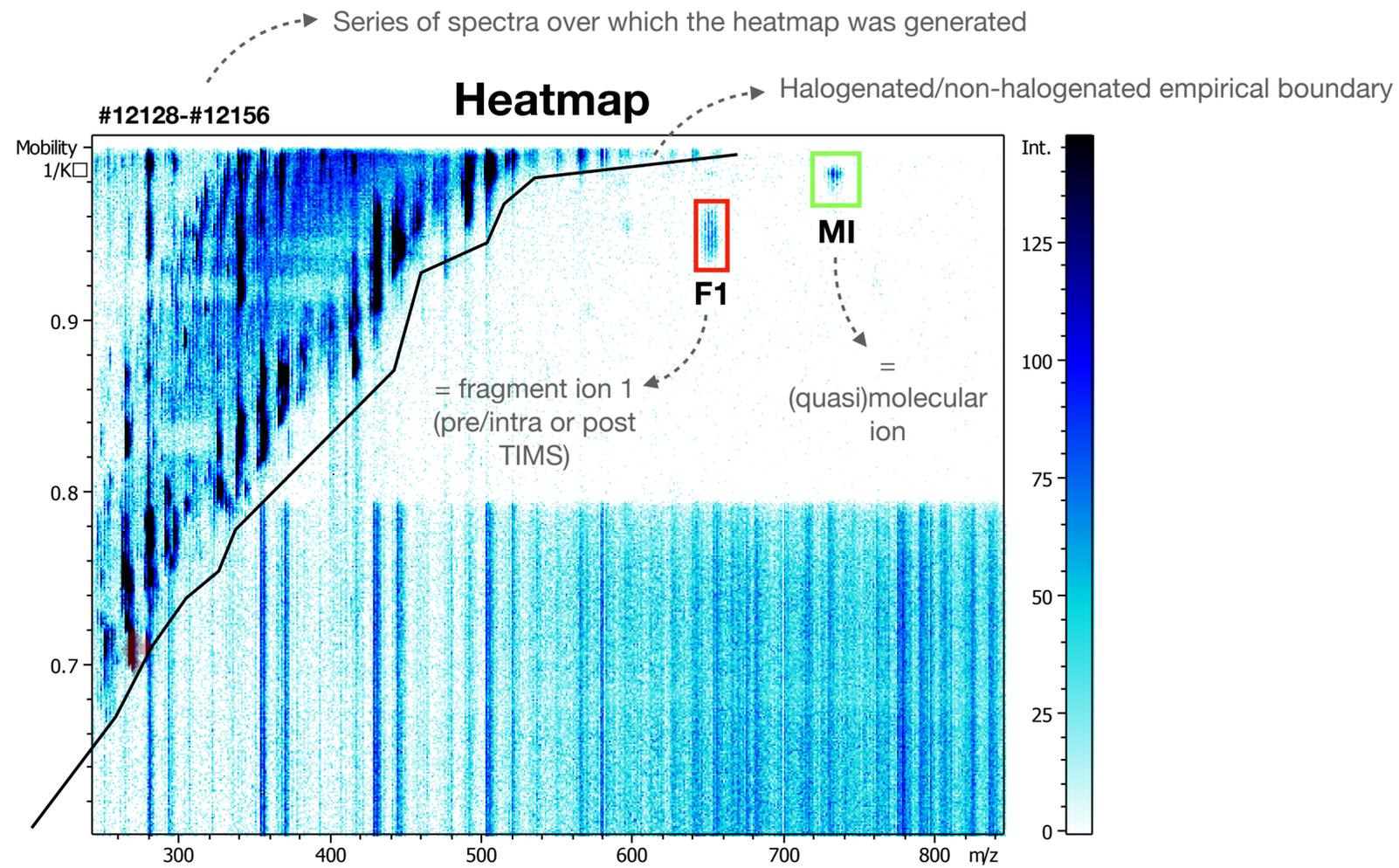
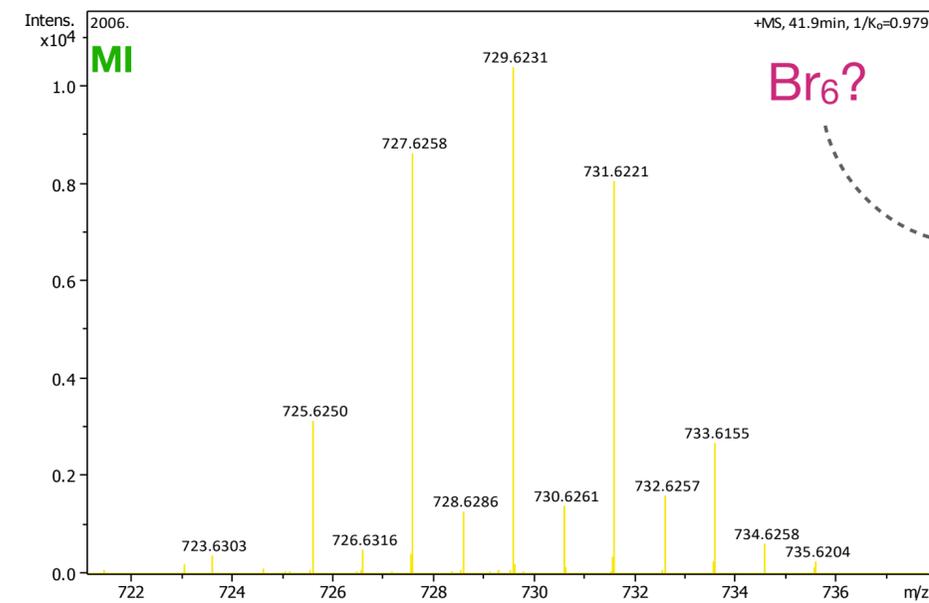


Annex A

Experimental data of chemical features identified
in the blubber of the stranded killer whale



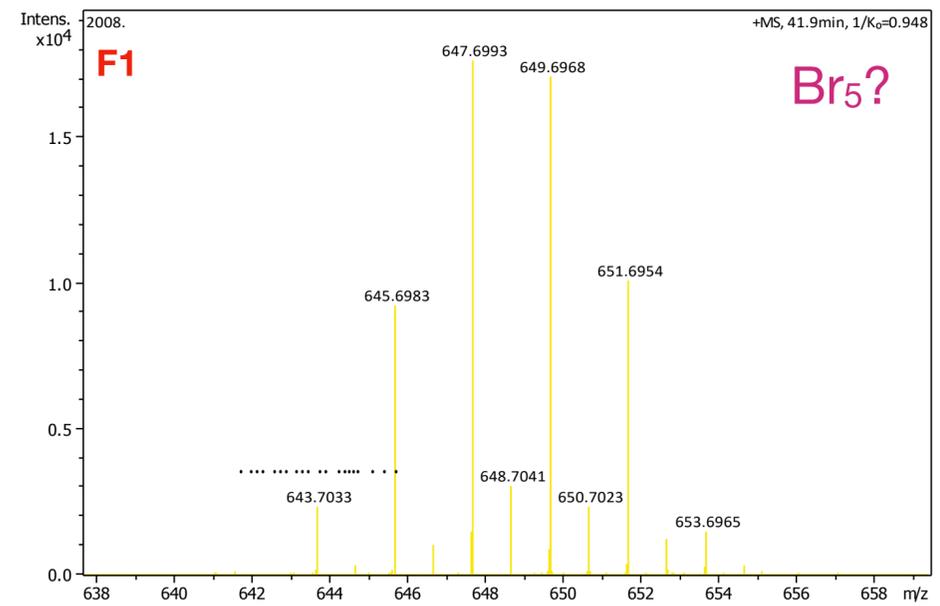
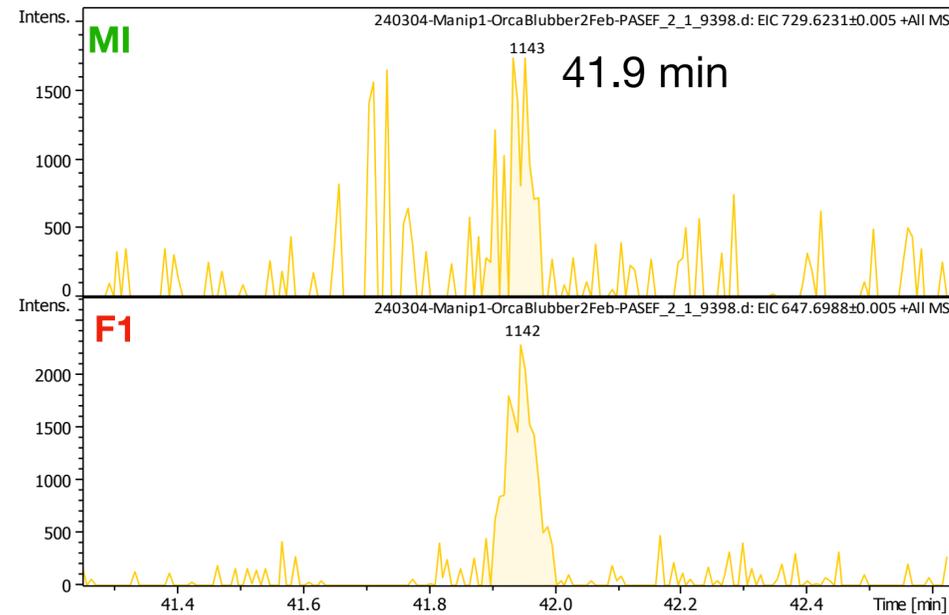
Mass spectra & isotopic profile



Tentative halogenated composition

- HBr?

Chromatogram

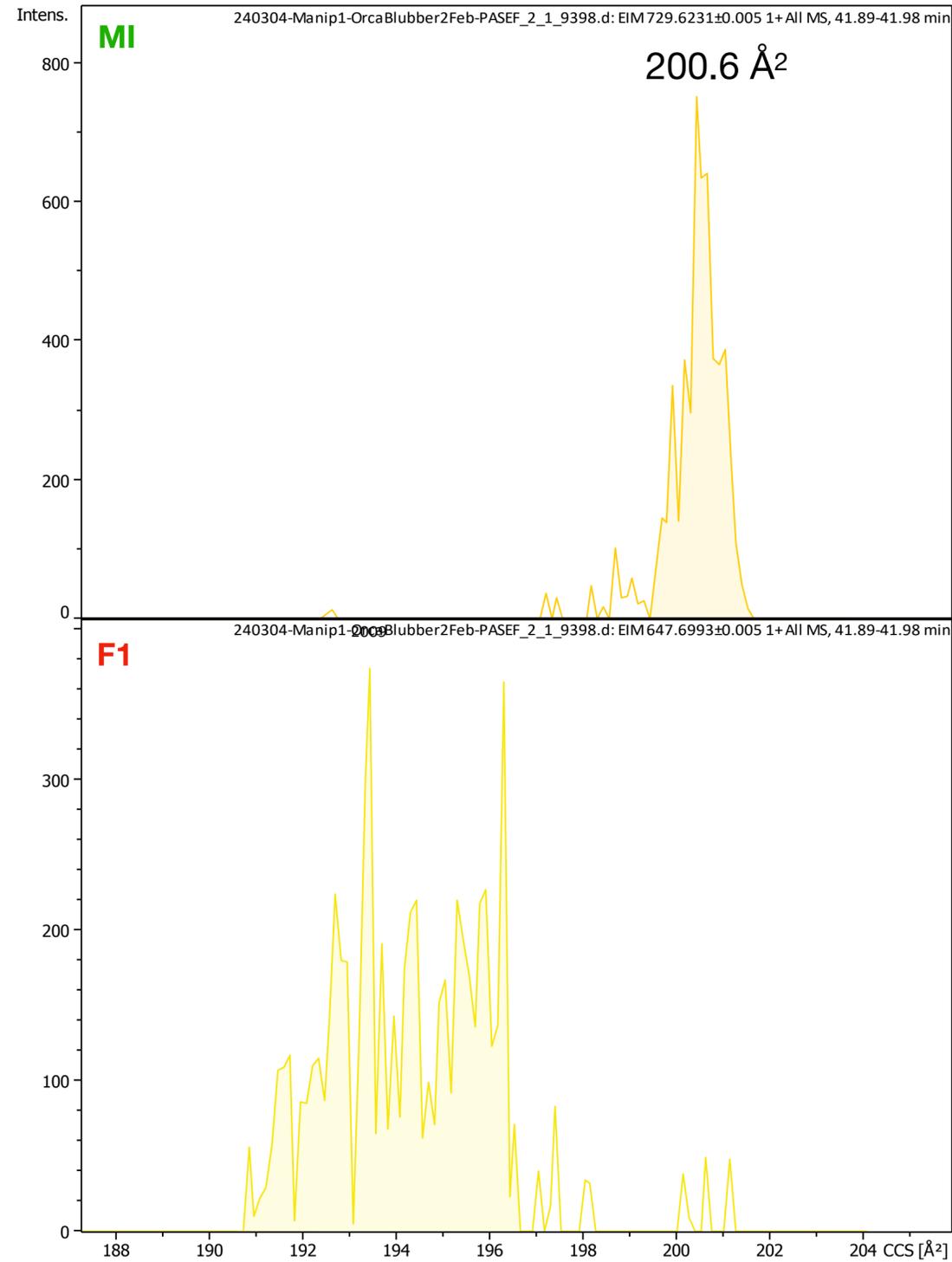


Feature #1

EIC 729.6231

Feature number and corresponding class

Ion mobility spectra



Tandem mass spectrum

/ Not available

Tentative candidate(s)

PubChem

/

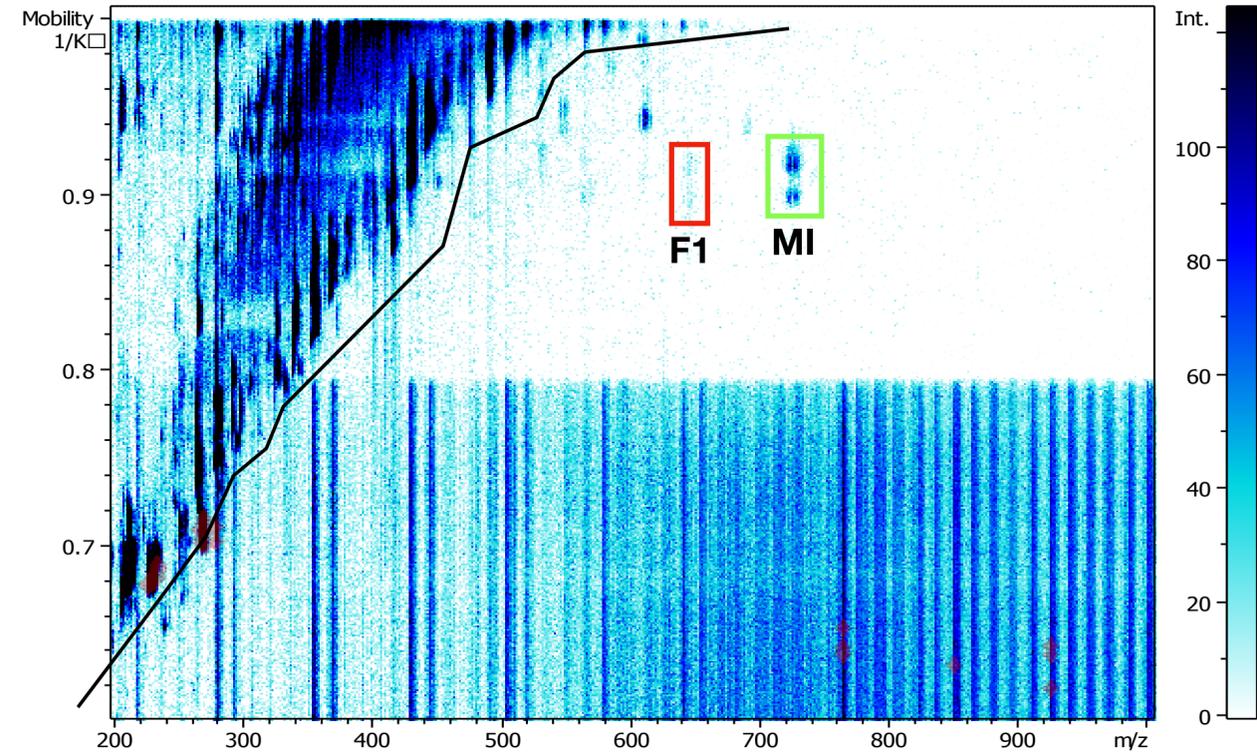
Confidence level

5

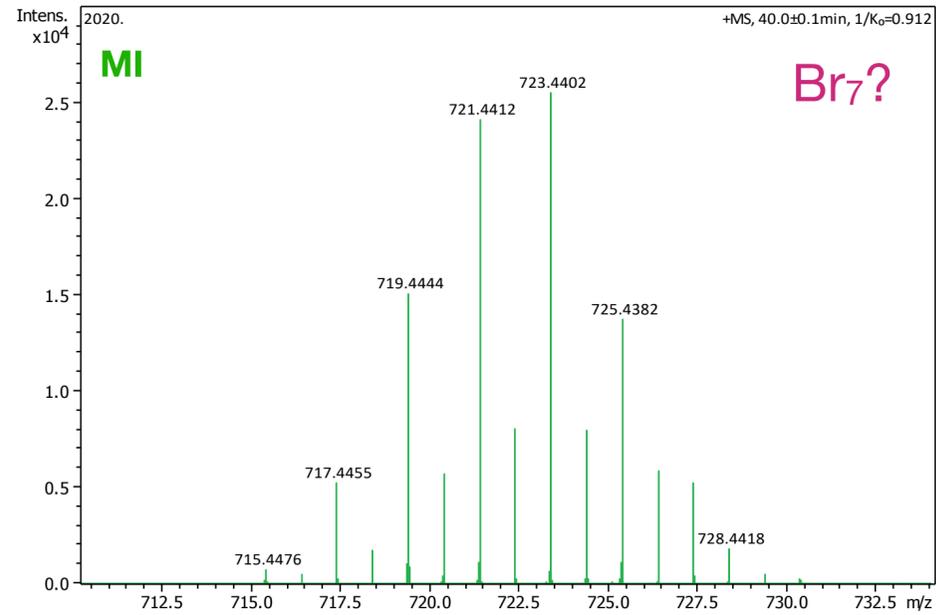
Based on Schymanski classification

Heatmap

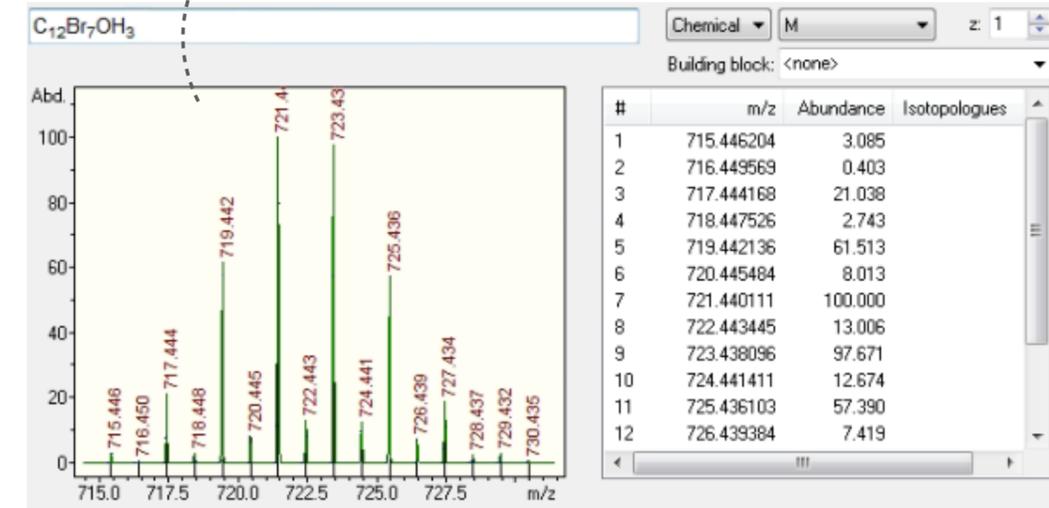
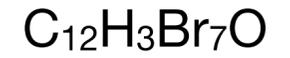
#11562-#11596



Mass spectra & isotopic profile

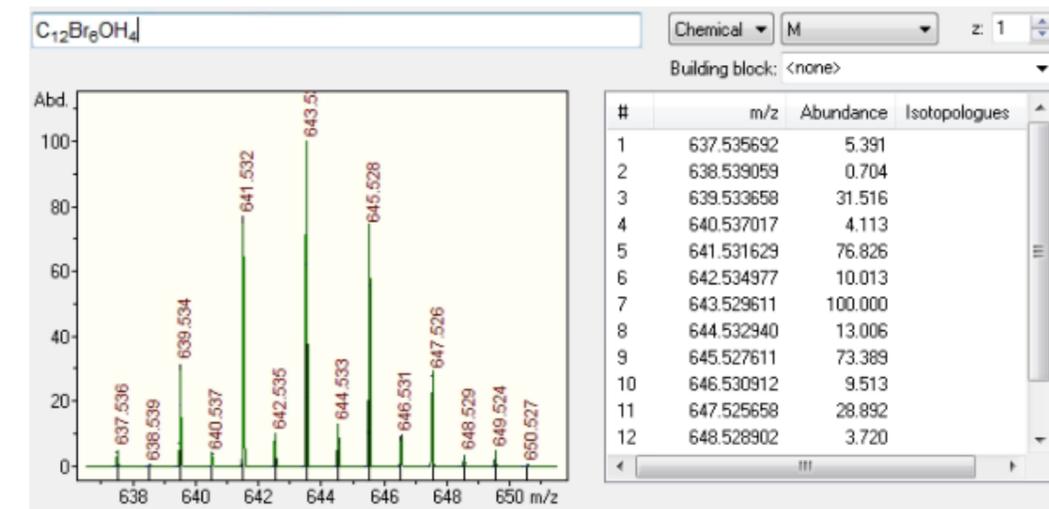
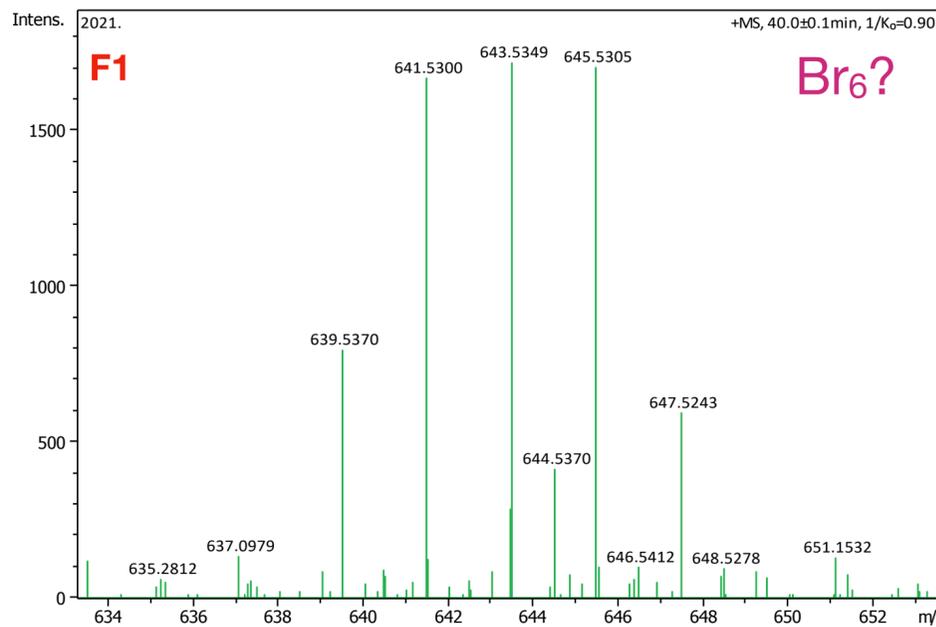
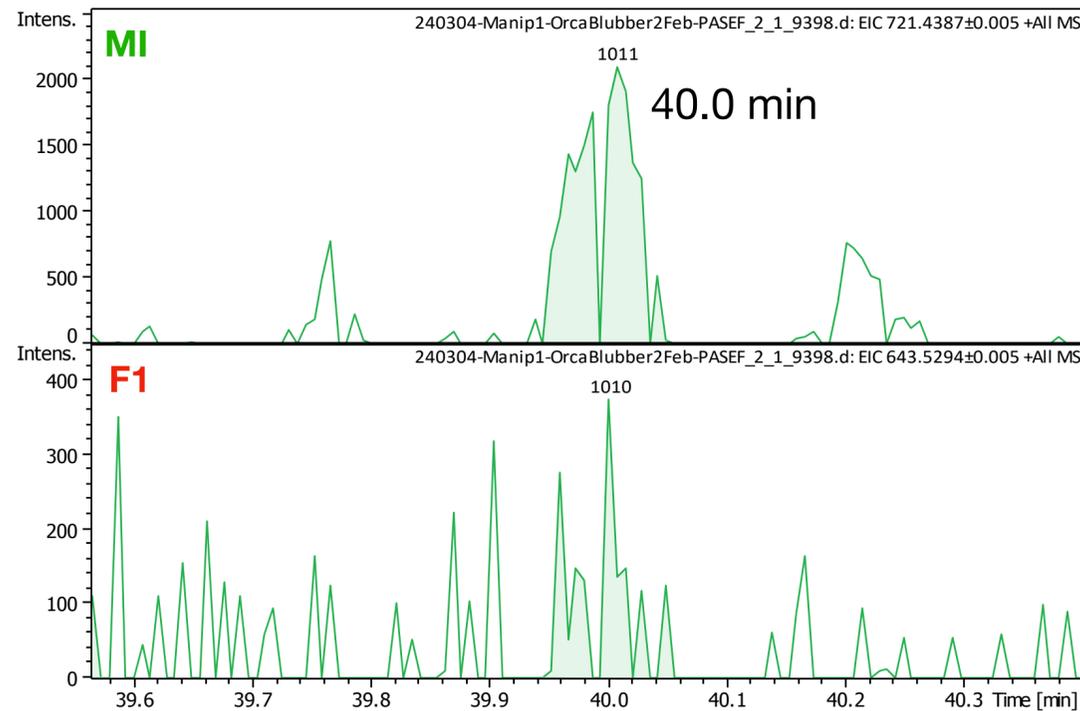


Theoretical isotopic pattern



- Br
+ H

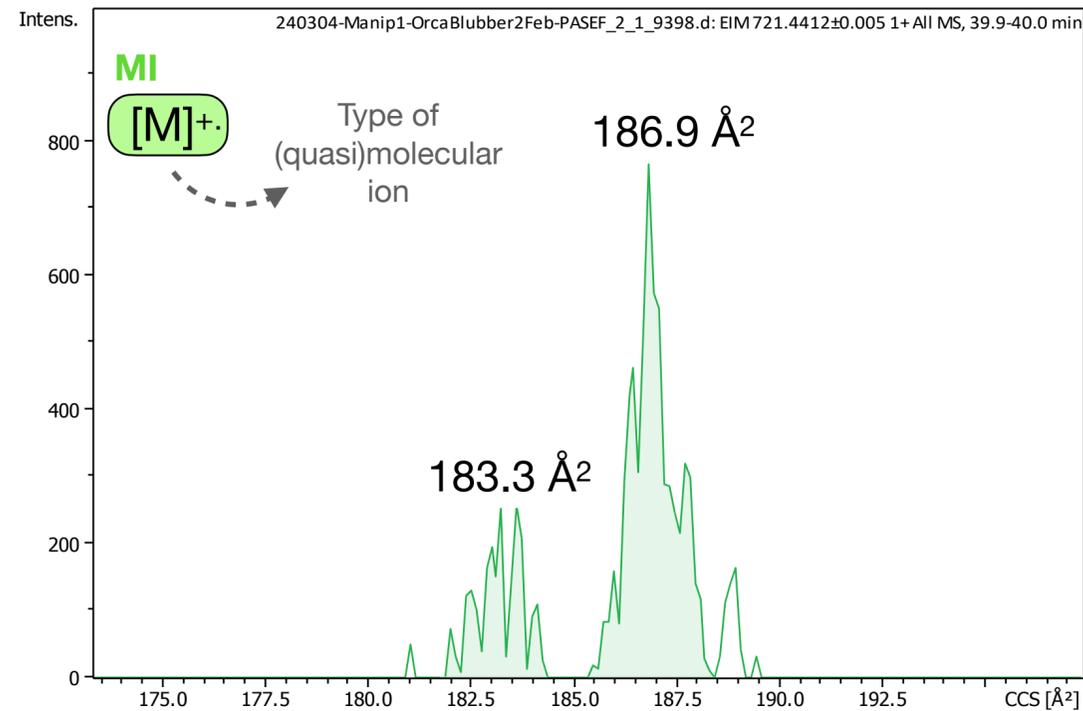
Chromatogram



Tandem mass spectrum

/

Ion mobility spectrum

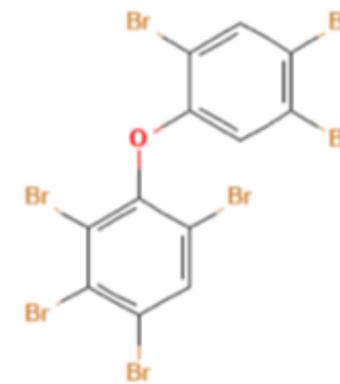


⇒ 2 isomers?

Comment

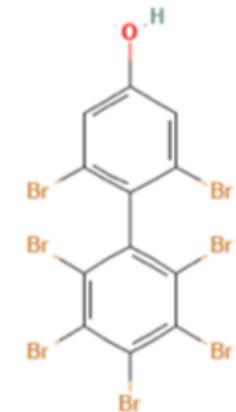
Tentative candidate(s)

PubChem

C₁₂H₃Br₇O

HpBDE (24 isomers)

⇒ Not HpBDE 183

(database CCS = 188.3 Å²)C₁₂H₃Br₇O

3,5-Dibromo-4-(2,3,4,5,6-pentabromophenyl)phenol

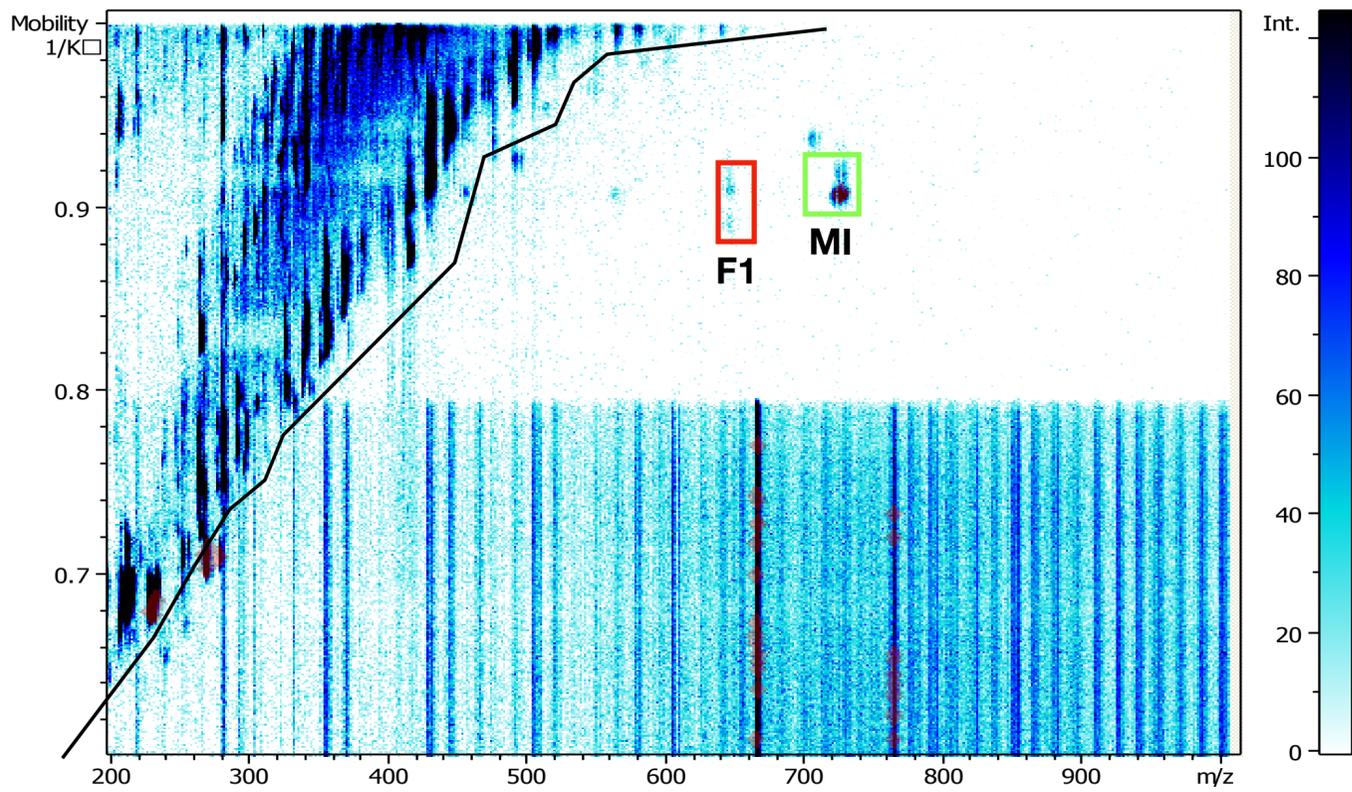
⇒ Phenol group not GC amenable

Confidence level

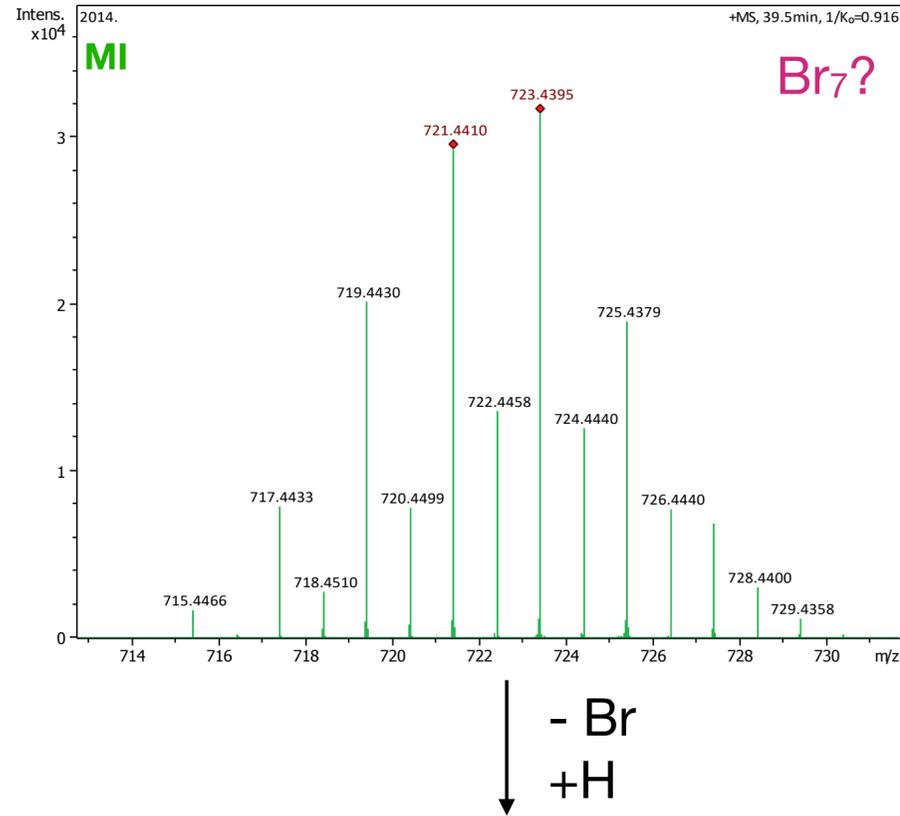
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CCS pred HpBDE isomers: see Figure S6.7A (manuscript)

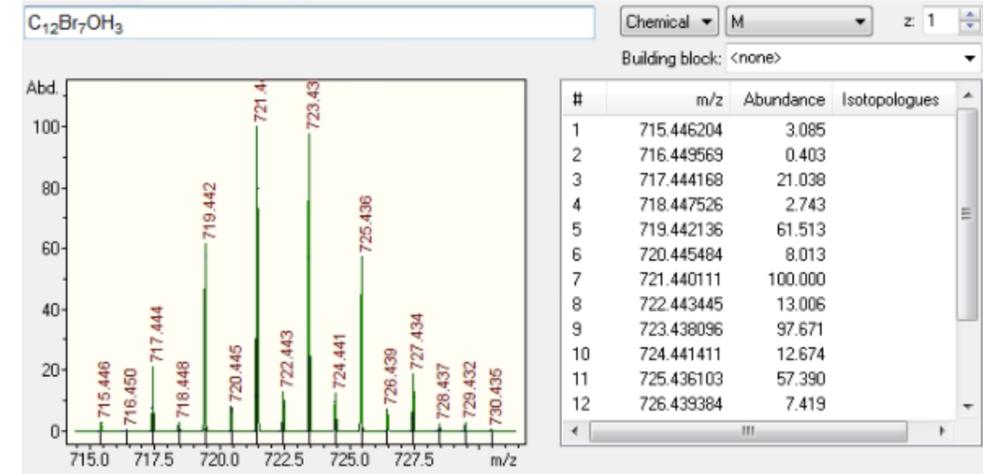
#11436-#11454 Heatmap



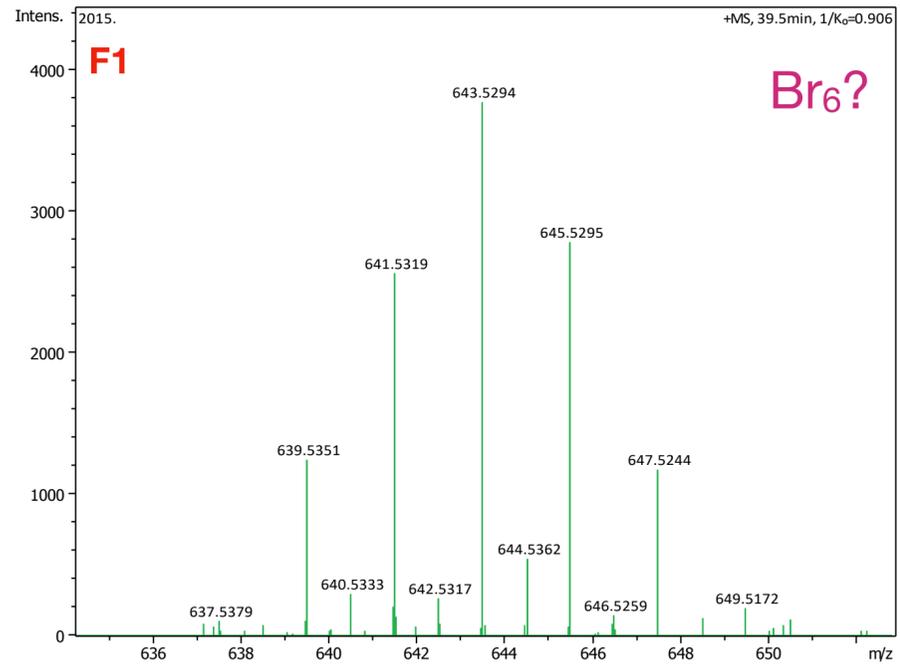
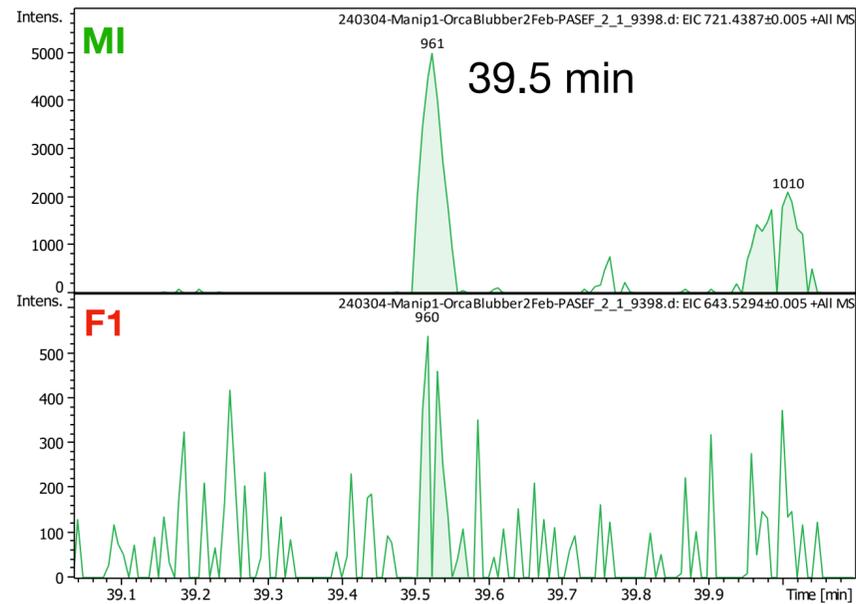
Mass spectra & isotopic profile



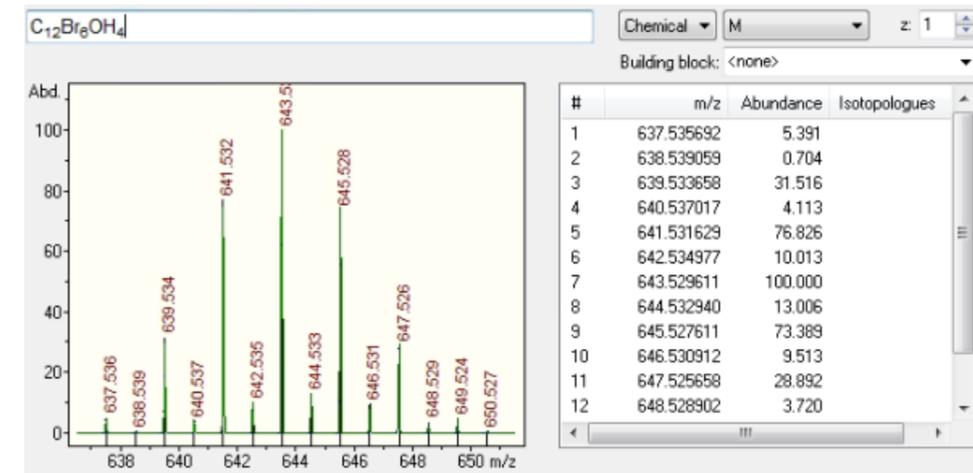
C₁₂H₃Br₇O



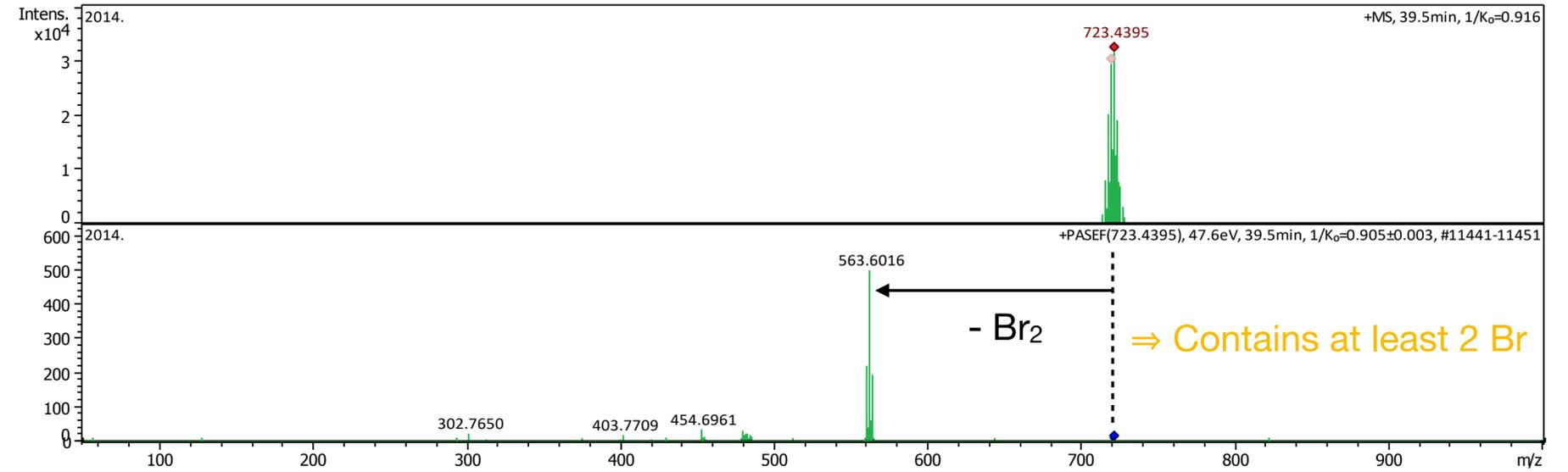
Chromatogram



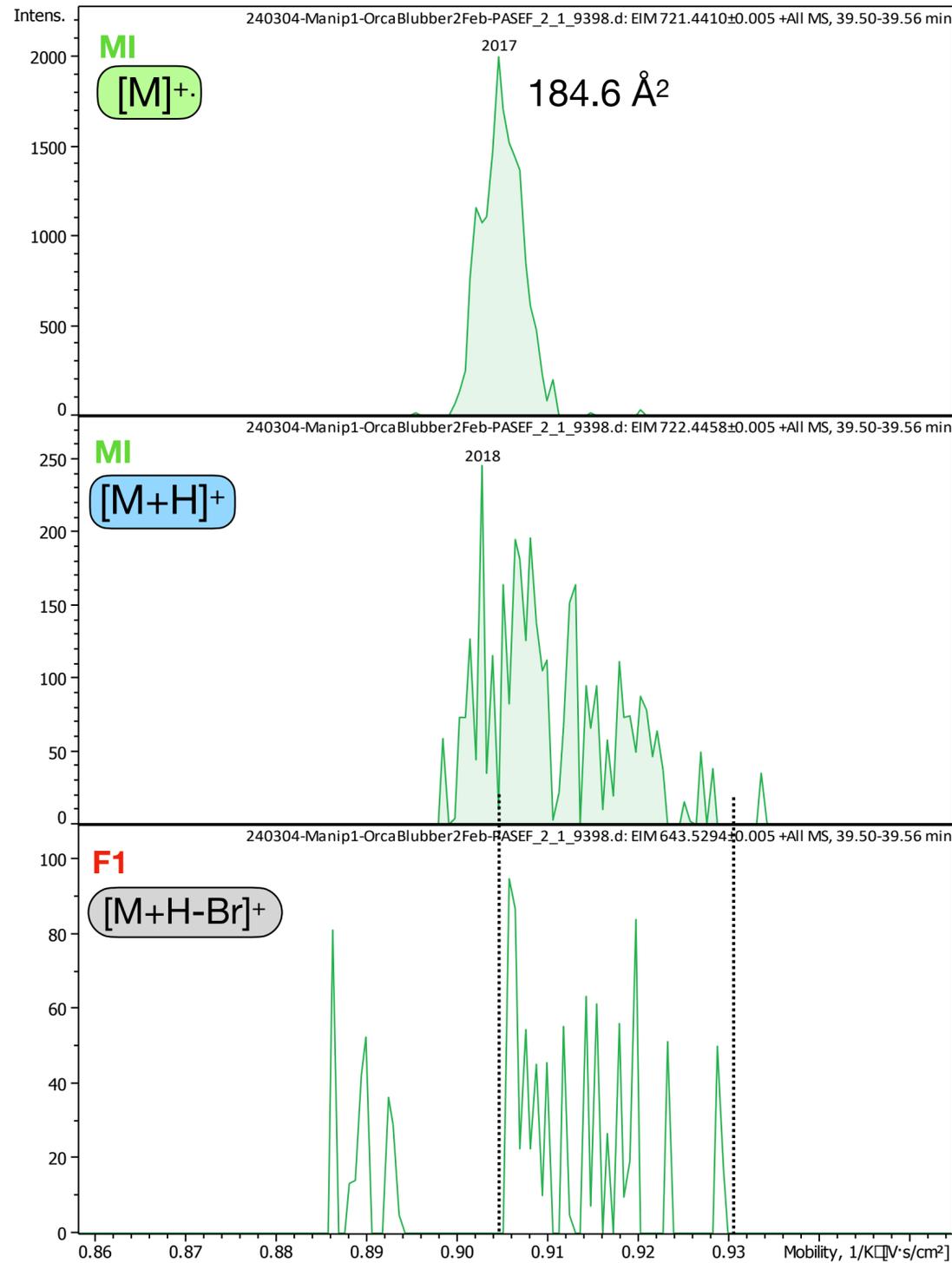
C₁₂H₄Br₆O



Tandem mass spectrum

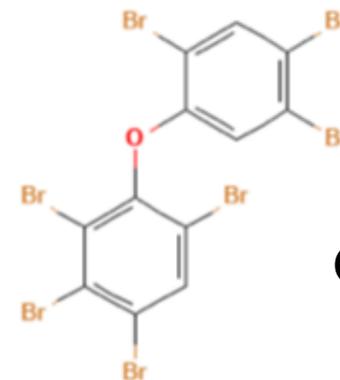


Ion mobility spectra



Tentative candidate(s)

PubChem



Confidence level

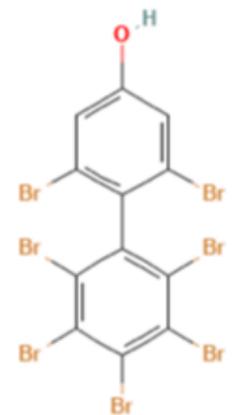
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C₁₂H₃Br₇O
HpBDE (24 isomers)

⇒ Not HpBDE 183

(database CCS = 188.3 Å²)

CCS pred HpBDE isomers: see Figure S6.7A (manuscript)

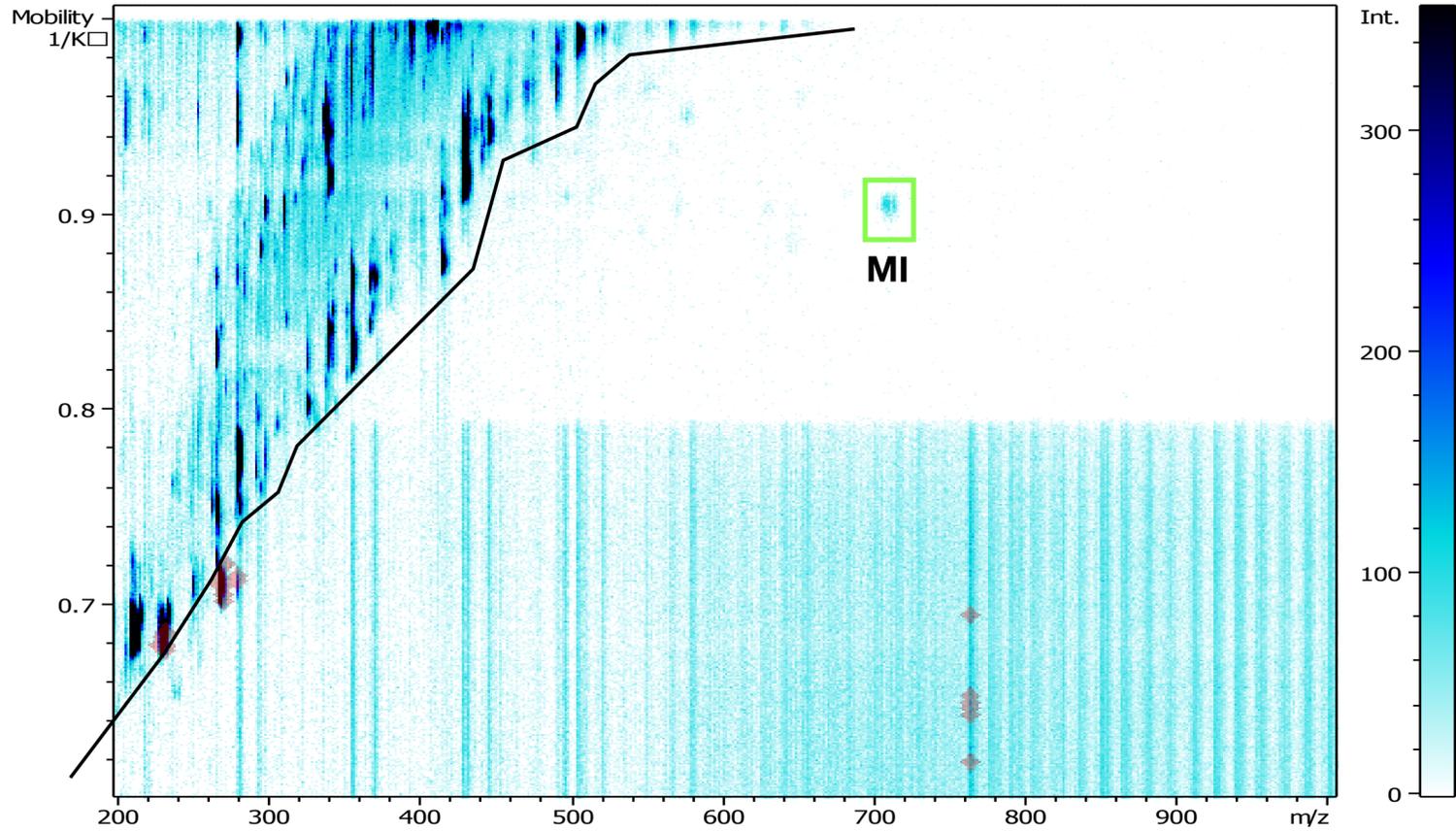


C₁₂H₃Br₇O

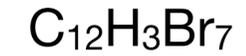
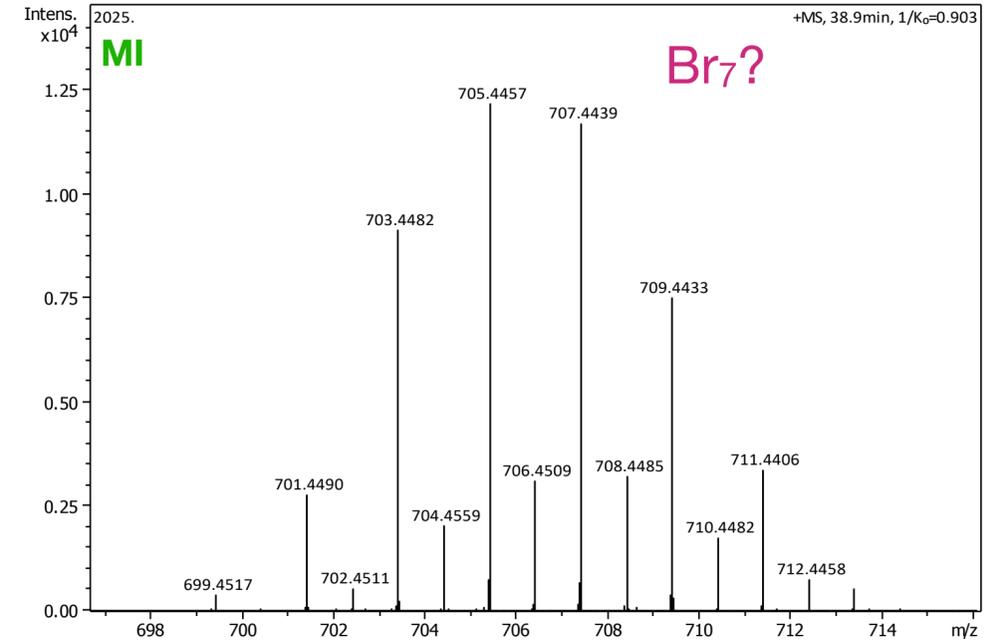
3,5-Dibromo-4-(2,3,4,5,6-pentabromophenyl)phenol
⇒ Phenol group not GC amenable

Heatmap

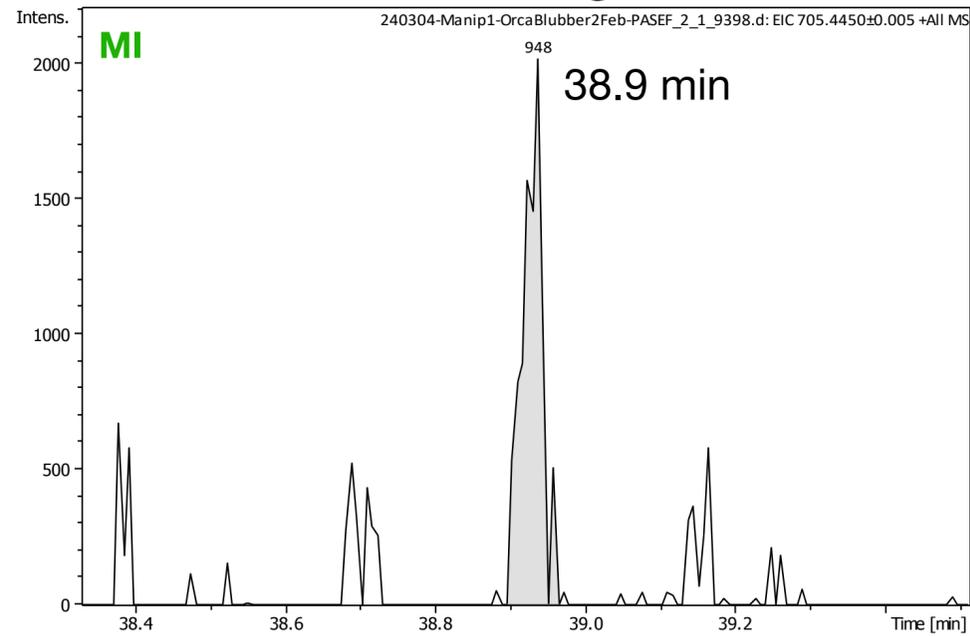
#11262-#11282



Mass spectrum & isotopic profile



Chromatogram



C12Br7H3 Chemical M z 1 Building block: <none>

#	m/z	Abundance	Isotopologues
1	699.451290	3.089	
2	700.454652	0.402	
3	701.449252	21.058	
4	702.452607	2.738	
5	703.447217	61.548	
6	704.450563	7.994	
7	705.445188	100.000	
8	706.448520	12.969	
9	707.443168	97.587	
10	708.446480	12.627	
11	709.441166	57.259	
12	710.444445	7.381	

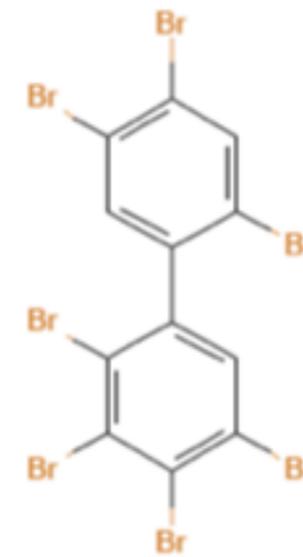
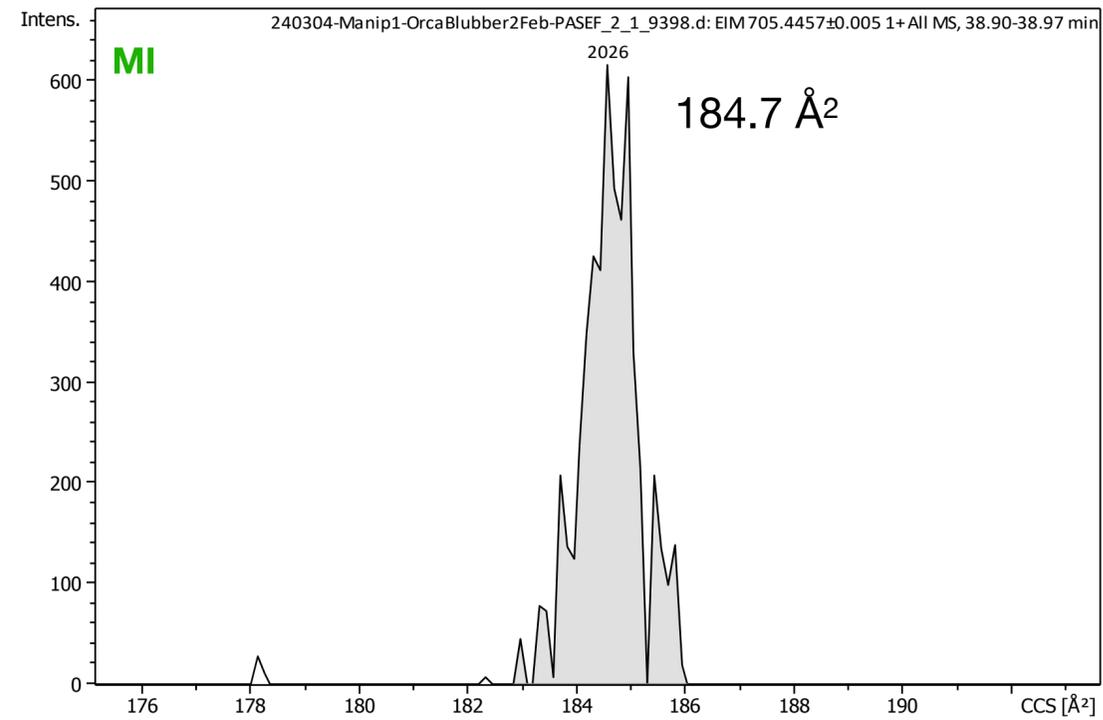
Tandem mass spectrum

/

Tentative candidate(s)

PubChem

Ion mobility spectrum

C12H3Br7

HpBB (24 isomers)

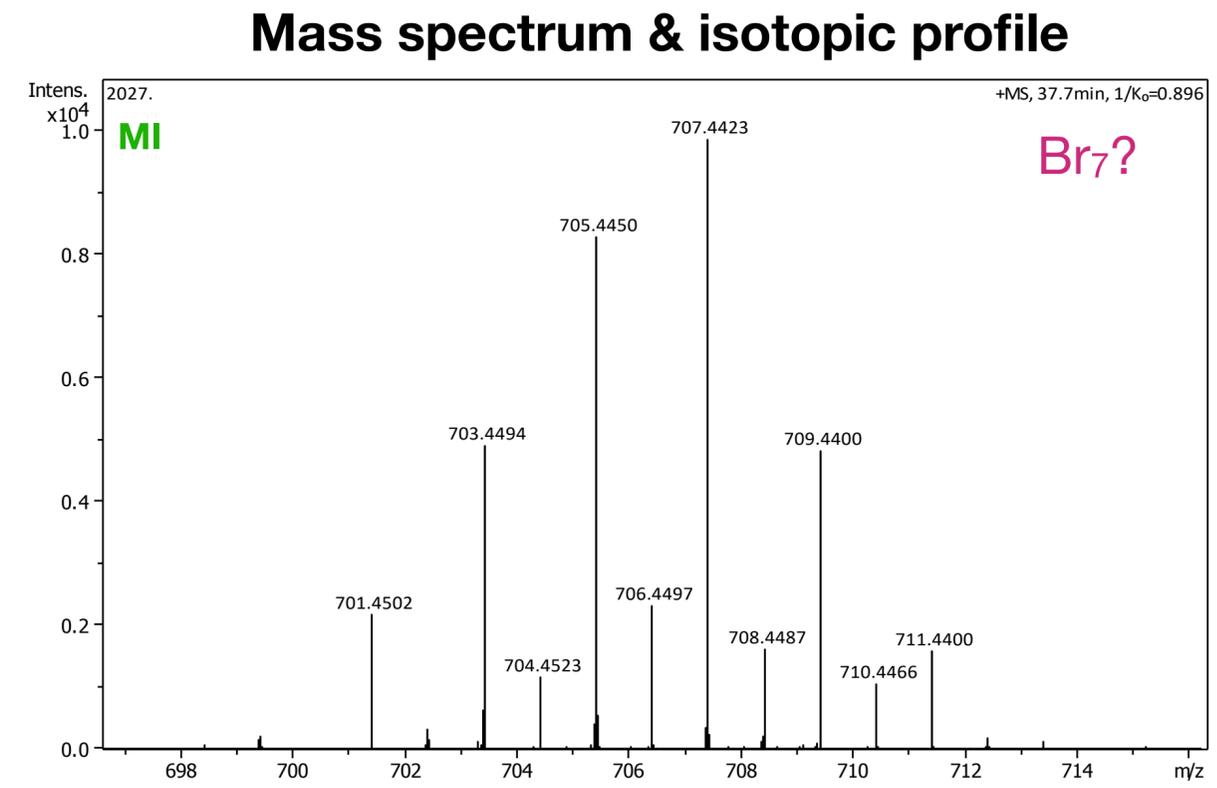
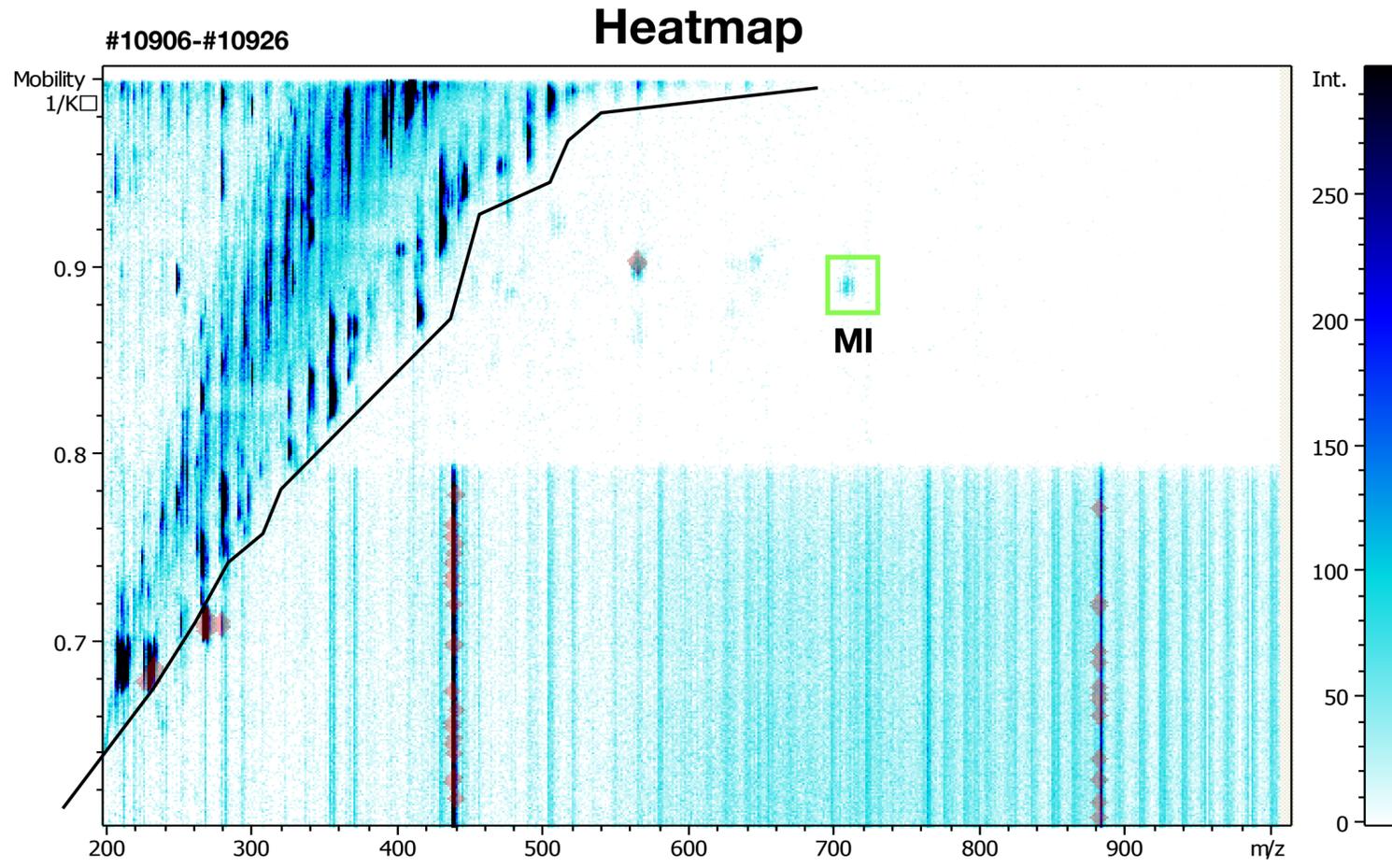
⇒ Not HpBB 180

(database CCS = 186.6 Å²)

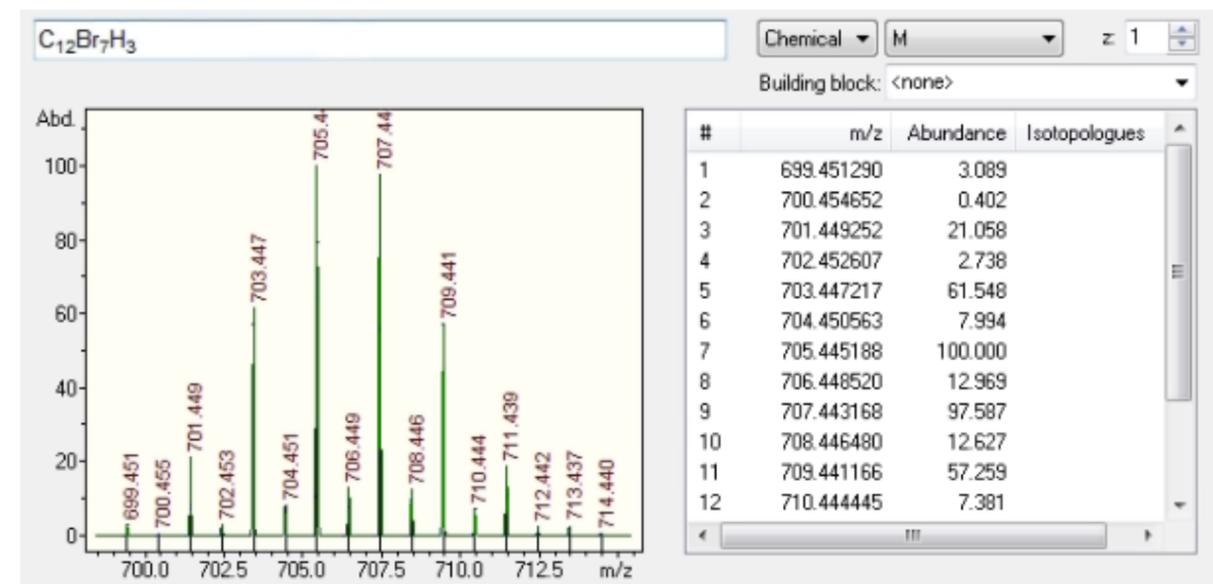
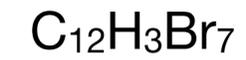
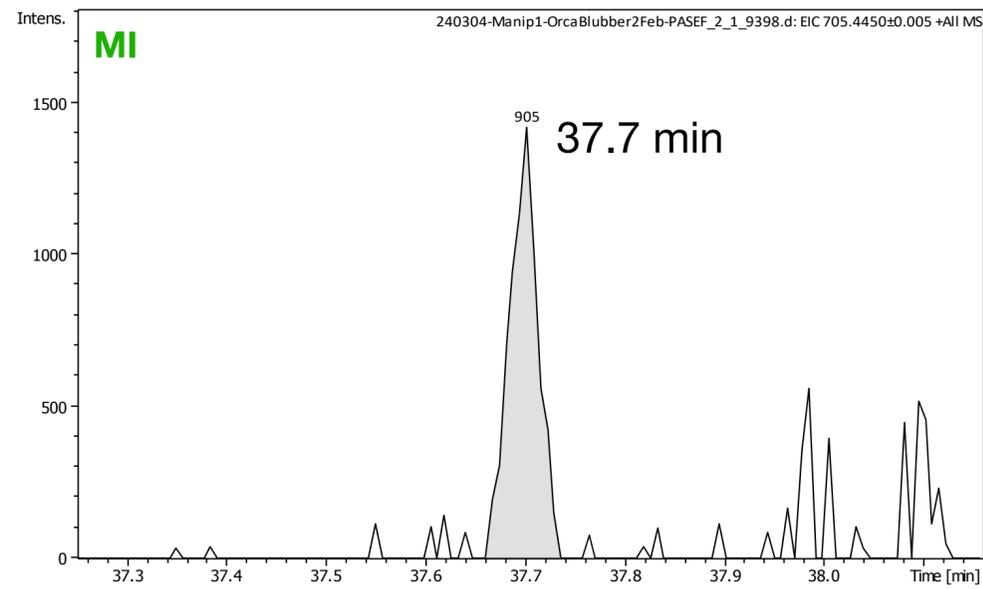
Confidence level

3

CCS pred HpBB isomers: see Figure
S6.7B (manuscript)



Chromatogram

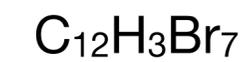
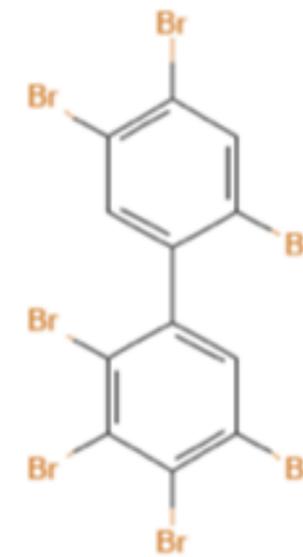


Tandem mass spectrum

/

Tentative candidate(s)

PubChem



HpBB (24 isomers)

⇒ Not HpBB 180

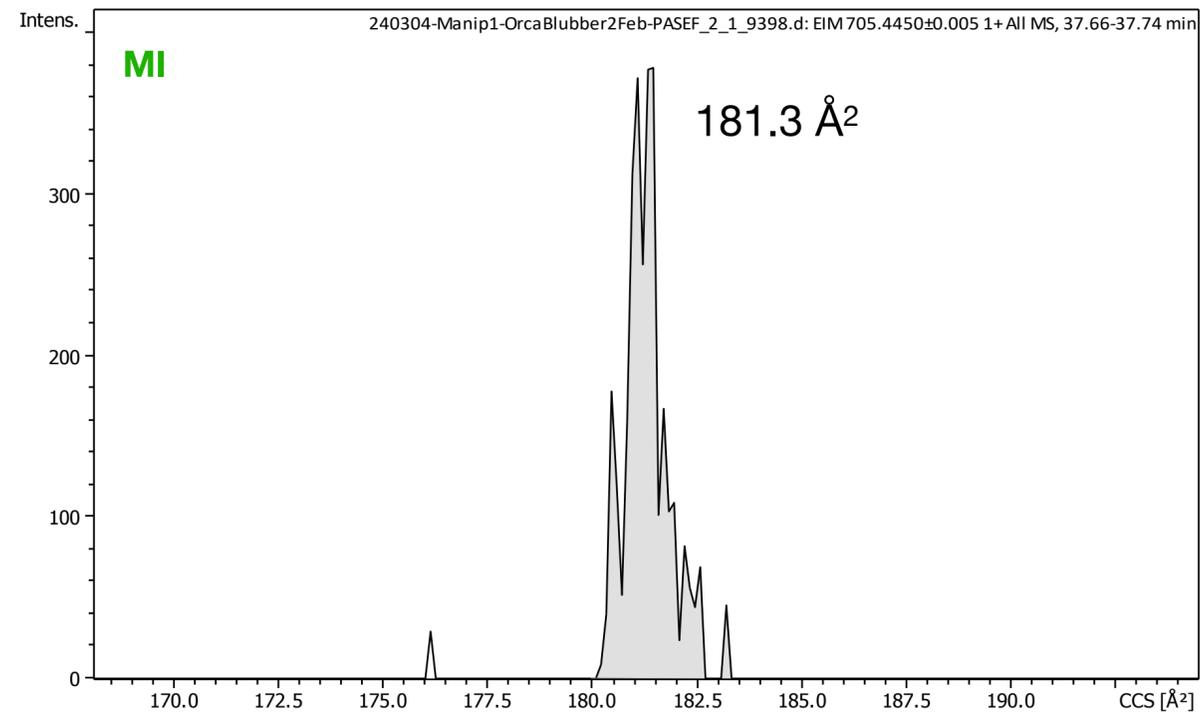
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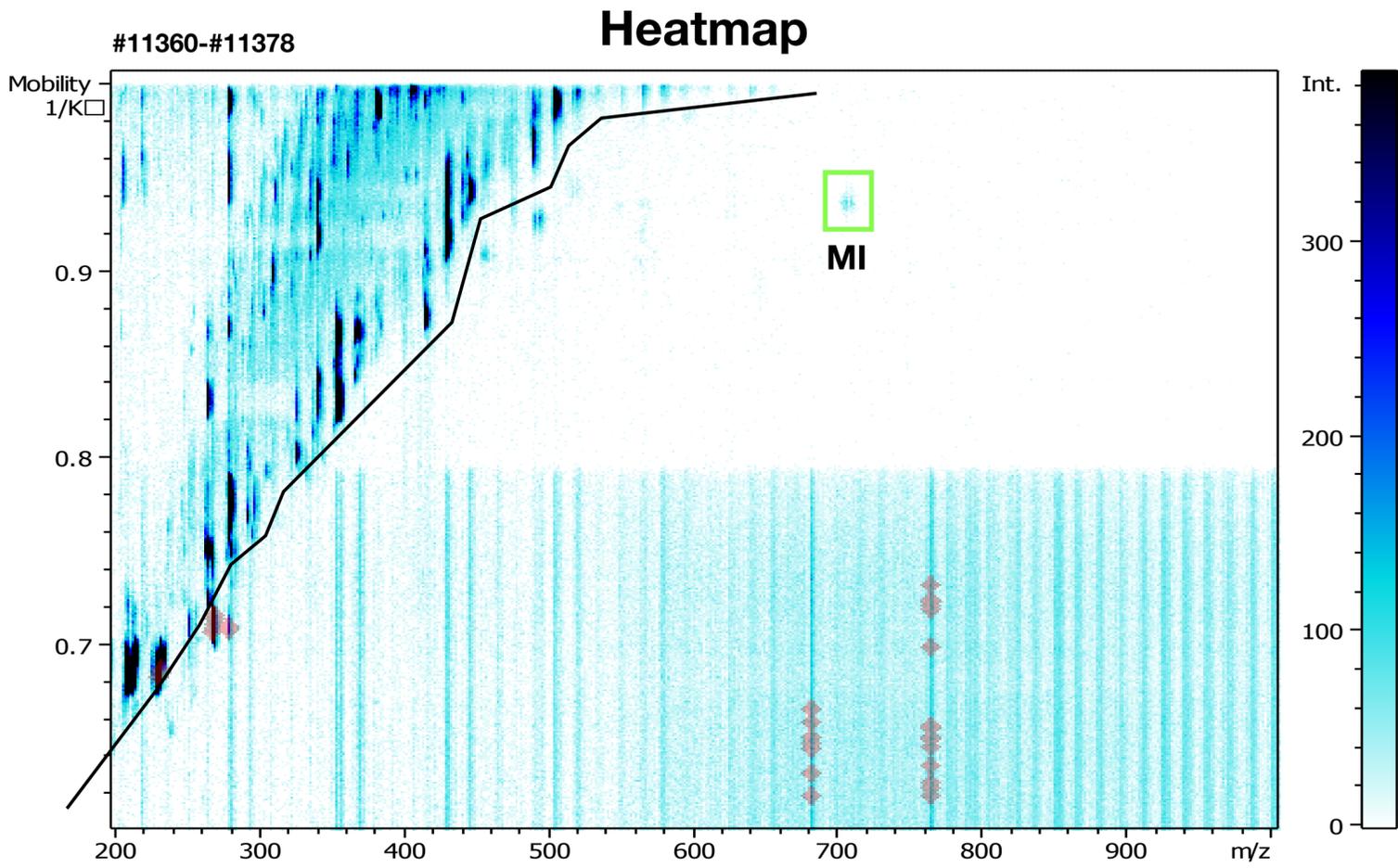
Confidence level

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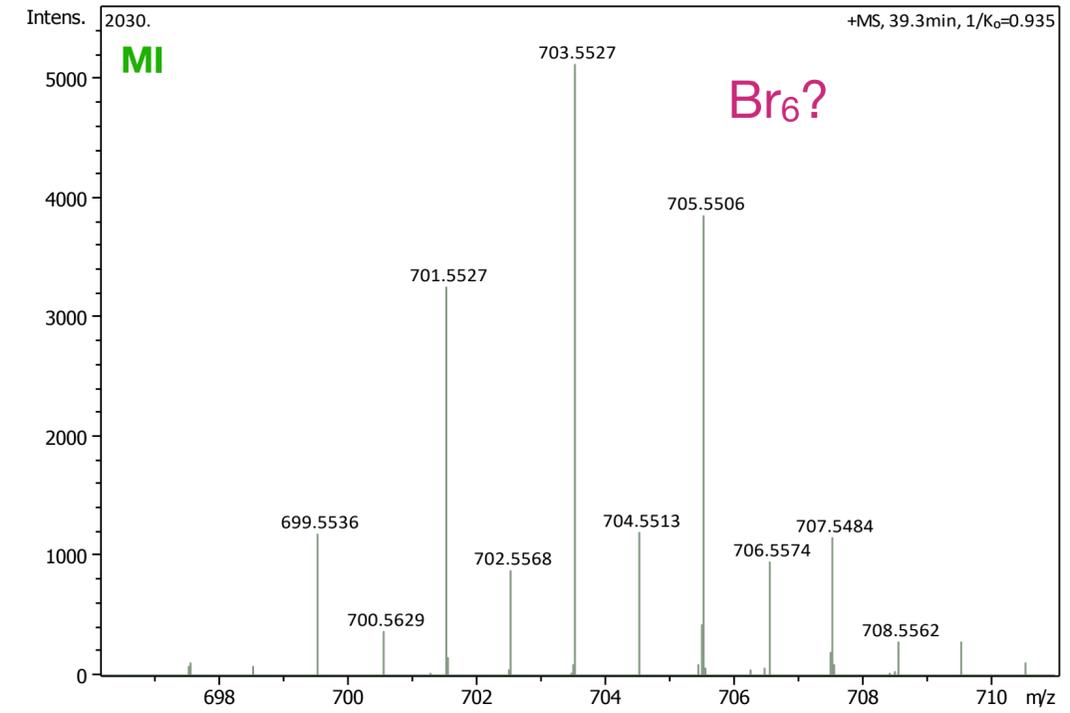
CCS pred HpBB isomers: see Figure
S6.7B (manuscript)

Ion mobility spectrum

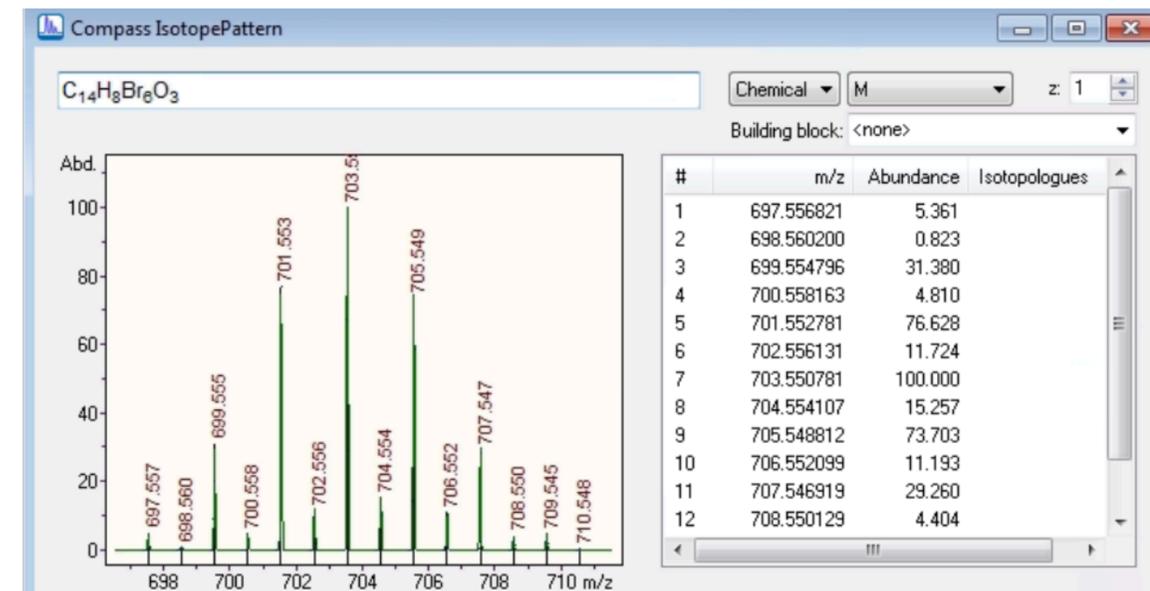
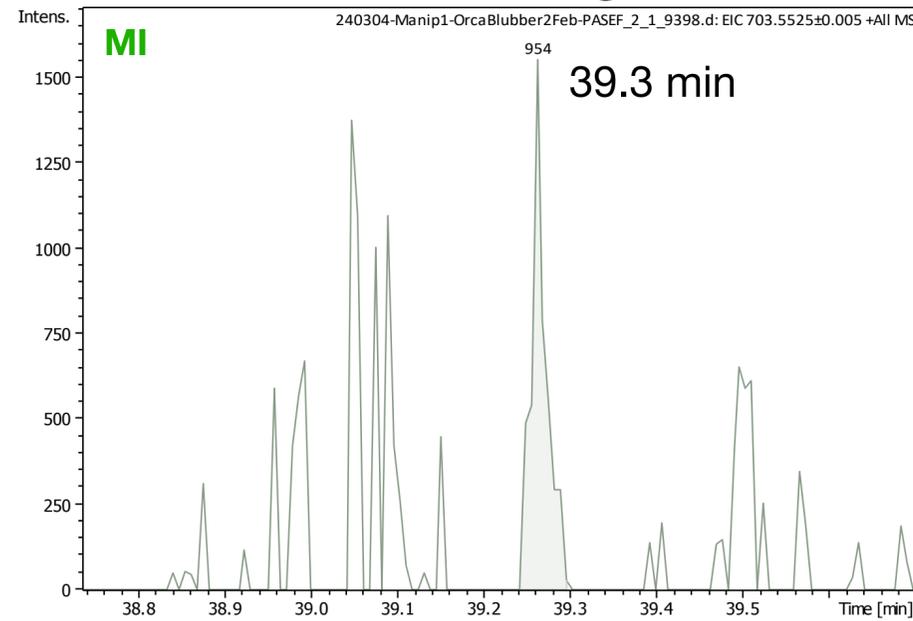




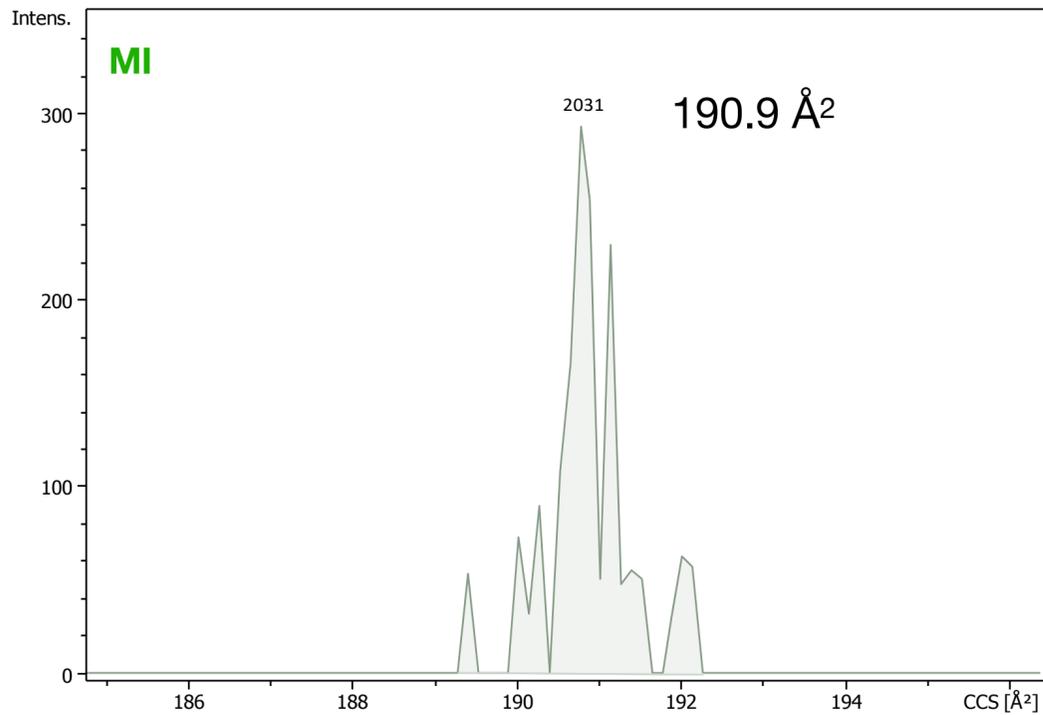
Mass spectrum & isotopic profile



Chromatogram



Ion mobility spectrum

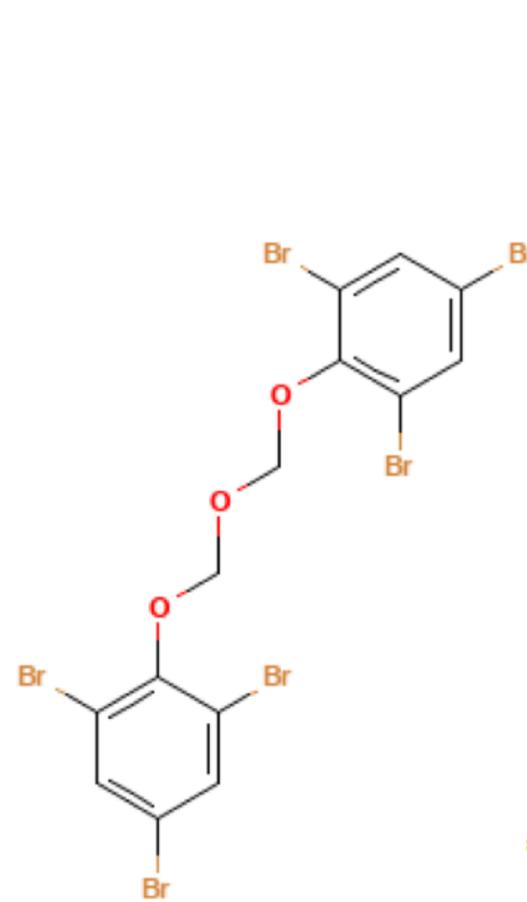


Tandem mass spectrum

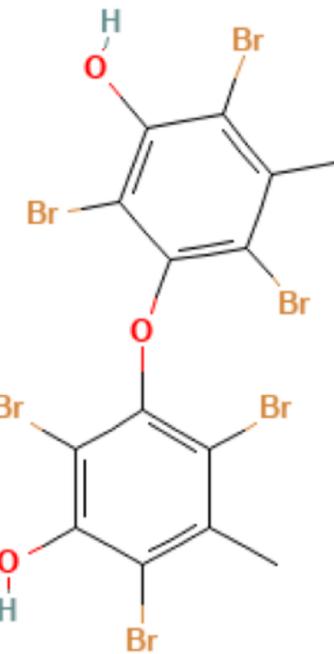
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Tentative candidate(s)

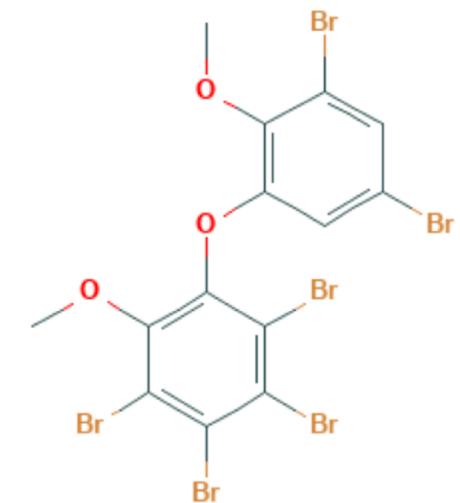
PubChem

C₁₄H₈Br₆O₃

Benzene, 1,1'-
[oxybis(methyleneoxy)]bis[2,4,6-tribromo-
CCS pred: 216.0 Å² (+13.1%)



