

Boosting annotation confidence in untargeted lipidomics experiments by the use of complementary chemical properties

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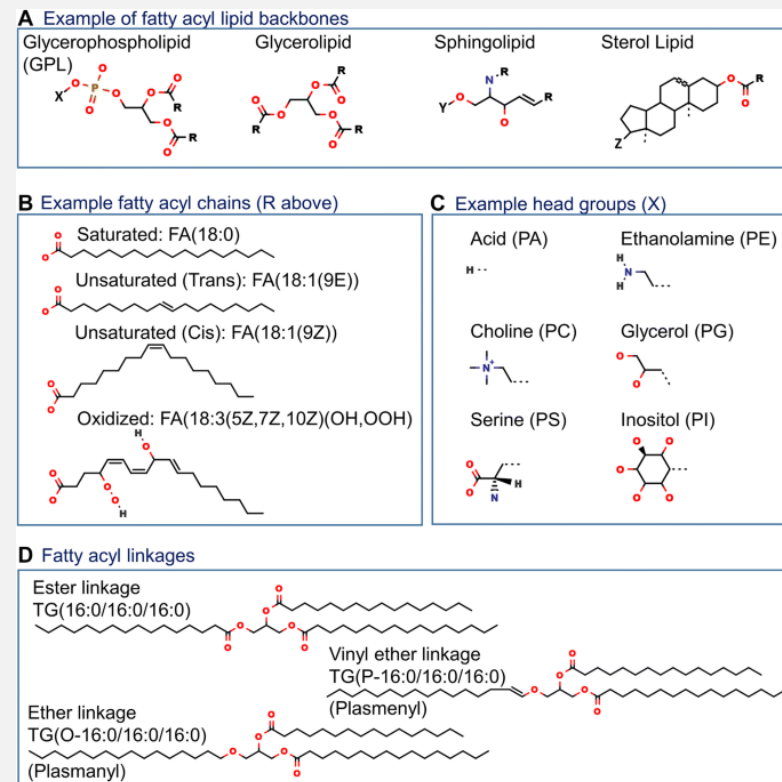
mar.garcia@fmach.it – github: mar-garcia

Italian Metabolomics Network General Meeting 2023 | <https://github.com/mar-garcia/IMN2023>

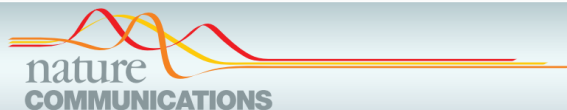
Introduction:

Lipids are typically composed of various building blocks:

- the lipid backbone
- fatty acyl chains
- head groups
- various linkages between backbone and fatty acyl constituents



Koelmel, J.P., Napolitano, M.P., Ulmer, C.Z. et al. *Metabolomics* 16, 56 (2020).
<https://doi.org/10.1007/s11306-020-01665-3>



MATTERS ARISING

<https://doi.org/10.1038/s41467-021-24984-y>

OPEN



Quality control requirements for the correct annotation of lipidomics data

Harald C. Köfeler^{1✉}, Thomas O. Eichmann², Robert Ahrends³, John A. Bowden⁴, Niklas Danne-Rasche⁵, Edward A. Dennis⁶, Maria Fedorova^{7,8}, William J. Griffiths⁹, Xianlin Han¹⁰, Jürgen Hartler^{6,11}, Michal Holčápek¹², Robert Jirásko¹², Jeremy P. Koelmel¹³, Christer S. Ejsing^{14,15}, Gerhard Liebisch¹⁶, Zhixu Ni^{7,8}, Valerie B. O'Donnell¹⁷, Oswald Quehenberger⁶, Dominik Schwudke^{18,19,20}, Andrej Shevchenko²¹, Michael J. O. Wakelam²², Markus R. Wenk²³, Denise Wolrab¹² & Kim Ekroos^{12,24}

ARISING FROM M. Mann et al. *Nature Communications* <https://doi.org/10.1038/s41467-019-14044-x> (2020).

Manually created with data from analytical standards. Information:

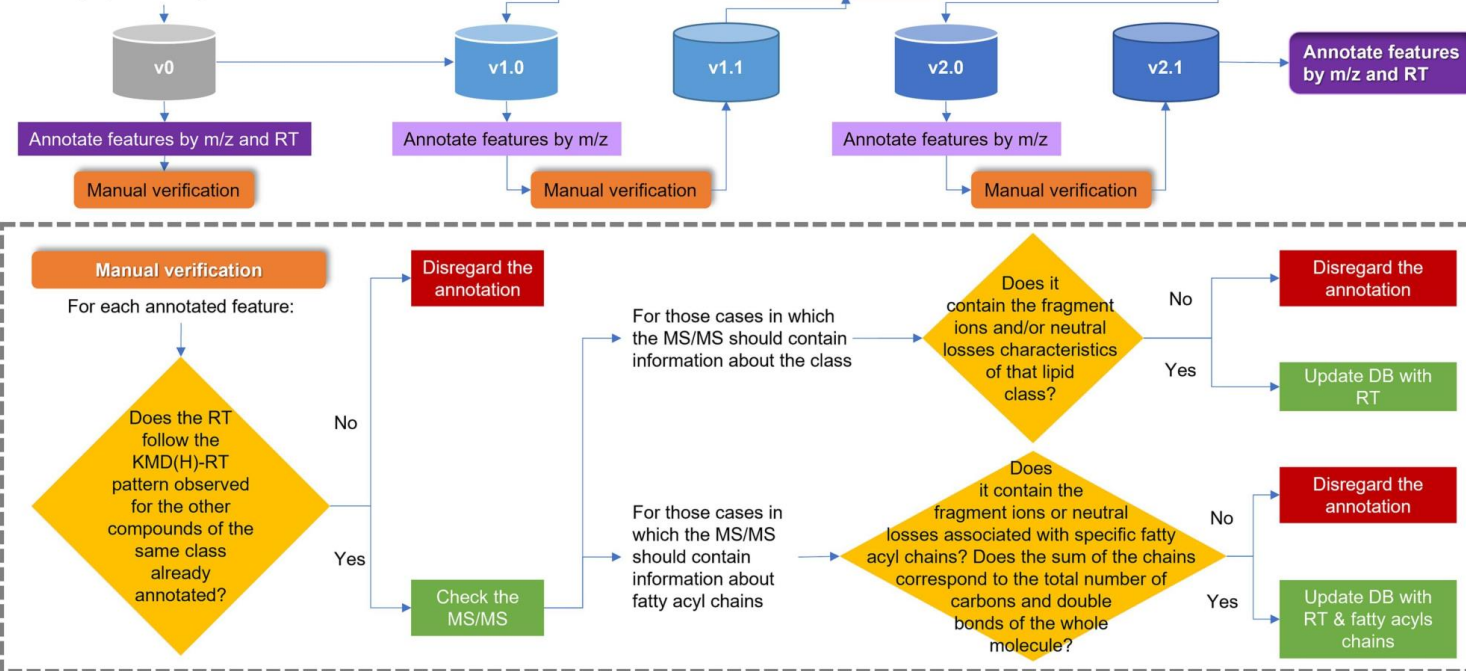
- Compound name at molecular species level (i.e., PA 16:0_18:2)
- Formula (i.e., $C_{37}H_{69}O_8P$)
- Adduct (i.e., $[M+NH_4]^+$, $[M-H]^-$)
- RT (i.e., 16.25 min)

Automatically created with data from classes for which there was available at least 1 analytical standard. Information:

- Compound name at species level (i.e., PA 36:2)
- Formula (i.e., $C_{39}H_{73}O_8P$)
- Adduct (i.e., $[M+NH_4]^+$, $[M-H]^-$)

Among non-annotated features:

- Search for possible m/z matches in dedicated databases such as LIPID MAPS
- De novo identification of groups of features showing similar MS2 patterns, as well as potential visually grid-like patterns for associations between RT and KMD(H)



Untargeted lipidomic profiling of grapes highlights the importance of modified lipid species beyond the traditional compound classes

Mar Garcia-Aloy^{a,*}, Domenico Masuero^a, Giulia Chitarrini^a, Domen Škrab^{a,b}, Paolo Sivilotti^b, Graziano Guella^c, Urska Vrhovsek^a, Pietro Franceschi^d

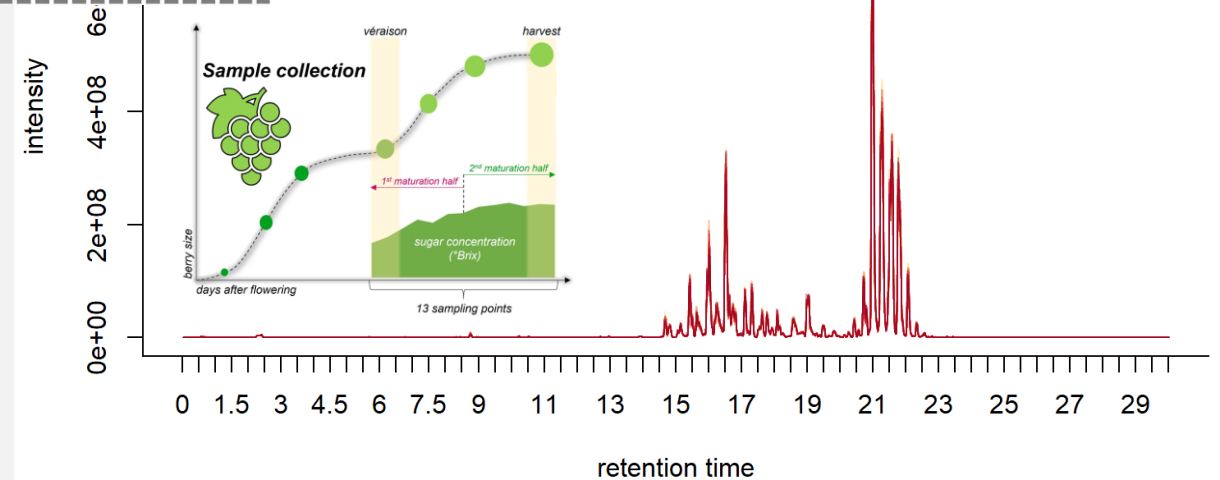
^a Metabolomics Unit, Research and Innovation Centre, Fondazione Edmund Mach, 38098 San Michele all'Adige, Italy

^b Department of Agricultural, Food, Environmental and Animal Sciences, University of Udine, 33100 Udine, Italy

^c Bioorganic Chemistry Laboratory, Department of Physics, University of Trento, 38123 Trento, Italy

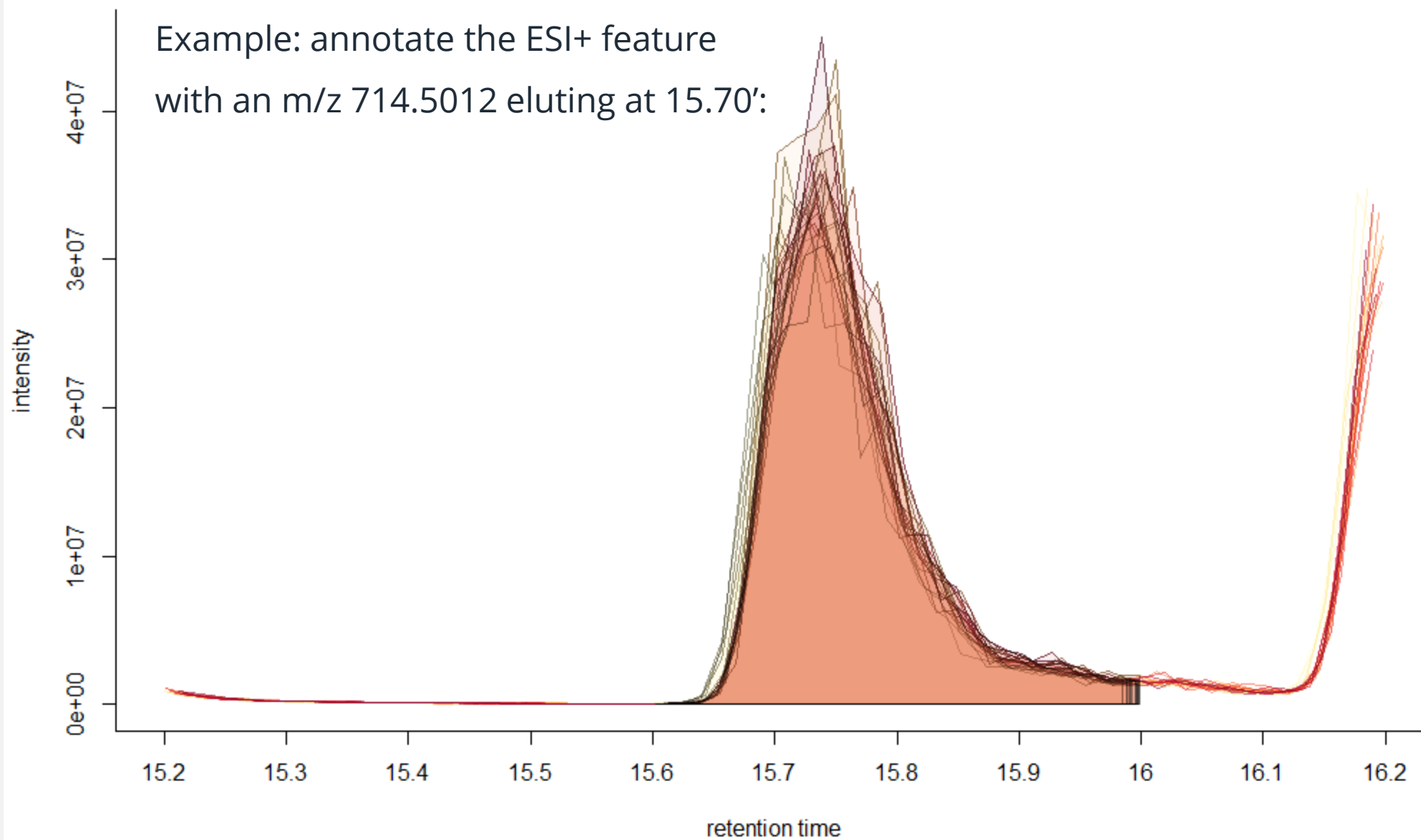
^d Unit of Computational Biology, Research and Innovation Centre, Fondazione Edmund Mach, 38098 San Michele all'Adige, Italy

Base Peak Chromatogram, ESI+



714.4687 - 714.6019

Example: annotate the ESI+ feature
with an m/z 714.5012 eluting at 15.70':



Isomeric and isobaric overlap:

	Lipid	Adduct	Formula	m/z	ppm
1	PA 36:4	[M+NH4] ⁺	C39H69O8P+NH4 ⁺	714.5068	7.84
2	PE 34:3	[M+H] ⁺	C39H72NO8P+H	714.5068	7.84
3	PC 31:3	[M+H] ⁺	C39H72NO8P+H	714.5068	7.84
4	MGDG 30:3	[M+NH4] ⁺	C39H68O10	714.5151	19.45
5	PA 36:5	2(13C)[M+NH4] ⁺	C39H67O8P	714.4975	5.18
6	PE 34:4	2(13C)[M+H] ⁺	C39H70NO8P	714.4975	5.18
7	PC 31:4	2(13C)[M+H] ⁺	C39H70NO8P	714.4975	5.18
8	MGDG 30:4	2(13C)[M+NH4] ⁺	C39H66O10	714.5057	6.30
9	PA 37:3	13C[M+H] ⁺	C40H73O8P	714.5150	19.31
10	PC 30:5	13C[M+NH4] ⁺	C38H66NO8P	714.4897	16.10
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Isomeric and isobaric overlap:

