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Overall study design

Title of the study	Four-dimensional Lipidomic Mobility Mass Spectrometr	Four-dimensional Lipidomics Profiling in X-linked Adrenoleukodystrophy using Trapped Ion Mobility Mass Spectrometry		
Document creation date	04/15/2024	Corresponding Email	y.r.jaspers@amsterdamumc.nl	
Principle investigator	Yorrick R.J. Jaspers	Is the workflow targeted or untargeted?	Untargeted	
Institution	Amsterdam UMC	Clinical	No	

Lipid extraction

Extraction method	1-phase system	1-phase system	1:1 (v/v) methanol:chloroform
Derivatization	-	Were internal standards added prior extraction?	Yes
pH adjustment	None		

Analytical platform

Ionizaton additives	Ammonium acetate, Formic acid	MS Level	MS2
Number of separation dimensions	One dimension	Mass window for precursor ion isolation (in Da total isolation window)	1
Separation type 1	LC	Mass resolution for detected ion at MS2	High resolution
Separation mode 1 (liquid)	RP	Resolution at m/z 200 at MS2	60000
Detector	Mass spectrometer	Mass accuracy in ppm at MS2	4
MS type	timsTOF Pro2	Recording mode of raw data at MS2	Profile mode
MS vendor	Bruker	Was/Were additional dimension/techniques used	Yes
lon source	HESI		

Quality control

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

Method qualification and validation

Method validation

No

Reporting

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

Sample Descriptions

Fibroblasts / Human / Cells

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Provided information	-	Additives	None
Temperature handling original sample	Unknown	Were samples stored under inert gas?	No
Instant sample preparation	No	Additional preservation methods	No
Storage temperature	-80 °C	Biobank samples	No

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

Lipid class	LPC	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	sn Position	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
HG(PC,184)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	Yes	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

	DC.		N 1
	PC	Limit of detection	No
MS Level for identification	MS1, MS2	RI verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
HG(PC,184)			
-FA1 (+HO)			
-FA1 (-H)			
-FA2 (+HO)			
-FA2 (-H)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of bydrocarbon chains
Check isomer overlap	Yes		,

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	TG	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA(+HO) -TG(17)		-	
-TG(17)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	DG	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	Yes
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-(H2O+NH3,35)		_	
-FA1(-H)-(H2O+NH3)			
-FA2(-H)-(H2O+NH3)		_	
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		•

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	CE	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA1 (+HO) -CE(17)		-	
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	Yes	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.

Check isomer overlap

Yes

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	Cer	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-(H2O,18)		-	
LCB(-HO)			
LCB(-H3O2)			
LCB(-CH3O2)			
Isotope correction at MS1	No		CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		·

6) Cer[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

7) AC[M+H]+ / Lipid identification

Lipid class	AC	RT verified by standard	No
MS Level for identification	MS1	Separation of isobaric/isomeric interferece confirmed	No
Identification level	Species level	Model for separation prediction	No
Polarity mode	Positive	Additional dimension/techniques	IMS
Type of positive (precursor)ion	[M+H]+	CCS verified by standard	No
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
MS1 verified by standard	No	Was a model used to predict lipid molecule separation?	No
Background check at MS1	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
Did you presume assumptions for identification?	No	Data manipulation	-
Check isomer overlap	Yes	Nomenclature for intact lipid molecule	Yes
Limit of detection	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.

7) AC[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

8) DG O[M+NH4]+ / Lipid identification

Lipid class	DG O	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	Yes
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA (-H)-(H2O+NH3)		-	
-(H2O+NH3,35)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains
Check isomer overlap	Yes		