2,4,6,2',4',6'-
Hexabromodiorcinol
⇒ Alcohols, not GC amenable

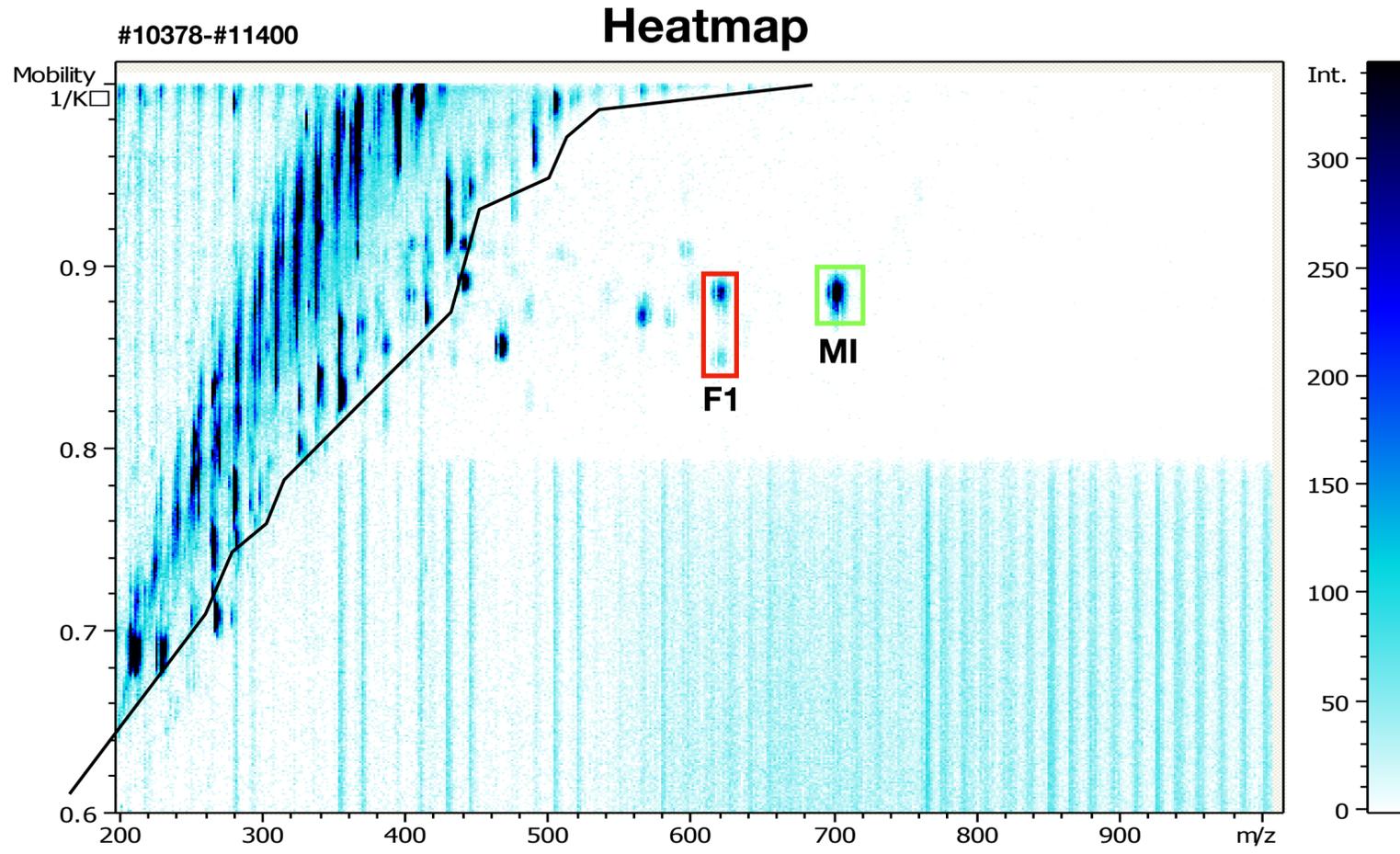


1,2,3,4-Tetrabromo-5-(3,5-
dibromo-2-methoxyphenoxy)-6-
methoxybenzene

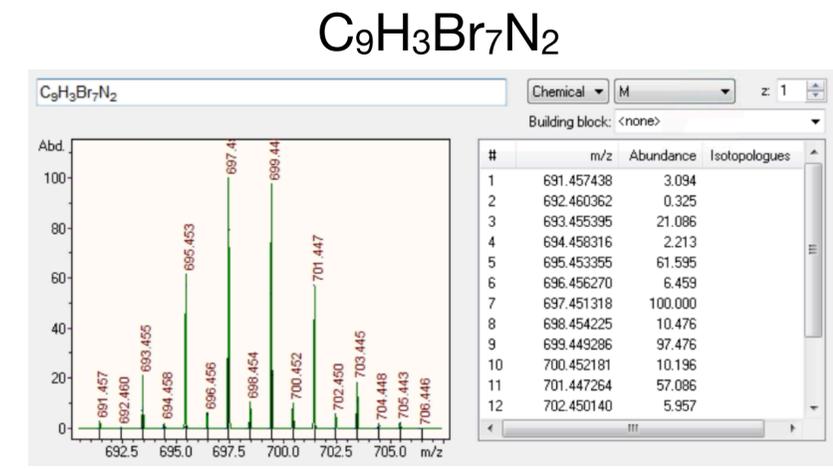
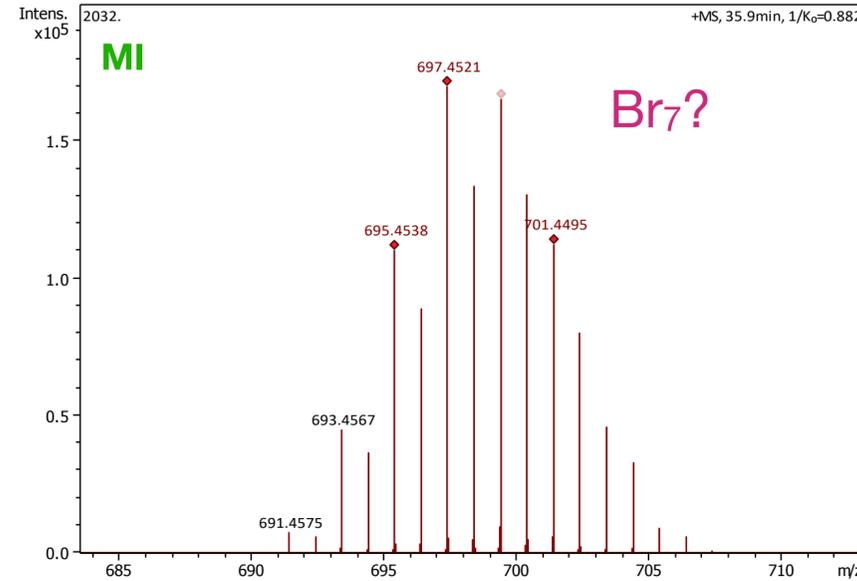
⇒ HNP?
CCS pred: 196.4 Å² (+2.9%)

Confidence level

3

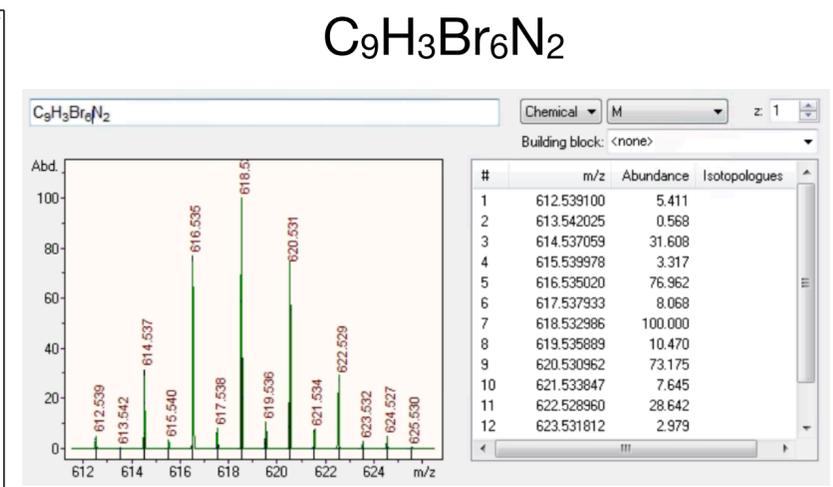
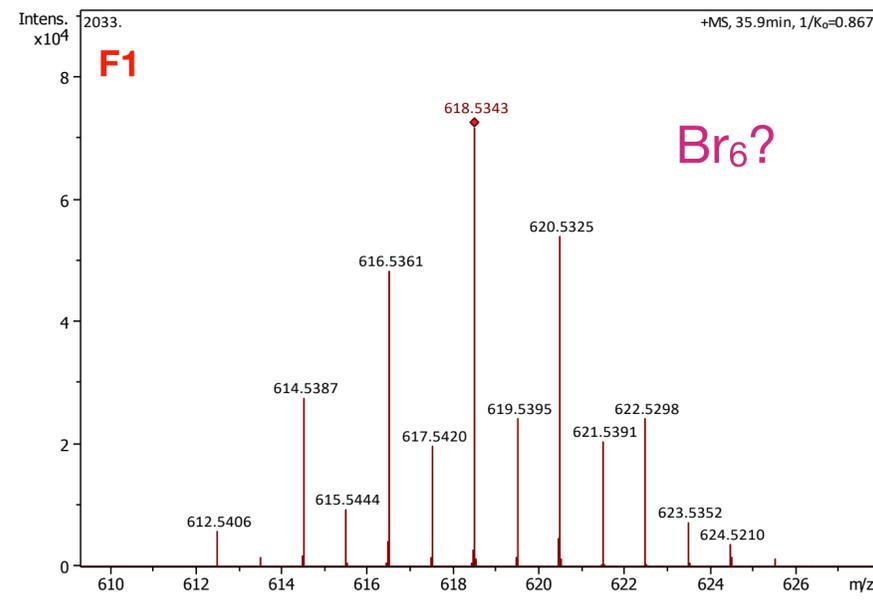
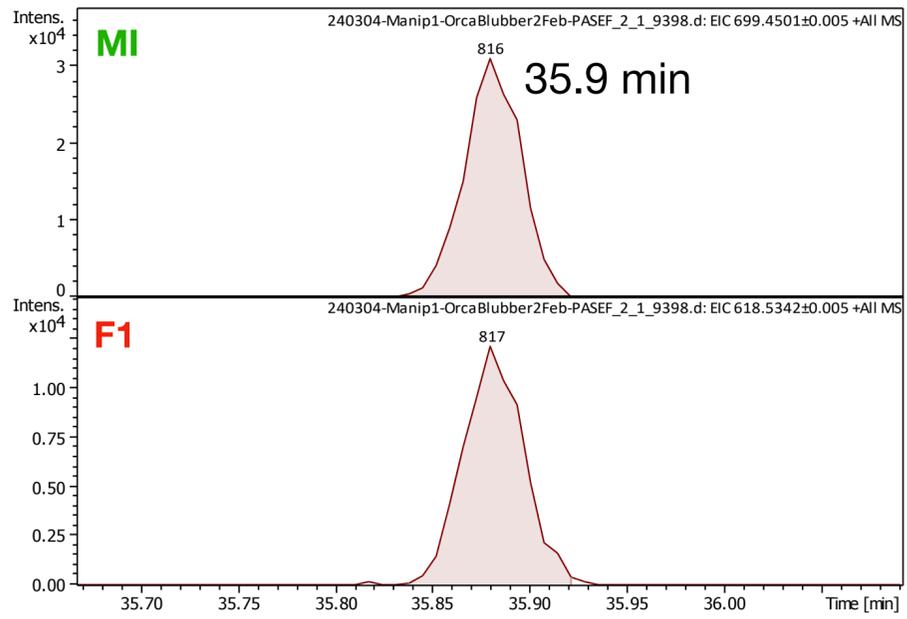


Mass spectra & isotopic profile

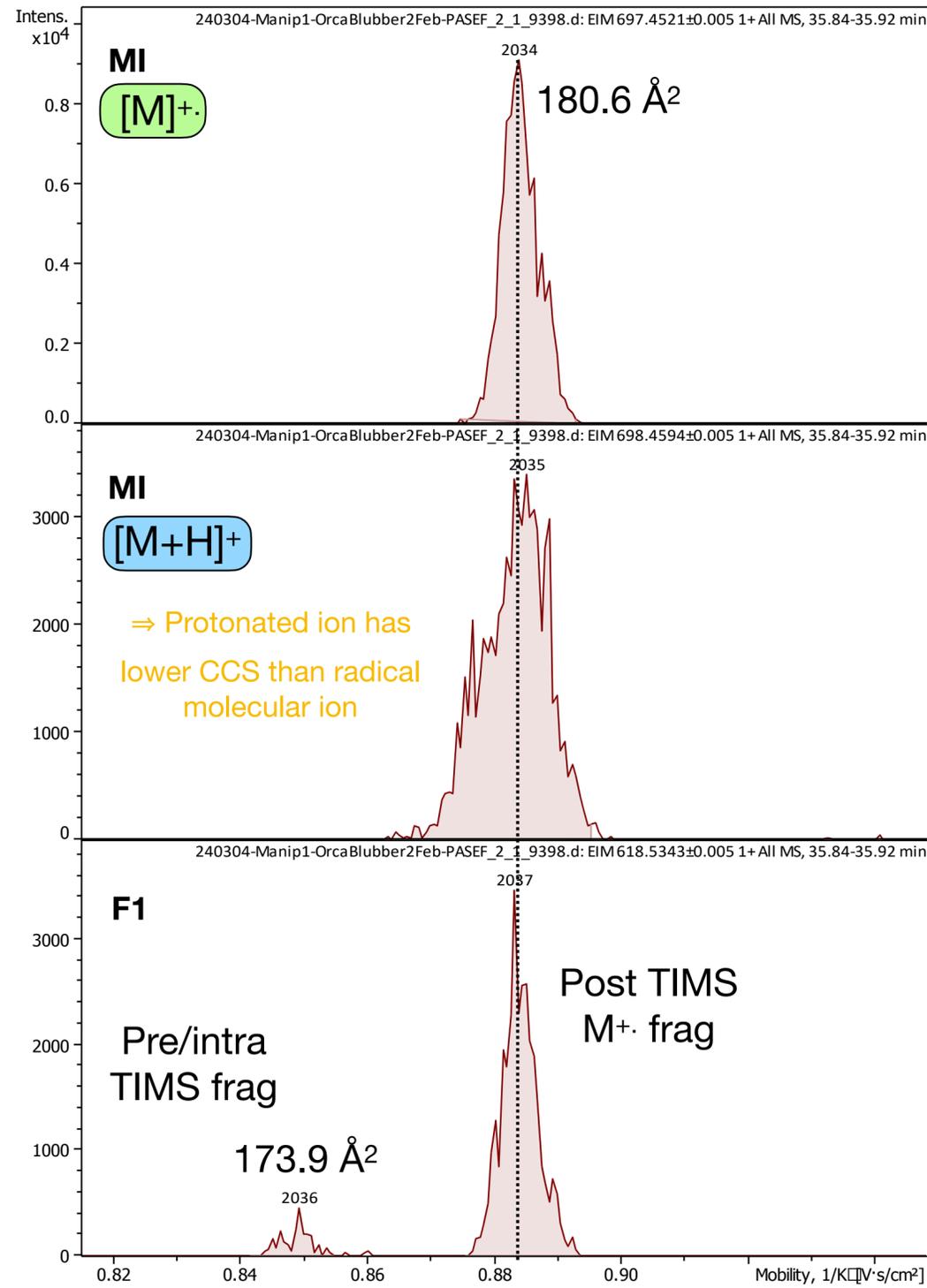


- Br

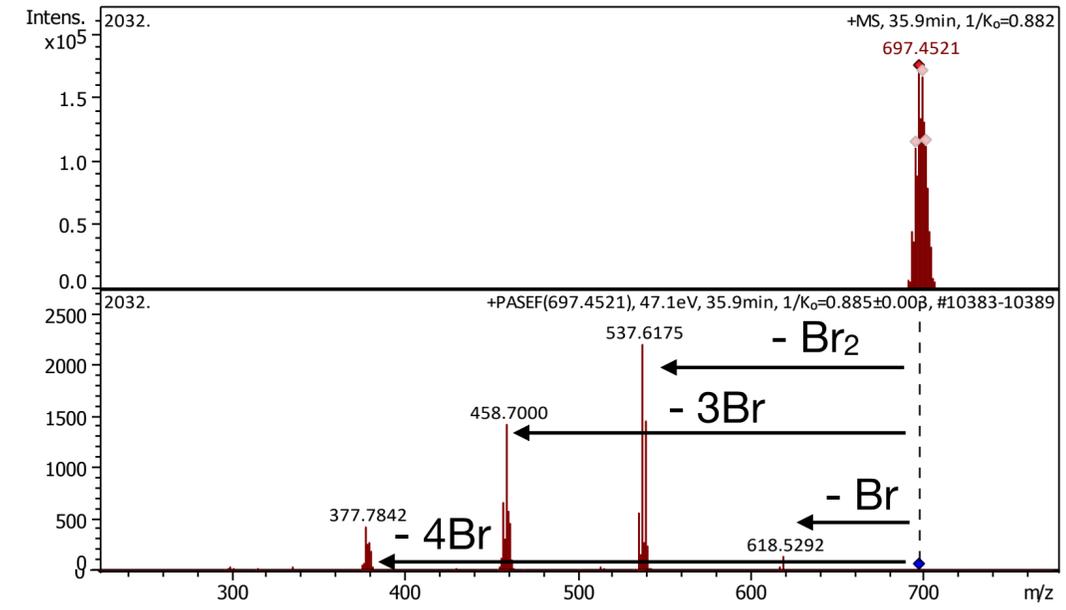
Chromatogram



Ion mobility spectra



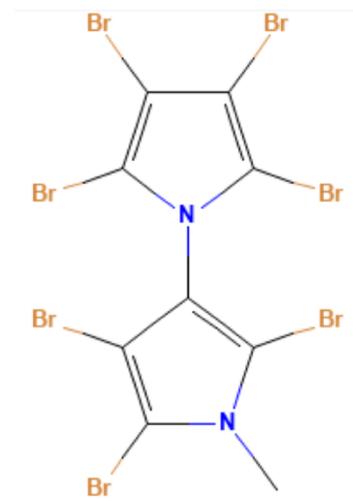
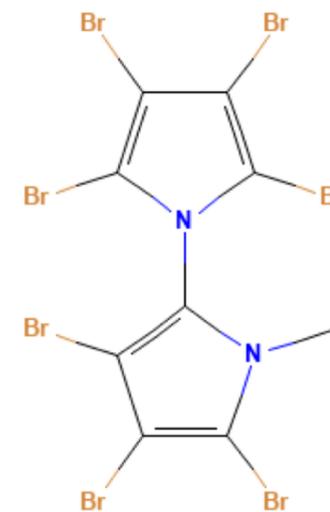
Tandem mass spectrum



⇒ Contains at least 4 Br

Tentative candidate(s)

PubChem



Confidence level

3

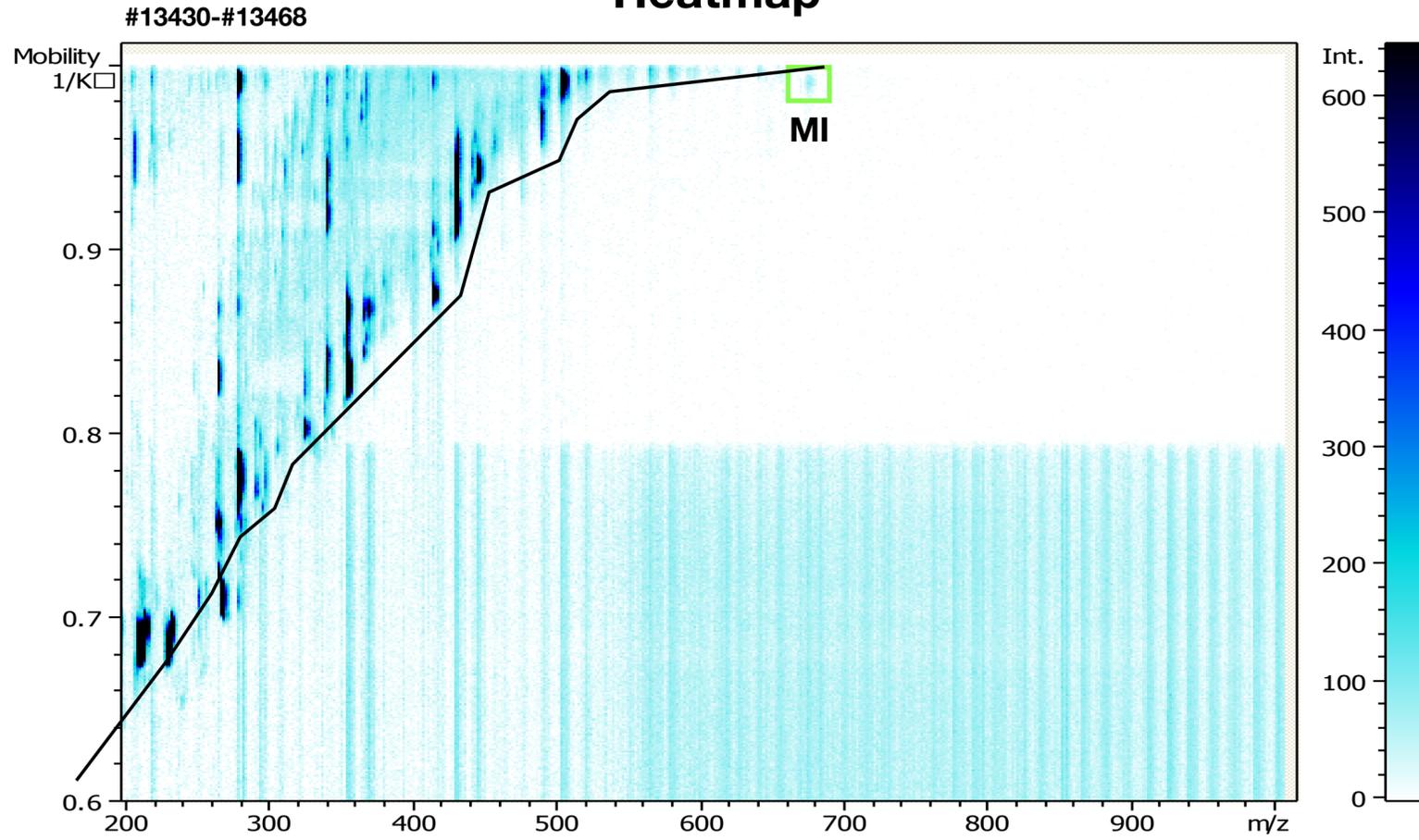
2,3,4,5-Tetrabromo-1-(3,4,5-tribromo-1-methylpyrrol-2-yl)pyrrole

CCS pred: 174.4 Å² (-3.4%)

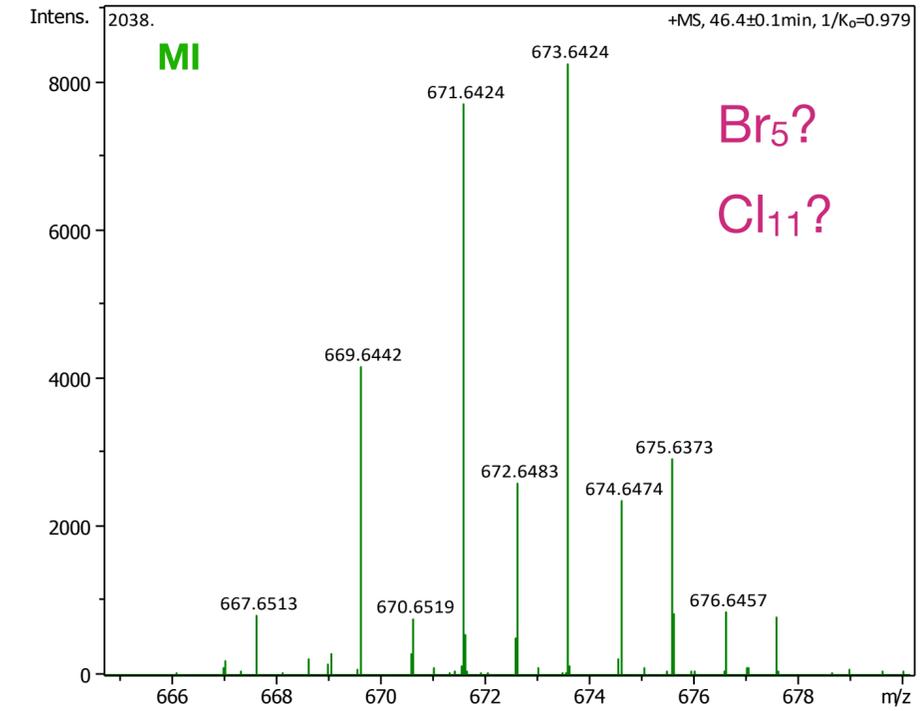
2,3,4,5-Tetrabromo-1-(2,4,5-tribromo-1-methylpyrrol-3-yl)pyrrole

CCS pred: 170.9 Å² (-5.4%)

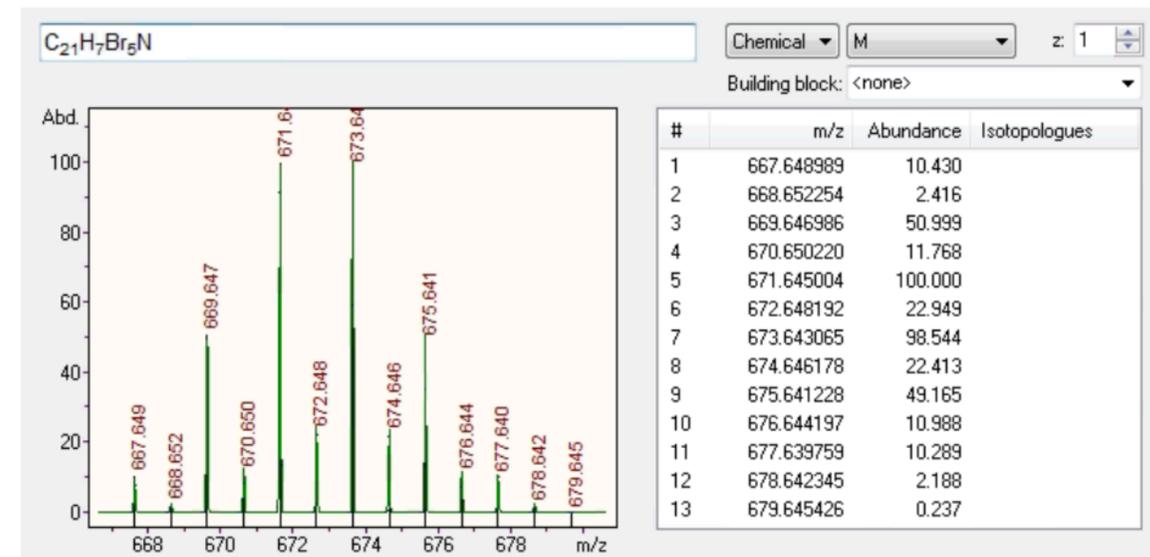
Heatmap



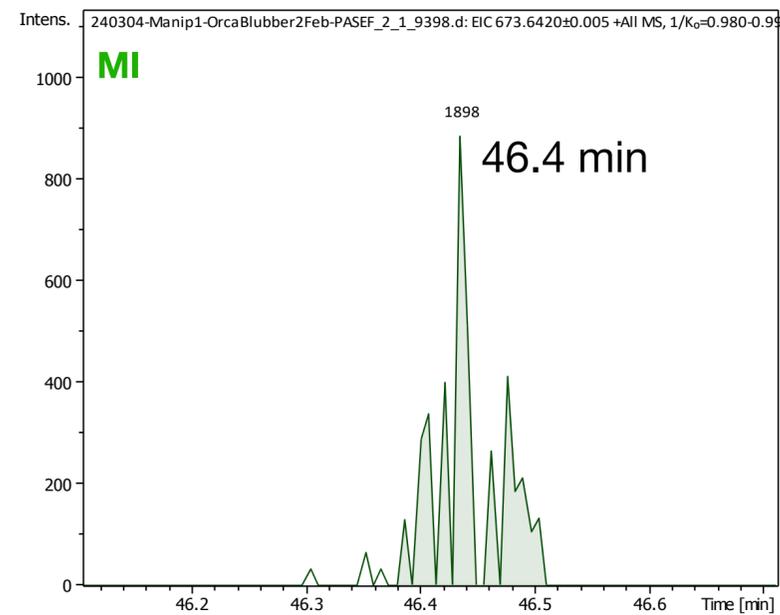
Mass spectrum & isotopic profile



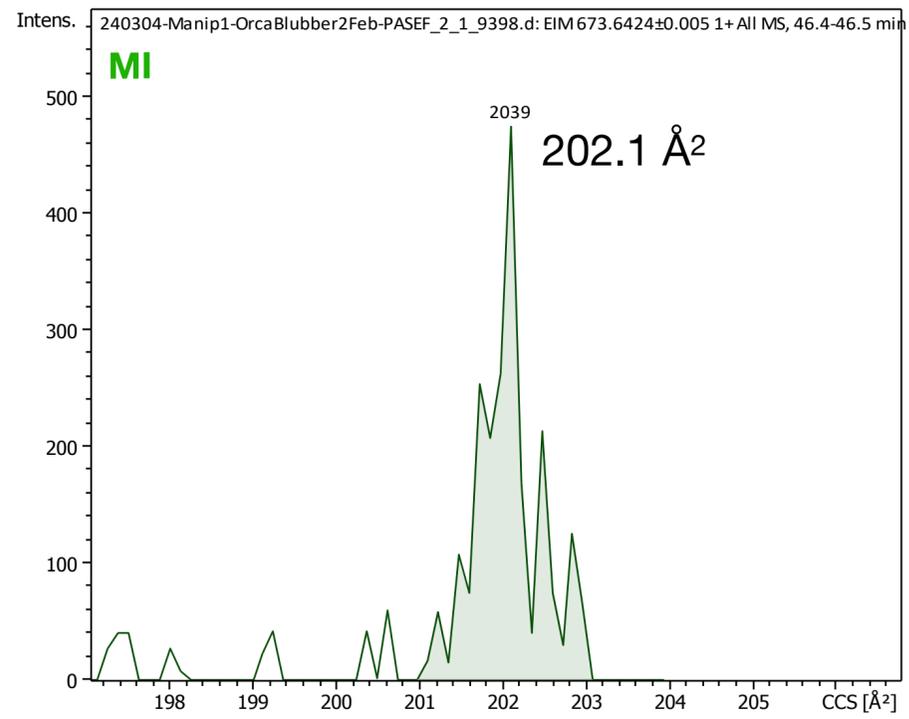
SmartFormula C₂₁H₇Br₅NH?



Chromatogram



Ion mobility spectrum



Tandem mass spectrum

/

Tentative candidate(s)

PubChem

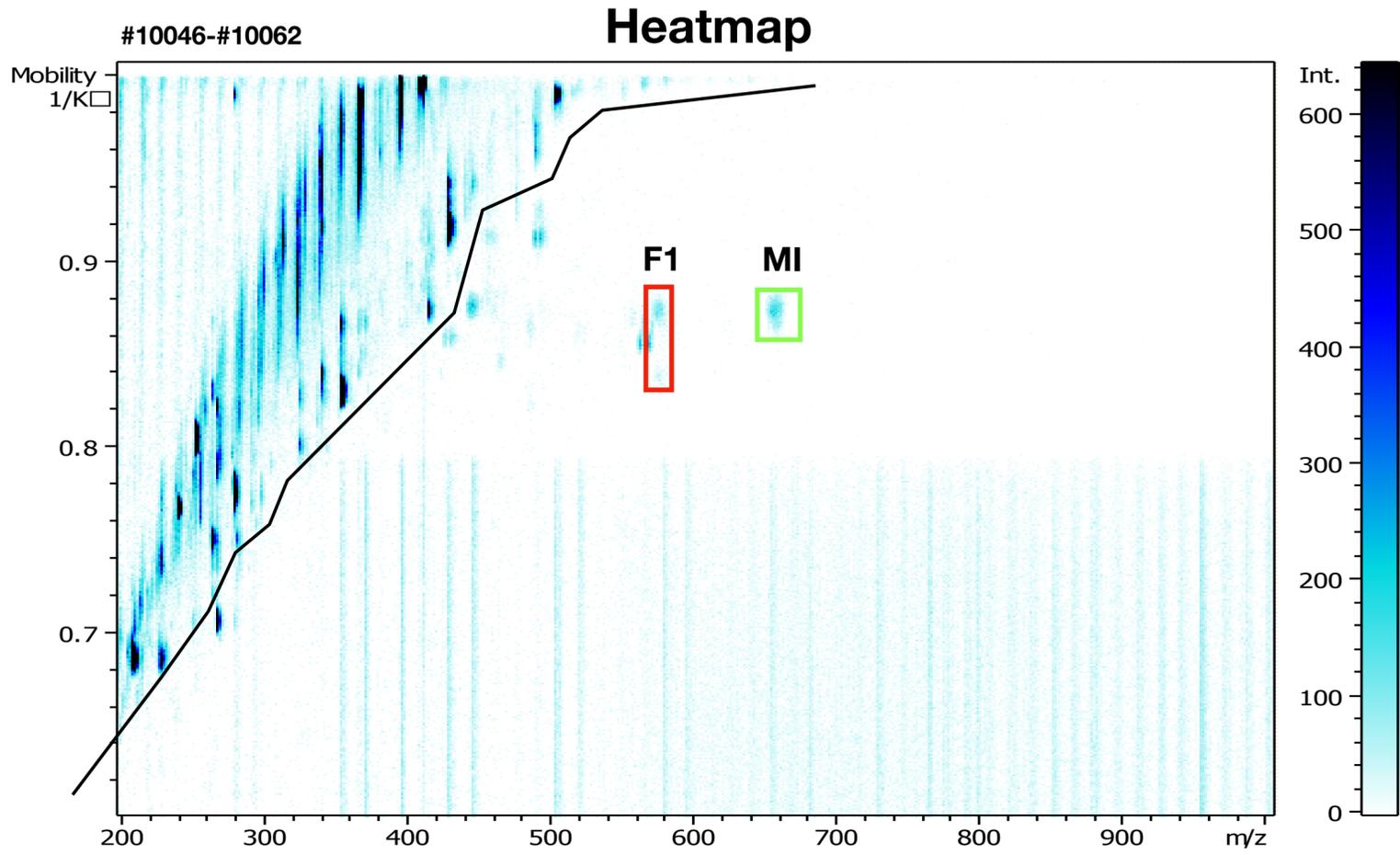
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Confidence level

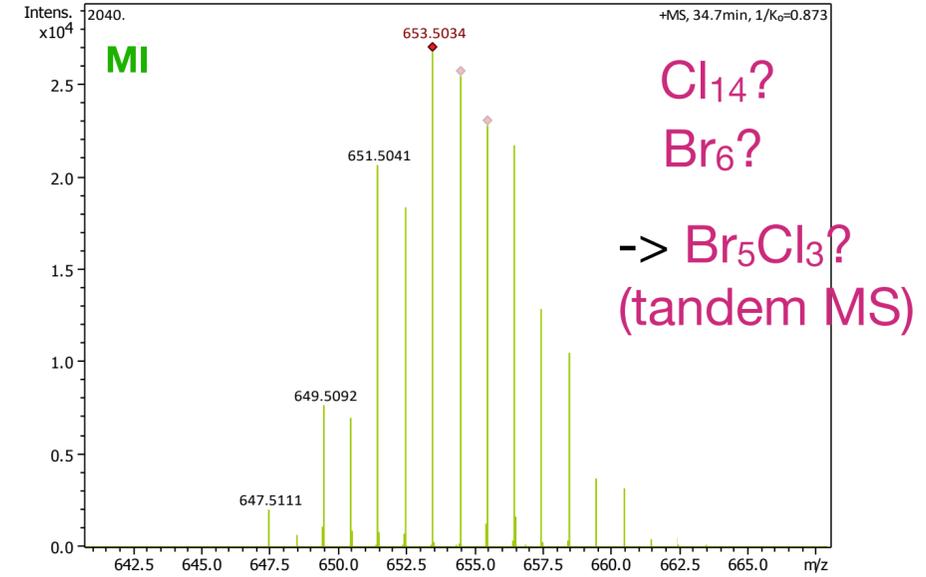
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Feature #9

- EIC 653.5023
- EIC 618.5329
- EIC 572.5851

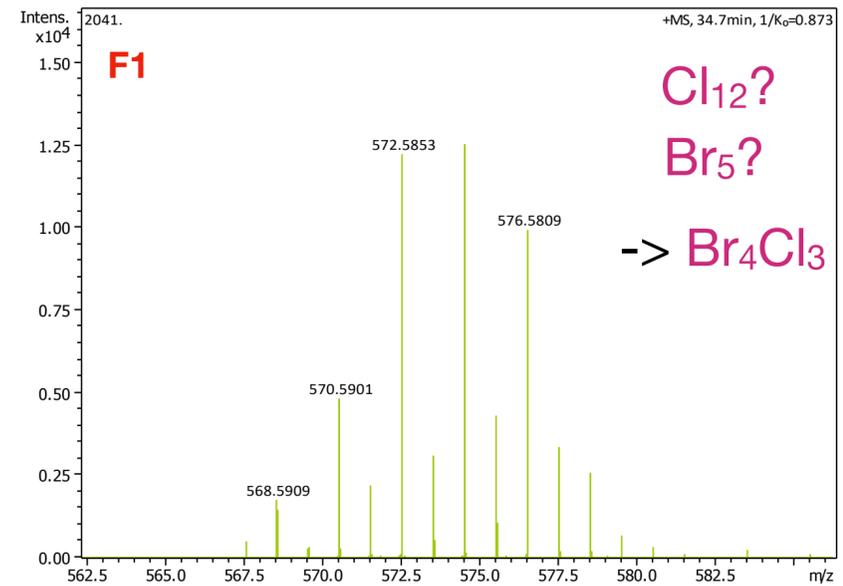
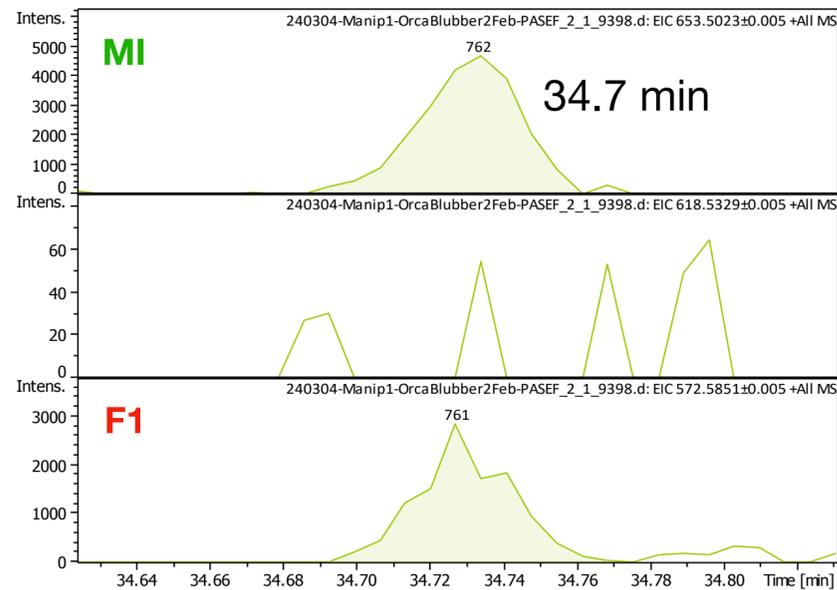


Mass spectra & isotopic profile

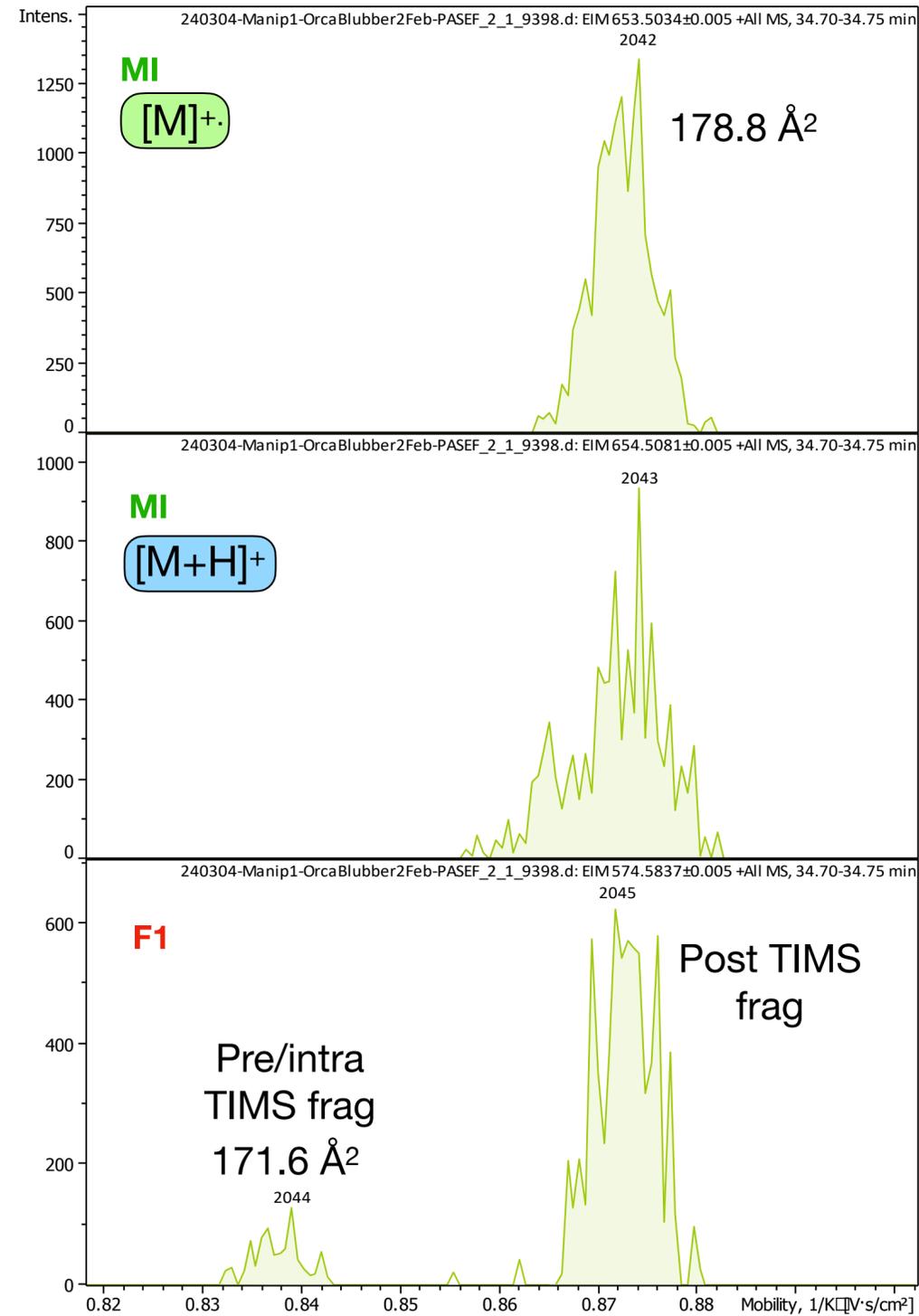


- Br

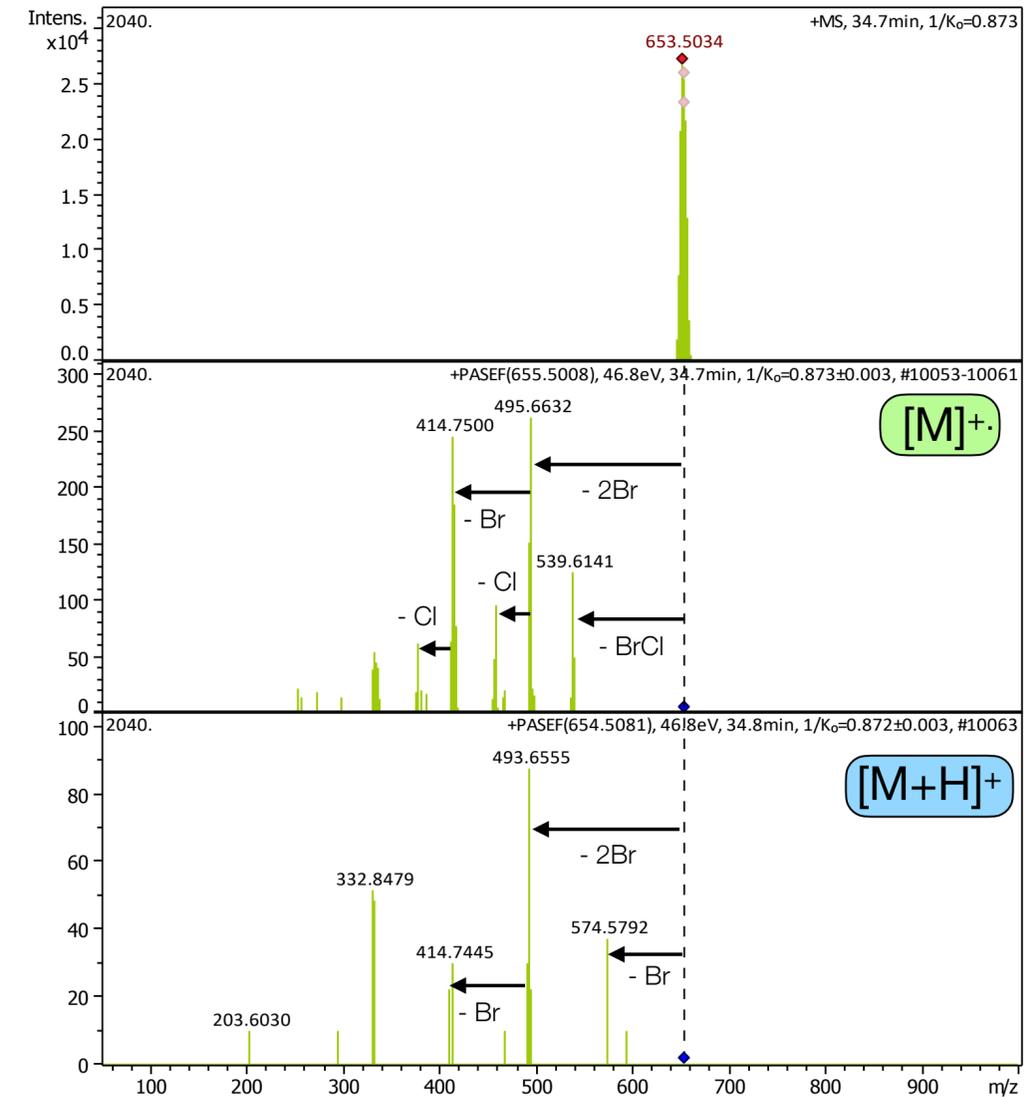
Chromatogram



Ion mobility spectra



Tandem mass spectra



⇒ Contains at least 3 Br and 1 Cl

Tentative candidate(s)

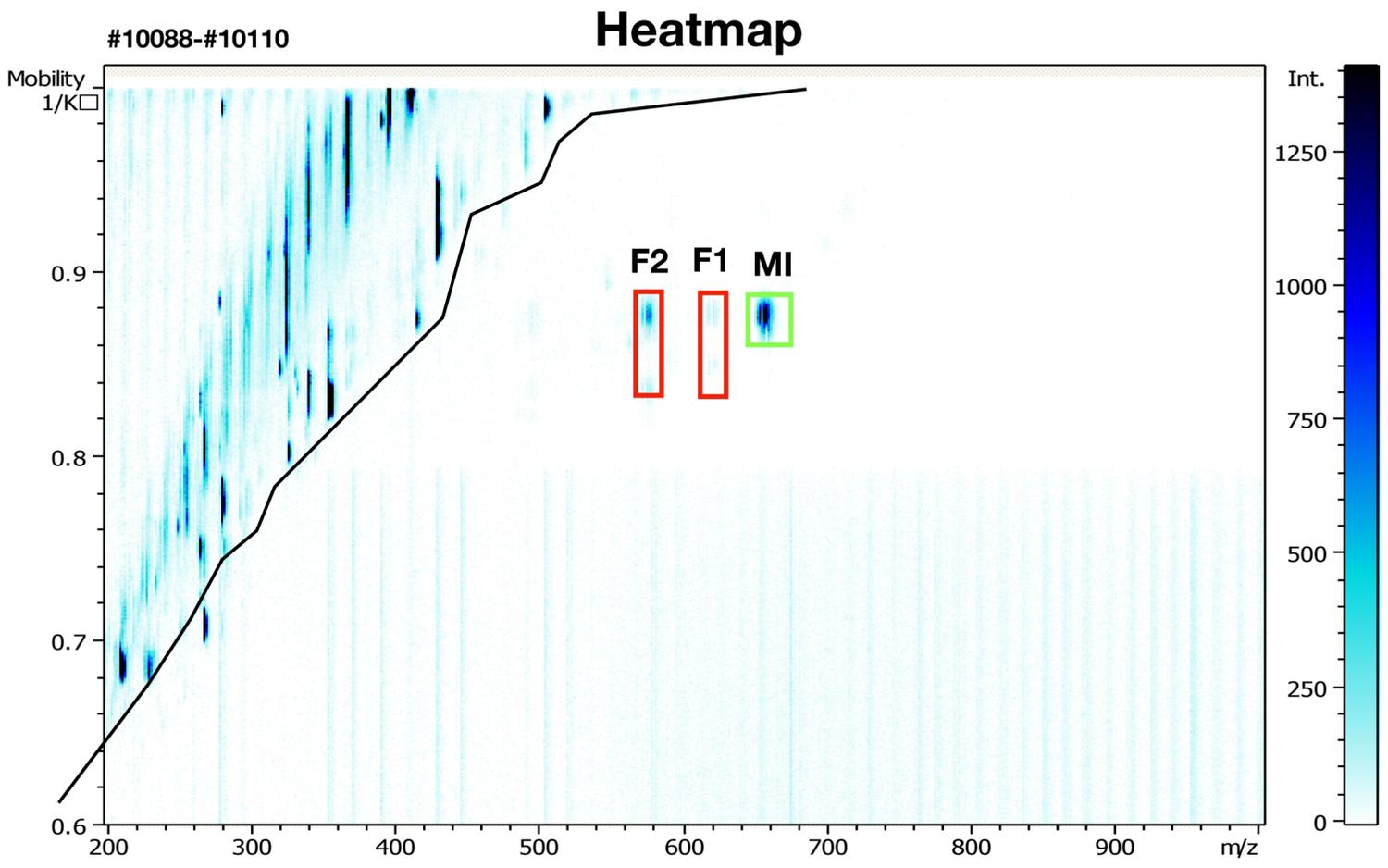
PubChem

Confidence level

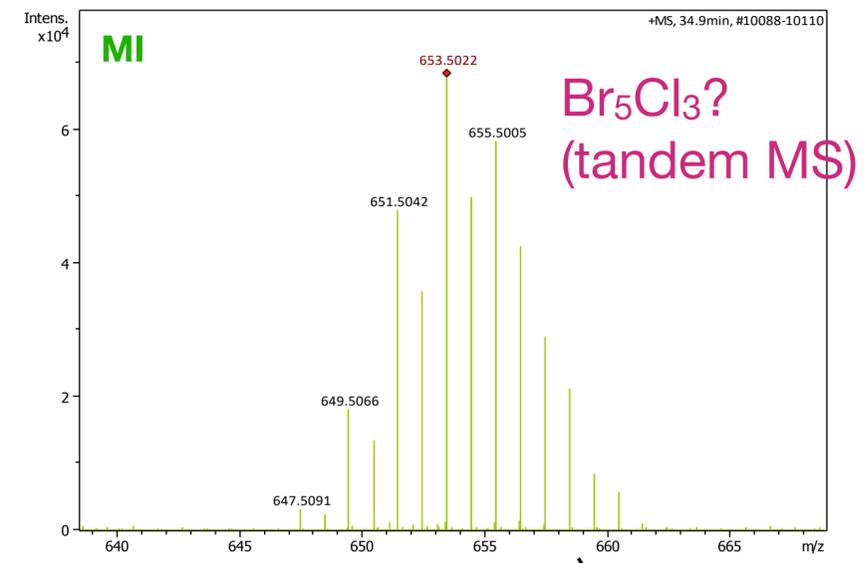
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/

- EIC 653.5023
- EIC 618.5329
- EIC 572.5851



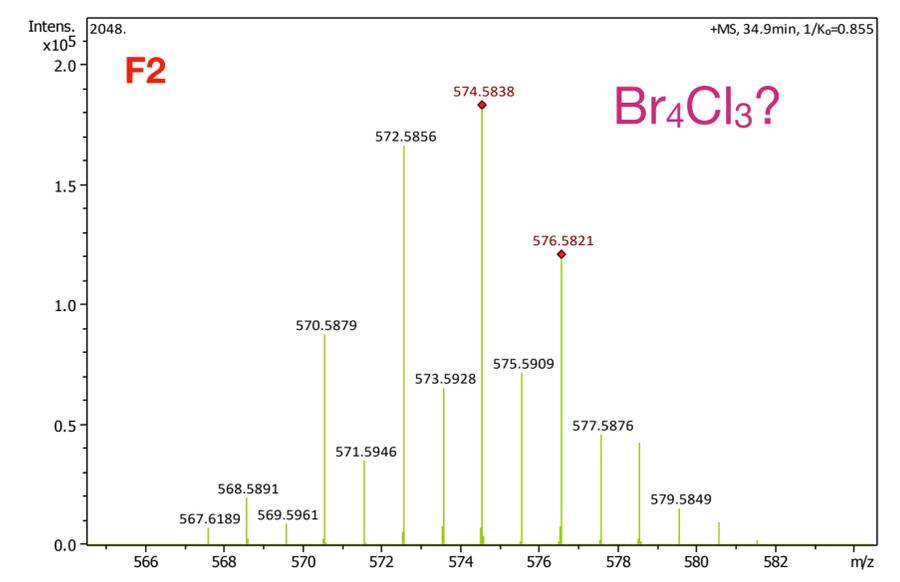
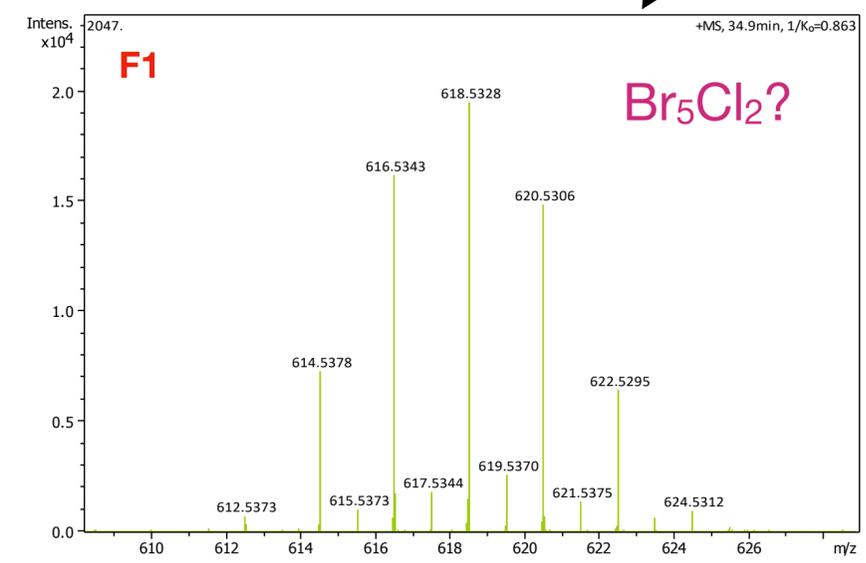
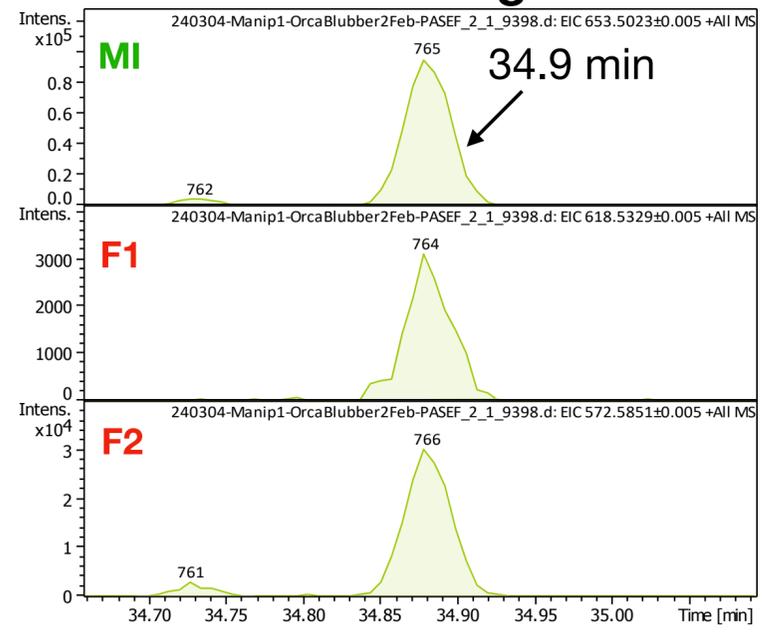
Mass spectra & isotopic profile



- Cl

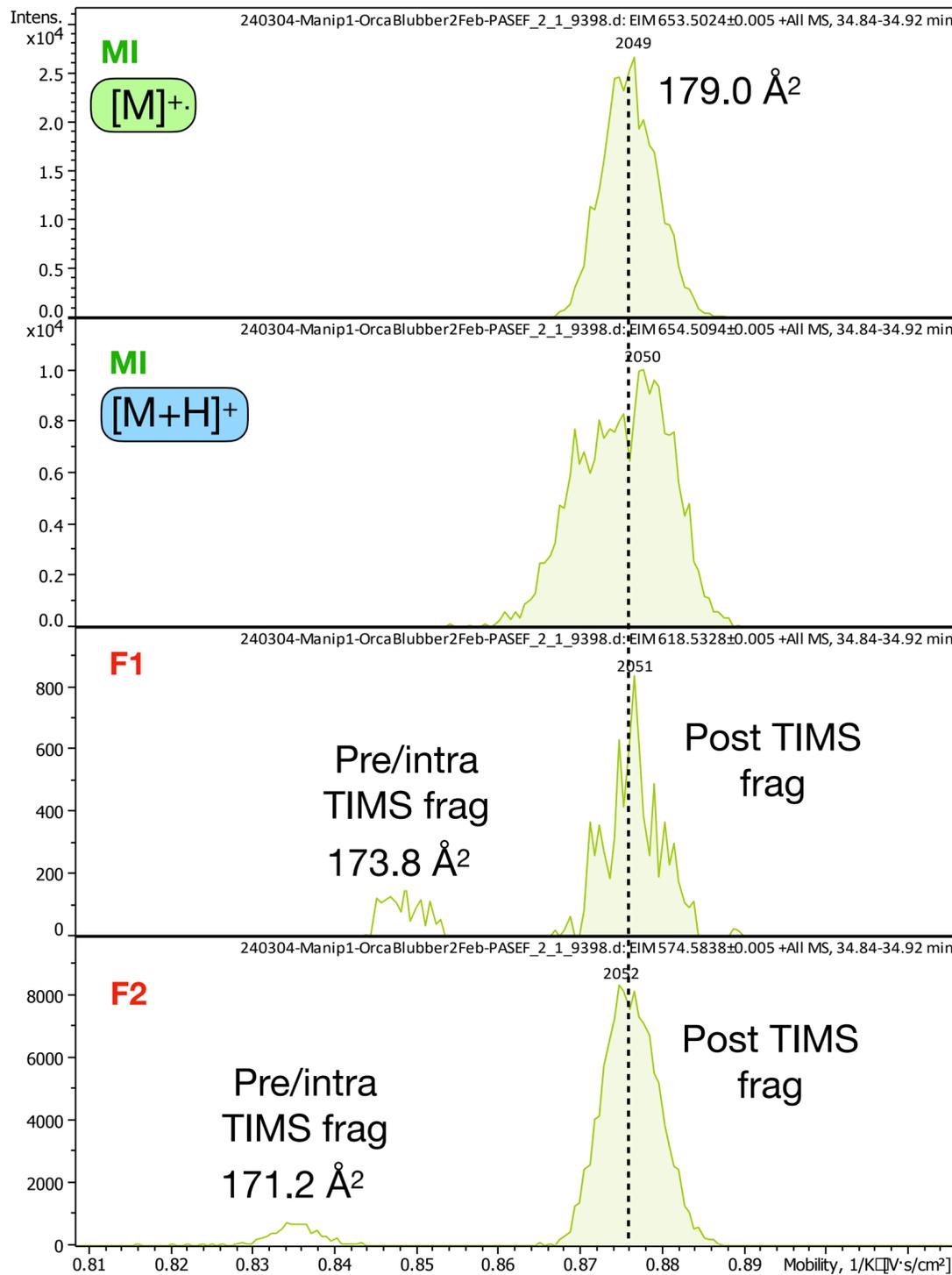
- Br

Chromatogram

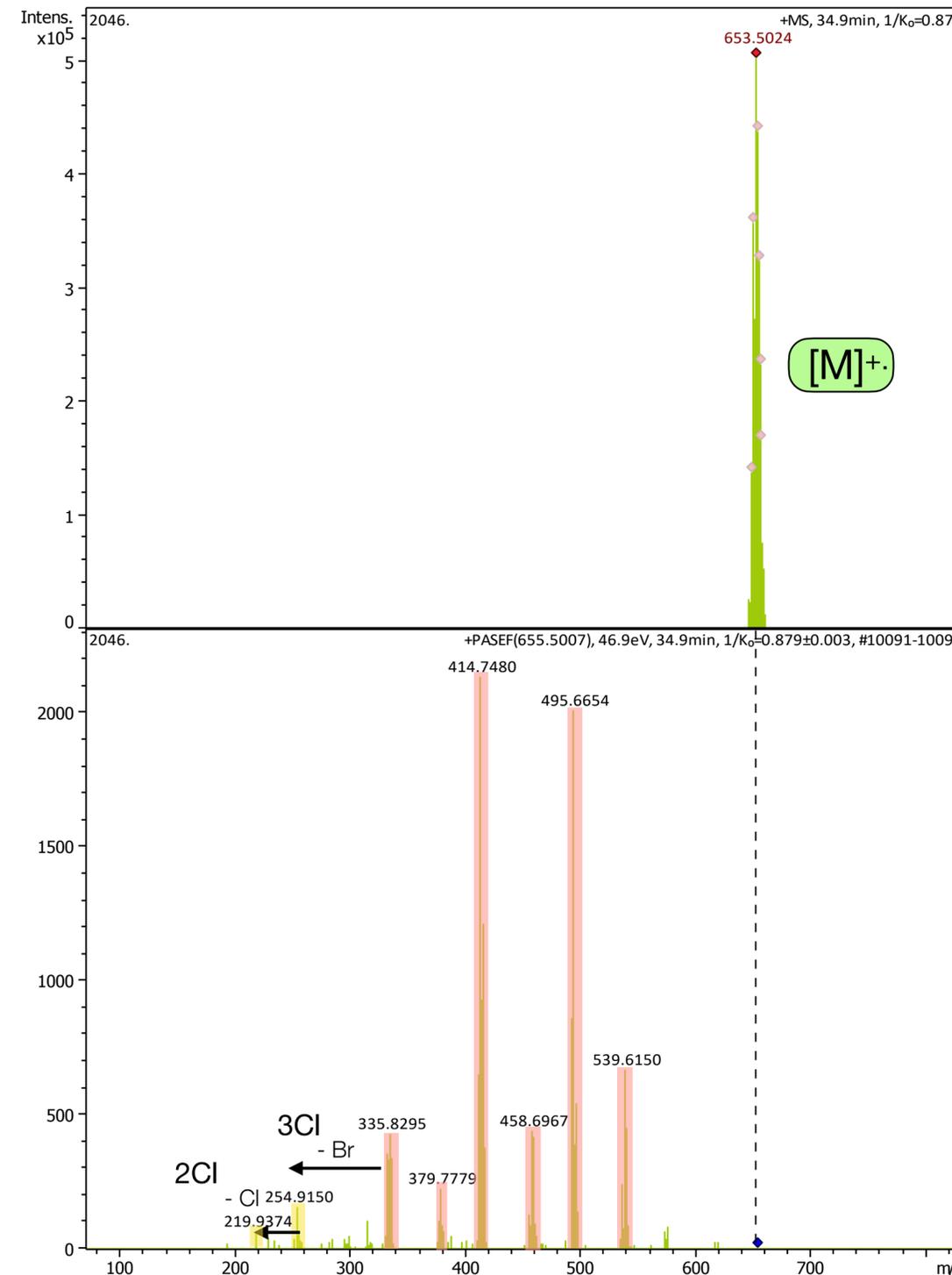


Tandem mass spectra

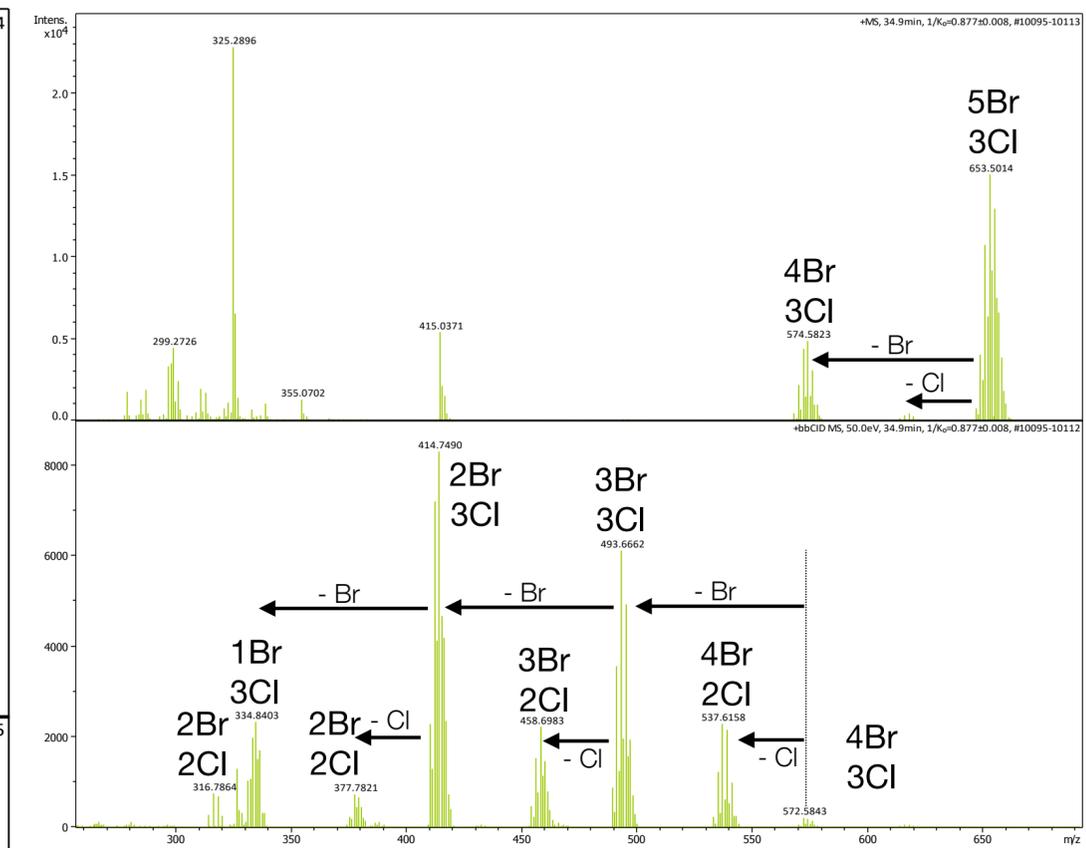
Ion mobility spectra



PASEF DDA



IM filtered bbCID



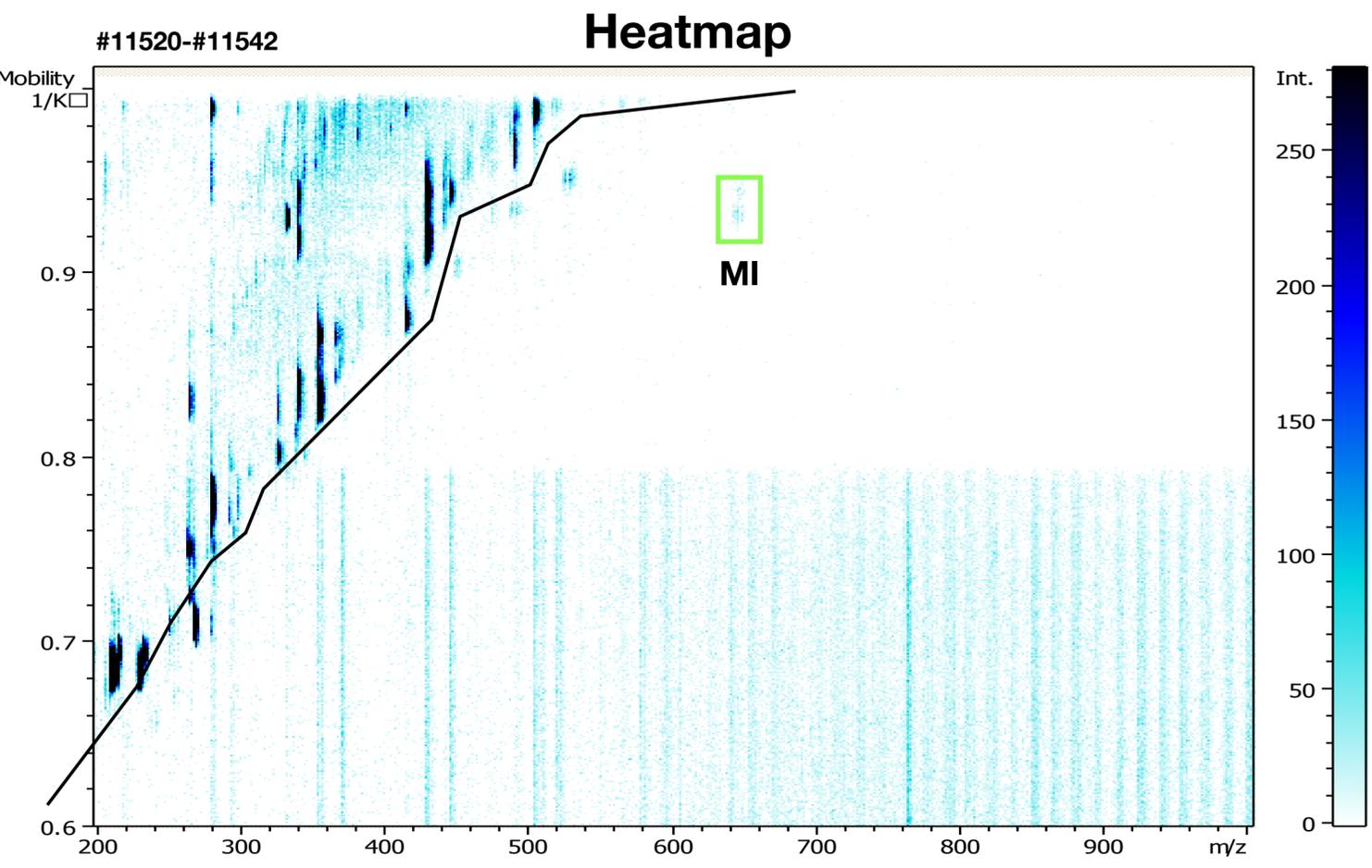
⇒ Contains at least 5 Br and 1 Cl
⇒ Confirmed by isotopic pattern of fragments (bbCID tandem mass spectrum)

Tentative candidate(s)

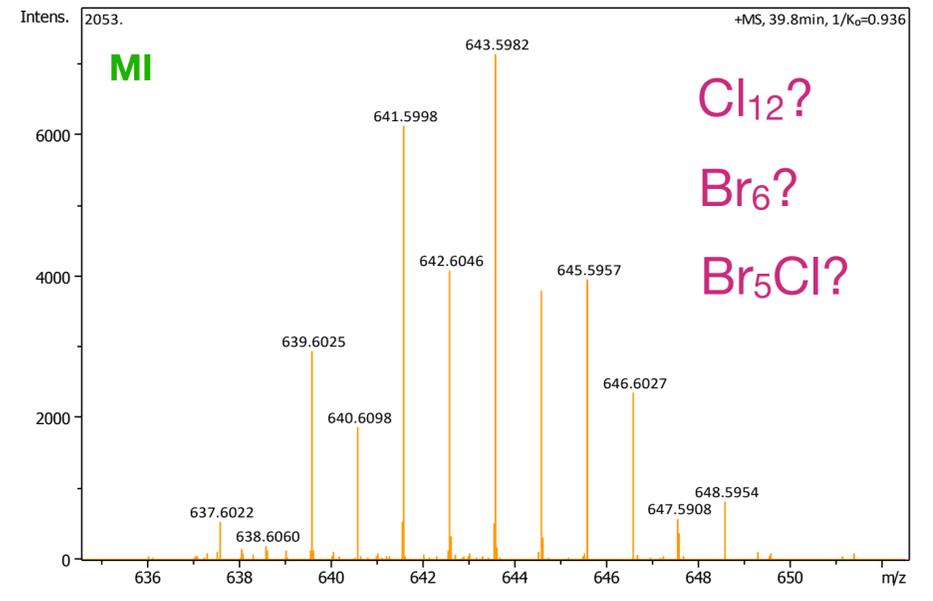
PubChem

Confidence level

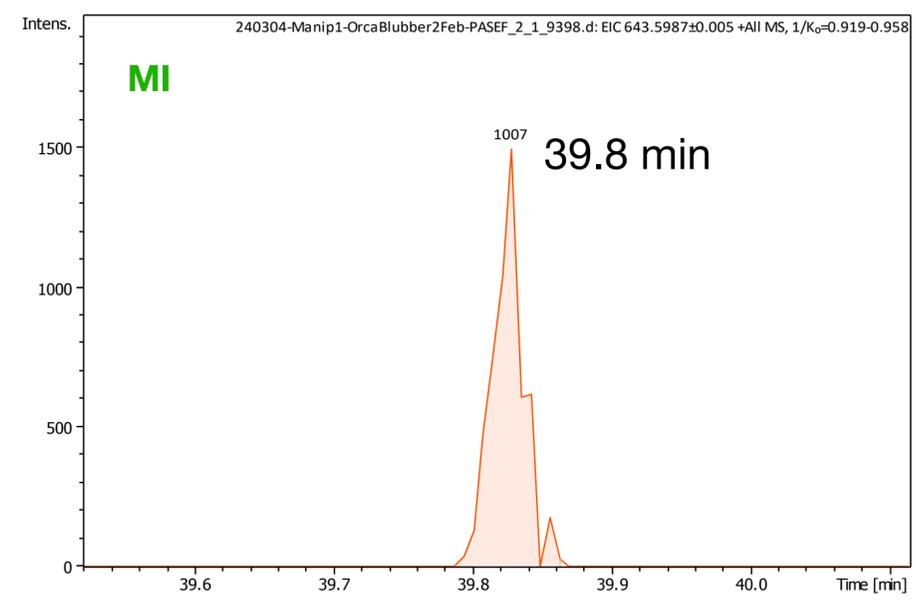
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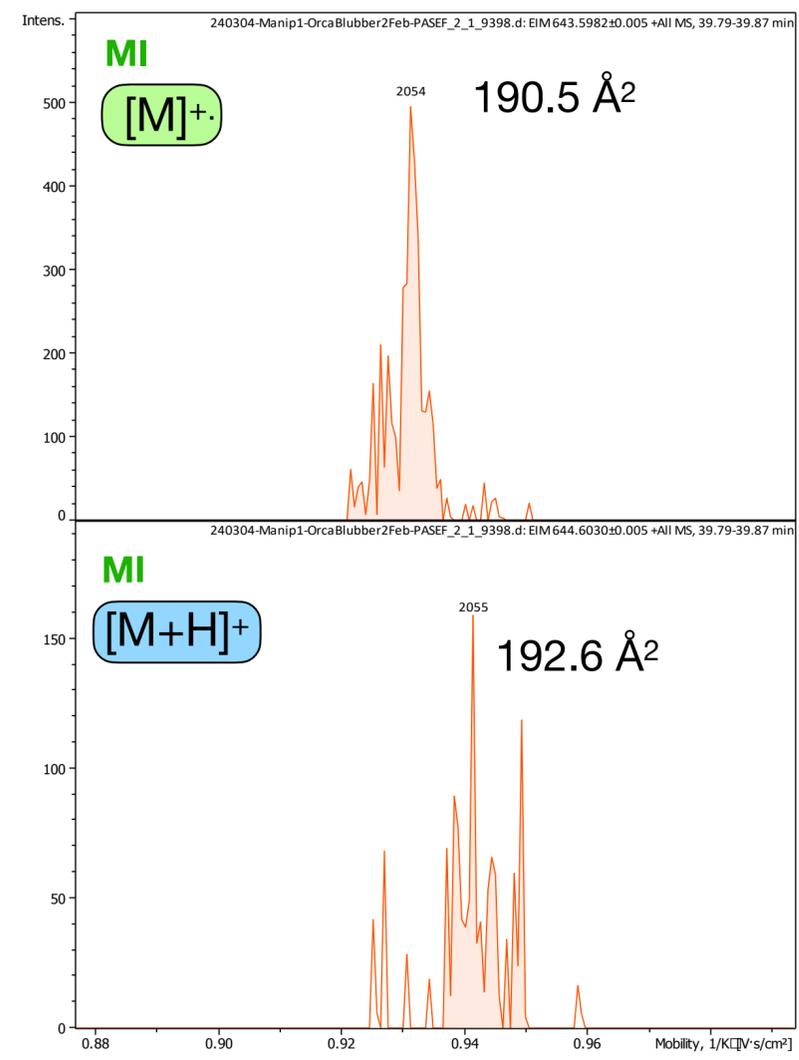
Mass spectrum & isotopic profile



Chromatogram



Ion mobility spectra



Tandem mass spectrum

/

Tentative candidate(s)



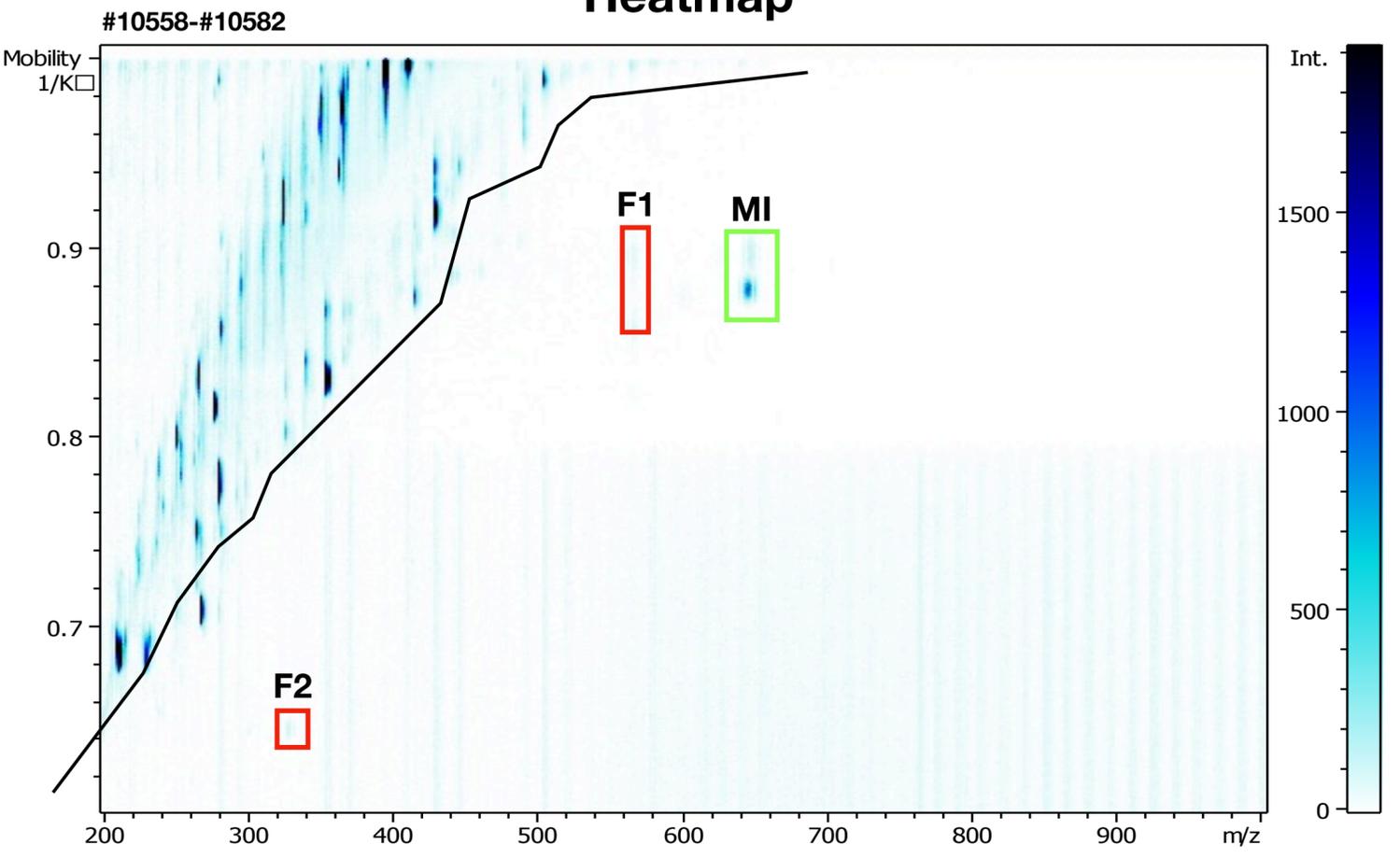
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Confidence level

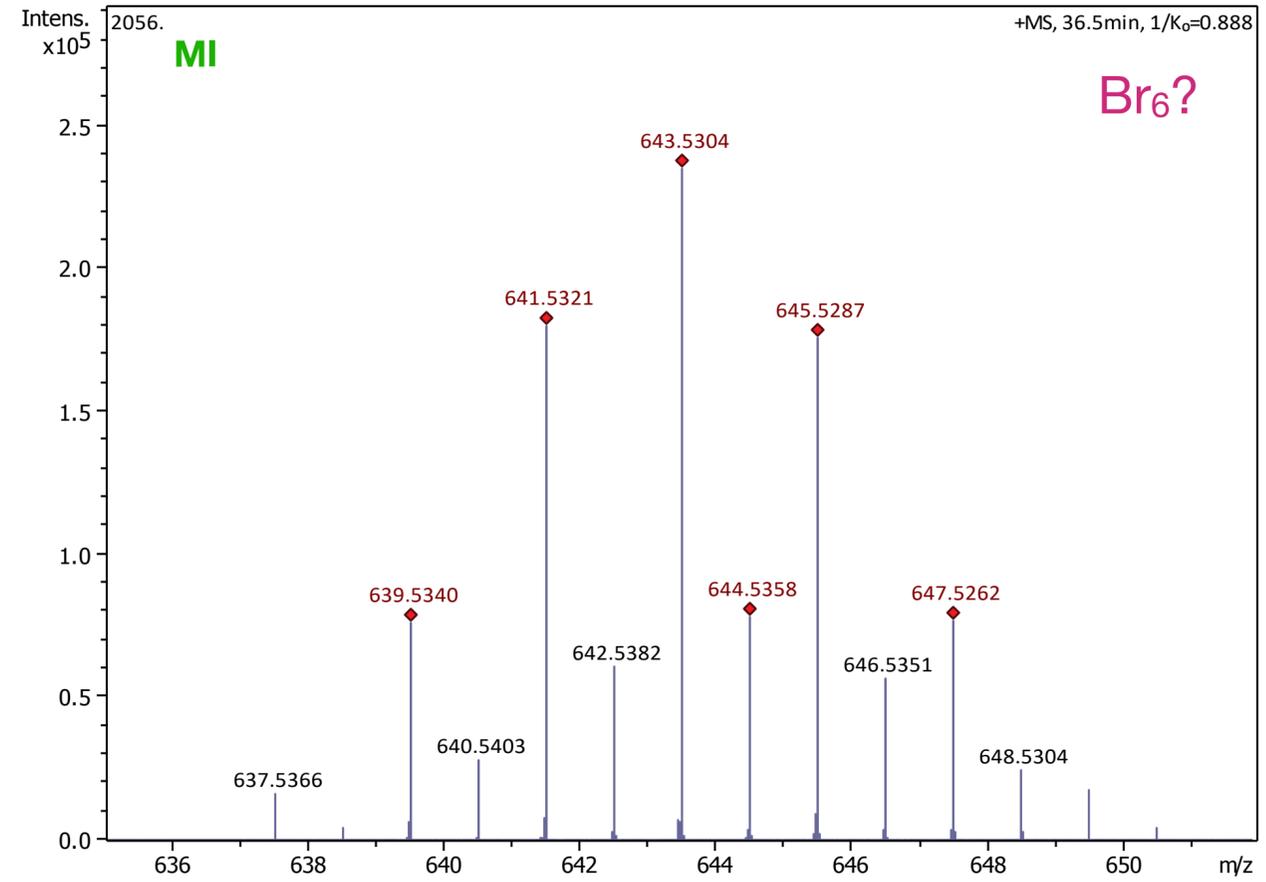


- EIC 643.5302
- EIC 563.6212
- EIC 328.7613

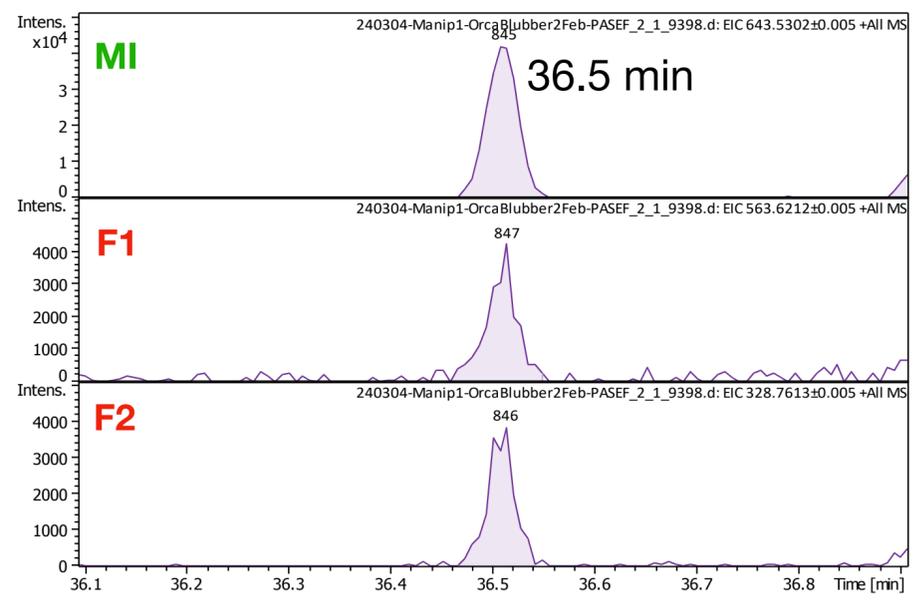
Heatmap



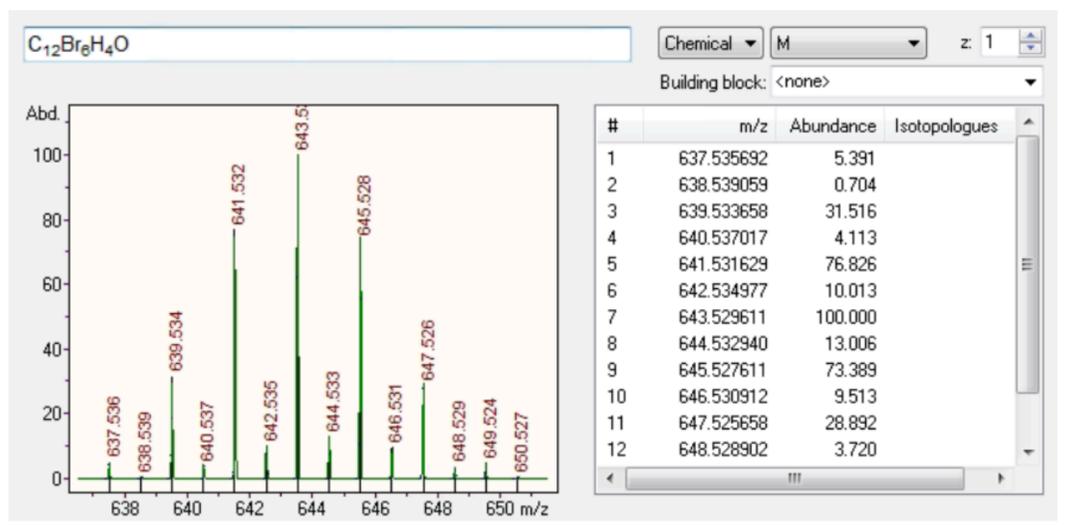
Mass spectra & isotopic profile



Chromatogram

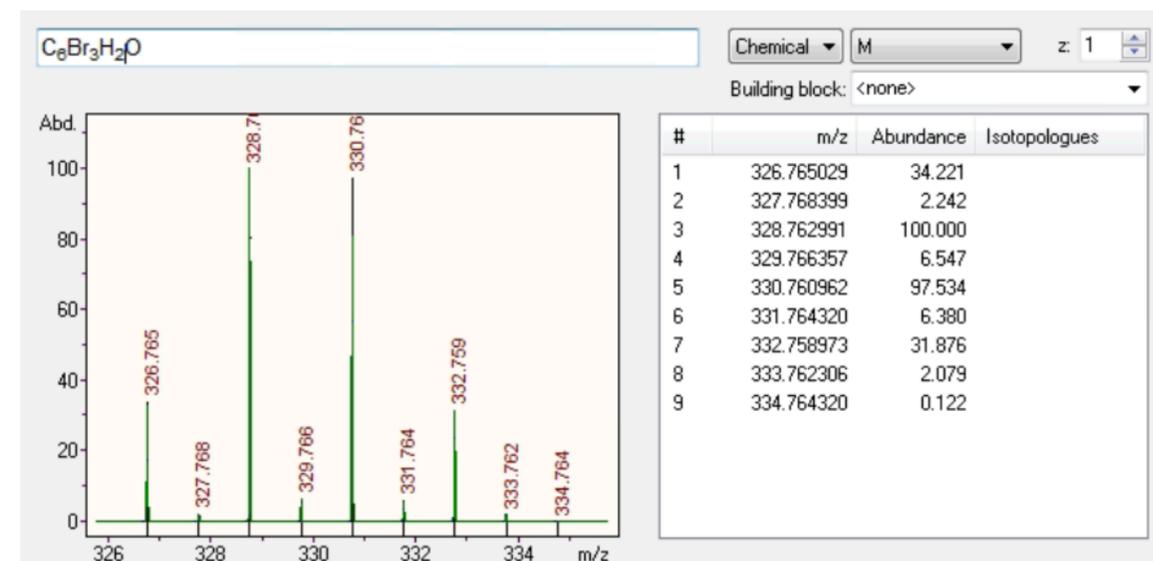
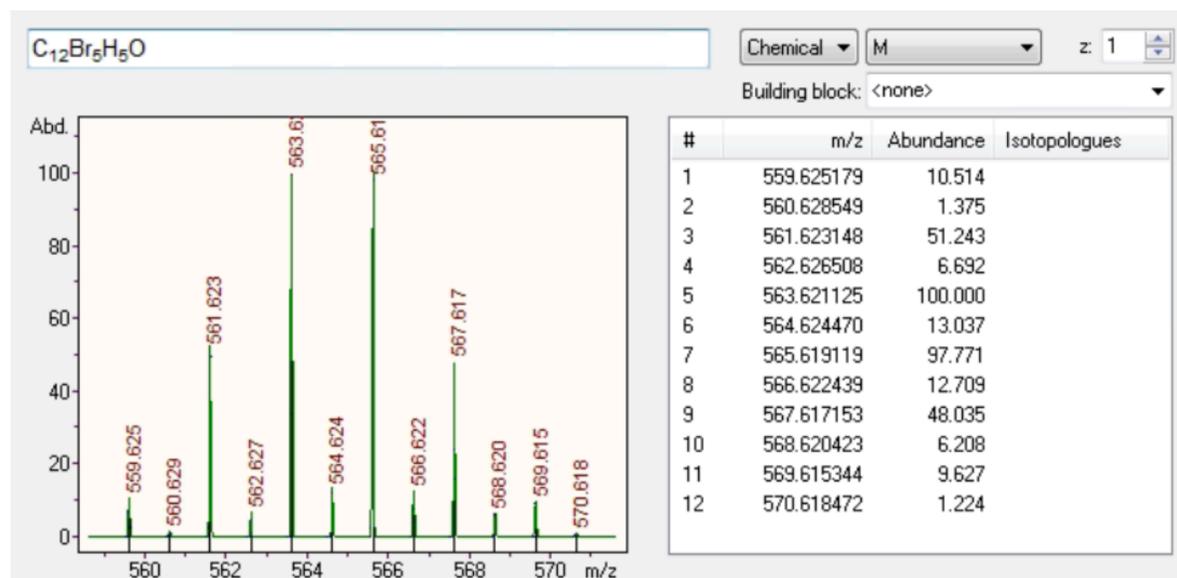
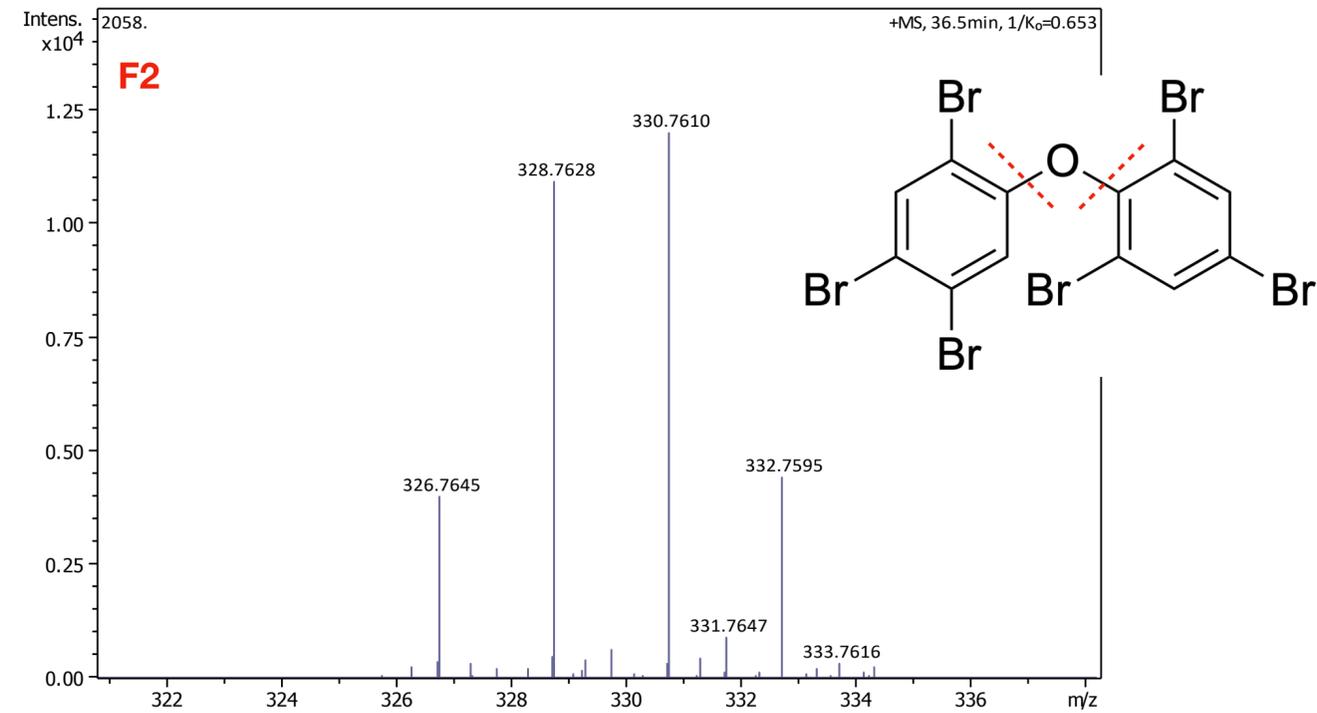
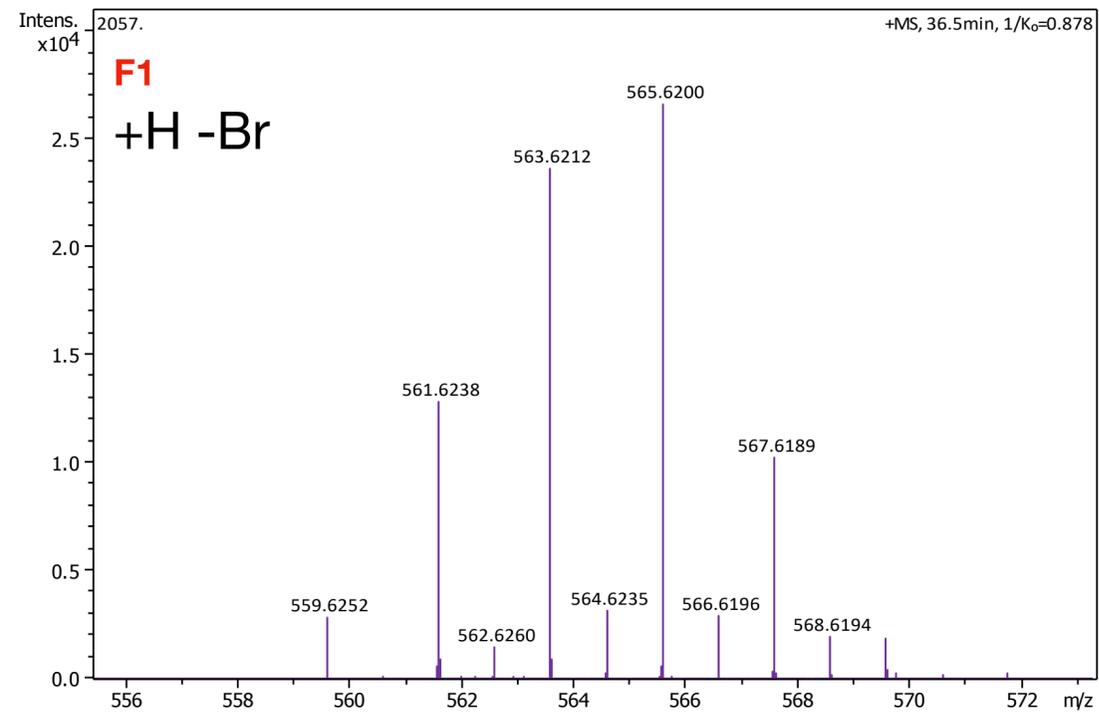


