCB(-H3O2)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

28) SHexCer / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
SHexCer 18:1;O2/12:0	LCB(-H3O2)	all SHexCer	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

29) SM / Lipid identification

Lipid class	SM	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
HG(PC,184)			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation	Further identification remarks	Annotated from additional fragmentation studies on pooled sample. Annotations aligned using rts. Some reported as species level, some at molecular species level

29) SM / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
SM 18:1;O2/15:0 d9HG(PC,184)	all SM		
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

30) SPBP / Lipid identification

Lipid class	SPBP	Limit of detection	No
MS Level for identification	MS ²	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name sphingoid base specific			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes
Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation		

30) SPBP / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard Fragment(s) Endogenous subclass SPBP 18:1;O2 d7 PI, 271.3 Da all SPBP			
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

31) TG[M+NH4]⁺ / Lipid identification

Lipid class	TG	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name -FA1(+HO)-(NH3) SIM			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

31) TG[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)	Endogenous subclass	
TG 48:1-d7 (IS)	-FA1(+HO)-(NH3)	all TG NLs	
TG 48:1-d7 (IS)	SIM	all TG SIMs	
TG 48:1-d7 (IS)	-FA1(+HO)-(NH3)	all TG(O)s	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

32) BA[M+NH₄]⁺ / Lipid identification

Lipid class	BA	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH ₄] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification	Model for separation prediction	No	
Fragment name			
NL 71 Da			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

32) BA[M+NH₄]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²	Normalization to reference	Yes	
Internal standard	Fragment(s)	Endogenous subclass	
Cholic Acid d4	NL 71 Da	all bile acids	
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC

33) SE[M+NH4]⁺ / Lipid identification

Lipid class	SE	Check on:	Isomeric overlap, Isobaric overlap, In-source fragmentation
MS Level for identification	MS ²	Limit of detection	No
Identification level	Species level	RT verified by standard	Yes
MS ² adduct	[M+NH4] ⁺	Separation of isobaric/isomeric interferece confirmed	Yes
Fragments for identification		Model for separation prediction	No
Fragment name			
sterol head group			
Isotope correction at MS ²	No	Lipid Identification Software	Homemade
MS ² verified by standard	Yes	Data manipulation	Smoothing
Background check at MS ²	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification?	No	Nomenclature for fragment ions	Yes

33) SE[M+NH4]⁺ / Lipid quantification

Quantitative	Yes	Type I isotope correction	No
MS Level for quantification	MS ²	Limit of quantification	No
Internal lipid standard(s) MS ²		Normalization to reference	Yes
Internal standard	Fragment(s)		
CE 18:0 d6	sterol head group	Endogenous subclass	all sterol esters
Type of quantification	Internal standard amount	Lipid Quantification Software	Homemade
Response correction	No	Batch correction	Normalization by reference material/QC