8) DG O[M+NH4]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	-

9) Hex2Cer[M+H]+ / Lipid identification

Lipid class Hex/Ler Limit of detection No MS Level for identification MS1, MS2 RT verified by standard Yes Identification level Species level Separation of isobaric/isomeric imreferece confirmed No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragment name				
MS Level for identification MS1, MS2 R T verified by standard Yes Identification level Species level Separation of isobaric/isomeric interferece confirmed No Polarity mode Positive Model for separation prediction No Pregments for identification MS Kongenet interferece confirmed No Pregments for identification MS CCS verified by standard No Pregments for identification MS CCS verified by standard No ILCB(-HO) LCB(-HOO) CCS verified by standard No LCB(-HOO) LCB(-HOO) MS CCS verified by standard No Isotope correction at MS1 No Mo was/were the additional dimension(s) used? Was a model used to predict lipid No MS1 verified by standard No Was a model used to predict lipid No No MS1 verified by standard No Lipid Identification Software Lipid identification was done using MetaboScape 2023b (Bruker Dataonics) utiling an in-house generated retention inter and n/2 database, true-based lipid annotation and the MS DLAL MS/MS library LipidBlast (version 68). MS2 verified by standard No No Data manipulation - Background check at MS1 <td>Lipid class</td> <td>Hex2Cer</td> <td>Limit of detection</td> <td>No</td>	Lipid class	Hex2Cer	Limit of detection	No
Identification level Spearation of isobaric/isomeric interference confirmed No Polarity mode Positive Model for separation prediction No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragment name	MS Level for identification	MS1, MS2	RT verified by standard	Yes
Polarity mode Positive Model for separation prediction No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragments for identification CCS verified by standard No (H20,18) CCS verified by standard No LCB(-H00) LCB(Hac2,322) HG(Hac2,324) -HG(Hac2,324) How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of potential isobaric/isomeric interference. Isotope correction at MS1 No Was a model used to predict lipid Mo MS1 verified by standard No Was a model used to predict lipid Mo MS1 verified by standard No Data manipulation MS2 verified by standard	Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragments for identification CCS verified by standard No -(H2O,18) CCS (H3O2) ICER(-H3O2) LCB(-H3O2) ICER(-H3O2) ICER(-H3O2) -HG(Hex2,322) -HG(Hex2,324) -HG(Hex2,324) Image: Comparison of positive (precursor) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at MS1 No Sotope correction at MS2 No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard	Polarity mode	Positive	Model for separation prediction	No
Fragment name CCS verified by standard No (H2O,18) LCB(-H3O2) LCB(-H3O2) HG(Hex2,342) HG(Hex2,324) HG(Hex2,324) How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at MS1 No Was a model used to predict lipid Momental isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid Momental isobaric/isomeric interference. Lipid Identification of Diads, separation? Isotope correction at MS2 No Was a model used to predict lipid Momental isobaric/isomeric interference. Ipid Identification of Diads, separation? MS1 verified by standard No Uipid Identification Software Lipid Identification, and the MS DIAL MS/MS library LipidBlast (version 68). No MS2 verified by standard No Data manipulation - Background check at MS1 Yes Nomenclature for intact lipid molecules Ves Modeule No Nomenclature for fragment ions N/A Environmental lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to	Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragment name -(H2O,18) LCB(-H0) LCB(-H3O2) LCB(-H3O2) -HG(Hex2,342) -HG(Hex2,324) Isotope correction at MS1 No Botope correction at MS2 No Was a model used to predict lipid molecule separation of potential isobaric/isomeric interference. Was a model used to predict lipid No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No <tr< td=""><td>Fragments for identification</td><td></td><td>CCS verified by standard</td><td>No</td></tr<>	Fragments for identification		CCS verified by standard	No
-(H2O,18) LCB(-H3O) LCB(-CH3O2) -HG(Hex2,342) -HG(Hex2,342) -HG(Hex2,324) Isotope correction at MS1 No Isotope correction at MS1 No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No MS3 verified by standard No MS4 verified by standard No MS4 verified by standard No MS5 verified by standard No MS6 verified by standard No MS7 verified by standard No MS6 verified by standard No MS6 verified by standard No MS6 verified by standard No MS6 verified by standard No MS7 verified by standard No MS7 verified by stand	Fragment name			