C₁₂Br₆H₄O

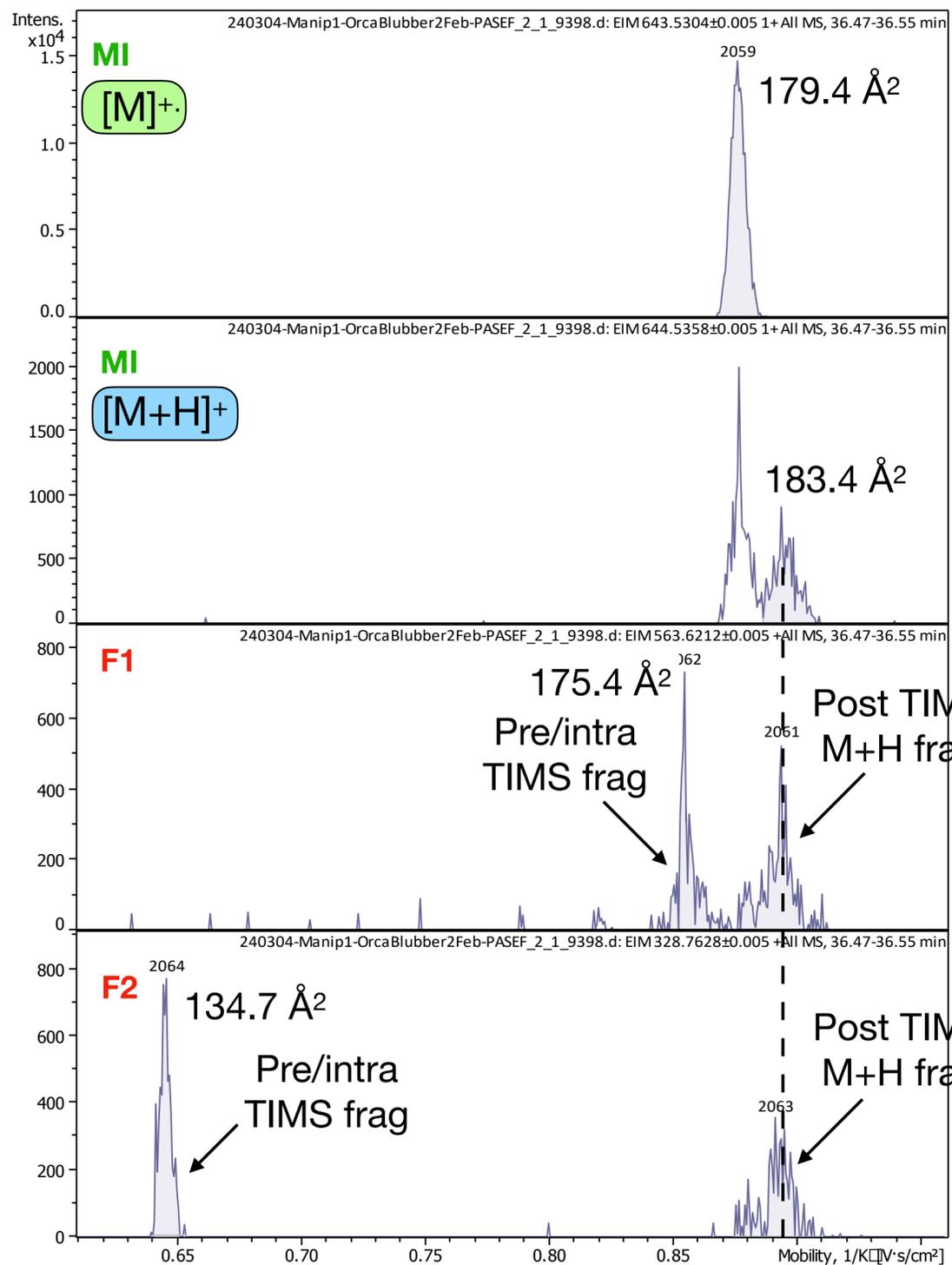


Feature #12

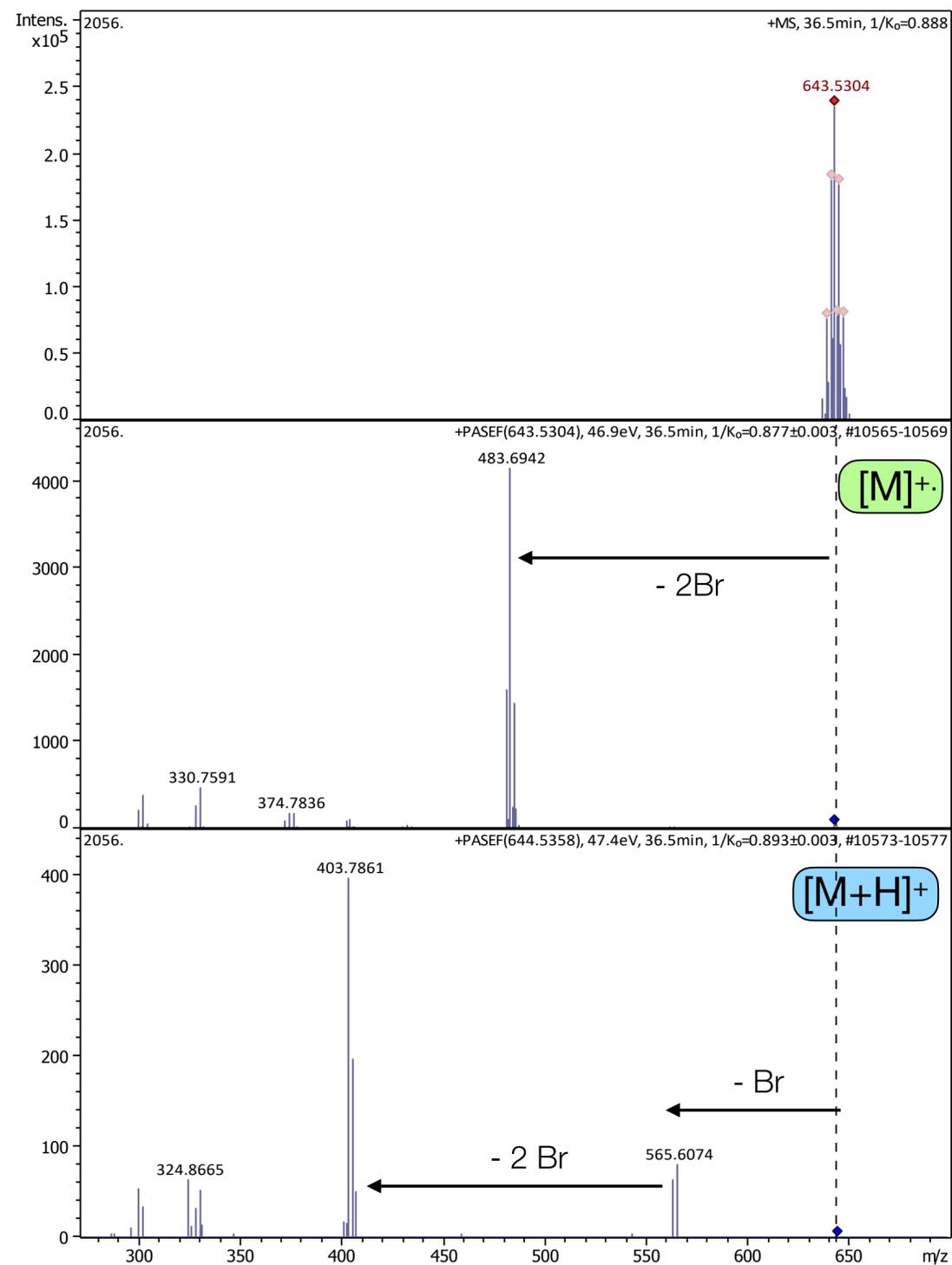
 EIC 643.5302
 EIC 563.6212
 EIC 328.7613



Ion mobility spectra

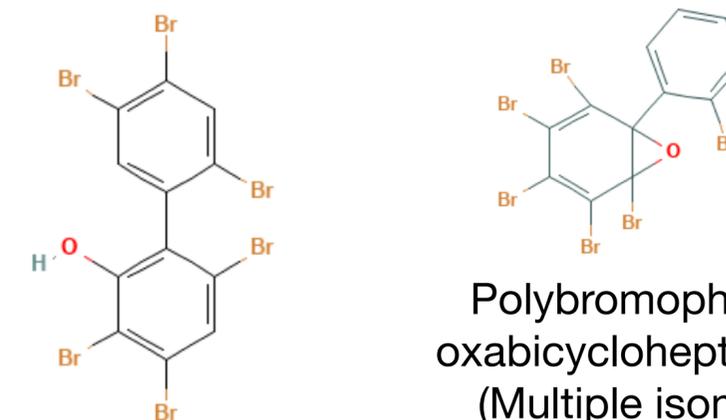


Tandem mass spectra



Tentative candidate(s)

PubChem

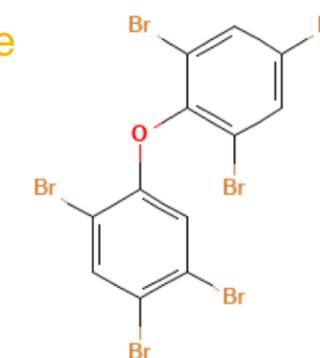


Hexabromobiphenylol
(Multiple isomers)

⇒ Not GC amenable

Polybromophenyl-oxabicycloheptadiene
(Multiple isomers)

CCS pred: 179.2 Å²
(-0.1%)



HxBDE (42 isomers)

⇒ Well-known POP class

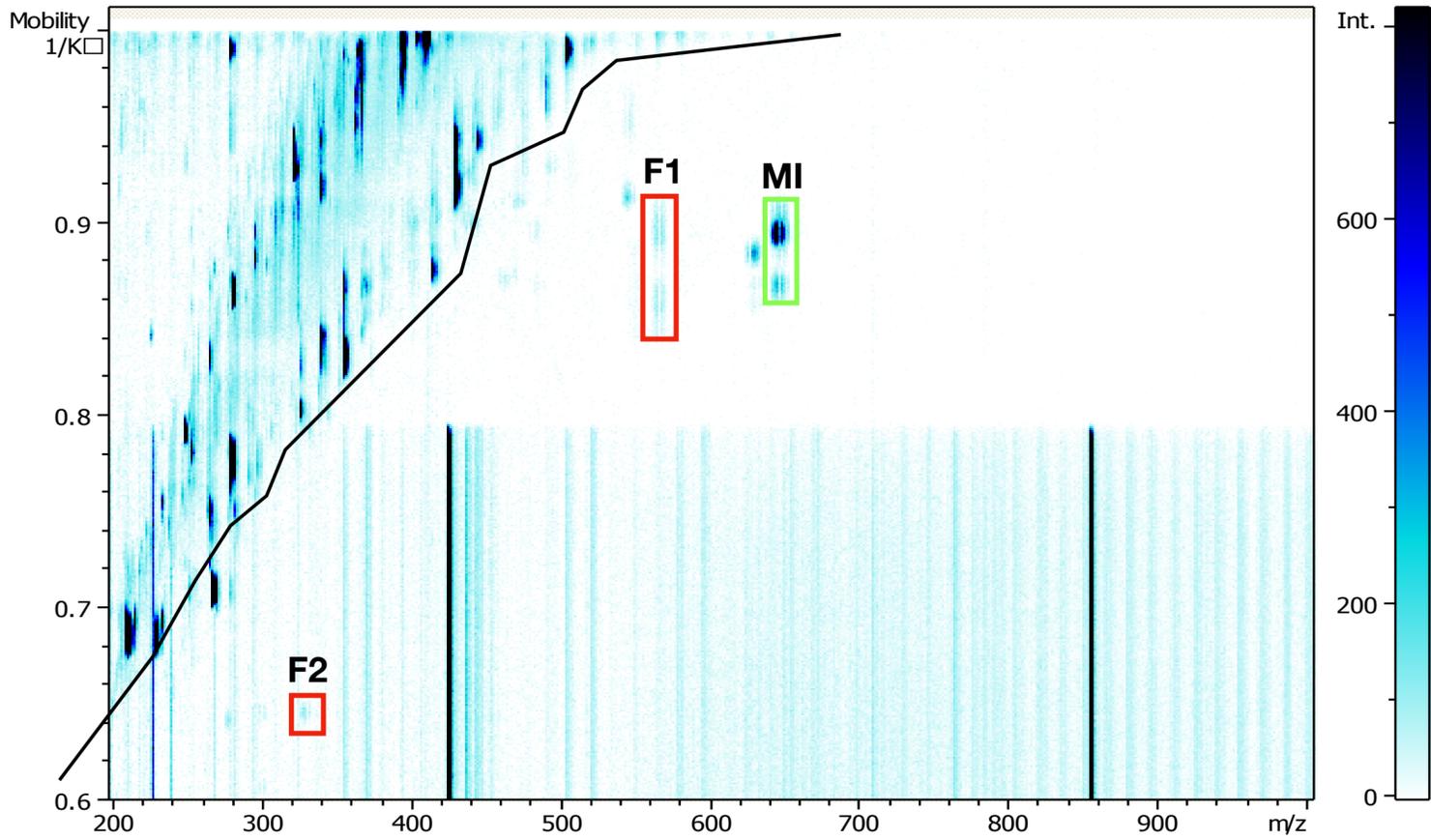
Confidence level

3

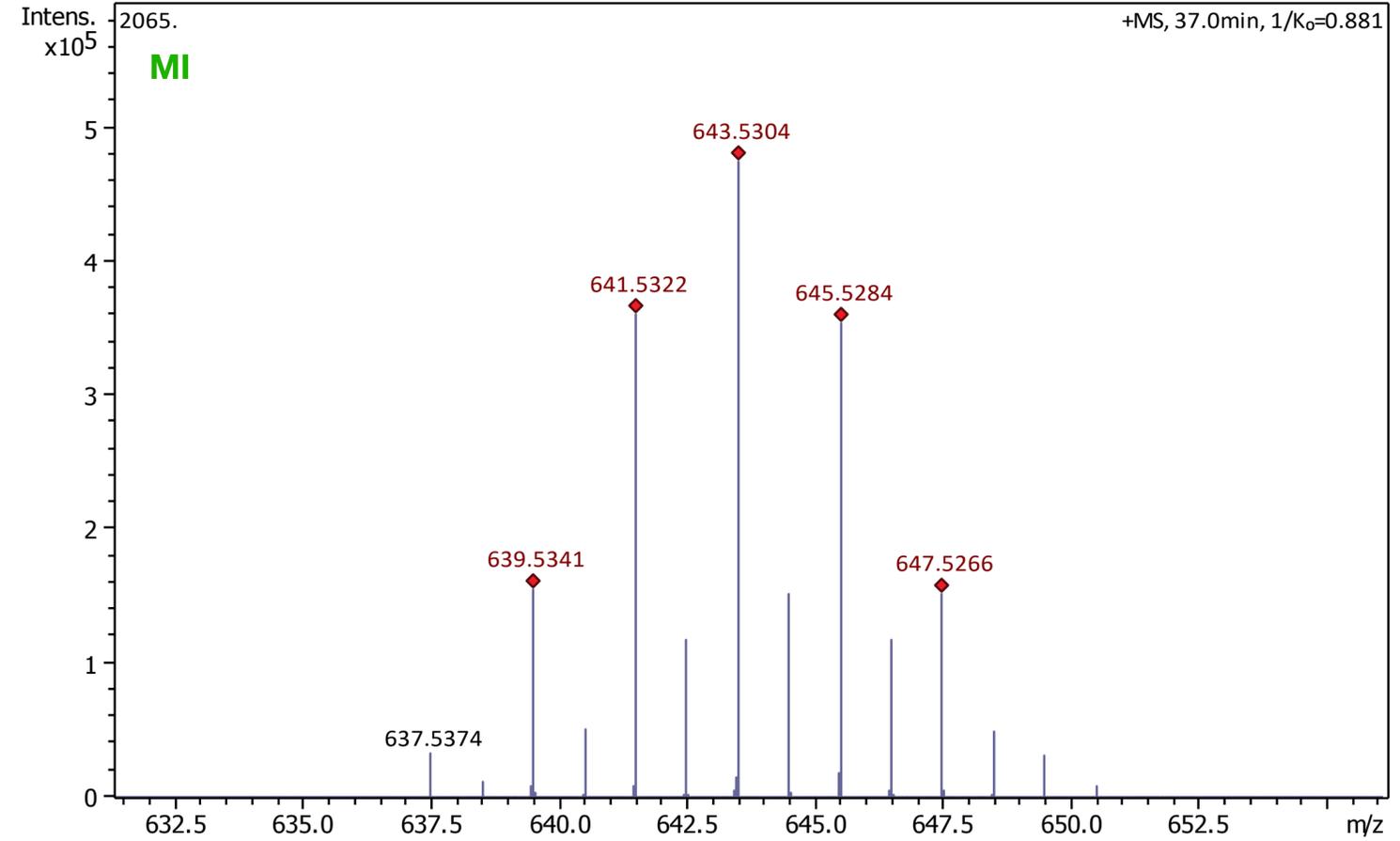
CCS pred HxBDE isomers: see
Figure S6.7A (manuscript)

Heatmap

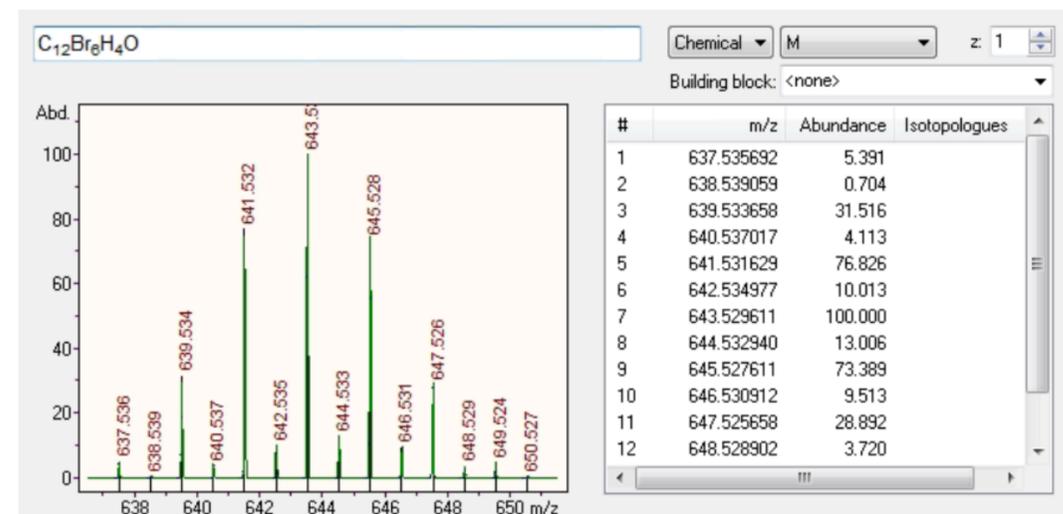
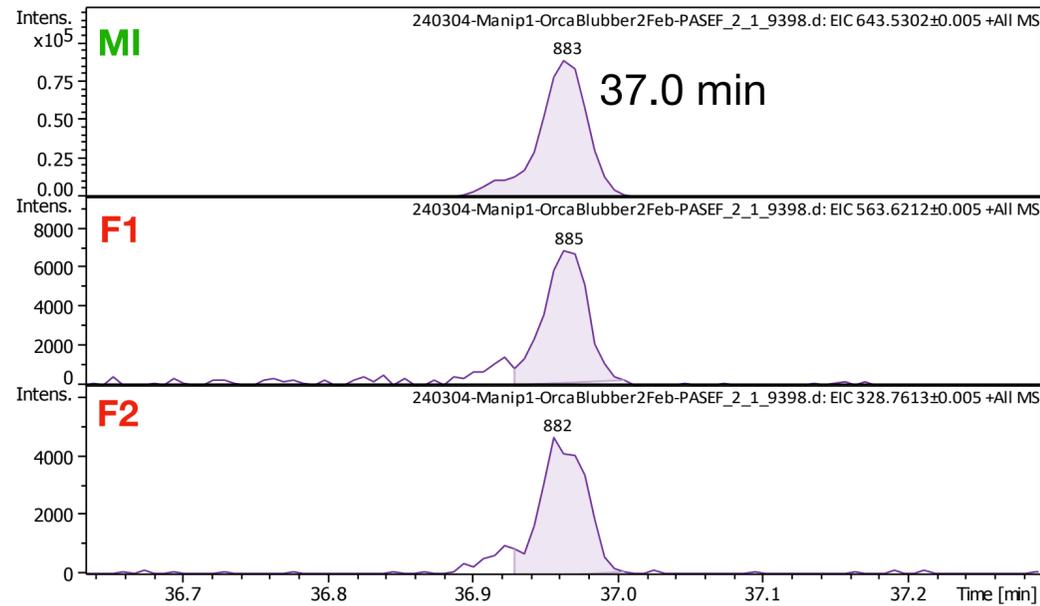
#10694-#10716



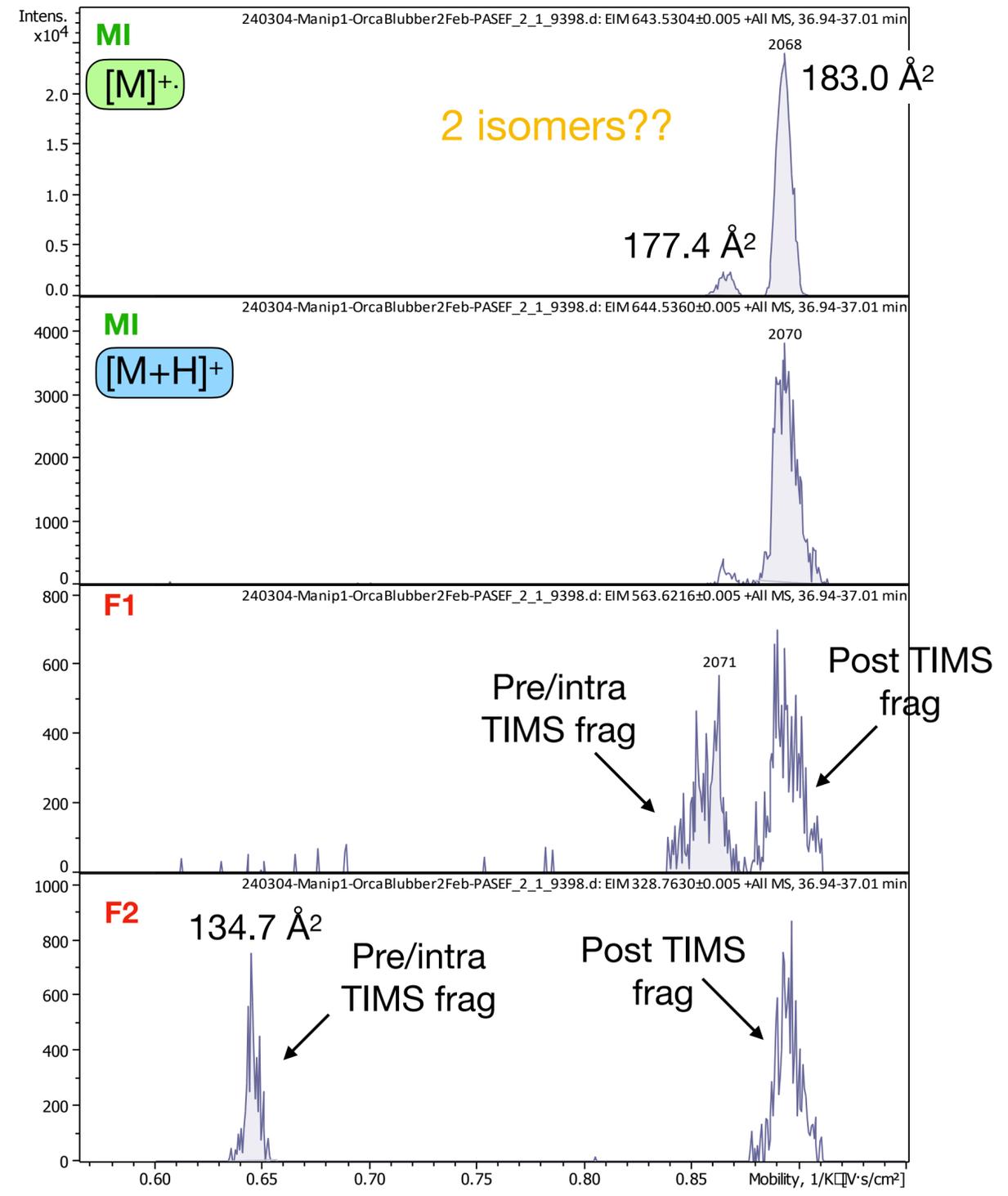
Mass spectrum & isotopic profile



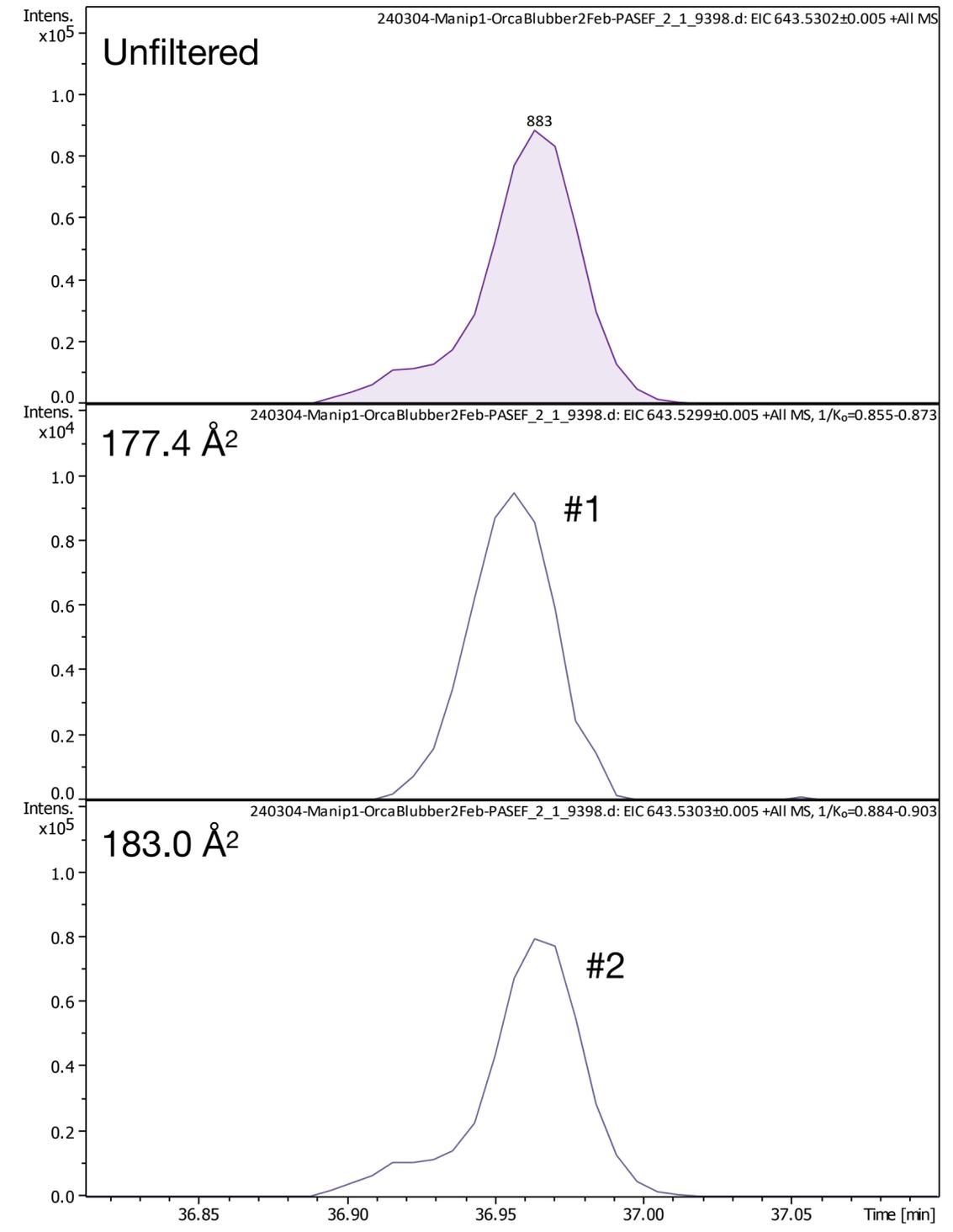
Chromatogram



Ion mobility spectra

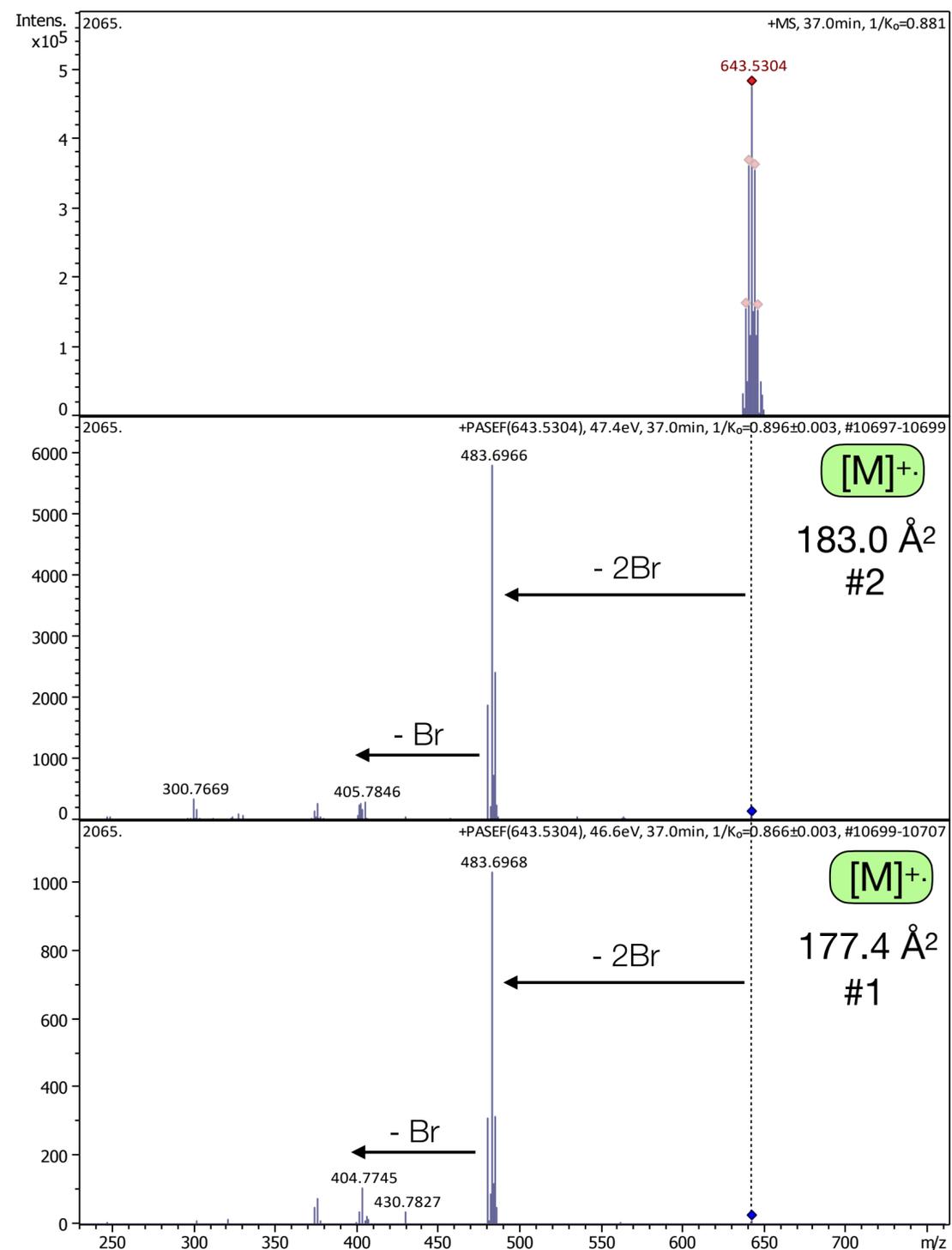


IM filtered chromatogram



\Rightarrow 2 isomers??

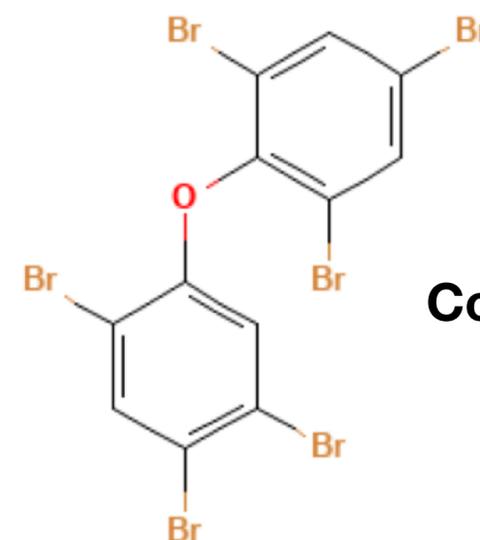
Tandem mass spectra



⇒ Both tentative isomers were isolated and fragmented separately thanks to the PASEF mode

Tentative candidate(s)

PubChem



Confidence level

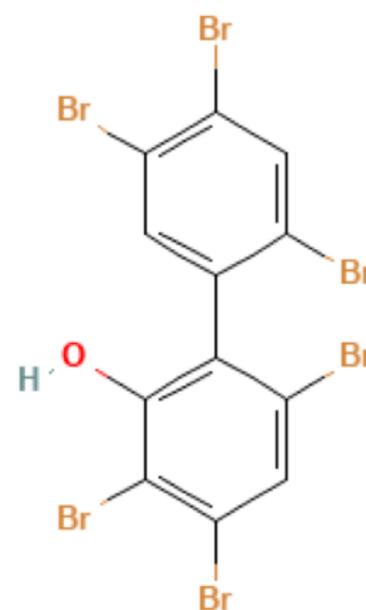
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HxBDE (42 isomers)

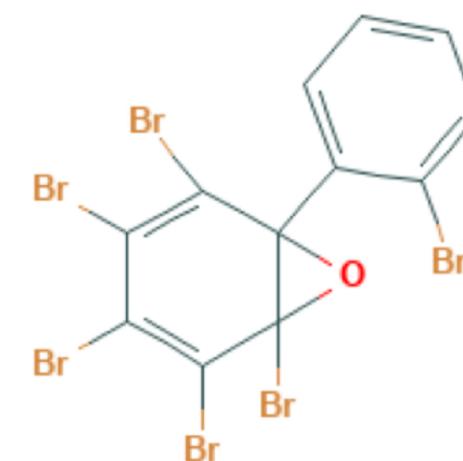
⇒ HxBDE 154 (#2)?

(database CCS = 182.8 Å²)

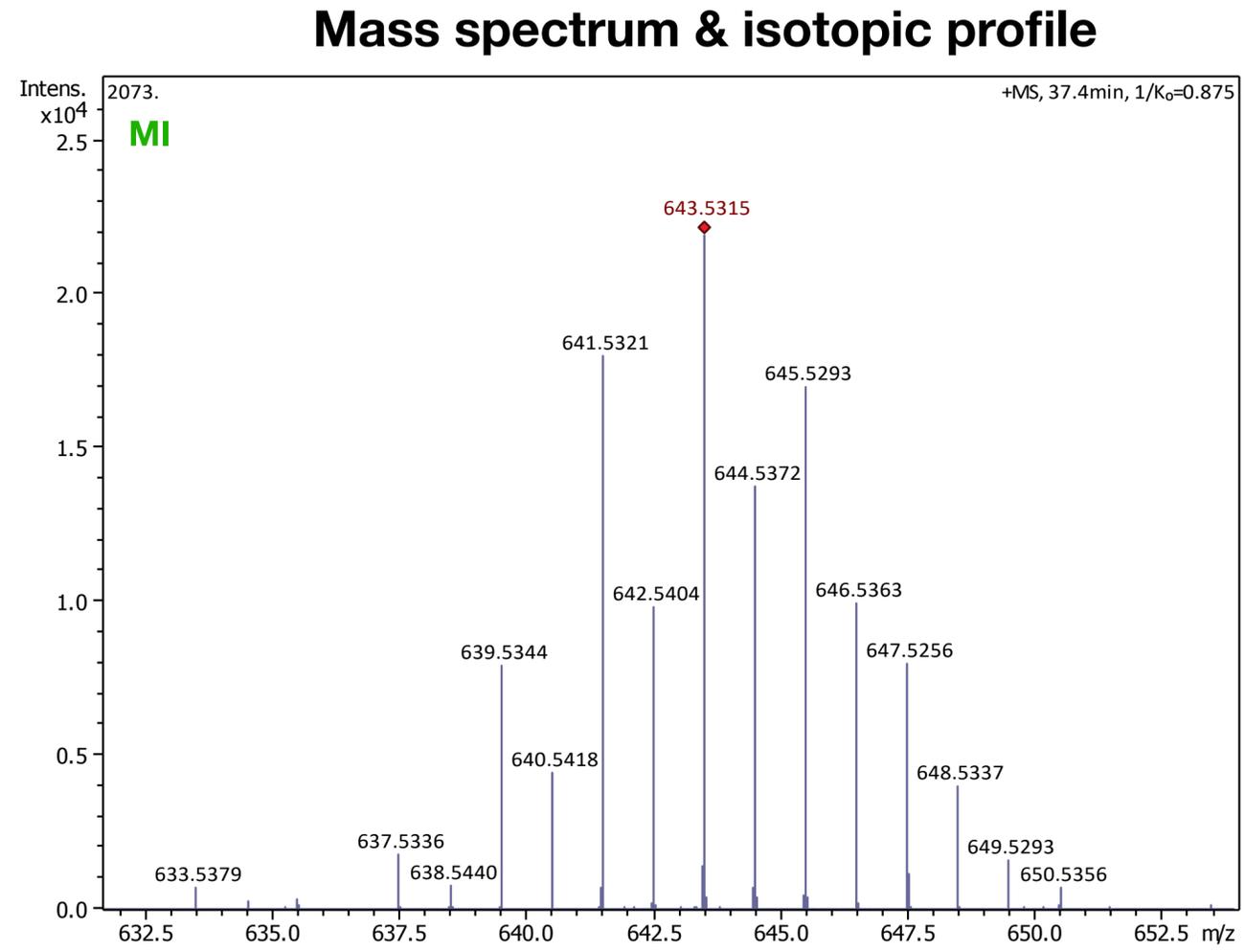
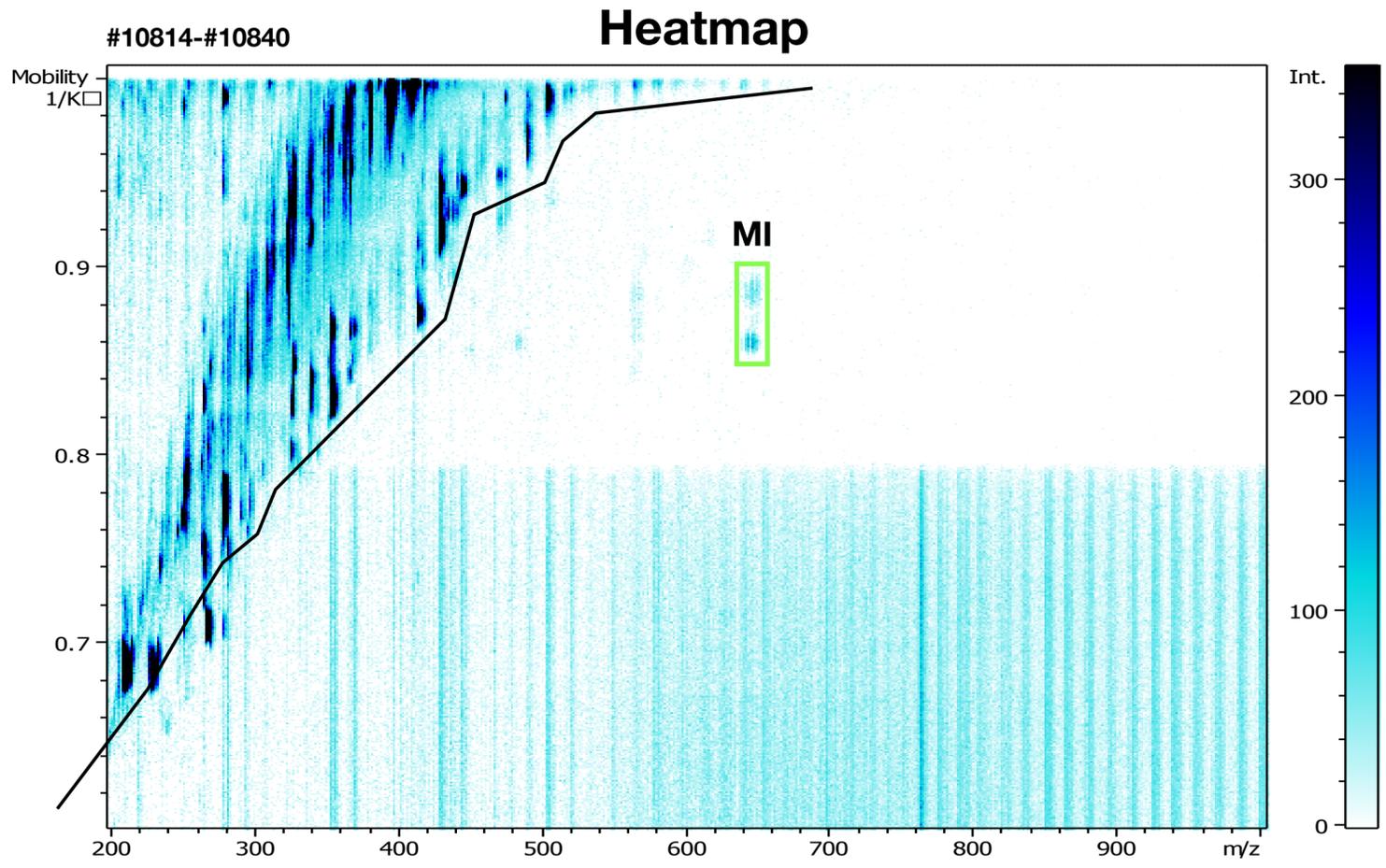
CCS pred HxBDE isomers: see Figure S6.7A (manuscript)

Hexabromobiphenylol
(Multiple isomers)

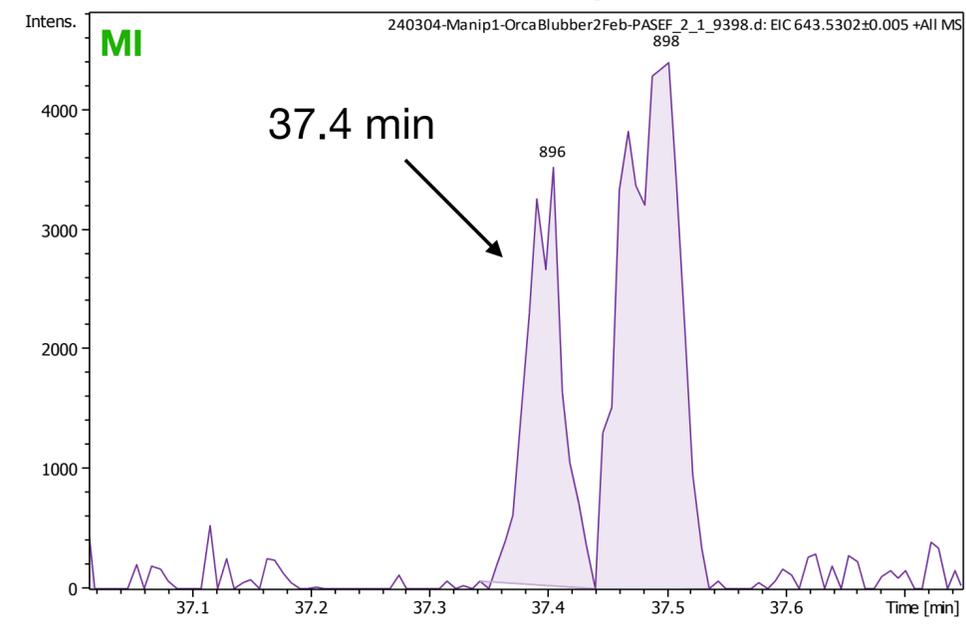
⇒ Not GC amenable

Polybromophenyl-oxabicycloheptadiene
(Multiple isomers)CCS pred: 179.2 Å² (+1.0%)CCS pred: 179.2 Å² (-2.1%)

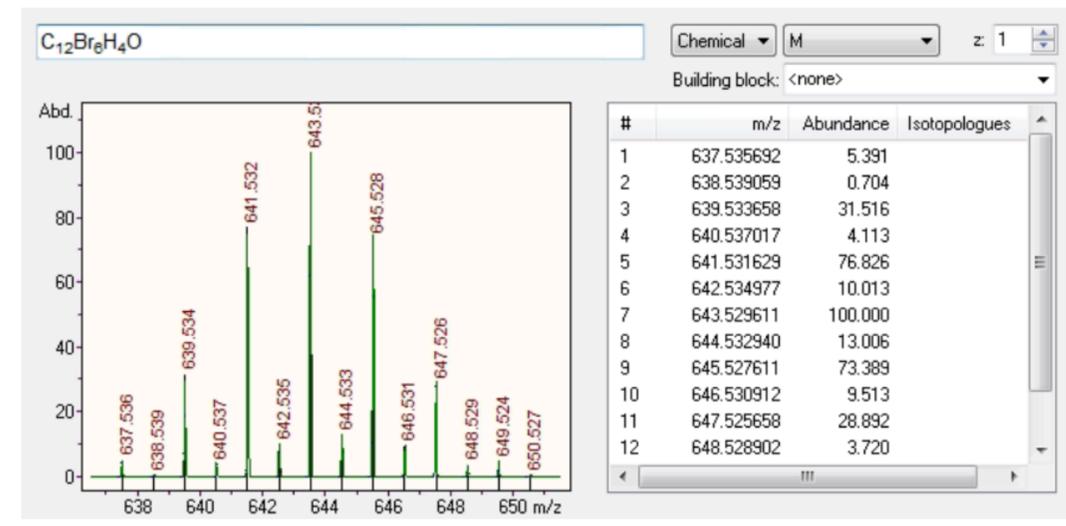
-  EIC 643.5302
-  EIC 563.6212
-  EIC 328.7613



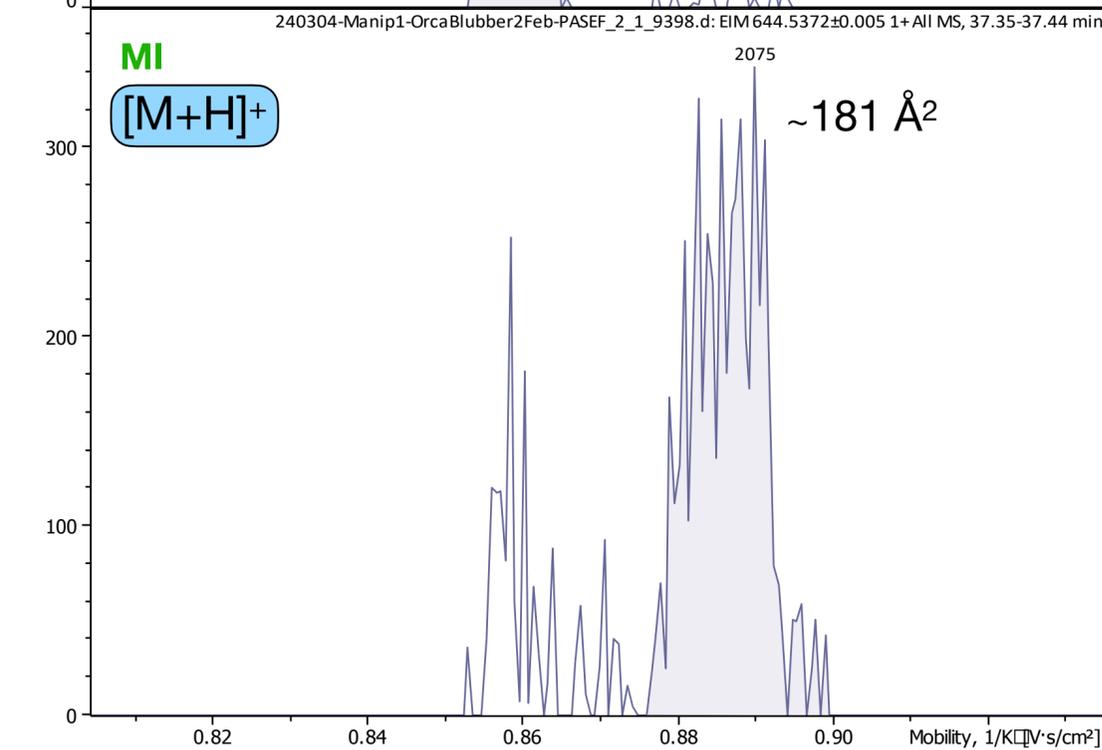
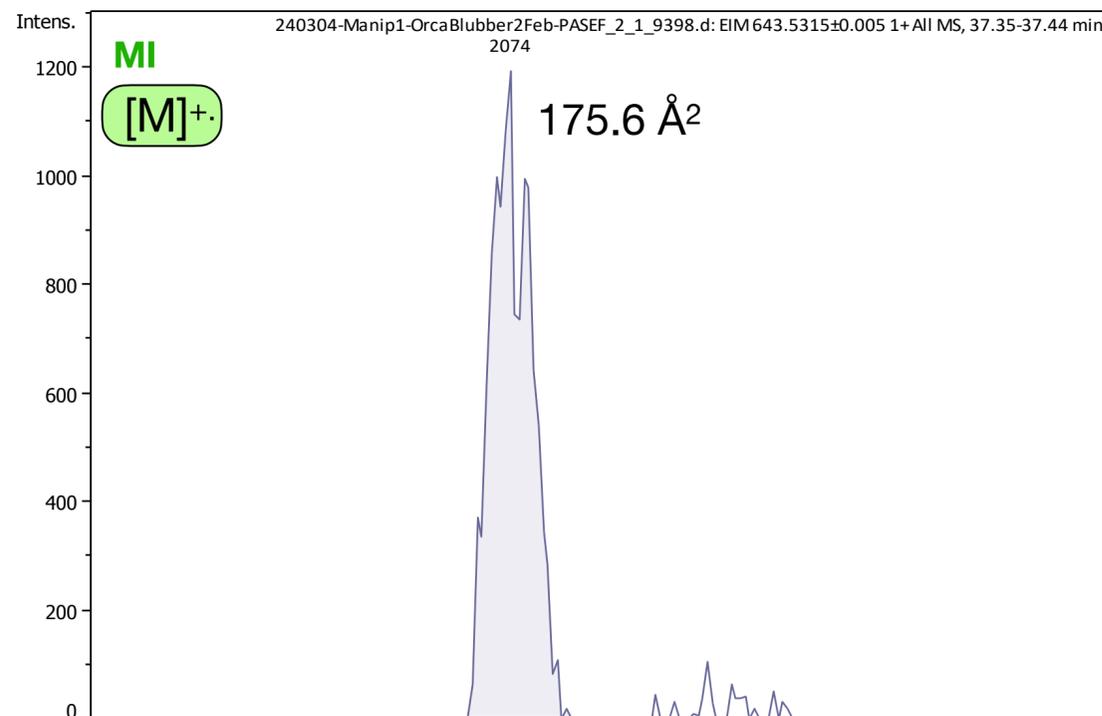
Chromatogram



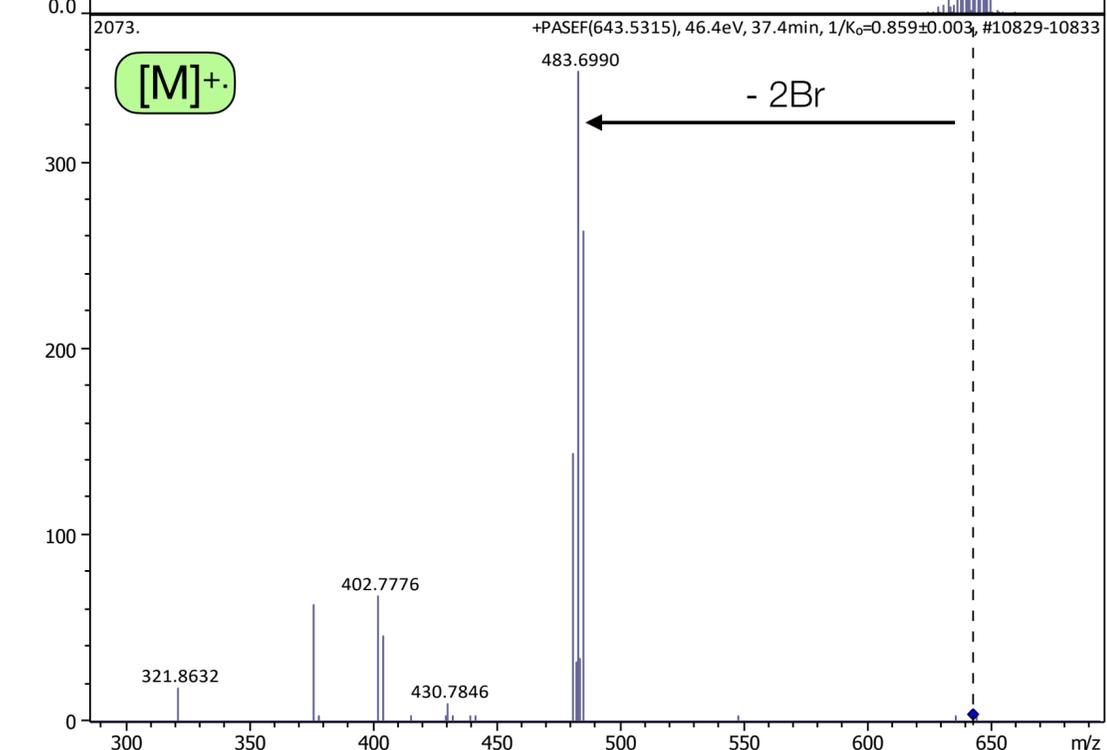
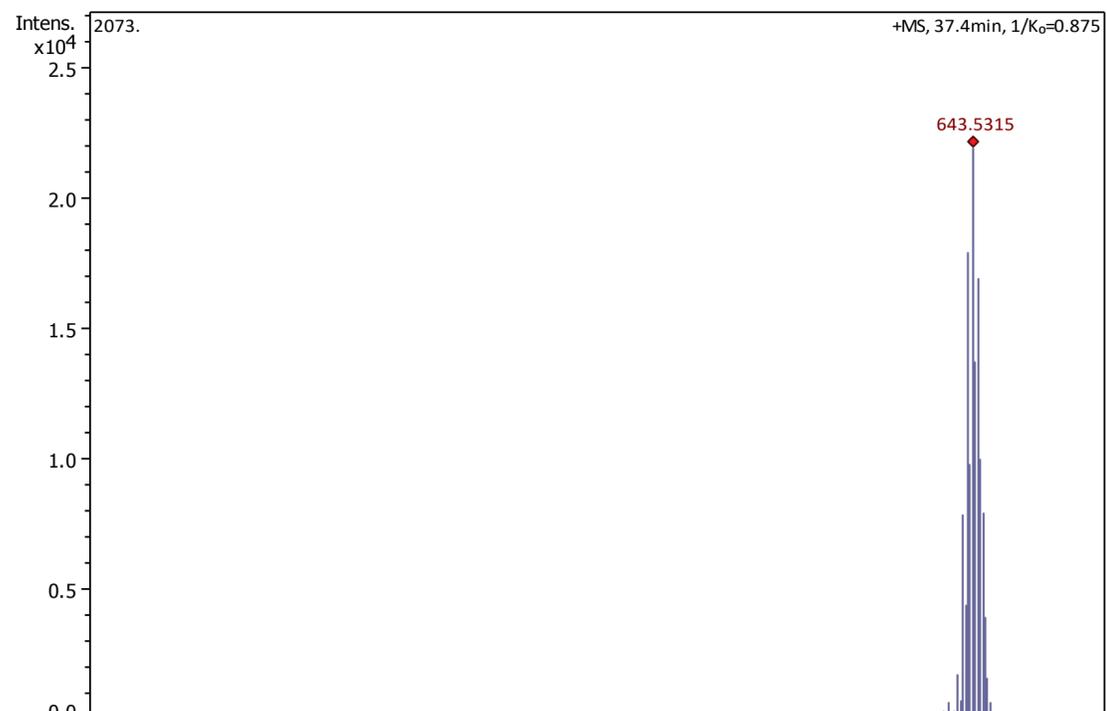
C₁₂Br₆H₄O



Ion mobility spectra

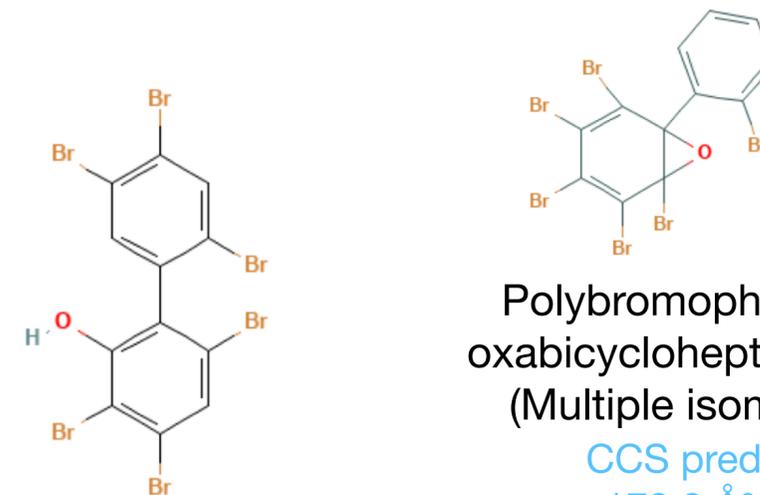


Tandem mass spectrum



Tentative candidate(s)

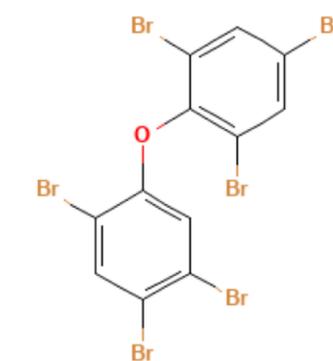
PubChem



CCS pred:
179.2 Å²
(+2.1%)

Hexabromobiphenylol
(Multiple isomers)

⇒ Not GC amenable

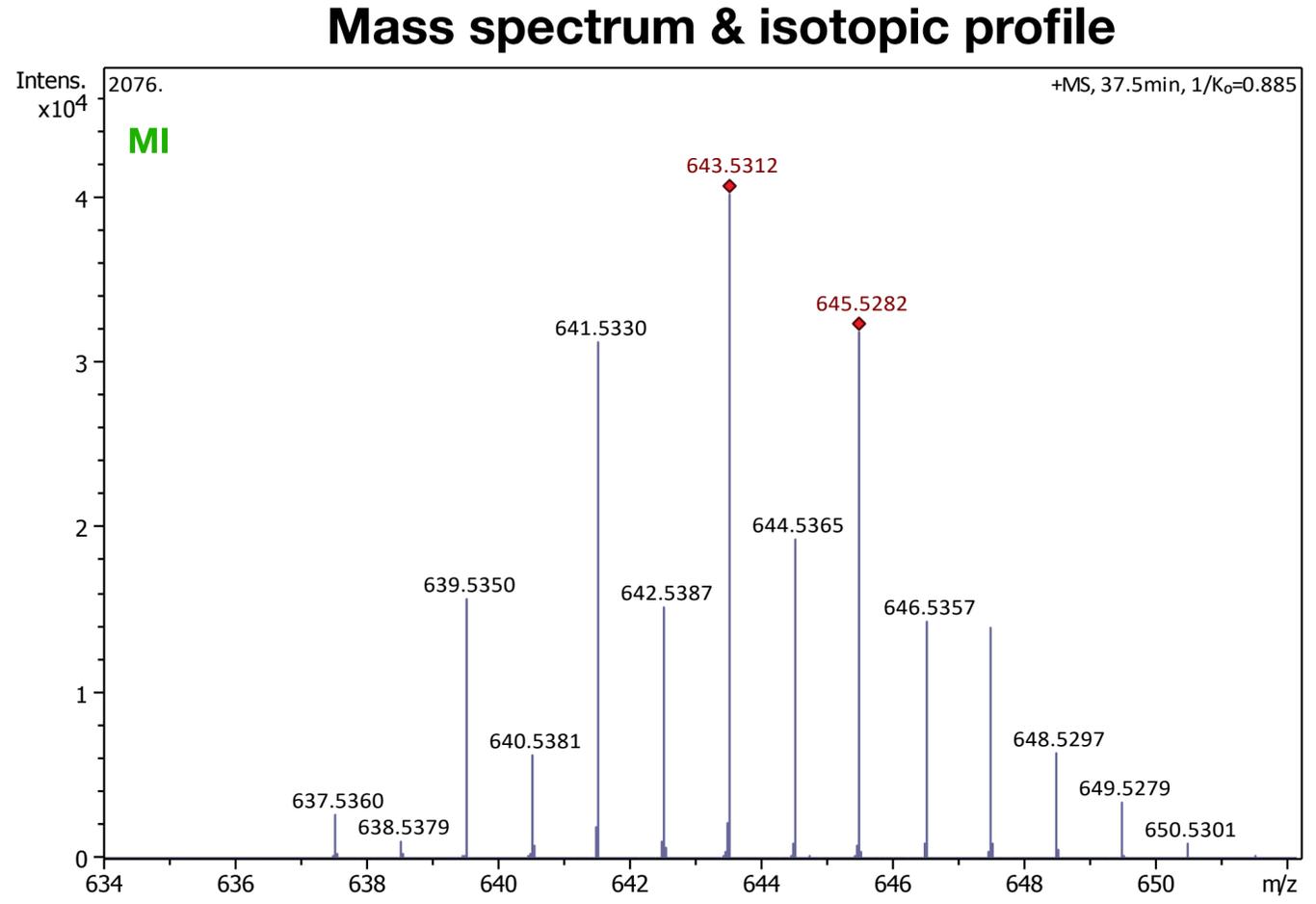
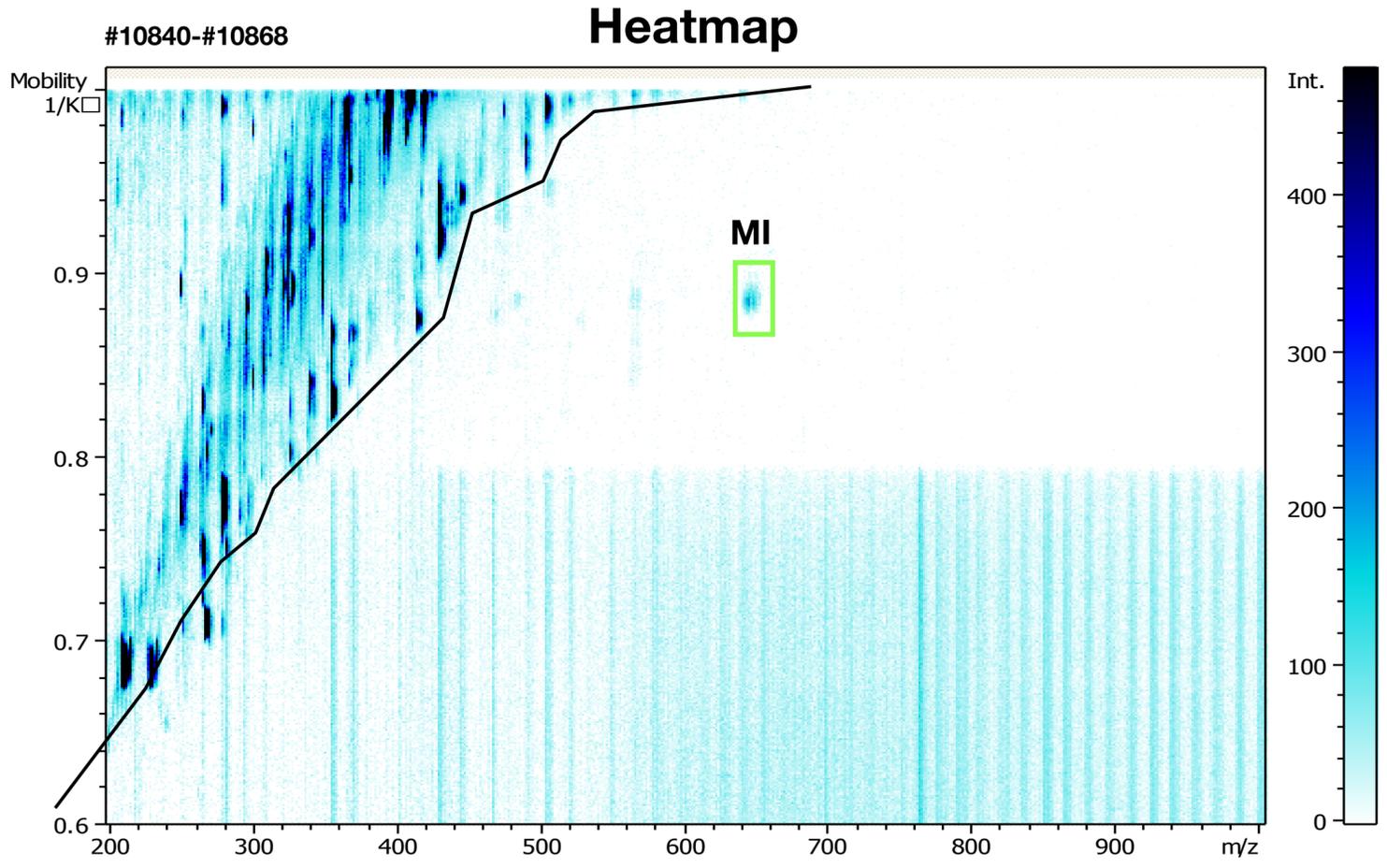


Confidence level

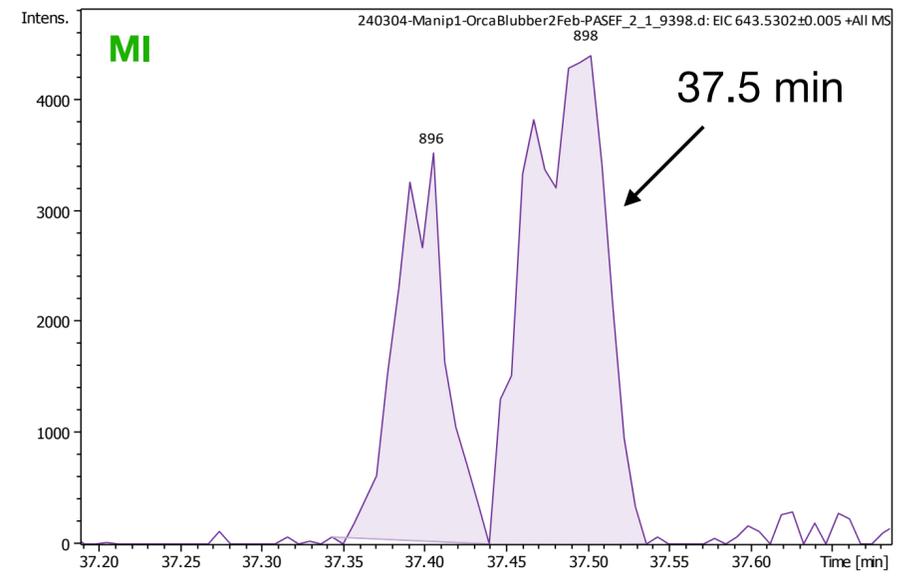
3

⇒ Well-known POP class

CCS pred HxBDE isomers: see
Figure S6.7A (manuscript)



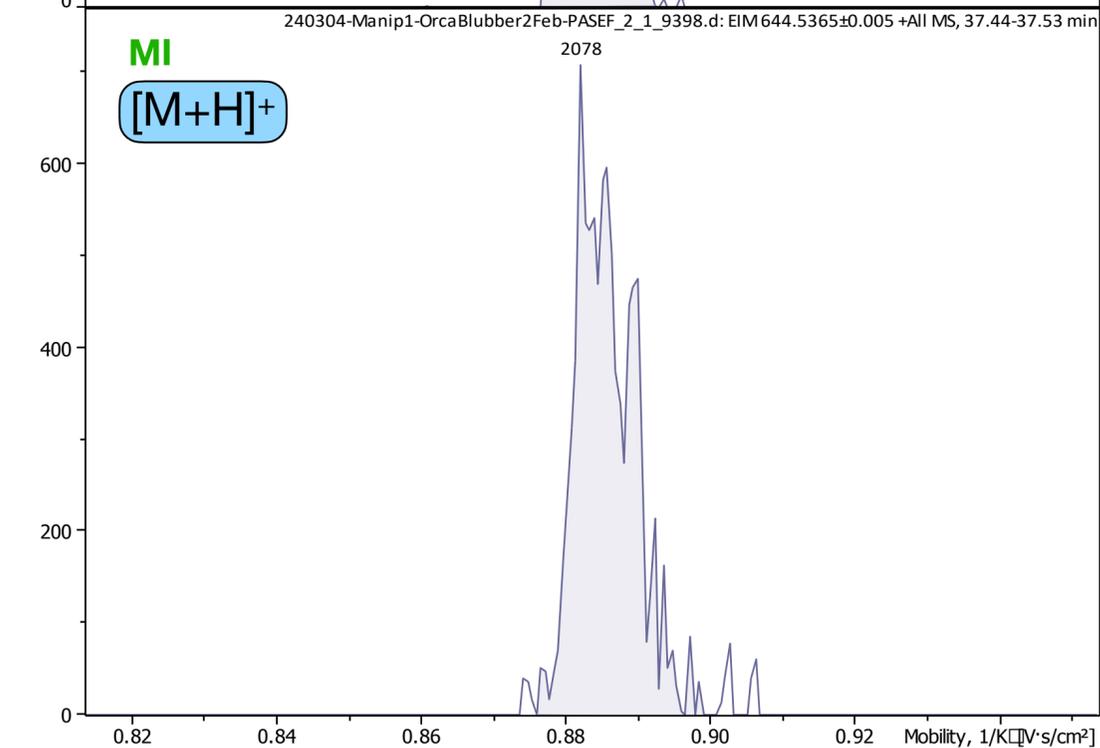
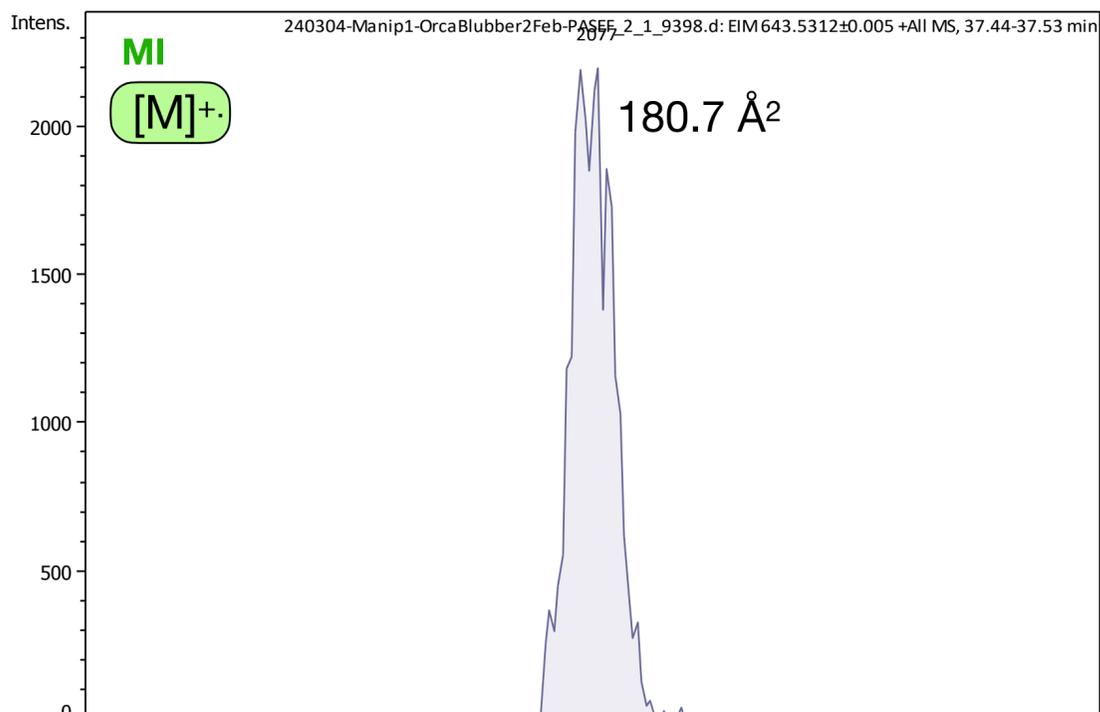
Chromatogram



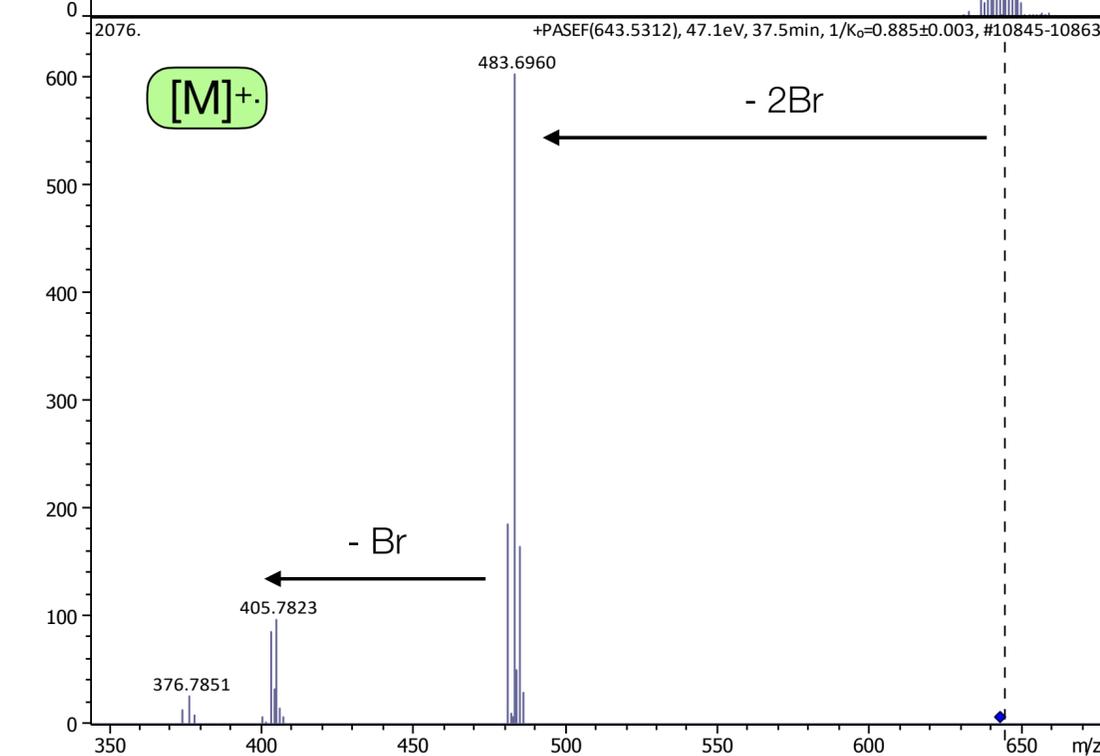
C12Br6H4O Chemical M z 1 Building block: <none>

#	m/z	Abundance	Isotopologues
1	637.535692	5.391	
2	638.539059	0.704	
3	639.533658	31.516	
4	640.537017	4.113	
5	641.531629	76.826	
6	642.534977	10.013	
7	643.529611	100.000	
8	644.532940	13.006	
9	645.527611	73.389	
10	646.530912	9.513	
11	647.525658	28.892	
12	648.528902	3.720	

Ion mobility spectra

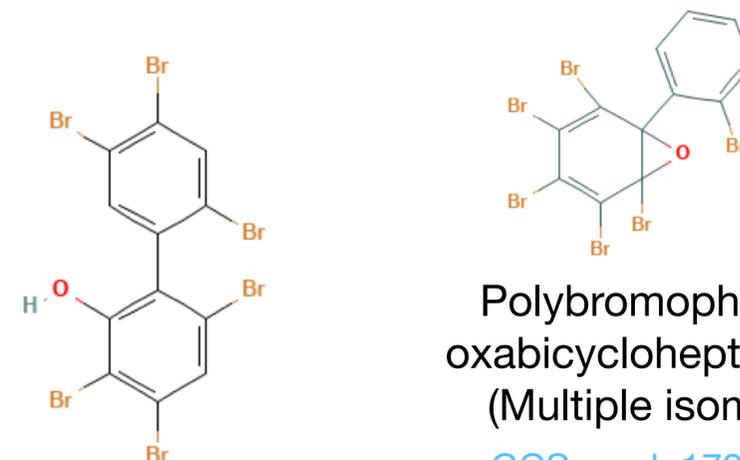


Tandem mass spectrum



Tentative candidate(s)

PubChem



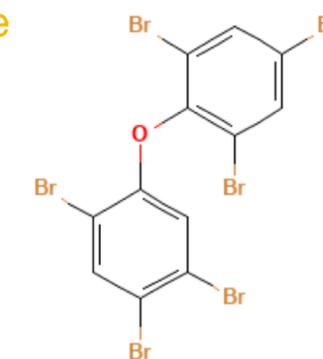
CCS pred: 179.2 Å²
(-0.8%)

Hexabromobiphenylol
(Multiple isomers)

⇒ Not GC amenable

Confidence level

3

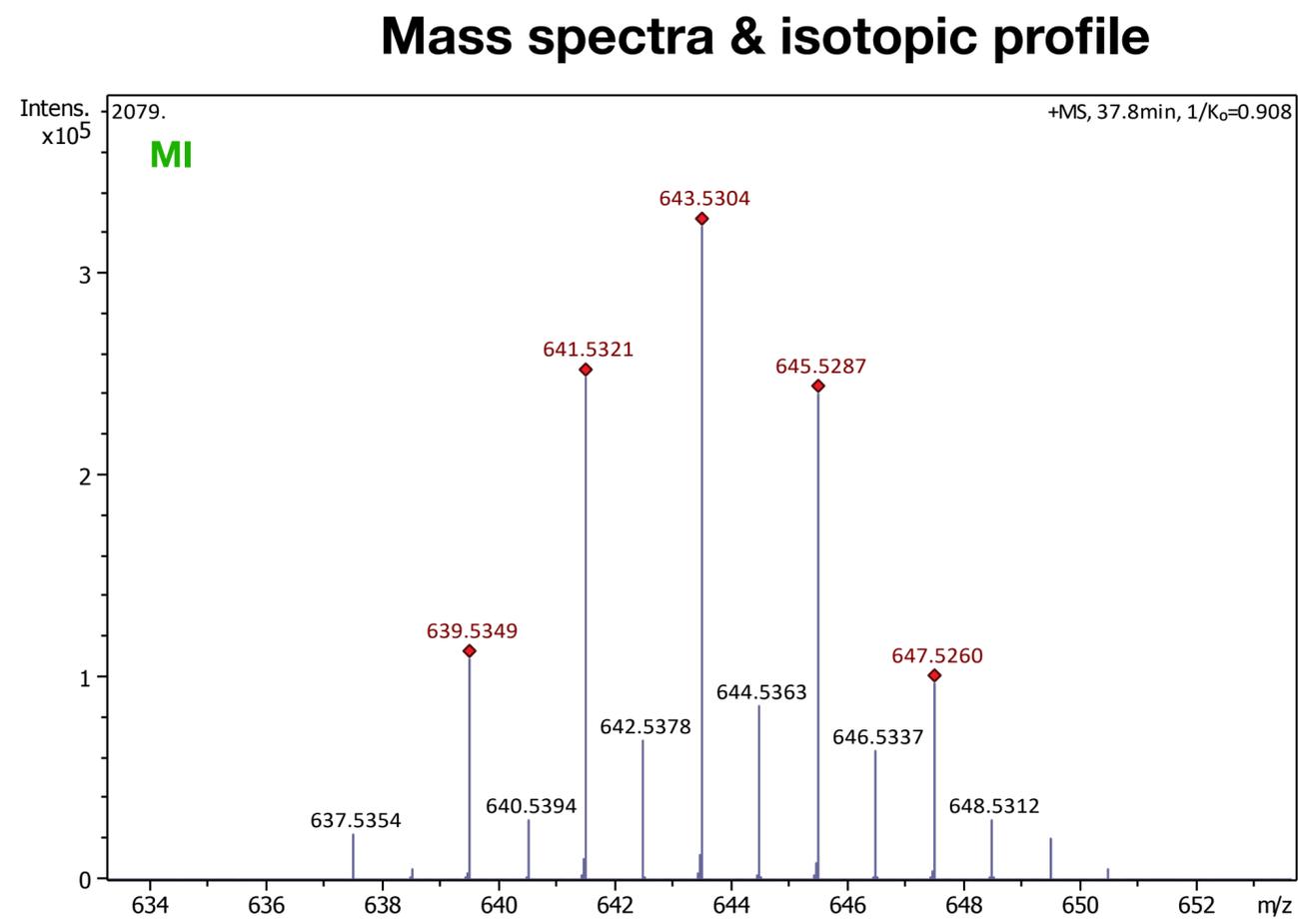
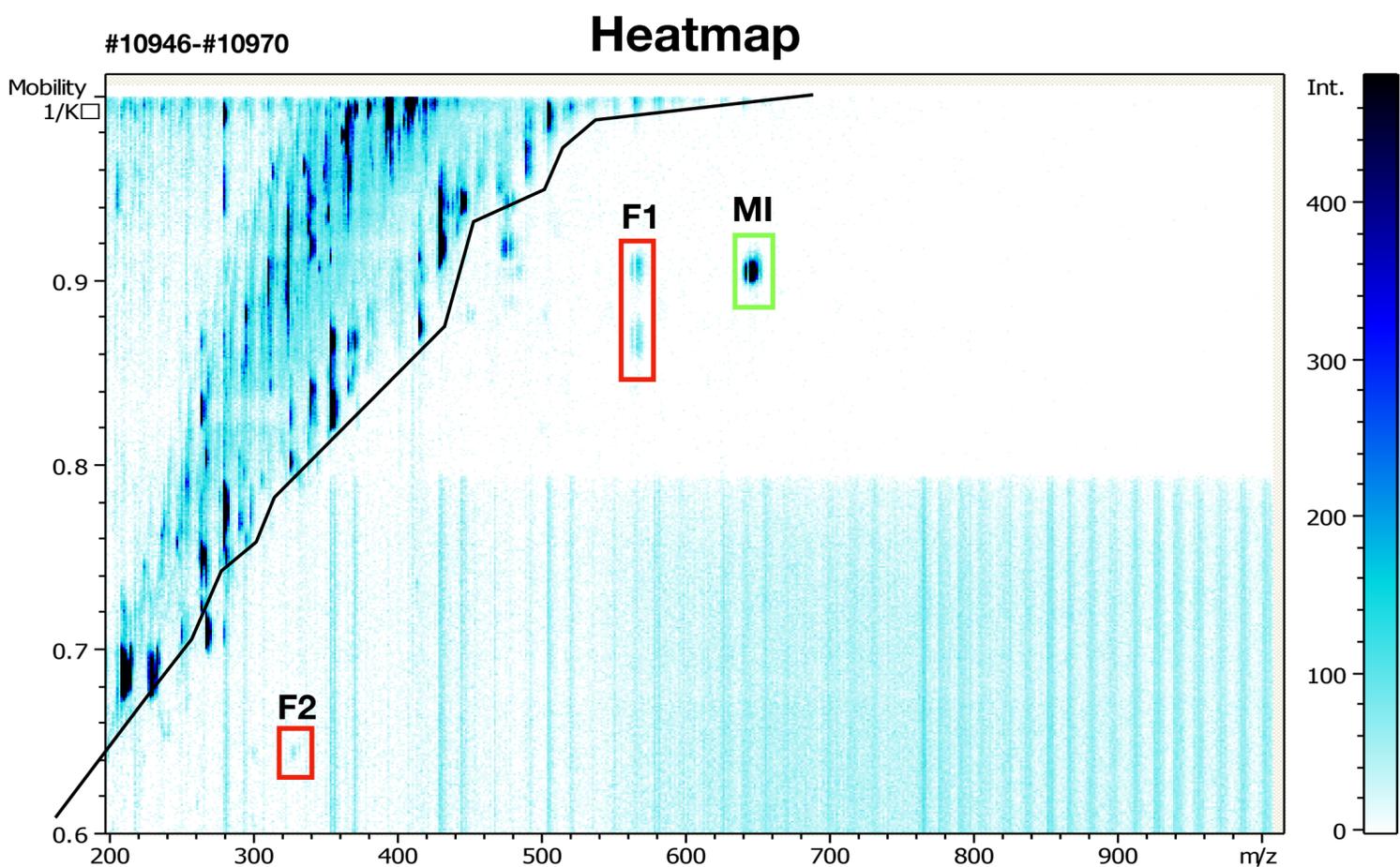


⇒ Well-known POP class

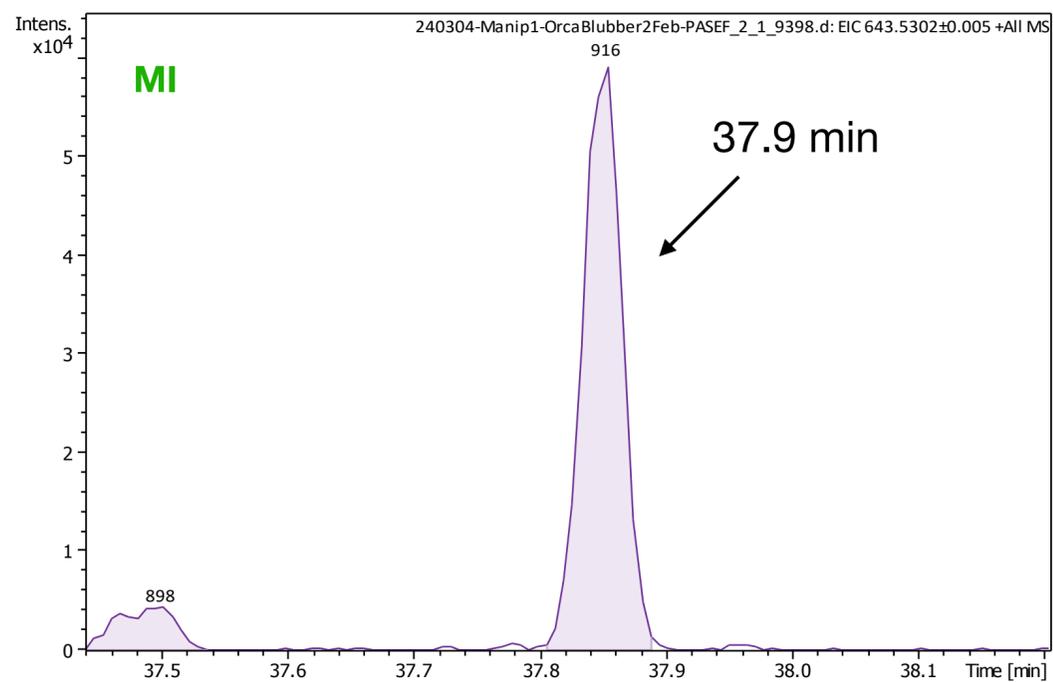
CCS pred HxBDE isomers: see
Figure S6.7A (manuscript)