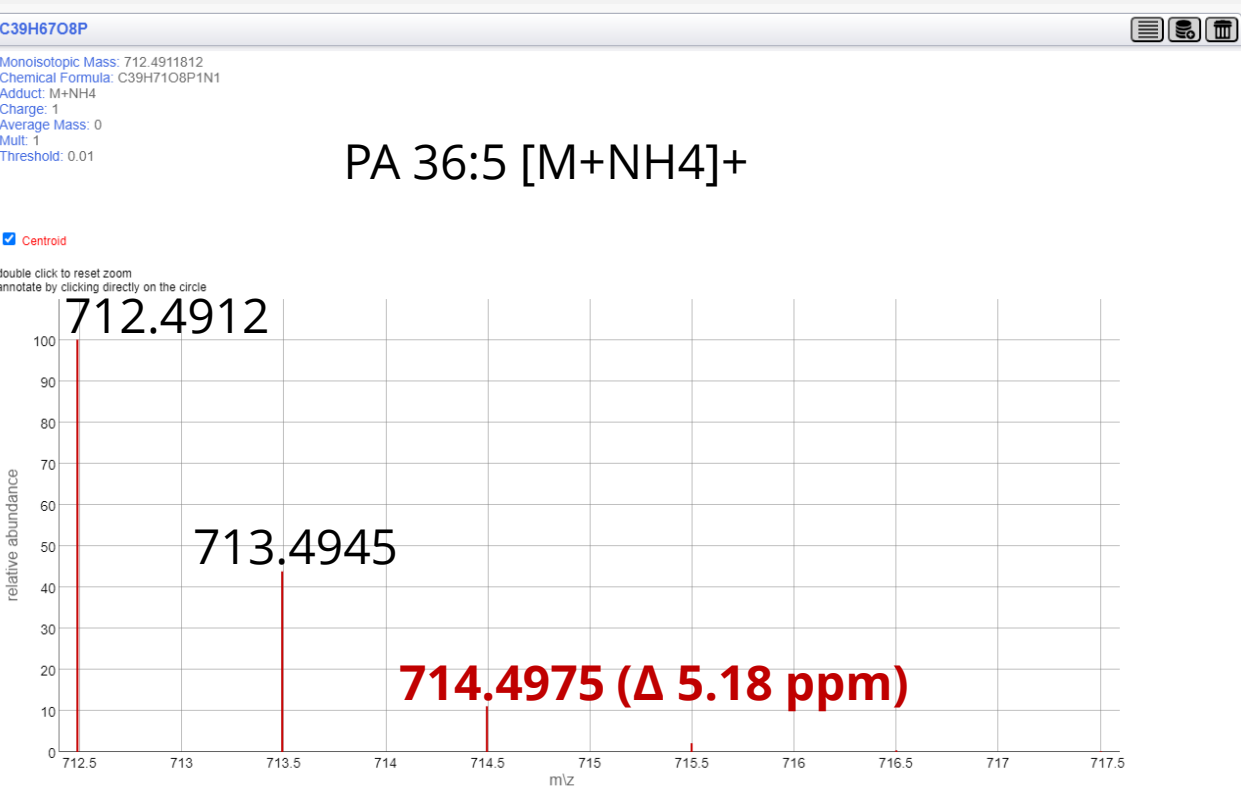
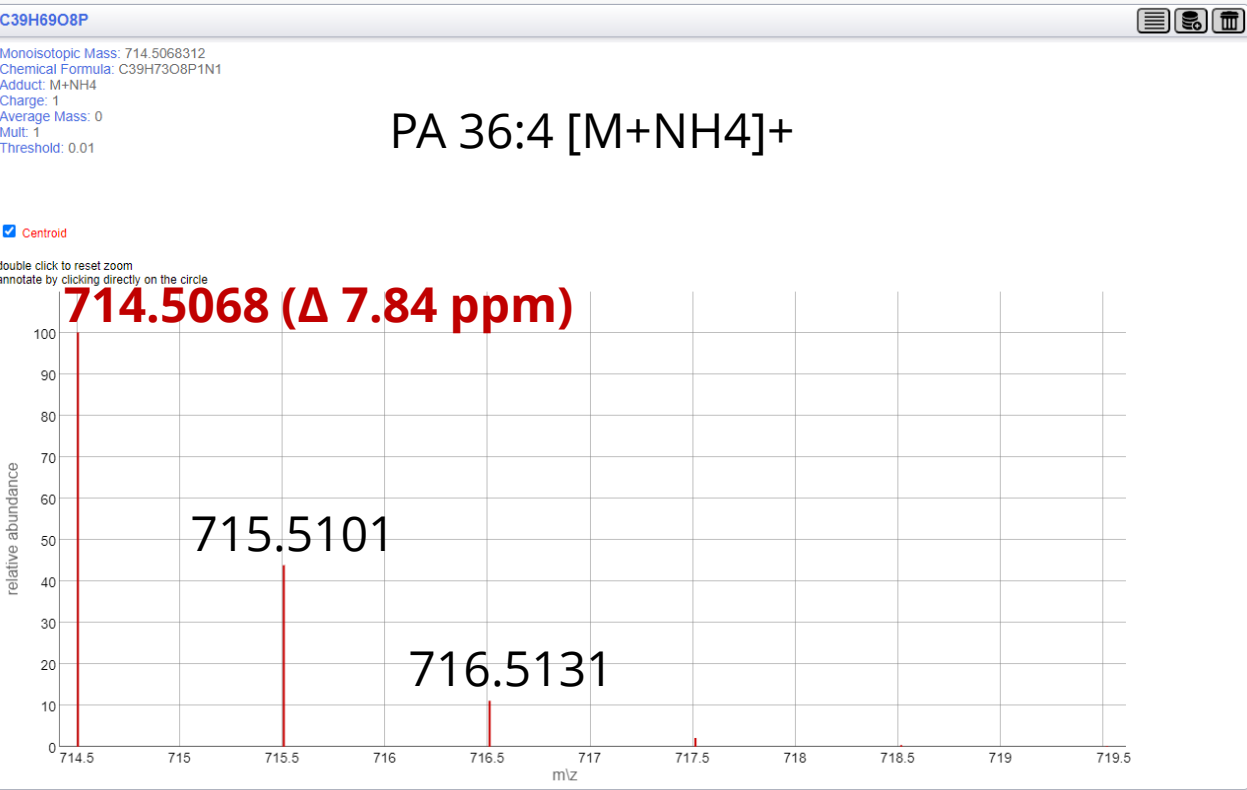
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Type II overlap:

	Lipid	Adduct	Formula	m/z	ppm
1	PA 36:4	[M+NH4] ⁺	C39H69O8P+NH4 ⁺	714.5068	7.84
2	PE 34:3	[M+H] ⁺	C39H72NO8P+H	714.5068	7.84
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- 1. Main ion species for each lipid class**
- 2. Isotopic pattern**
- 3. Complementarity of main ion species for each lipid class in each polarity mode**
- 4. Fragmentation pattern**
- 5. Retention time dependences**

Main ion



Isotopic pattern



Complementarity



MS/MS pattern



RT dependences

1. Main ion species for each lipid class

	Lipid	Adduct	Formula	m/z	ppm
1	PA 36:4	[M+NH ₄] ⁺	C ₃₉ H ₆₉ O ₈ P	714.5068	7.84
2	PE 34:3	[M+H] ⁺	C ₃₉ H ₇₂ NO ₈ P	714.5068	7.84
3	PC 31:3	[M+H] ⁺	C ₃₉ H ₇₂ NO ₈ P	714.5068	7.84
4	MGDG 30:3	[M+NH ₄] ⁺	C ₃₉ H ₆₈ O ₁₀	714.5151	19.45
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6	PE 34:4	2(13C)[M+H] ⁺	C ₃₉ H ₇₀ NO ₈ P	714.4975	5.18
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9	PA 37:3	13C[M+H] ⁺	C ₄₀ H ₇₃ O ₈ P	714.5150	19.31
10	PC 30:5	13C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10
11	PE 33:5	13C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10

Main ion



Isotopic pattern



Complementarity



MS/MS pattern



RT dependences

1. Main ion species for each lipid class

	Lipid	Adduct
1	PA 36:4	[M+NH ₄] ⁺
2	PE 34:3	[M+H] ⁺
3	PC 31:3	[M+H] ⁺
4	MGDG 30:3	[M+NH ₄] ⁺
5	PA 36:5	2(13C)[M+NH ₄] ⁺
6	PE 34:4	2(13C)[M+H] ⁺
7	PC 31:4	2(13C)[M+H] ⁺
8	MGDG 30:4	2(13C)[M+NH ₄] ⁺
9	PA 37:3	13C[M+H] ⁺
10	PC 30:5	13C[M+NH ₄] ⁺
11	PE 33:5	13C[M+NH ₄] ⁺

Lipid class	Positive
Fatty acid, FA	–
(Lyso)Phosphatidic acid, (L)PA	[M+NH ₄] ⁺
(Lyso)Phosphatidylcholine, (L)PC	[M+H] ⁺
(Lyso)Phosphatidylethanolamine, (L)PE	[M+H] ⁺
(Lyso)Phosphatidylglycerol, (L)PG	[M+NH ₄] ⁺
(Lyso)Phosphatidylinositol, (L)PI	[M+NH ₄] ⁺
(Lyso)Phosphatidylserine, (L)PS	[M+H] ⁺
Monogalactosyldiacylglycerol, MGDG	[M+NH ₄] ⁺
Digalactosyldiacylglycerol, DGDG	[M+NH ₄] ⁺
Diacylglycerol, DG	[M+NH ₄] ⁺
Triacylglycerol, TG	[M+NH ₄] ⁺
C ₄₀ H ₇₃ O ₈ P	714.5150 19.31
C ₃₈ H ₆₆ NO ₈ P	714.4897 16.10
C ₃₈ H ₆₆ NO ₈ P	714.4897 16.10

Main ion



Isotopic pattern



Complementarity



MS/MS pattern



RT dependences

1. Main ion species for each lipid class

	Lipid	Adduct
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Lipid class	Positive
Fatty acid, FA	–
(Lyso)Phosphatidic acid, (L)PA	[M+NH ₄] ⁺
(Lyso)Phosphatidylcholine, (L)PC	[M+H] ⁺
(Lyso)Phosphatidylethanolamine, (L)PE	[M+H] ⁺
(Lyso)Phosphatidylglycerol, (L)PG	[M+NH ₄] ⁺
(Lyso)Phosphatidylinositol, (L)PI	[M+NH ₄] ⁺
(Lyso)Phosphatidylserine, (L)PS	[M+H] ⁺
Monogalactosyldiacylglycerol, MGDG	[M+NH ₄] ⁺
Digalactosyldiacylglycerol, DGDG	[M+NH ₄] ⁺
Diacylglycerol, DG	[M+NH ₄] ⁺
Triacylglycerol, TG	[M+NH ₄] ⁺

C ₄₀ H ₇₃ O ₈ P	714.5150	19.31
C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10
C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10

Main ion



Isotopic pattern



Complementarity



MS/MS pattern

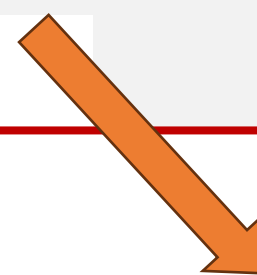
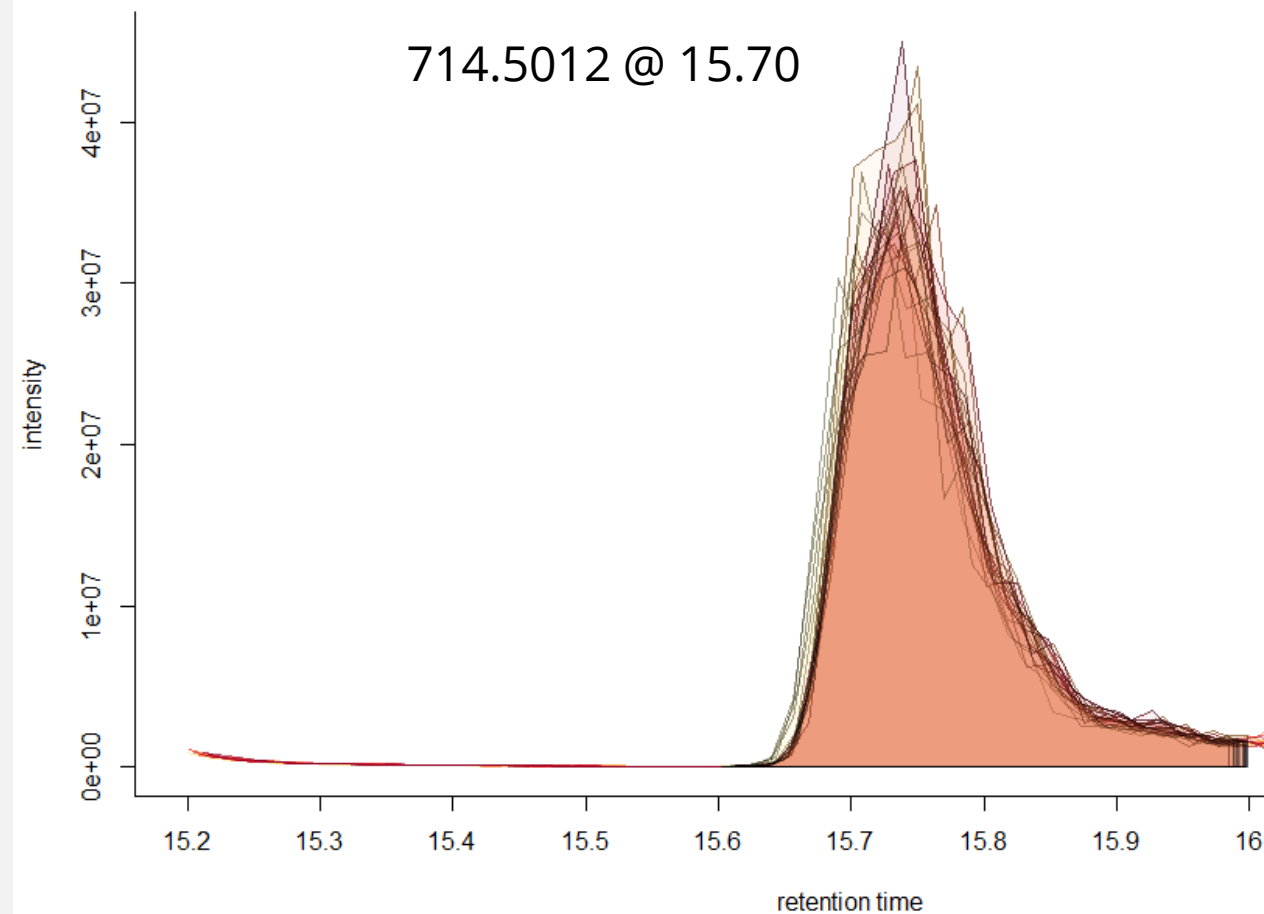