LCB(-H0) LCB(-H302) LCB(-CH302) -HG(Hex2,342) -HG(Hex2,324) Isotope correction at MS1 No Bocope correction at MS1 No Was a model used to predict lipid identification of potential isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid molecule separation of potential isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid molecule separation? Lipid Identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, an in-house generated retention time and m/z database. MS2 verified by standard No MS2 verified by standard No MS2 verified by standard No Data manipulation - Background check at MS1 Yes Did you presume assumptions for No No Did you presume assumptions for No No Did you presume assumptions for No No Check isomer overlap Yes	-(H2O,18)			
LCB(-H302) -HG(Hex2,342) -HG(Hex2,324) Isotope correction at M51 No Botope correction at M51 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at M52 No MS1 verified by standard No MS1 verified by standard No MS2 verified by st	LCB(-HO)			
LCB(-CH302) -HG(Hex2, 342) -HG(Hex2, 324) Isotope correction at MS1 No Botope correction at MS1 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of potential isobaric/isomeric interference. Isotope correction at MS2 No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No Background check at MS1 Yes Momenclature for intact lipid molecule Yes More clature for fragment ions N/A Did you presume assumptions for No No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-spr	LCB(-H3O2)			
-HG(Hex2,342) -HG(Hex2,360) -HG(Hex2,324) Isotope correction at M51 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at M52 No Was a model used to predict lipid Monolecule separation? No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No Did you presume assumptions for identification? No Check isomer overlap Yes	LCB(-CH3O2)			
-HG(Hex2,360) -HG(Hex2,324) Isotope correction at MS1 No Move was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of potential isobaric/isomeric interference. Isotope correction at MS2 No MS1 verified by standard No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No Did you presume assumptions for identification? No Did you presume assumptions for identification? No No No Further identification remarks For lipid identification? No More clause For lipid identification, the lipid species-specific fragment the lipid species-specific fragments to determine the lipid species-specific fragments to determine the lipid species-specific fragments for the annotation of hydrocarbon chains.	-HG(Hex2,342)			
-HG(Hex2,324) Isotope correction at MS1 No Botope correction at MS1 No Isotope correction at MS2 No Botope correction at MS2 No Was a model used to predict lipid molecule separation? No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No Background check at MS1 Yes Did you presume assumptions for No Did you presume assumptions for No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species-and molecular lipid species-and molecular lipid species-and molecular lipid species-and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. <td>-HG(Hex2,360)</td> <td></td> <td></td> <td></td>	-HG(Hex2,360)			
Isotope correction at MS1 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at MS2 No MS1 verified by standard No MS1 verified by standard No MS2 verified by standard No Background check at MS1 Yes Did you presume assumptions for identification if was end used for fragment ions N/A Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, erigidelines were followed, eriging specisan dimetellars in the lipid specisan dim otec	-HG(Hex2,324)			
Isotope correction at MS2NoWas a model used to predict lipid molecule separation?NoMS1 verified by standardNoLipid Identification SoftwareLipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).MS2 verified by standardNoData manipulation-Background check at MS1YesNoData manipulation-Background check at MS2NoNoNomenclature for intact lipid moleculeYesDid you presume assumptions for identification?NoFurther identification remarks lipid species and molecular lipid species specific fragments for the annotation of hydrocarbo	Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
MS1 verified by standardNoLipid Identification SoftwareLipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).MS2 verified by standardNoData manipulation-Background check at MS1YesNoNomenclature for intact lipid moleculeYesDid you presume assumptions for identification?NoNoFurther identification remarksFor lipid identification, the Lipidwidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species and molecular	Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS2 verified by standard No Data manipulation - Background check at MS1 Yes Nomenclature for intact lipid molecule Yes Background check at MS2 No Nomenclature for fragment ions N/A Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
Background check at MS1 Yes Nomenclature for intact lipid molecule Yes Background check at MS2 No Nomenclature for fragment ions N/A Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	MS2 verified by standard	No	Data manipulation	-
Background check at MS2 No Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	Background check at MS2	No	Nomenclature for fragment ions	N/A
Check isomer overlap Yes	Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
	Check isomer overlap	Yes		