Feature #16

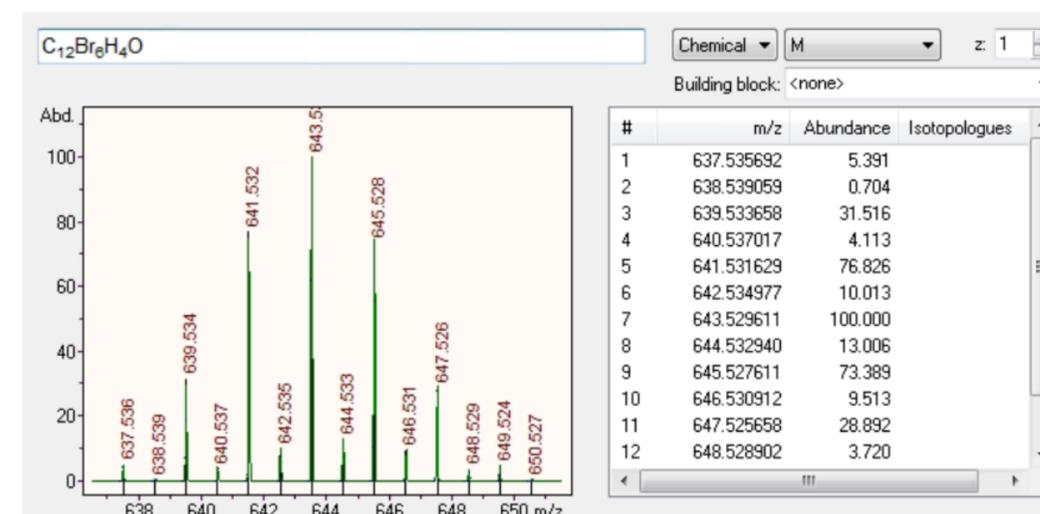
EIC 643.5302
EIC 563.6212
EIC 328.7613

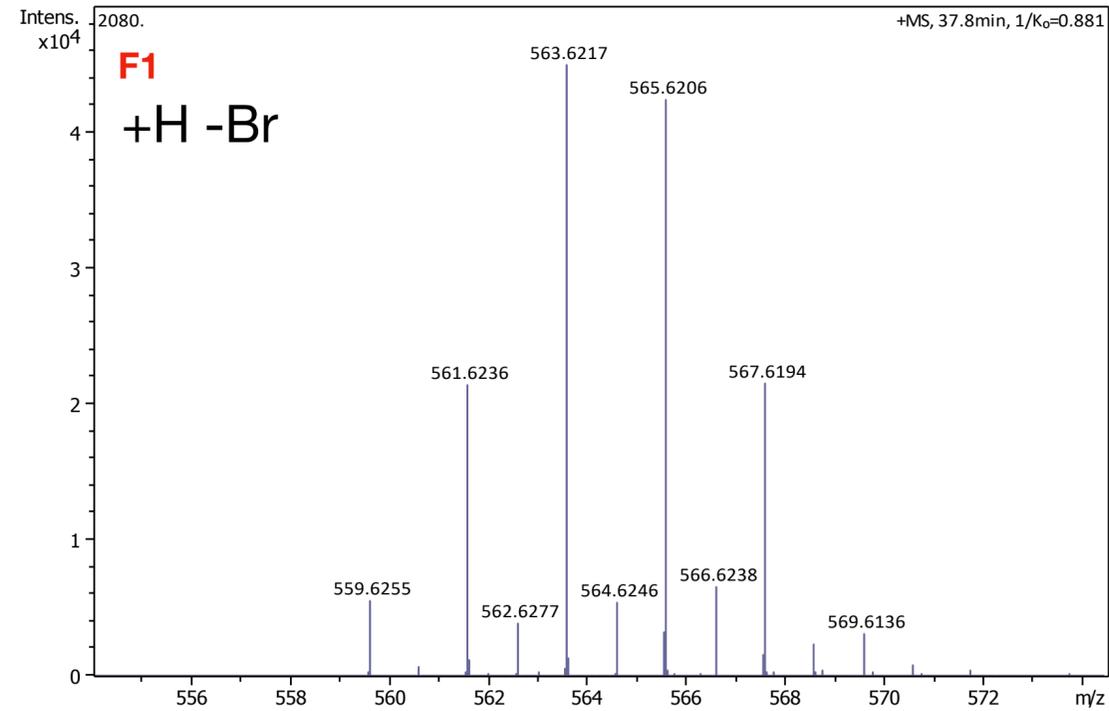


Chromatogram

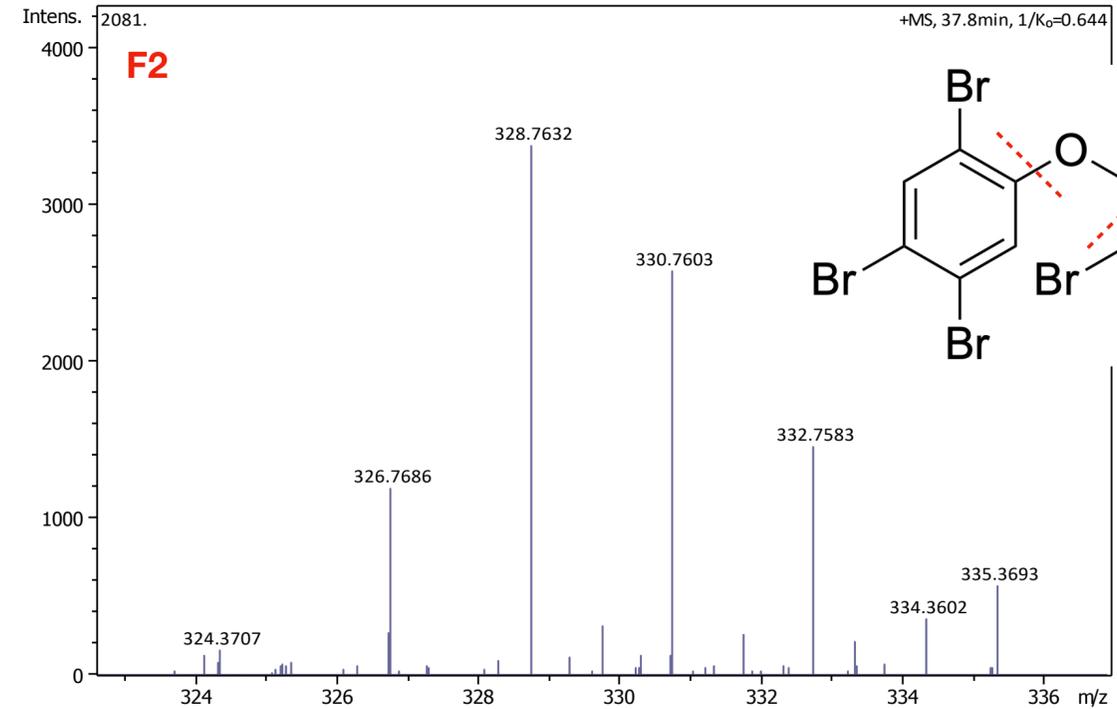


C₁₂Br₆H₄O

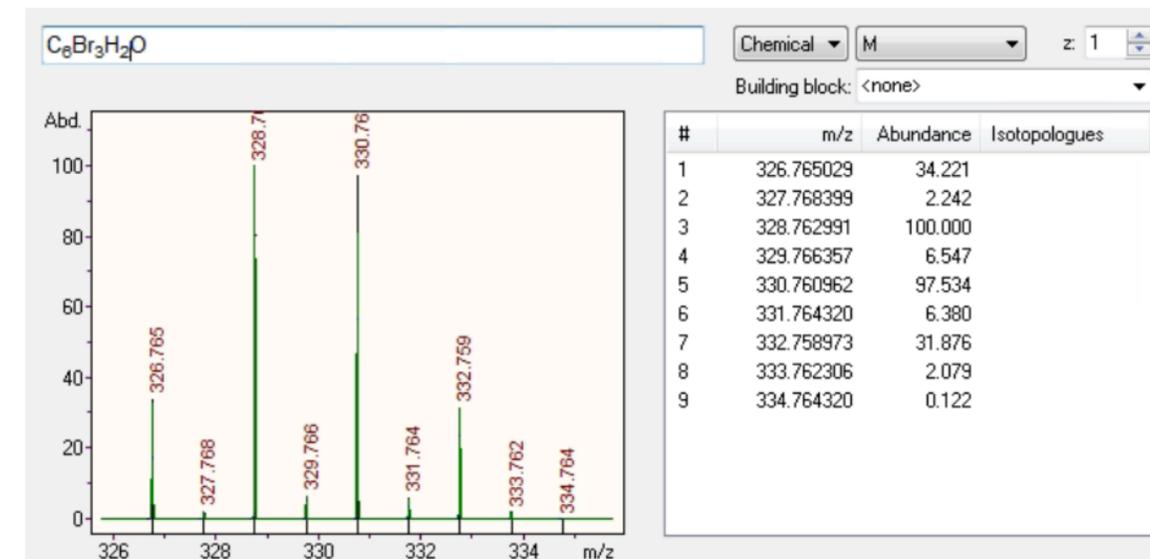
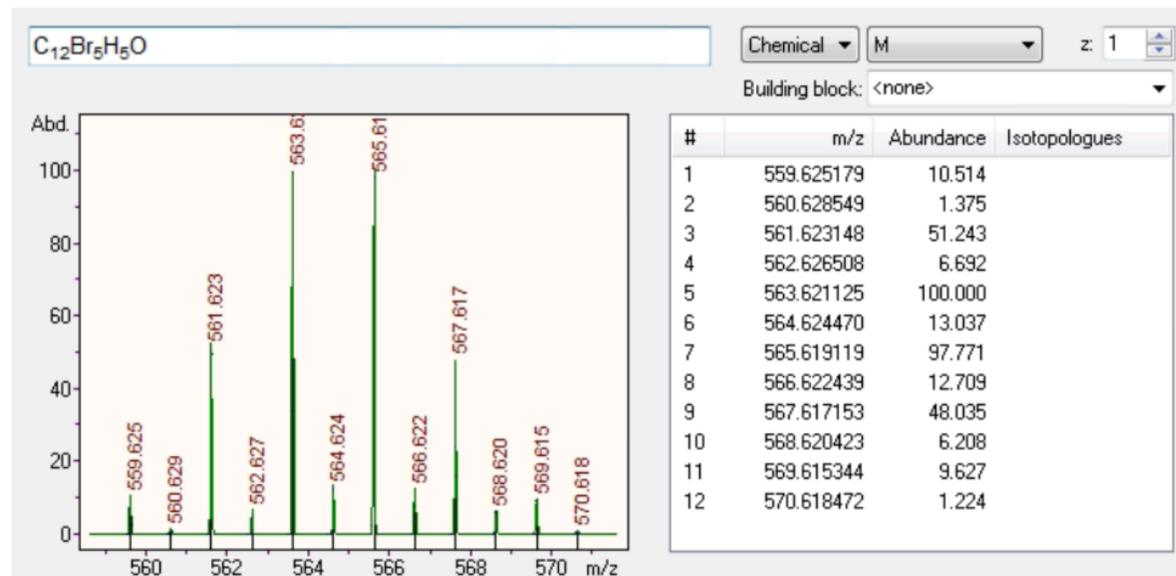




$C_{12}Br_5H_5O$



$C_6Br_3H_2O$

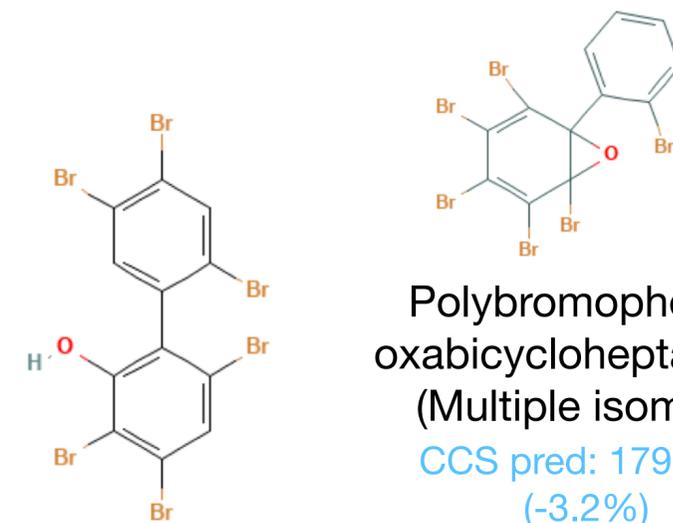


Ion mobility spectra

Tandem mass spectrum

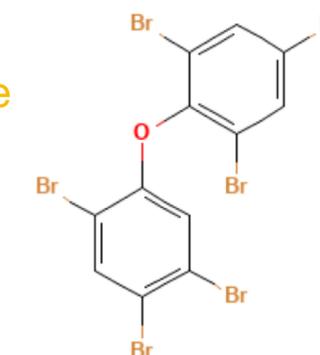
Tentative candidate(s)

PubChem



Hexabromobiphenylol (Multiple isomers)

⇒ Not GC amenable



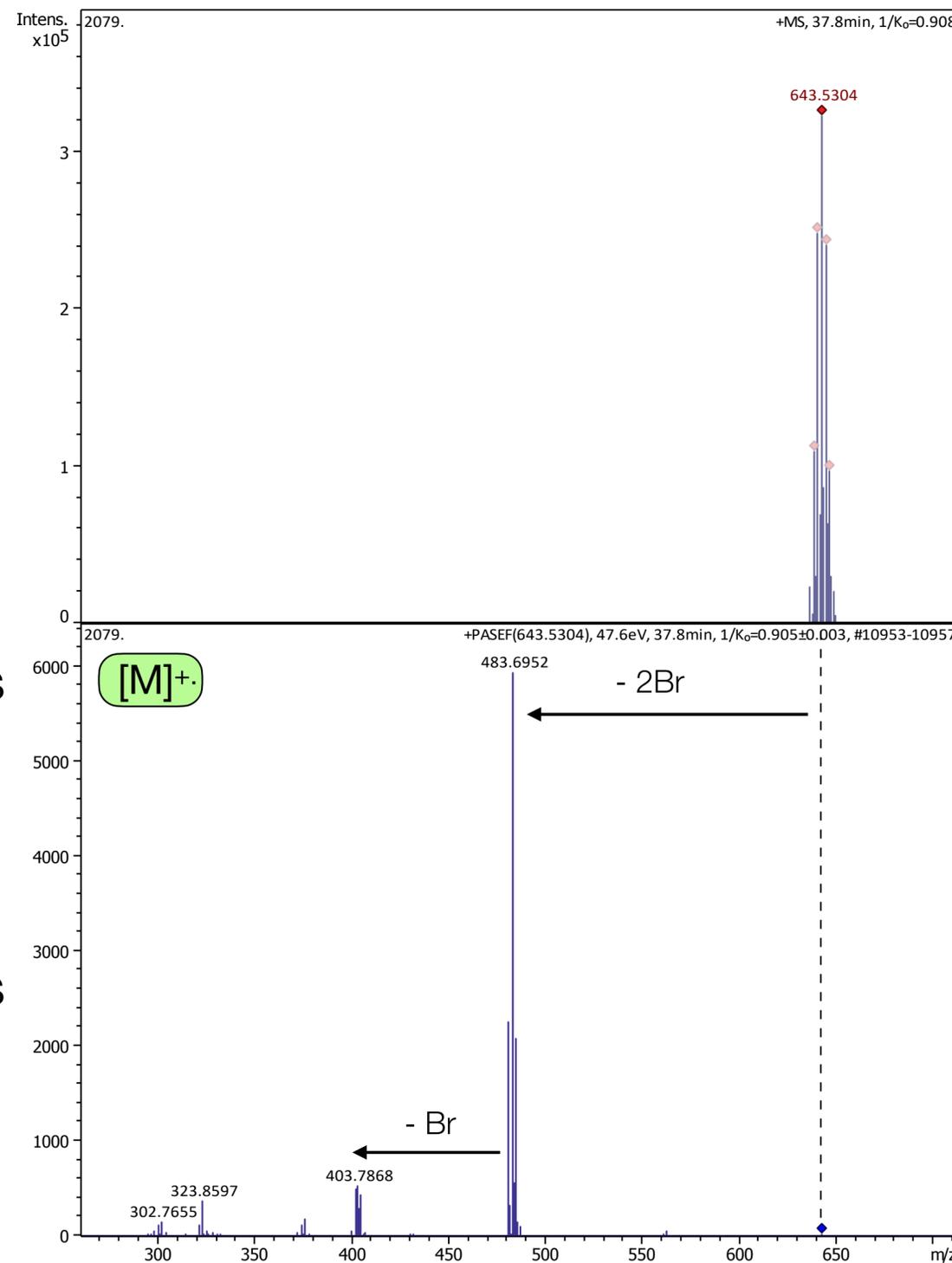
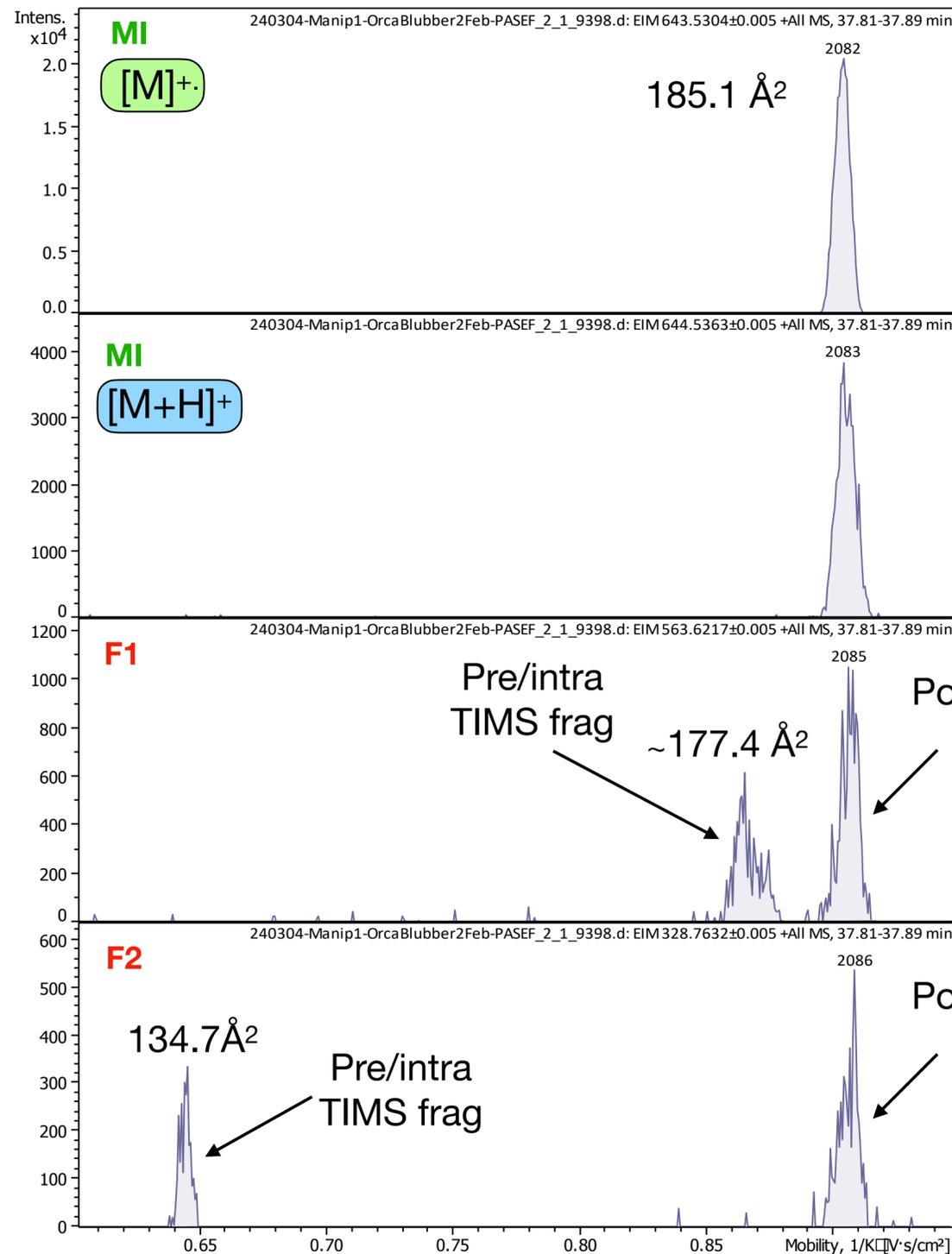
Confidence level

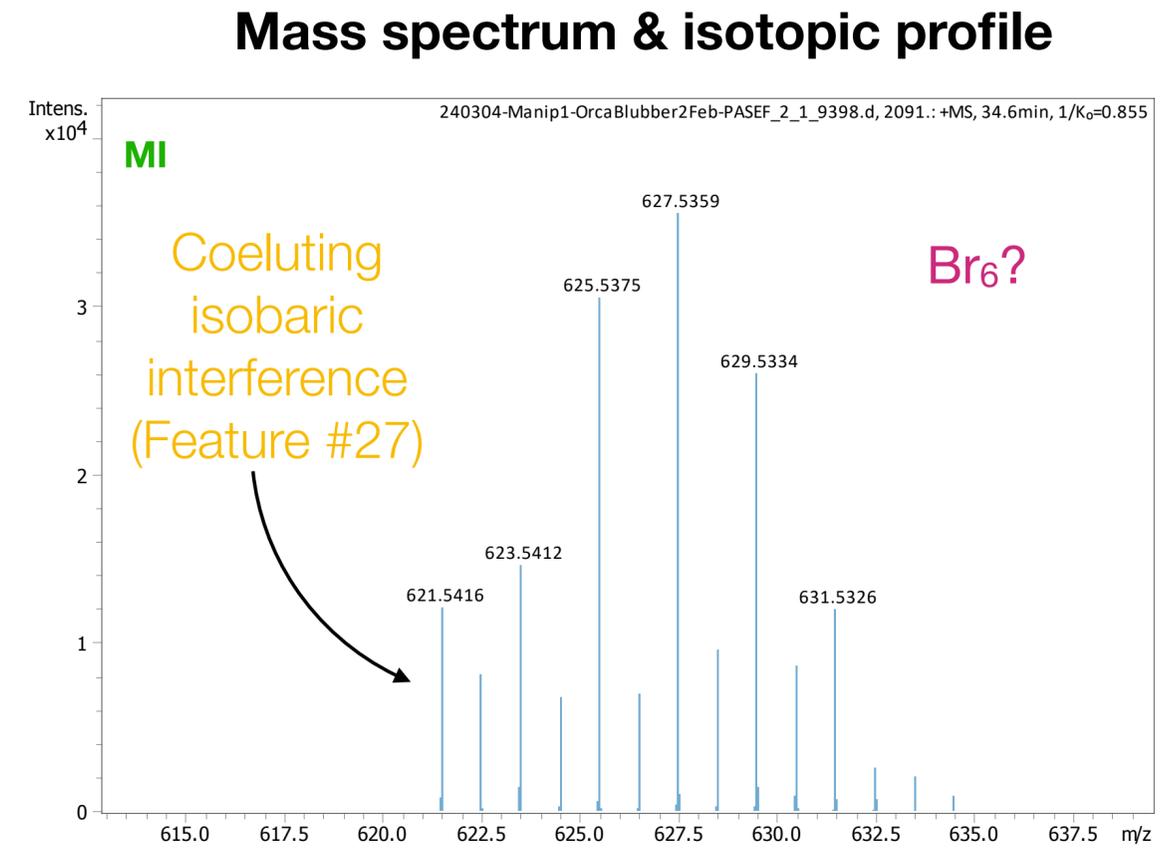
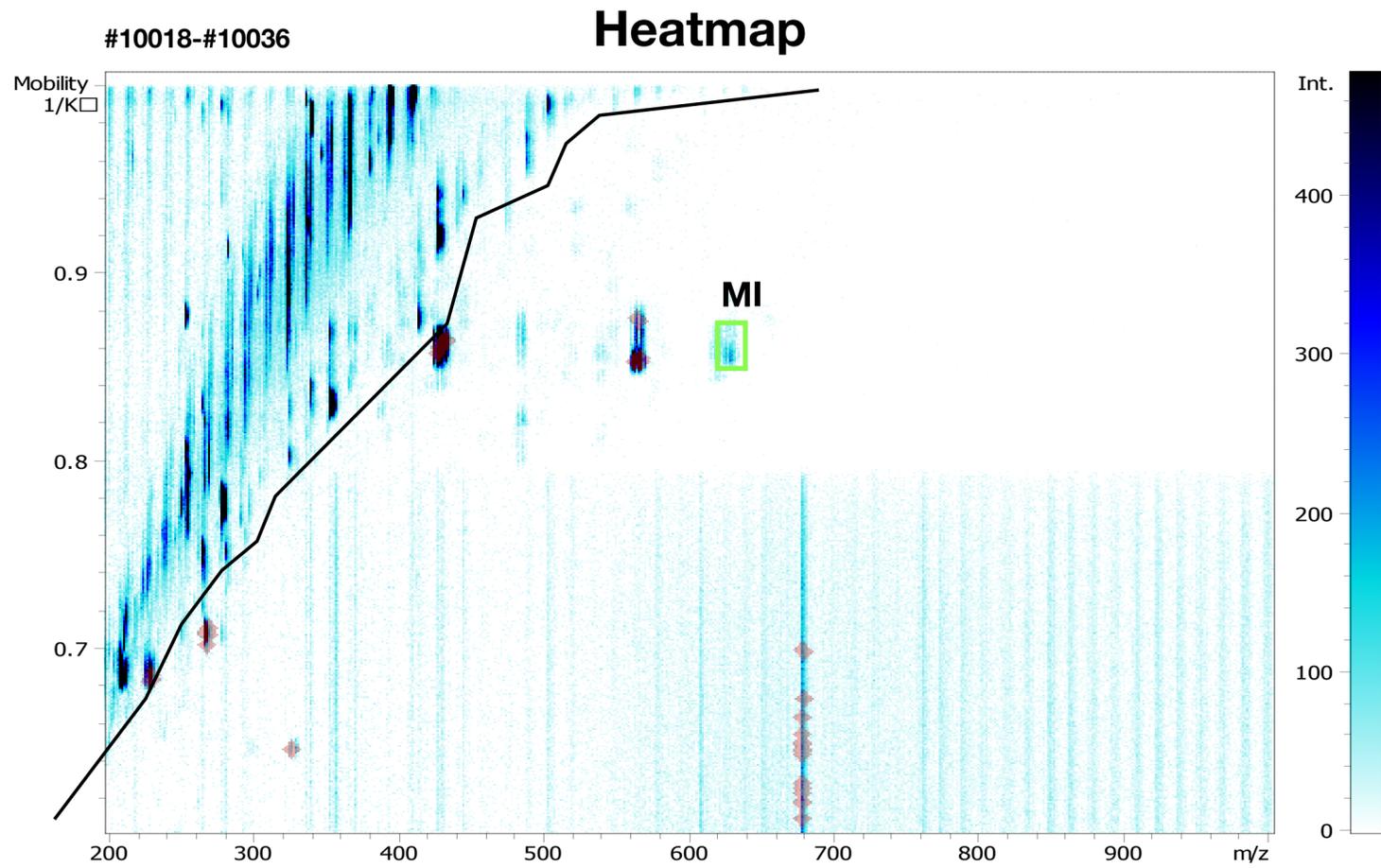
3

HxBDE (42 isomers)

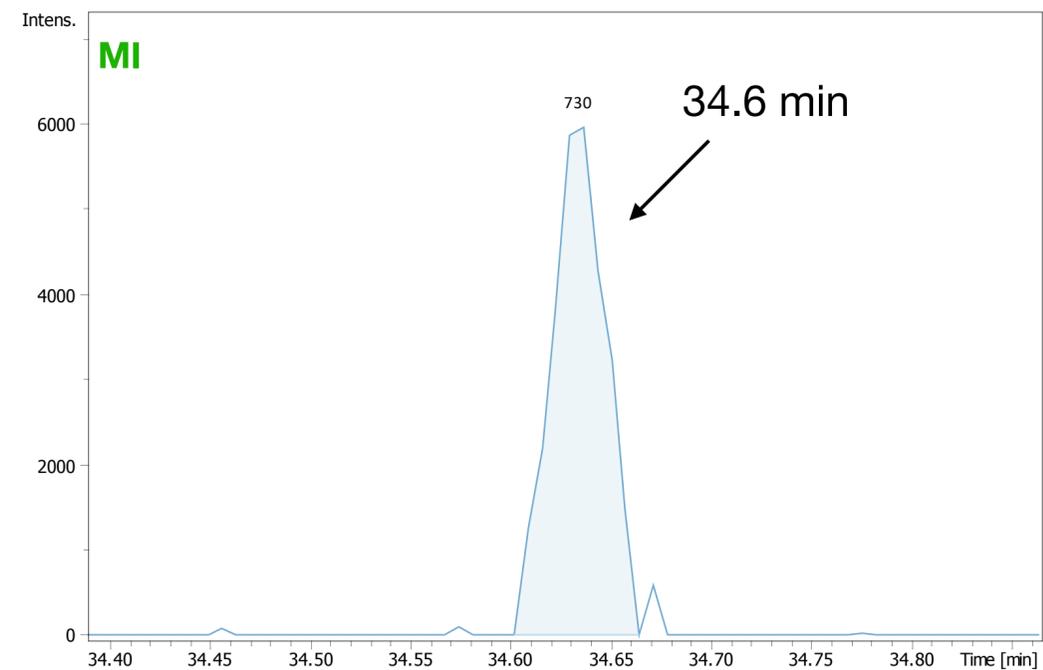
⇒ Well-known POP class

CCS pred HxBDE isomers: see Figure S6.7A (manuscript)

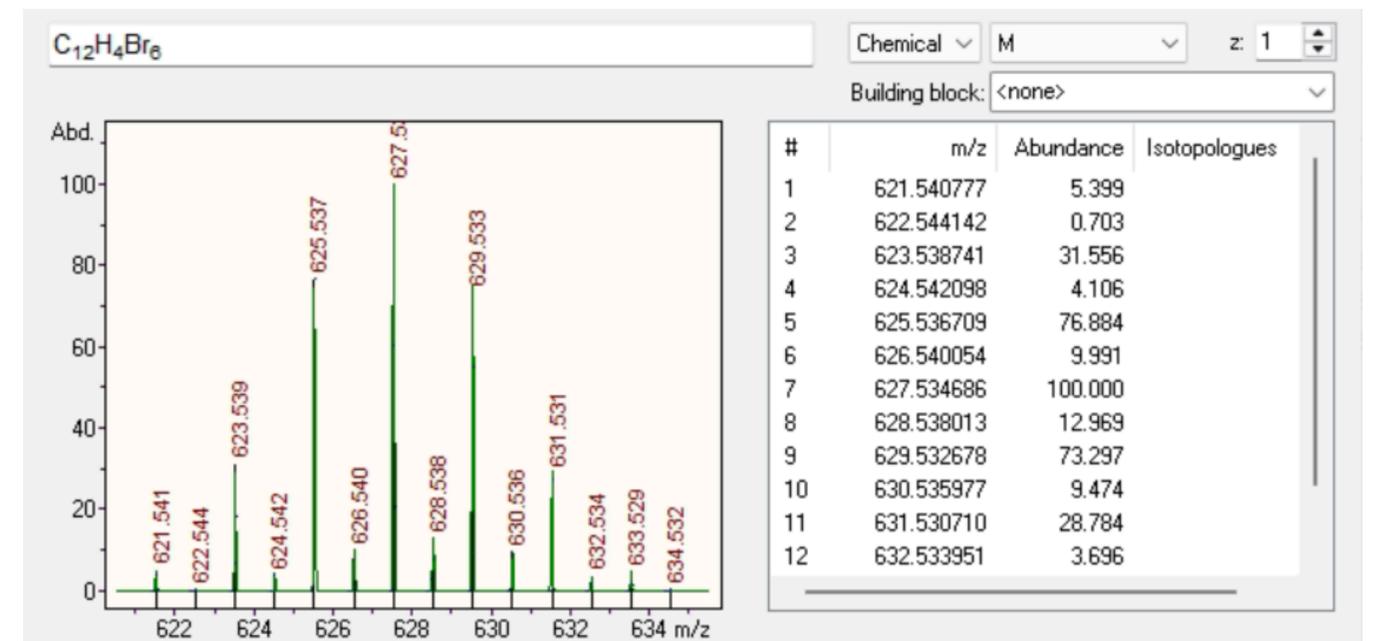




Chromatogram



C₁₂Br₆H₄



Tandem mass spectrum

/

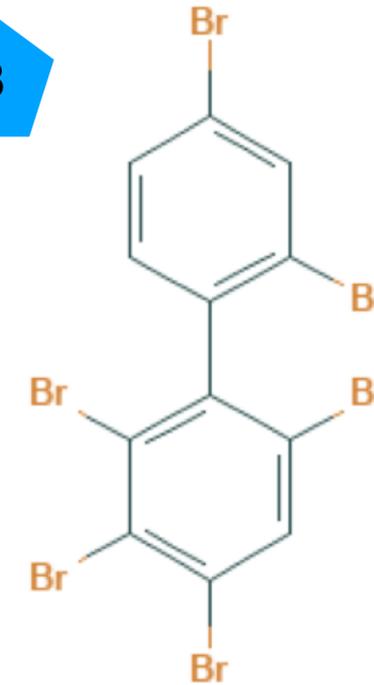
Tentative candidate(s)

PubChem

C₁₂Br₆H₄

Confidence level

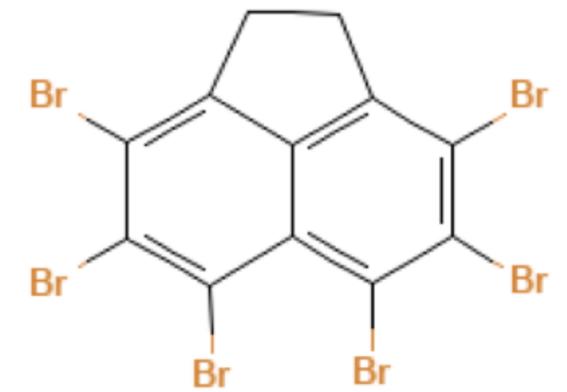
3



HxBBs (42 isomers)

⇒ Well known POP class

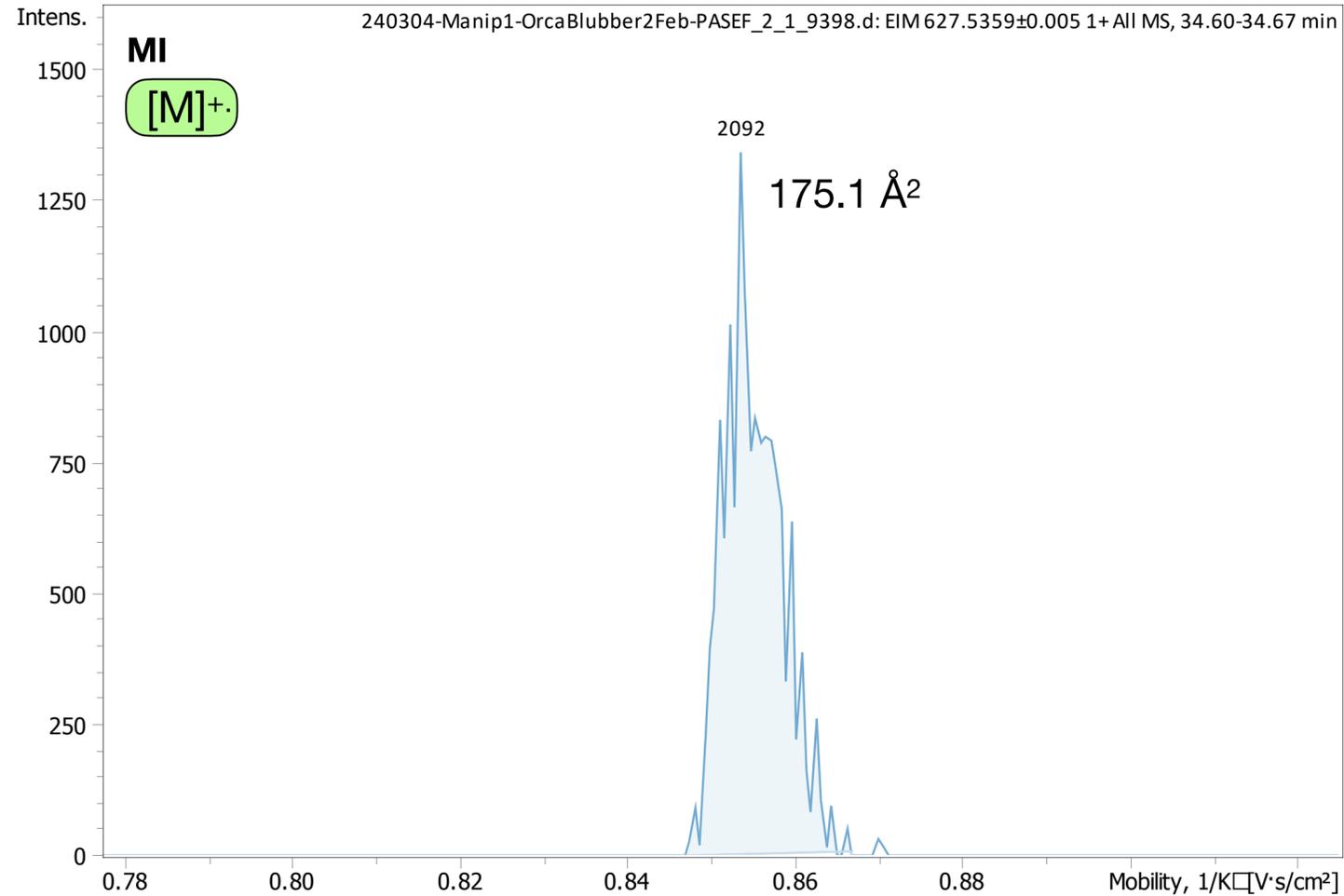
CCS pred HxBB
isomers: see Figure
S6.7B (manuscript)



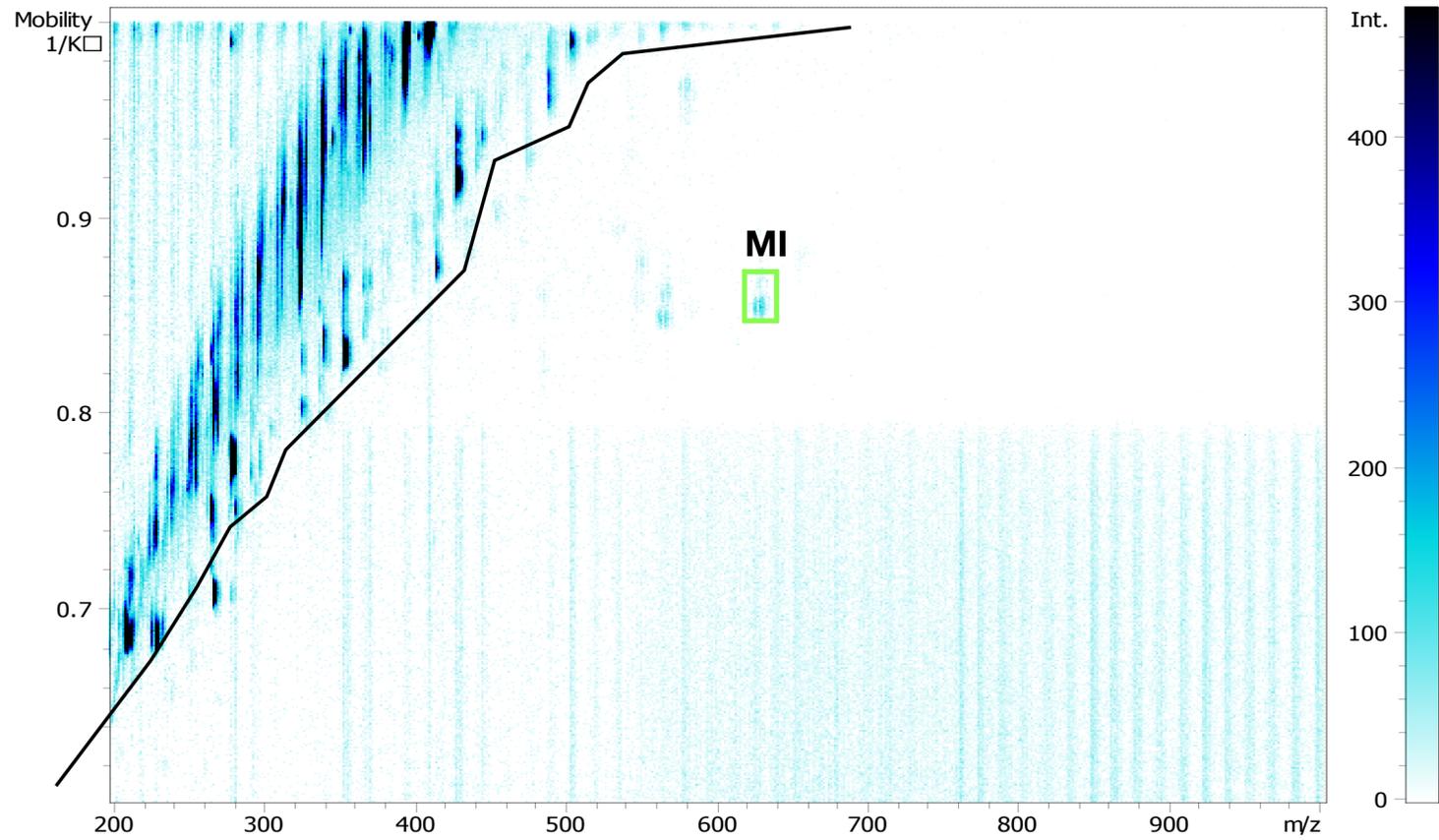
Hexabromoacenaphthene

CCS pred: 173.7 Å² (-0.8%)

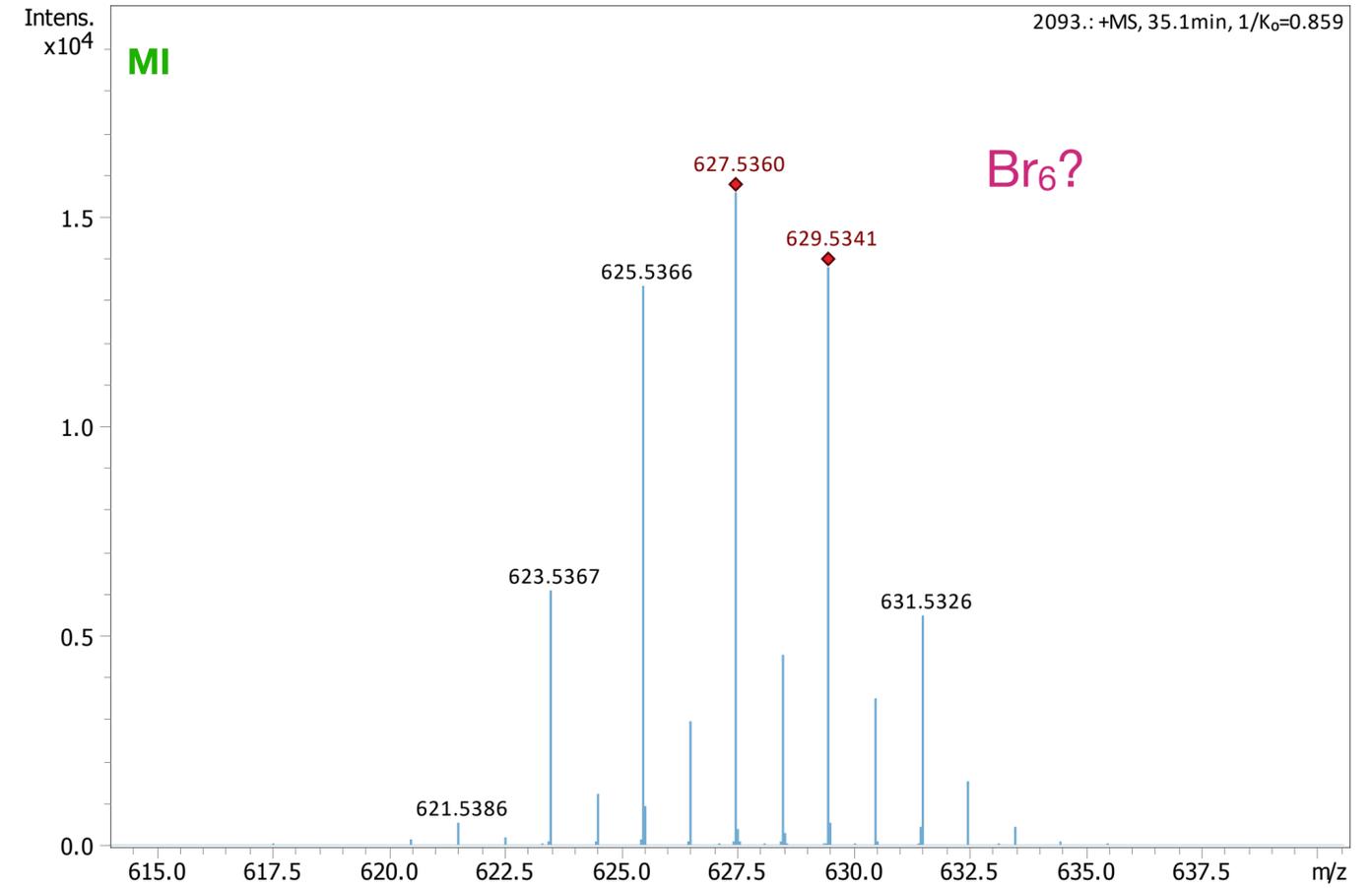
Ion mobility spectrum



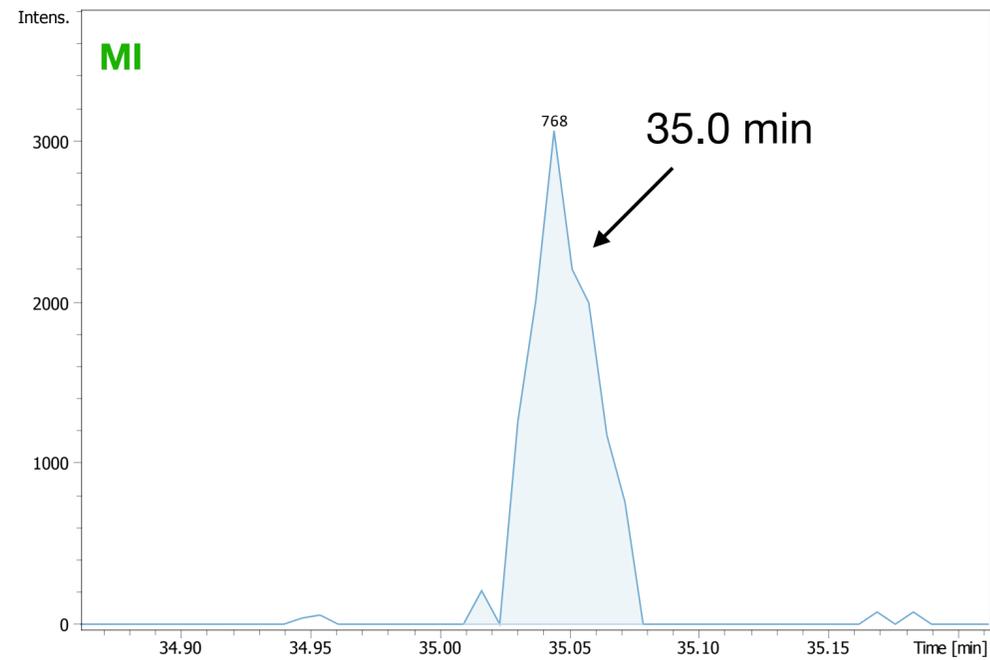
#10140-#10156 Heatmap



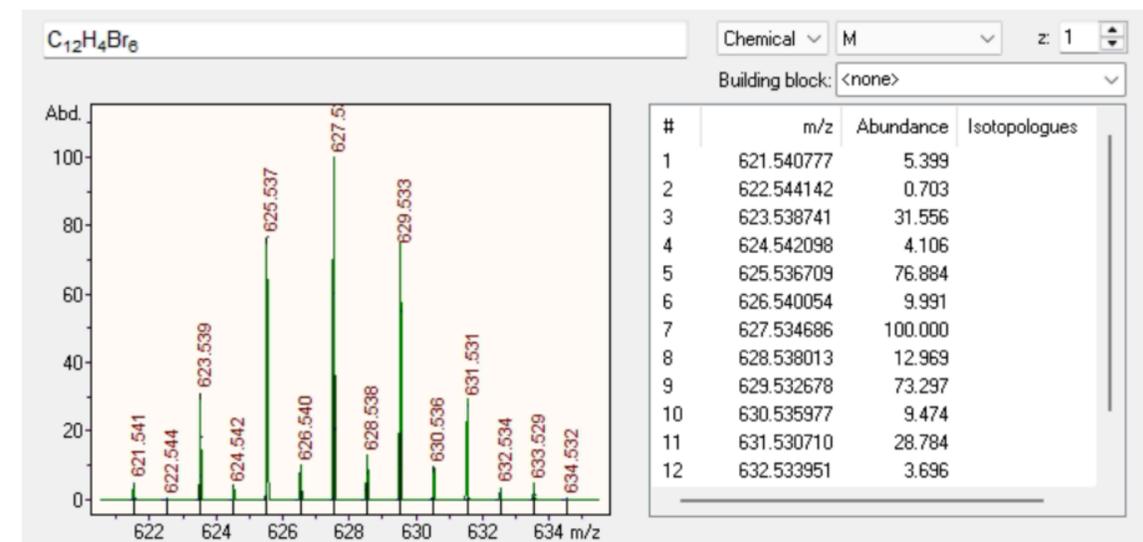
Mass spectrum & isotopic profile



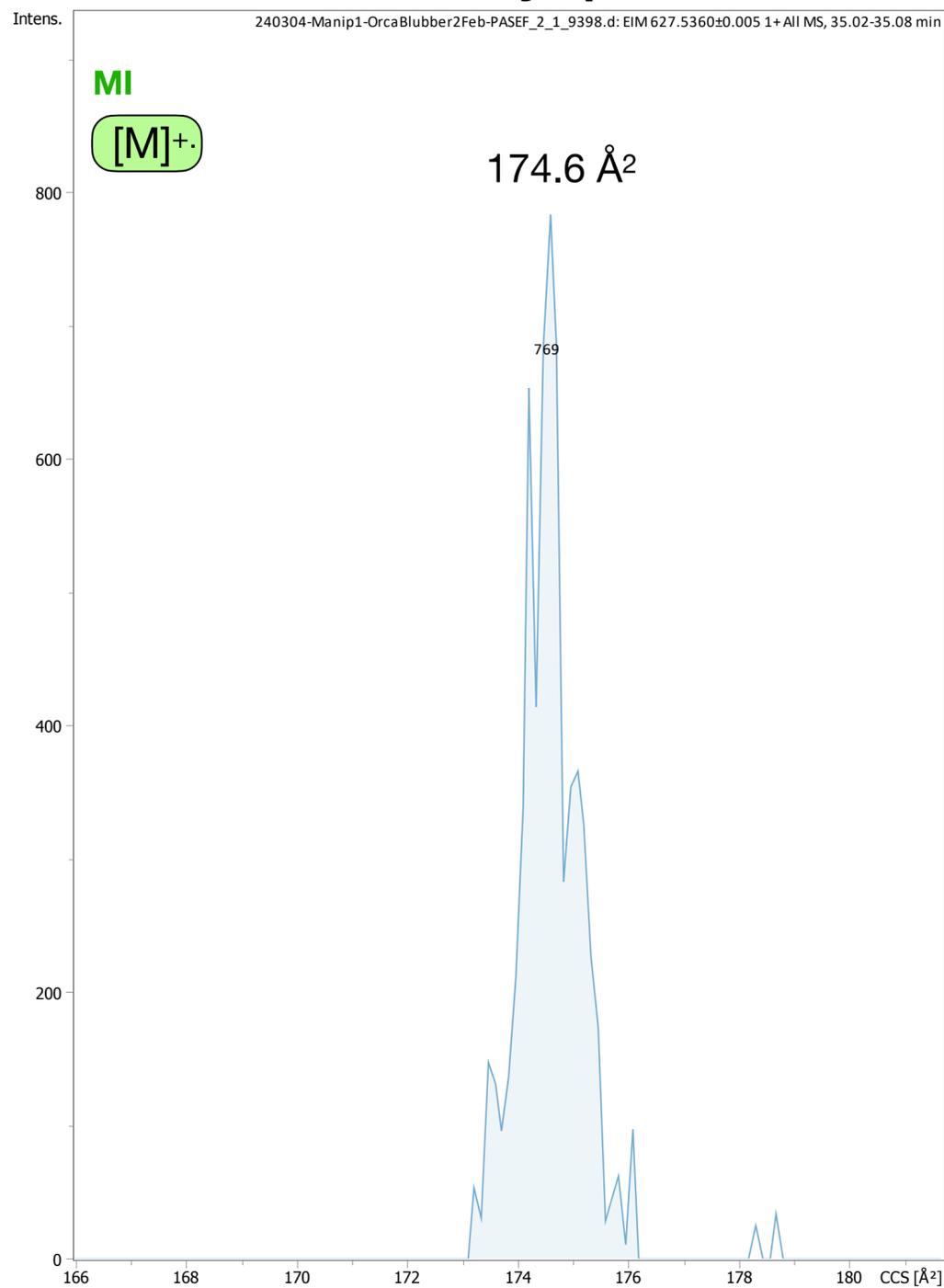
Chromatogram



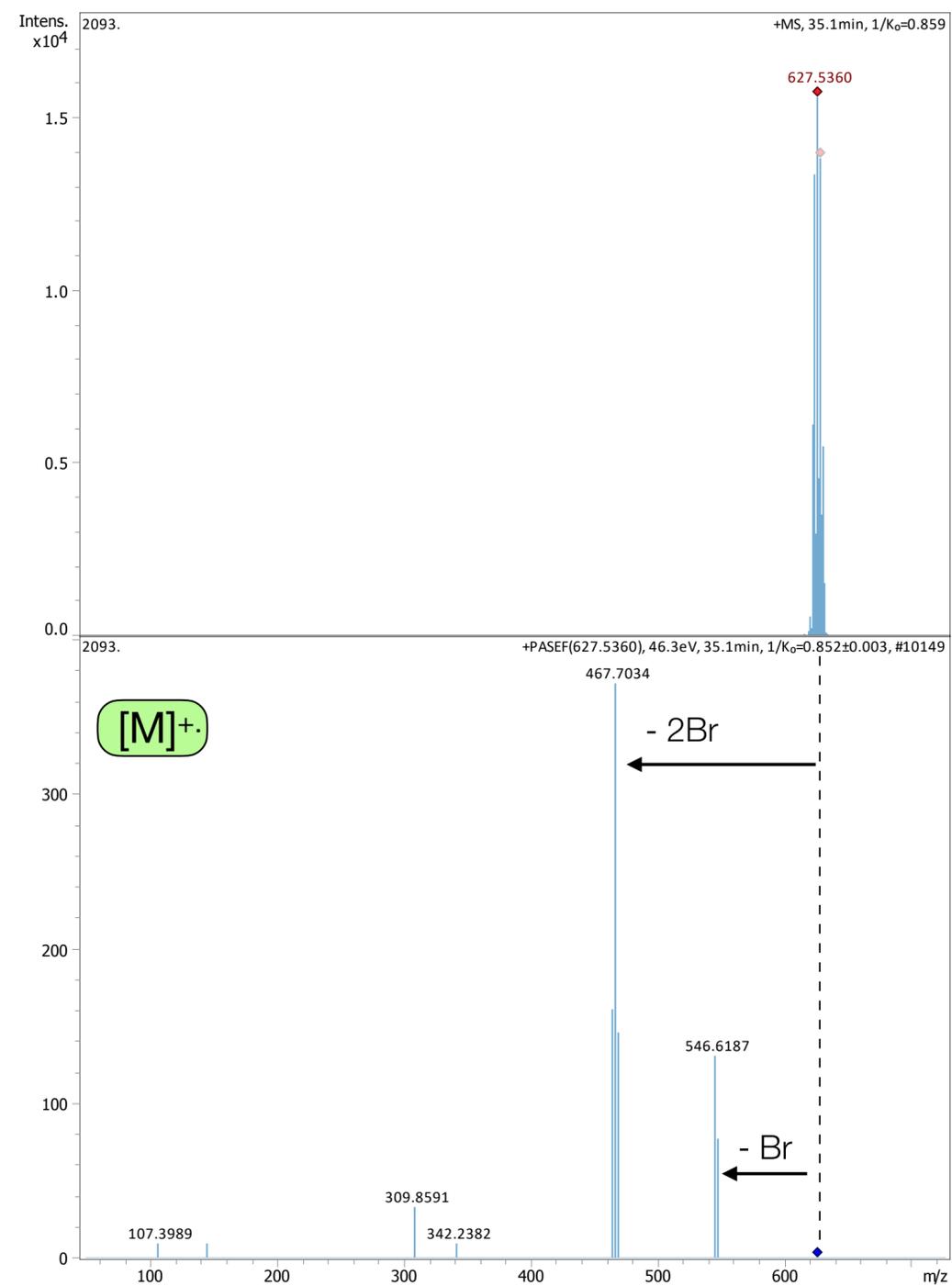
C₁₂Br₆H₄



Ion mobility spectrum

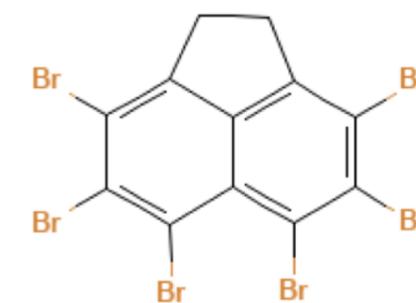


Tandem mass spectrum



Tentative candidate(s)

PubChem

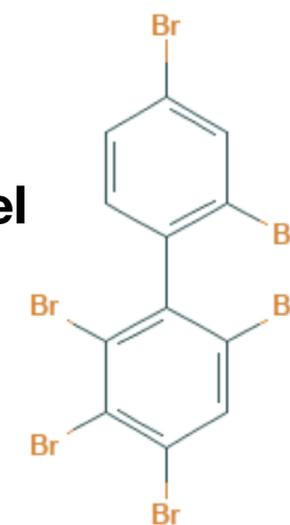
C₁₂Br₆H₄

Hexabromoacenaphthene

CCS pred: 173.7 Å² (-0.5%)

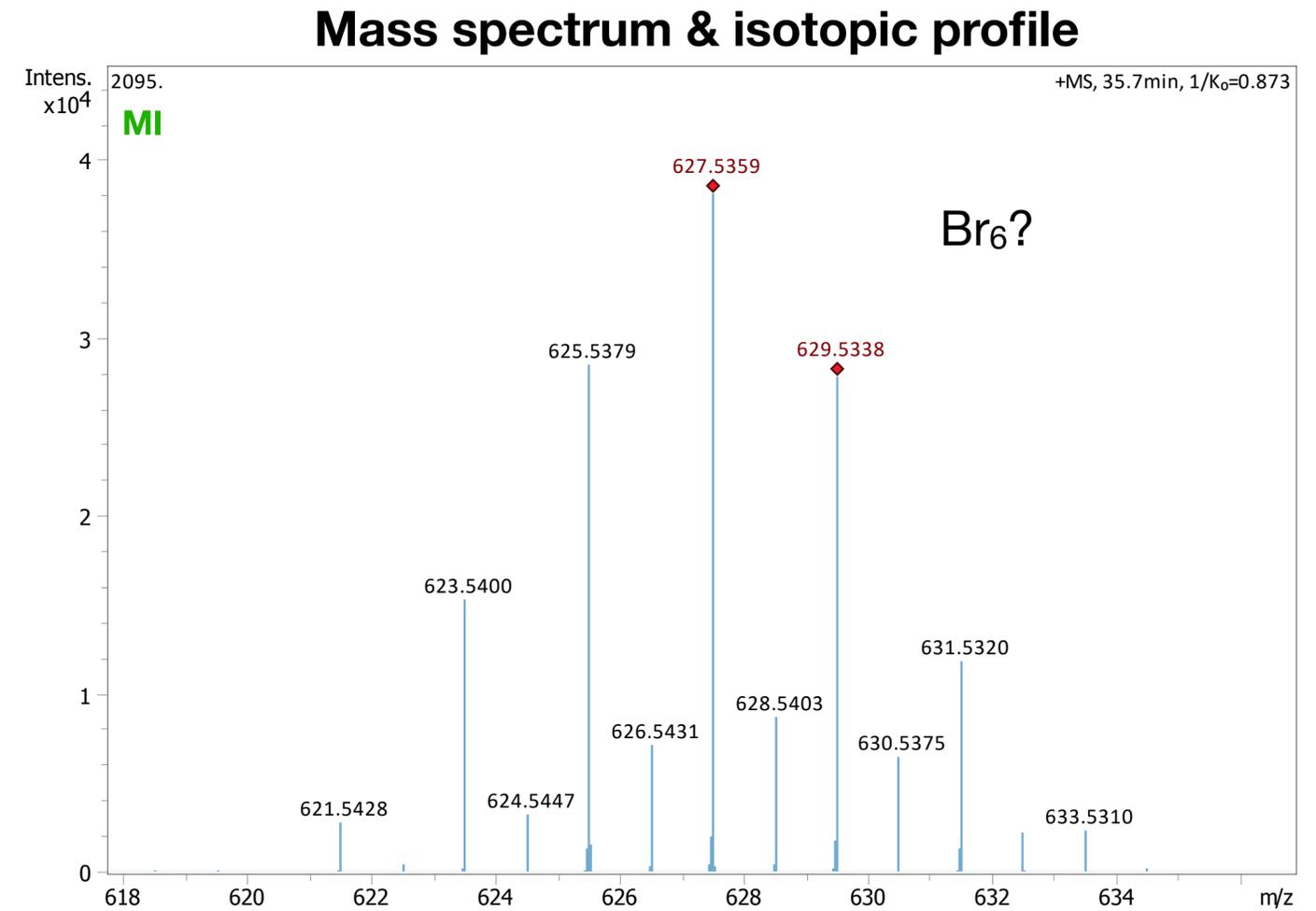
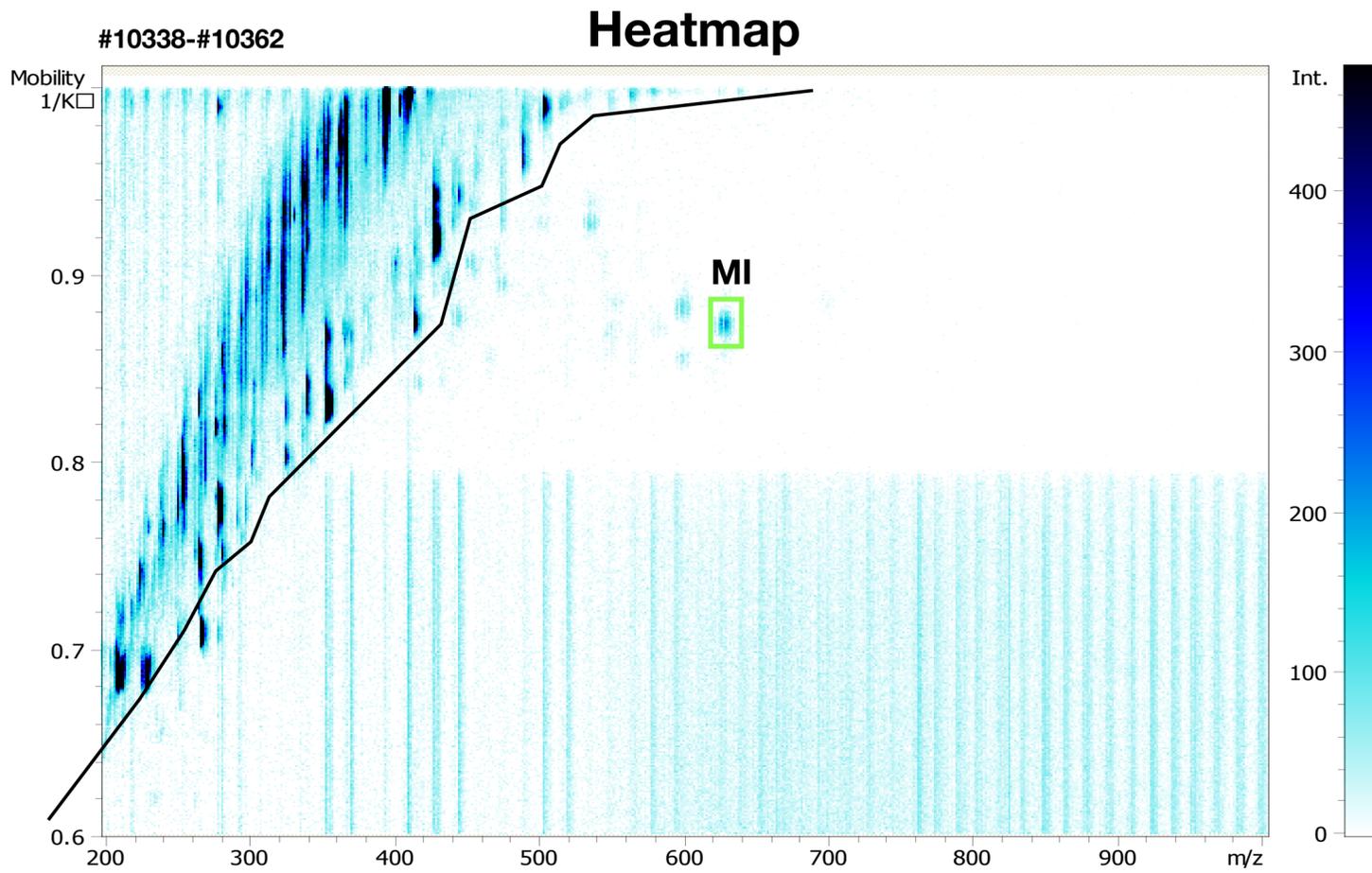
Confidence level

3

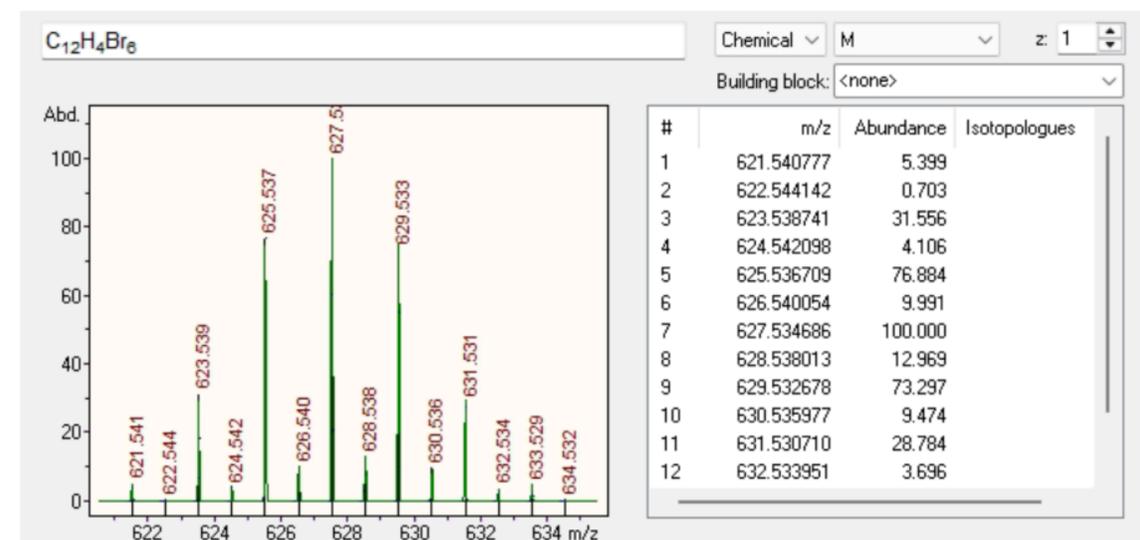
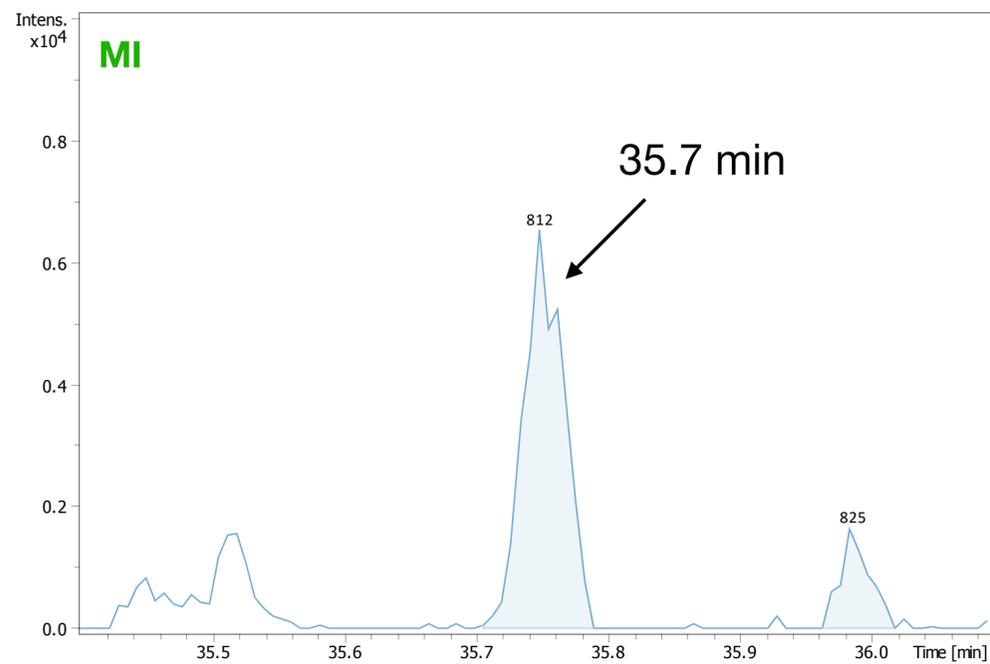


HxBBs (42 isomers)

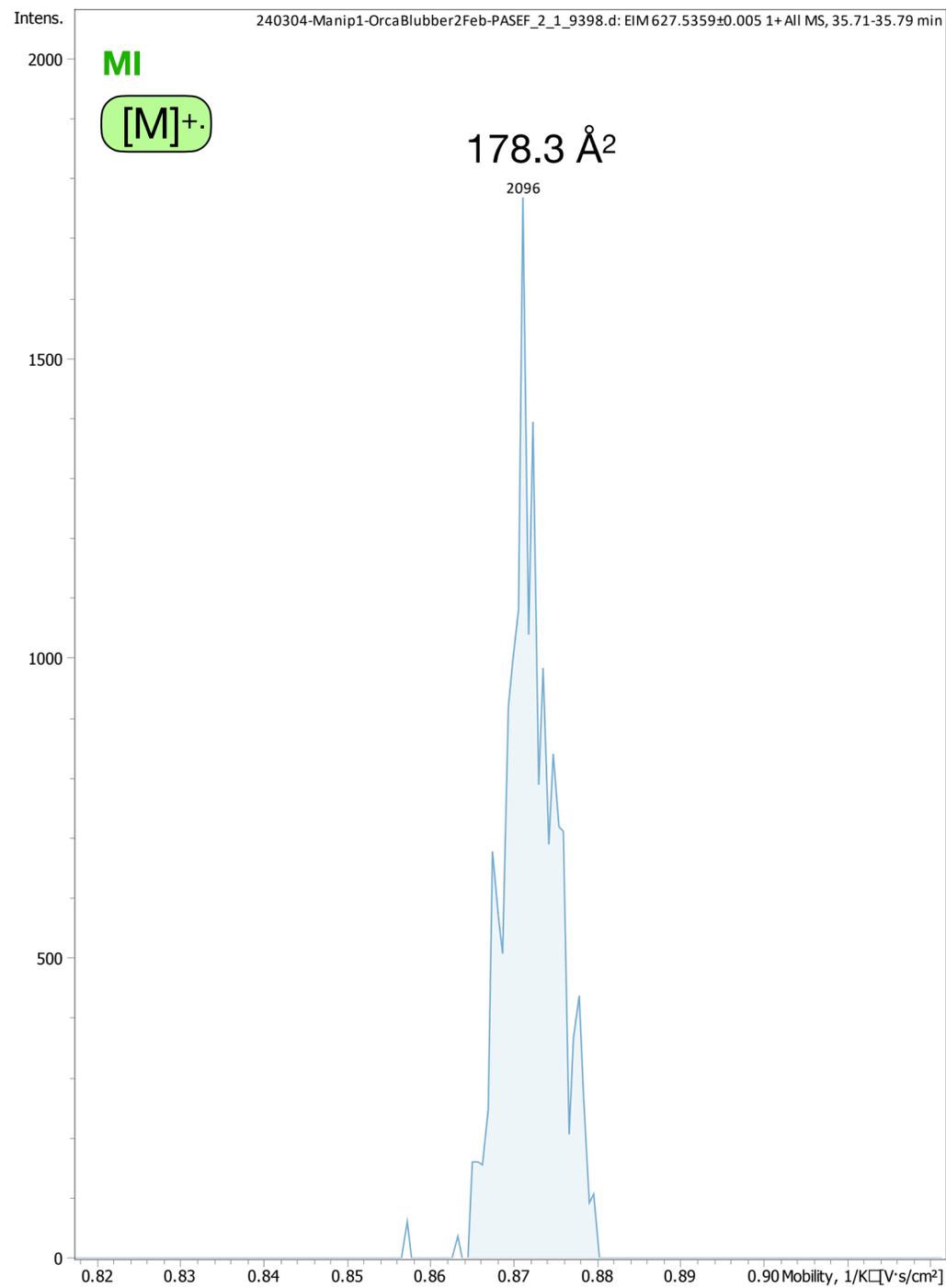
CCS pred HxBB
isomers: see Figure
S6.7B (manuscript)



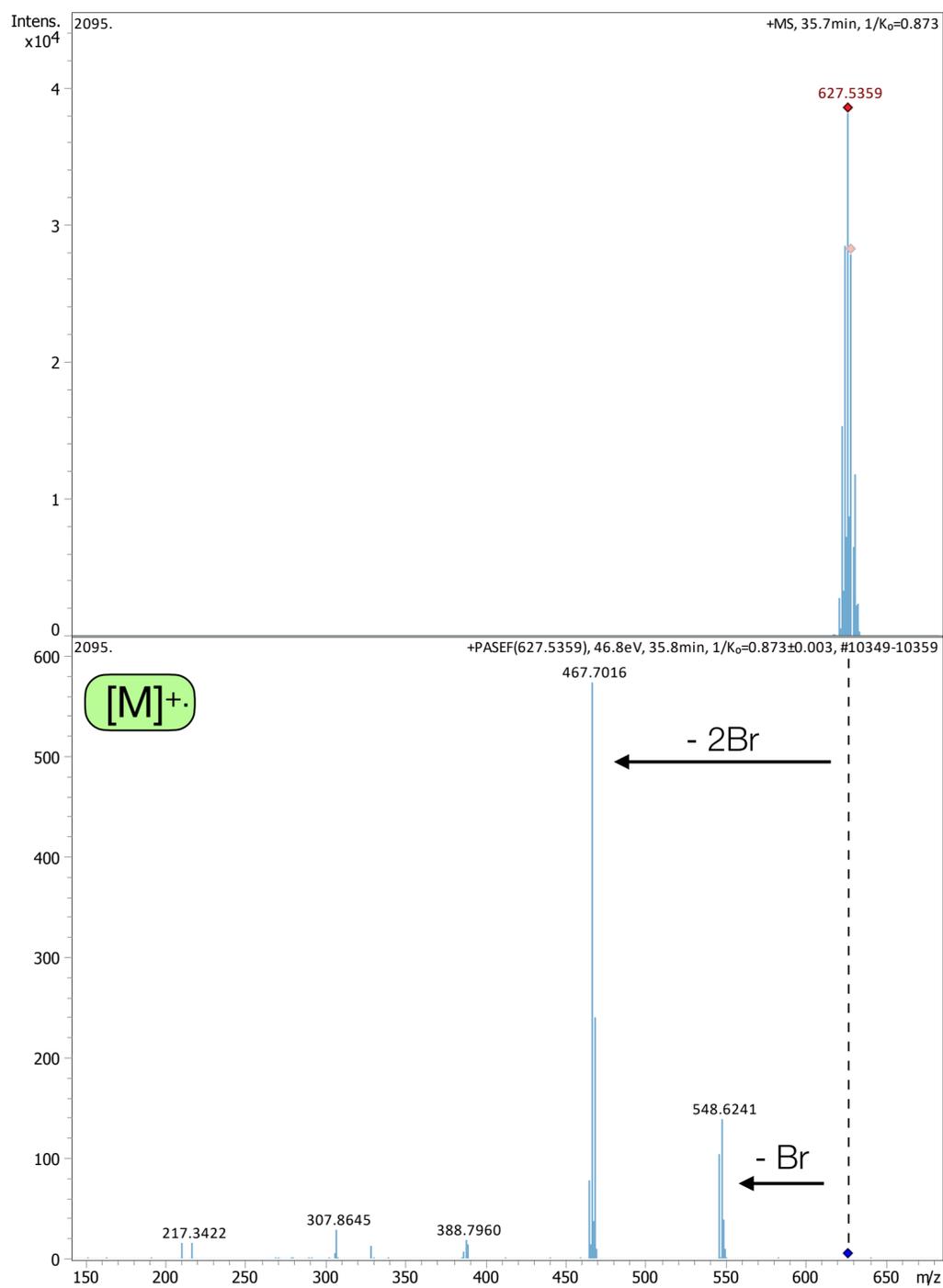
Chromatogram



Ion mobility spectrum

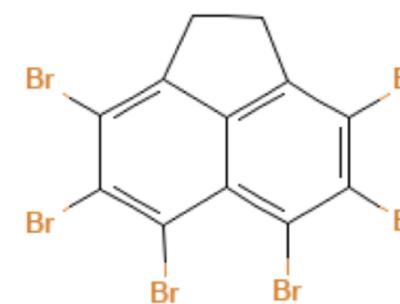


Tandem mass spectrum



Tentative candidate(s)

PubChem

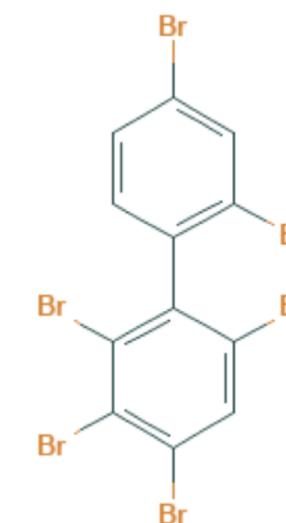
C₁₂Br₆H₄

Hexabromoacenaphthene

CCS pred: 173.7 Å² (-2.6%)

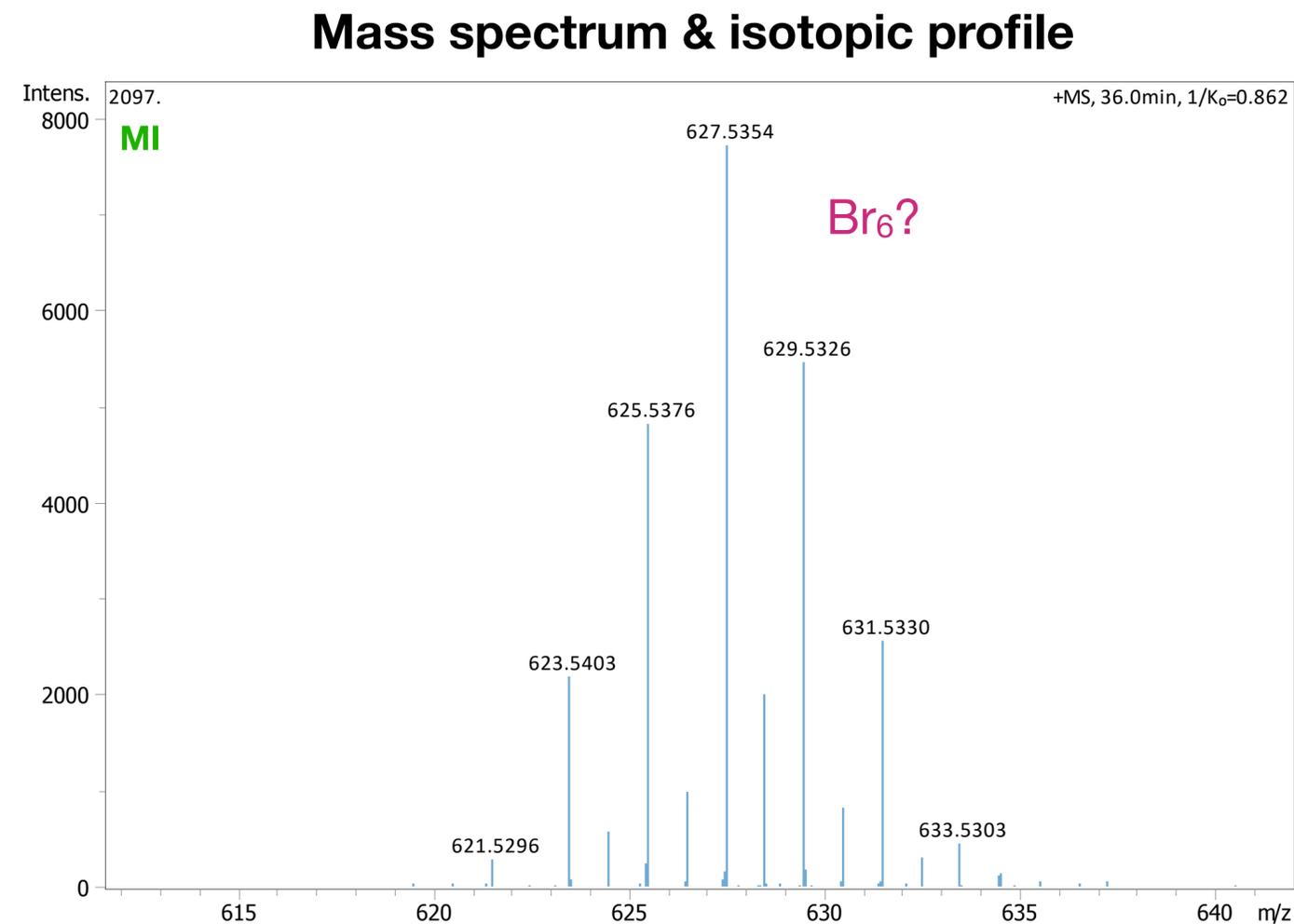
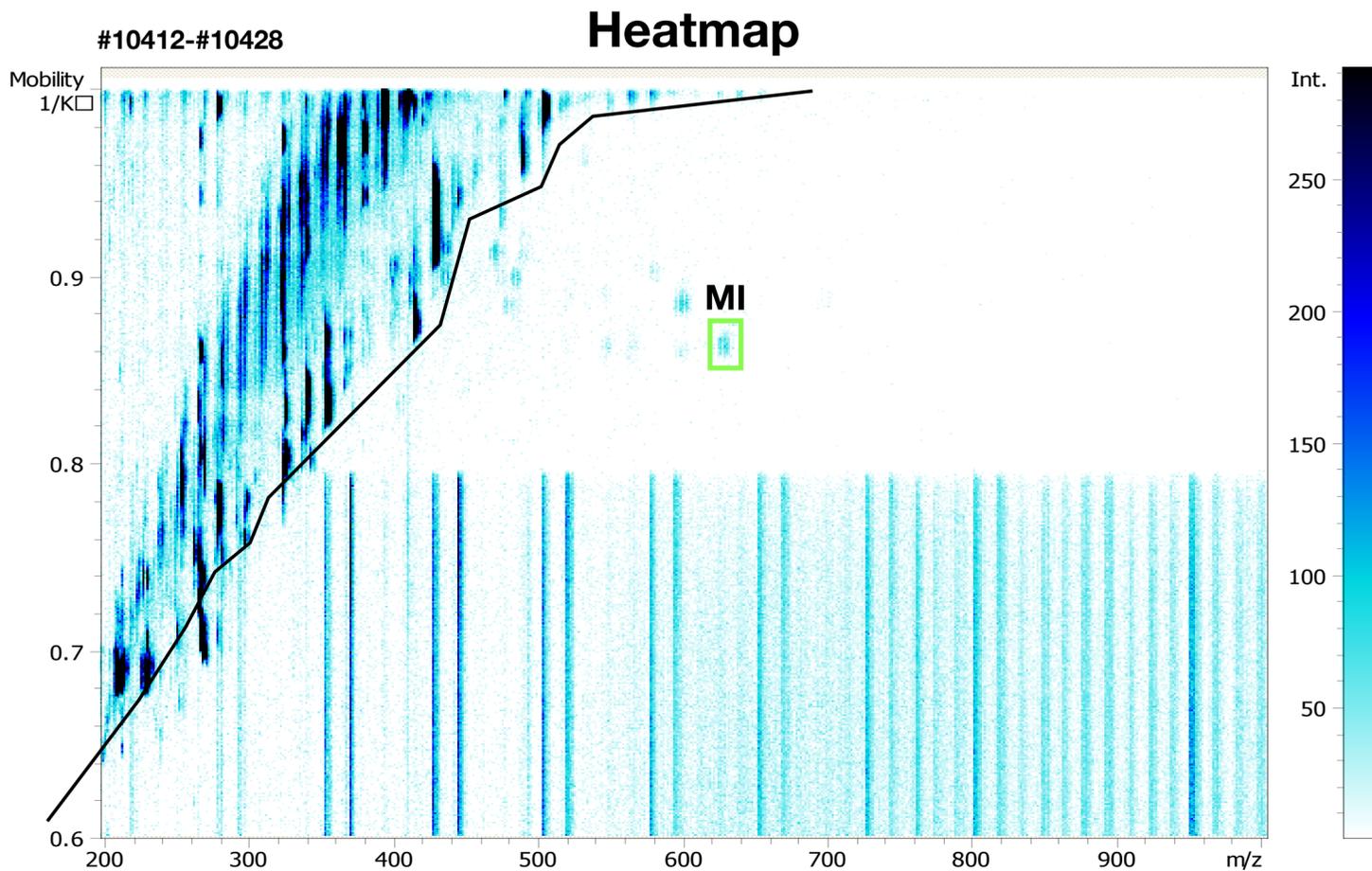
Confidence level

3

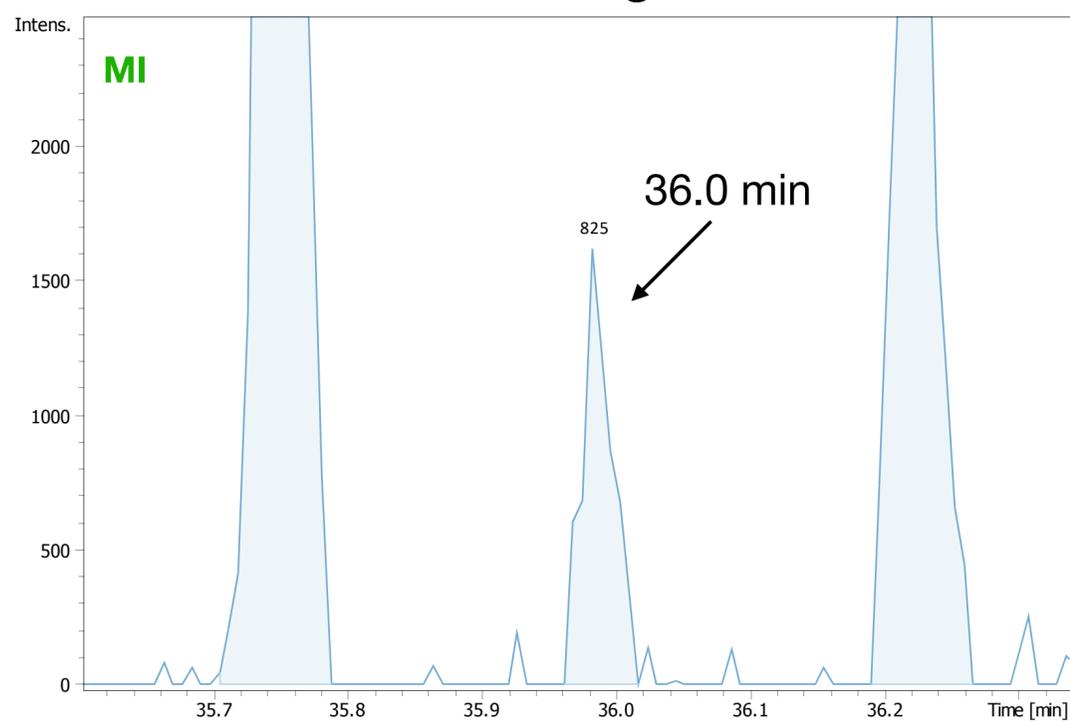


HxBBs (42 isomers)

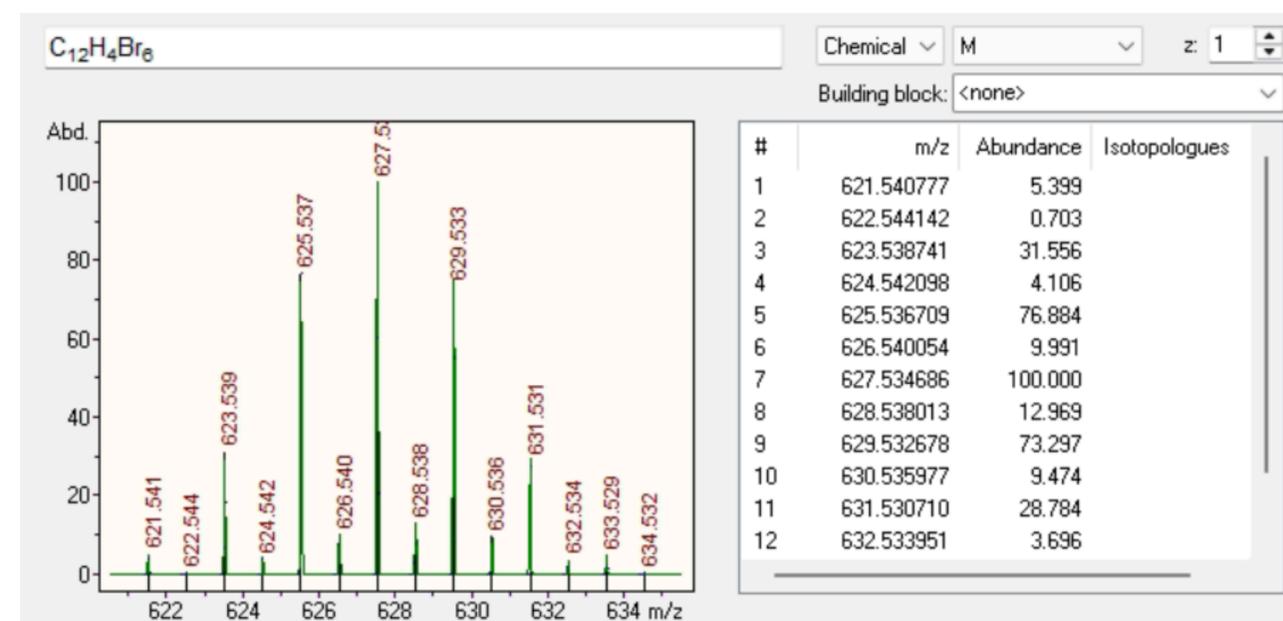
CCS pred HxBB isomers: see Figure S6.7B (manuscript)



Chromatogram



C₁₂Br₆H₄



Tandem mass spectrum

/

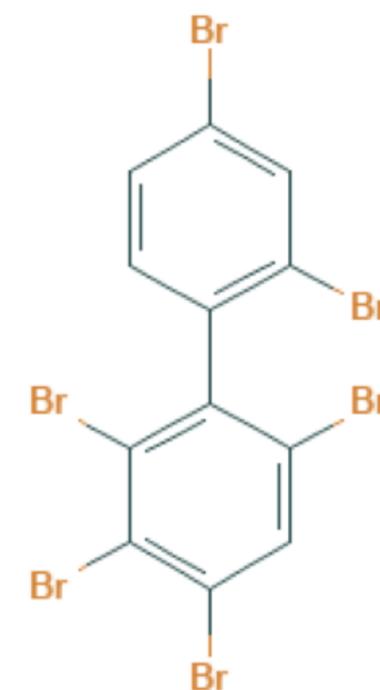
Tentative candidate(s)