RT dependences

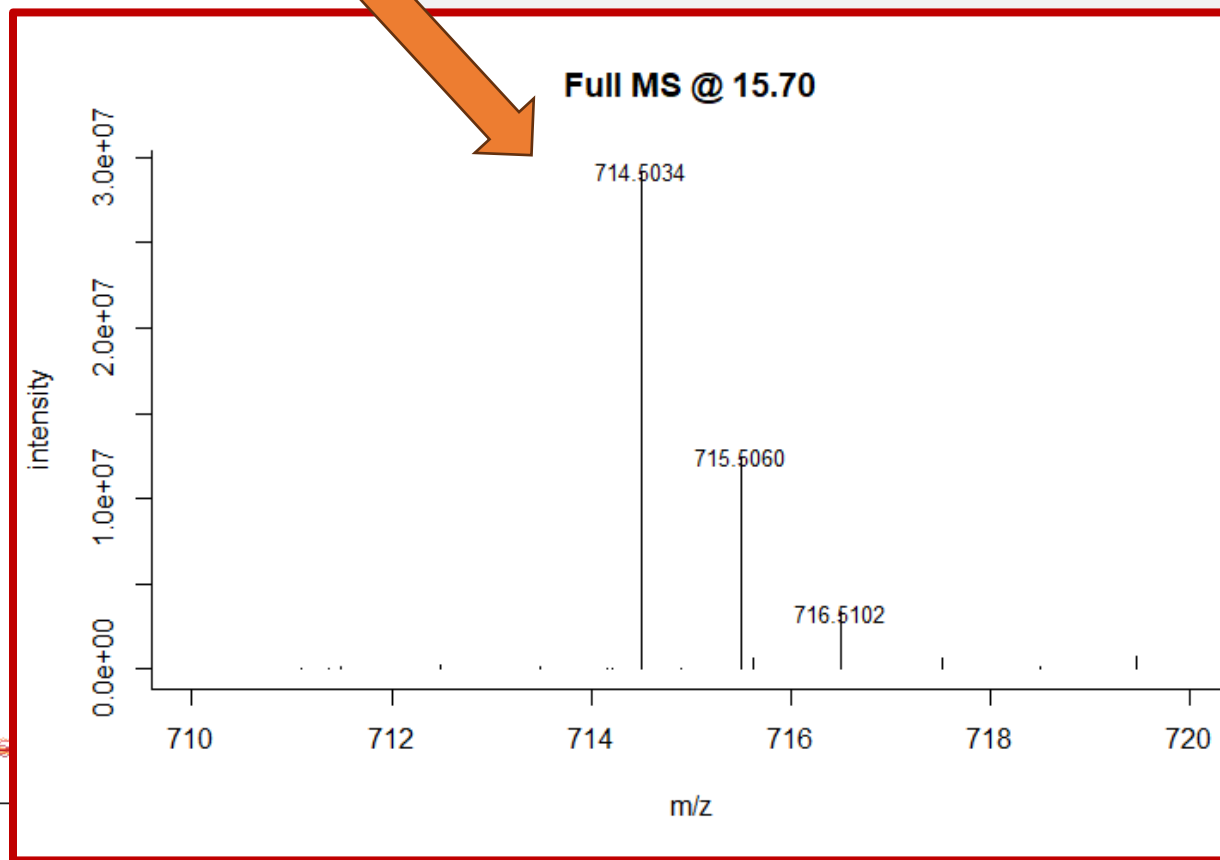
2. Isotopic pattern

714.4687 - 714.6019

714.5012 @ 15.70



Full MS @ 15.70



Main ion



Isotopic pattern



Complementarity



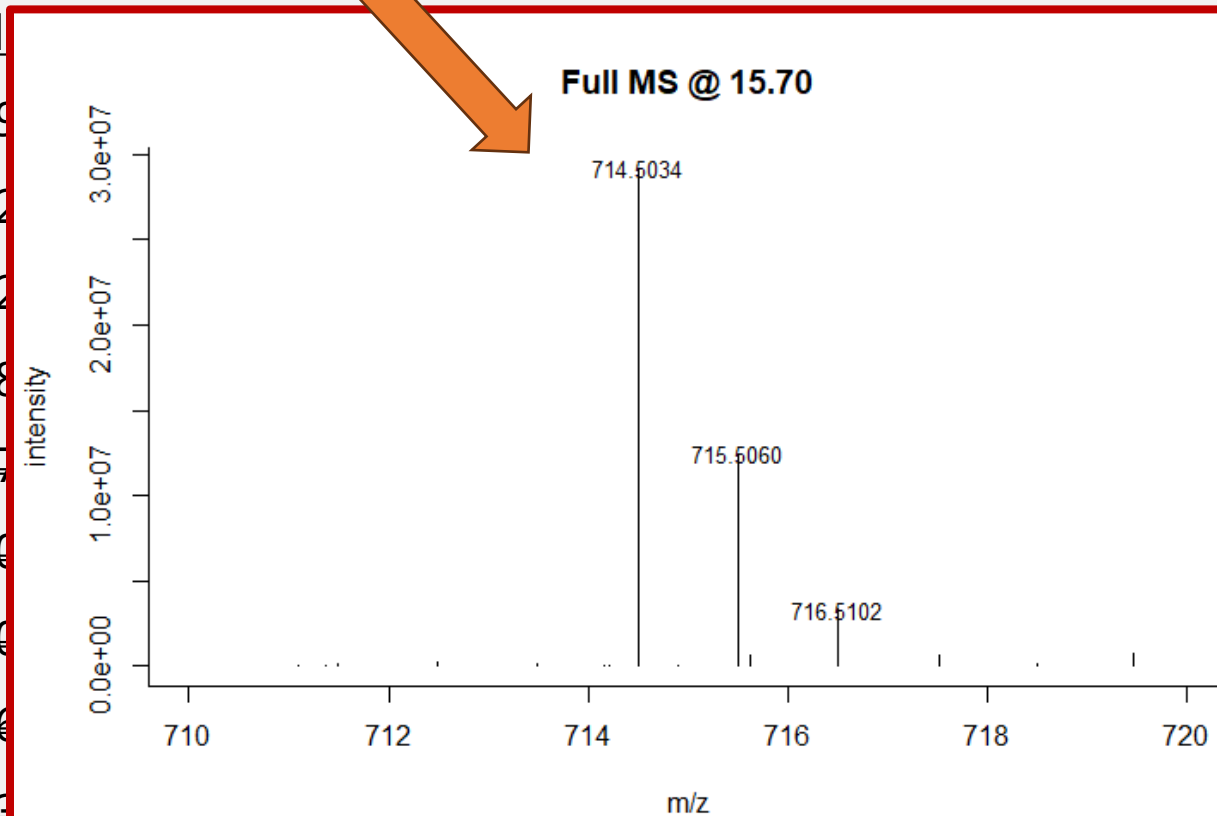
MS/MS pattern



RT dependences

2. Isotopic pattern

	Lipid	Adduct	Formula
1	PA 36:4	[M+NH ₄] ⁺	C ₃₉ H ₆₉ N
2	PE 34:3	[M+H] ⁺	C ₃₉ H ₇₂ O
3	PC 31:3	[M+H] ⁺	C ₃₉ H ₇₂ O ₂
4	MGDG 30:3	[M+NH ₄] ⁺	C ₃₉ H ₆₈ O ₇ N
5	PA 36:5	2(13C)[M+NH₄]⁺	C₃₉H₆₇N
6	PE 34:4	2(13C)[M+H]⁺	C₃₉H₇₀O
7	PC 31:4	2(13C)[M+H]⁺	C₃₉H₇₀O₂
8	MGDG 30:4	2(13C)[M+NH₄]⁺	C₃₉H₆₆O₇N
9	PA 37:3	¹³ C[M+H] ⁺	C ₄₀ H ₇₃ O
10	PC 30:5	¹³ C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P
11	PE 33:5	¹³ C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P



Main ion



Isotopic pattern



Complementarity

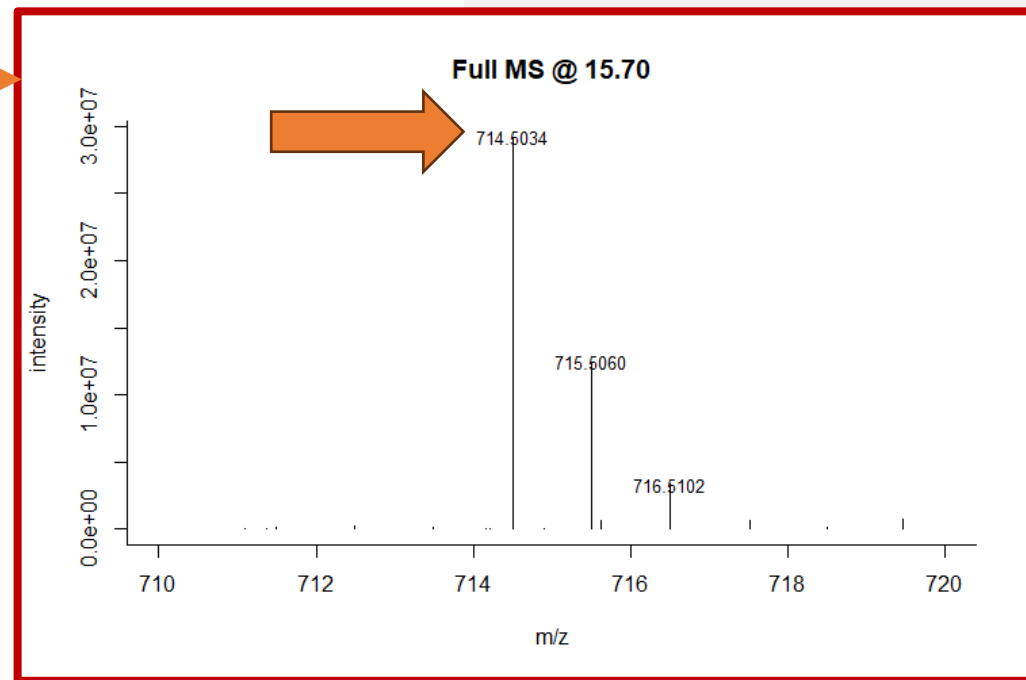
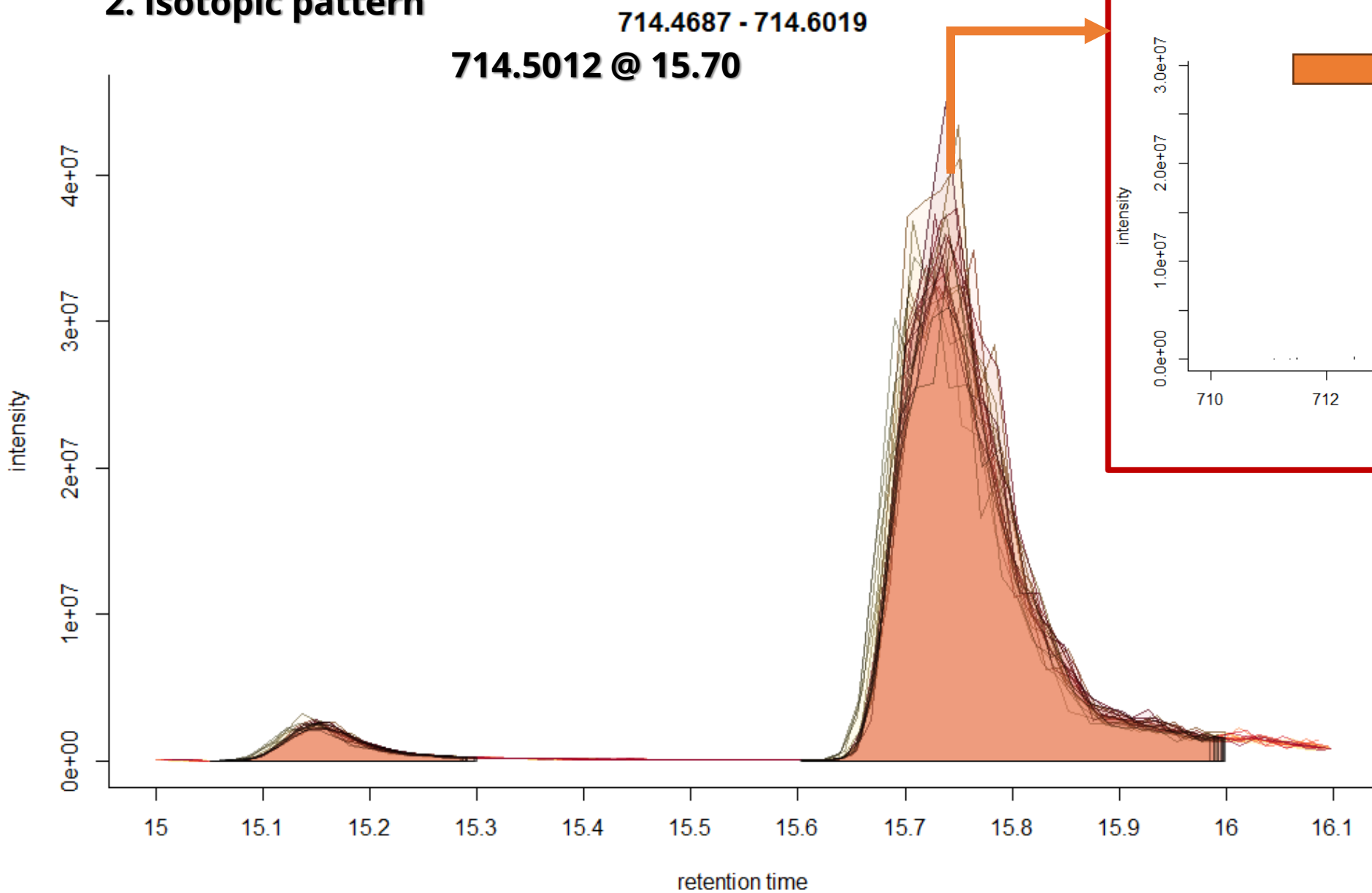


MS/MS pattern



RT dependences

2. Isotopic pattern



Main ion



Isotopic pattern



Complementarity



MS/MS pattern

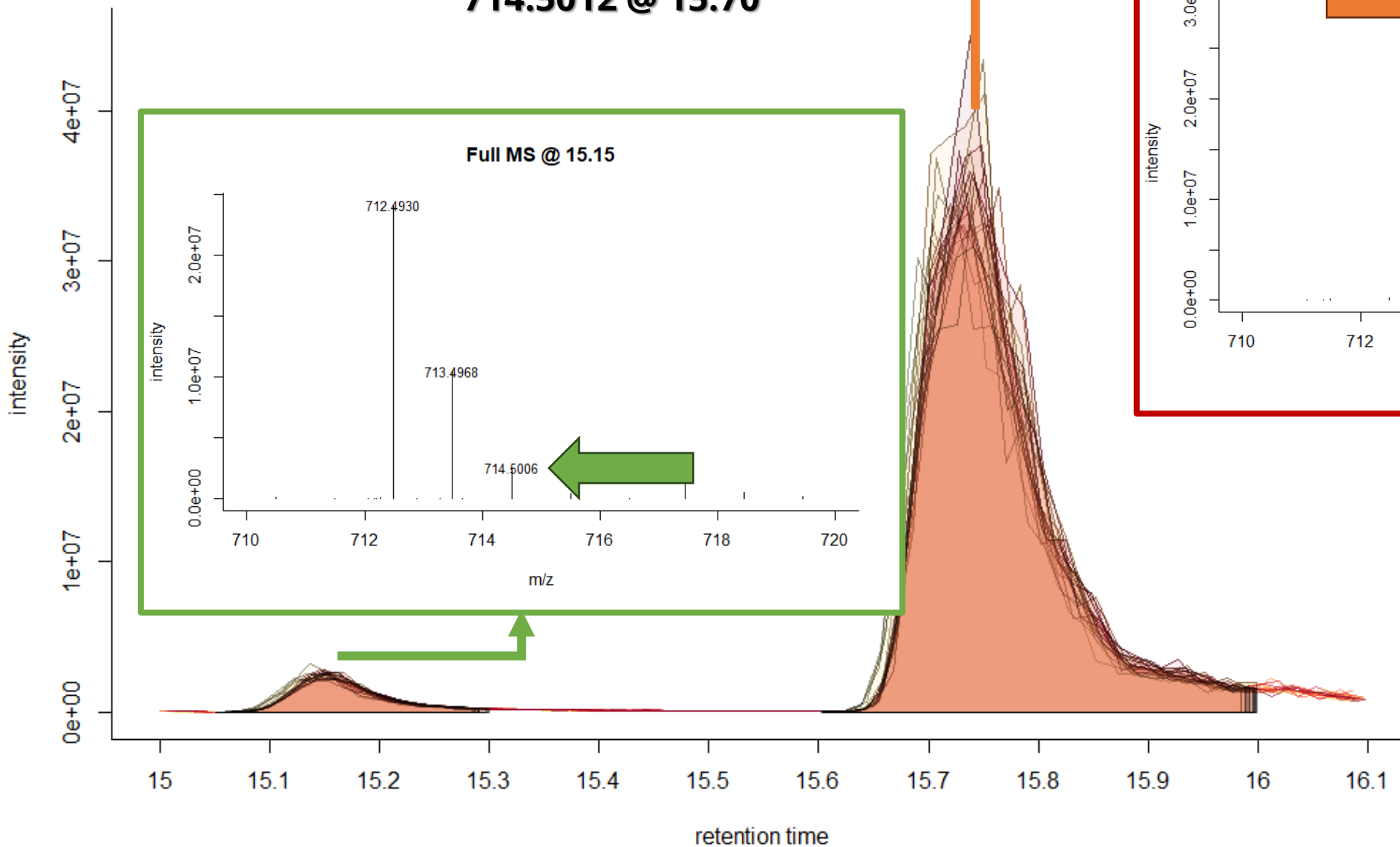


RT dependences

2. Isotopic pattern

714.4687 - 714.6019

714.5012 @ 15.70



Main ion



Isotopic pattern



Complementarity



MS/MS pattern



RT dependences

3. Complementarity of main ion species for each lipid class in each polarity mode

	Lipid	Adduct	Formula	m/z	ppm
1	PA 36:4	[M+NH ₄] ⁺	C ₃₉ H ₆₉ O ₈ P	714.5068	7.84
2	PE 34:3	[M+H] ⁺	C ₃₉ H ₇₂ NO ₈ P	714.5068	7.84
3	PC 31:3	[M+H] ⁺	C ₃₉ H ₇₂ NO ₈ P	714.5068	7.84
4	MGDG 30:3	[M+NH ₄] ⁺	C ₃₉ H ₆₈ O ₁₀	714.5151	19.45
5	PA 36:5	2(13C)[M+NH₄]⁺	C₃₉H₆₇O₈P	714.4975	5.18
6	PE 34:4	2(13C)[M+H]⁺	C₃₉H₇₀NO₈P	714.4975	5.18
7	PC 31:4	2(13C)[M+H]⁺	C₃₉H₇₀NO₈P	714.4975	5.18
8	MGDG 30:4	2(13C)[M+NH₄]⁺	C₃₉H₆₆O₁₀	714.5057	6.30
9	PA 37:3	¹³ C[M+H] ⁺	C ₄₀ H ₇₃ O ₈ P	714.5150	19.31
10	PC 30:5	¹³ C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10
11	PE 33:5	¹³ C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10