9) Hex2Cer[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

10) Hex3Cer[M+H]+ / Lipid identification

Linid class	Hay2Car	Limit of detection	Na
Lipid class	Hex3Cer	DT use if a days standard	No No
NIS Level for Identification		RT verified by standard	No.
Identification level	Species level	interferece confirmed	INO
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-(H2O,18)			
LCB(-HO)			
LCB(-H3O2)			
LCB(-CH3O2)			
-HG(Hex3,504)			
-HG(Hex3,522)			
-HG(Hex3,534)			
-HG(Hex2,342)			
-HG(Hex,180)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains
Check isomer overlap	Yes		

10) Hex3Cer[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	HexCer	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-(H2O,18)			
LCB(-HO)			
LCB(-H3O2)			
LCB(-CH3O2)			
-HG(Hex,180)			
-HG(Hex,198)			
-HG(Hex,162)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	LPE	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA1(-H)-(H2O)			
-FA1(-H)			
GP(153)			
FA1(+O)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

13) LPE[M+H]+ / Lipid identification

Lipid class	LPE	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-HG(PE,141)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

13) LPE[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

14) LPE O[M-H]- / Lipid identification

Lipid class	LPE O	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA1(-H)			
GP(153)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		,

14) LPE O[M-H]- / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

15) LPE O[M+H]+ / Lipid identification

Lipid class	LPE O	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-HG(PE,141)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

15) LPE O[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

16) PE[M-H]- / Lipid identification

Lipid class	PE	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
HG(PE,196)		_	
GP(153)			
FA1(+O)			
FA2(+O)			
-FA1(+HO)			
-FA2(+HO)			
-FA1(-H)			
-FA2(-H)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	No
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

16) PE[M-H]- / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	PE	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-HG(PE,141)		_	
FA1			
FA2		_	
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	No
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

18) PE O[M+H]+ / Lipid identification

Lipid class	PE O	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-HG(PE,141)		_	
FA2+(C3H6O2)			
Isotope correction at MS1	No		CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

18) PE O[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

19) PE O[M-H]- / Lipid identification

Lipid class	PE O	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
GP(153)			
GP(135)			
FA2(+O)			
-FA2(+HO)			
-FA2(-H)			
FA2 -(CO)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		<u> </u>

19) PE O[M-H]- / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	PI	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA1(-H)			
FA1(+O)			
-FA1(+HO)			
-FA2(-H)			
FA2(+O)			
-FA2(+HO)			
HG(PI,241)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

21) PI[M+NH4]+ / Lipid identification

Lipid class	PI	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-HG(PI,260)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Charle in an entropy of	V.		

Check isomer overlap

Yes

21) PI[M+NH4]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

22) PS[M-H]- / Lipid identification

Lipid class	PS	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-FA1(-H)-(C3H5NO2)			
FA1(+O)			
-FA1(+HO)-(C3H5NO2)			
-FA2(-H)-(C3H5NO2)			
FA2(+O)			
-FA2(+HO)-(C3H5NO2)			
-(C3H5NO2,87)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