PubChem

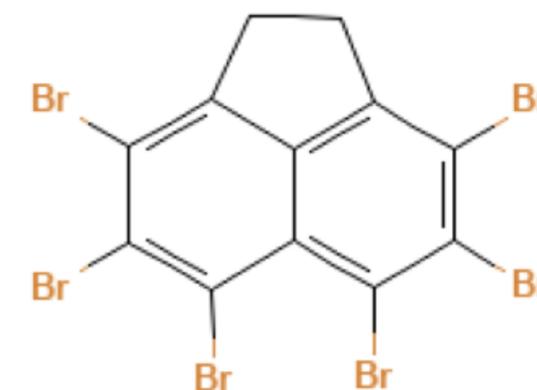
 $C_{12}Br_6H_4$

Confidence level

3



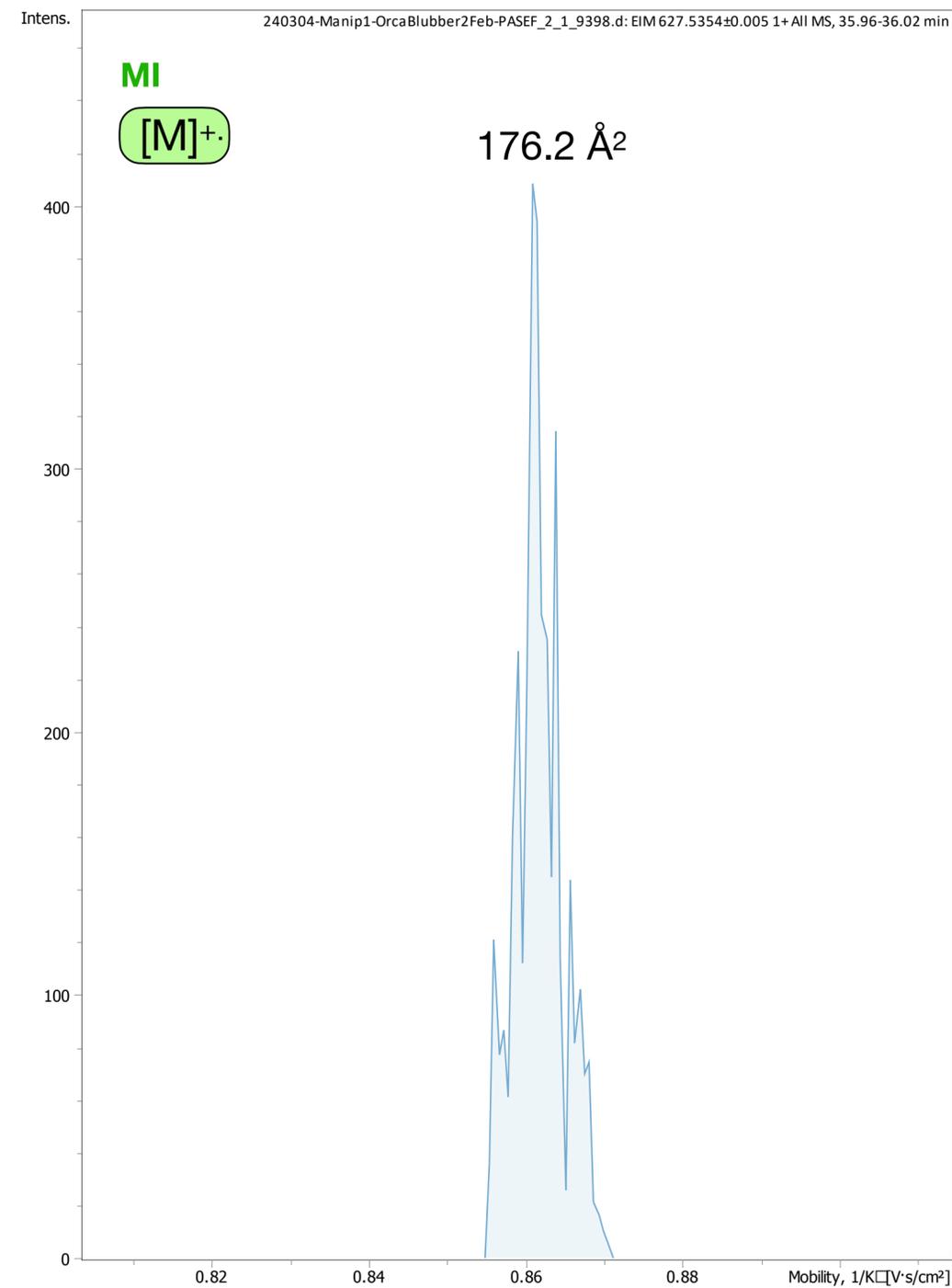
HxBBs (42 isomers)

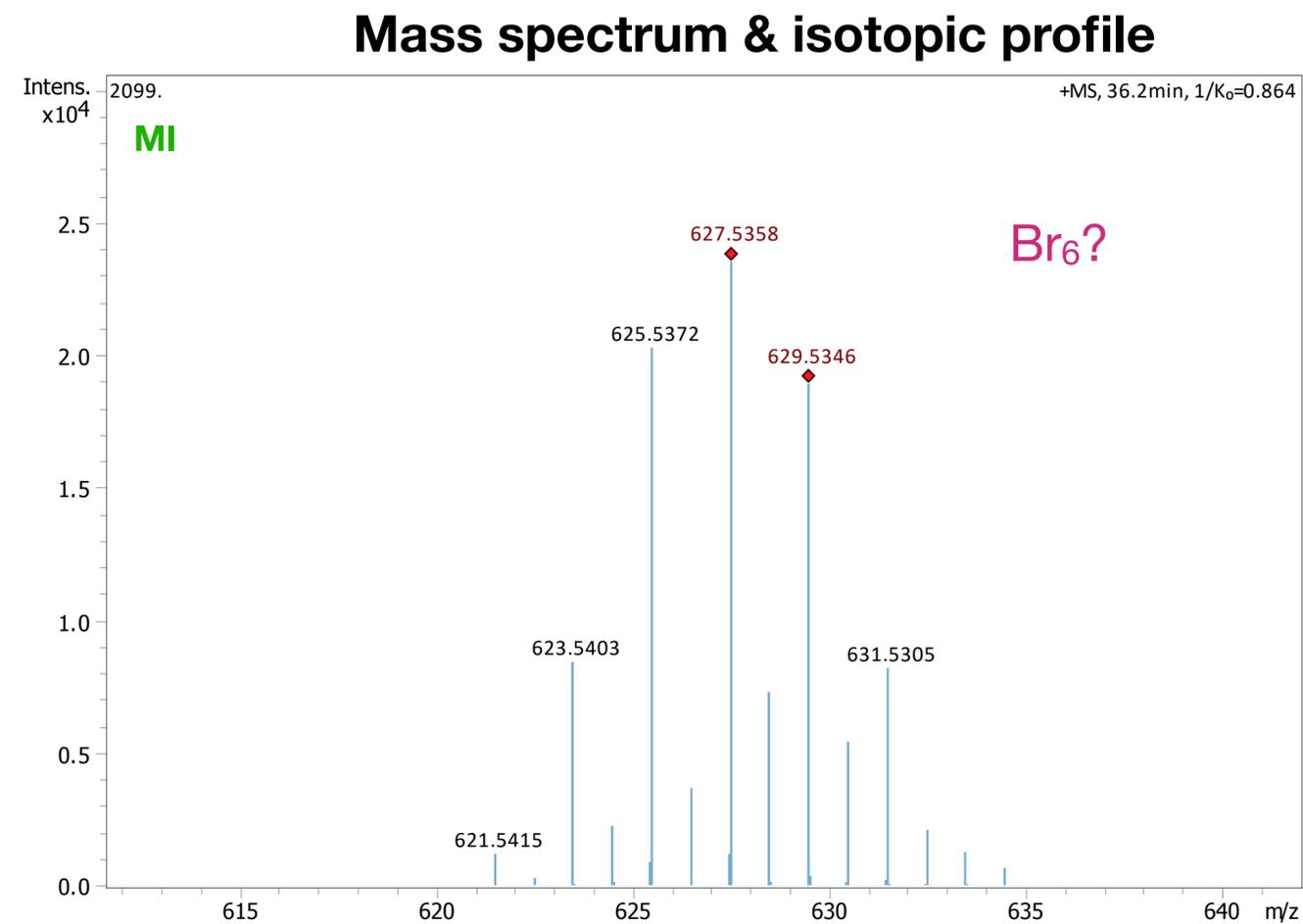
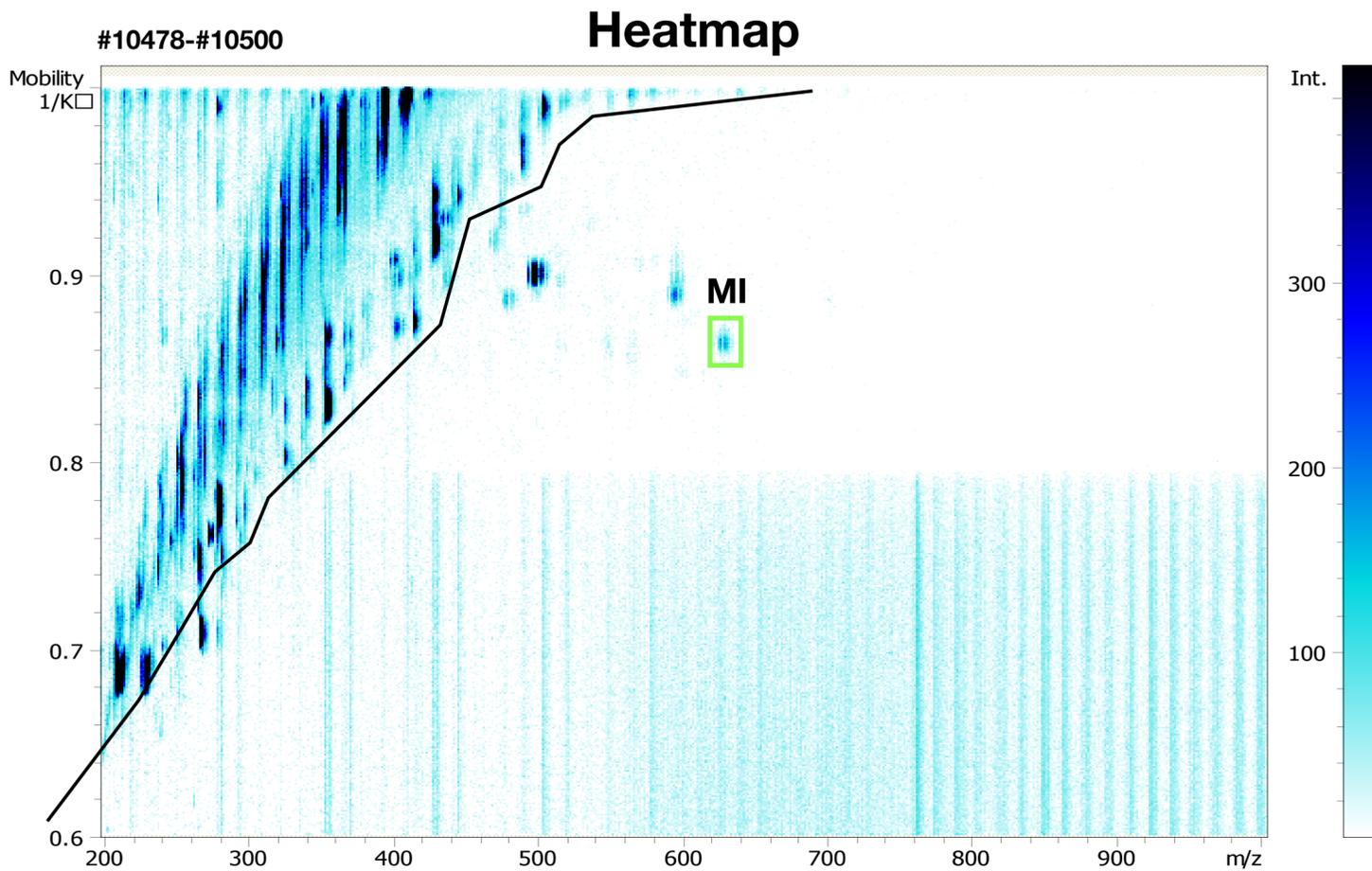
CCS pred HxBB
isomers: see Figure
S6.7B (manuscript)

Hexabromoacenaphthene

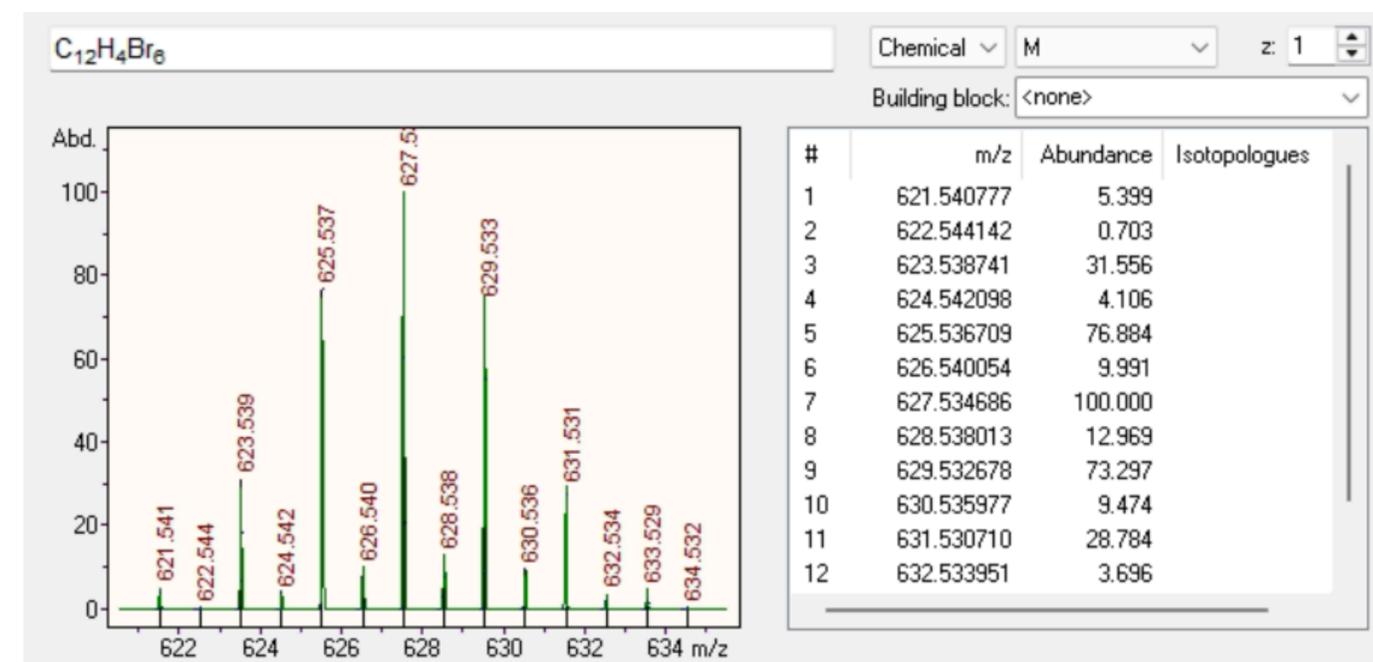
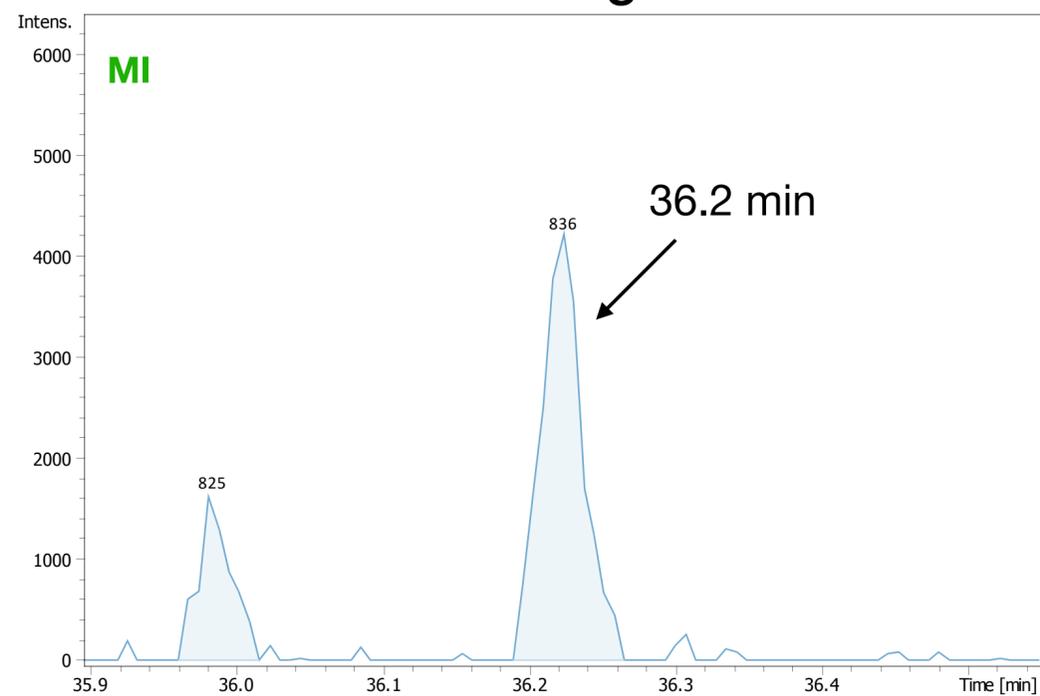
CCS pred: 173.7 Å² (-1.4%)

Ion mobility spectra

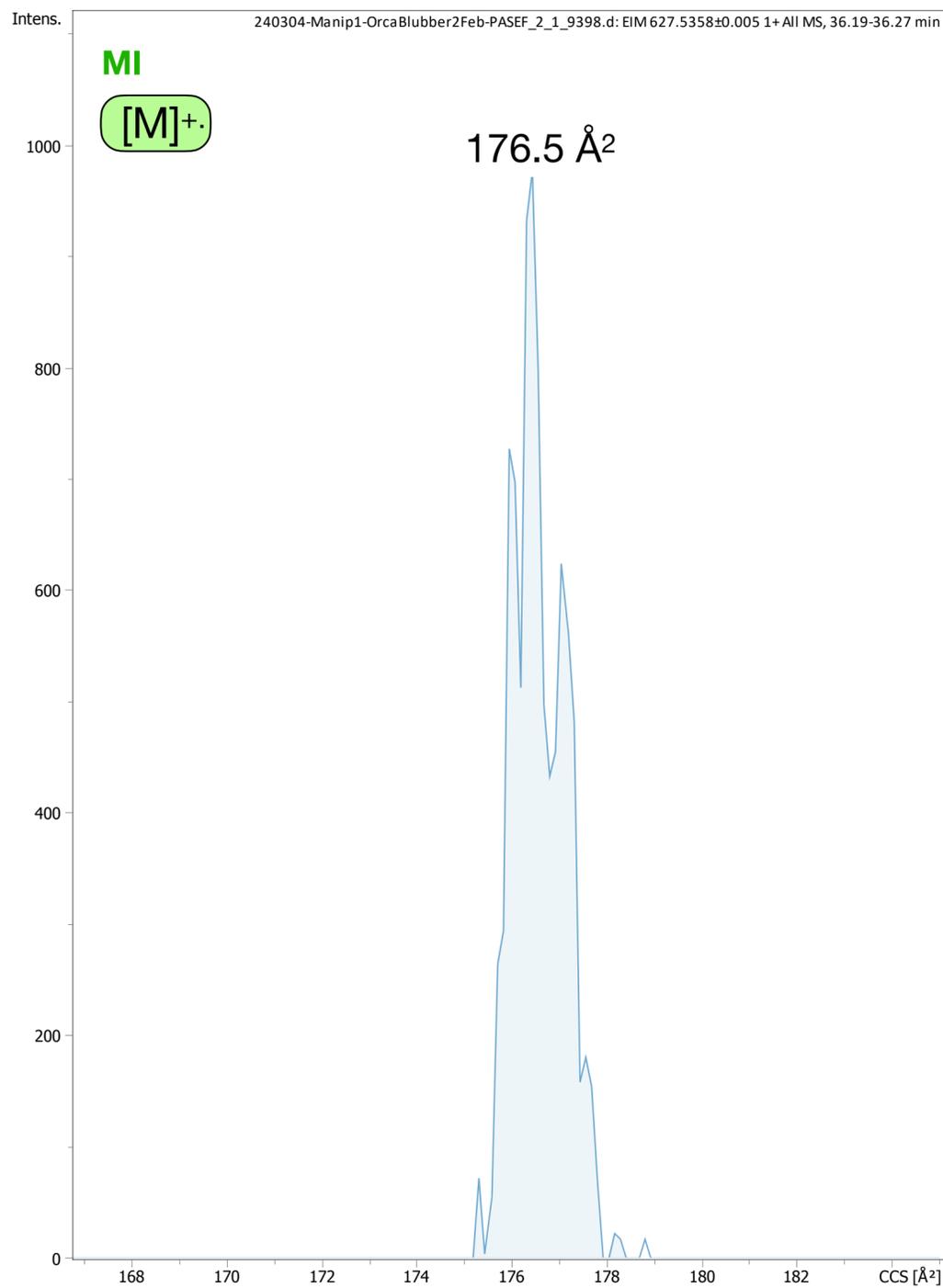




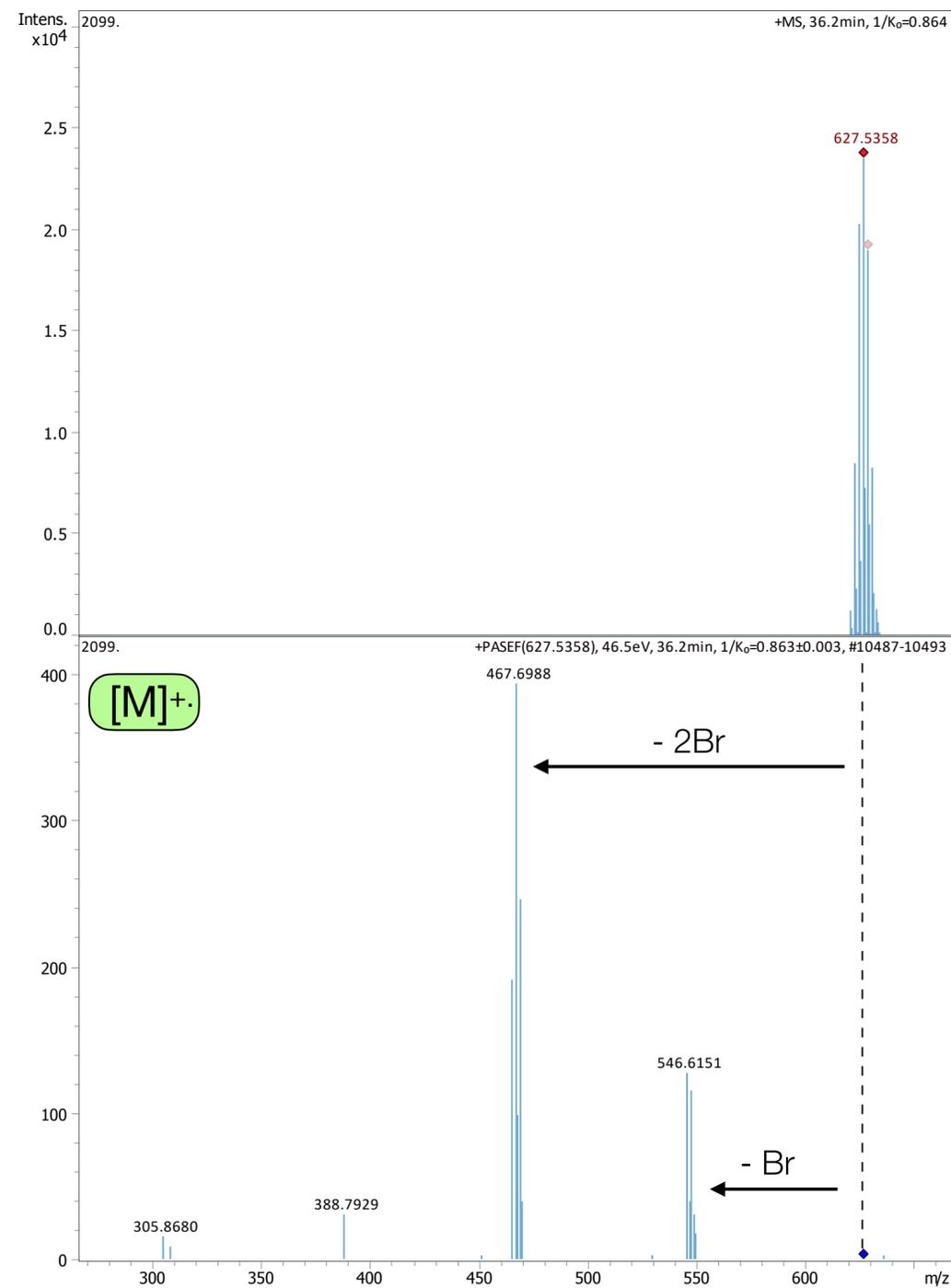
Chromatogram



Ion mobility spectrum

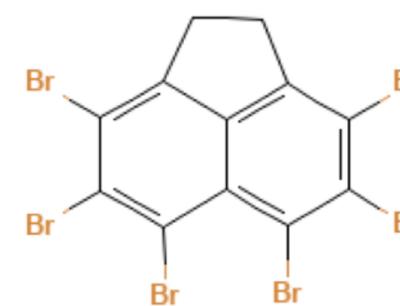


Tandem mass spectrum



Tentative candidate(s)

PubChem

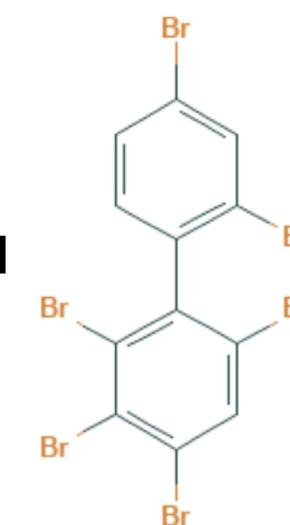
C₁₂Br₆H₄

Hexabromoacenaphthene

CCS pred: 173.7 Å² (-1.6%)

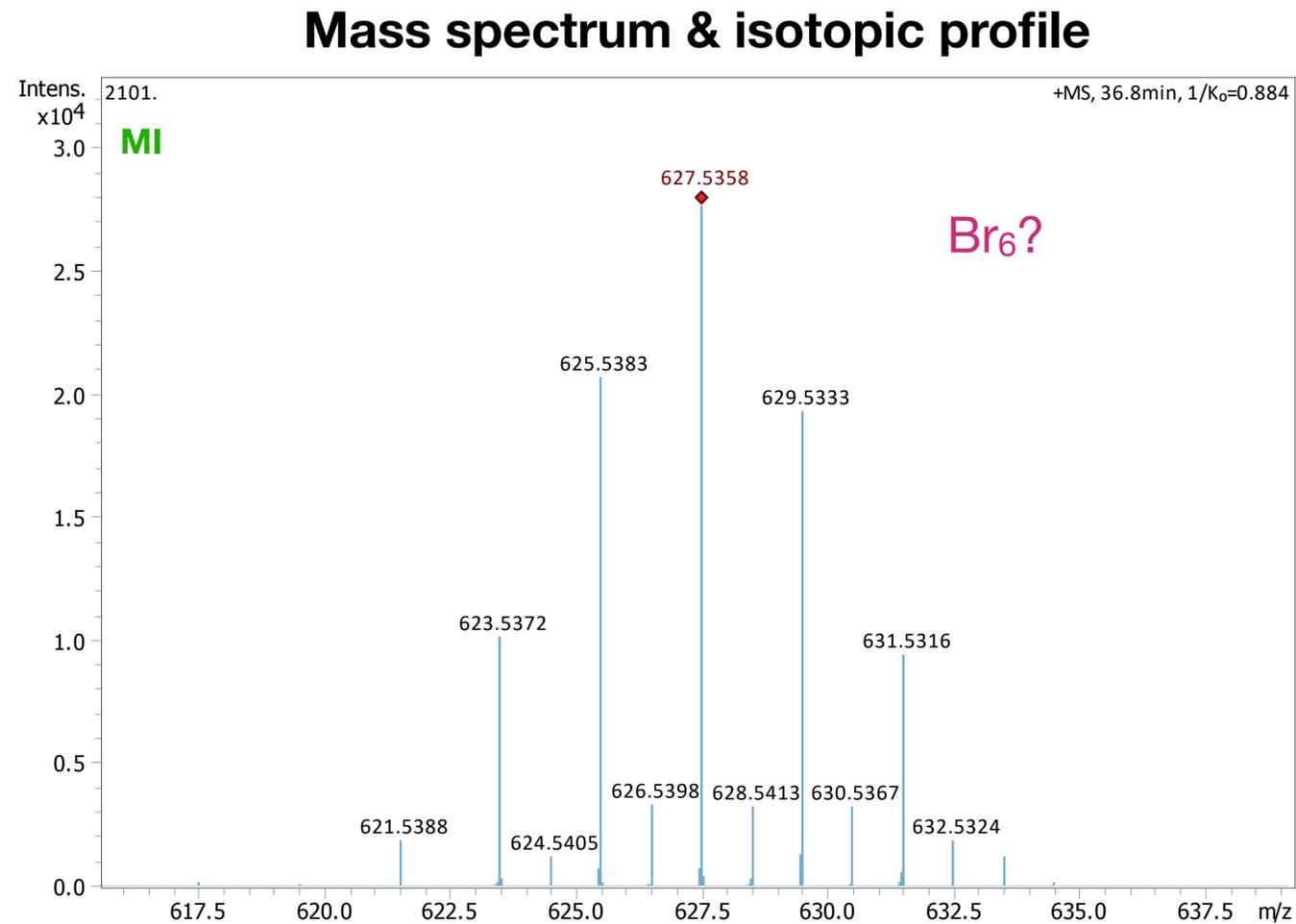
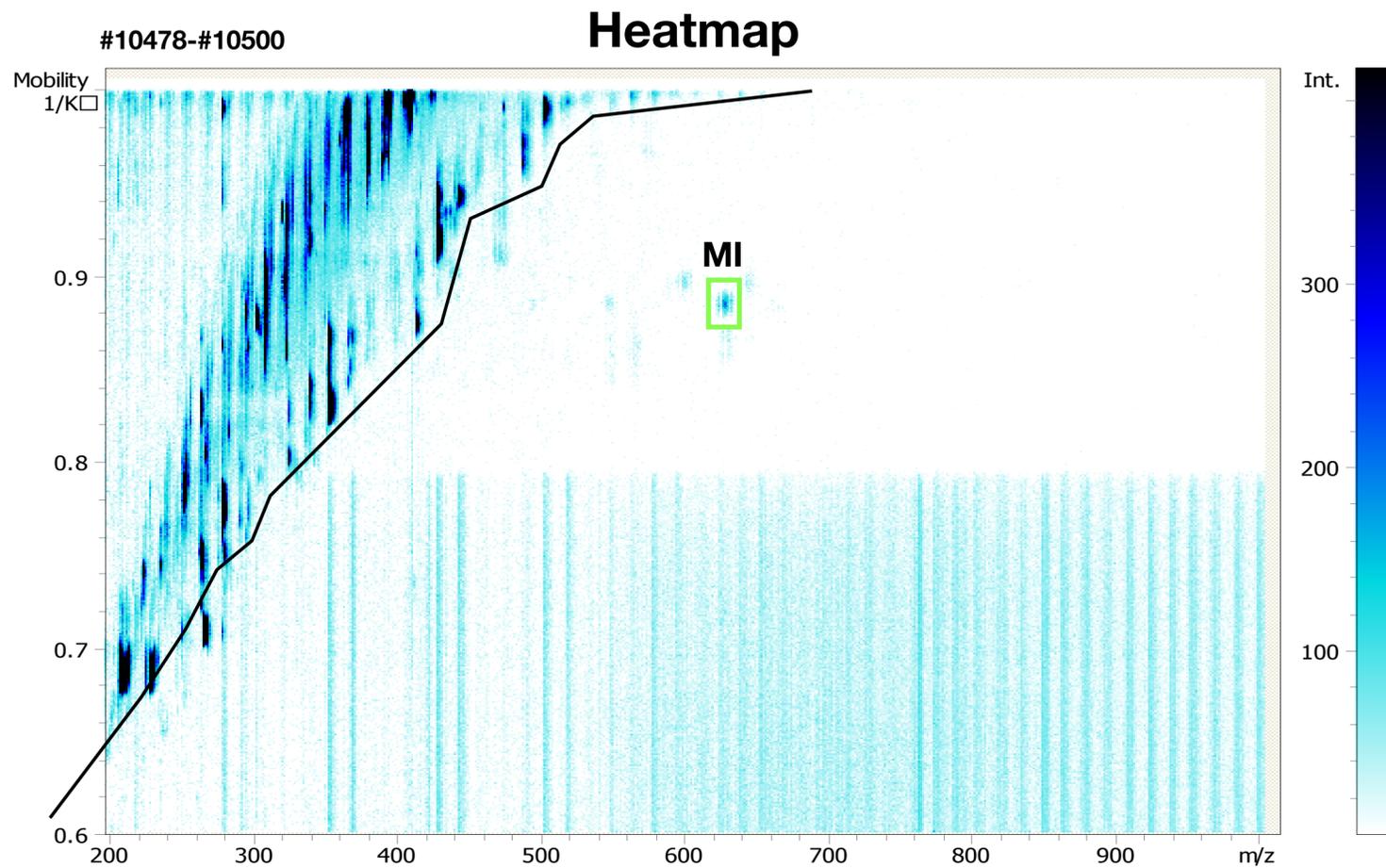
Confidence level

3

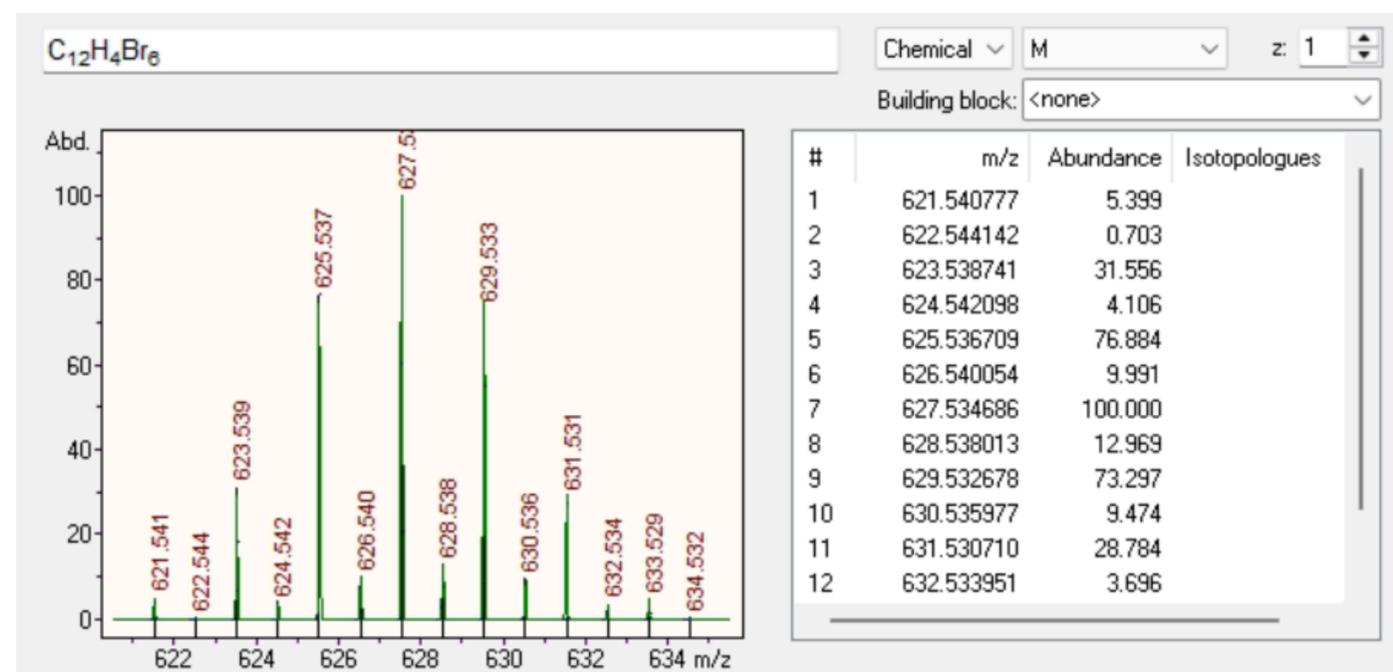
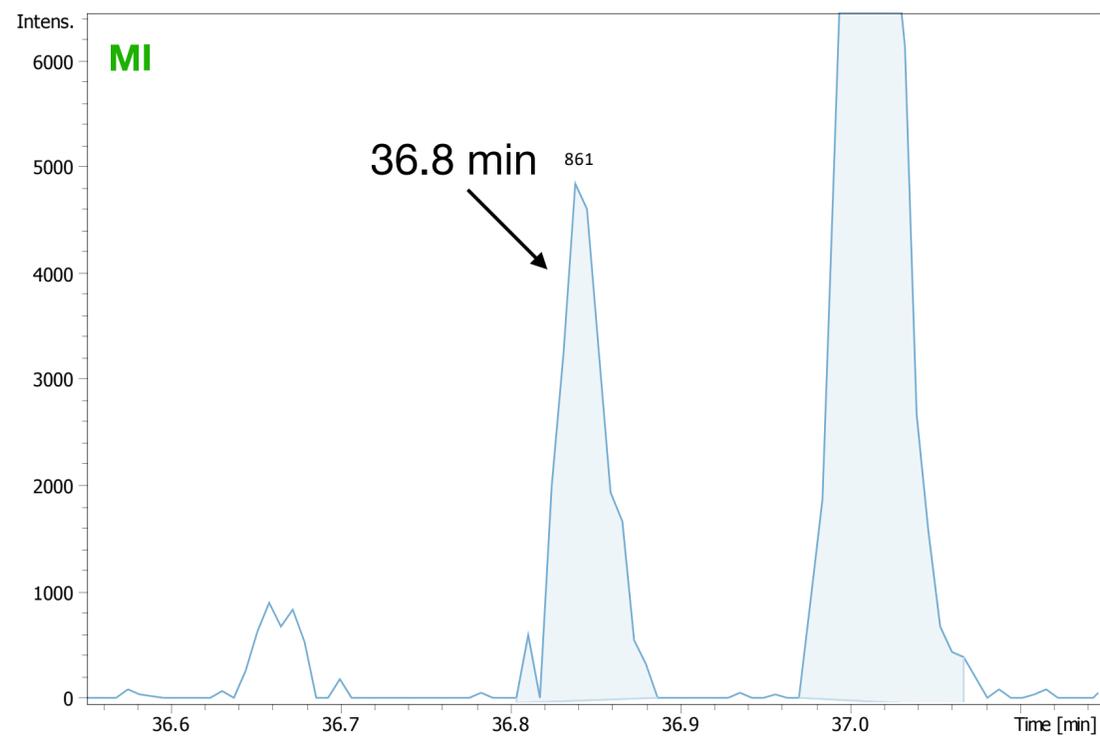


HxBBs (42 isomers)

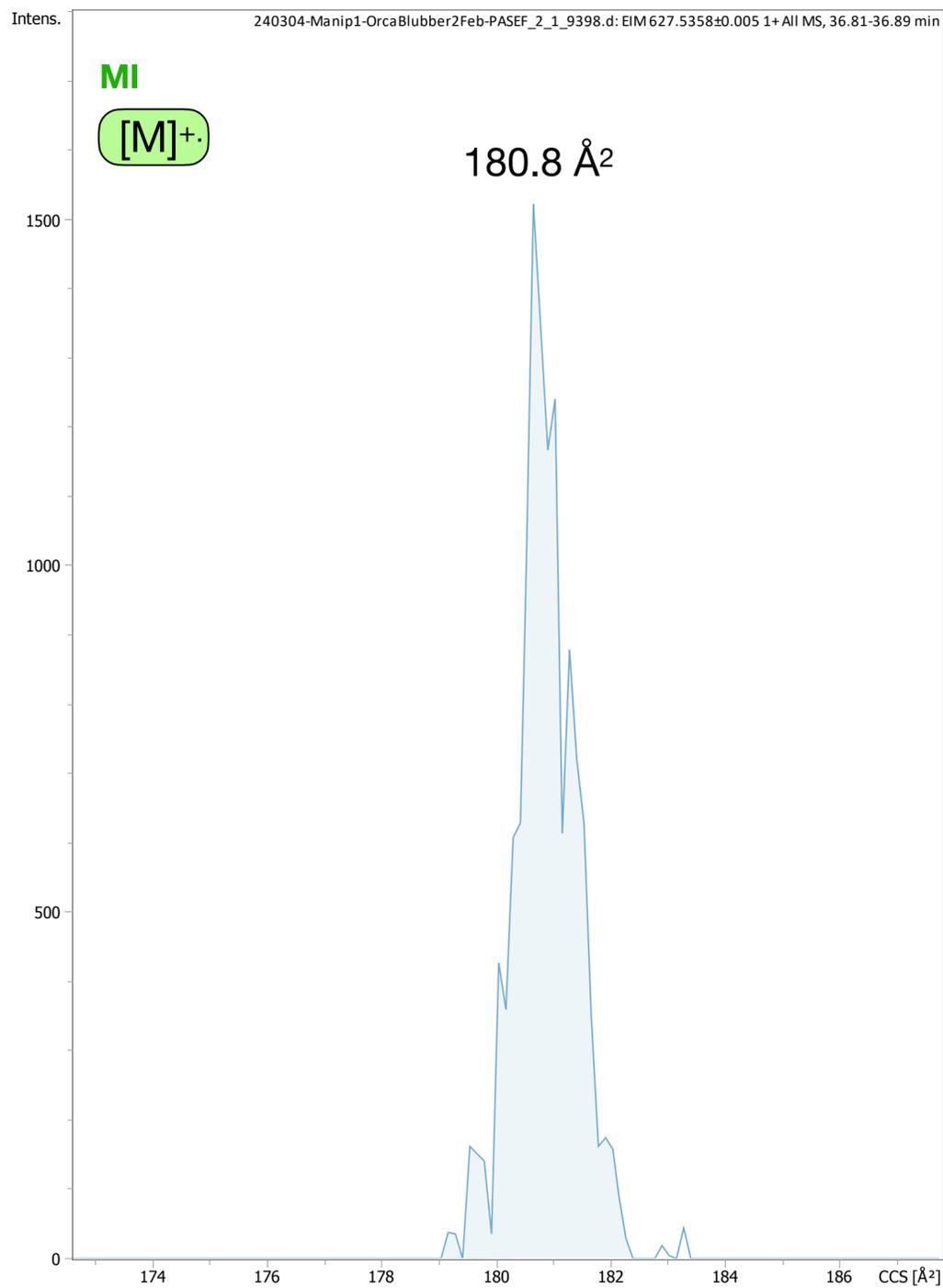
CCS pred HxBB
isomers: see Figure
S6.7B (manuscript)



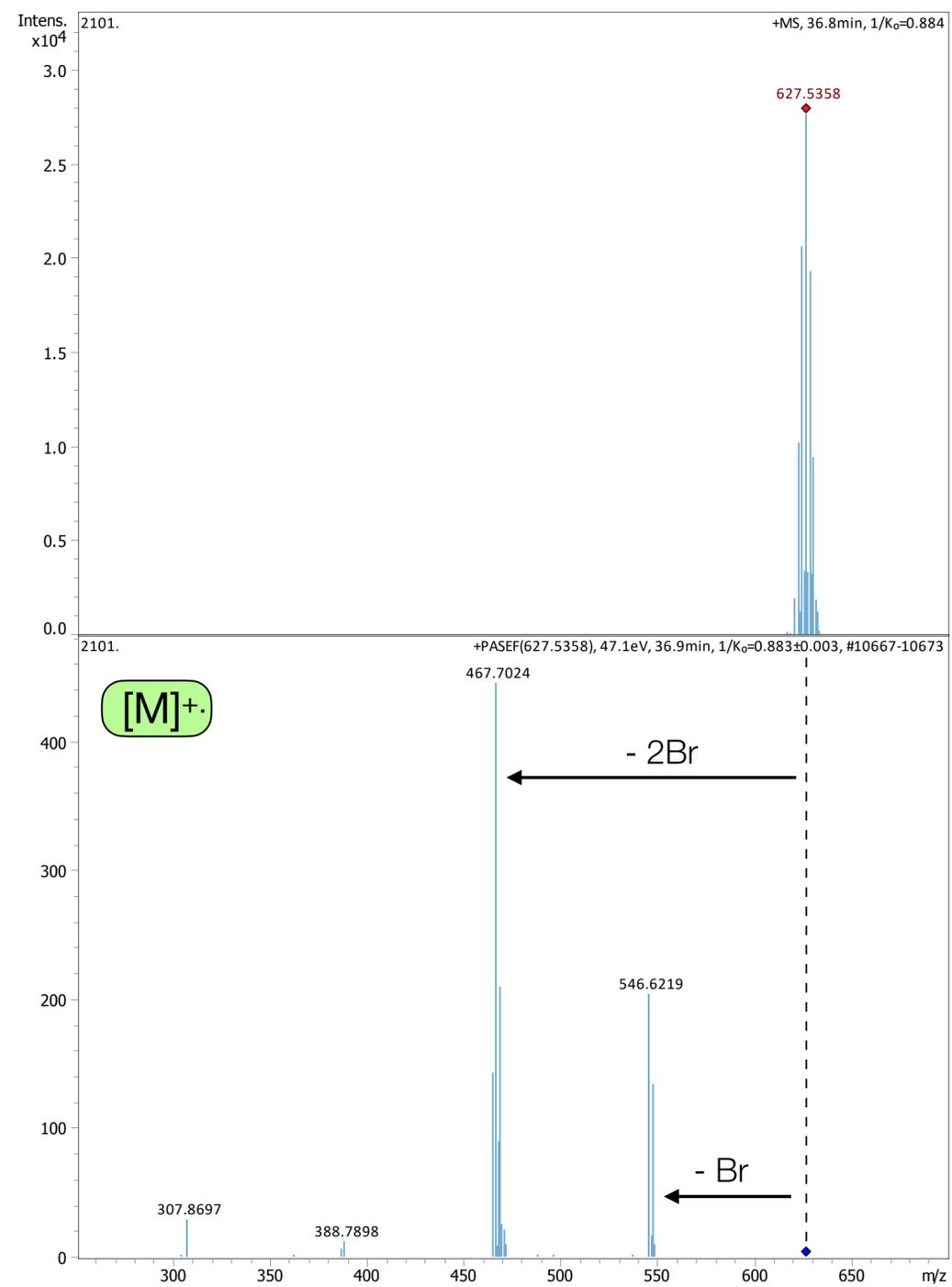
Chromatogram



Ion mobility spectrum

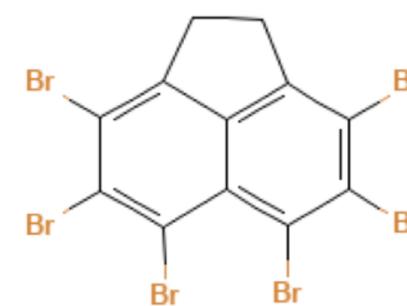


Tandem mass spectrum



Tentative candidate(s)

PubChem

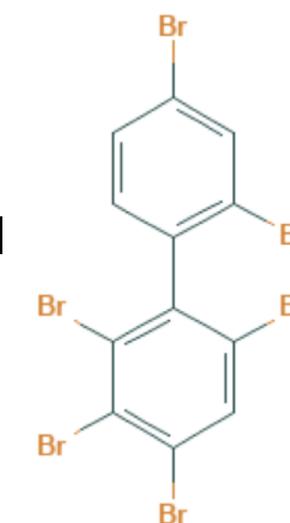
C₁₂Br₆H₄

Hexabromoacenaphthene

CCS pred: 173.7 Å² (-3.9%)

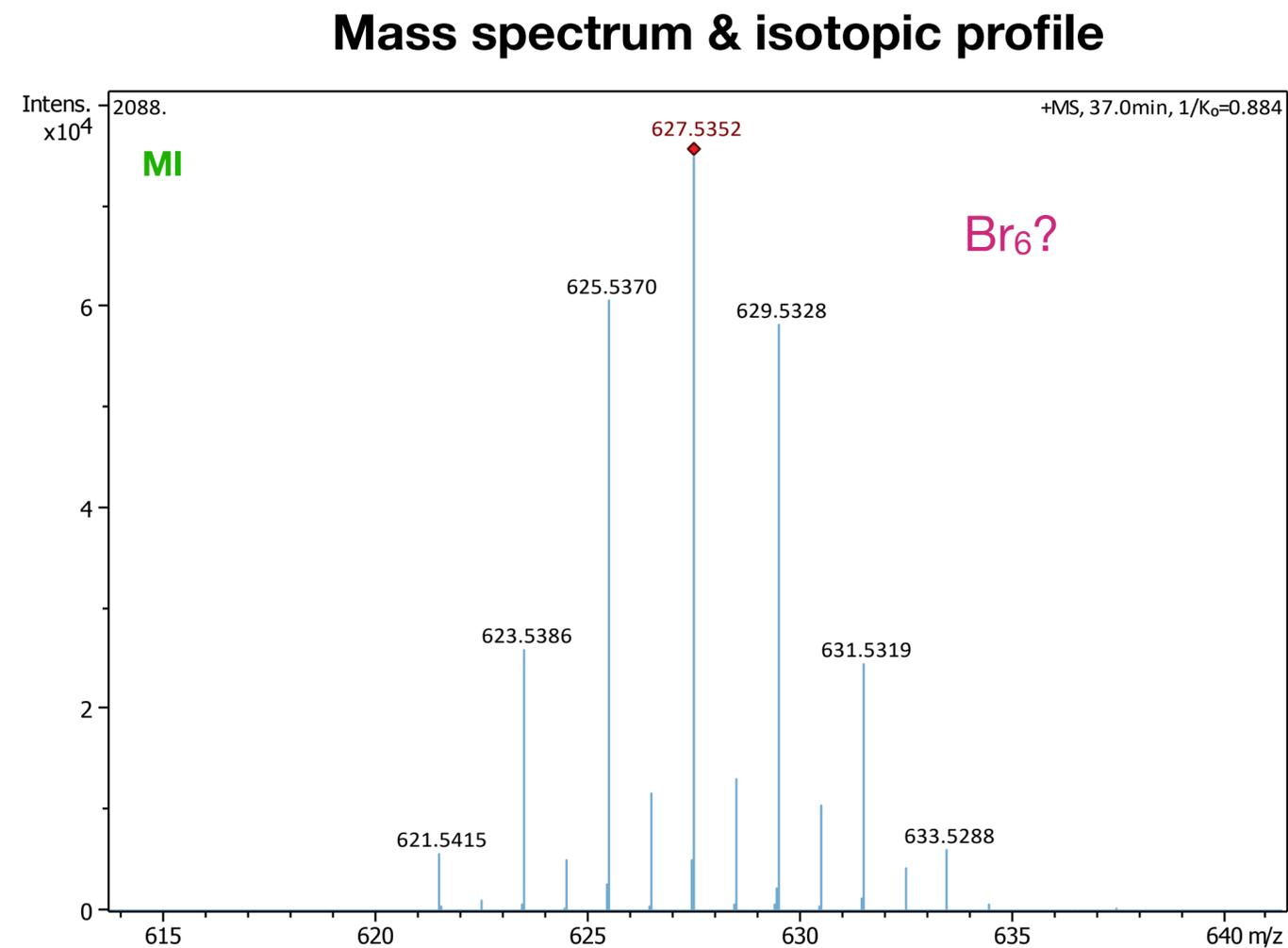
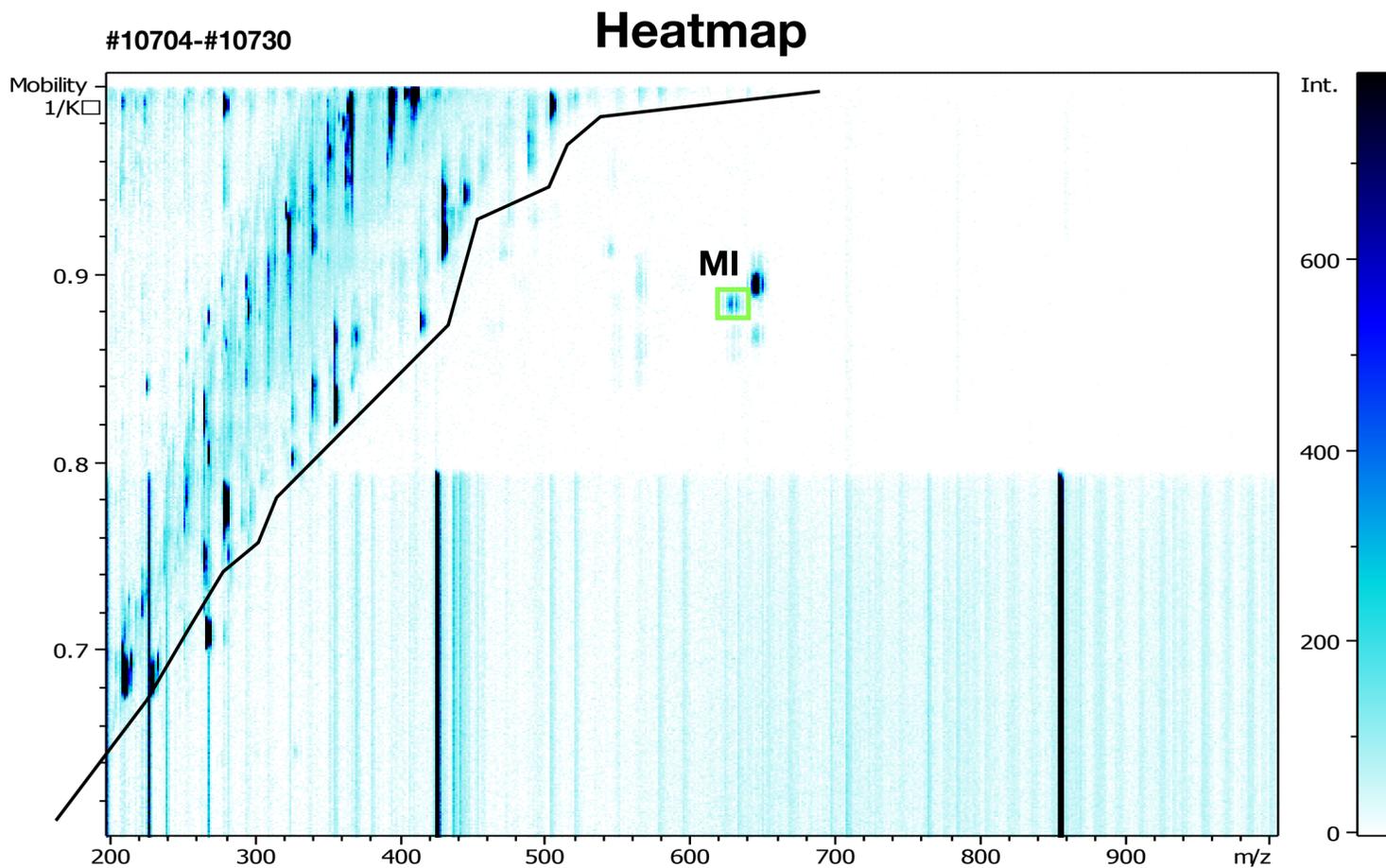
Confidence level

3

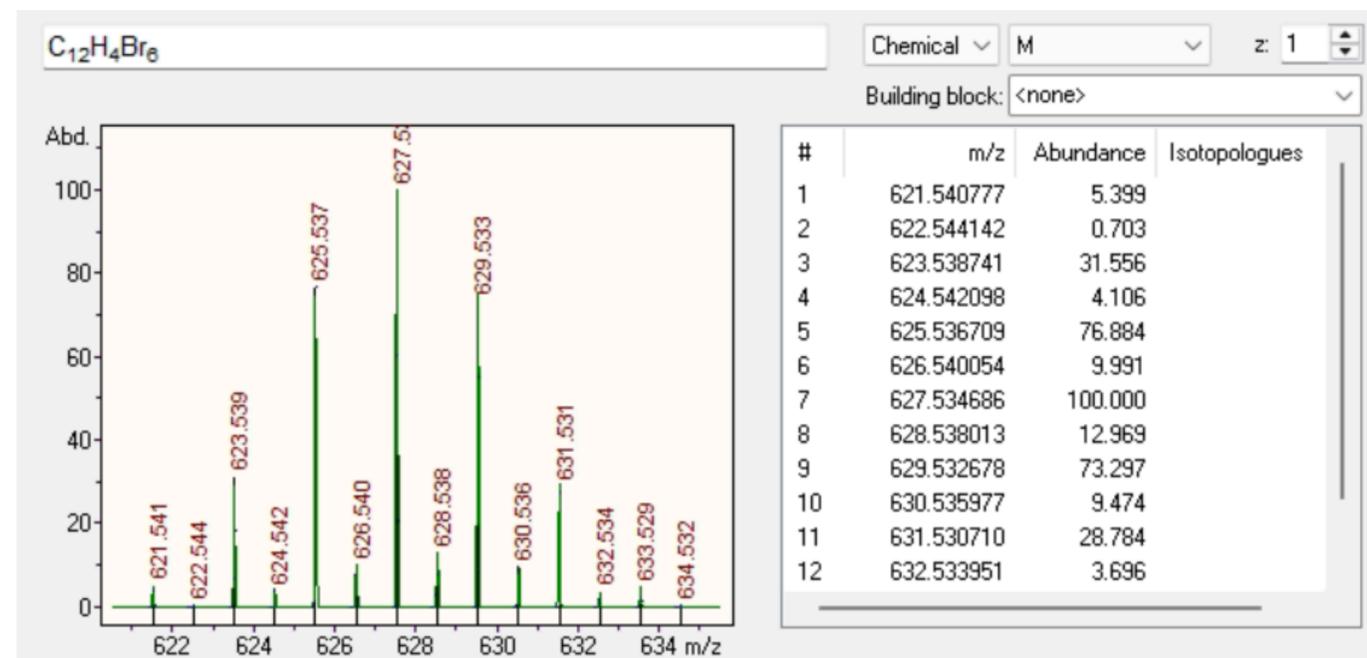
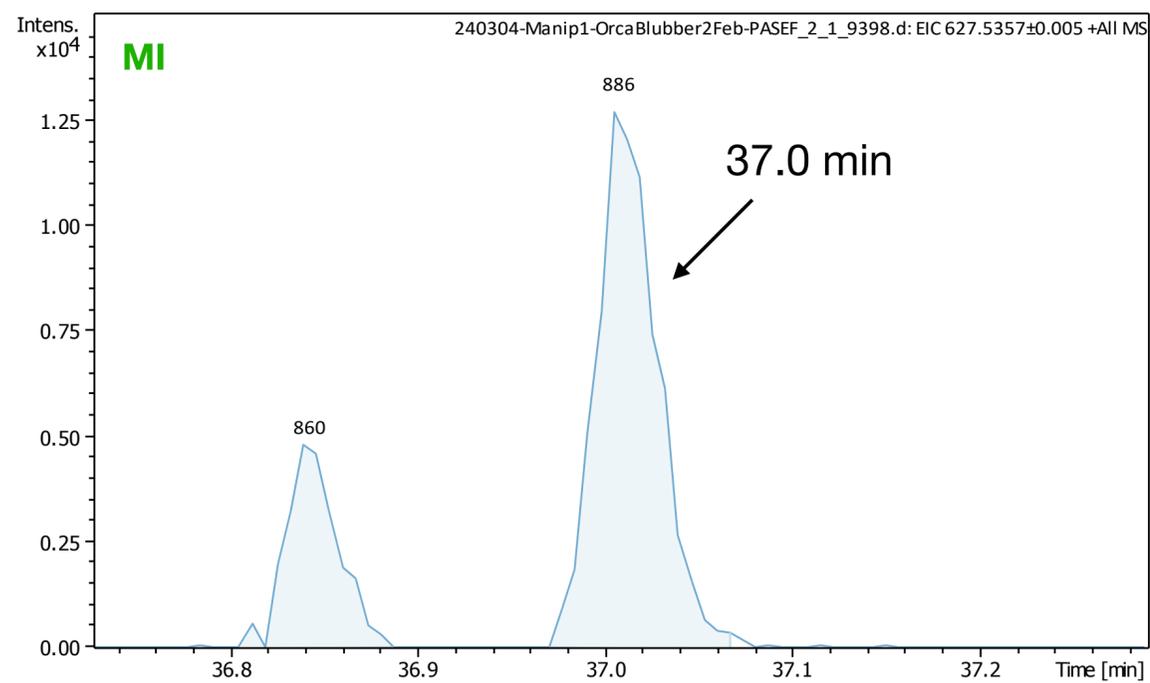


HxBBs (42 isomers)

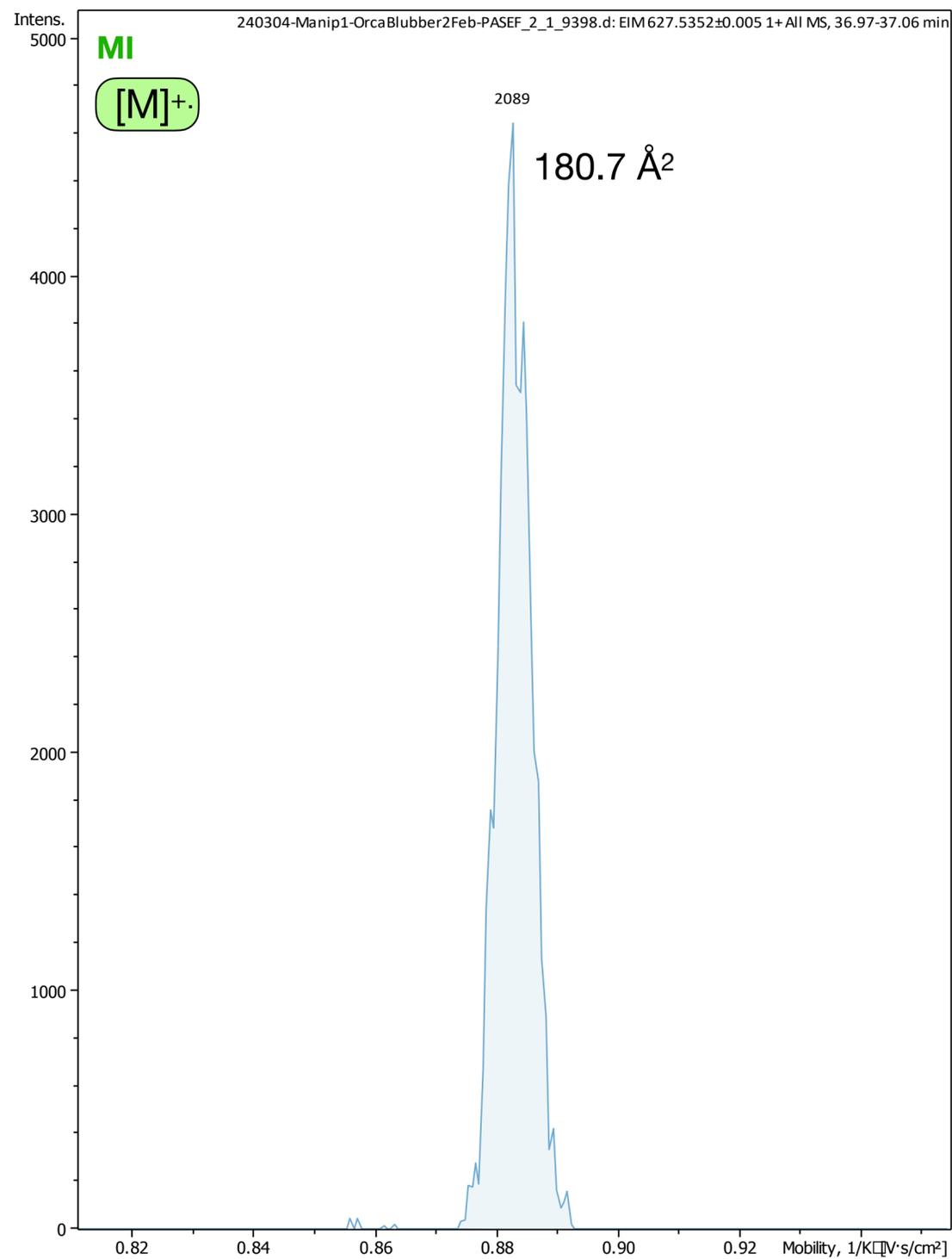
CCS pred HxBB
isomers: see Figure
S6.7B (manuscript)



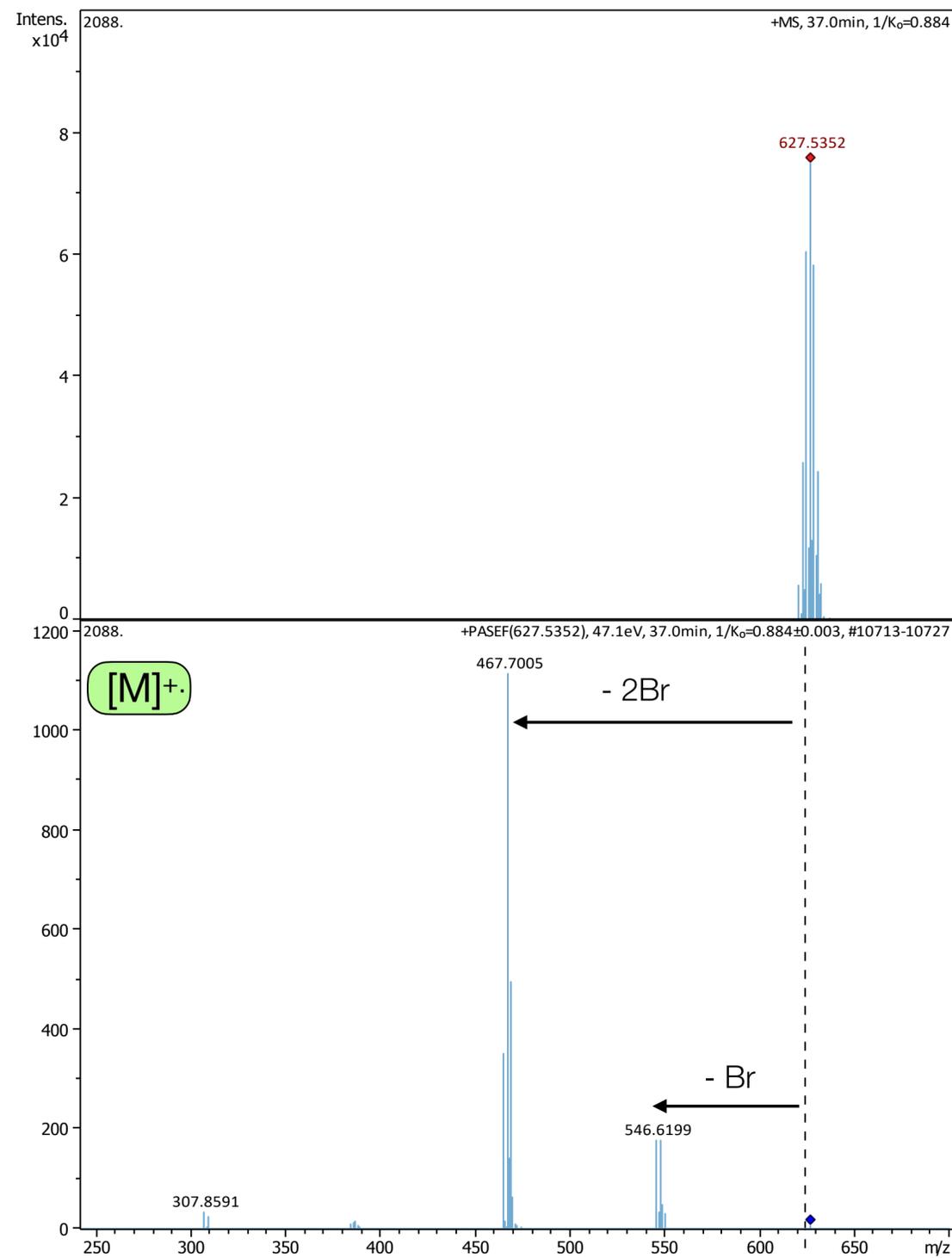
Chromatogram



Ion mobility spectrum

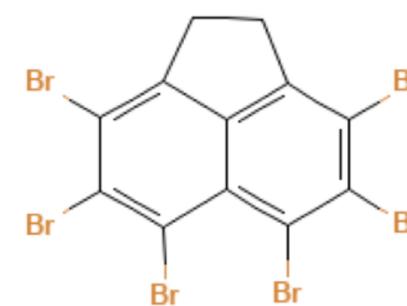


Tandem mass spectrum



Tentative candidate(s)

PubChem

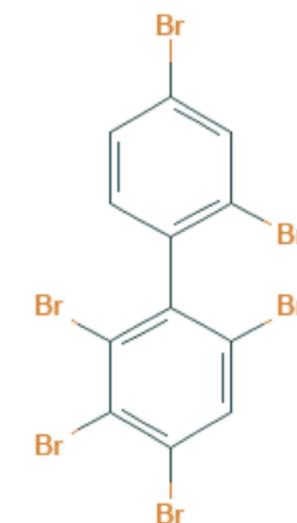
C₁₂Br₆H₄

Hexabromoacenaphthene

CCS pred: 173.7 Å² (-3.9%)

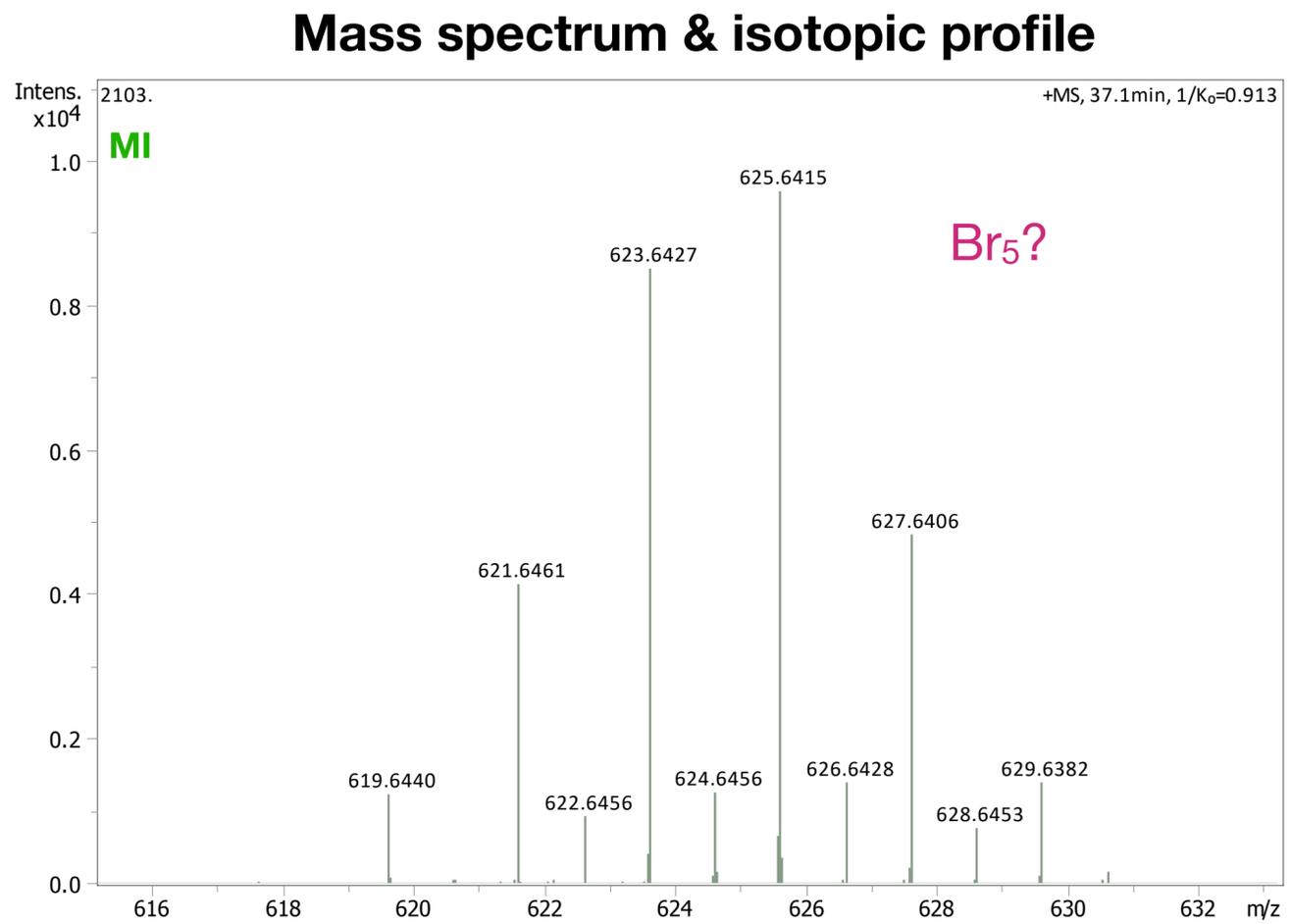
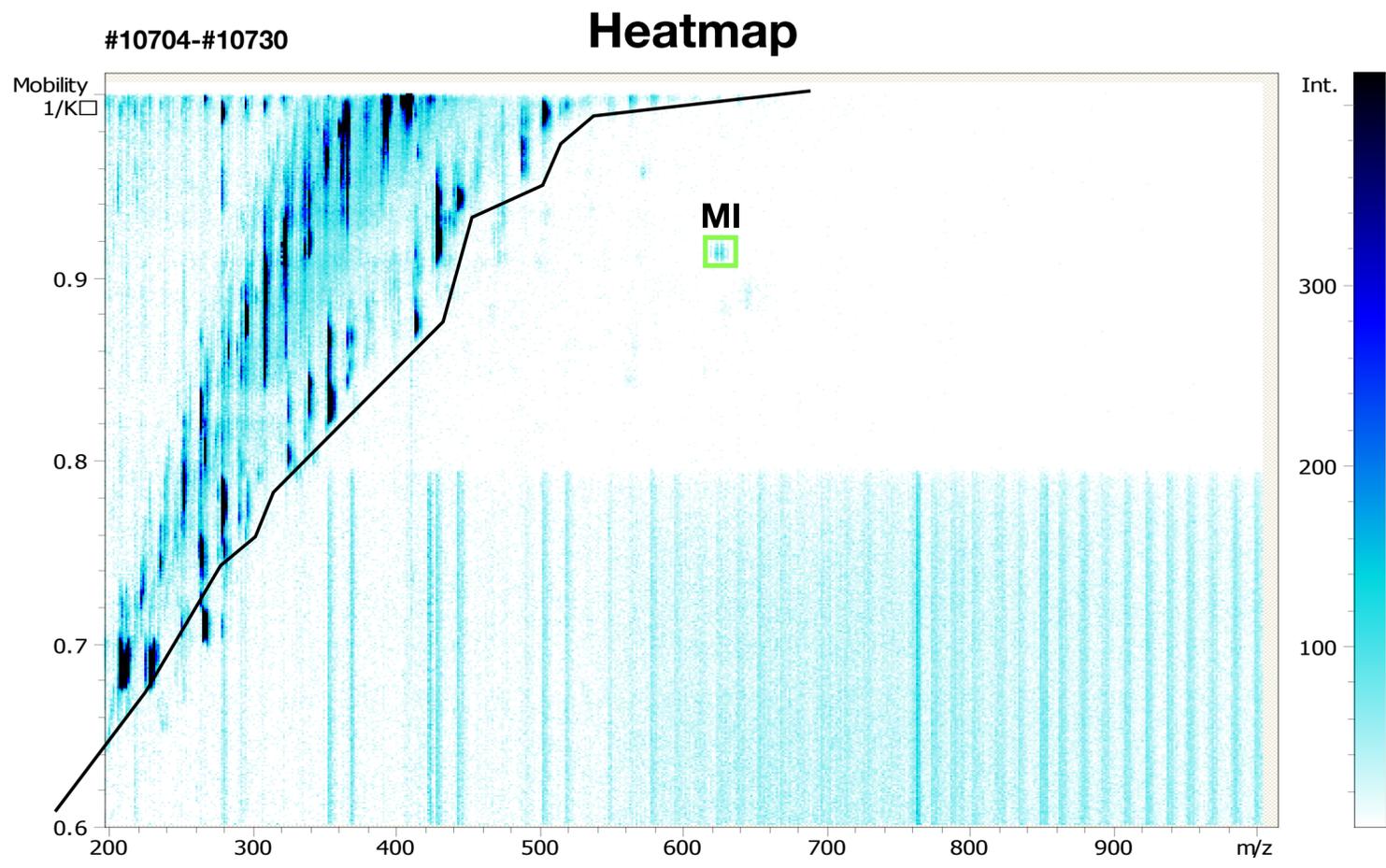
Confidence level

3

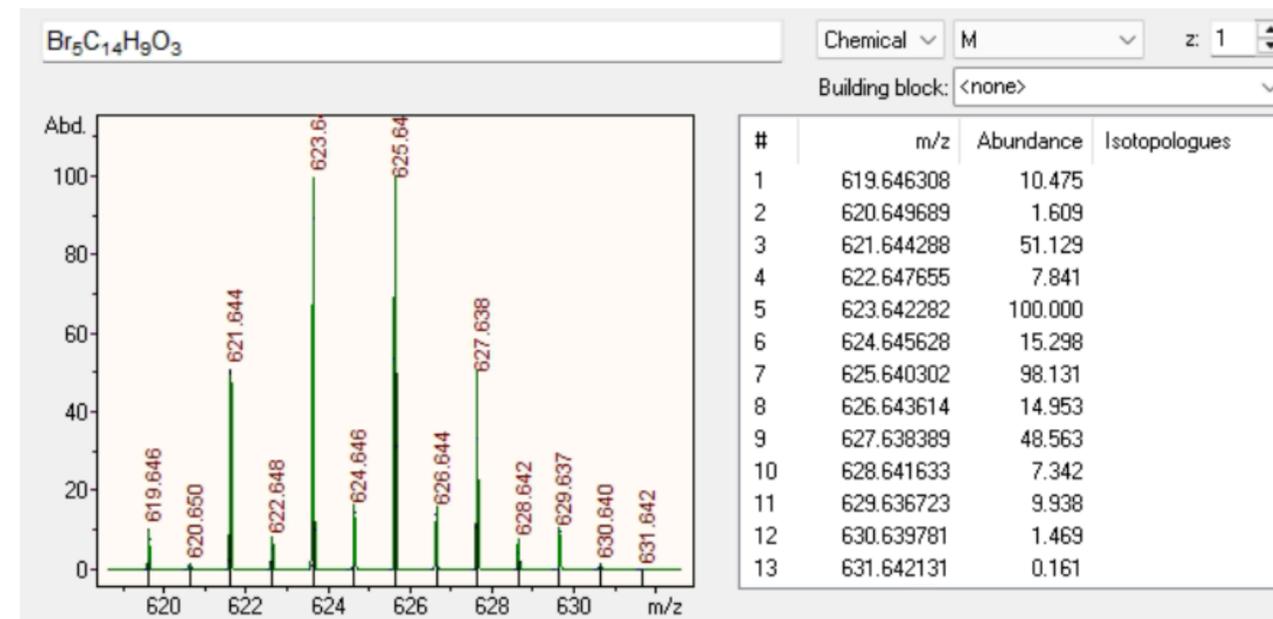
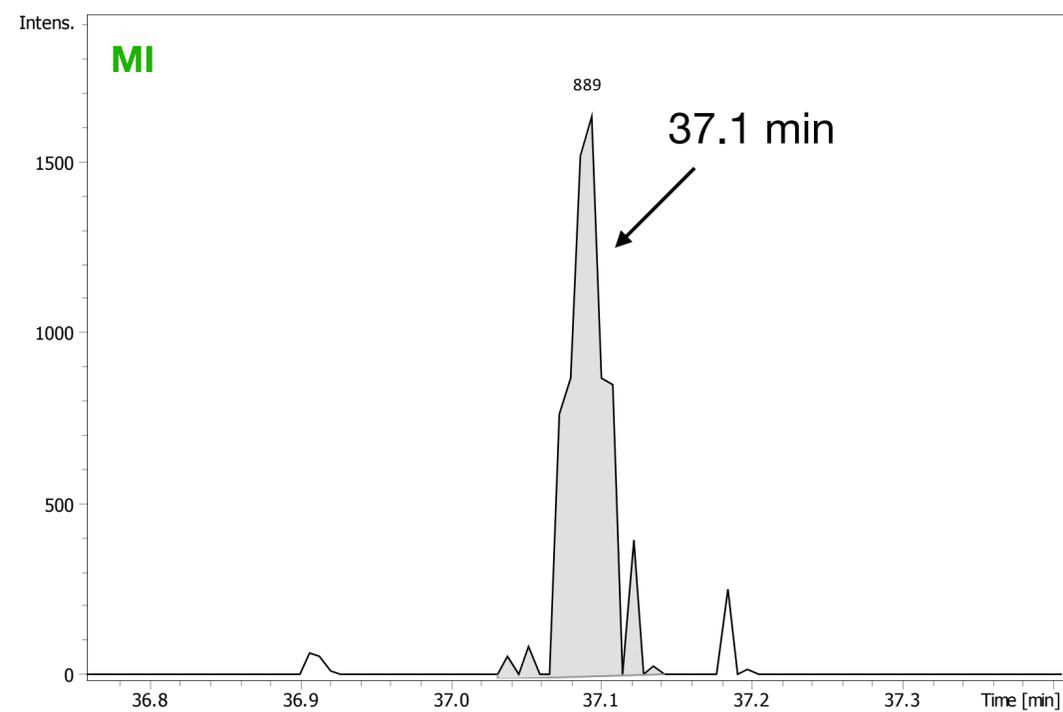


HxBBs (42 isomers)

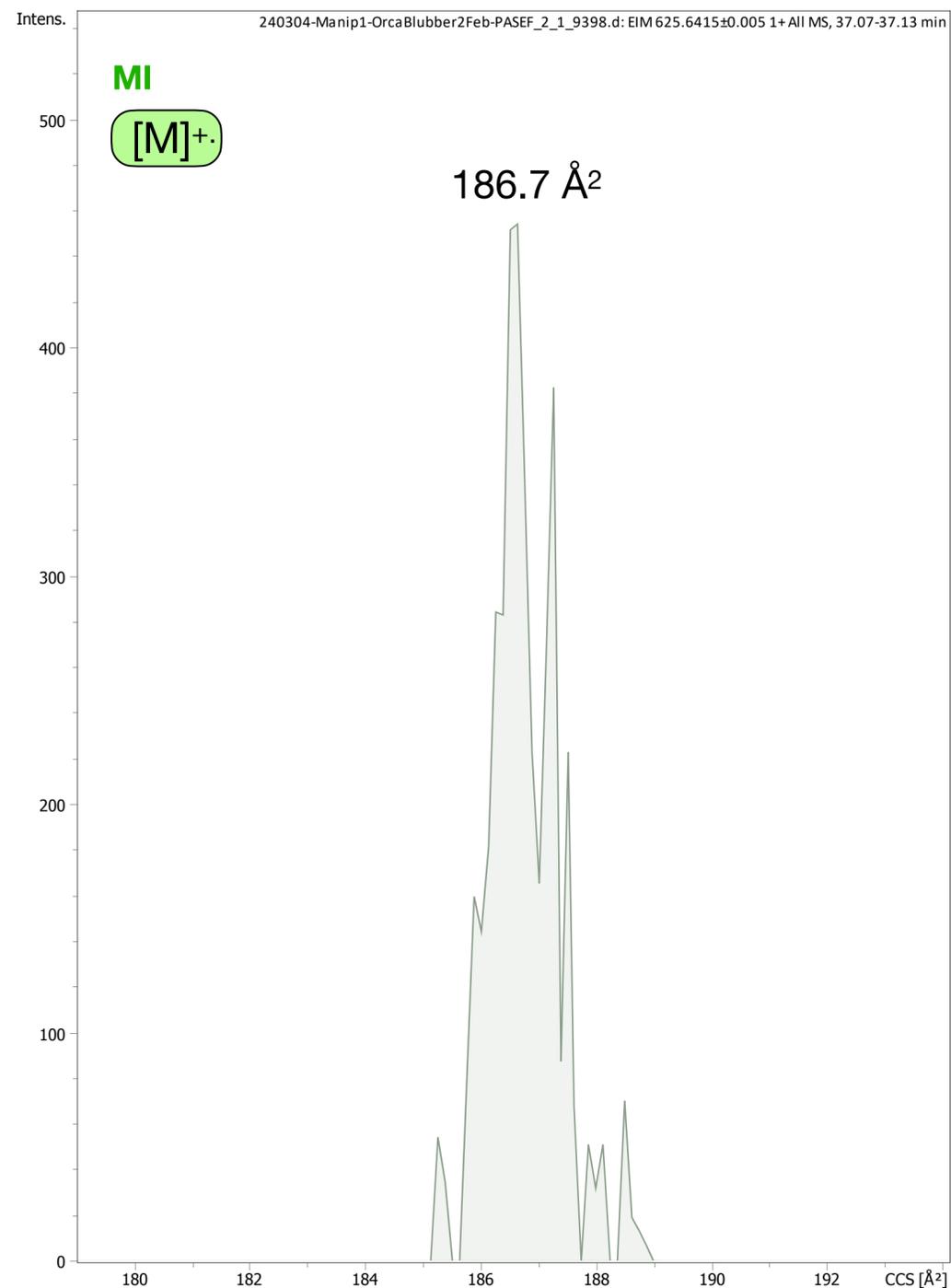
CCS pred HxBB
isomers: see Figure
S6.7B (manuscript)



Chromatogram



Ion mobility spectrum

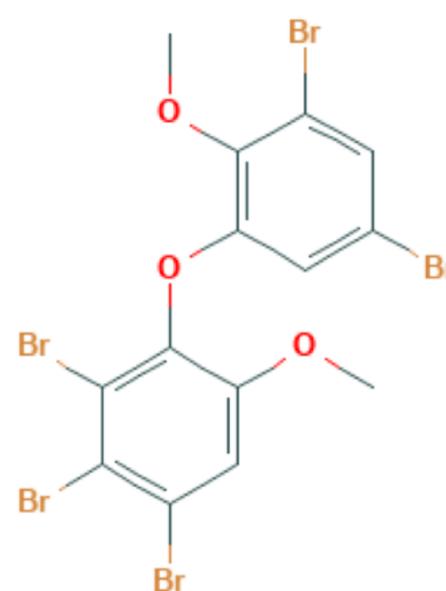


Tandem mass spectrum

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Tentative candidate(s)

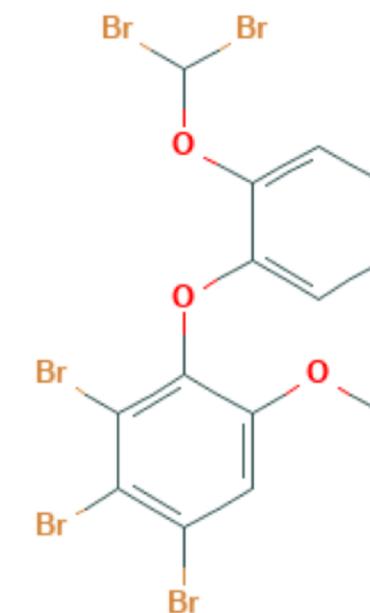
PubChem

C₁₄H₉O₃Br₅CCS pred (isomer 1): 193.9 Å²
(+3.9%)CCS pred (isomer 2): 193.8 Å²
(+3.8%)CCS pred (isomer 3): 193.8 Å²
(+3.8%)CCS pred (isomer 4): 193.8 Å²
(+3.8%)Pentabromodimethoxydiphenyl ethers
(multiple isomers)

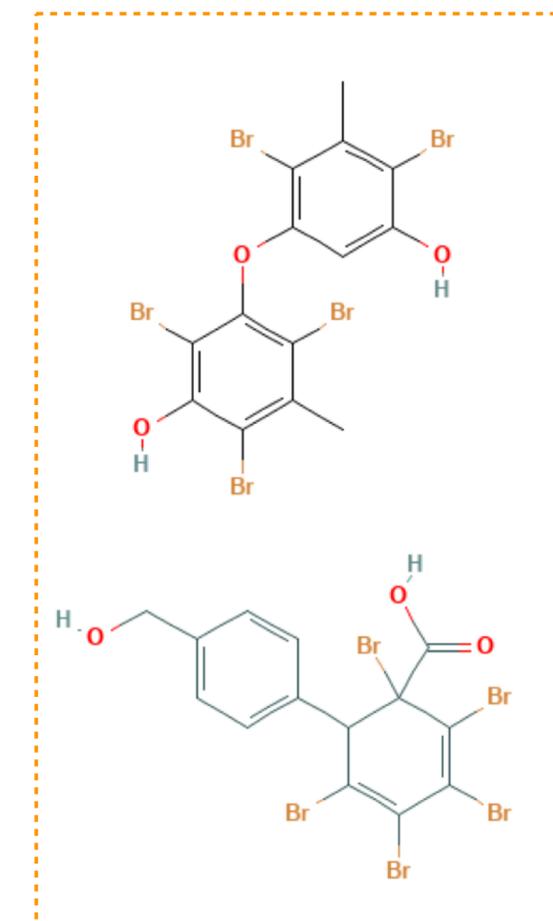
⇒ NHC?