Main ion

Isotopic pattern

Complementarity

MS/MS pattern

RT dependences

3. Complementarity of main ion species for each lipid class in each polarity mode

			Lipid class	Positive	Negative
	Lipid	Adduct			
			Fatty acid, FA	–	[M-H] ⁻
1	PA 36:4	[M+NH ₄] ⁺	(Lyso)Phosphatidic acid, (L)PA	[M+NH ₄] ⁺	[M-H] ⁻
2	PE 34:3	[M+H] ⁺	(Lyso)Phosphatidylcholine, (L)PC	[M+H] ⁺	[M+CHO ₂] ⁻
3	PC 31:3	[M+H] ⁺	(Lyso)Phosphatidylethanolamine, (L)PE	[M+H] ⁺	[M-H] ⁻
4	MGDG 30:3	[M+NH ₄] ⁺	(Lyso)Phosphatidylglycerol, (L)PG	[M+NH ₄] ⁺	[M-H] ⁻
5	PA 36:5	2(13C)[M+NH₄]⁺	(Lyso)Phosphatidylinositol, (L)PI	[M+NH ₄] ⁺	[M-H] ⁻
6	PE 34:4	2(13C)[M+H]⁺	(Lyso)Phosphatidylserine, (L)PS	[M+H] ⁺	[M-H] ⁻
7	PC 31:4	2(13C)[M+H]⁺	Monogalactosyldiacylglycerol, MGDG	[M+NH ₄] ⁺	[M+CHO ₂] ⁻
8	MGDG 30:4	2(13C)[M+NH₄]⁺	Digalactosyldiacylglycerol, DGDG	[M+NH ₄] ⁺	[M+CHO ₂] ⁻
9	PA 37:3	13C[M+H] ⁺	Diacylglycerol, DG	[M+NH ₄] ⁺	–
10	PC 30:5	13C[M+NH ₄] ⁺	Triacylglycerol, TG	[M+NH ₄] ⁺	–
11	PE 33:5	13C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10

Main ion



Isotopic pattern



Complementarity



MS/MS pattern



RT dependences

3. Complementarity of main ion species for each lipid class in each polarity mode

	Lipid	Adduct	Negative	m/z	
1	PA 36:4	[M+NH ₄] ⁺	[M-H] ⁻	695.4657	
2	PE 34:3	[M+H] ⁺	[M-H] ⁻	712.4923	
3	PC 31:3	[M+H] ⁺	[M+CHO ₂] ⁻	758.4978	
4	MGDG 30:3	[M+NH ₄] ⁺	[M+CHO ₂] ⁻	741.4794	
5	PA 36:5	2(13C)[M+NH₄]⁺	C₃₉H₆₇O₈P	714.4975	5.18
6	PE 34:4	2(13C)[M+H]⁺	C₃₉H₇₀NO₈P	714.4975	5.18
7	PC 31:4	2(13C)[M+H]⁺	C₃₉H₇₀NO₈P	714.4975	5.18
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9	PA 37:3	13C[M+H] ⁺	C ₄₀ H ₇₃ O ₈ P	714.5150	19.31
10	PC 30:5	13C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10
11	PE 33:5	13C[M+NH ₄] ⁺	C ₃₈ H ₆₆ NO ₈ P	714.4897	16.10

Main ion

Isotopic pattern

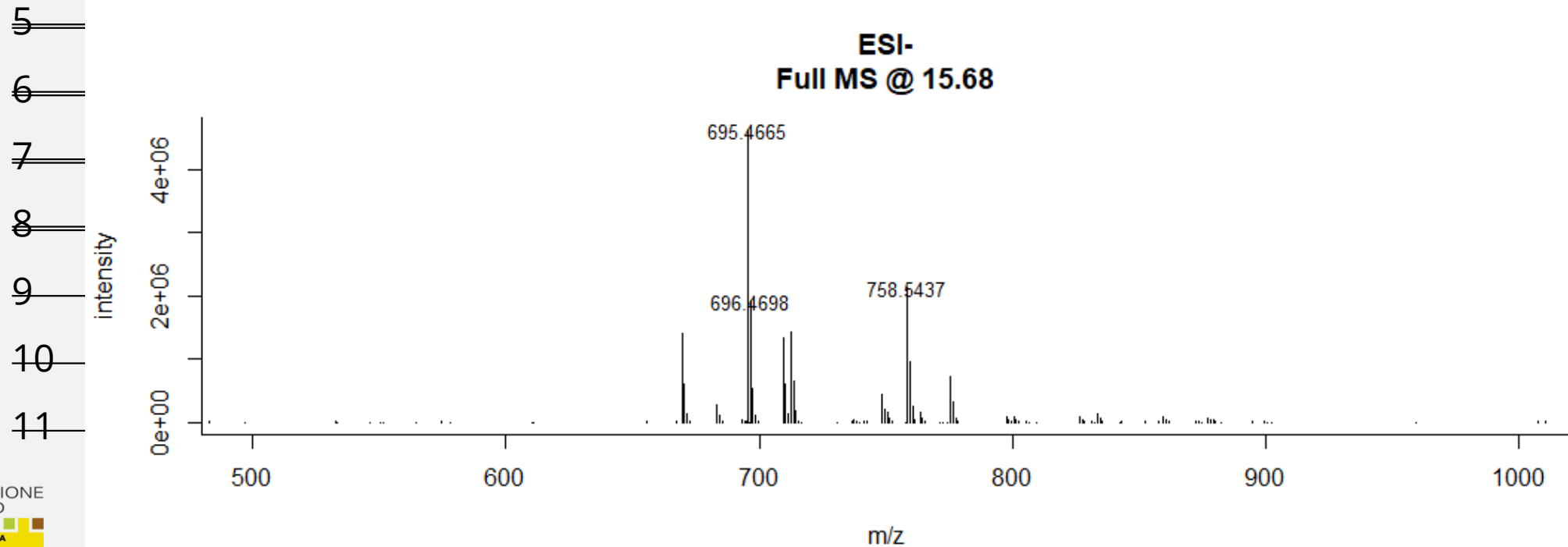
Complementarity

MS/MS pattern

RT dependences

3. Complementarity of main ion species for each lipid class in each polarity mode

	Lipid	Adduct	Negative	m/z
1	PA 36:4	[M+NH ₄] ⁺	[M-H] ⁻	695.4657
2	PE 34:3	[M+H] ⁺	[M-H] ⁻	712.4923
3	PC 31:3	[M+H] ⁺	[M+CHO ₂] ⁻	758.4978
4	MGDG 30:3	[M+NH ₄] ⁺	[M+CHO ₂] ⁻	741.4794



Main ion

Isotopic pattern

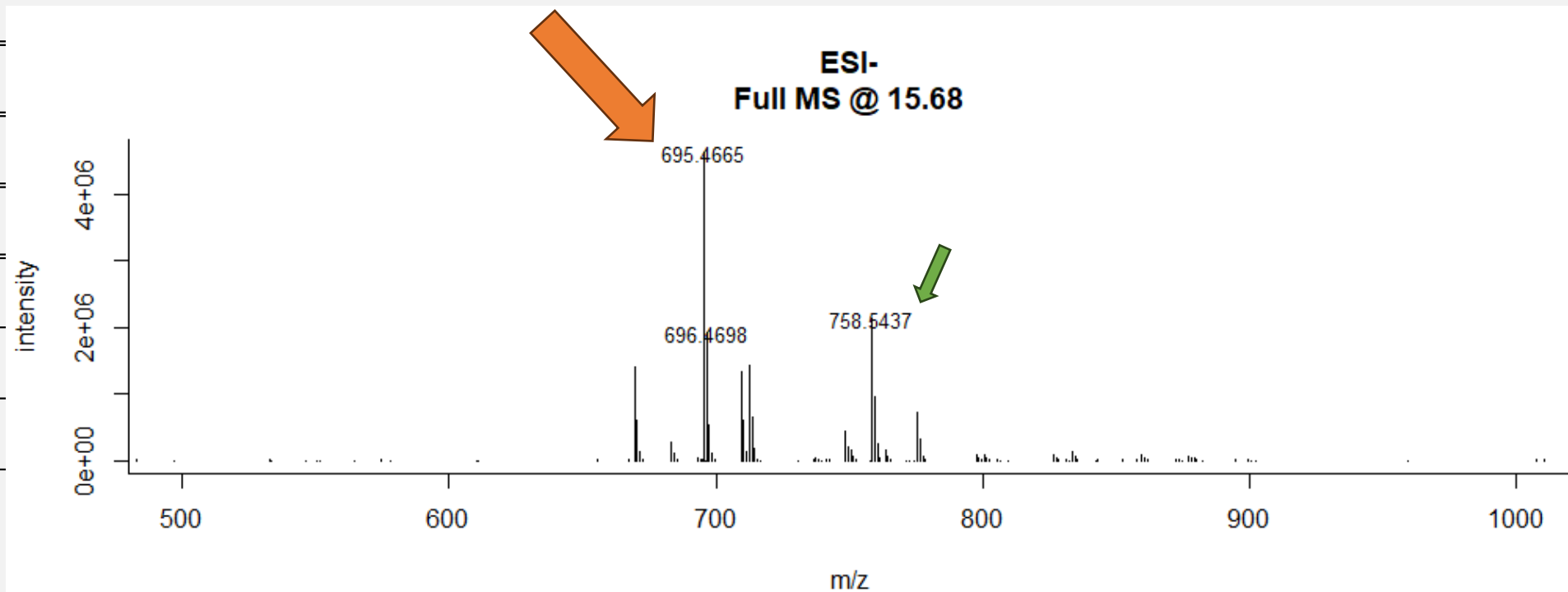
Complementarity

MS/MS pattern

RT dependences

3. Complementarity of main ion species for each lipid class in each polarity mode

	Lipid	Adduct	Negative	m/z
1	PA 36:4	[M+NH ₄] ⁺	[M-H] ⁻	695.4657
2	PE 34:3	[M+H] ⁺	[M-H] ⁻	712.4923
3	PC 31:3	[M+H] ⁺	[M+CHO ₂] ⁻	758.4978
4	MGDG 30:3	[M+NH ₄] ⁺	[M+CHO ₂] ⁻	741.4794



Main ion

Isotopic pattern

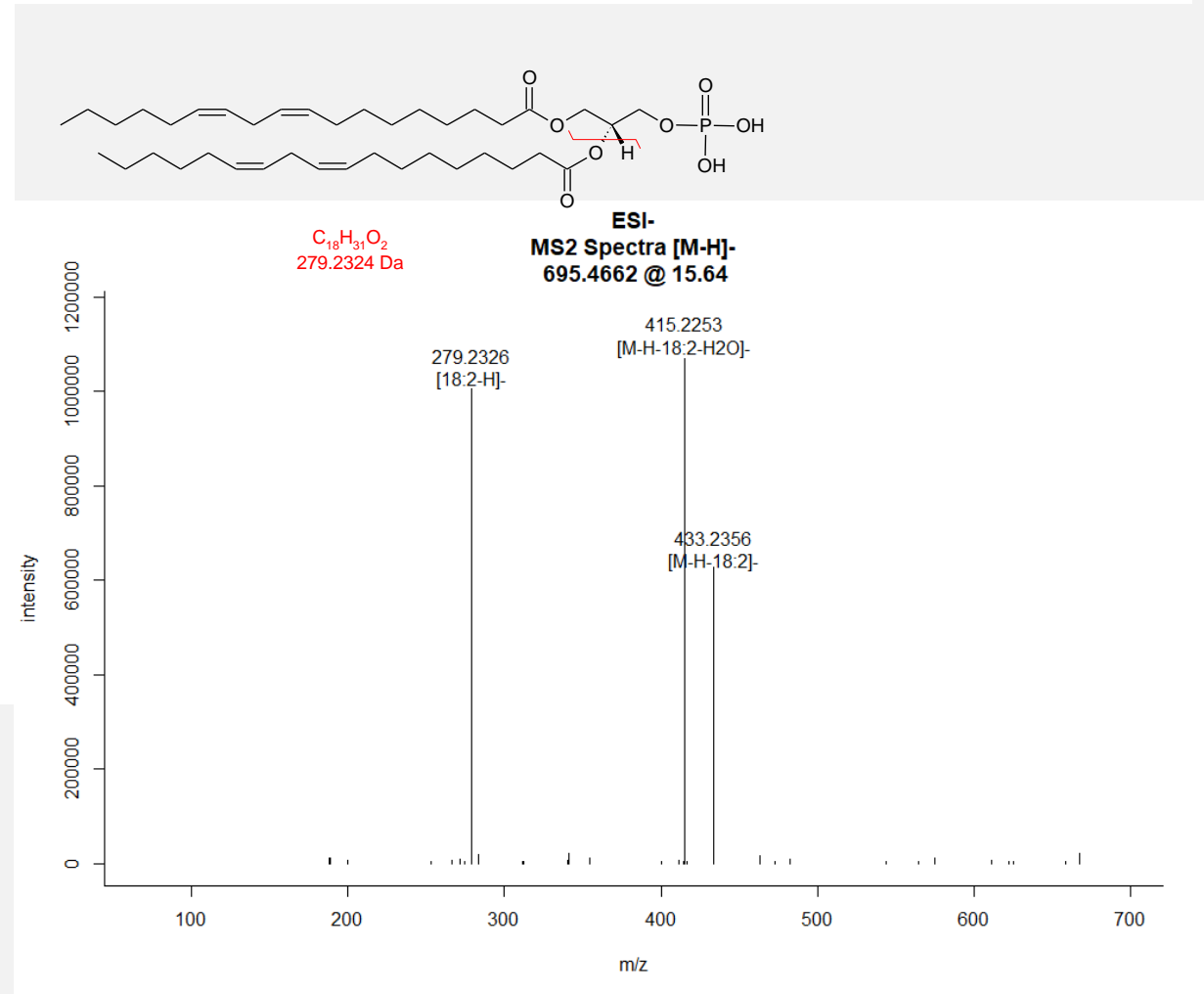
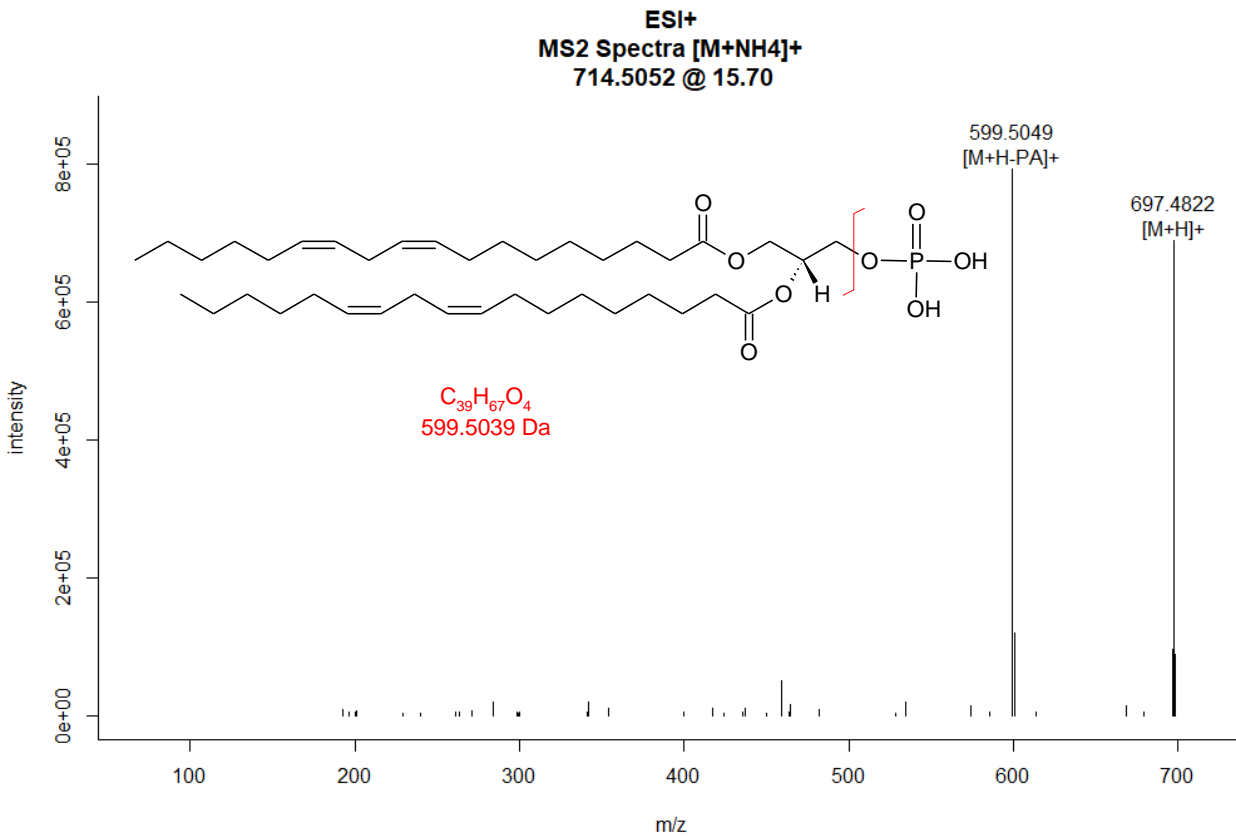
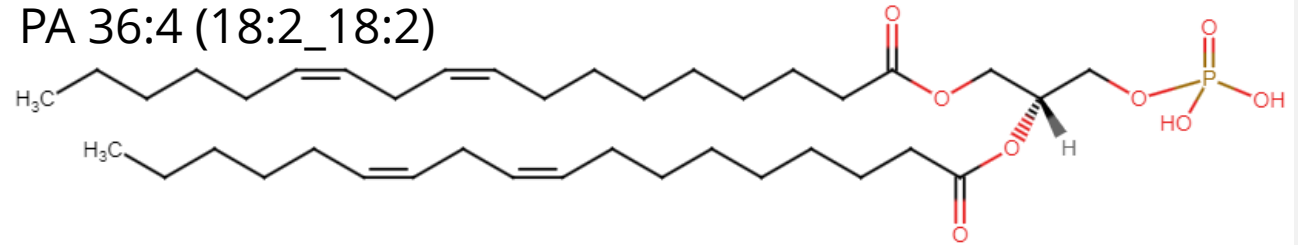
Complementarity