22) PS[M-H]- / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class PS Limit of detection No MS Level for identification MS1, MS2 RT verified by standard Yes Identification level Molecular species level Separation of isobaric/isomeric No Polarity mode Positive Model for separation prediction No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragments for identification CCS verified by standard No Polarity mode Positive How was/were the additional dimension/techniques MS -HG(PS,185) Isotope correction at MS1 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at MS1 No Was a model used to predict lipid molecule separation? No MS1 verified by standard Yes Uipid Identification Software Lipid identification was done using MetaboScape 2023b (Bruker Dationcis) utiling anotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Data manipulation - MS2 verified by standard Yes Nomenclature for intact lipid molecule No MS2 verified by standard Yes No Nomenclature for fragment ions N/A <tr< th=""><th></th><th></th><th></th><th></th></tr<>				
MS Level for identification MS1, MS2 RT verified by standard Yes Identification level Molecular species level Separation of isobaric/isomeric interferee confirmed No Polarity mode Positive Model for separation prediction No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragments for identification	Lipid class	PS	Limit of detection	No
Identification level Molecular species level Separation of isobaric/isomeric interferece confirmed No Polarity mode Positive Model for separation prediction No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragment name -HG(PS,185) CCS verified by standard No Isotope correction at MS1 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid molecule separation? No MS1 verified by standard Yes Lipid Identification Software using MetaboScape 2023b (Bruker Datonics) utilising an in-house generated retention ime and my2 database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Data manipulation - Background check at MS1 Yes Nomenclature for intact lipid molecule Yes Background check at MS2 No Nomenclature for fragment ions N/A Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipid byscies and molecula employing lipid class-specific fragments to determine the lipid species and molecular ipid species and molecular ipid species and molecular ipid species specific fragments for the anno	MS Level for identification	MS1, MS2	RT verified by standard	Yes
Polarity mode Positive Model for separation prediction No Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragments for identification	Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Type of positive (precursor)ion [M+H]+ Additional dimension/techniques IMS Fragment name -HG(PS,185) CCS verified by standard No Isotope correction at MS1 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of potential isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid noisecule separation? No MS1 verified by standard Yes Lipid Identification Software Lipid Identification was done using MetaboScape 2023b (Bruker Datonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Data manipulation - Background check at MS1 Yes No Nomenclature for fragment ions N/A Did you presume assumptions for No No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines sepecific fragments to determine the lipid species-specific fragments for the annotation of hydrocarbon chains. MS2 verified by standard Yes For lipid identification, the LipidOmics Standards Initiative guidelines were followed, employing lipid class-specific fragments for the annotation of hydrocarbon chains.	Polarity mode	Positive	Model for separation prediction	No
Fragments for identification CCS verified by standard No Pragment name -HC(PS,185) No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of potential isobaric/isomeric interference. Isotope correction at MS1 No Was a model used to predict lipid molecule separation of potential isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid No MS1 verified by standard Yes Lipid Identification Software Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Data manipulation - Background check at MS1 Yes Nomenclature for intact lipid molecule N/A Did you presume assumptions for identification? No Nomenclature for fragment ions in the lipid identification, the Lipidomics Standards Initative guidelines were followed, employing lipid class-specific fragments to determine the lipid species-apecific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes Yes Nomenclature for check at MS1	Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragment name -HG(PS,185) Isotope correction at MS1 No Isotope correction at MS1 No Isotope correction at MS2 No Isotope correction at MS2 No Was a model used to predict lipid molecule separation of potential isobaric/isomeric interference. No MS1 verified by standard Yes MS1 verified by standard Yes Lipid Identification Software Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Background check at MS1 Yes Did you presume assumptions for identification? No No Nomenclature for intact lipid molecule For lipid identification, the Lipid identification, the Lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species-apecific fragments of the annotation of hydrocarbon chains.	Fragments for identification		CCS verified by standard	No
-HG(PS,185) Isotope correction at MS1 No Isotope correction at MS2 No Isotope correction at MS2 No Was a model used to predict lipid molecule separation? No MS1 verified by standard Yes MS1 verified by standard Yes Lipid Identification Software Lipid identification was done using MetaboScape 2023b (Bruker Datonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Background check at MS1 Yes Background check at MS2 No No Nomenclature for fragment ions Did you presume assumptions for identification? No Did you presume assumptions for identification? No Kiew Followed, employing lipid class-specific fragments to determine the lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	Fragment name			
Isotope correction at MS1 No How was/were the additional dimension(s) used? CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference. Isotope correction at MS2 No Was a model used to predict lipid No MS1 verified by standard Yes Lipid Identification Software Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68). MS2 verified by standard Yes Data manipulation - Background check at MS1 Yes No Nomenclature for intact lipid regression 68). Background check at MS2 No No Nodecule Did you presume assumptions for identification? No For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes Yes	-HG(PS,185)		_	
Isotope correction at MS2NoWas a model used to predict lipid molecule separation?NoMS1 verified by standardYesLipid Identification SoftwareLipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).MS2 verified by standardYesData manipulation-Background check at MS1YesNoNomenclature for intact lipid moleculeYesBackground check at MS2NoNomenclature for fragment ionsN/ADid you presume assumptions for identification?NoFurther identification remarksFor lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species-specific fragments for the annotation of hydrocarbon chains.Check isomer overlapYes	Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
MS1 verified by standardYesLipid Identification SoftwareLipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).MS2 verified by standardYesData manipulation-Background check at MS1YesNomenclature for intact lipid moleculeYesBackground check at MS2NoNomenclature for fragment ionsN/ADid you presume assumptions for identification?NoFurther identification remarksFor lipid identification, the Lipidolines Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species network chains.Check isomer overlapYes	Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS2 verified by standard Yes Data manipulation - Background check at MS1 Yes Nomenclature for intact lipid molecule Yes Background check at MS2 No Nomenclature for fragment ions N/A Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species and molecular lipid species and molecular lipid species of the annotation of hydrocarbon chains. Check isomer overlap Yes	MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
Background check at MS1 Yes Nomenclature for intact lipid Yes Background check at MS2 No Nomenclature for fragment ions N/A Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	MS2 verified by standard	Yes	Data manipulation	-
Background check at MS2 No Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Did you presume assumptions for identification? No Further identification remarks For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains. Check isomer overlap Yes	Background check at MS2	No	Nomenclature for fragment ions	N/A
Check isomer overlap Yes	Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
	Check isomer overlap	Yes		,