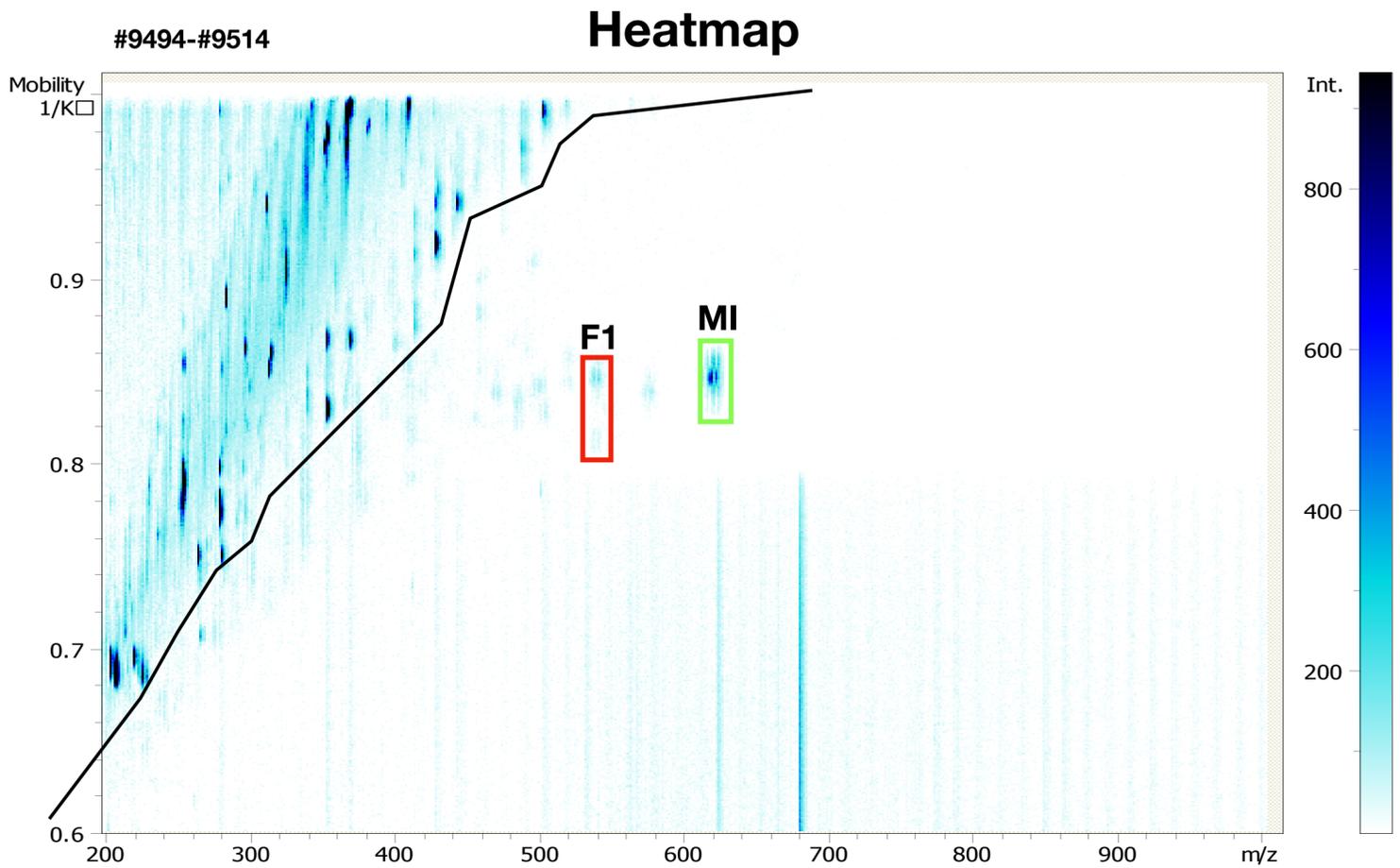
Confidence level

3



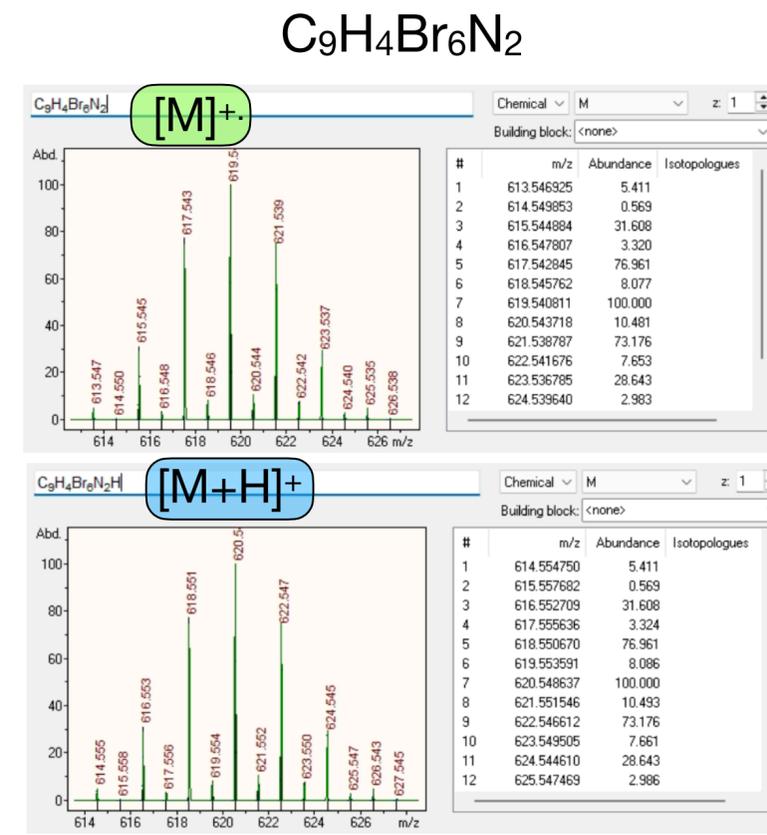
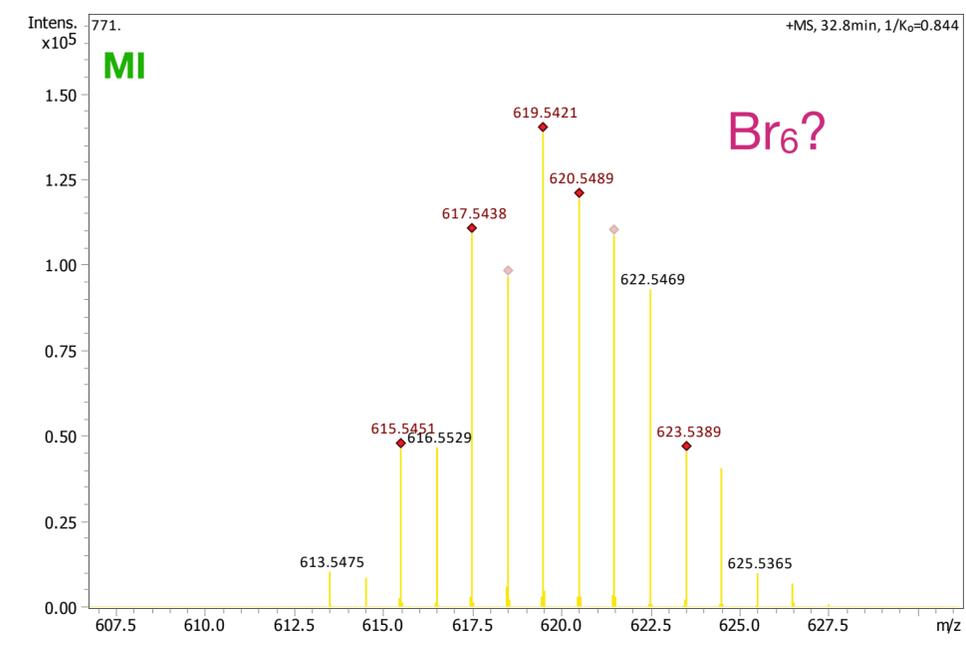
1,2,3-Tribromo-4-[2-(dibromomethoxy)phenoxy]-5-methoxybenzene

CCS pred: 190.0 Å² (+1.8%)⇒ Not GC amenable
(Alcohol groups)



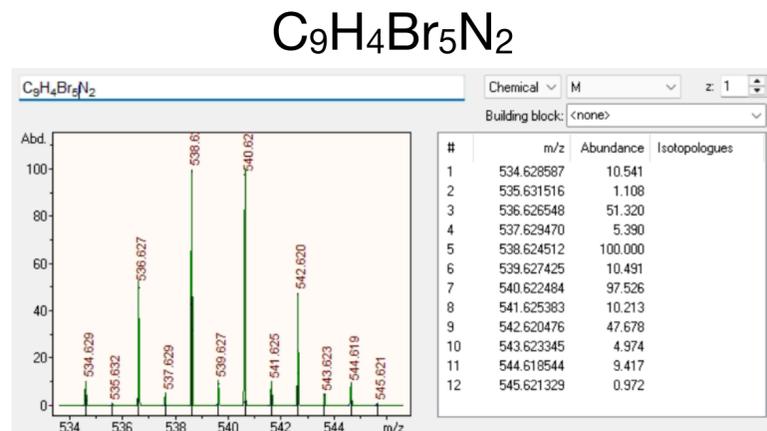
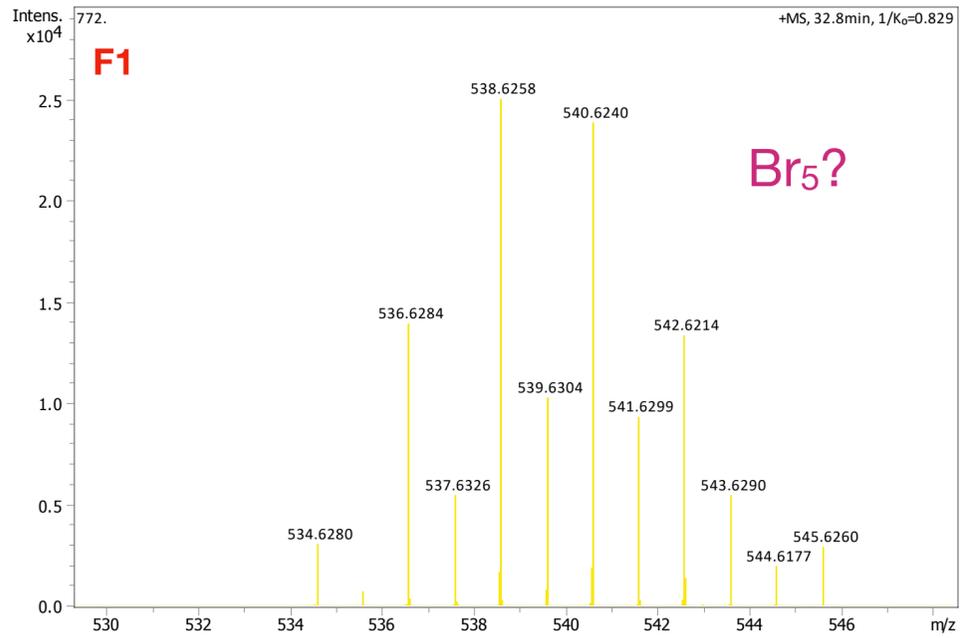
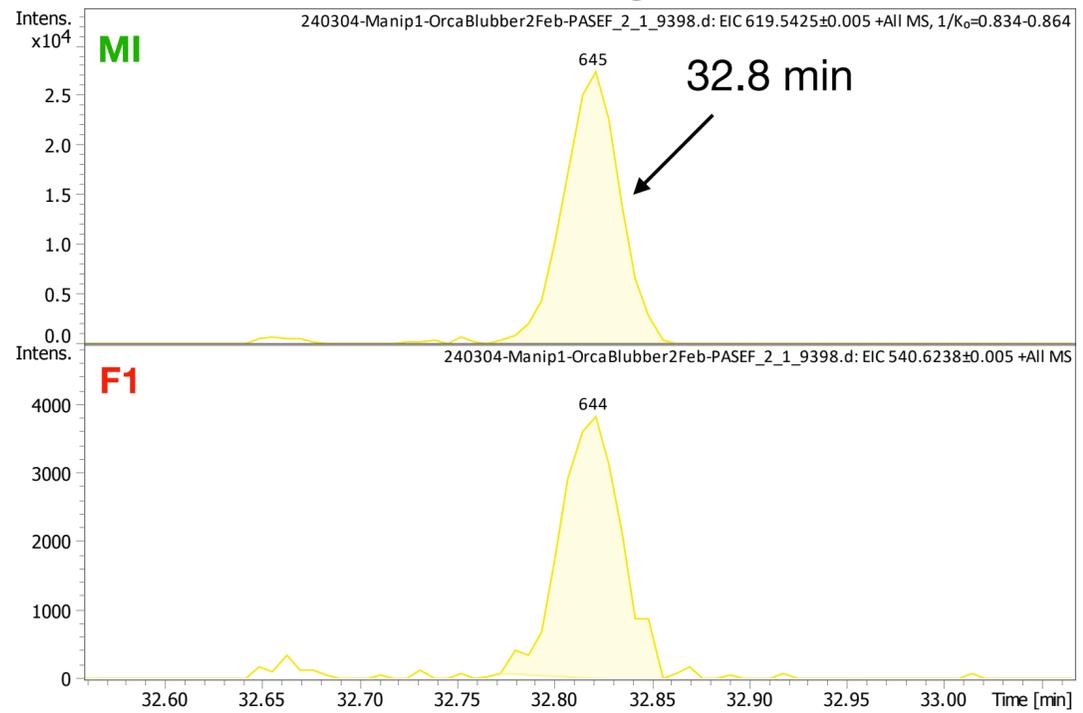
Mass spectra & isotopic profile

⇒ High proportion of protonation

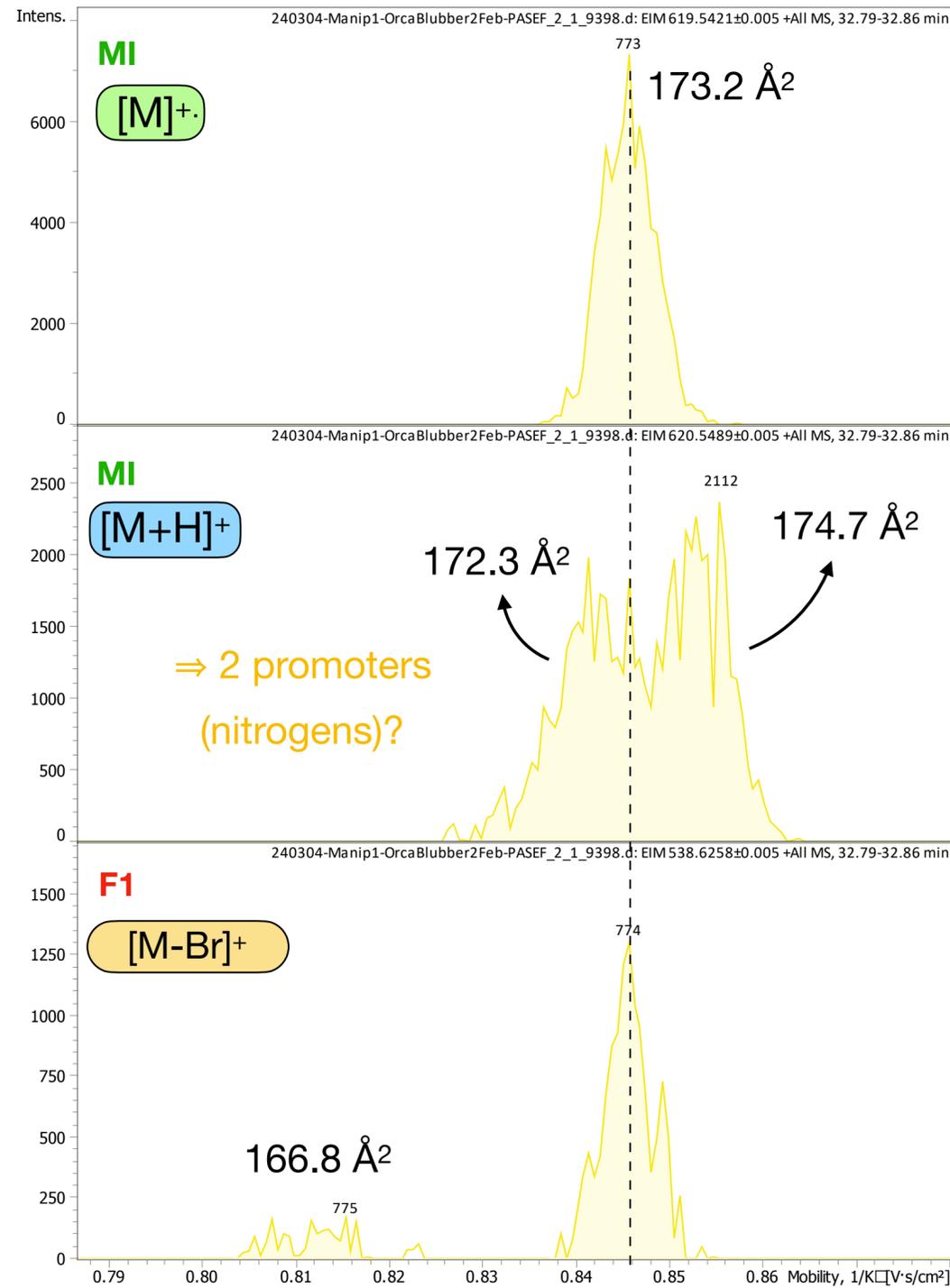


↓ -Br

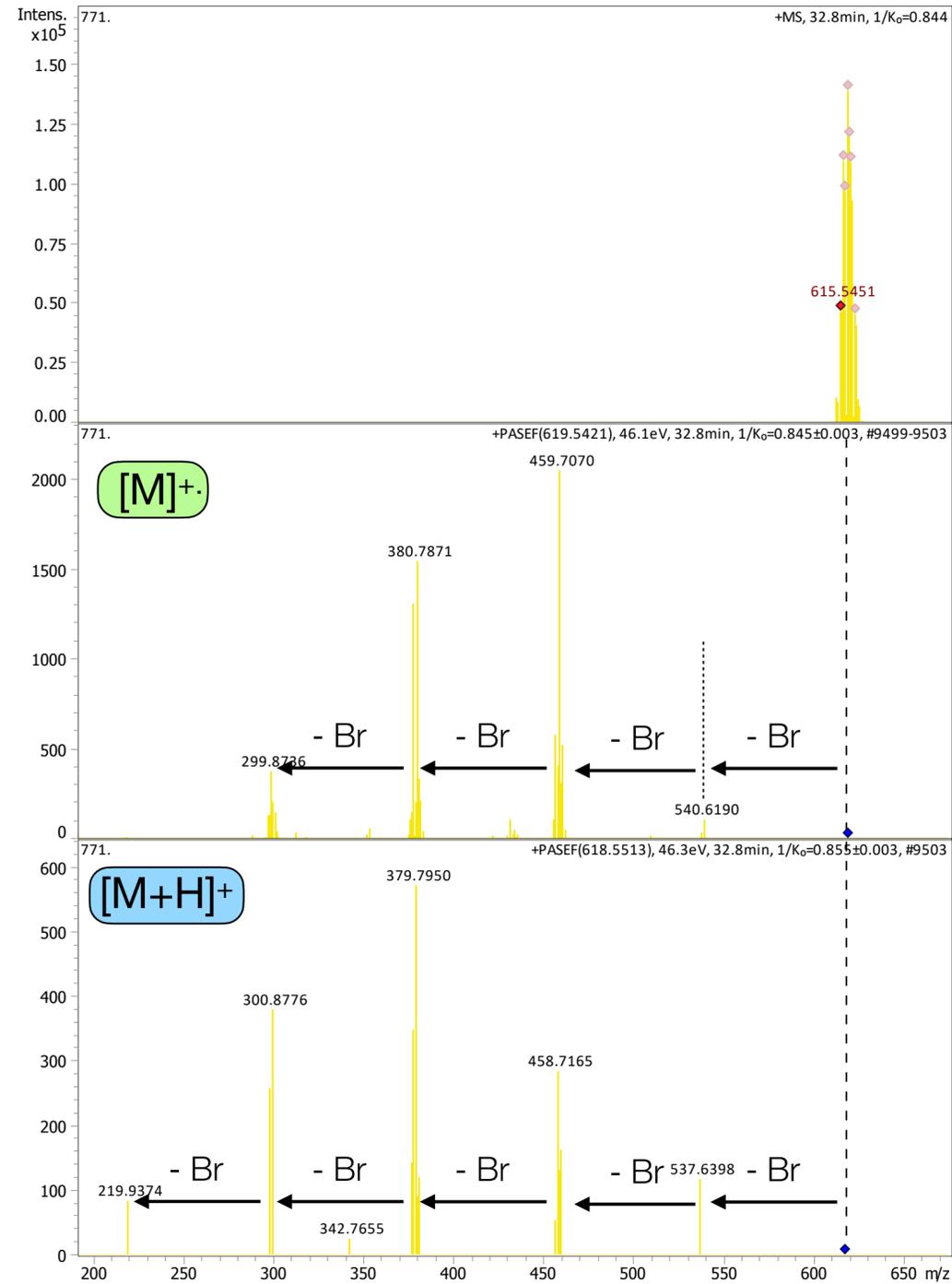
Chromatogram



Ion mobility spectra



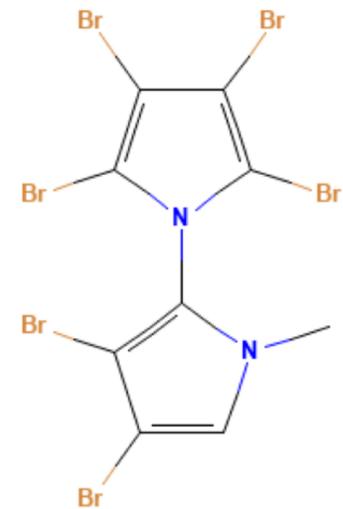
Tandem mass spectra



⇒ At least 5 Br

Tentative candidate(s)

PubChem



Hexabrominated methyl bipyrroles HxBMBPs (Multiple isomers)

⇒ HNPs?

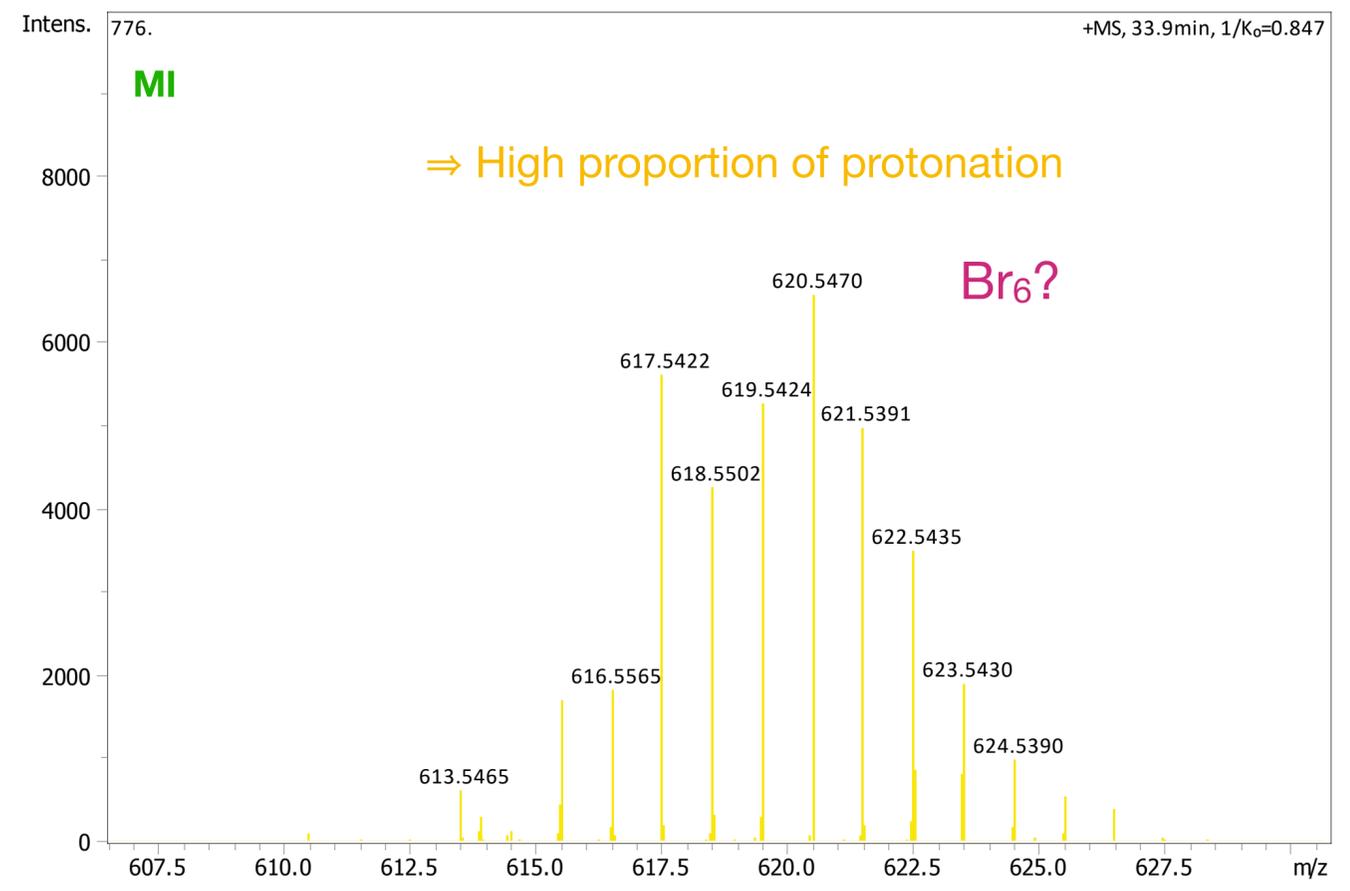
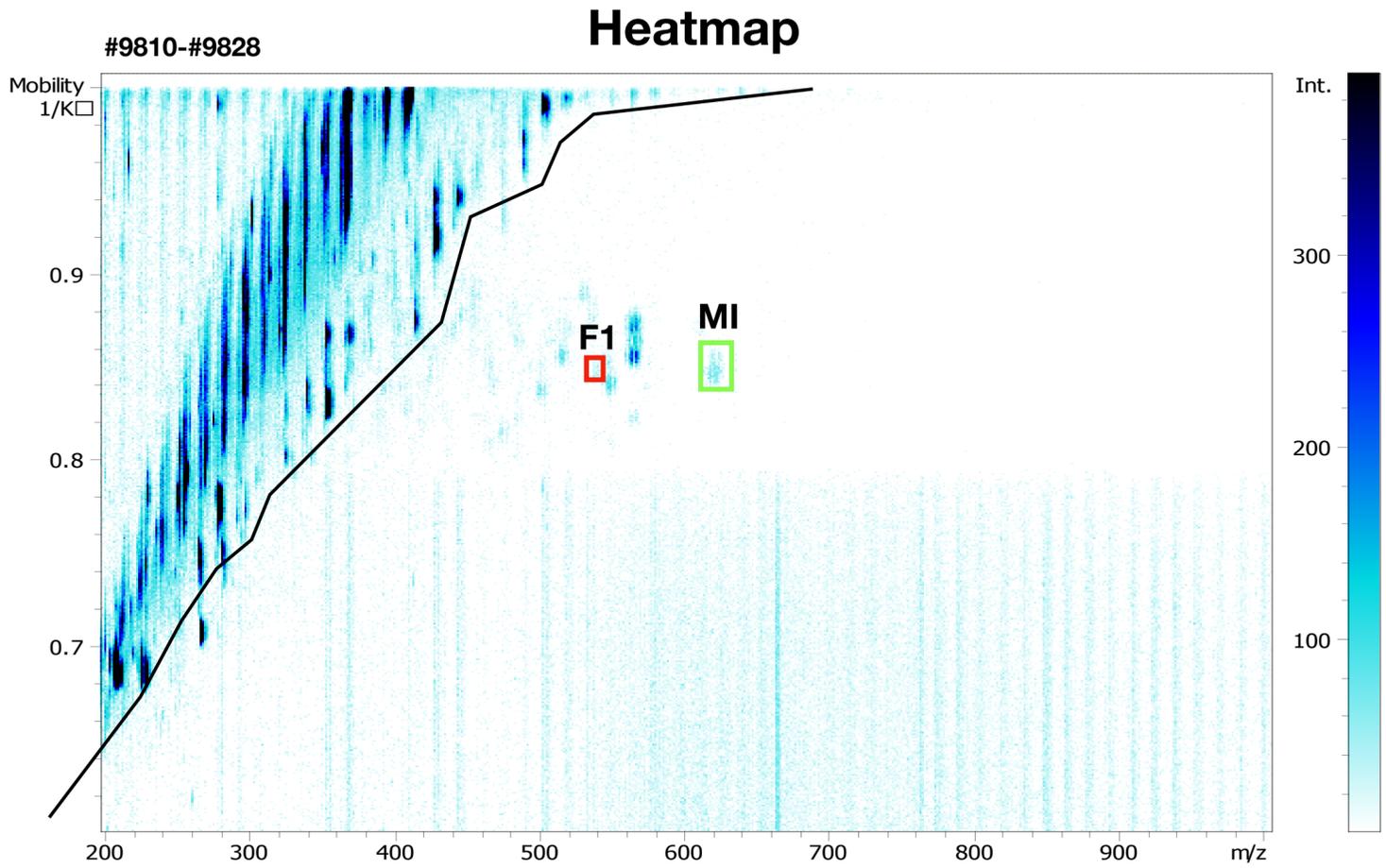
CCS pred (isomer 1): 170.8 Å² (-1.4%)

CCS pred (isomer 2): 170.2 Å² (-1.7%)

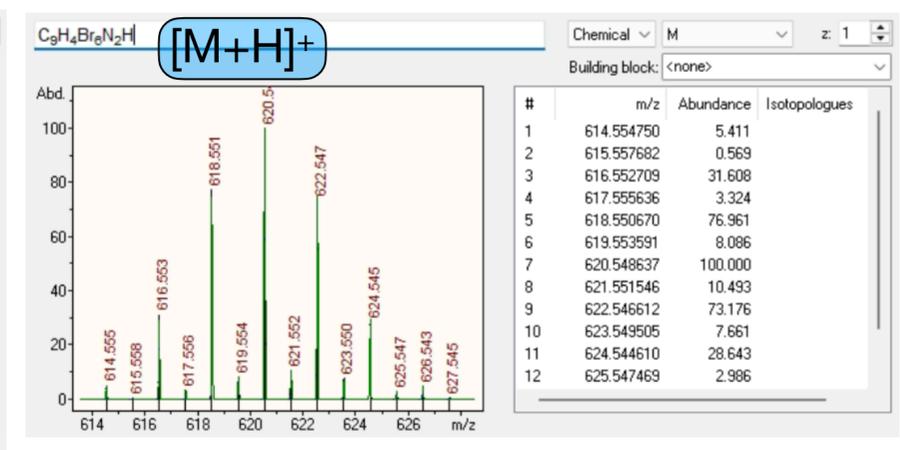
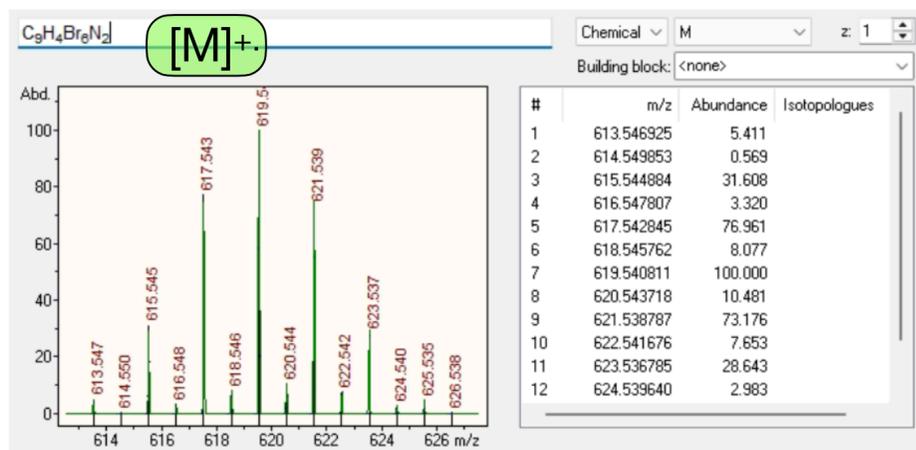
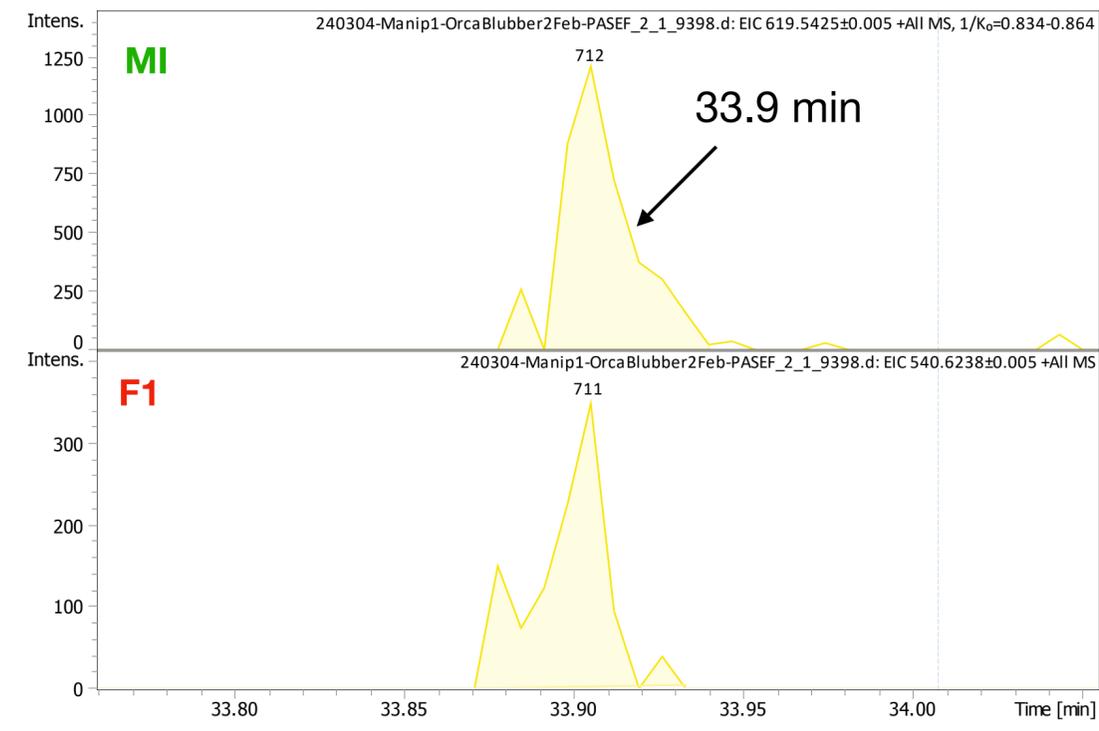
Confidence level

3

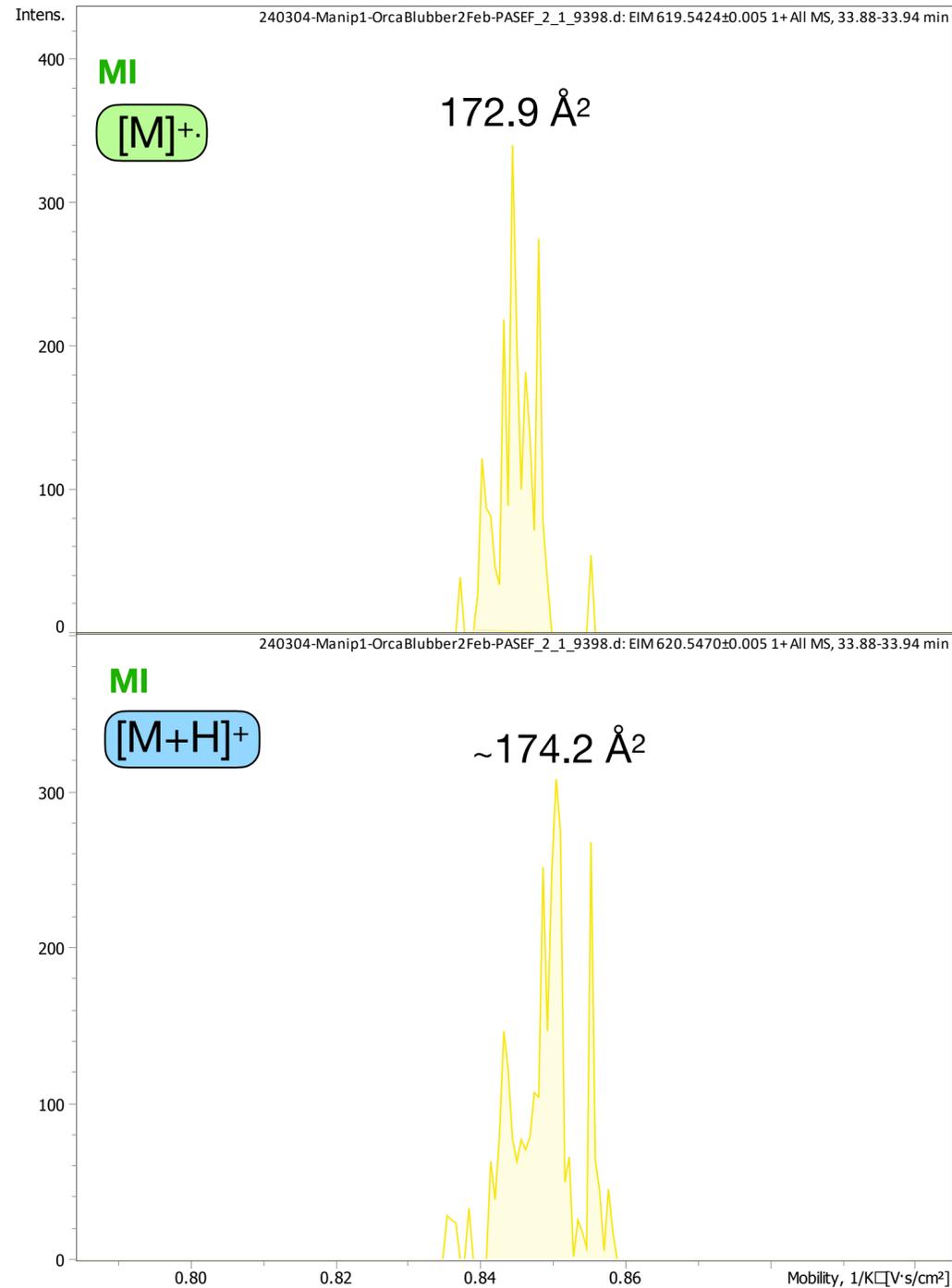
Mass spectrum & isotopic profile



Chromatogram



Ion mobility spectra

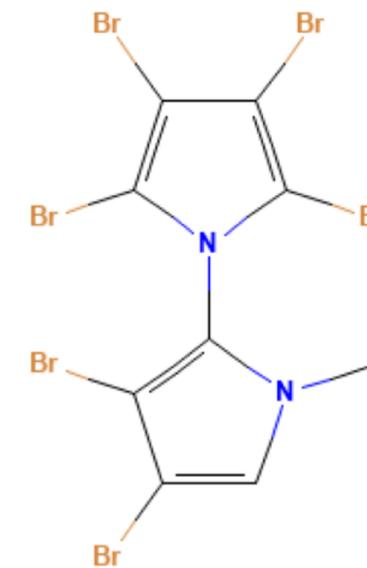


Tandem mass spectrum

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Tentative candidate(s)

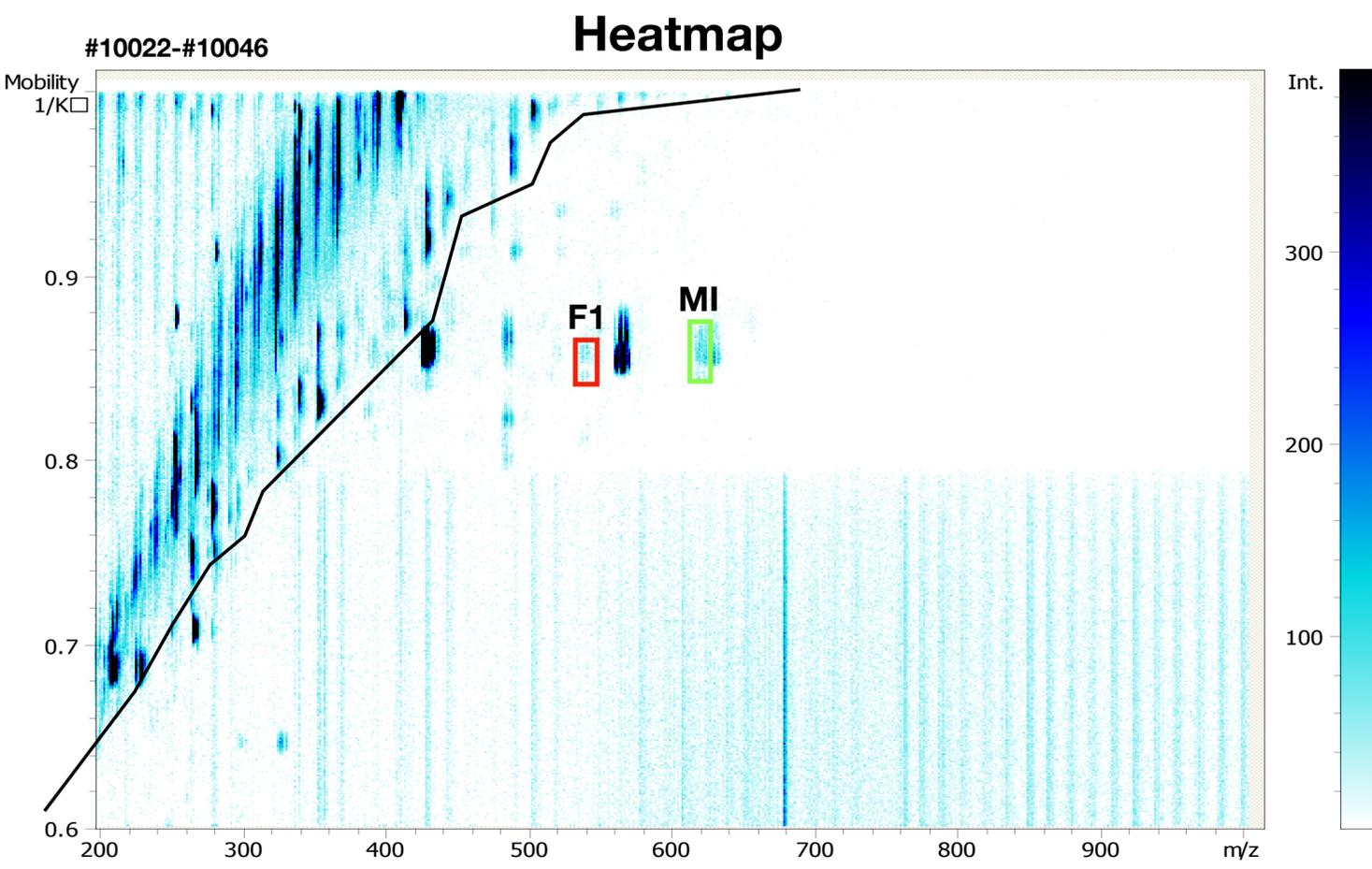
PubChem

C₉H₄Br₆N₂CCS pred (isomer 1):
170.8 Å² (-1.2%)CCS pred (isomer 2):
170.2 Å² (-1.6%)Hexabrominated
methyl bipyrroles
HxBMBPs (Multiple
isomers)

⇒ HNPs?

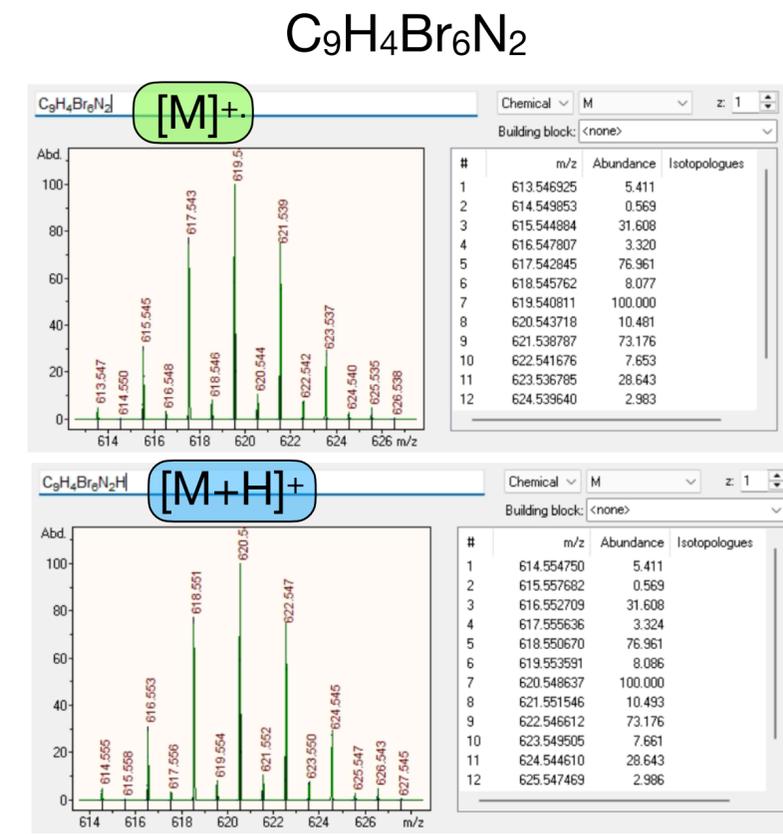
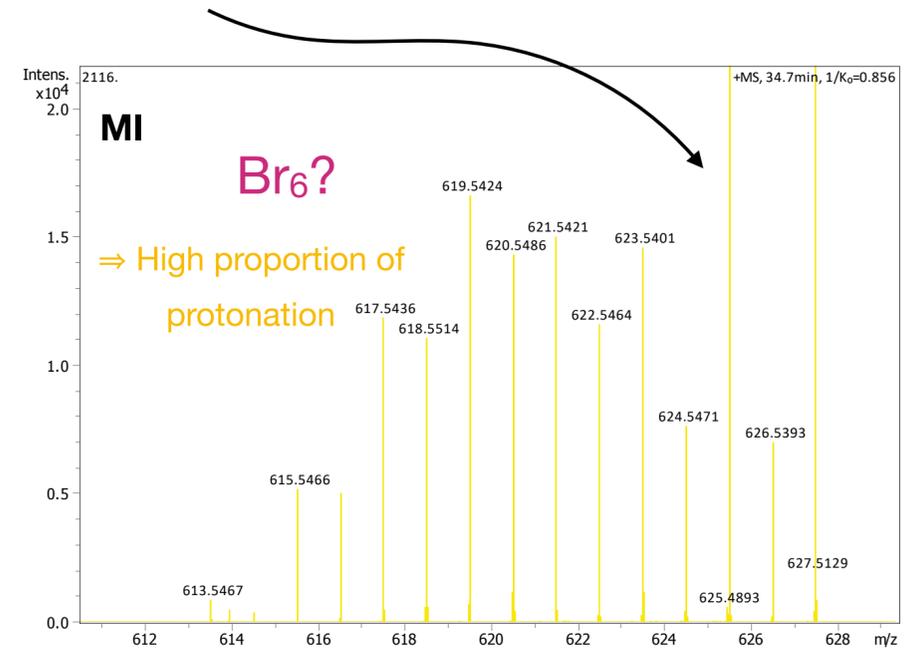
Confidence level

3

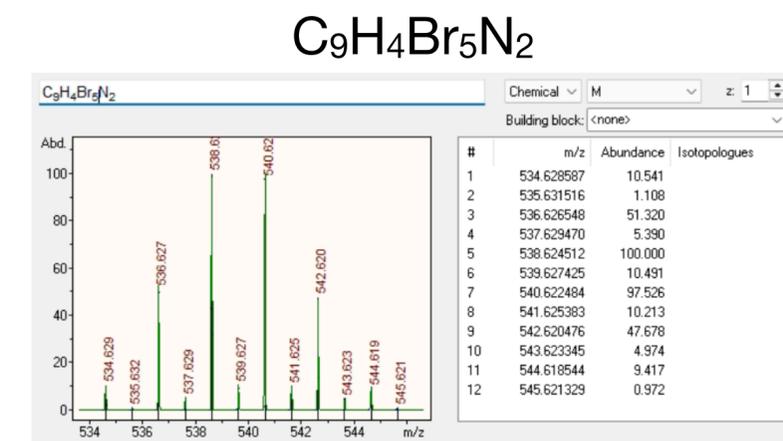
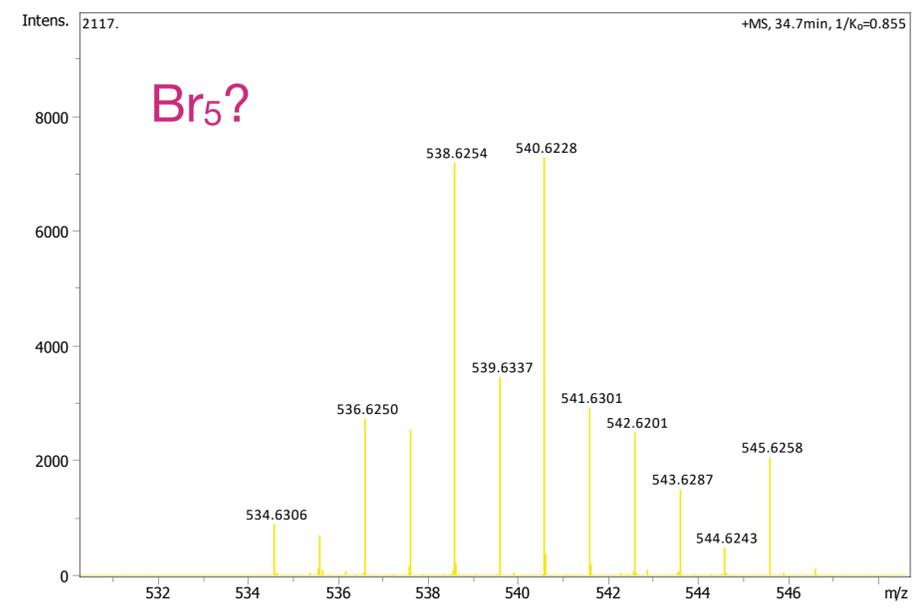


Coeluting isobaric interference (Feature #17)

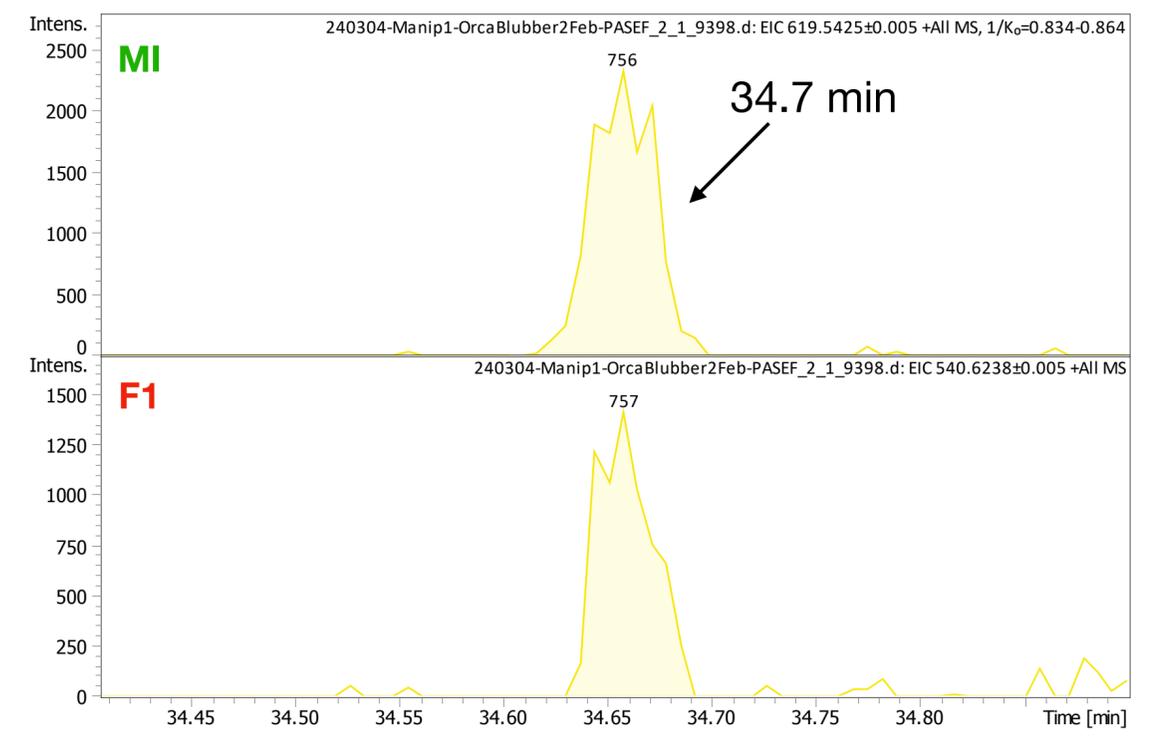
Mass spectra & isotopic profile



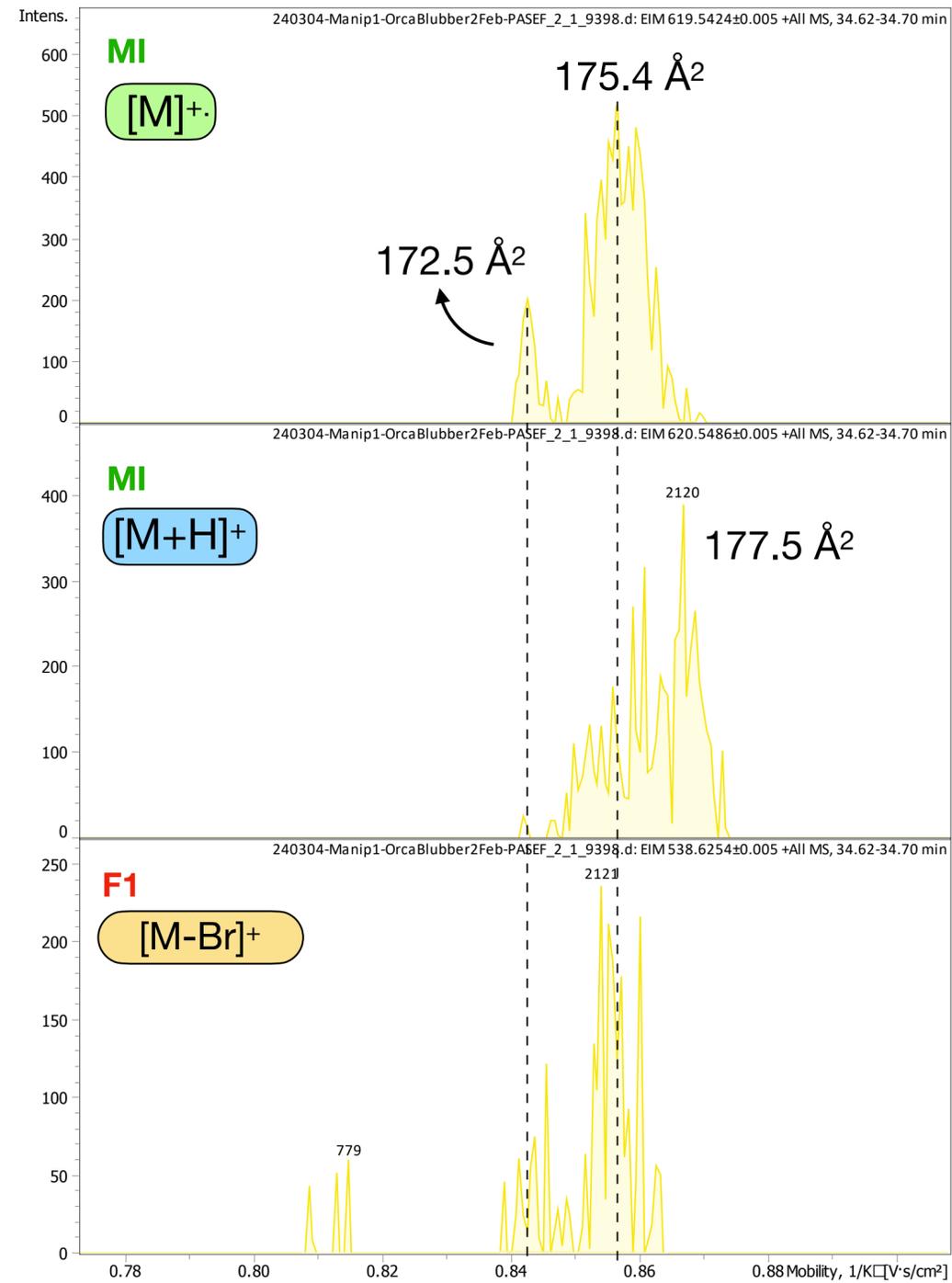
-Br



Chromatogram



Ion mobility spectra

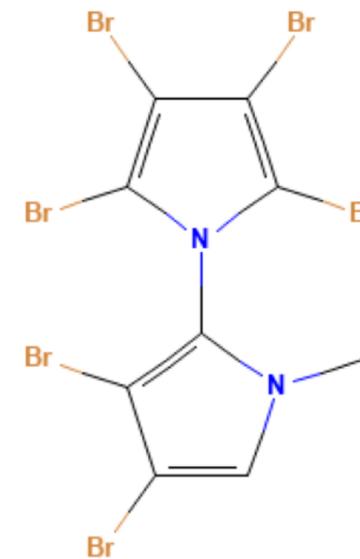


Tandem mass spectrum

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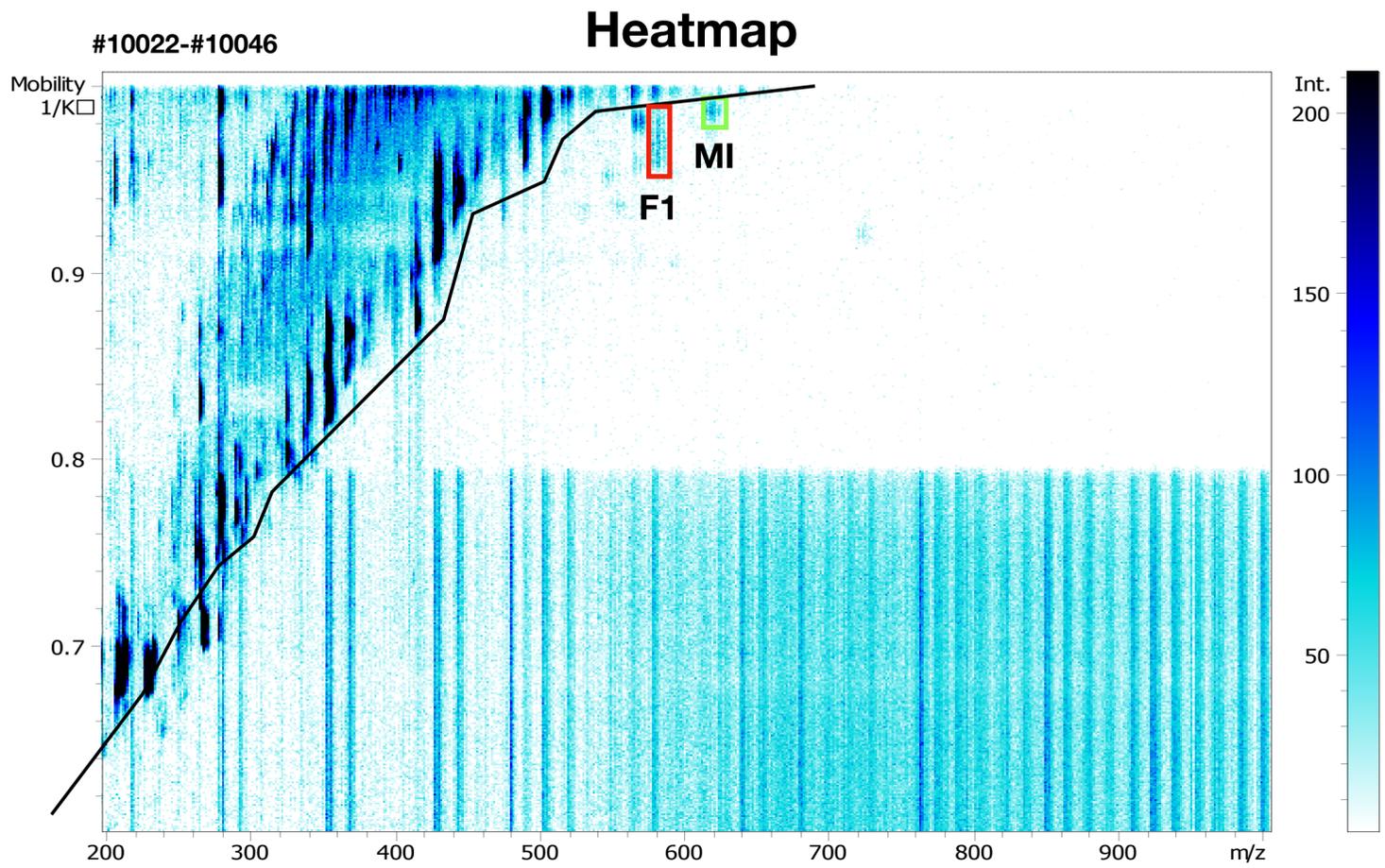
Tentative candidate(s)

PubChem

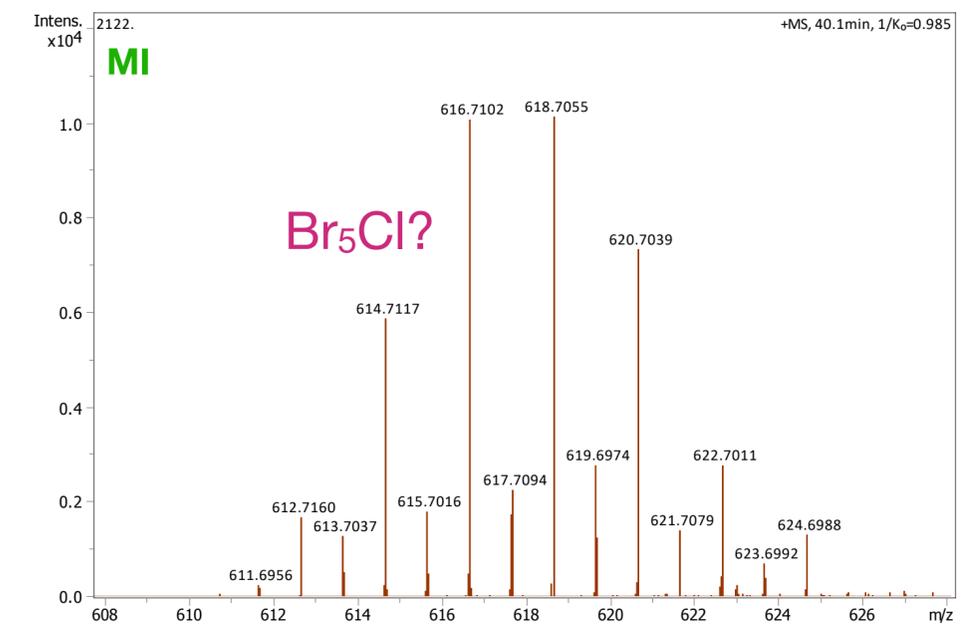
CCS pred (isomer 1):
170.8 Å \square (-2.6%)CCS pred (isomer 2):
170.2 Å \square (-3.0%)Hexabrominated
methyl bipyrroles
HxBMBPs (Multiple
isomers) \Rightarrow HNPs?

Confidence level

3

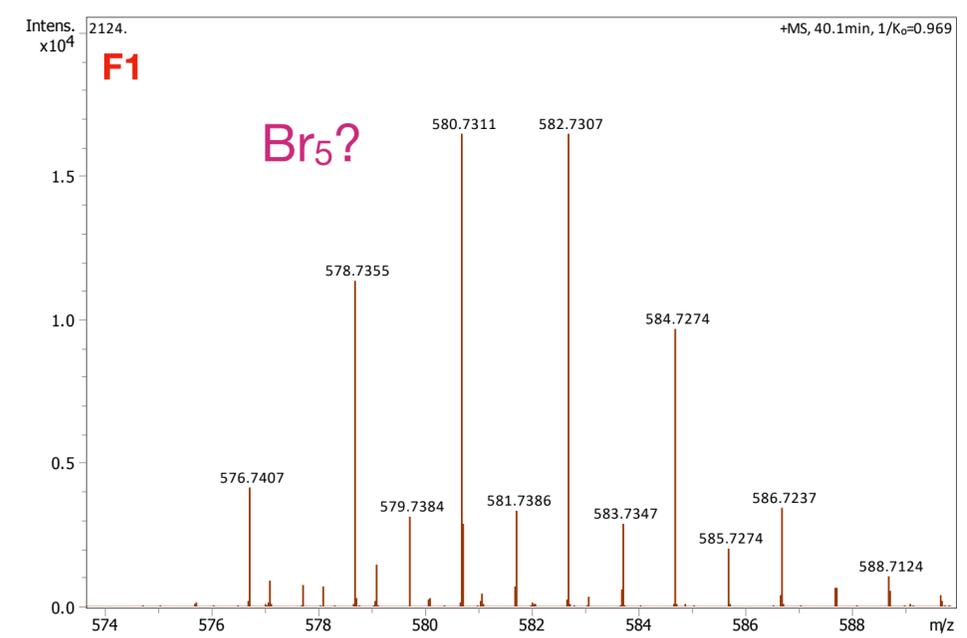
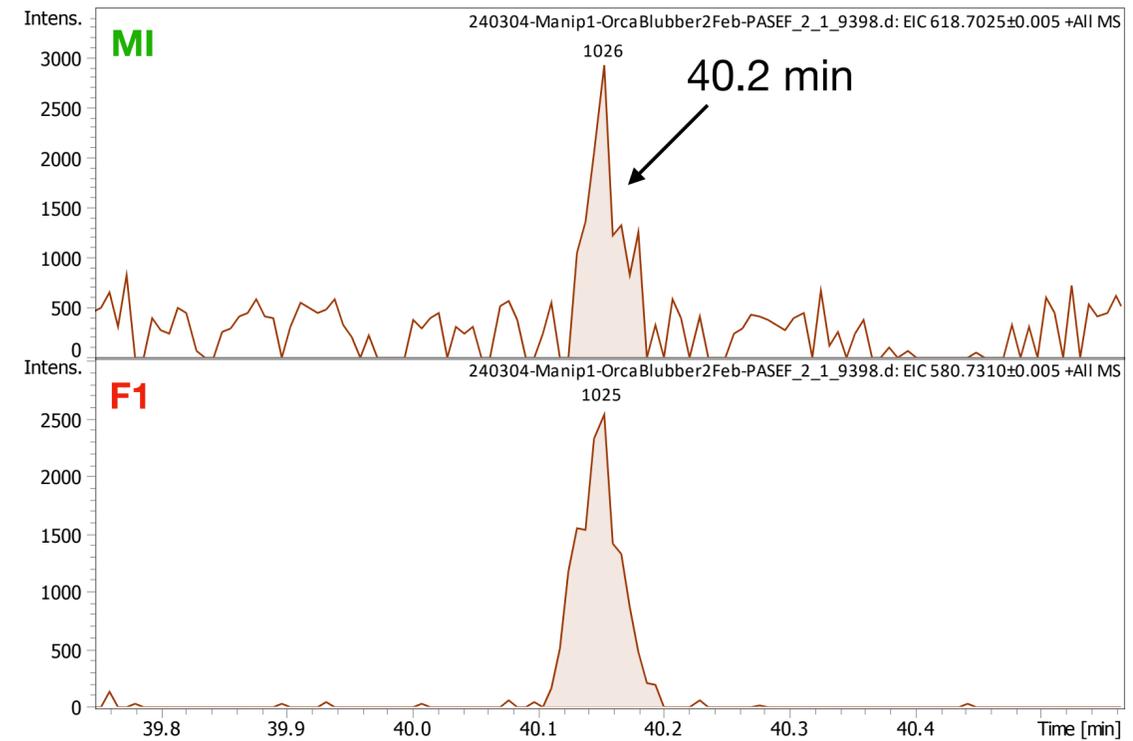


Mass spectra & isotopic profile

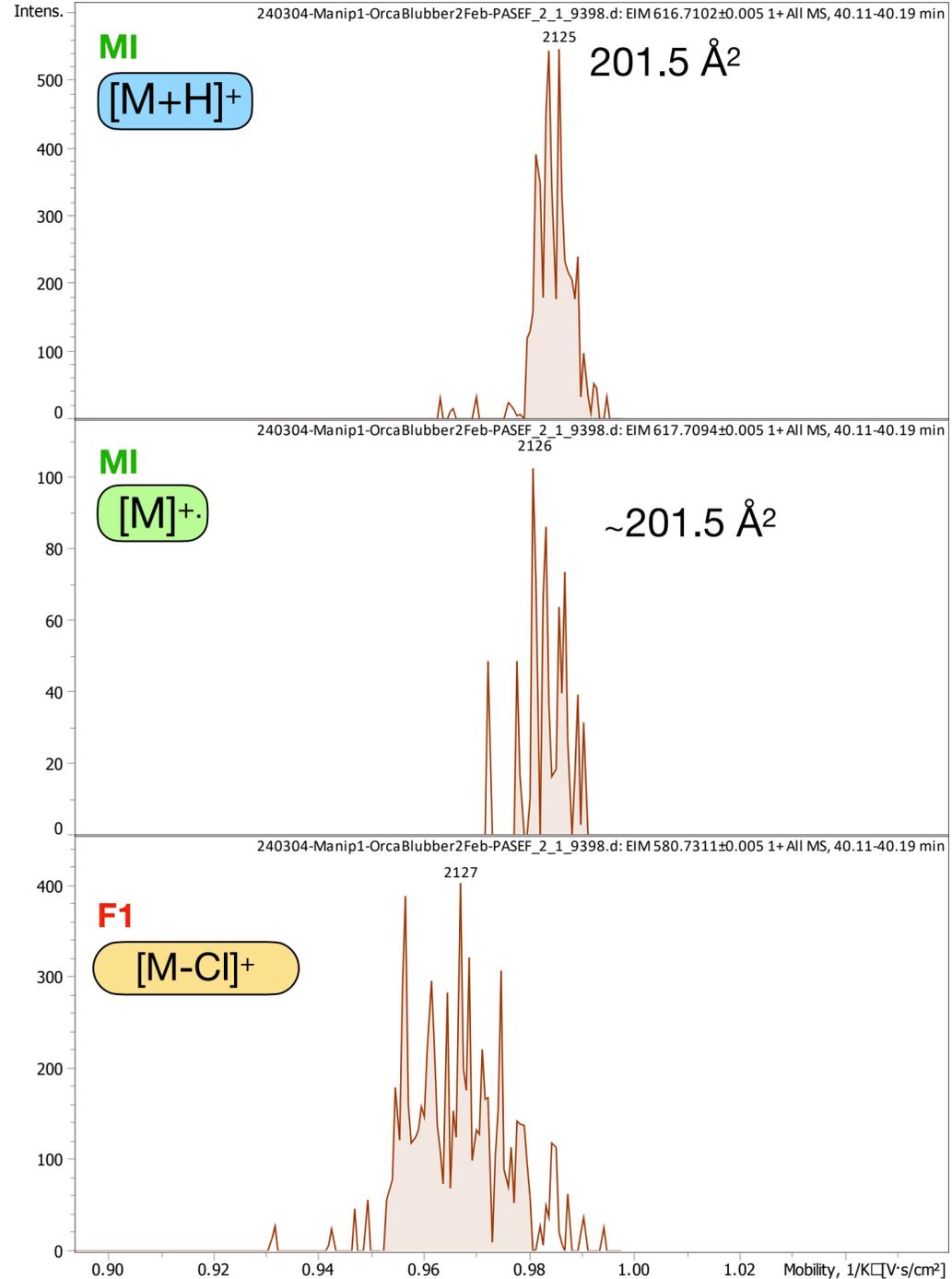


↓ -(H)Cl?

Chromatogram



Ion mobility spectra



Tandem mass spectrum

/

Tentative candidate(s)

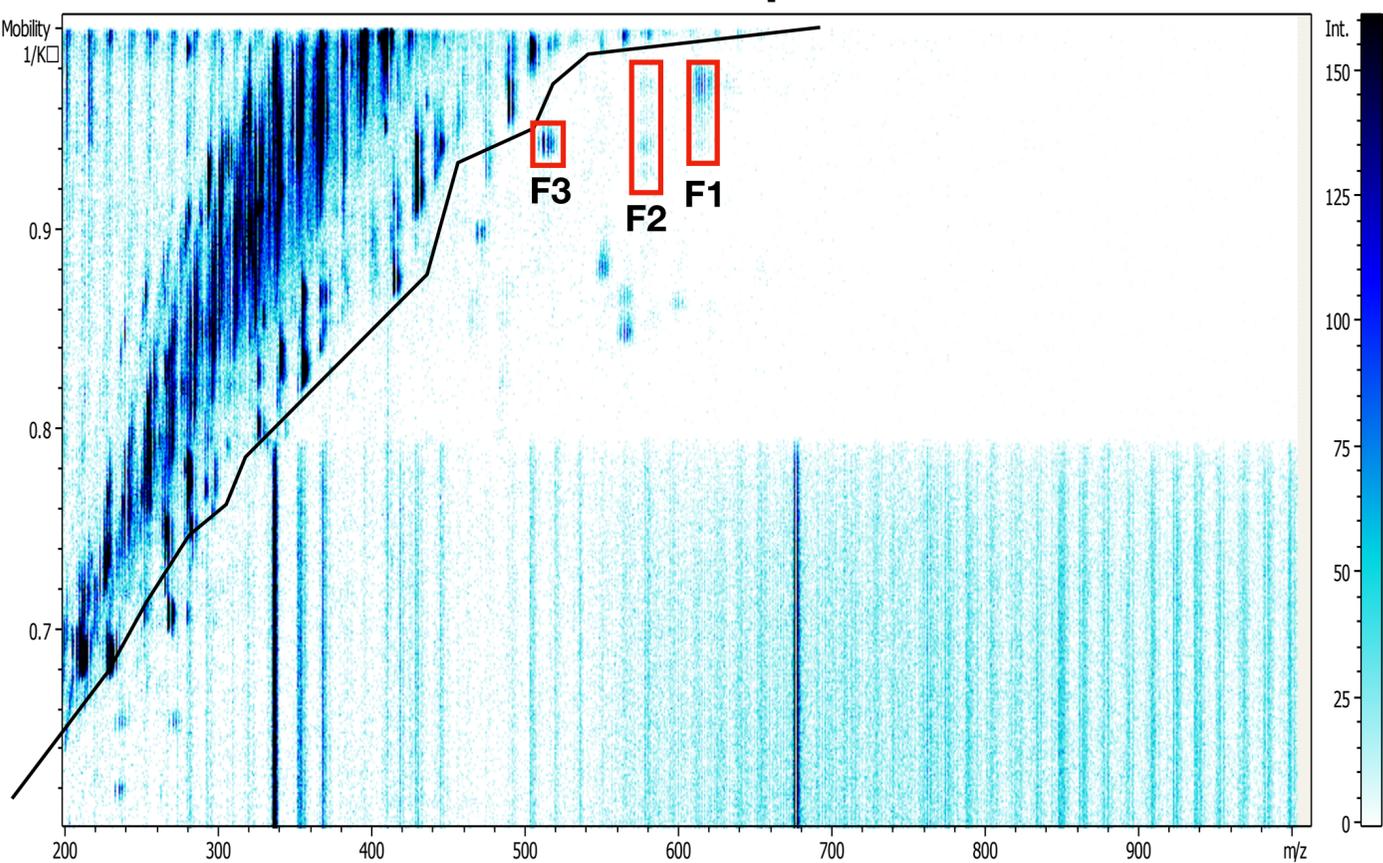


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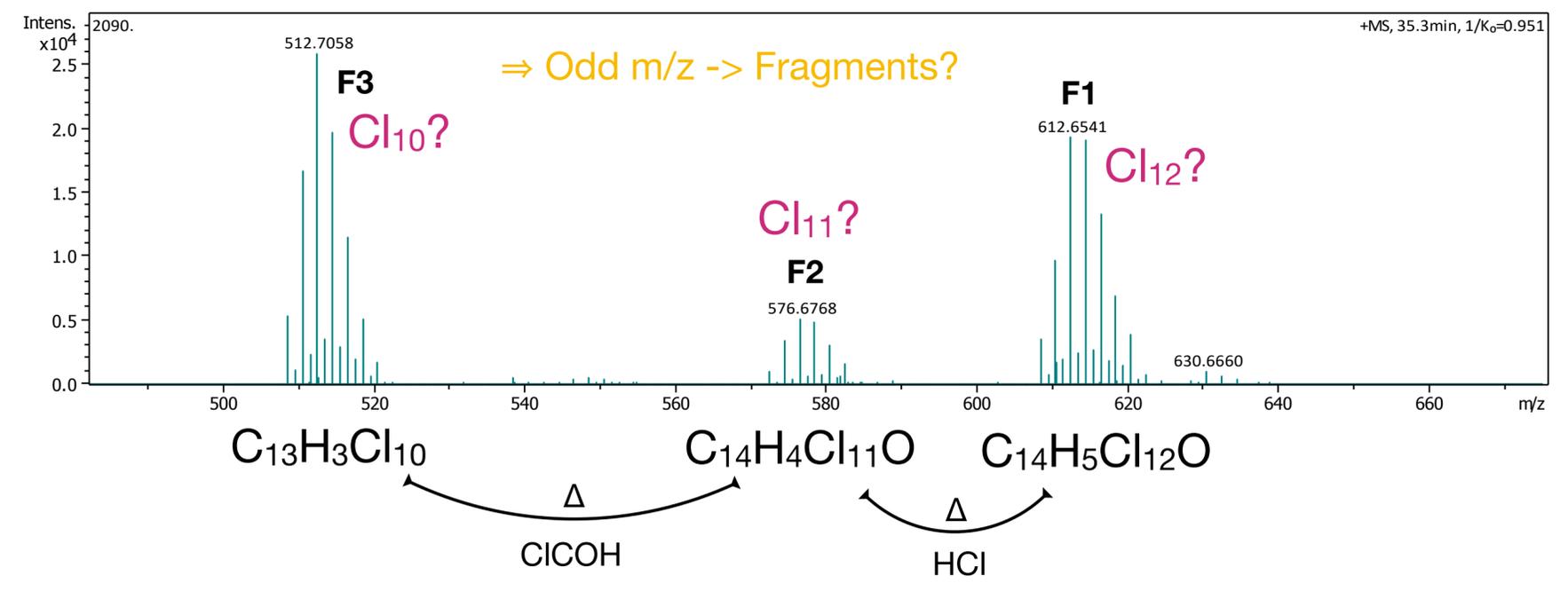
Confidence level



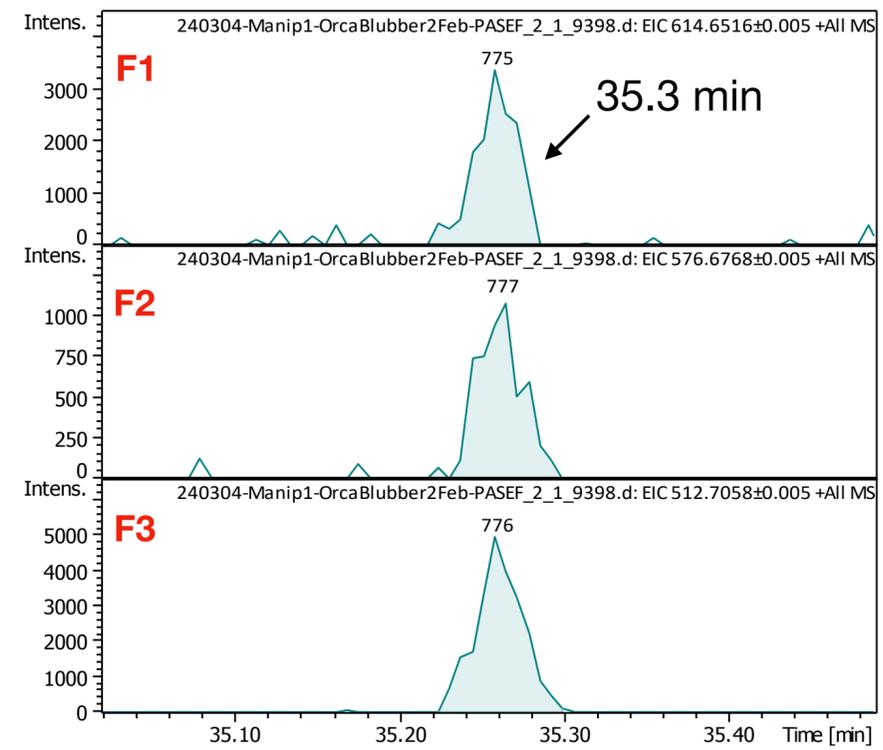
#10196-#10216 Heatmap



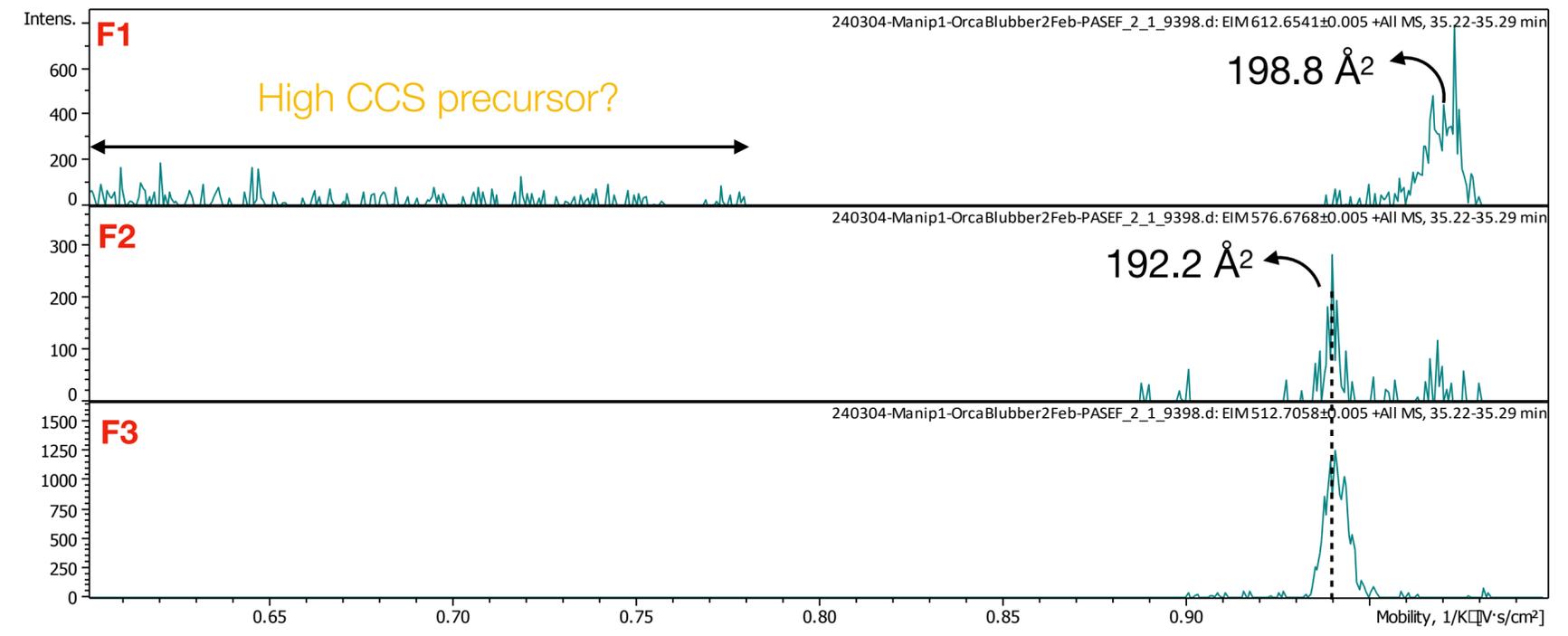
Mass spectra & isotopic profile



Chromatogram

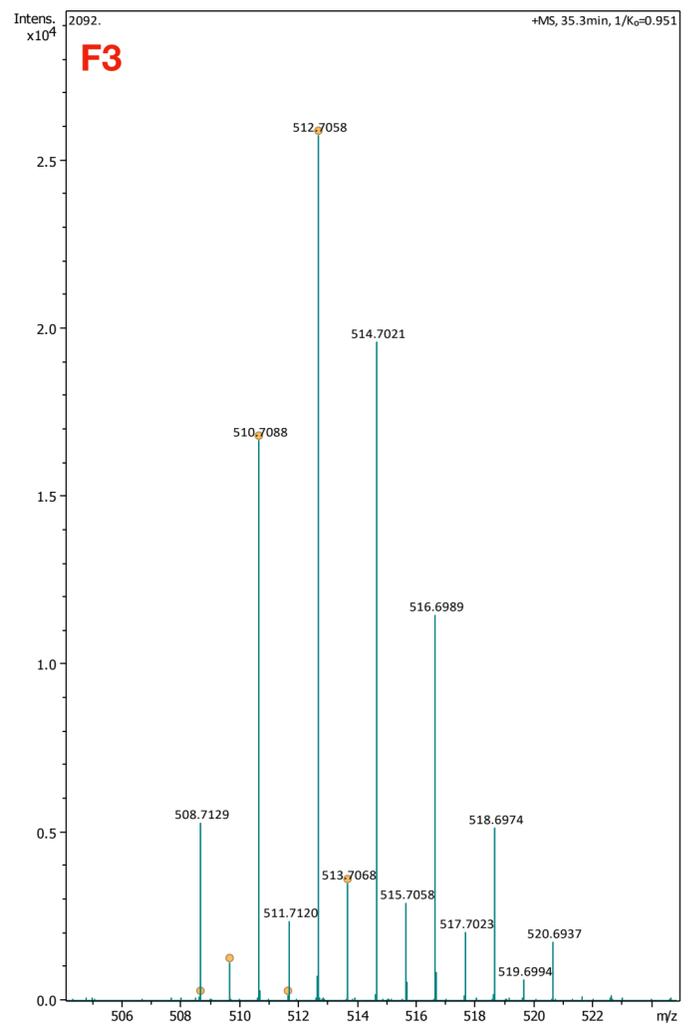
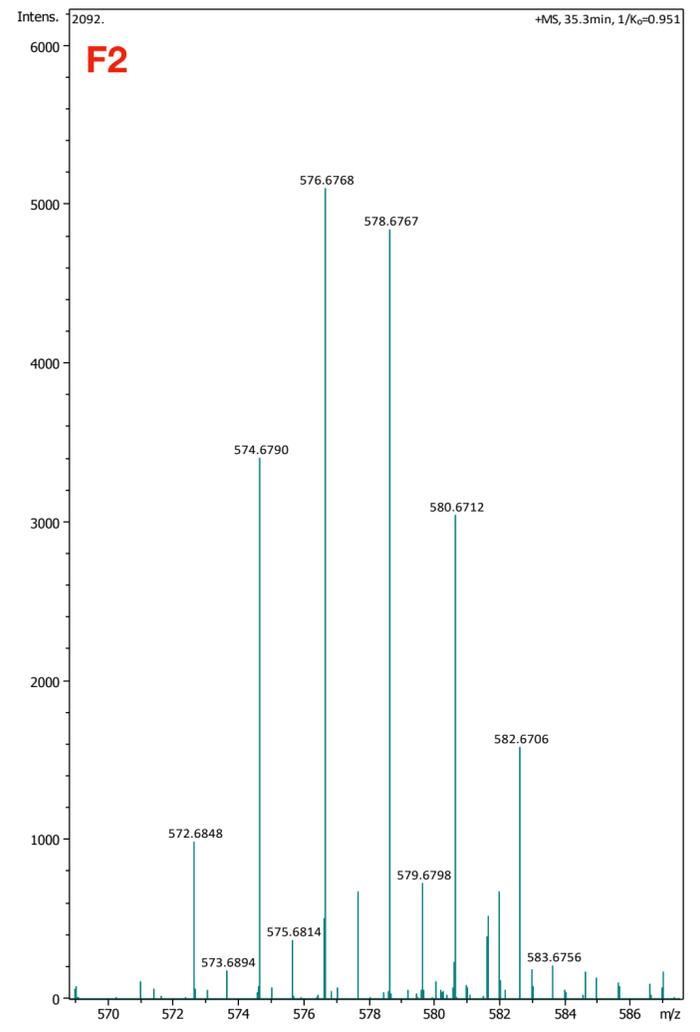
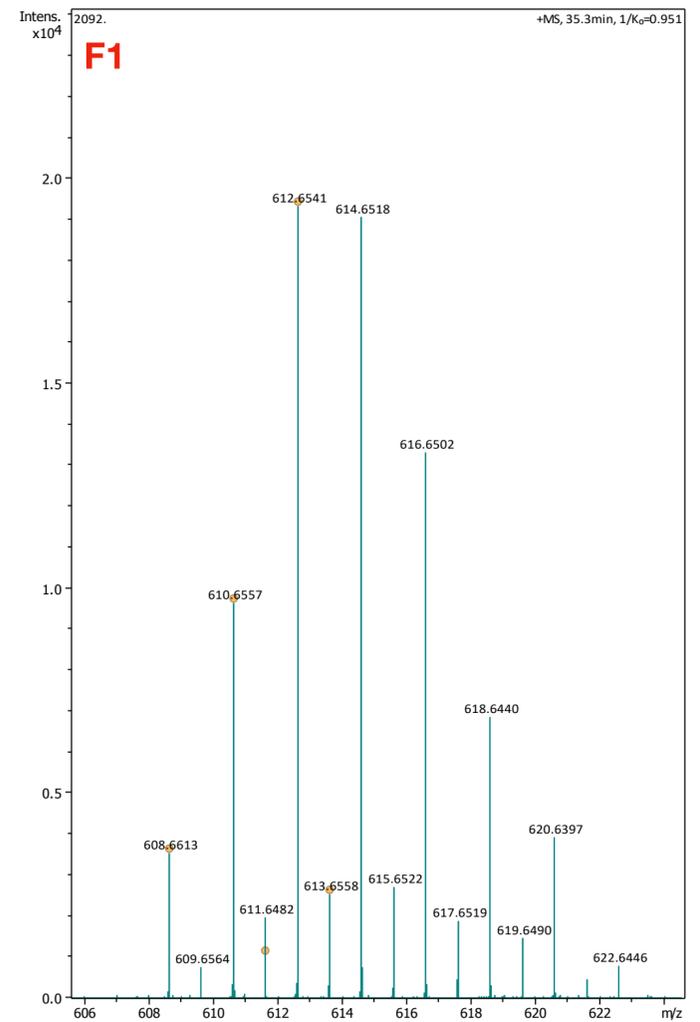


Ion mobility spectra

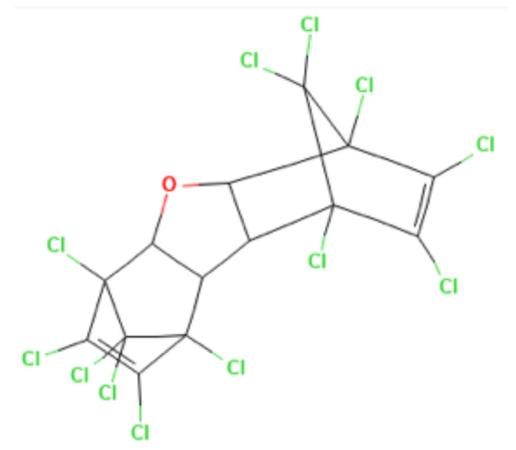


Mass spectra & isotopic profile

Tandem mass spectrum



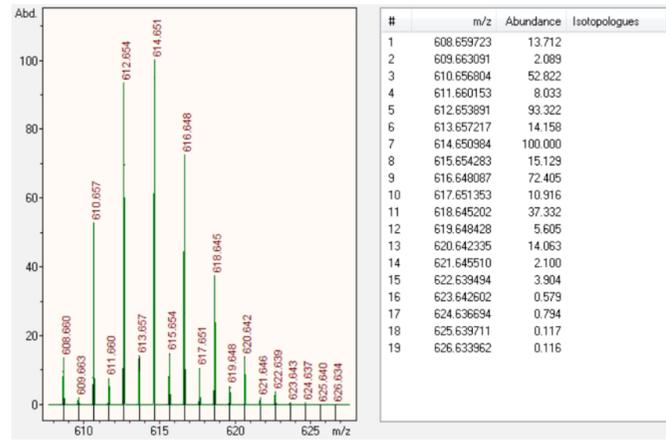
Tentative candidate(s)