MS/MS pattern

RT dependences

4. Fragmentation pattern

PA 36:4 (18:2_18:2)



Main ion



Isotopic pattern



Complementarity

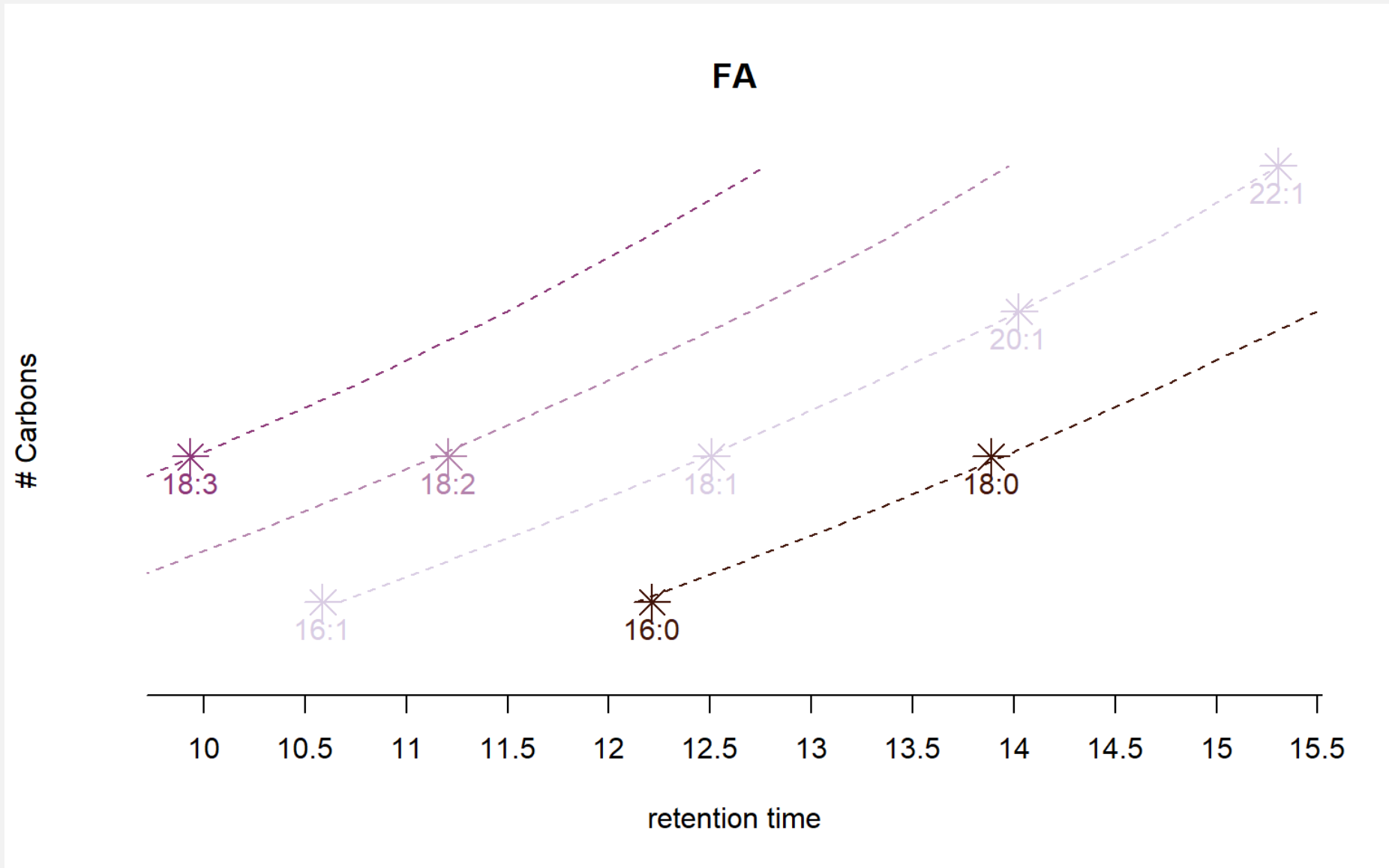


MS/MS pattern



RT dependences

5. Retention time dependences



Main ion

Isotopic pattern

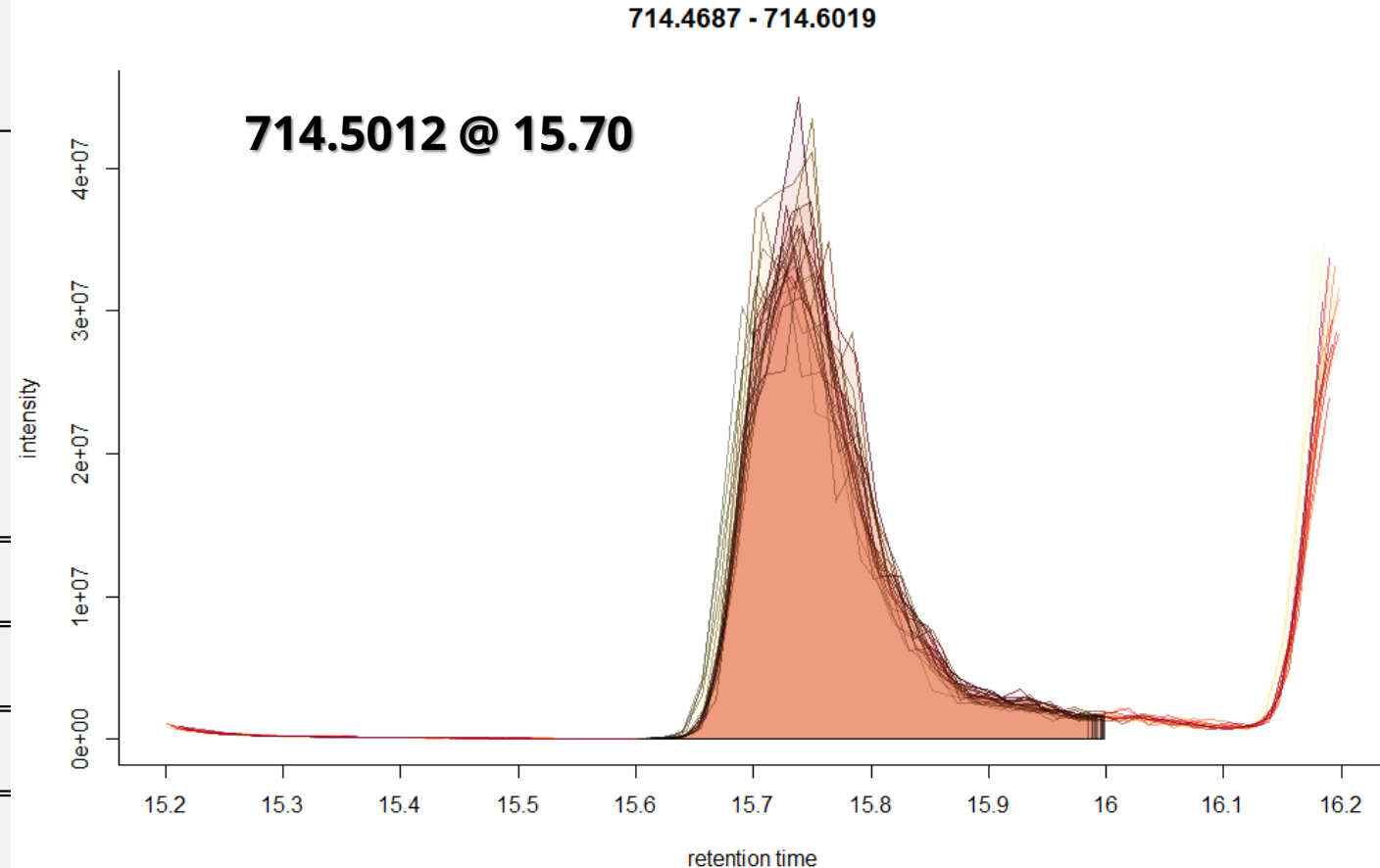
Complementarity

MS/MS pattern

RT dependences

5. Retention time dependences

	Lipid	Adduct
1	PA 36:4	[M+NH ₄] ⁺
2	PE 34:3	[M+H] ⁺
3	PC 31:3	[M+H] ⁺
4	MGDG 30:3	[M+NH ₄] ⁺
5	PA 36:5	2(13C)[M+NH₄]⁺
6	PE 34:4	2(13C)[M+H]⁺
7	PC 31:4	2(13C)[M+H]⁺
8	MGDG 30:4	2(13C)[M+NH₄]⁺
9	PA 37:3	13C[M+H] ⁺
10	PC 30:5	13C[M+NH ₄] ⁺
11	PE 33:5	13C[M+NH ₄] ⁺



C38H66NO8P	714.4897	16.10
C38H66NO8P	714.4897	16.10

Main ion



Isotopic pattern



Complementarity



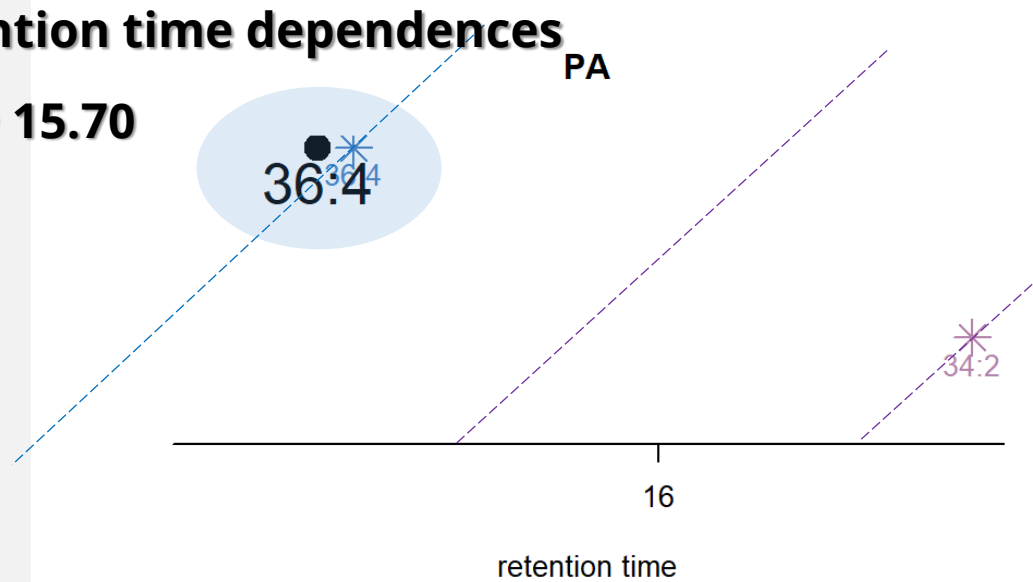
MS/MS pattern



RT dependences

5. Retention time dependences

714.5012 @ 15.70



Main ion



Isotopic pattern



Complementarity



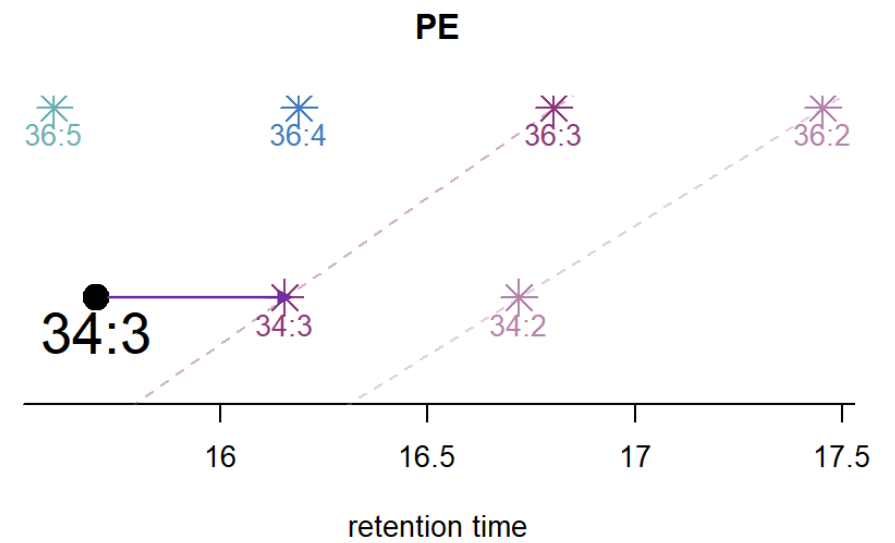
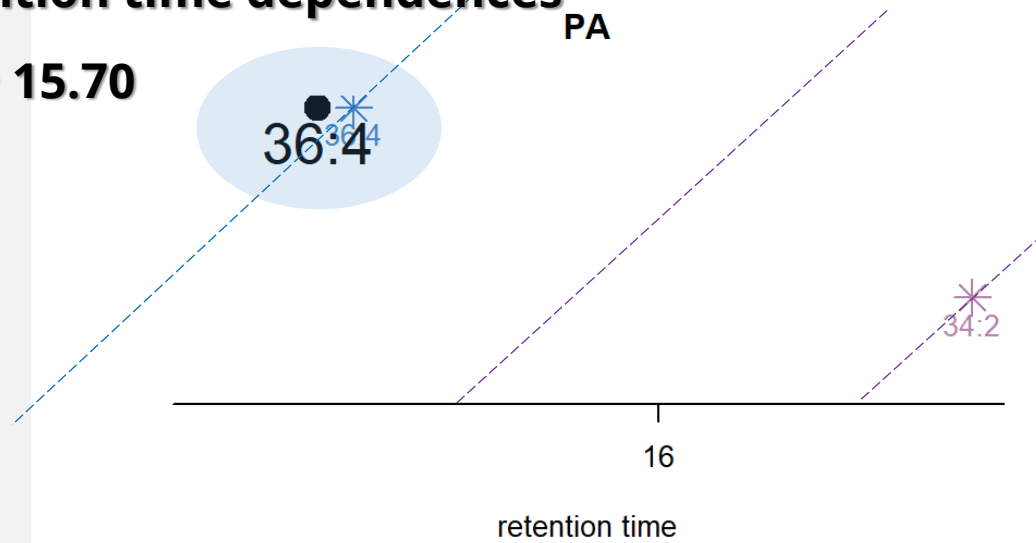
MS/MS pattern