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	SM	Limit of detection	No
MS Level for identification	MS1. MS2	RT verified by standard	Yes
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	No
Type of positive (precursor)ion	[M+H]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
HG(PC,184)		-	
LCB(-H3O2)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		,

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

25) TG O[M+NH4]+ / Lipid identification

Lipid class	TG O	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Positive	Model for separation prediction	Yes
Type of positive (precursor)ion	[M+NH4]+	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	Yes
Fragment name			
-FA(+HO) -TG(17)			
-TG(17)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	No
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	No		·

25) TG O[M+NH4]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

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

Lipid class	LPI	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
GP(153)			
HG(PI,241)			
-FA1(+HO)			
FA1(+O)			
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

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

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

27) LPS[M-H]- / Lipid identification

Lipid class	LPS	Limit of detection	No
MS Level for identification	MS1, MS2	RT verified by standard	No
Identification level	Molecular species level	Separation of isobaric/isomeric interferece confirmed	No
Polarity mode	Negative	Model for separation prediction	No
Type of negative (precursor)ion	[M-H]-	Additional dimension/techniques	IMS
Fragments for identification		CCS verified by standard	No
Fragment name			
-(C3H5NO2,87)		-	
FA1(+O)			
GP(153)		_	
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
Isotope correction at MS2	No	Was a model used to predict lipid molecule separation?	No
MS1 verified by standard	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
MS2 verified by standard	No	Data manipulation	-
Background check at MS1	Yes	Nomenclature for intact lipid molecule	Yes
Background check at MS2	No	Nomenclature for fragment ions	N/A
Did you presume assumptions for identification?	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.
Check isomer overlap	Yes		

27) LPS[M-H]- / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

28) LPS[M+H]+ / Lipid identification

linid alara	LDS	DT verified by standard	Na
MS Level for identification	MS1	Separation of isobaric/isomeric interferece confirmed	Yes
Identification level	Species level	Model for separation prediction	No
Polarity mode	Positive	Additional dimension/techniques	IMS
Type of positive (precursor)ion	[M+H]+	CCS verified by standard	No
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
MS1 verified by standard	No	Was a model used to predict lipid molecule separation?	No
Background check at MS1	Yes	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilizing an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
Did you presume assumptions for identification?	No	Data manipulation	-
Check isomer overlap	Yes	Nomenclature for intact lipid molecule	Yes
Limit of detection	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.

28) LPS[M+H]+ / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.

29) SLBPA[M-H]- / Lipid identification

Lipid class	SIRDA	PT verified by standard	No
MS Level for identification	MS1	Separation of isobaric/isomeric interferece confirmed	No
Identification level	Species level	Model for separation prediction	No
Polarity mode	Negative	Additional dimension/techniques	IMS
Type of negative (precursor)ion	[M-H]-	CCS verified by standard	No
Isotope correction at MS1	No	How was/were the additional dimension(s) used?	CCS was used (in combination with other parameters) in the identification of lipids, separation of potential isobaric/isomeric interference.
MS1 verified by standard	No	Was a model used to predict lipid molecule separation?	No
Background check at MS1	No	Lipid Identification Software	Lipid identification was done using MetaboScape 2023b (Bruker Daltonics) utilising an in-house generated retention time and m/z database, rule-based lipid annotation and the MS DIAL MS/MS library LipidBlast (version 68).
Did you presume assumptions for identification?	No	Data manipulation	-
Check isomer overlap	No	Nomenclature for intact lipid molecule	No
Limit of detection	No	Further identification remarks	For lipid identification, the Lipidomics Standards Initiative guidelines were followed, employing lipid class-specific fragments to determine the lipid species and molecular lipid species-specific fragments for the annotation of hydrocarbon chains.

29) SLBPA[M-H]- / Lipid quantification

Quantitative	No	Batch correction	No
Normalization to reference	No	Further quantification remarks	The reported lipid abundances were semi-quantitative, calculated by dividing the analyte response by that of the corresponding internal standard.