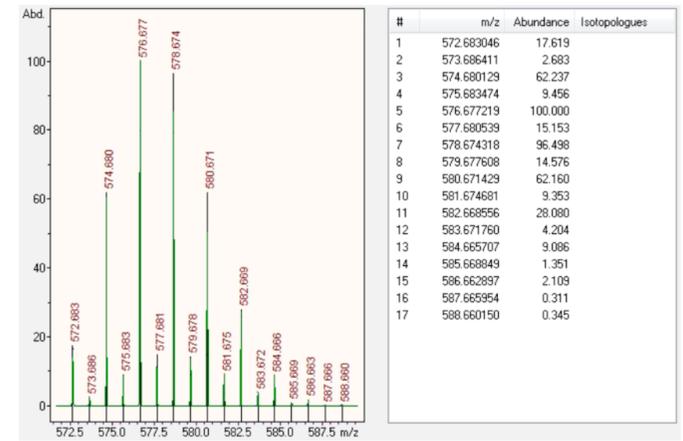
Dechlorane 602

⇒ Maybe compound similar to dechlorane 602

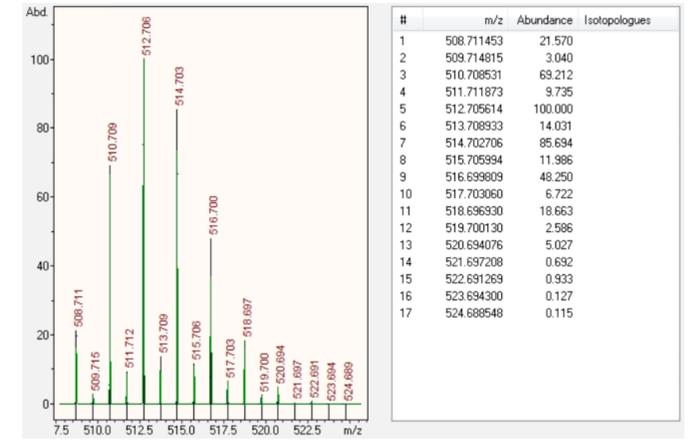
Confidence level



C14H5Cl12O

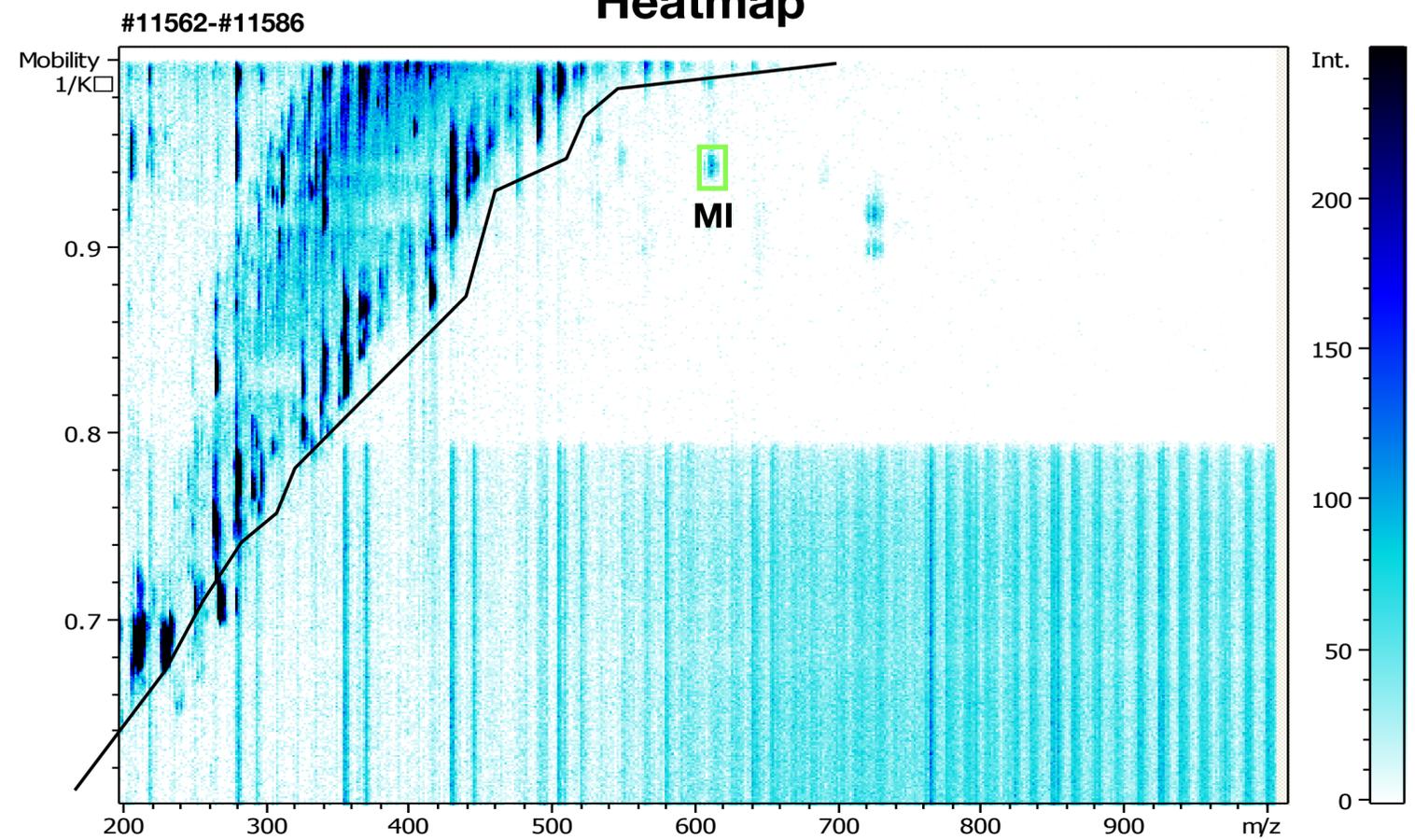


C14H4Cl11O

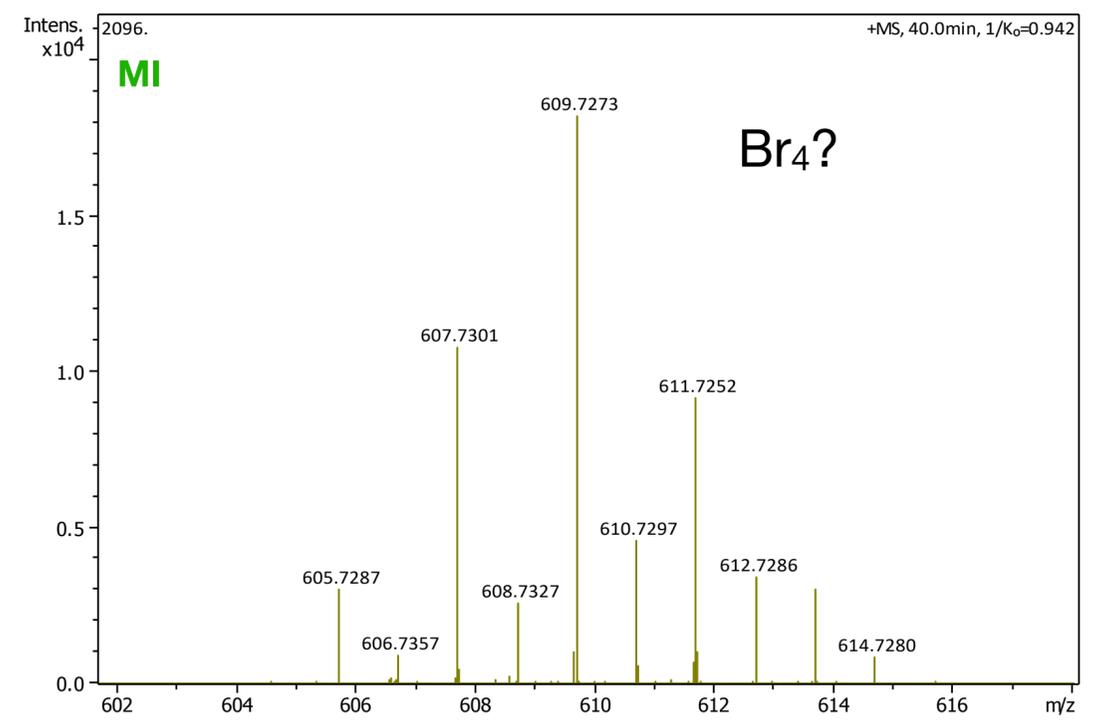


C13H3Cl10

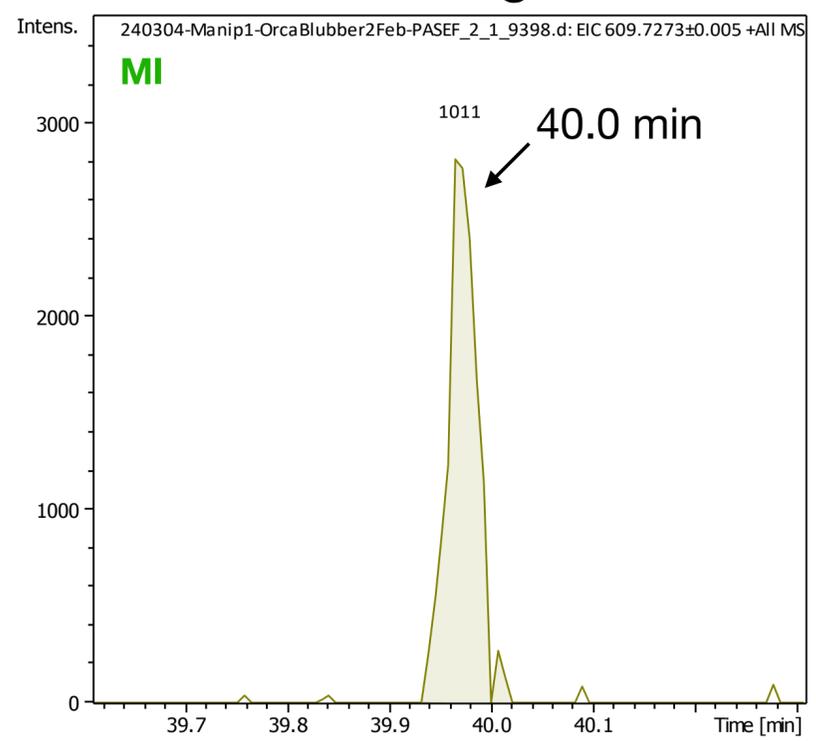
Heatmap



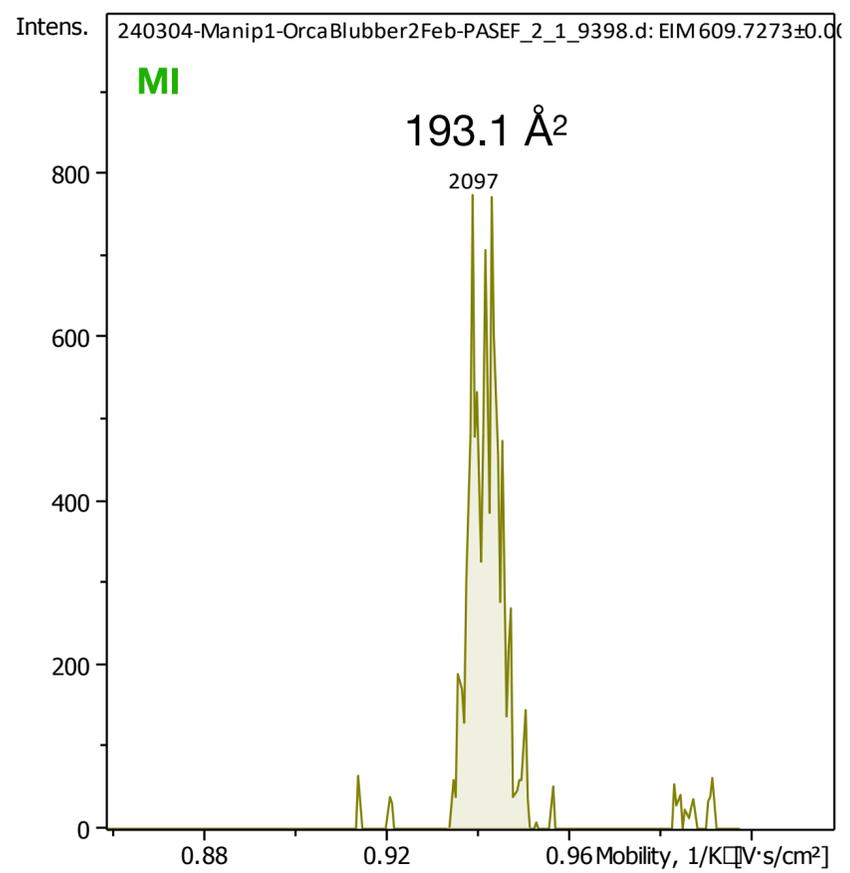
Mass spectrum & isotopic profile



Chromatogram



Ion mobility spectrum



Tandem mass spectrum

/

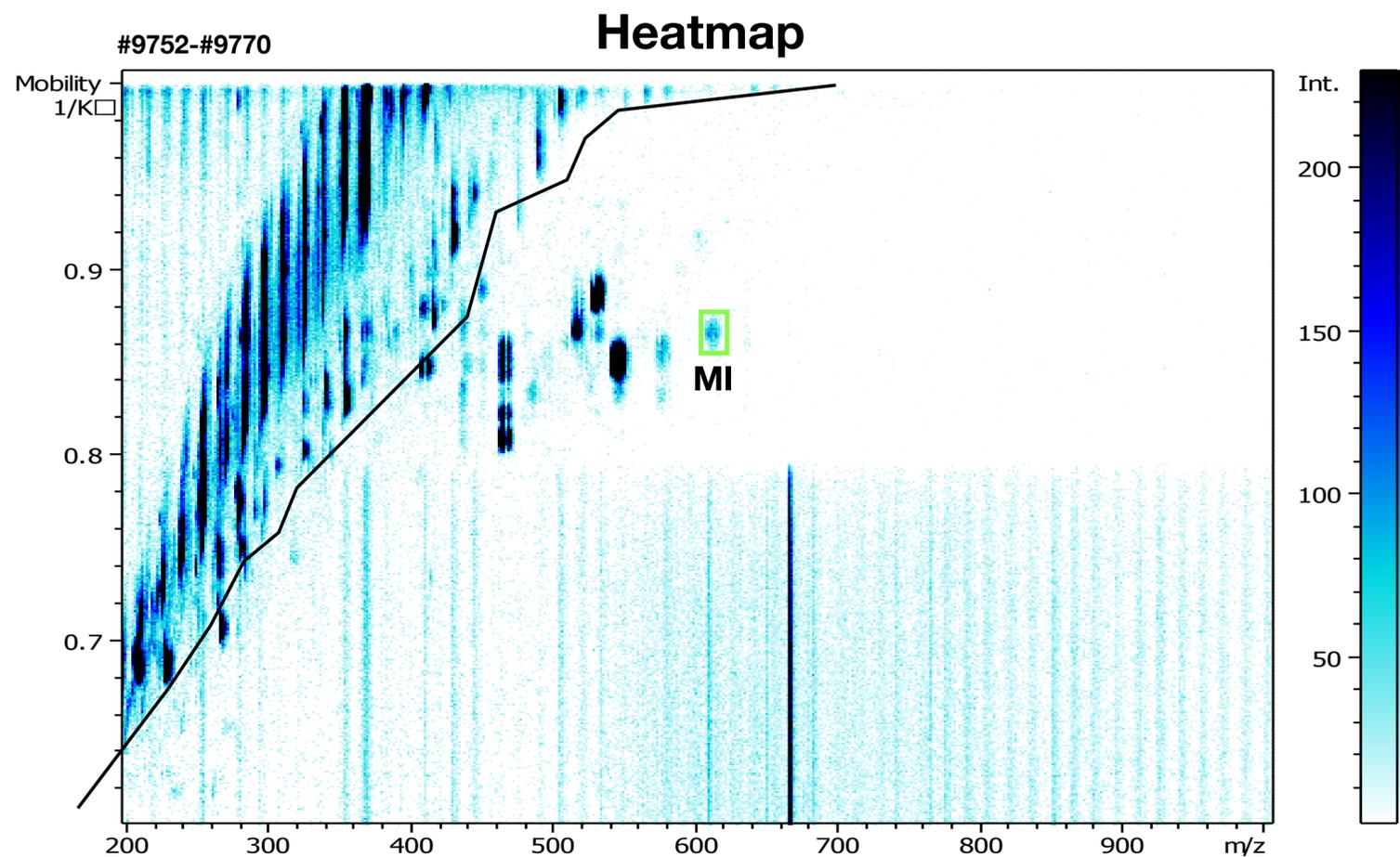
Tentative candidate(s)



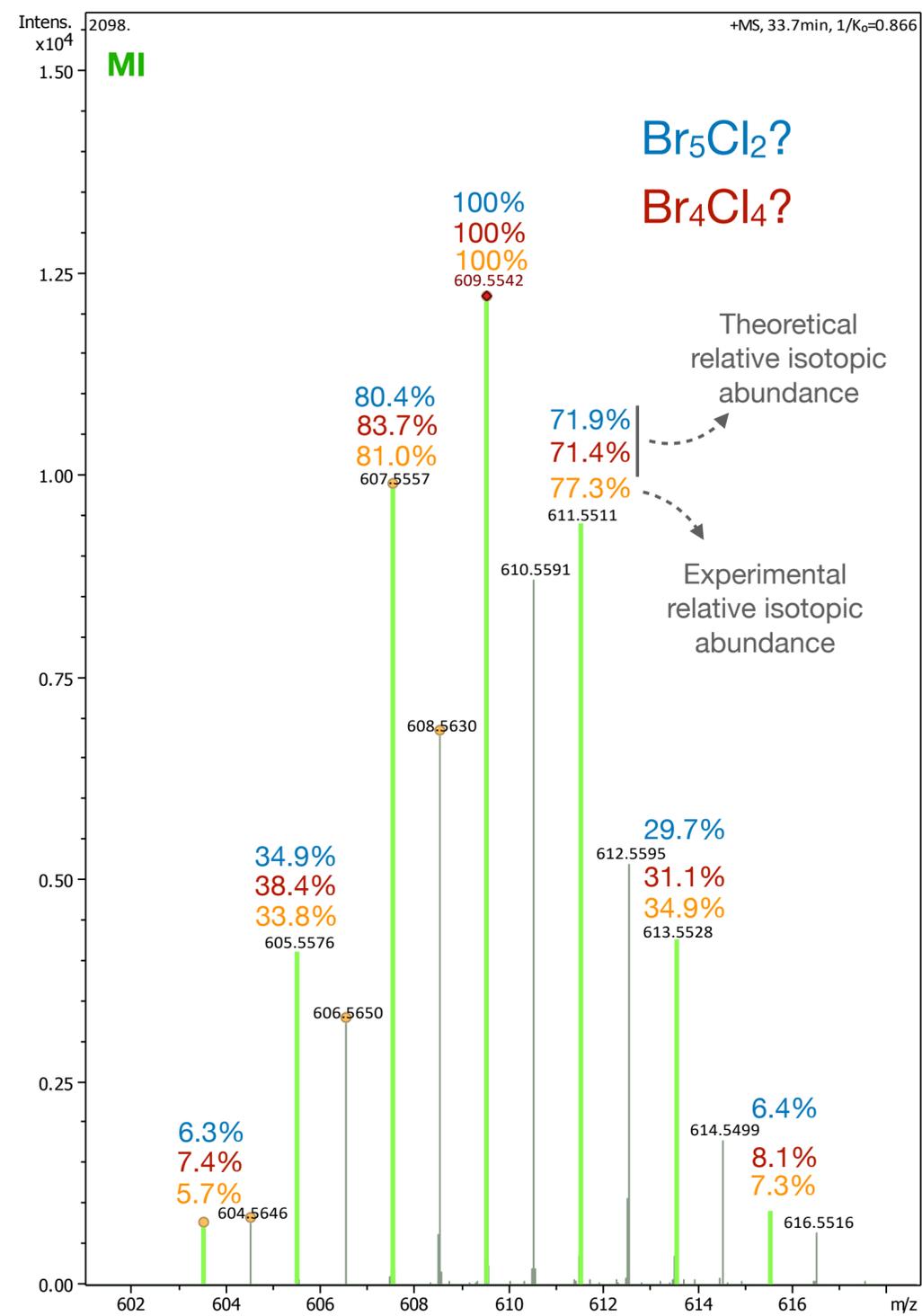
/

Confidence level

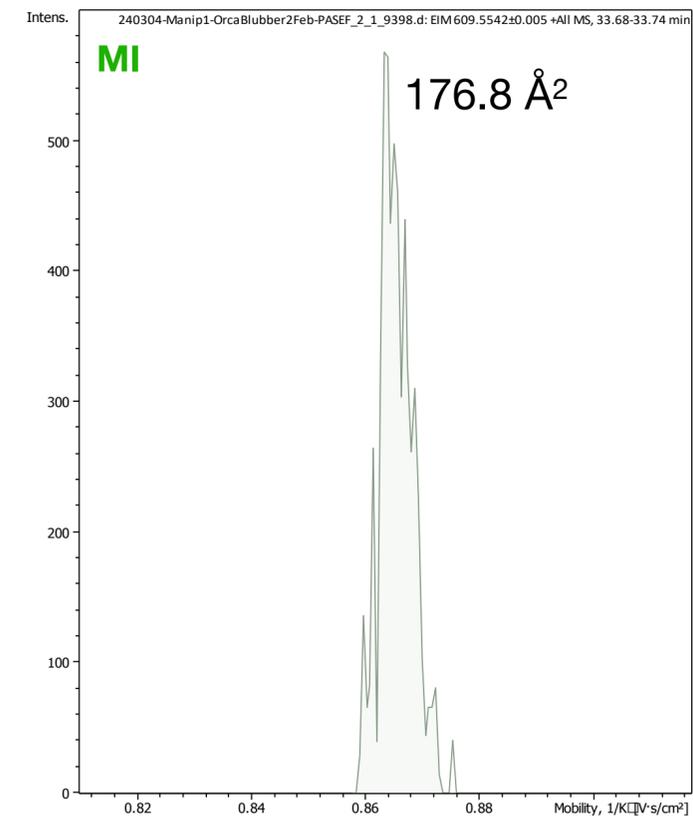




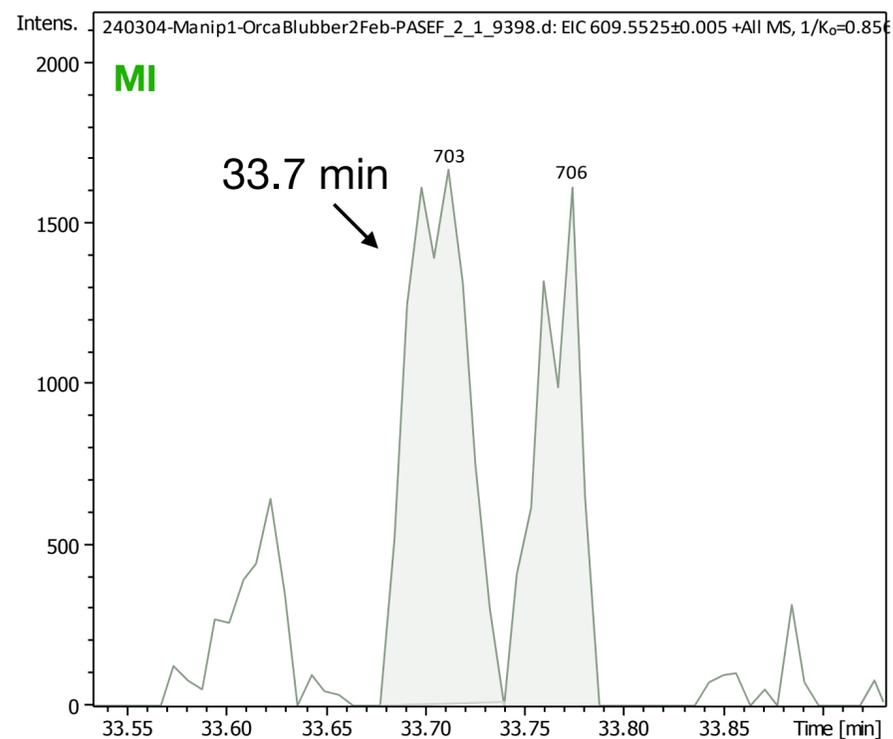
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



Tandem mass spectra

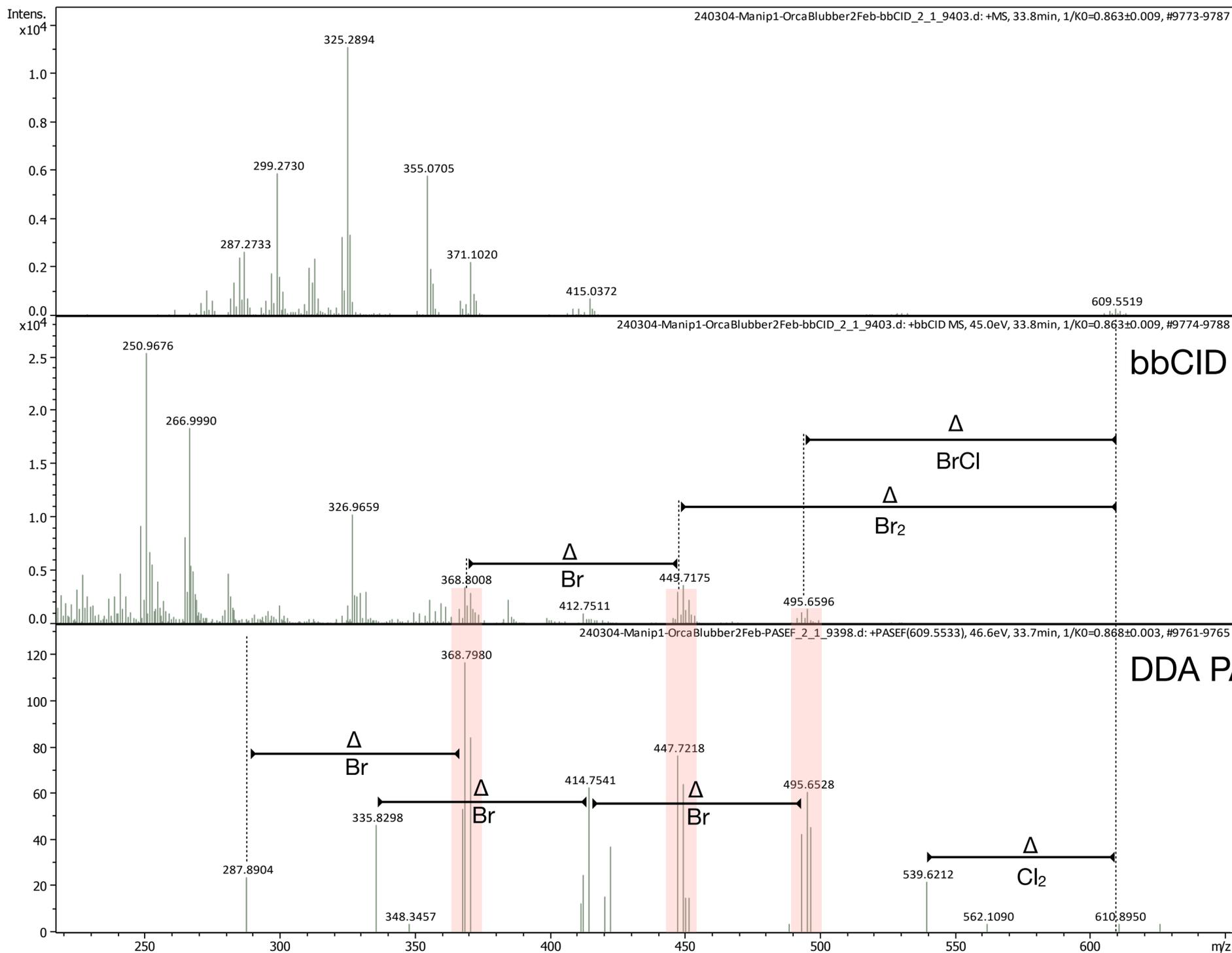
Tentative candidate(s)

PubChem

No PubChem hit

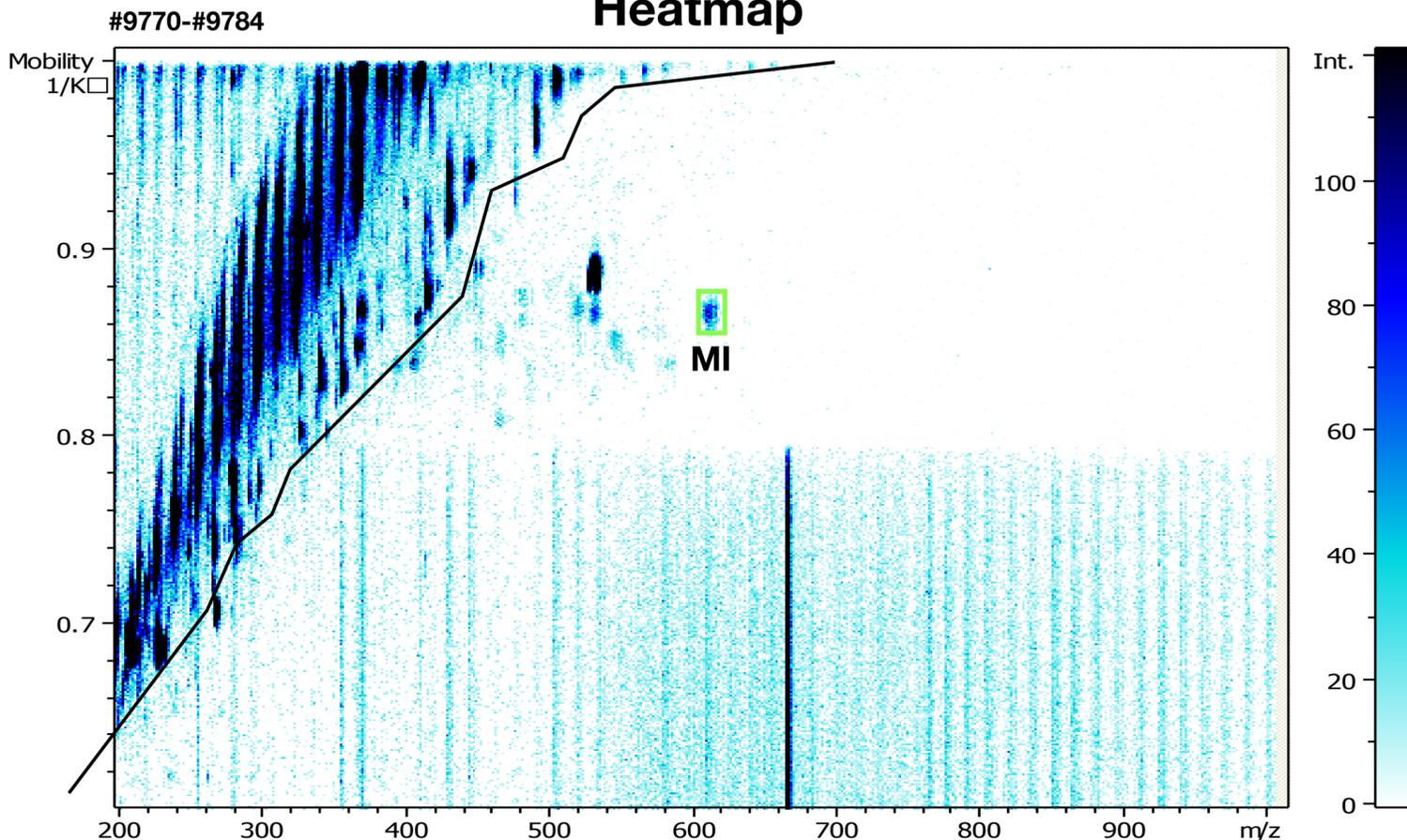
Confidence level

5

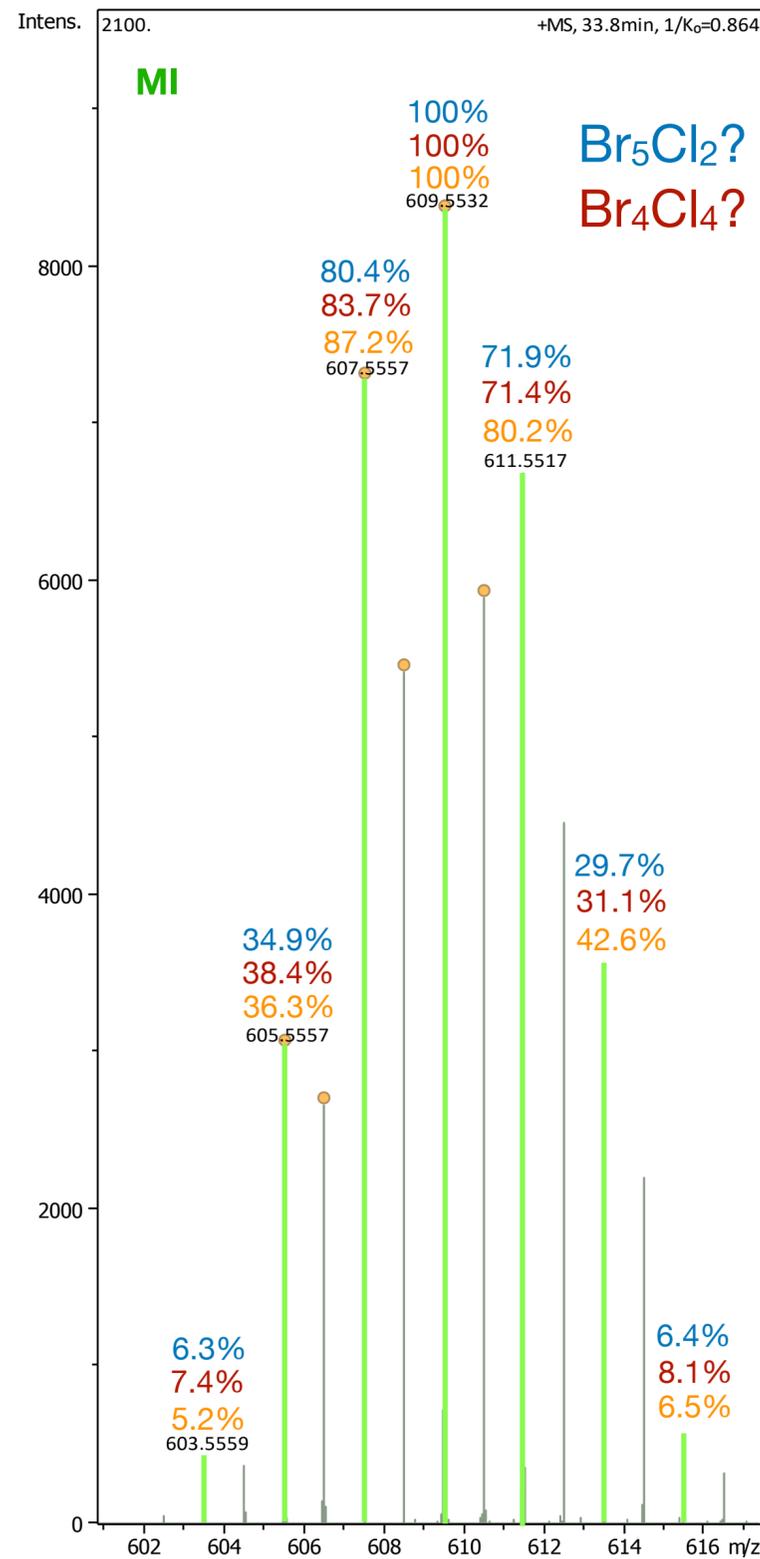


⇒ Contains at least Br₄Cl₂

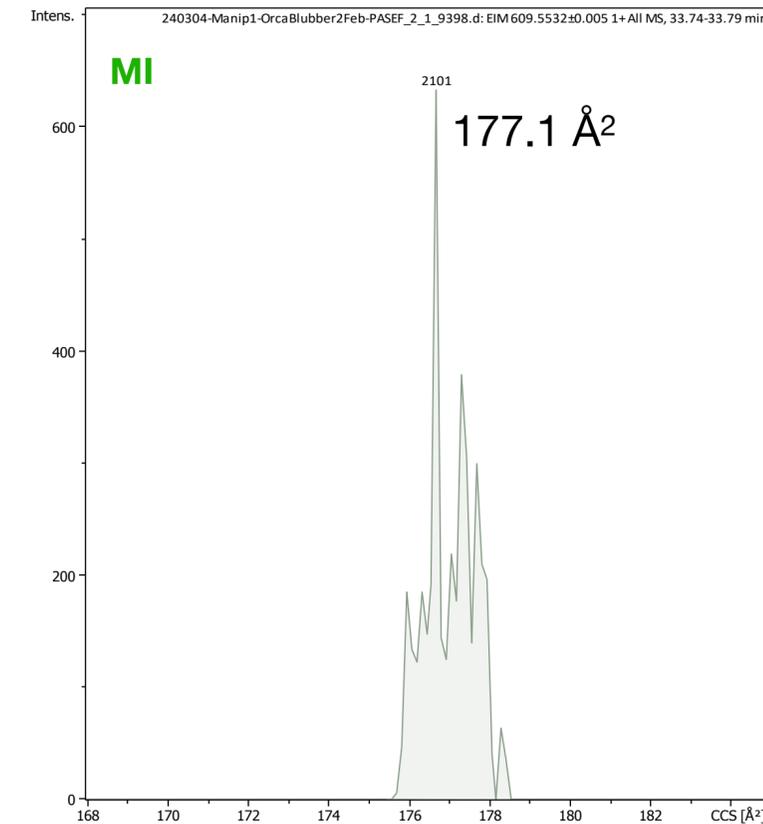
Heatmap



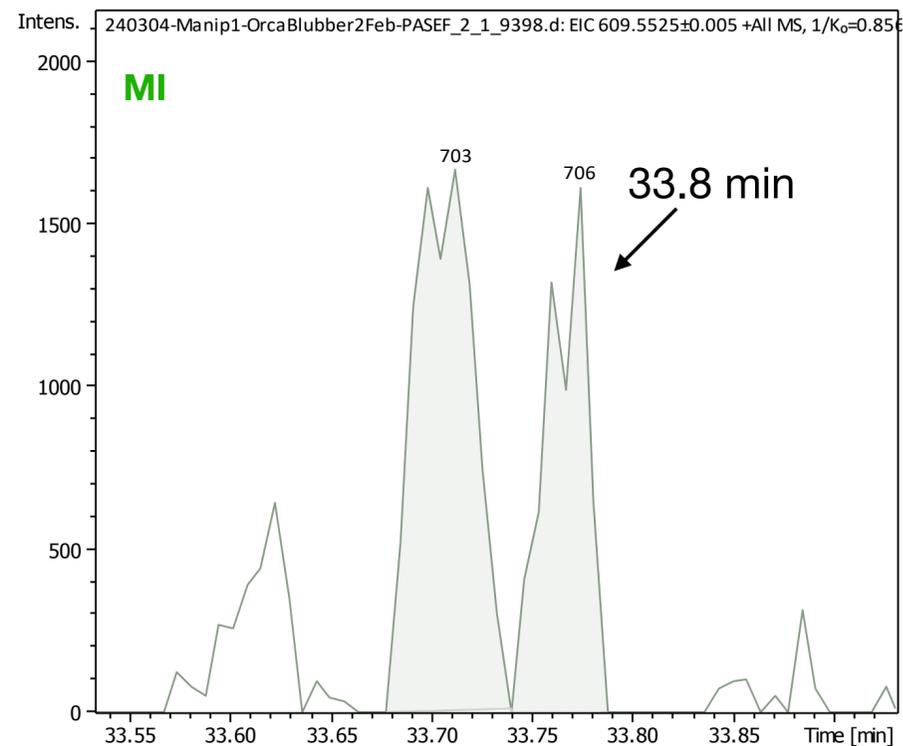
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



Tandem mass spectrum

Tentative candidate(s)

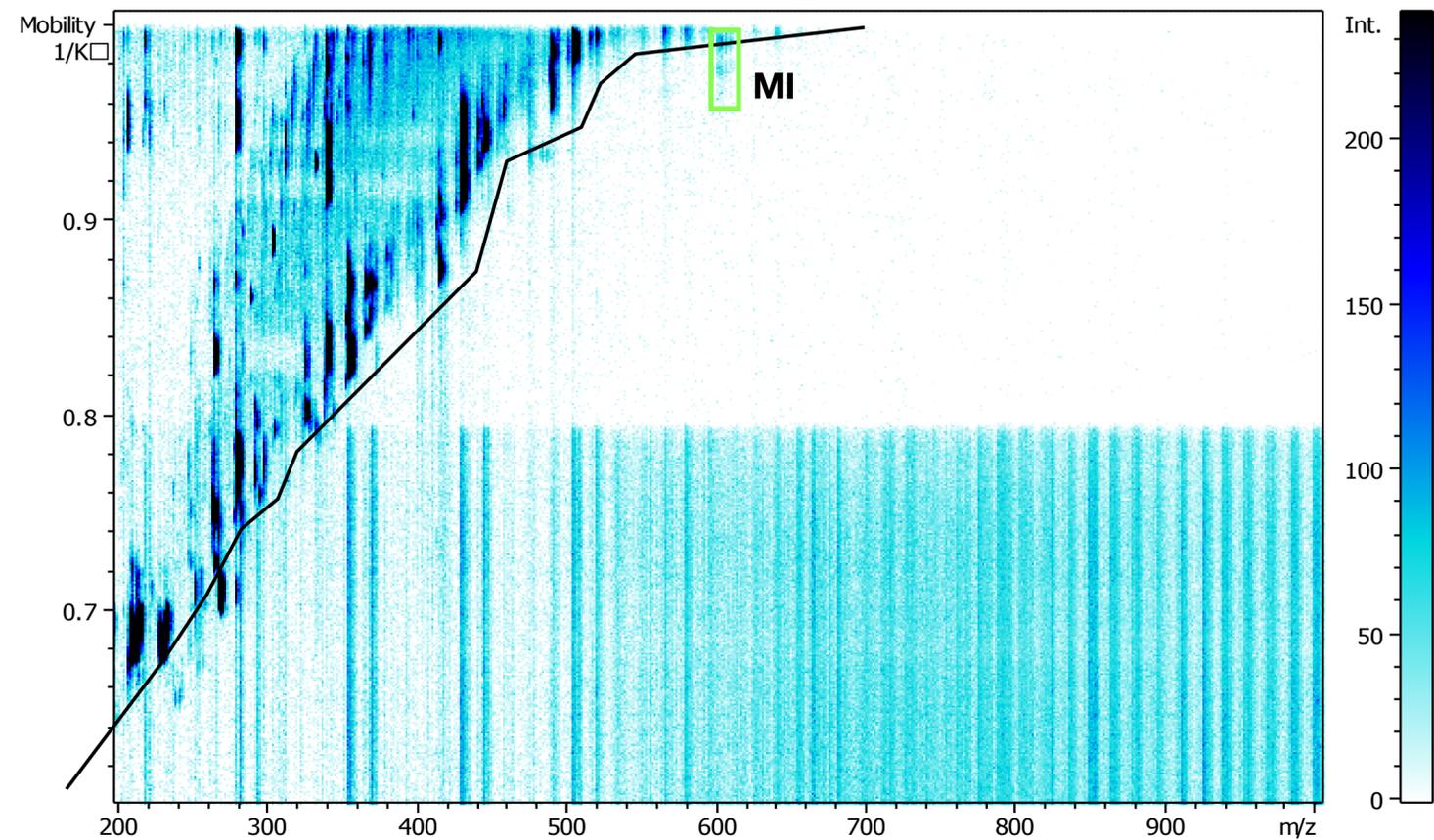
PubChem

Confidence level

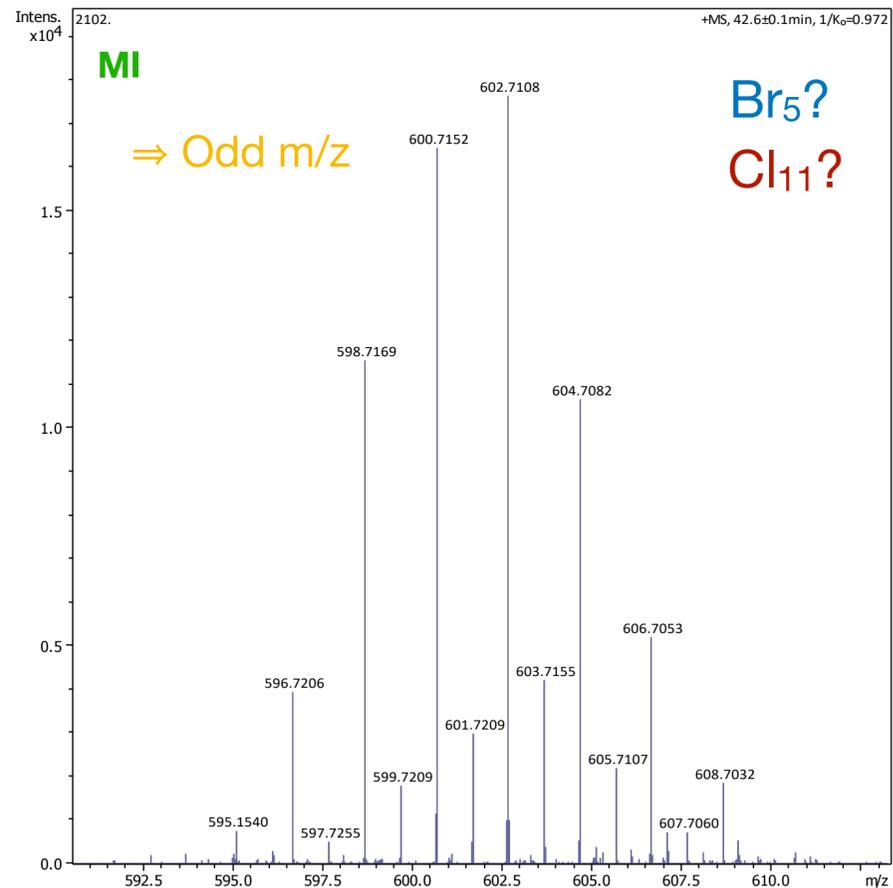
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Heatmap

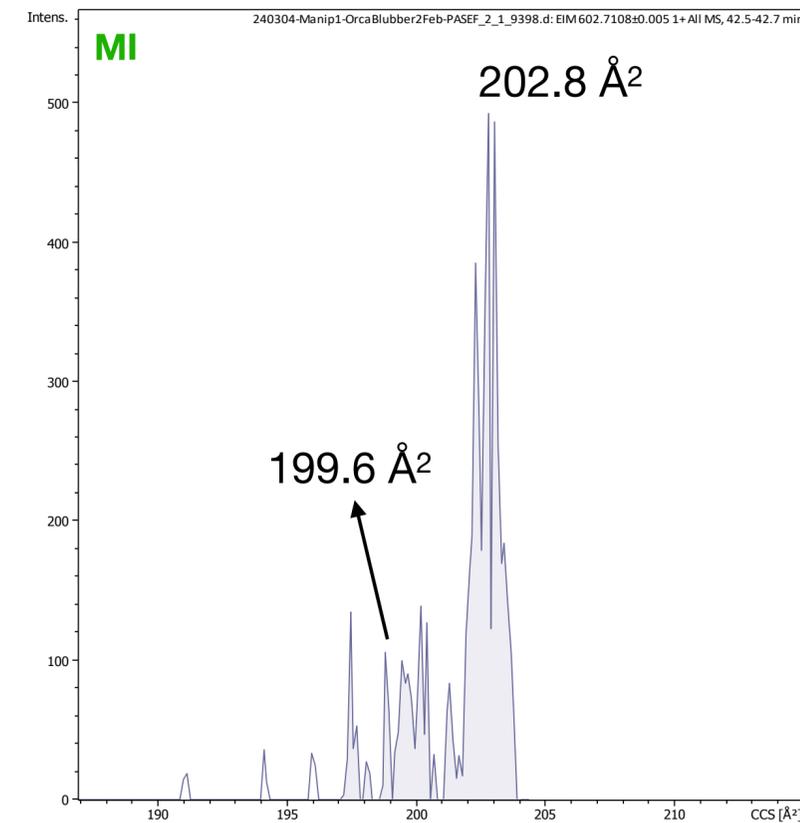
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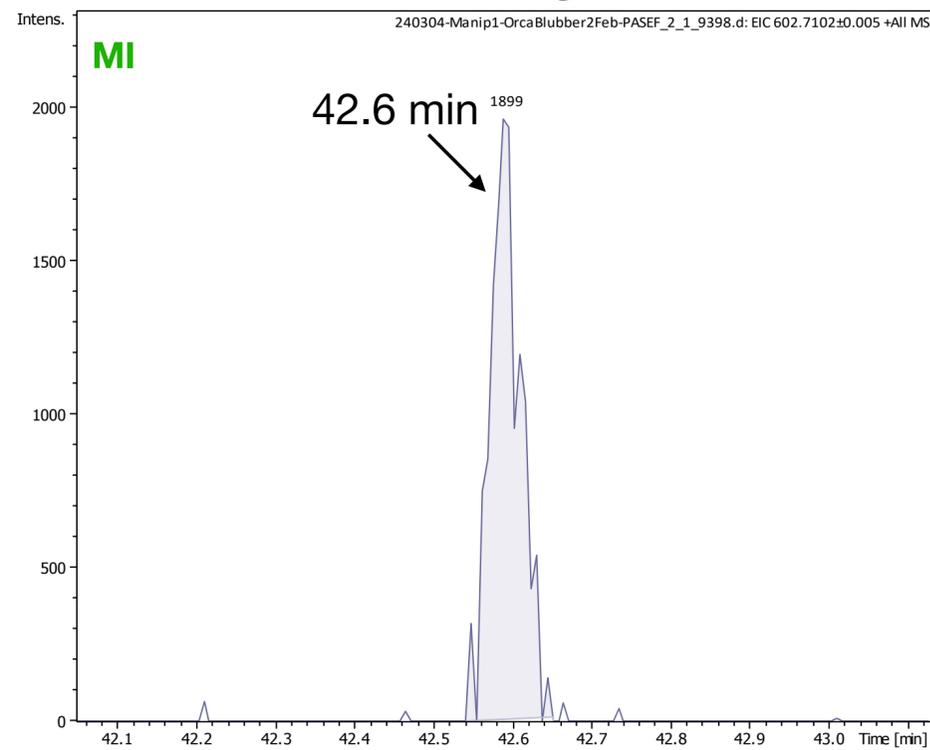
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



Tandem mass spectrum

Tentative candidate(s)

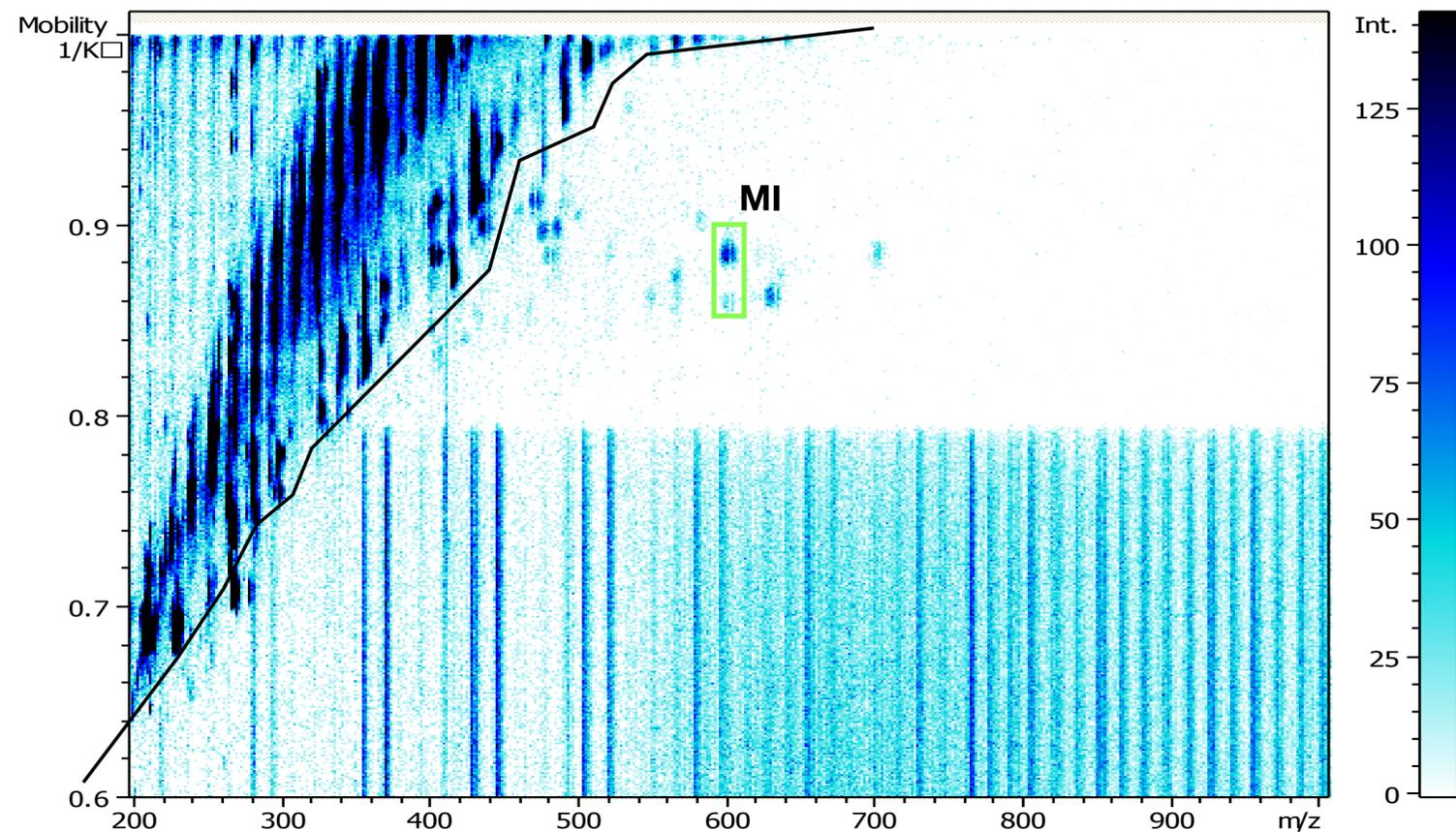
PubChem

Confidence level

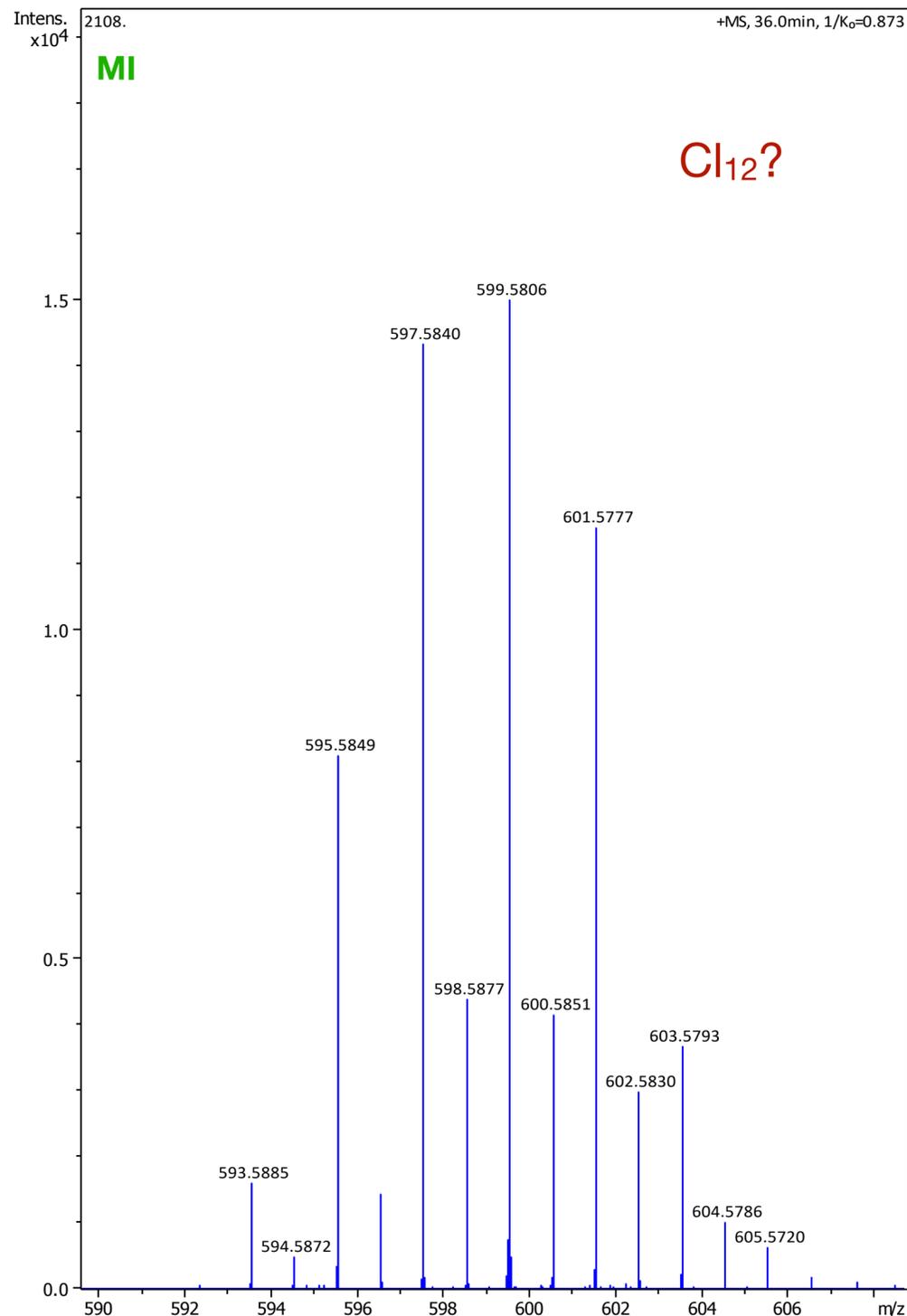
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Heatmap

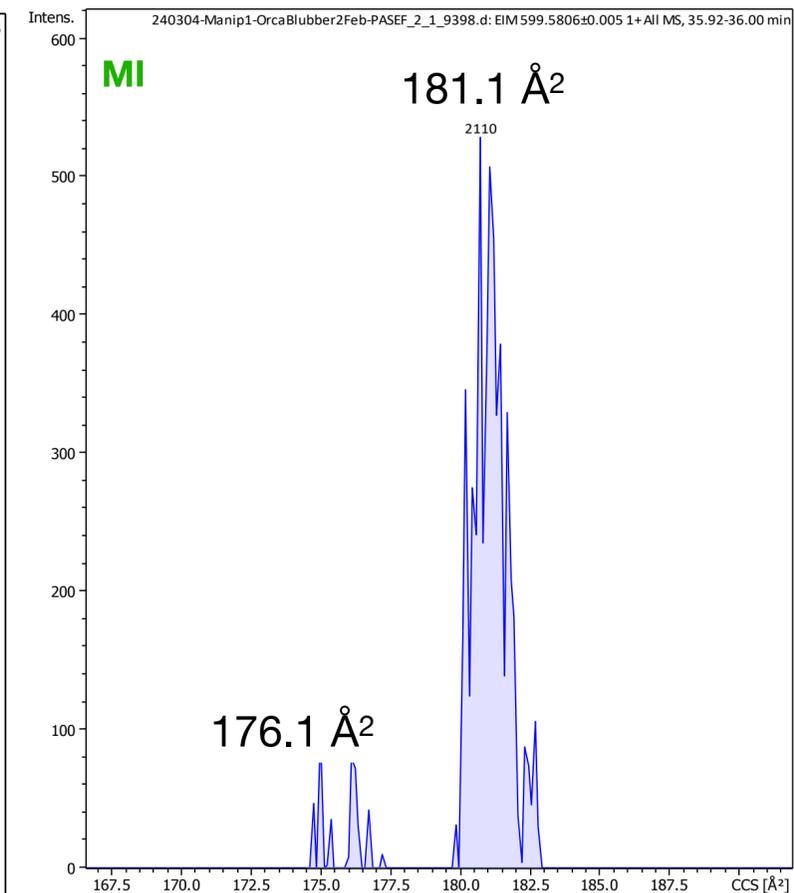
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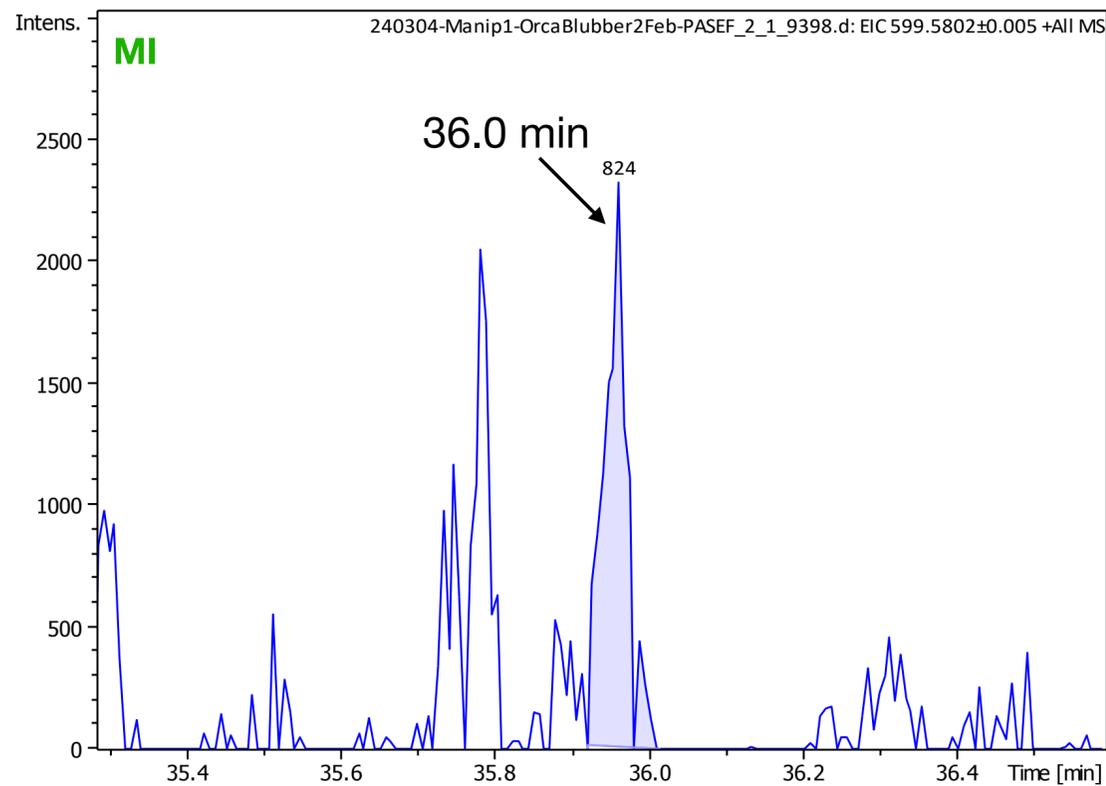
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



Tandem mass spectrum

/

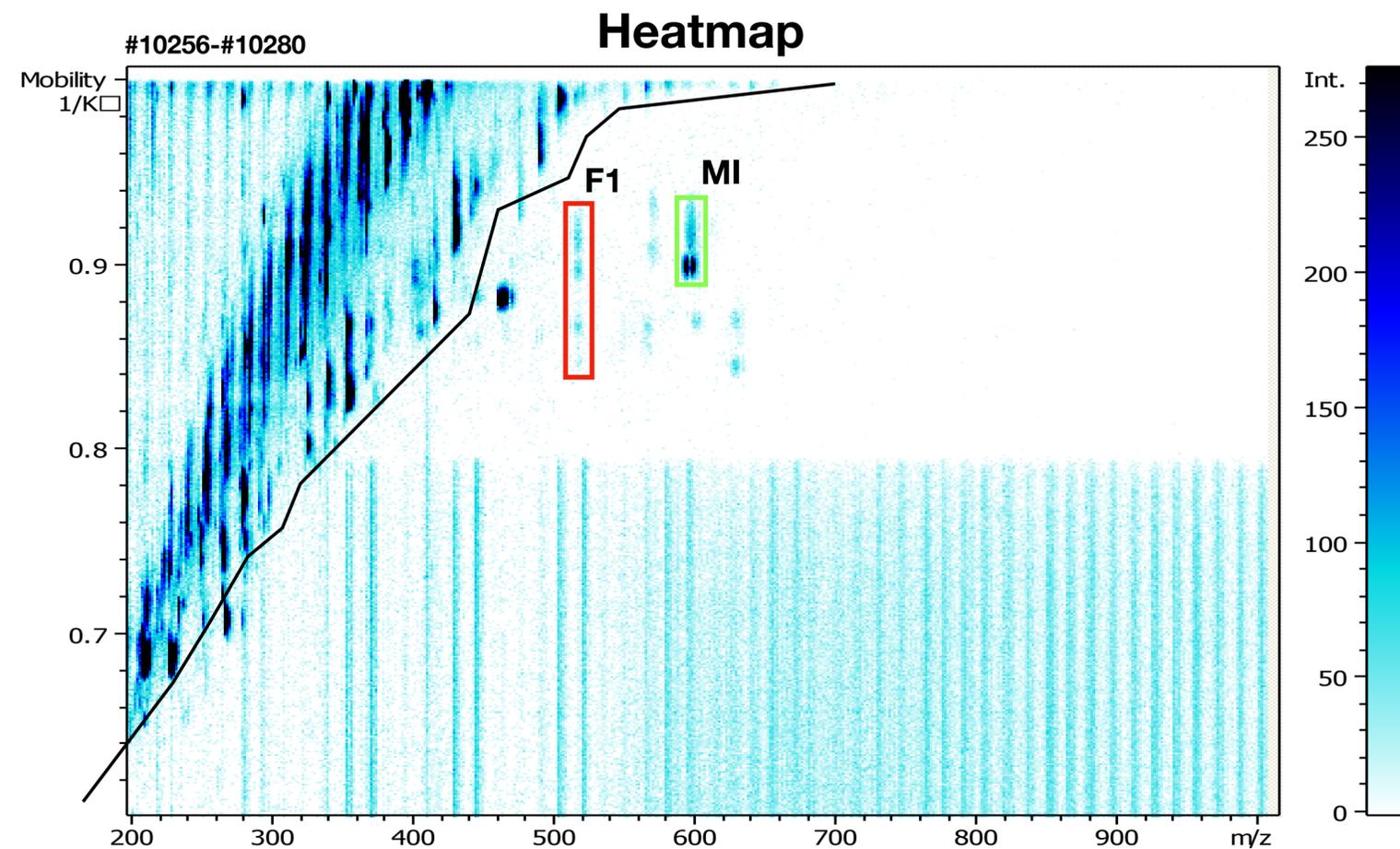
Tentative candidate(s)

PubChem

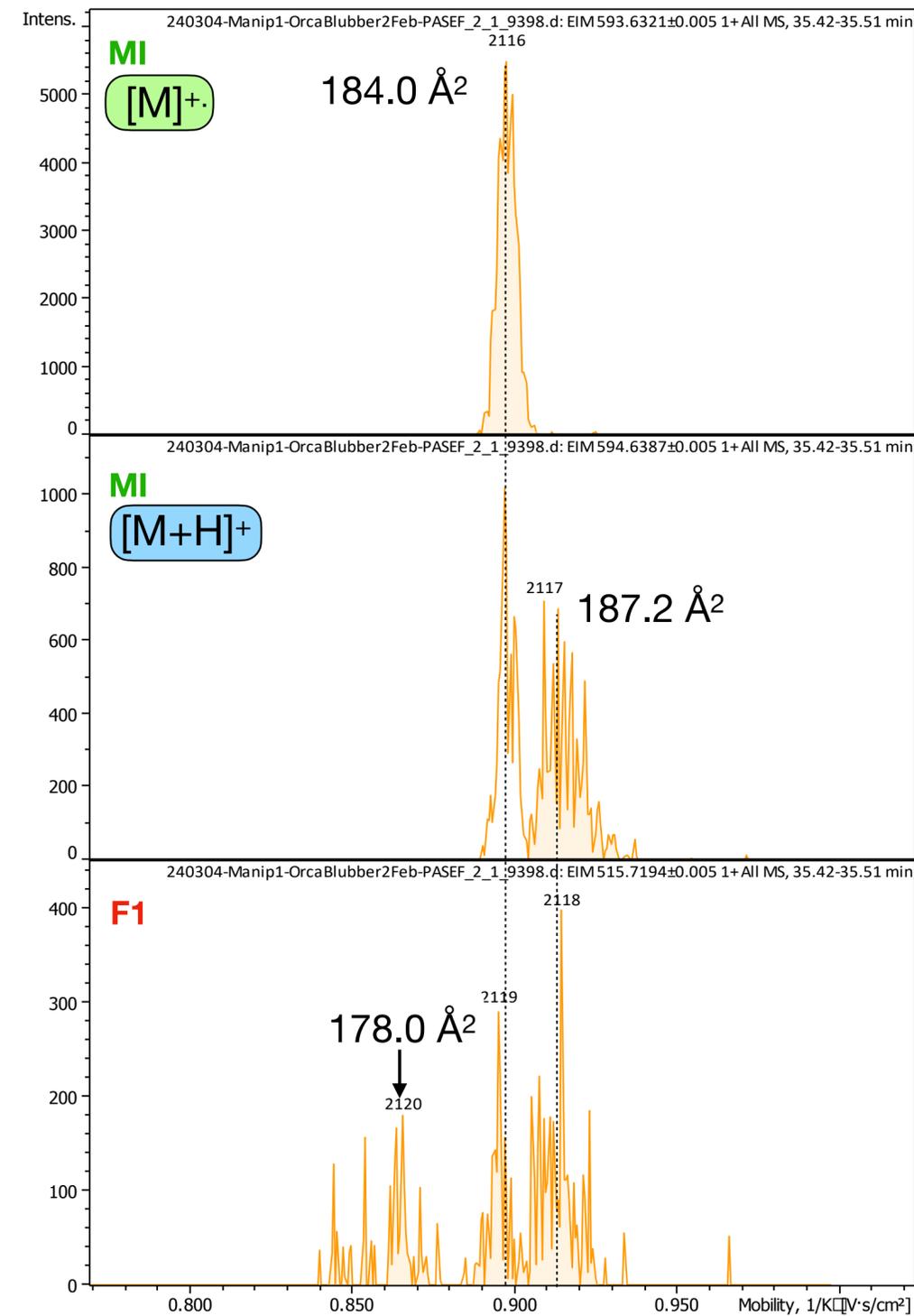
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Confidence level

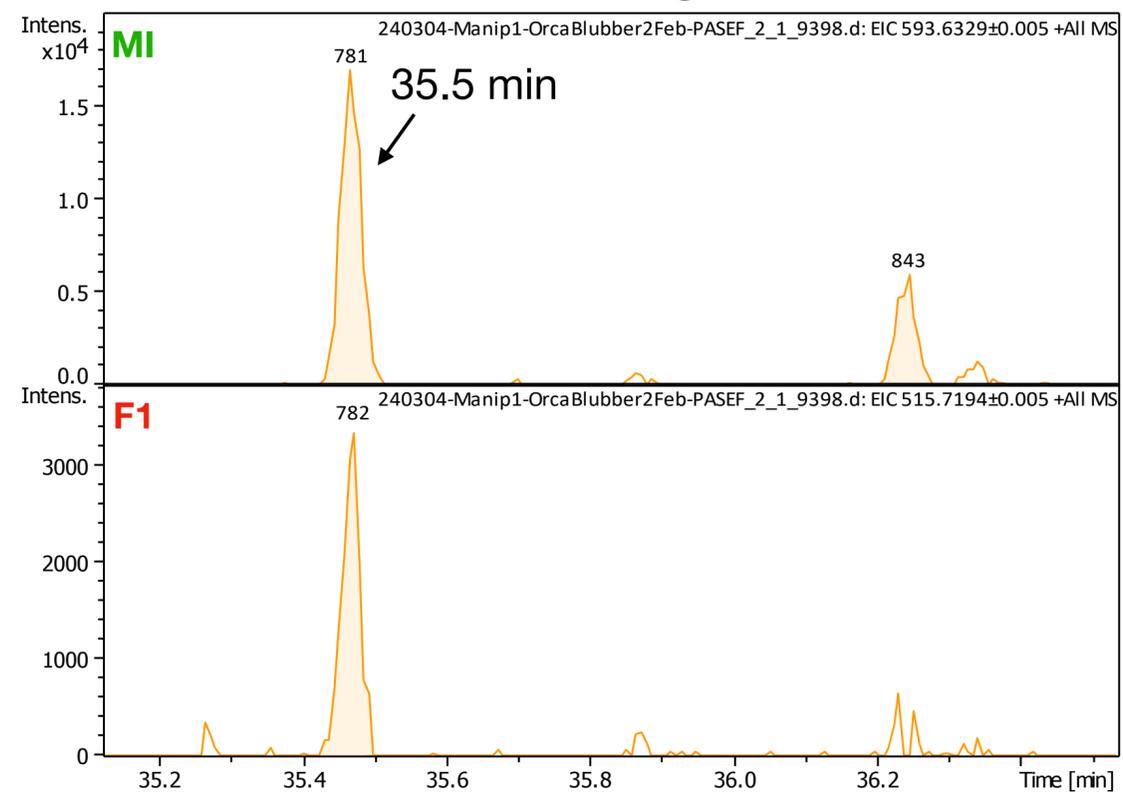
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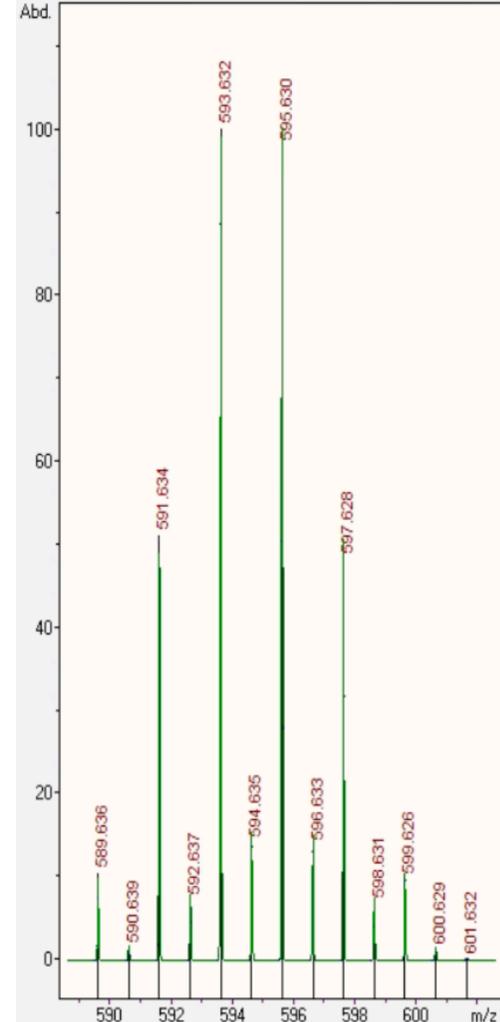
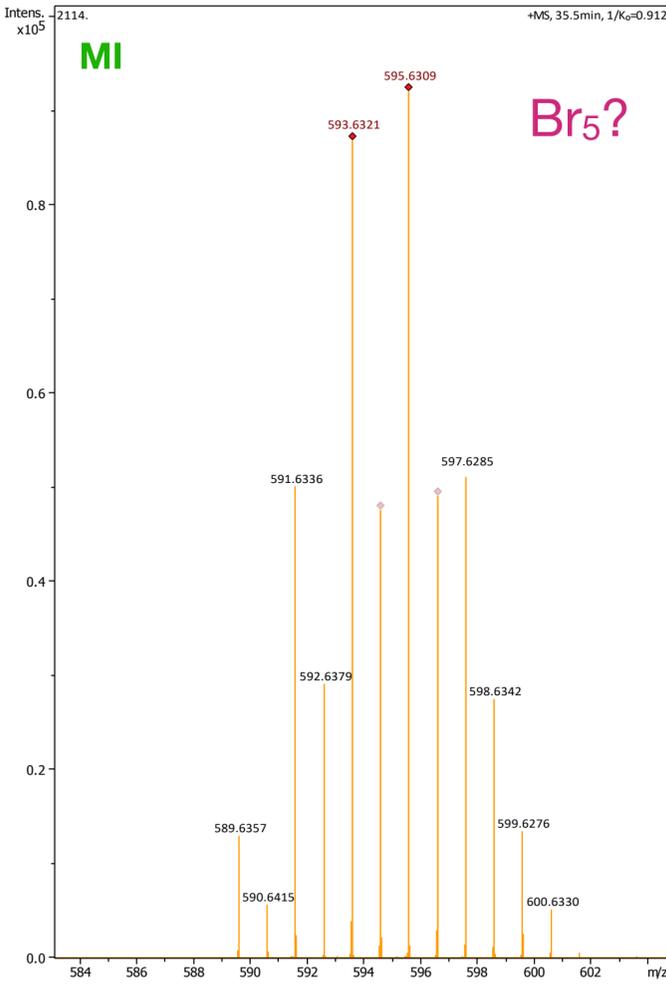
Ion mobility spectra



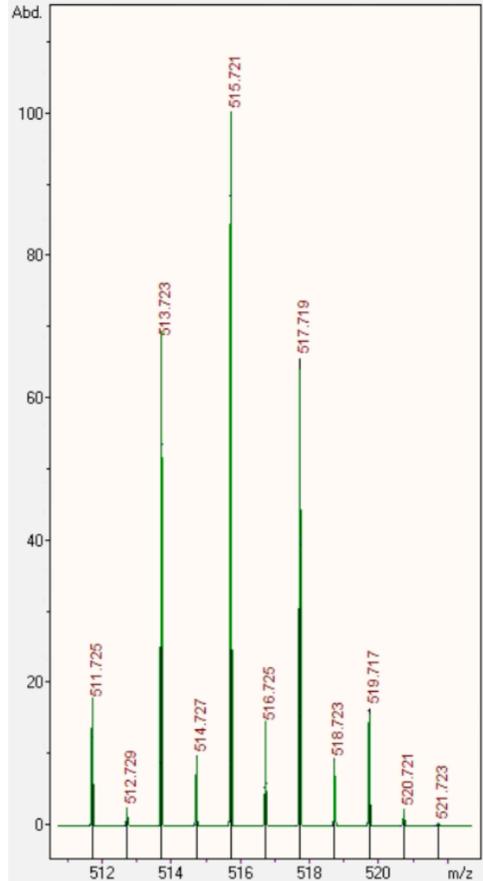
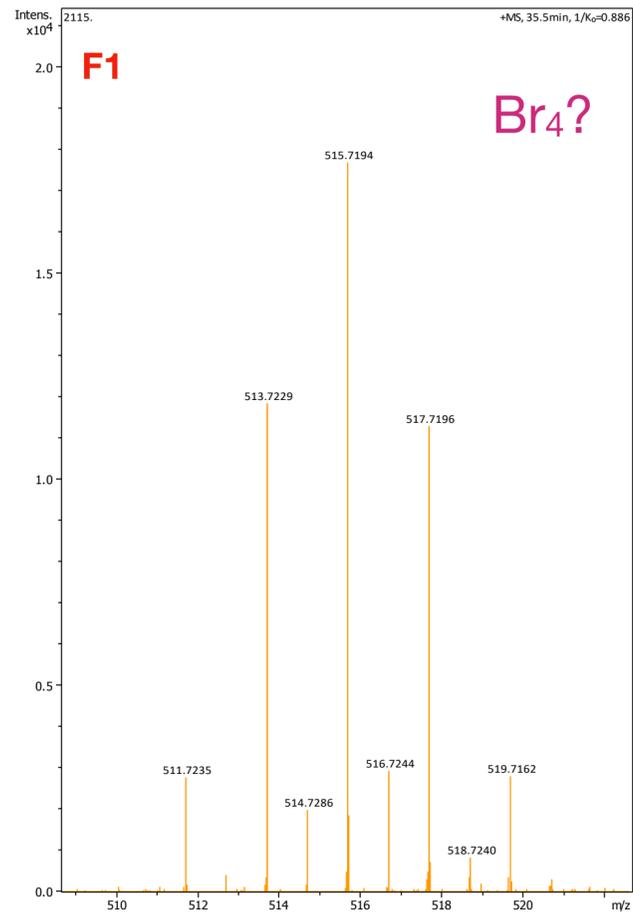
Chromatogram



Mass spectra & isotopic profile



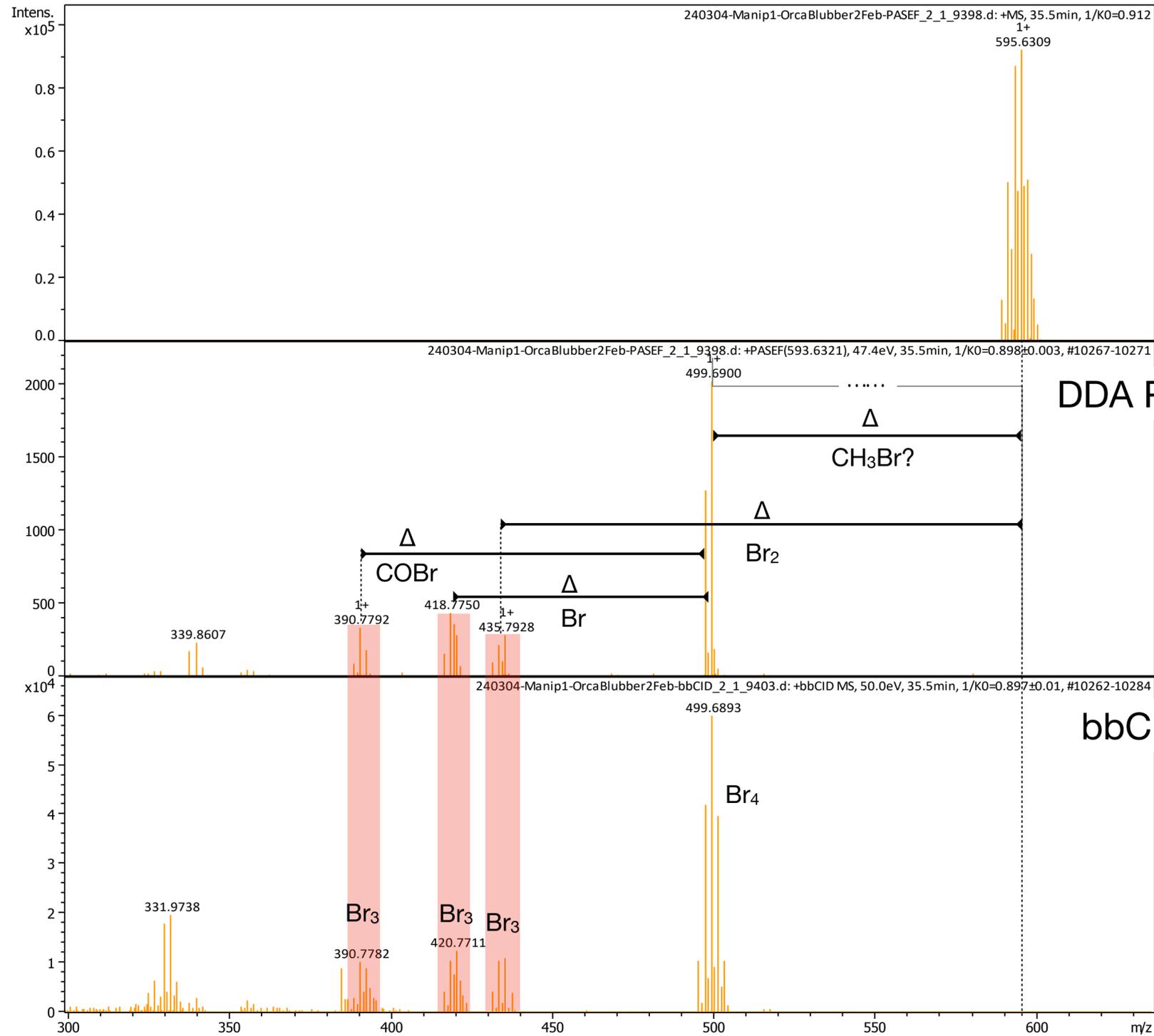
#	m/z	Abundance	Isotopologues
1	589.635744	10.495	
2	590.639120	1.492	
3	591.633718	51.187	
4	592.637082	7.267	
5	593.631703	100.000	
6	594.635049	14.168	
7	595.629710	97.948	
8	596.633026	13.830	
9	597.627770	48.295	
10	598.631028	6.773	
11	599.626032	9.779	
12	600.629127	1.345	
13	601.631639	0.126	



#	m/z	Abundance	Isotopologues
1	511.725231	17.451	
2	512.728610	2.483	
3	513.723211	68.140	
4	514.726574	9.679	
5	515.721209	100.000	
6	516.724547	14.164	
7	517.719252	65.596	
8	518.722541	9.238	
9	519.717467	16.498	
10	520.720616	2.285	
11	521.723150	0.214	



Tandem mass spectrum

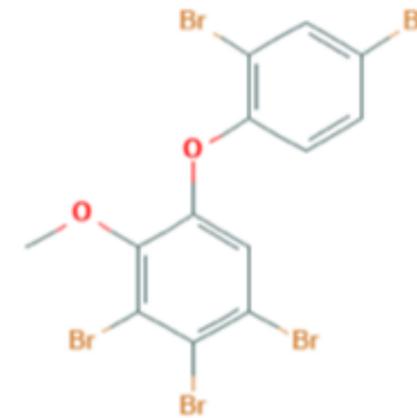
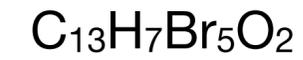


- 5 Br
- At least 2C, 3H and 1O

Tentative candidate(s)



16 isomers



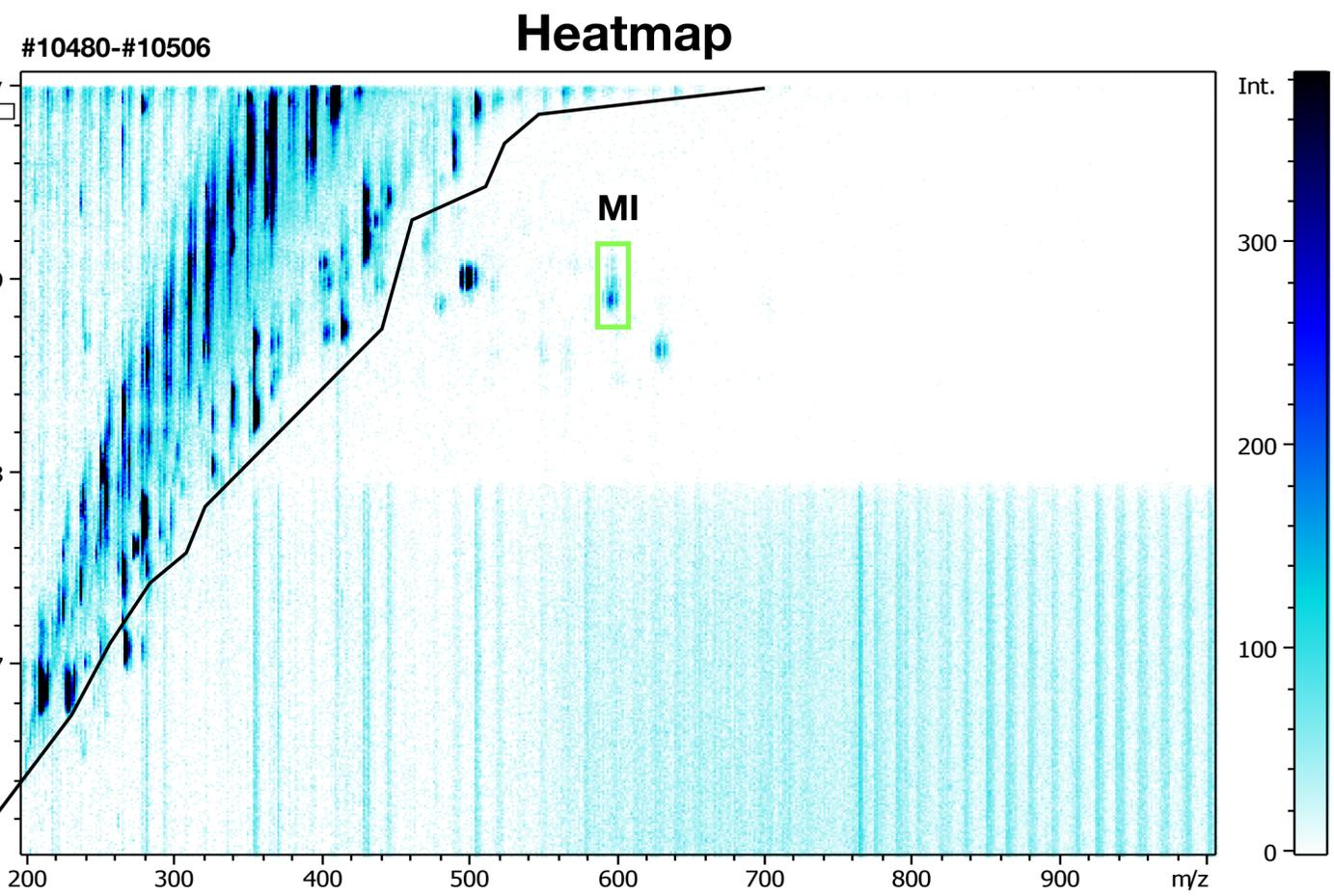
Methoxylated pentaBDEs (multiple isomers)

⇒ HNP?