RT dependences

5. Retention time dependences

714.5012 @ 15.70



Main ion



Isotopic pattern



Complementarity



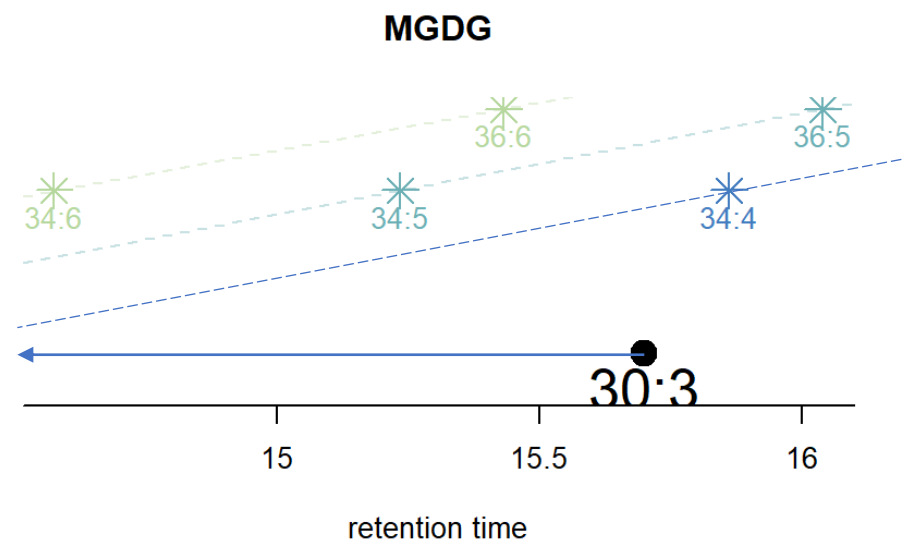
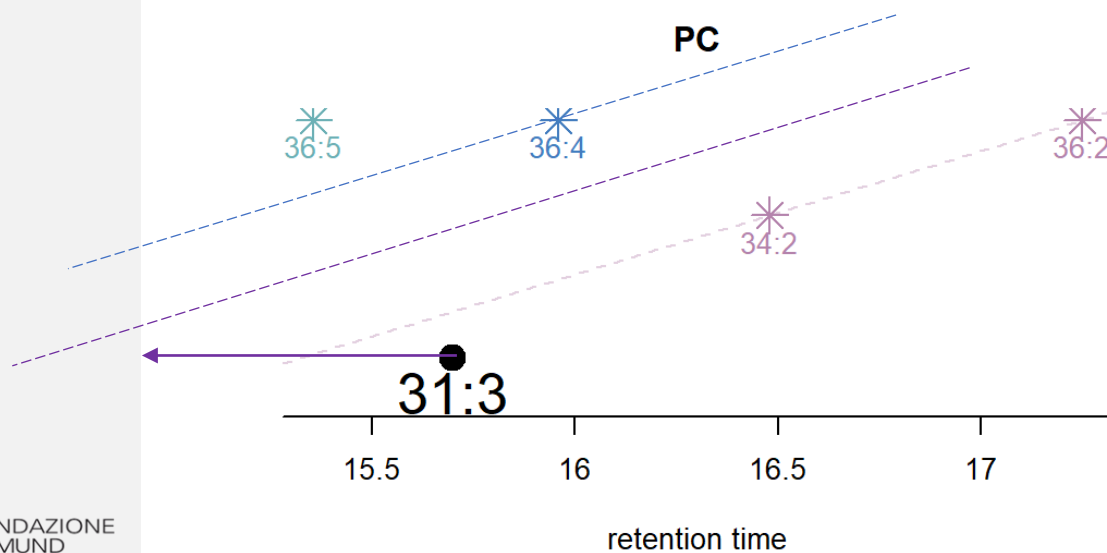
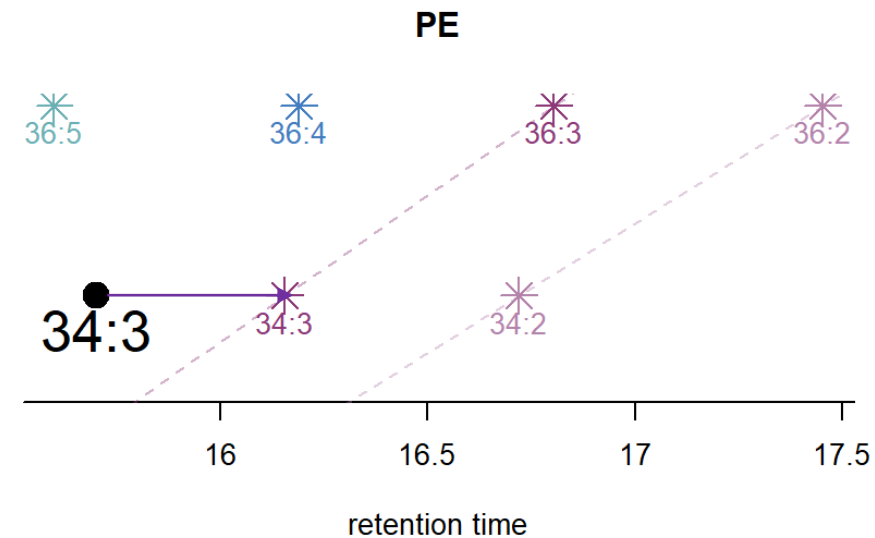
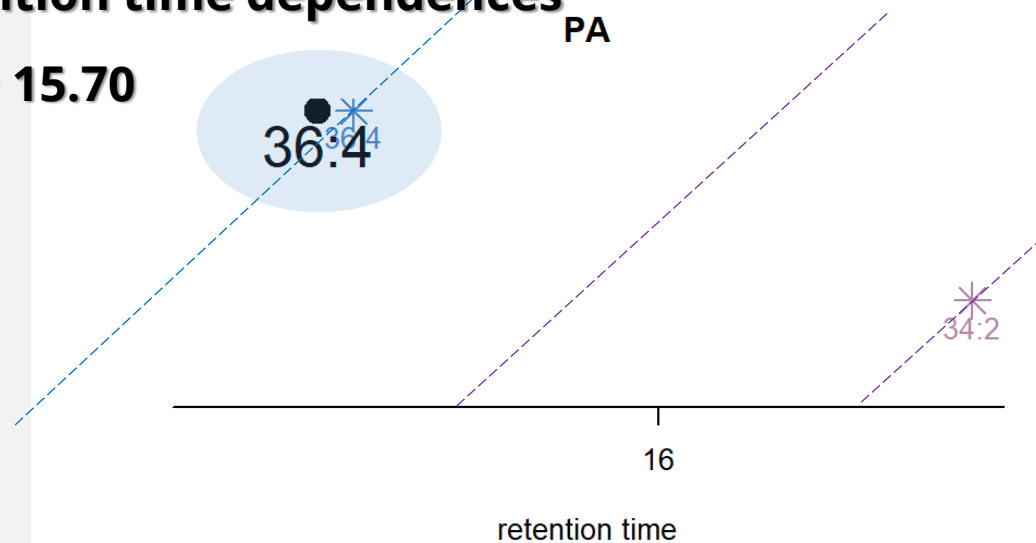
MS/MS pattern



RT dependences

5. Retention time dependences

714.5012 @ 15.70



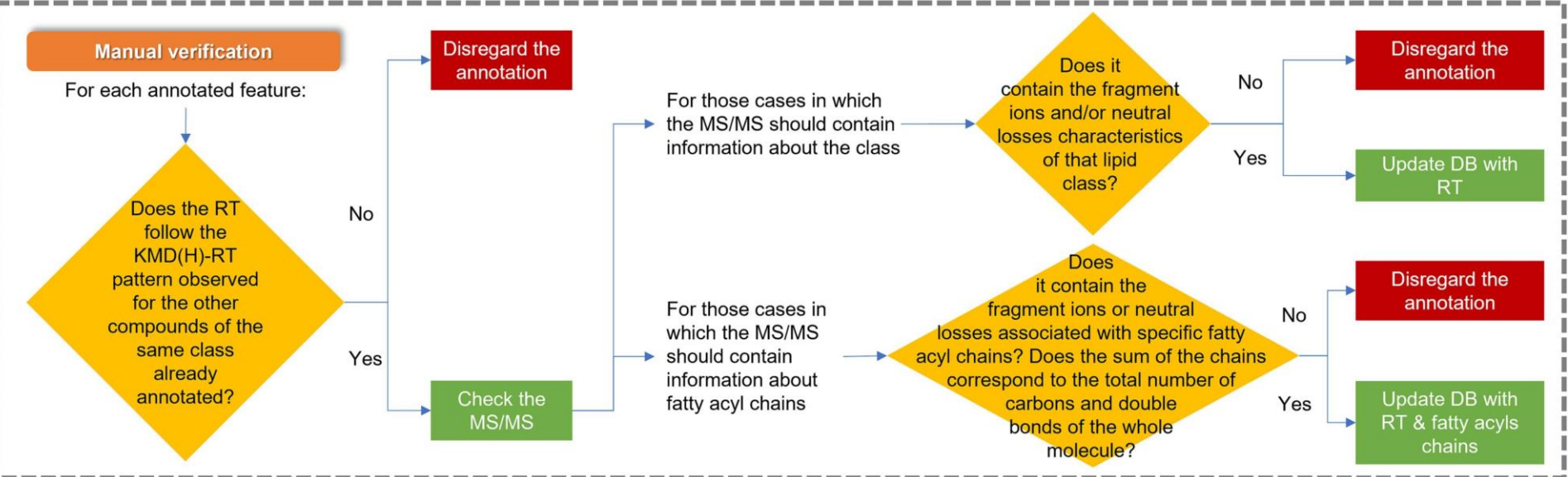
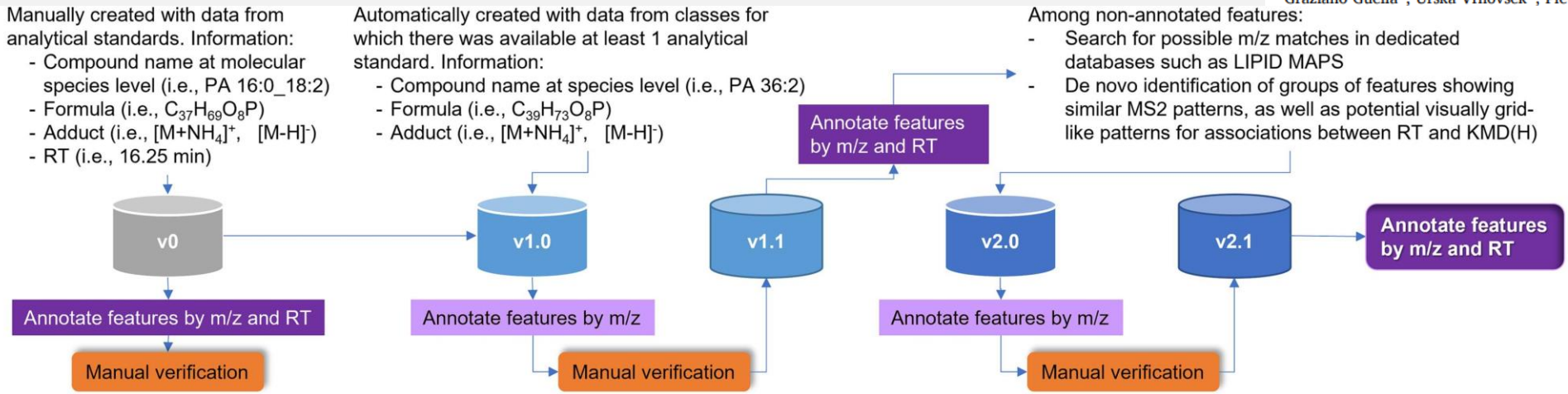
Designed pipeline :

Manually created with data from analytical standards. Information:

- Compound name at molecular species level (i.e., PA 16:0_18:2)
- Formula (i.e., $C_{37}H_{69}O_8P$)
- Adduct (i.e., $[M+NH_4]^+$, $[M-H]^-$)
- RT (i.e., 16.25 min)

Automatically created with data from classes for which there was available at least 1 analytical standard. Information:

- Compound name at species level (i.e., PA 36:2)
- Formula (i.e., $C_{39}H_{73}O_8P$)
- Adduct (i.e., $[M+NH_4]^+$, $[M-H]^-$)



Untargeted lipidomic profiling of grapes highlights the importance of modified lipid species beyond the traditional compound classes

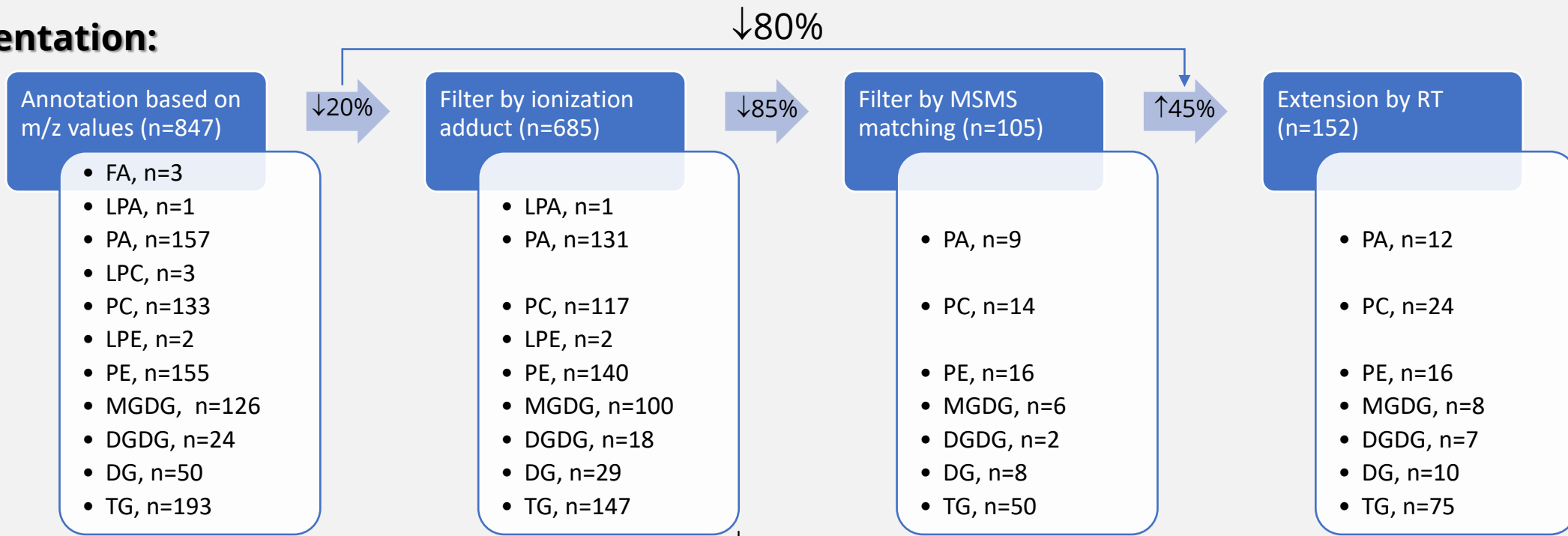
Mar Garcia-Aloy^{a,*}, Domenico Masuero^a, Giulia Chitarrini^a, Domen Škrab^{a,b}, Paolo Sivilotti^b, Graziano Guella^c, Urska Vrhovsek^a, Pietro Franceschi^d

^aEdmund Mach, 38098 San Michele all'Adige, Italy
^bUniversity of Udine, 33100 Udine, Italy
^cTrento, 38123 Trento, Italy
^dEdmund Mach, 38098 San Michele all'Adige, Italy

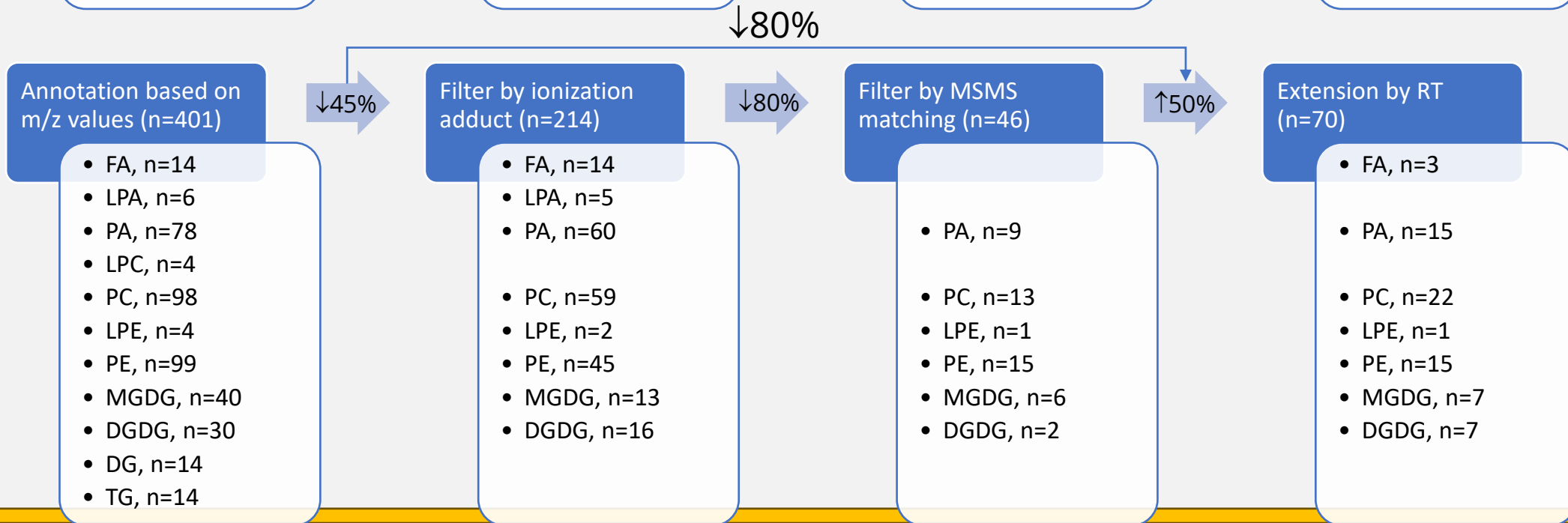


Pipeline implementation:

ESI+
n = 2,370

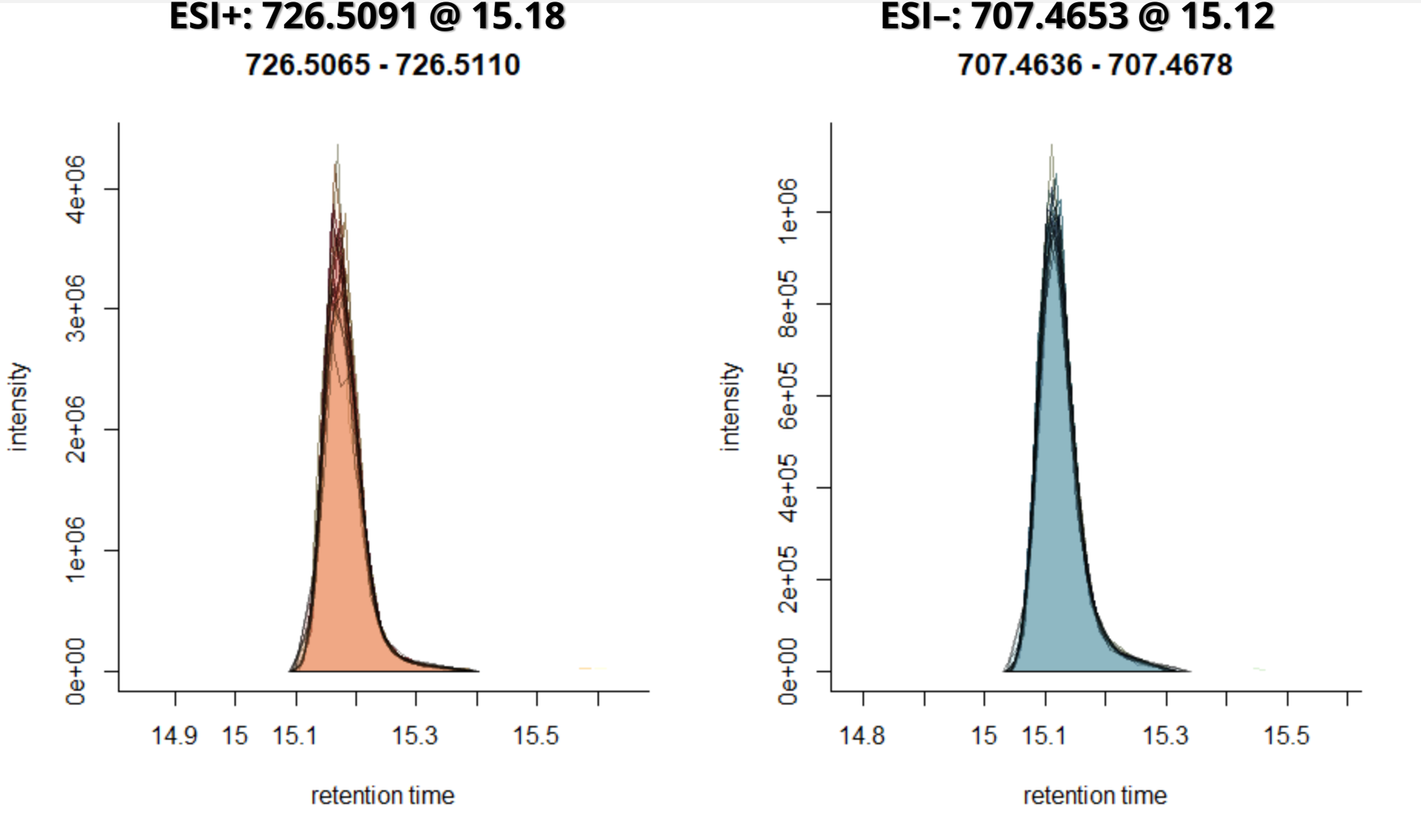


ESI-
n = 1,493



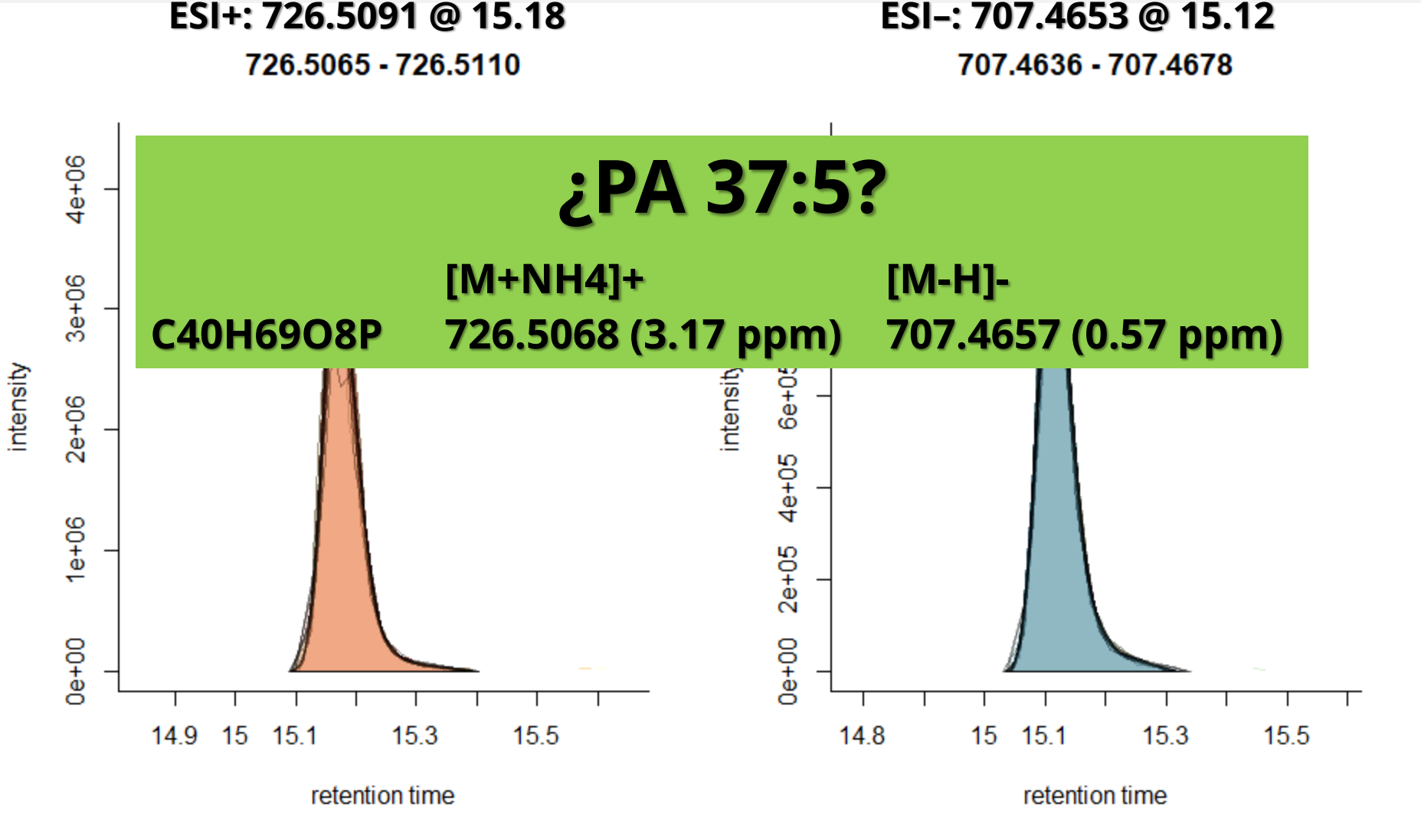
Annotation of less common lipid classes:

https://garciamar.shinyapps.io/lipidomics_tool/



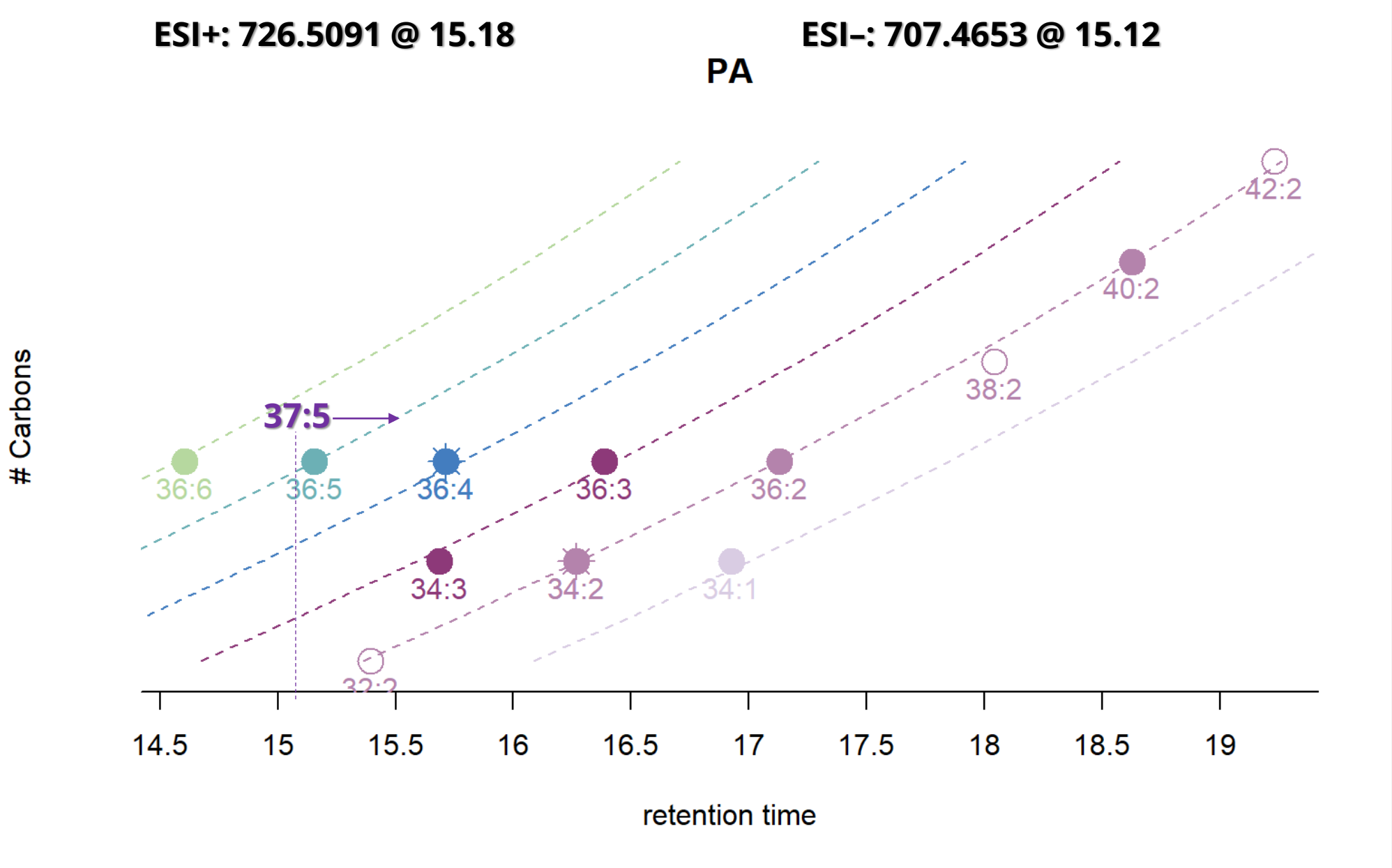
Annotation of less common lipid classes:

https://garciamar.shinyapps.io/lipidomics_tool/



Annotation of less common lipid classes:

https://garciamar.shinyapps.io/lipidomics_tool/



Annotation of less common lipid classes:

https://garciamar.shinyapps.io/lipidomics_tool/

Formula

Lipid class: PA

C37

db5

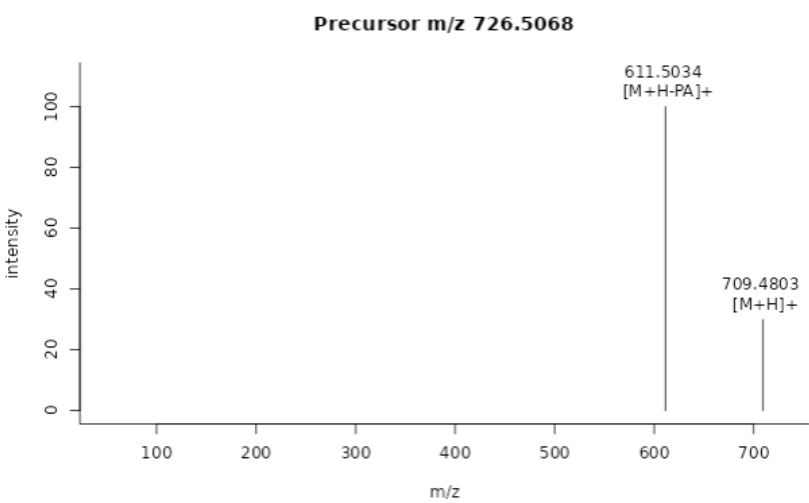
[1] "C40H69O8P"

Major adducts

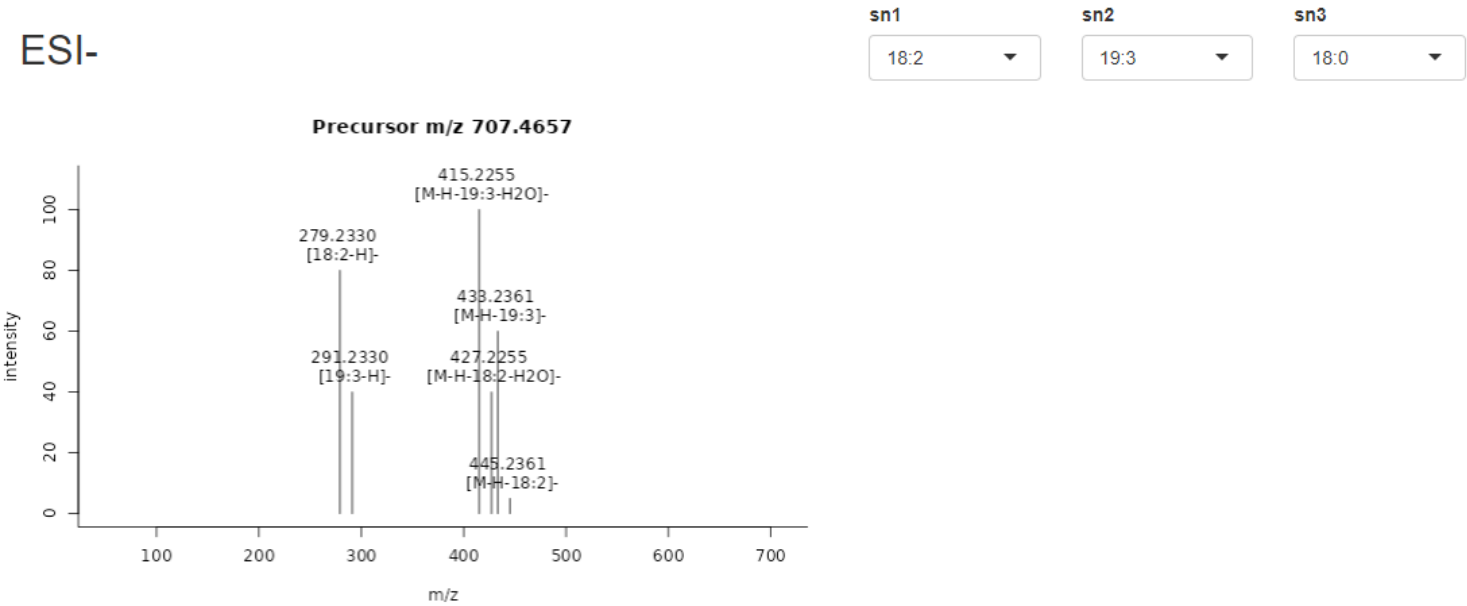
[M+NH4] ⁺	[M-H] ⁻
C40H69O8P 726.5068	707.4657

Theoretical MS2

ESI+



ESI-



Annotation of less common lipid classes:

https://garciamar.shinyapps.io/lipidomics_tool/

Lipidomics Main Panel MS2

Formula

Lipid class:

C

db

PA

37

5

[1] "C40H69O8P"

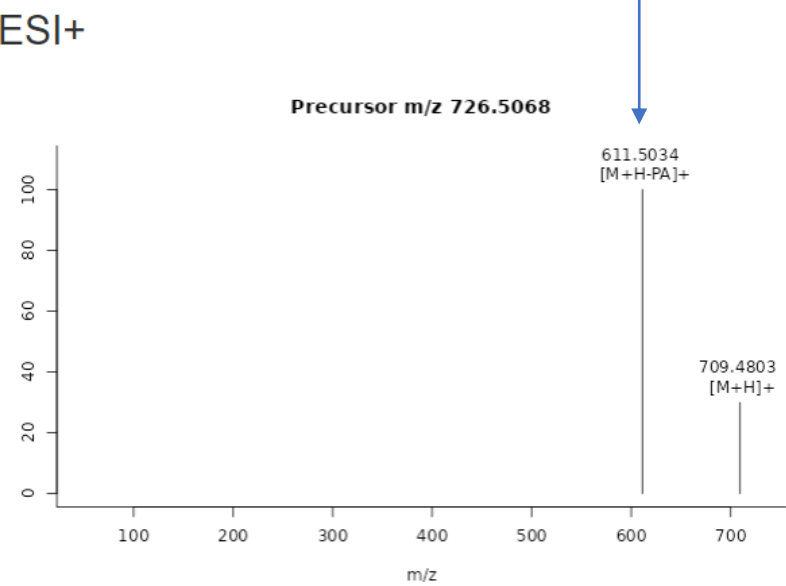
Major adducts

[M+NH4]⁺

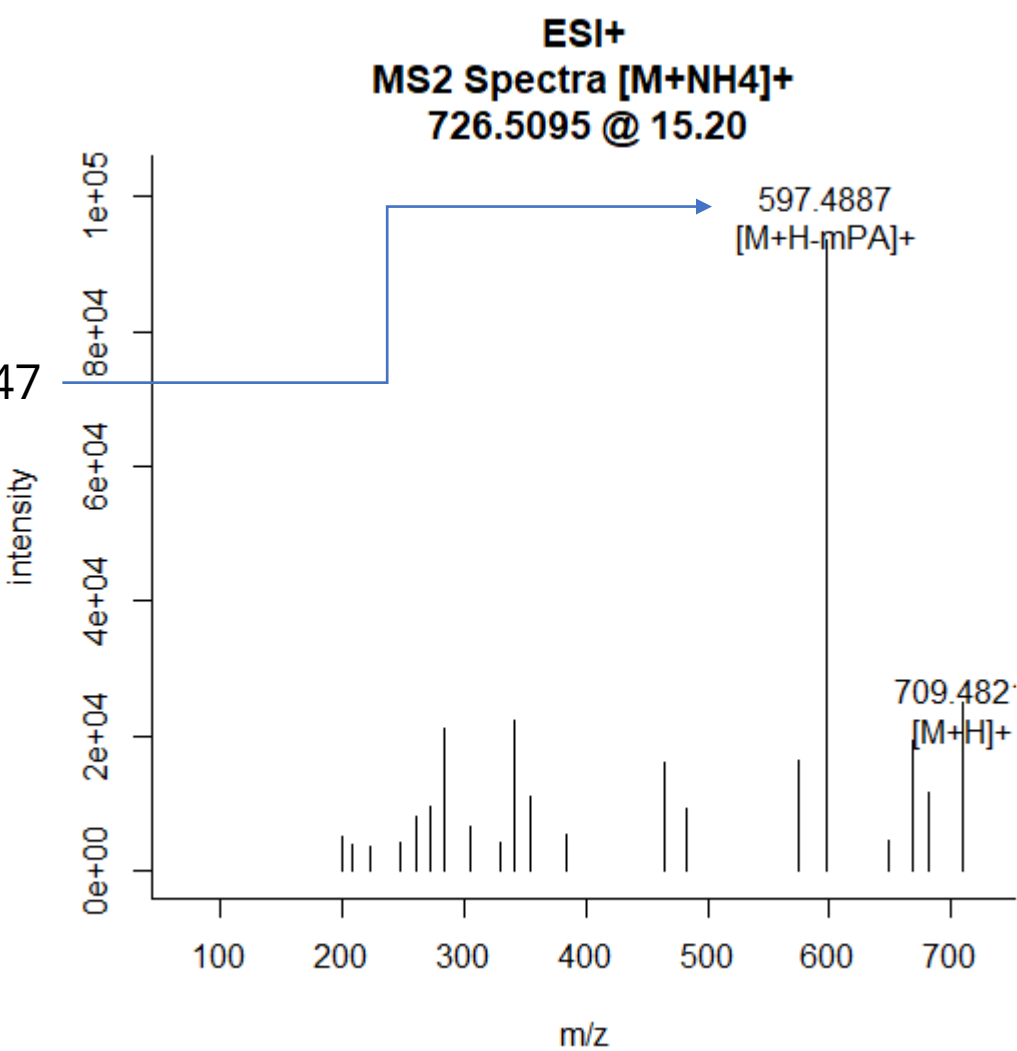
[M-H]⁻

C40H69O8P 726.5068 707.4657

Theoretical MS2



$\Delta 14.0147$



n2

19:3

sn3

18:0

Annotation of less common lipid classes:

https://garciamar.shinyapps.io/lipidomics_tool/

Formula

Lipid class:

PA

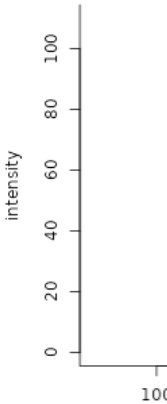
[1] "C40H69O"

Major adduc

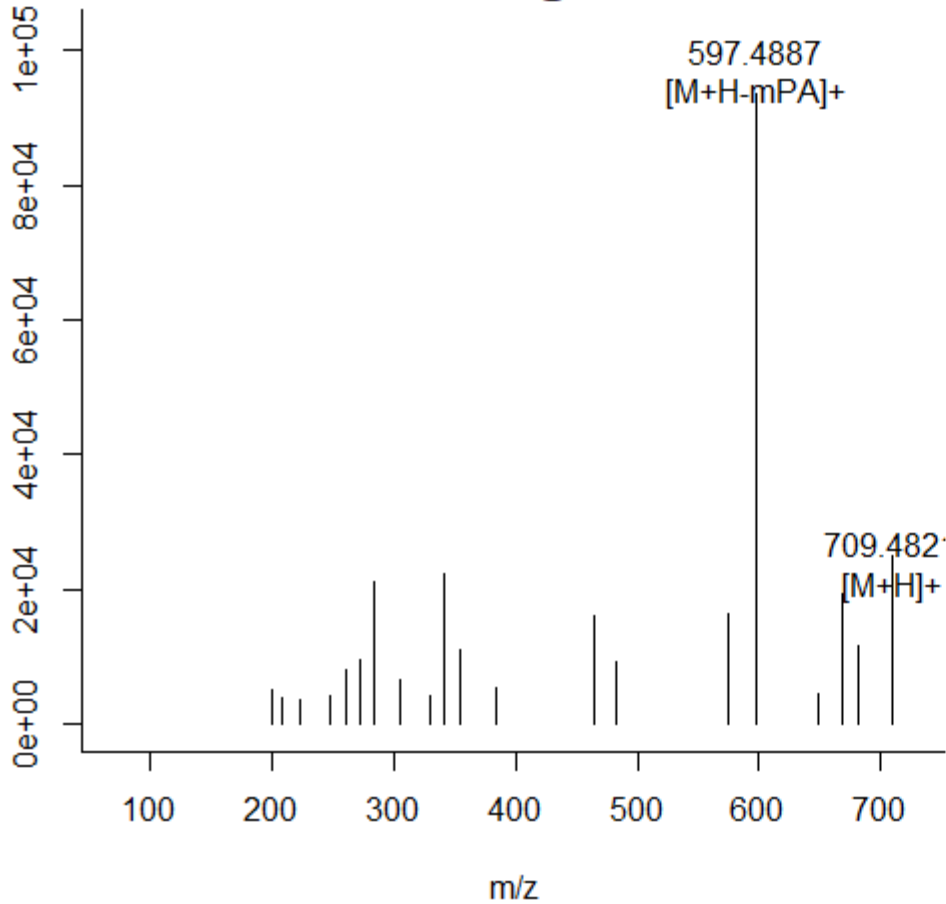
[M+NH4]
C40H69O8P 726.50

Theoretical

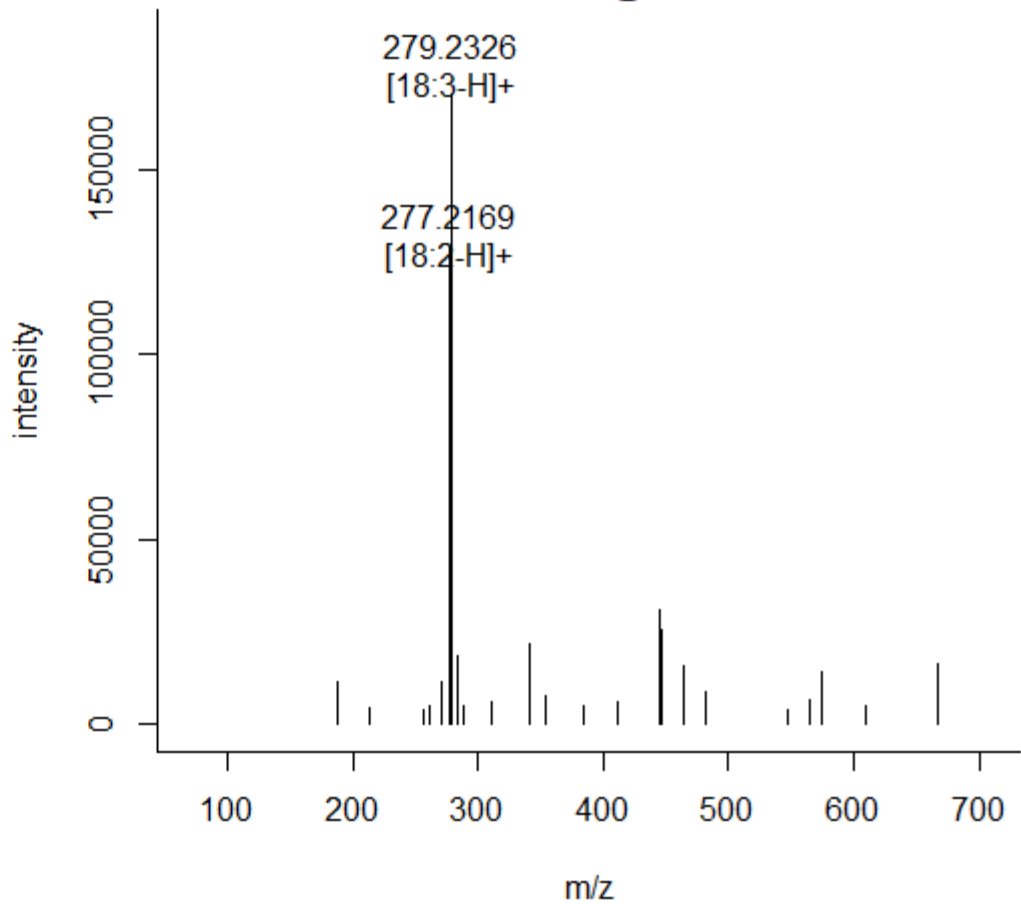
ESI+



ESI+
MS2 Spectra [M+NH4]
726.5095 @ 15.20



ESI-
MS2 Spectra [M-H]-
707.4656 @ 15.11



n3

18:0

Annotation of le

Lipidomics Main Panel MS2

Formula

Lipid class:

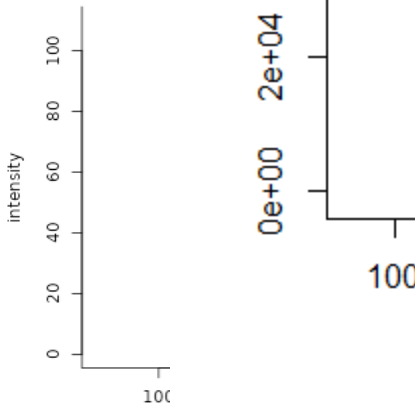
PA

[1] "C40H69O

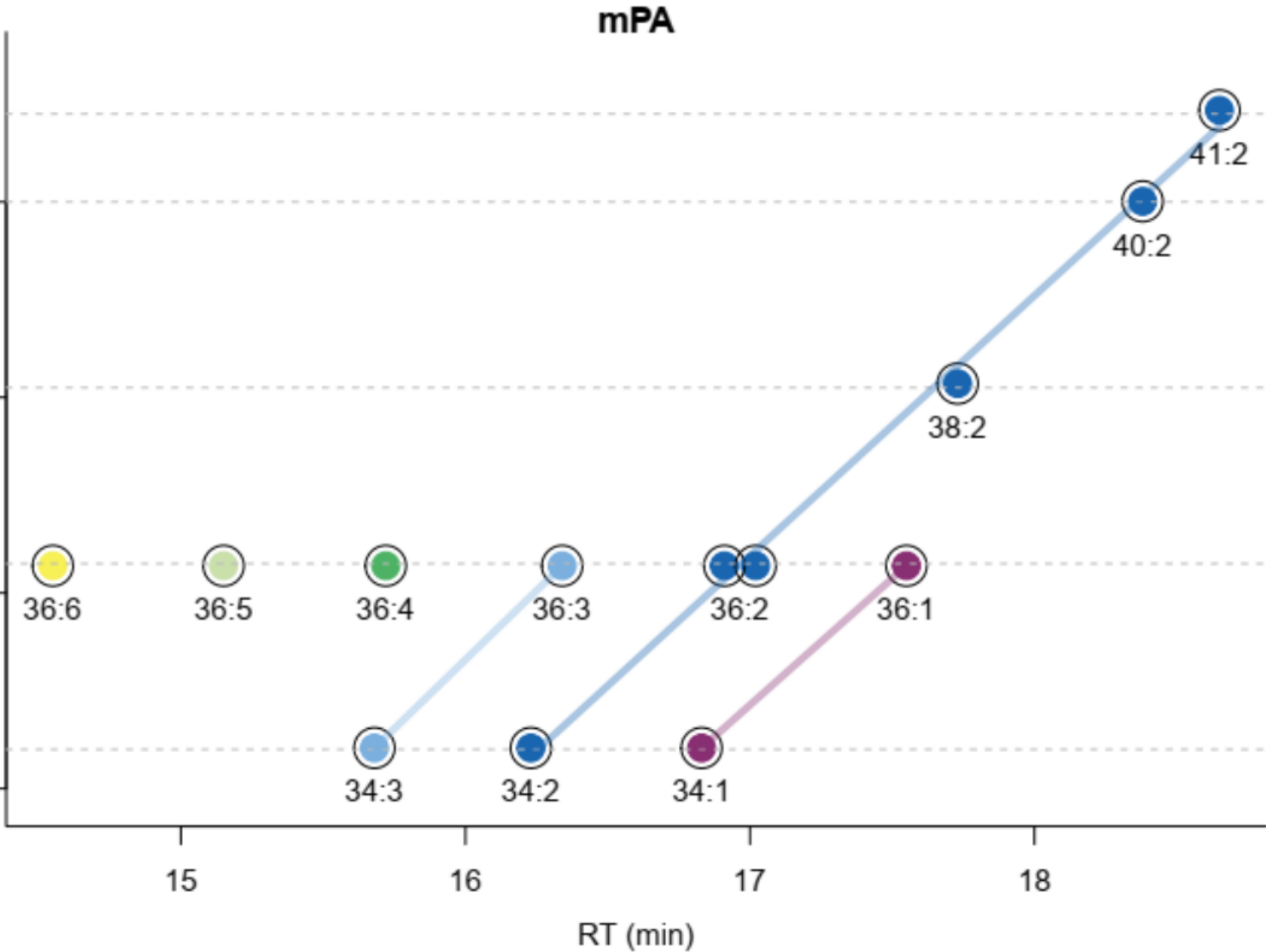
Major adduc

[M+NH4
C40H69O8P 726.50

Theoretical
ESI+



Carbons



n3

18:0

Thank you for your attention!

mar.garcia@fmach.it – github: mar-garcia

Italian Metabolomics Network General Meeting 2023 | <https://github.com/mar-garcia/IMN2023>