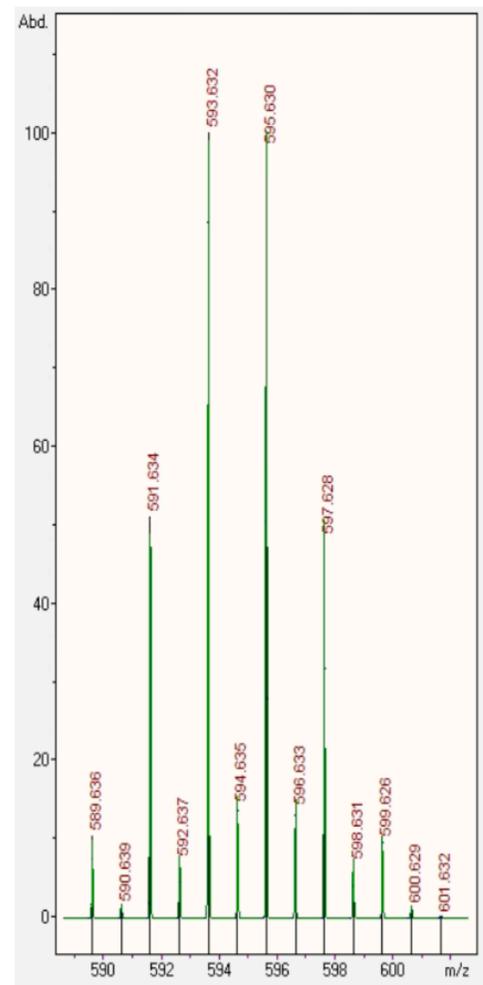
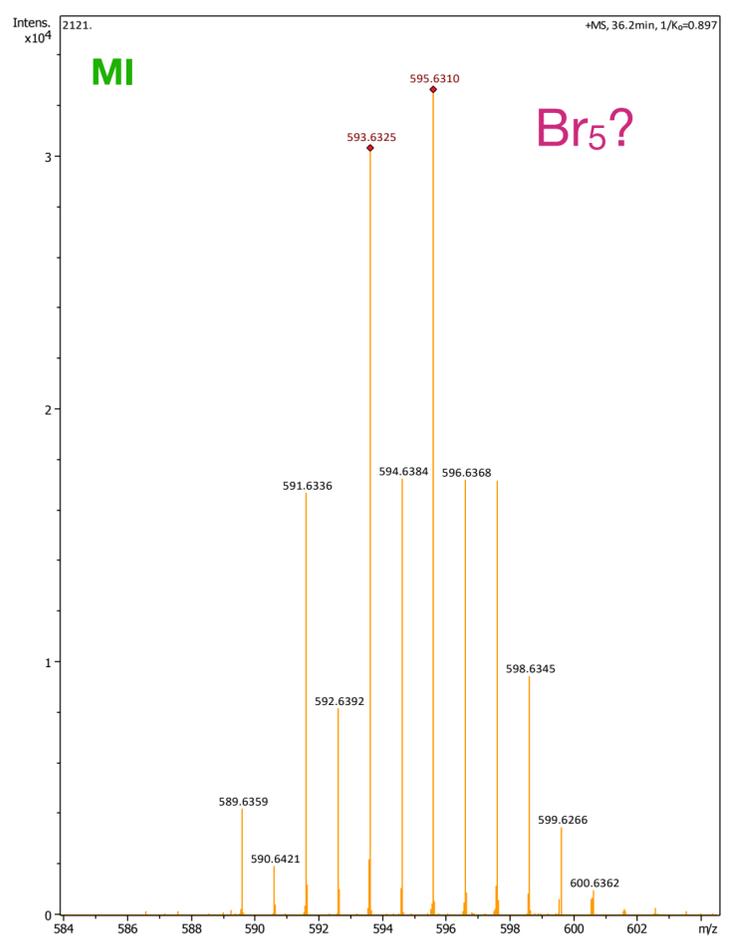
Confidence level



- CCS pred: 184.6 Å² (+0.3%)
- CCS pred: 184.8 Å² (+0.5%)
- CCS pred: 181.3 Å² (-1.5%)
- CCS pred: 182.1 Å² (-1.0%)
- CCS pred: 186.6 Å² (+1.4%)
- CCS pred: 183.0 Å² (-0.5%)
- CCS pred: 181.9 Å² (-1.1%)
- CCS pred: 183.7 Å² (-0.2%)
- CCS pred: 183.2 Å² (-0.4%)
- CCS pred: 185.6 Å² (+0.9%)
- CCS pred: 185.6 Å² (+0.9%)
- CCS pred: 183.5 Å² (-0.3%)
- CCS pred: 184.1 Å² (+0.1%)
- CCS pred: 184.2 Å² (+0.1%)
- CCS pred: 185.4 Å² (+0.8%)
- CCS pred: 182.3 Å² (-0.9%)



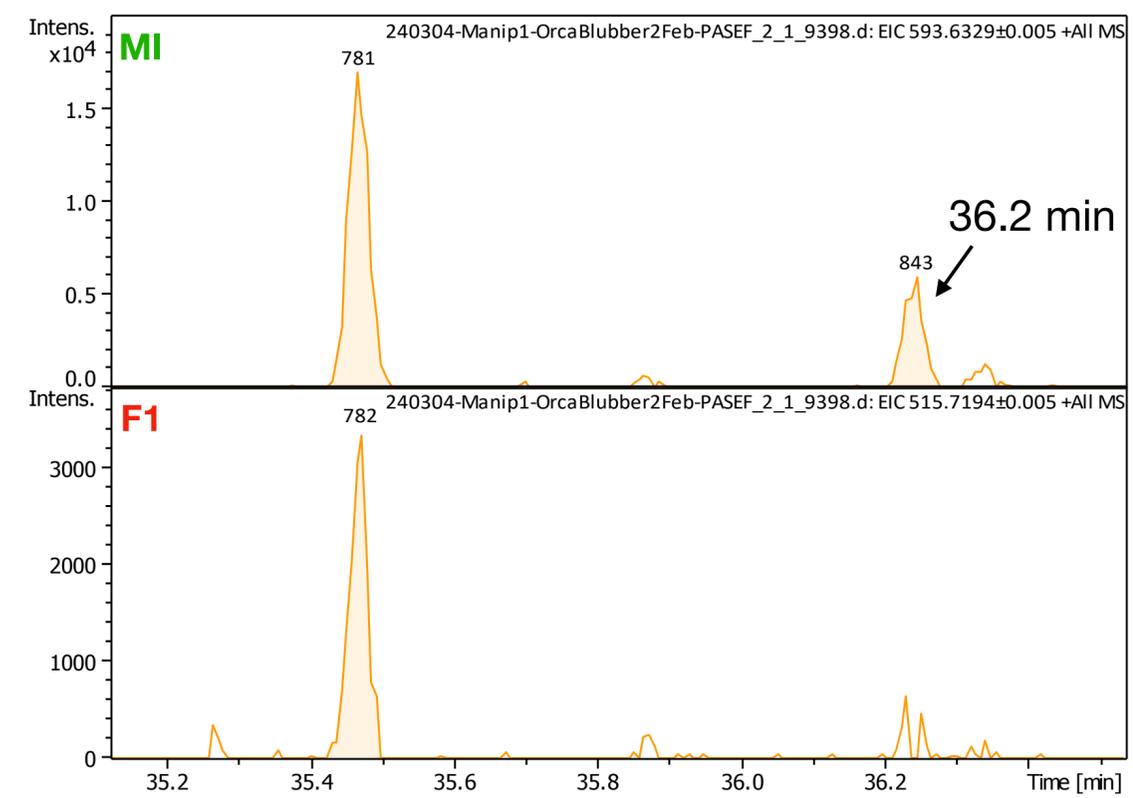
Mass spectrum & isotopic profile



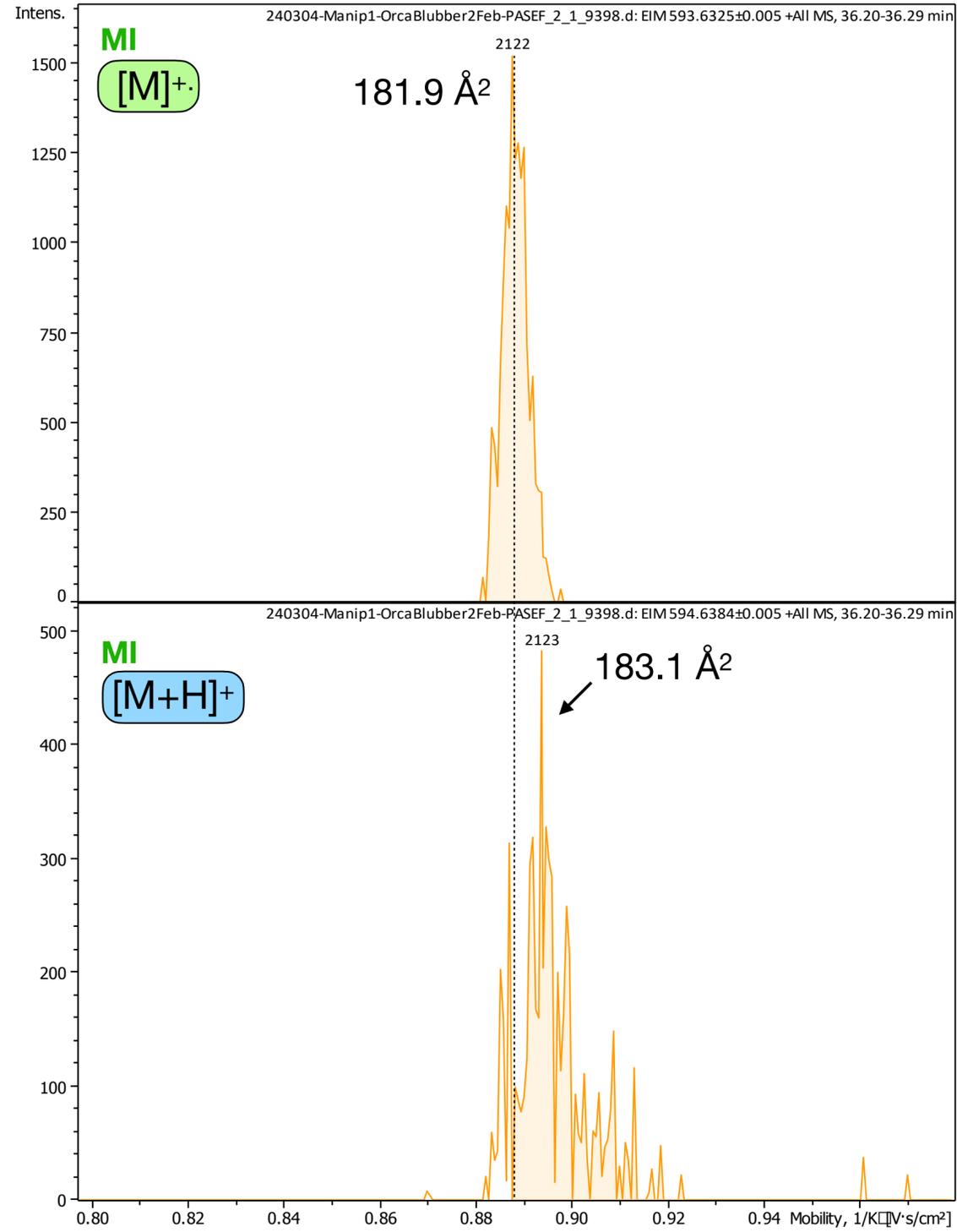
#	m/z	Abundance	Isotopologues
1	589.635744	10.495	
2	590.639120	1.492	
3	591.633718	51.187	
4	592.637082	7.267	
5	593.631703	100.000	
6	594.635049	14.168	
7	595.629710	97.948	
8	596.633026	13.830	
9	597.627770	48.295	
10	598.631028	6.773	
11	599.626032	9.779	
12	600.629127	1.345	
13	601.631639	0.126	



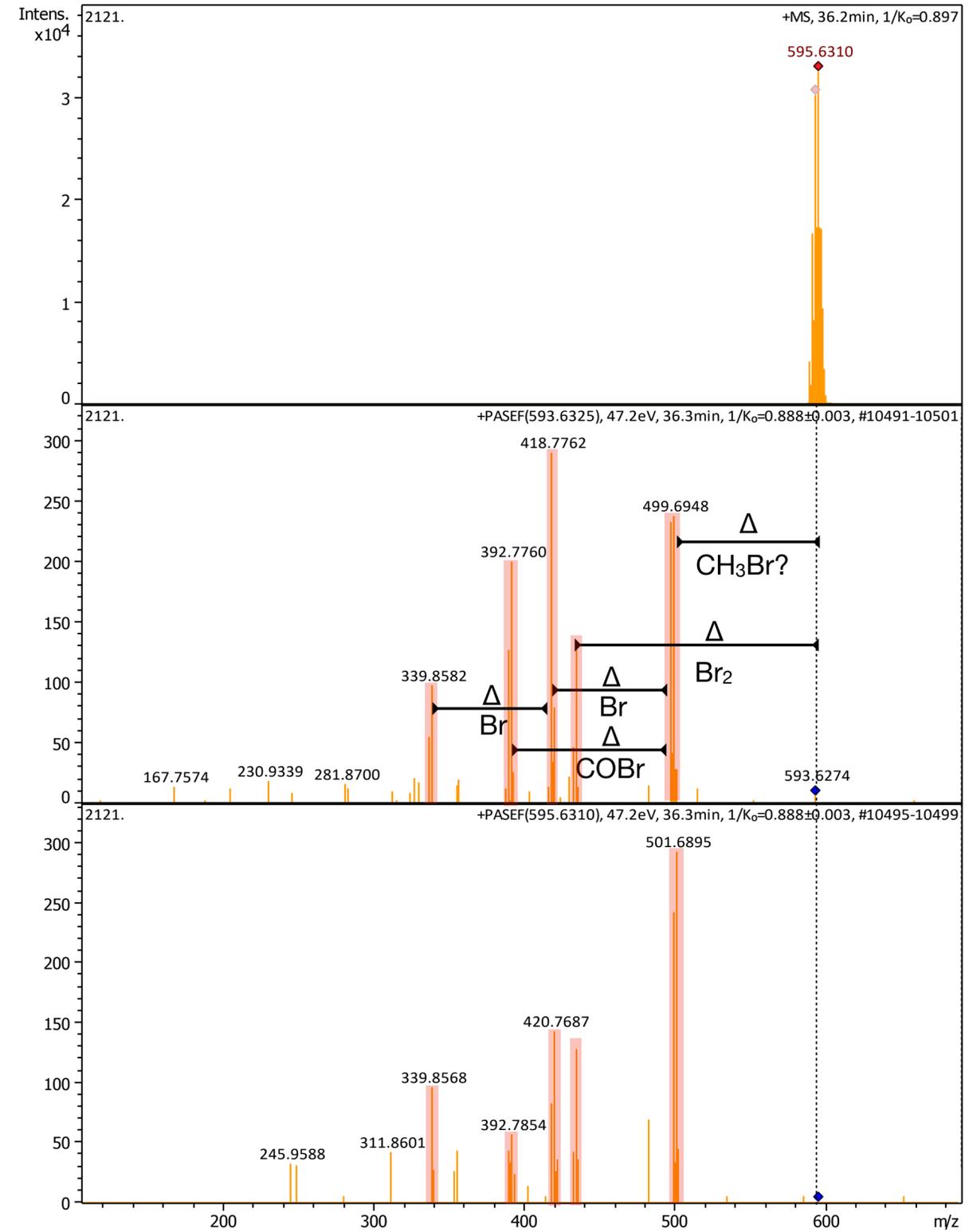
Chromatogram



Ion mobility spectra



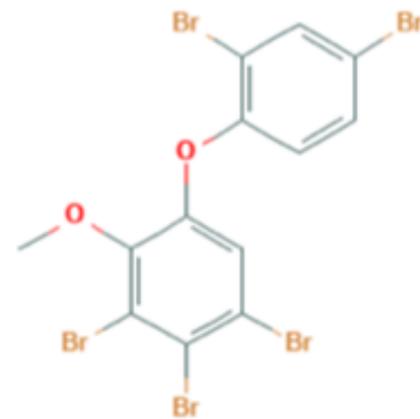
Tandem mass spectrum



- 5 Br
- At least 2C, 3H and 1O

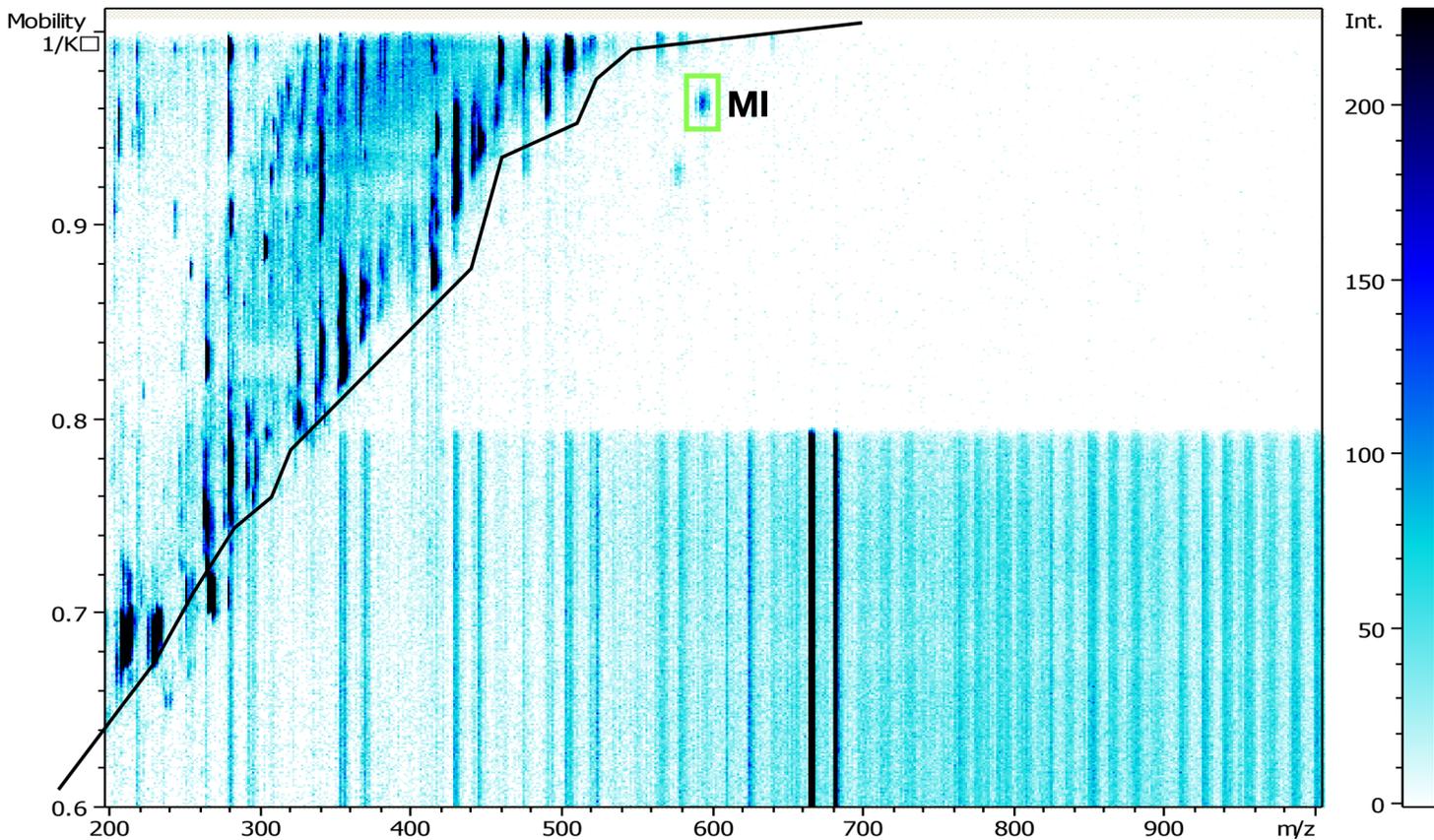
Putative candidate(s)

PubChem

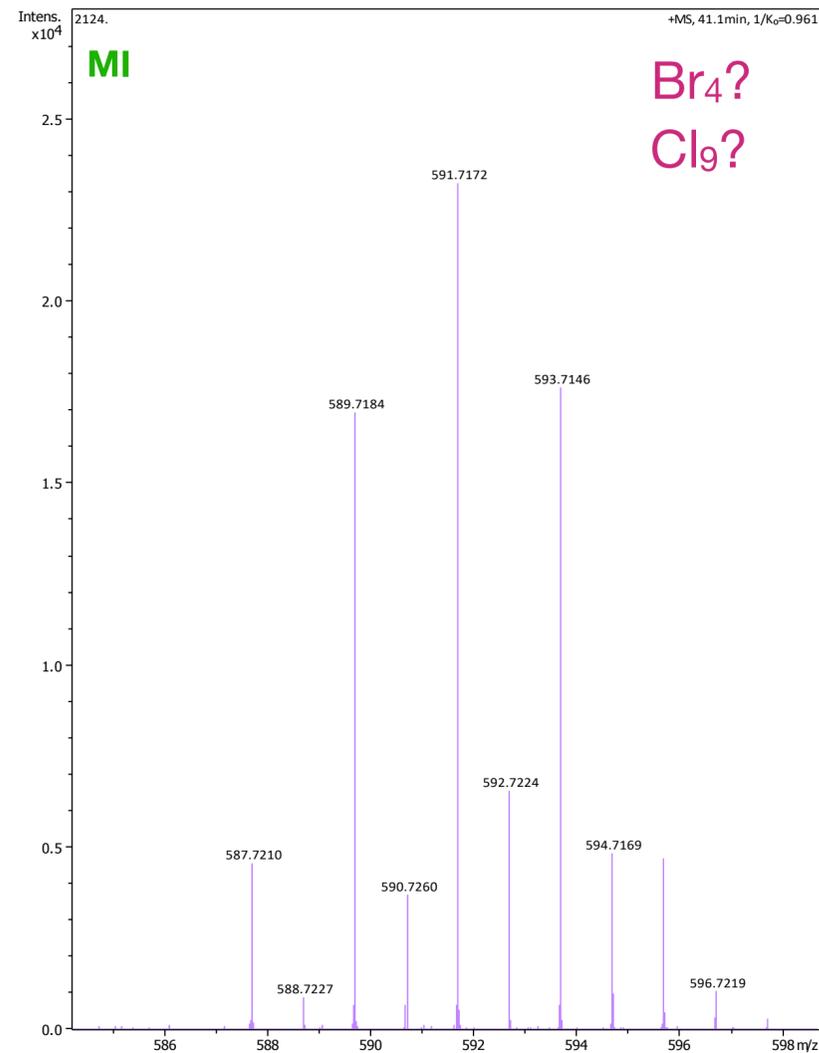
 $C_{13}H_7Br_5O_2$ Methoxylated
pentaBDEs
(multiple isomers)16 isomersCCS pred: 184.6 Å² (+1.5%)CCS pred: 184.8 Å² (+1.6%)CCS pred: 181.3 Å² (-0.3%)CCS pred: 182.1 Å² (+0.1%)CCS pred: 186.6 Å² (+2.6%)CCS pred: 183.0 Å² (+0.6%)CCS pred: 181.9 Å² (0.0%)CCS pred: 183.7 Å² (+1.0%)CCS pred: 183.2 Å² (+0.7%)CCS pred: 185.6 Å² (+2.0%)CCS pred: 185.6 Å² (+2.0%)CCS pred: 183.5 Å² (+0.9%)CCS pred: 184.1 Å² (+1.2%)CCS pred: 184.2 Å² (+1.3%)CCS pred: 185.4 Å² (+1.9%)CCS pred: 182.3 Å² (+0.2%)

Heatmap

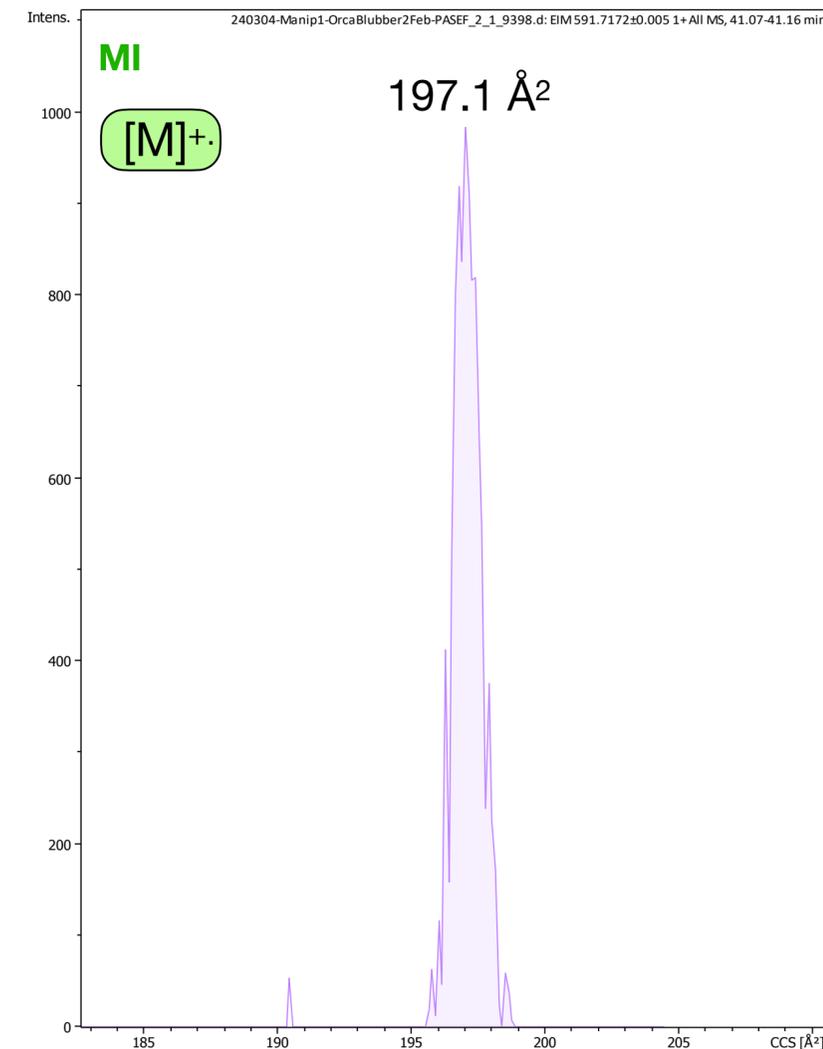
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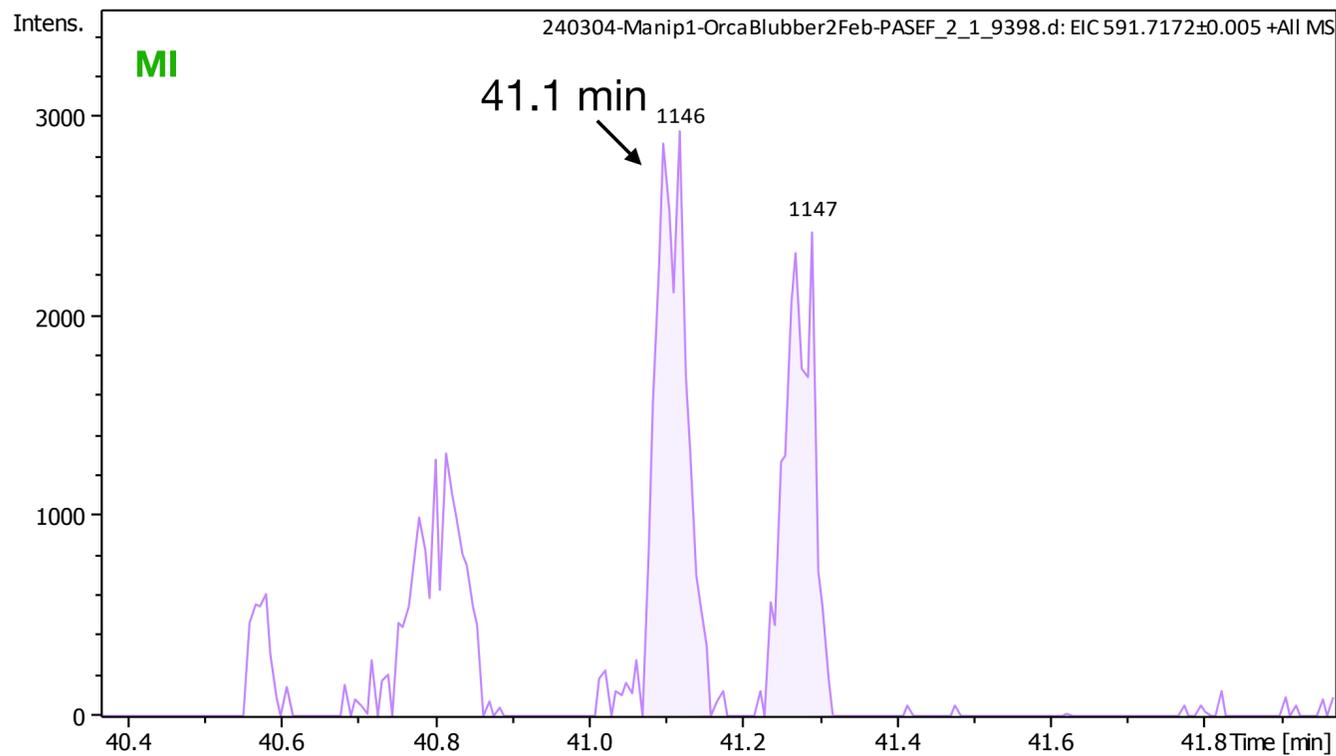
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



SmartFormula:
C15H11Br4ClNO2?

Tandem mass spectrum

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Tentative candidate(s)

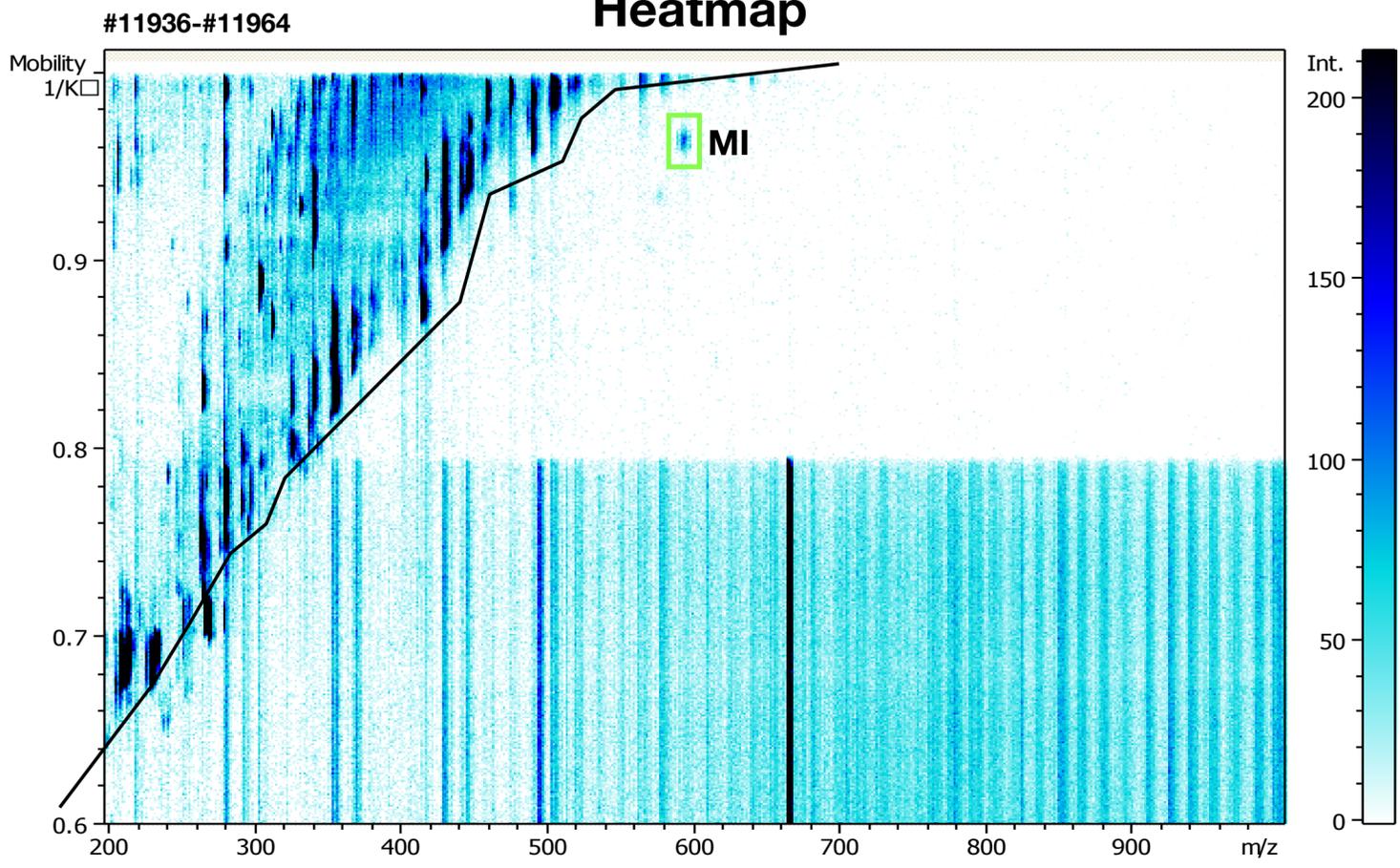
PubChem

/

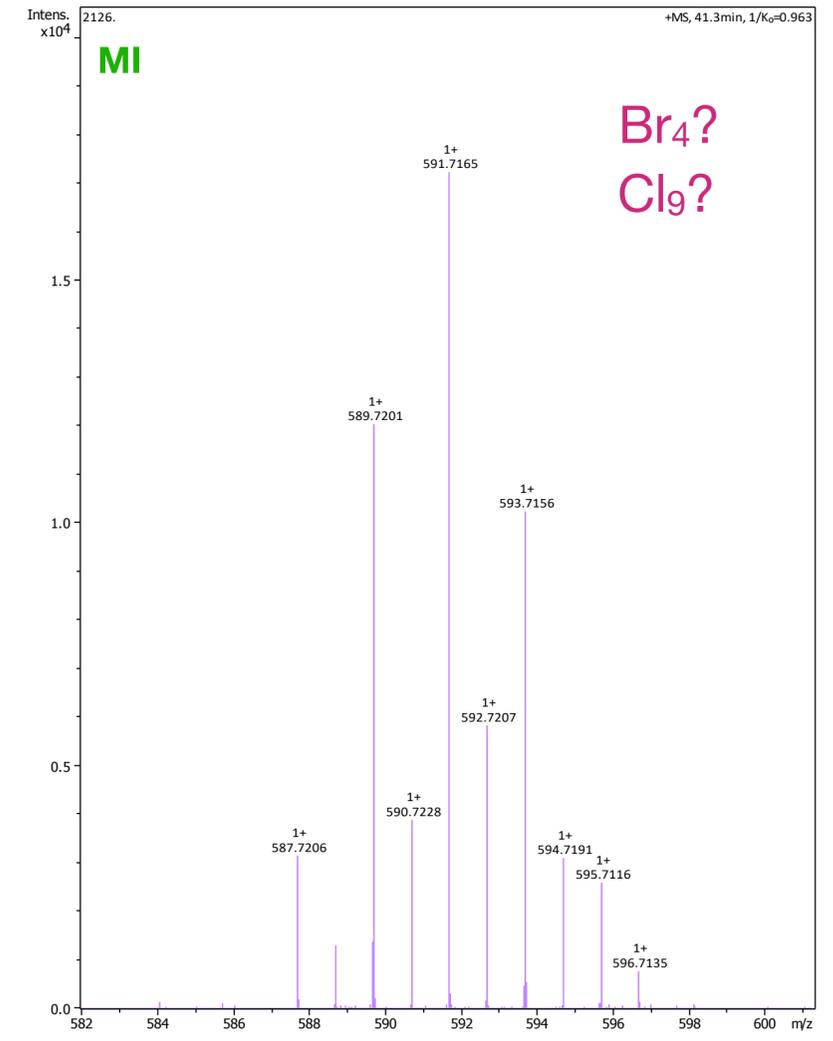
Confidence level

5

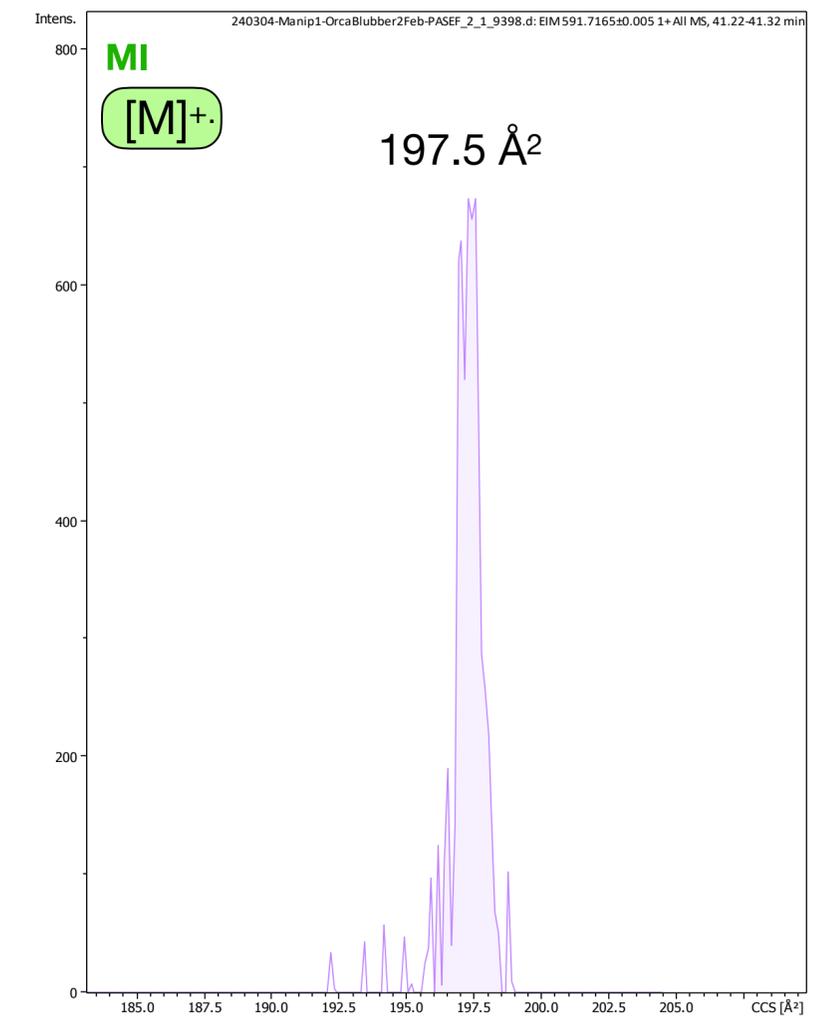
Heatmap



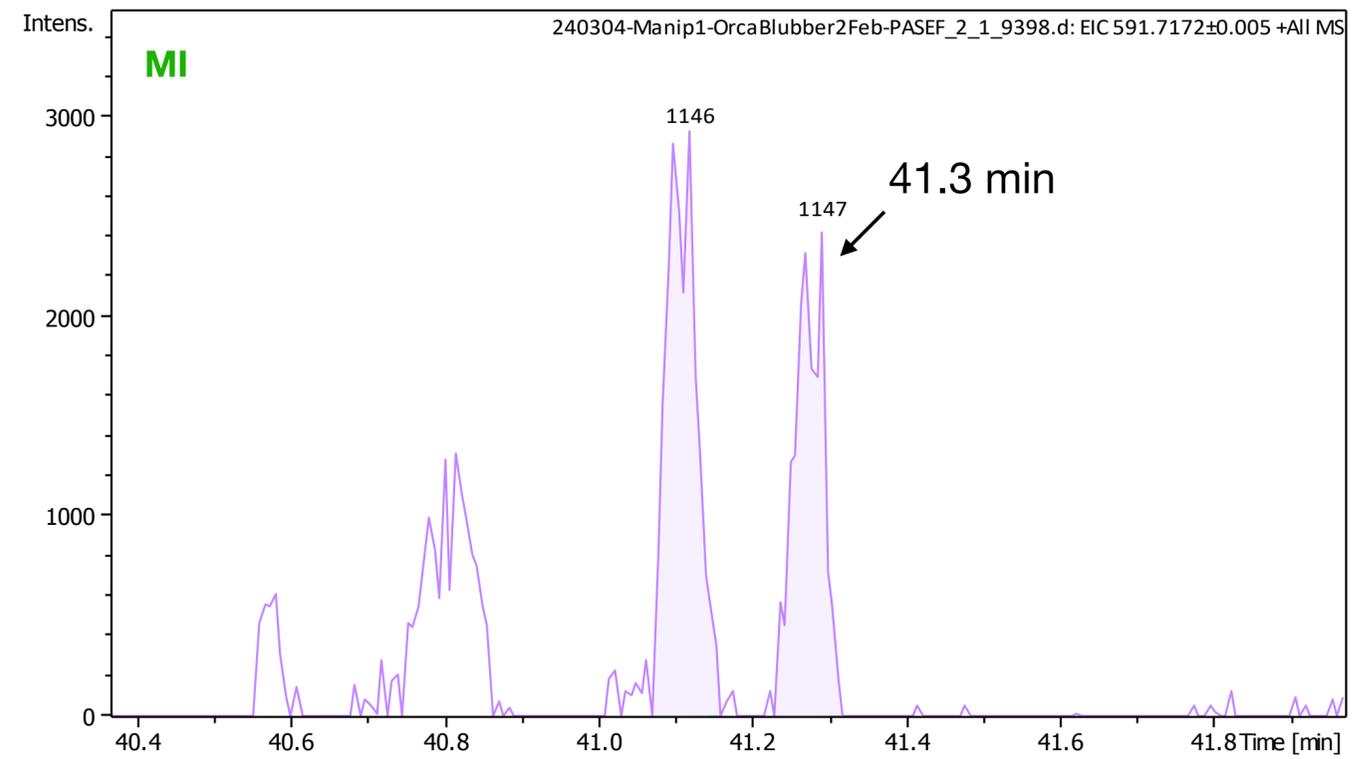
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



SmartFormula:
C15H11Br4ClNO2?

Tandem mass spectrum
 /

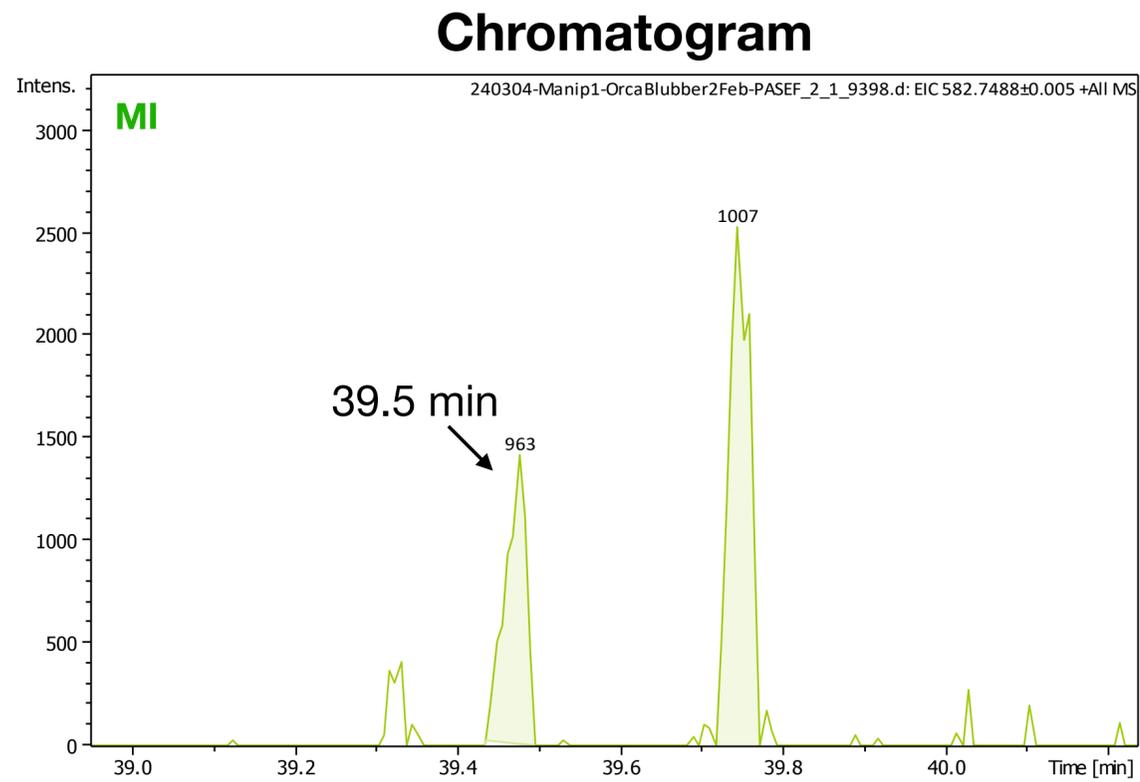
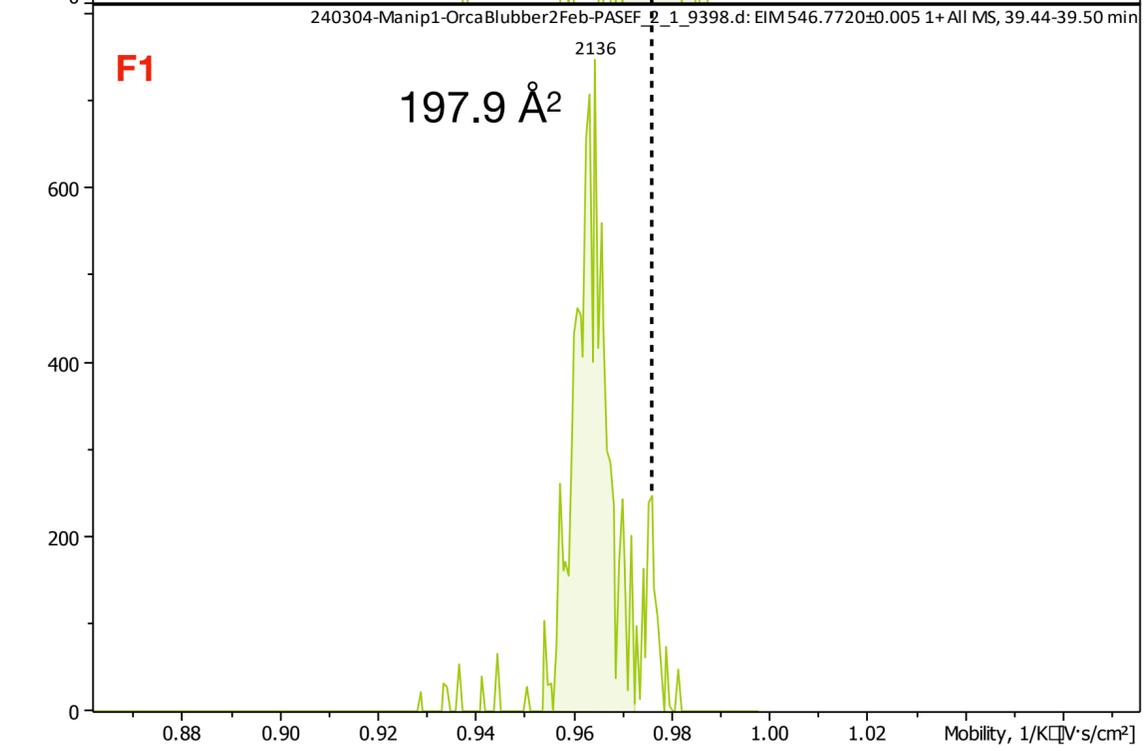
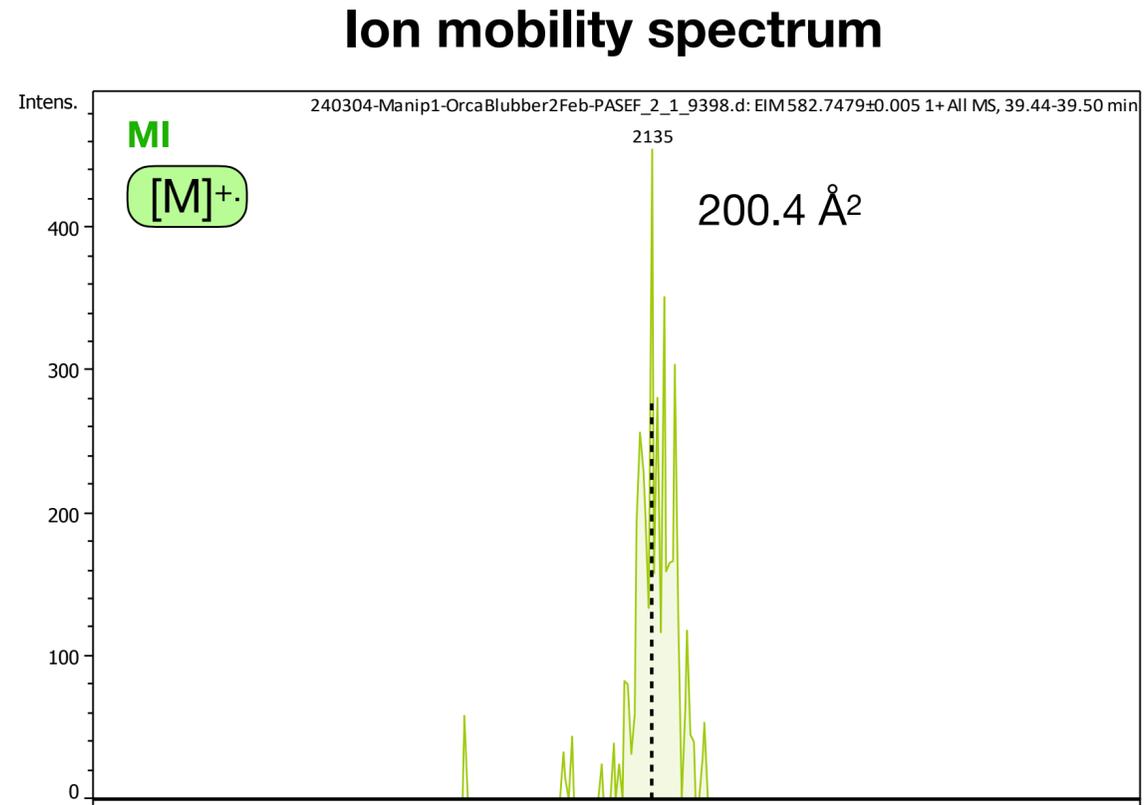
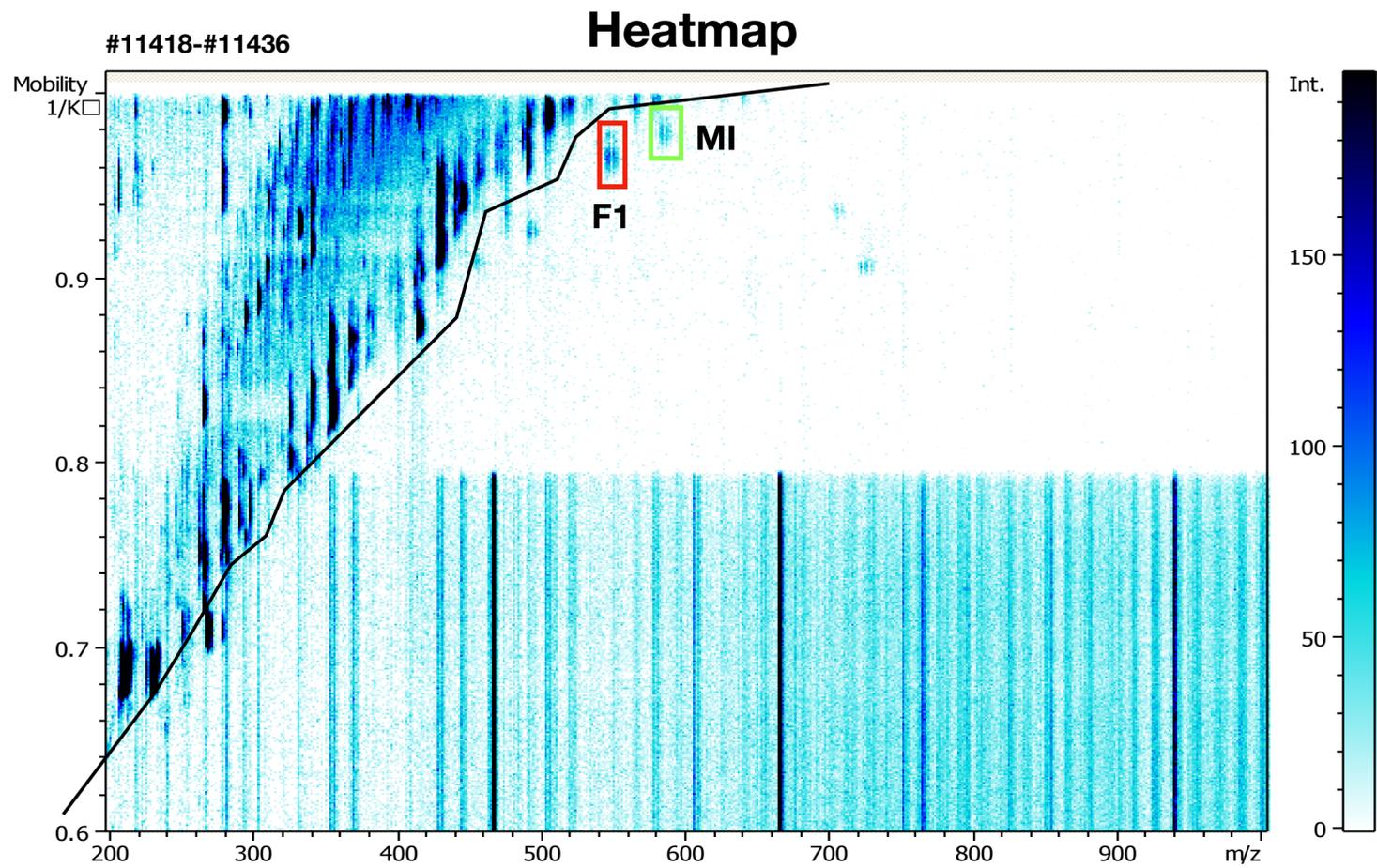
Tentative candidate(s)

PubChem

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Confidence level

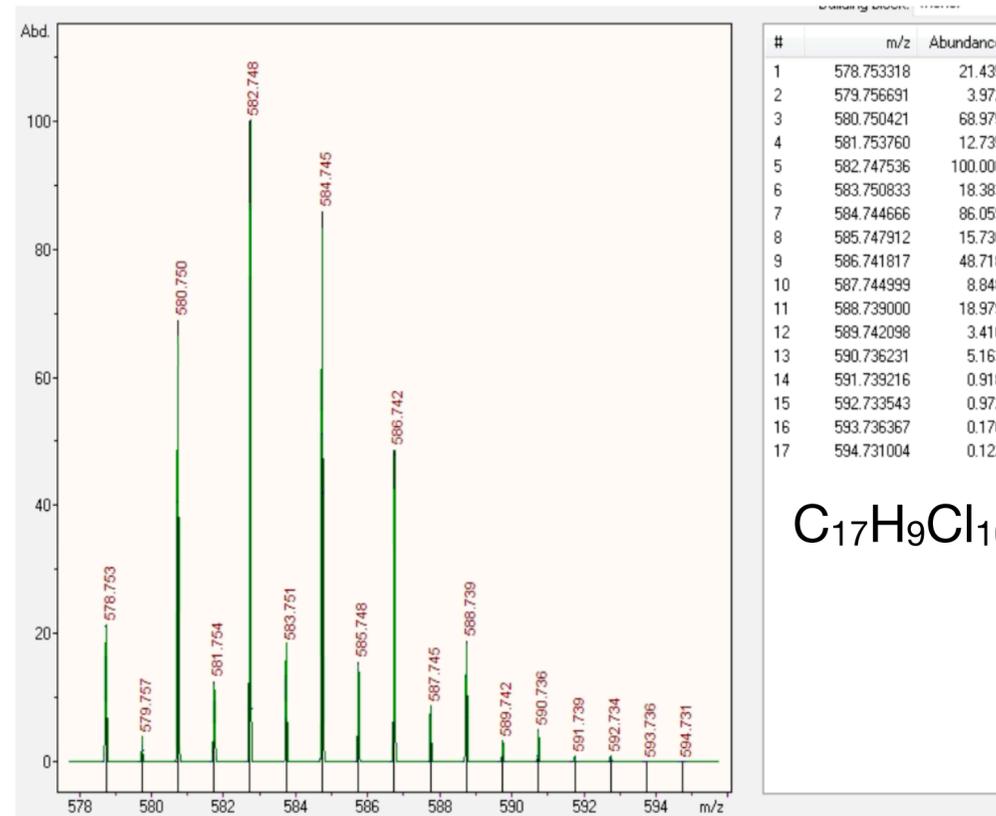
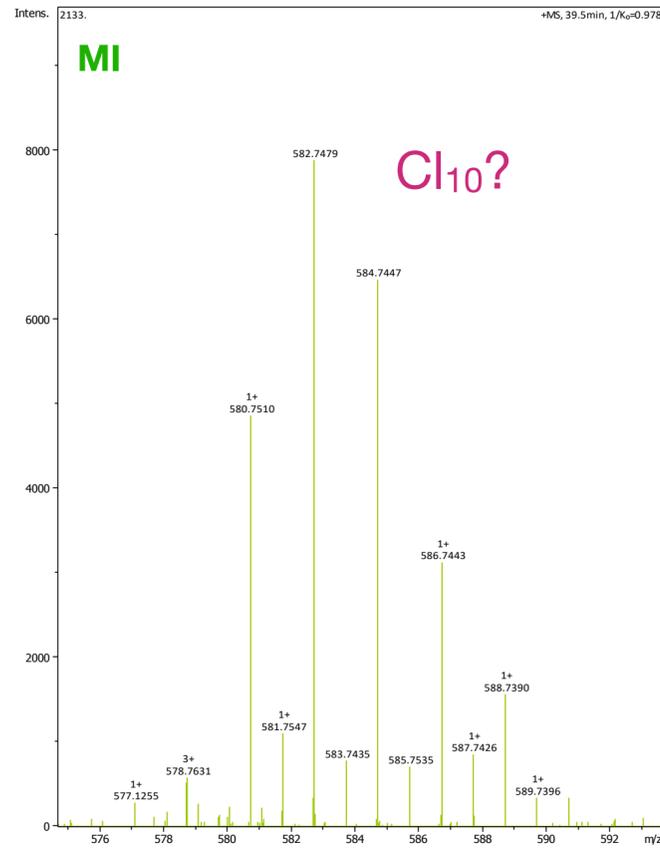
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Mass spectra & isotopic profile

Feature #39

EIC 582.7488:
EIC 546.7733:



Tandem mass spectrum

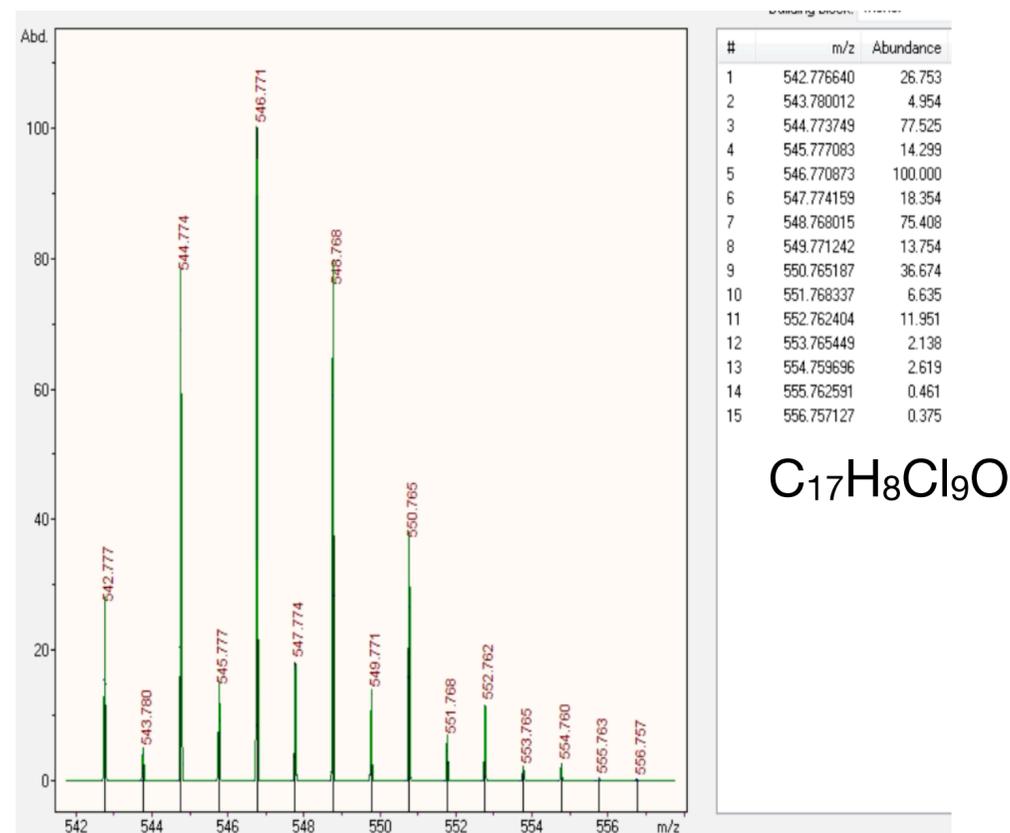
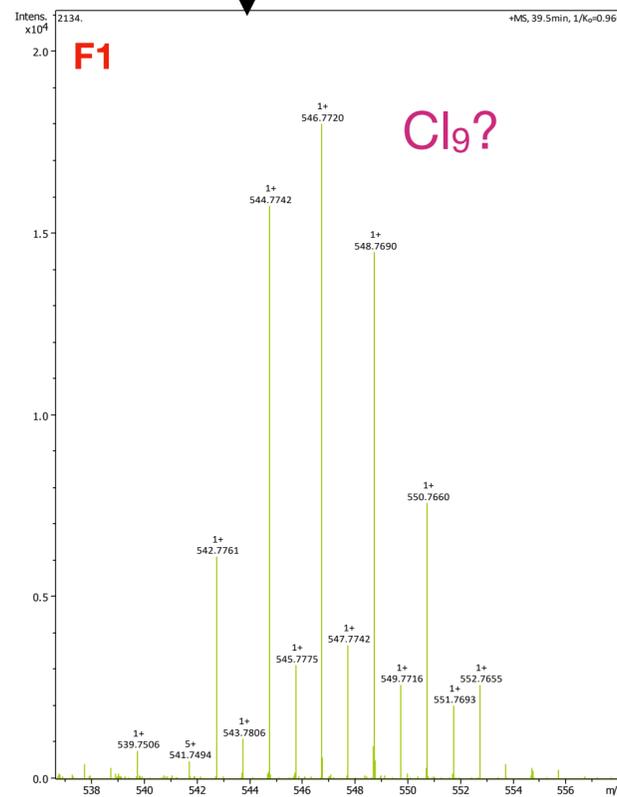
Tentative candidate(s)

PubChem

Confidence level

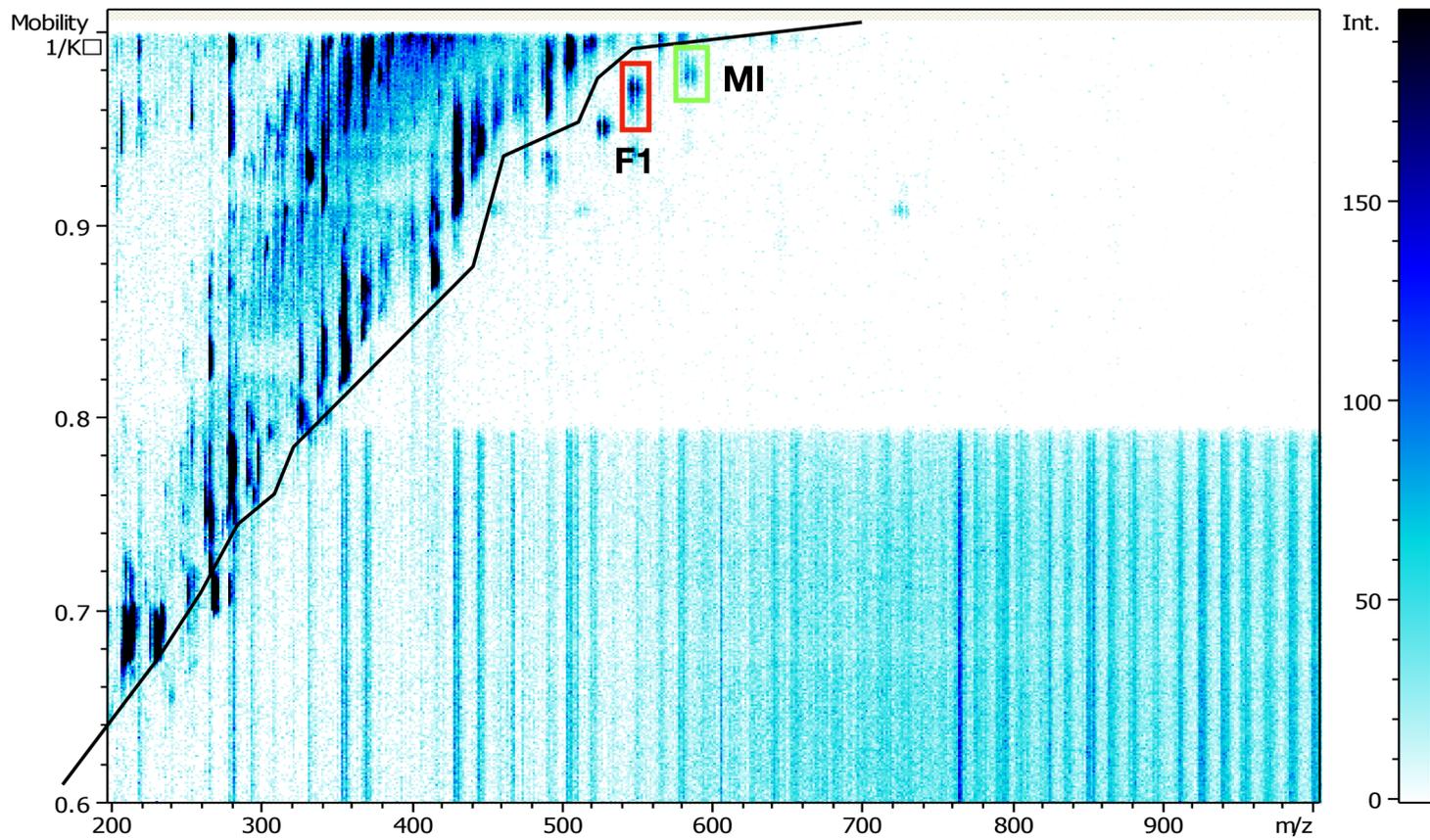
4

- HCl?

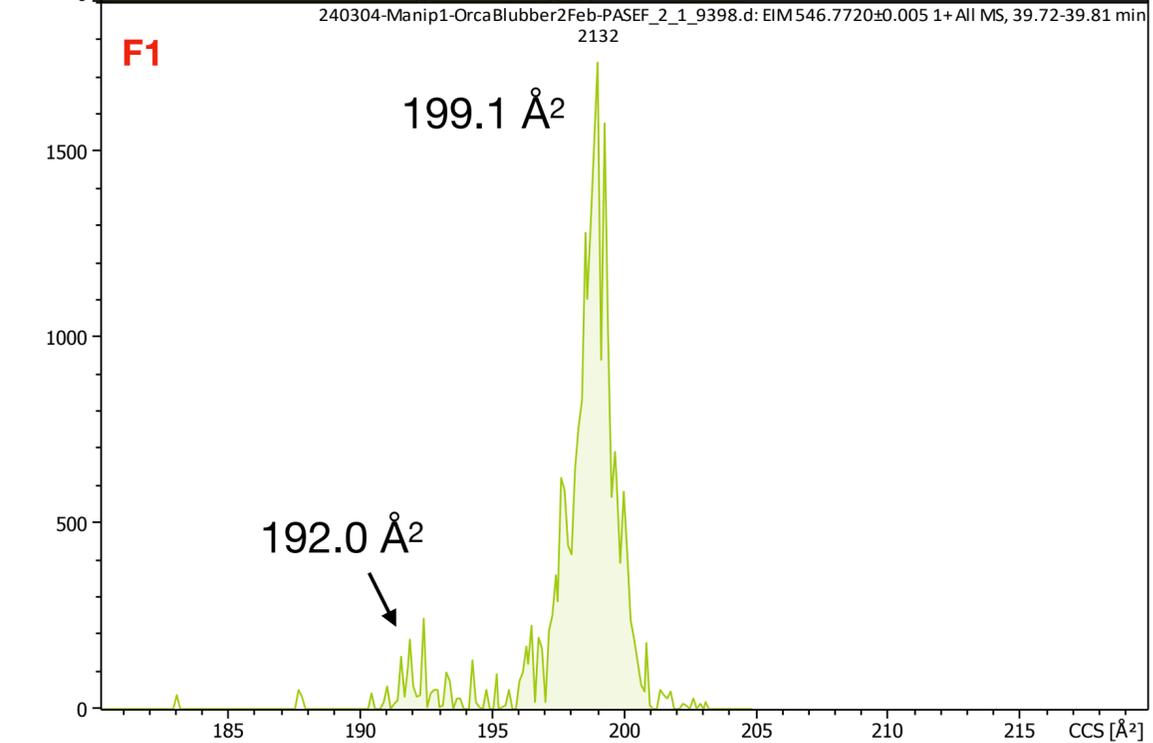
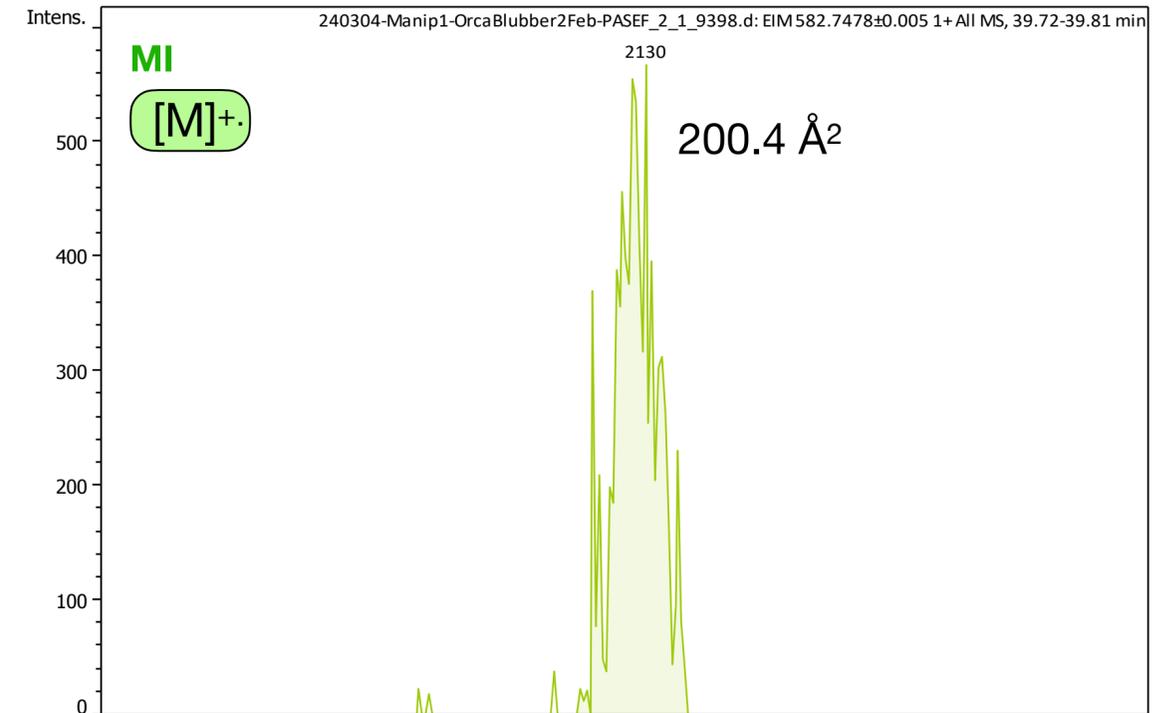


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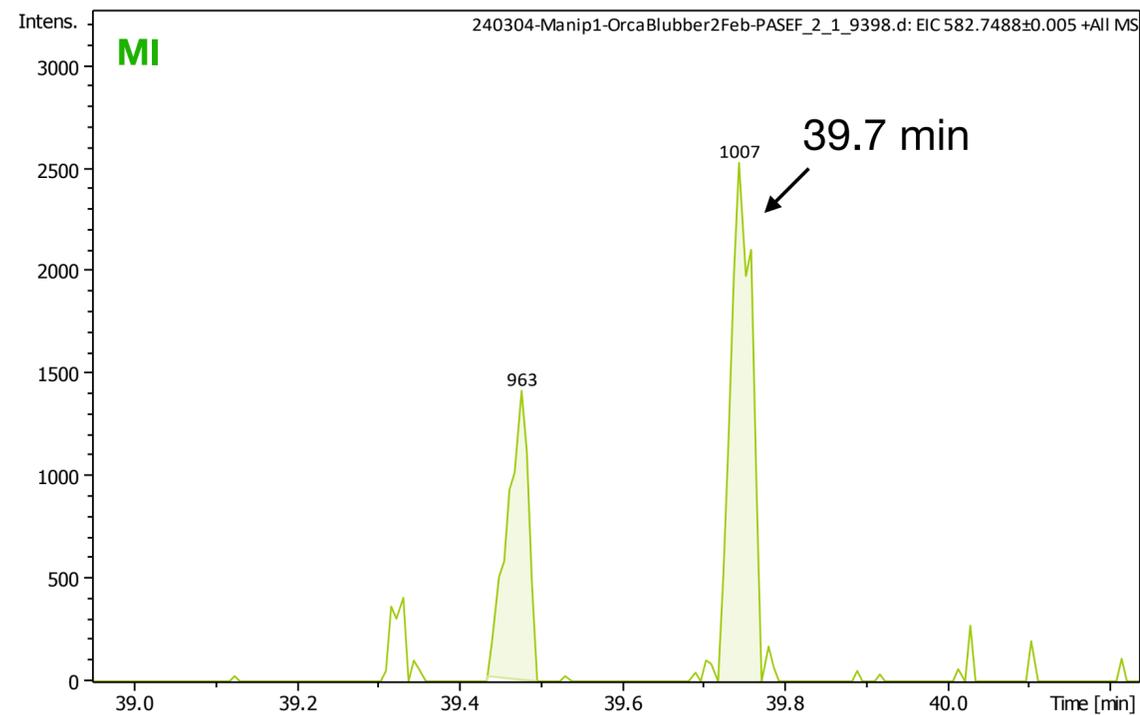
Heatmap



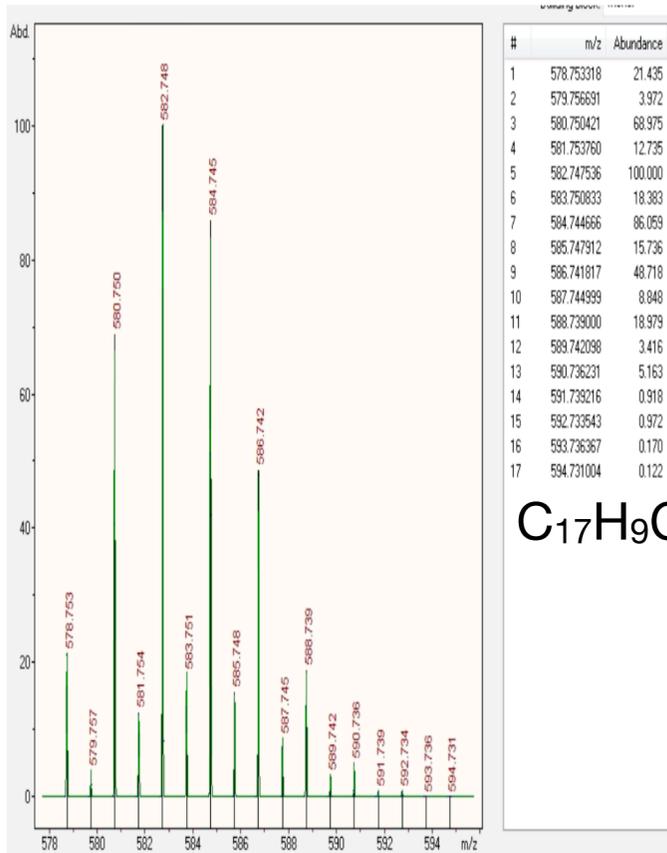
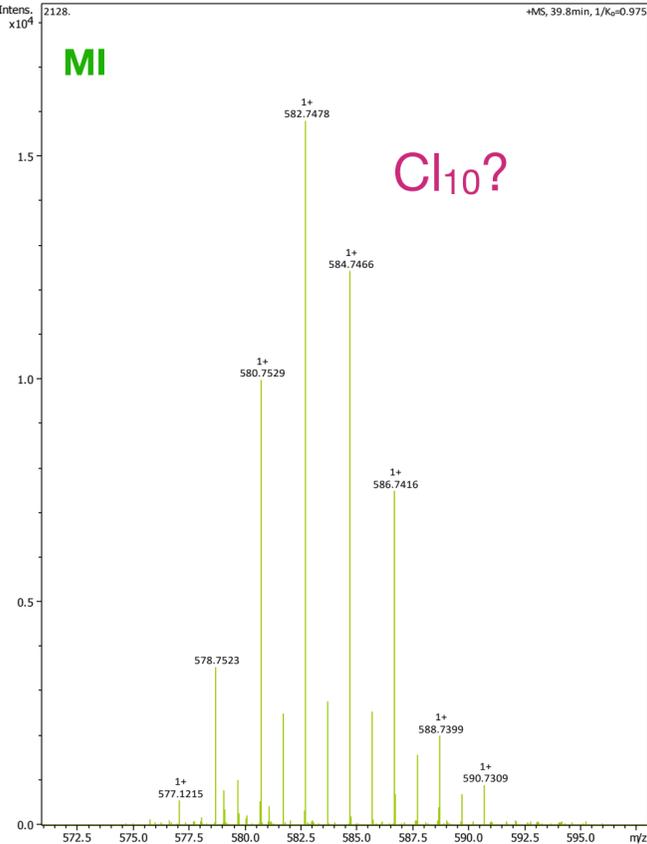
Ion mobility spectra



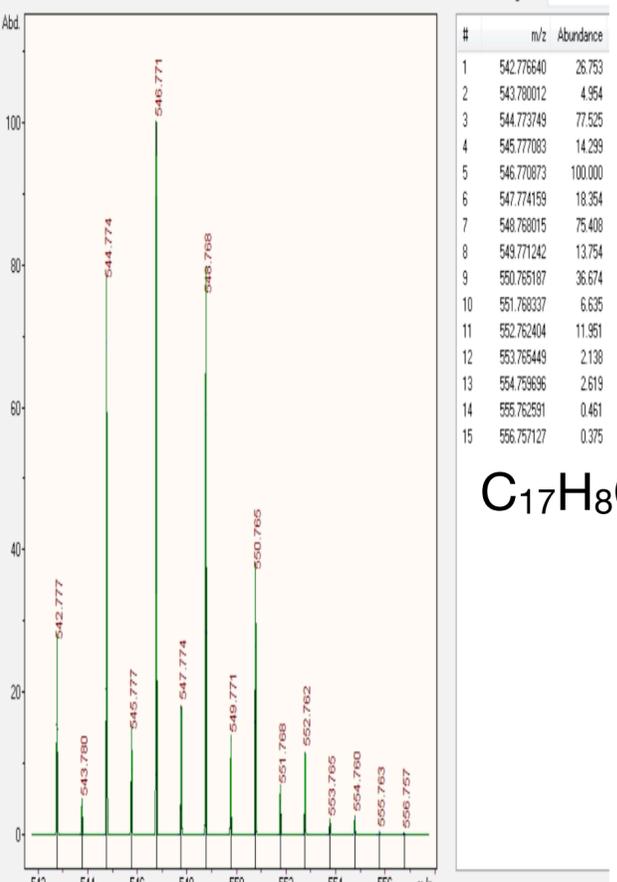
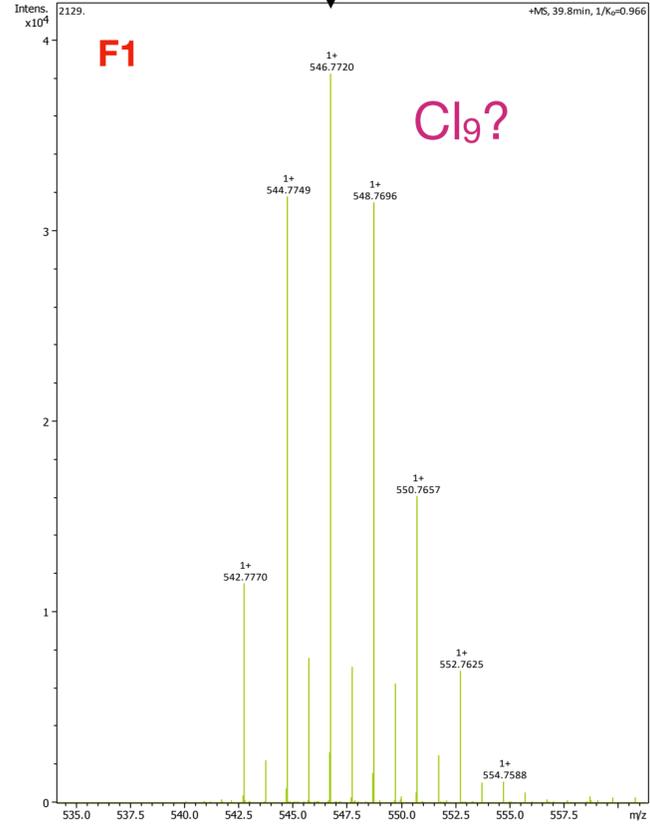
Chromatogram



Mass spectra & isotopic profile



- HCl?



Tandem mass spectrum

/

Tentative candidate(s)



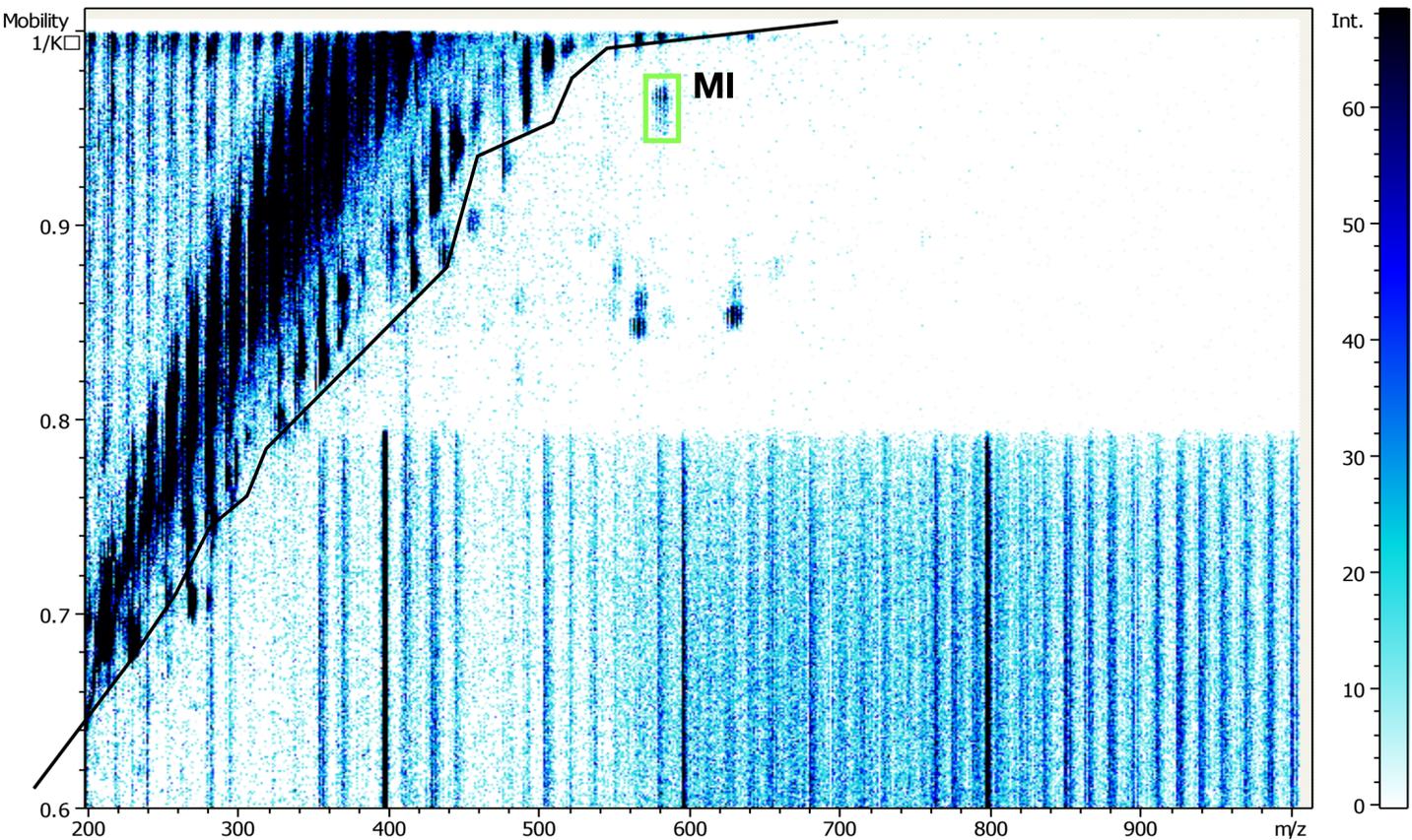
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Confidence level

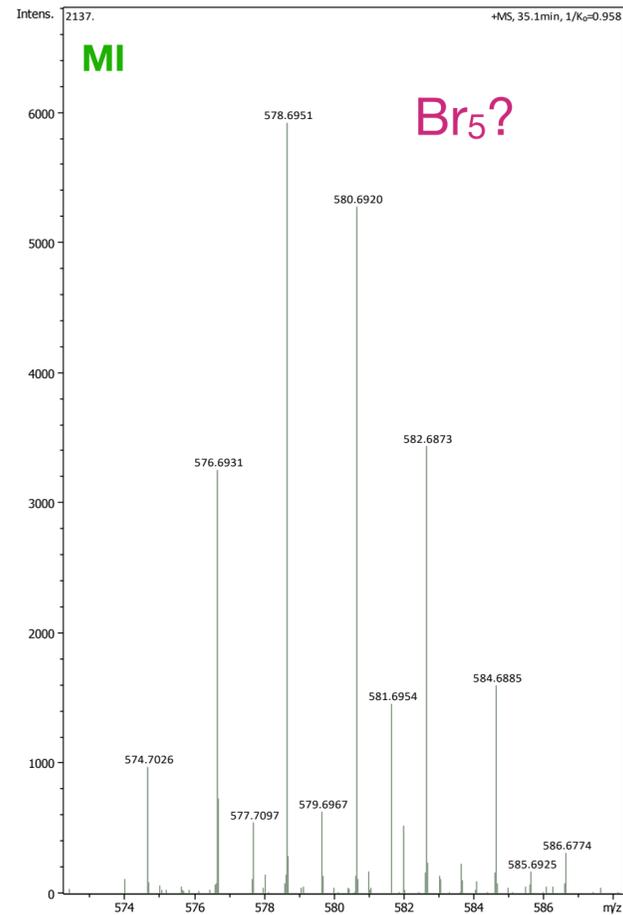


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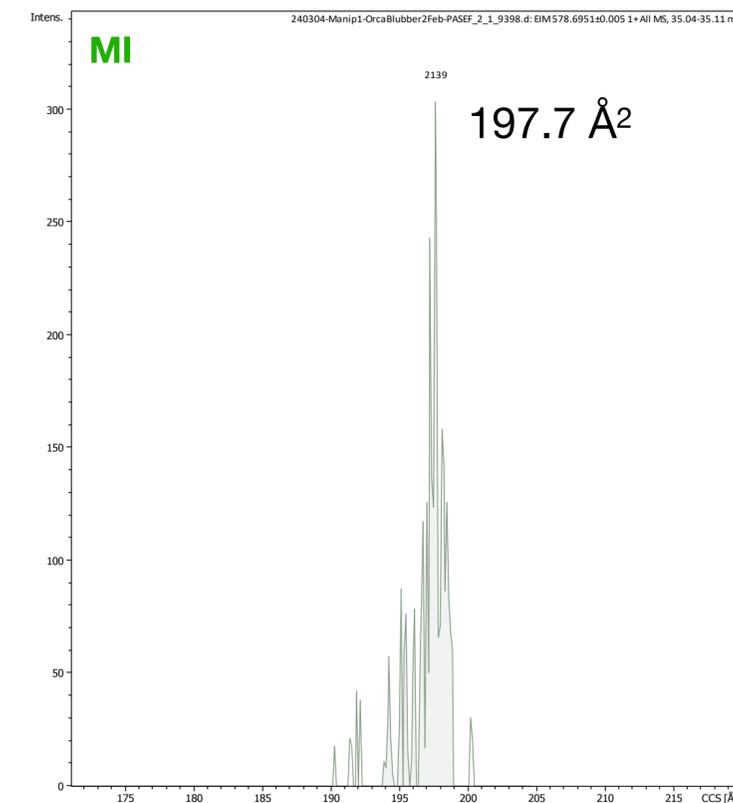
Heatmap



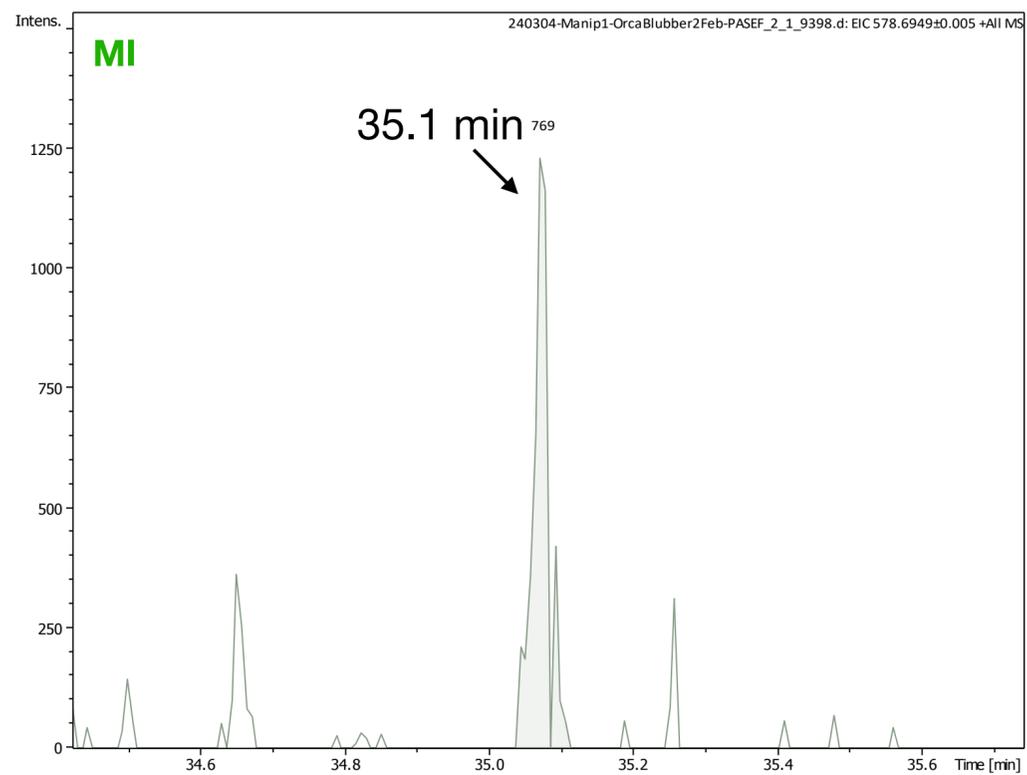
Mass spectrum & isotopic profile



Ion mobility spectrum



Chromatogram



Tandem mass spectrum

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Tentative candidate(s)

PubChem

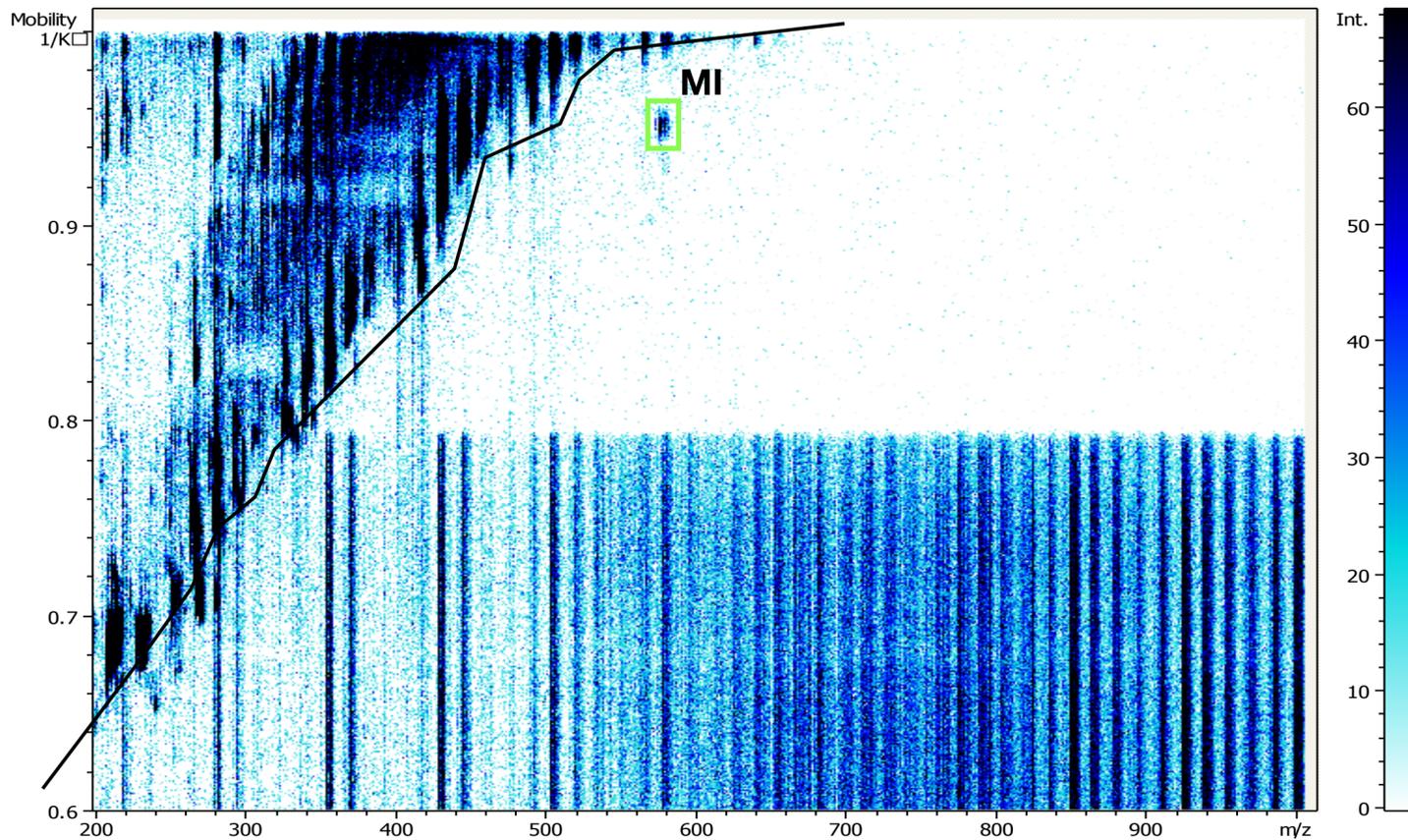
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Confidence level

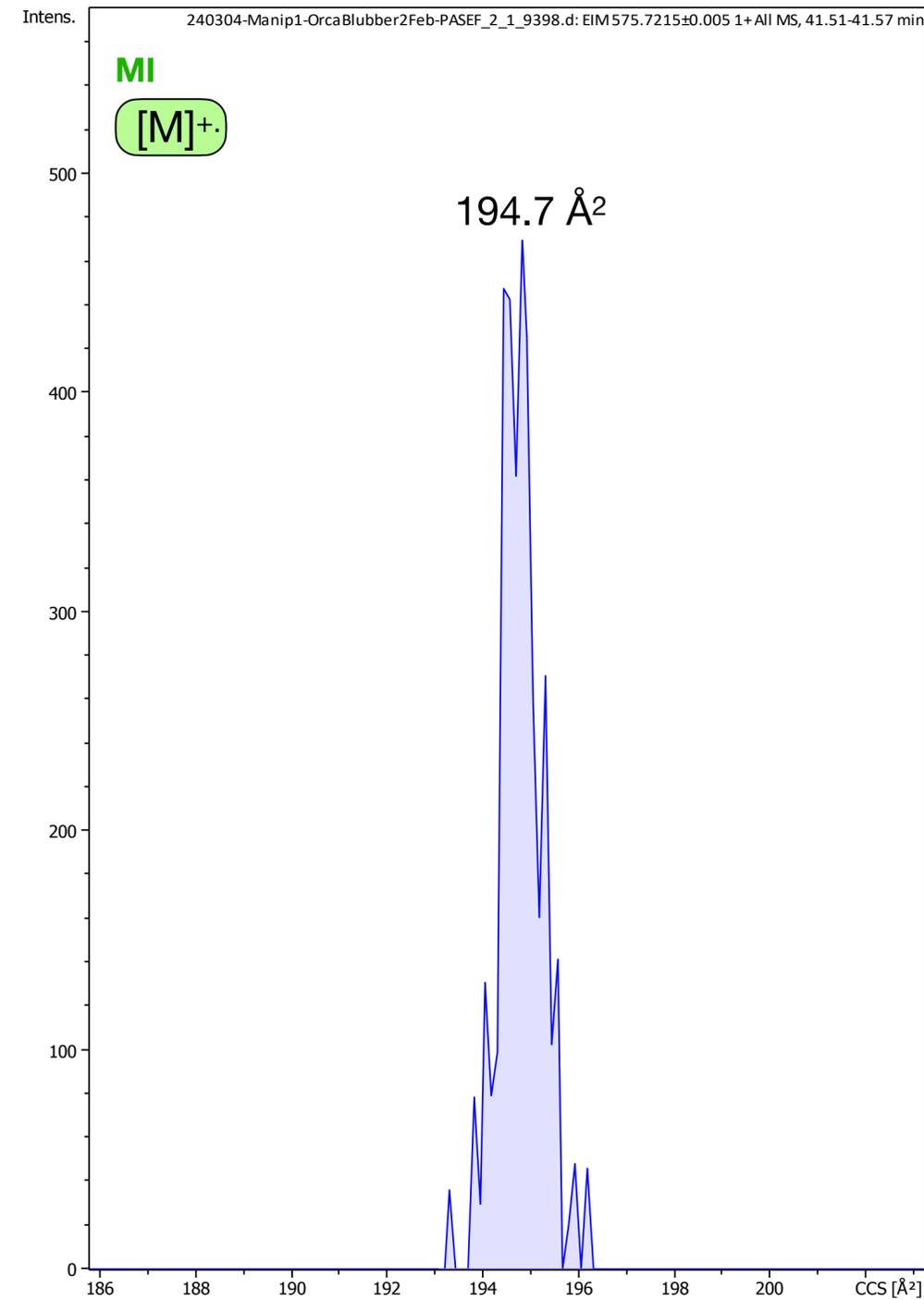
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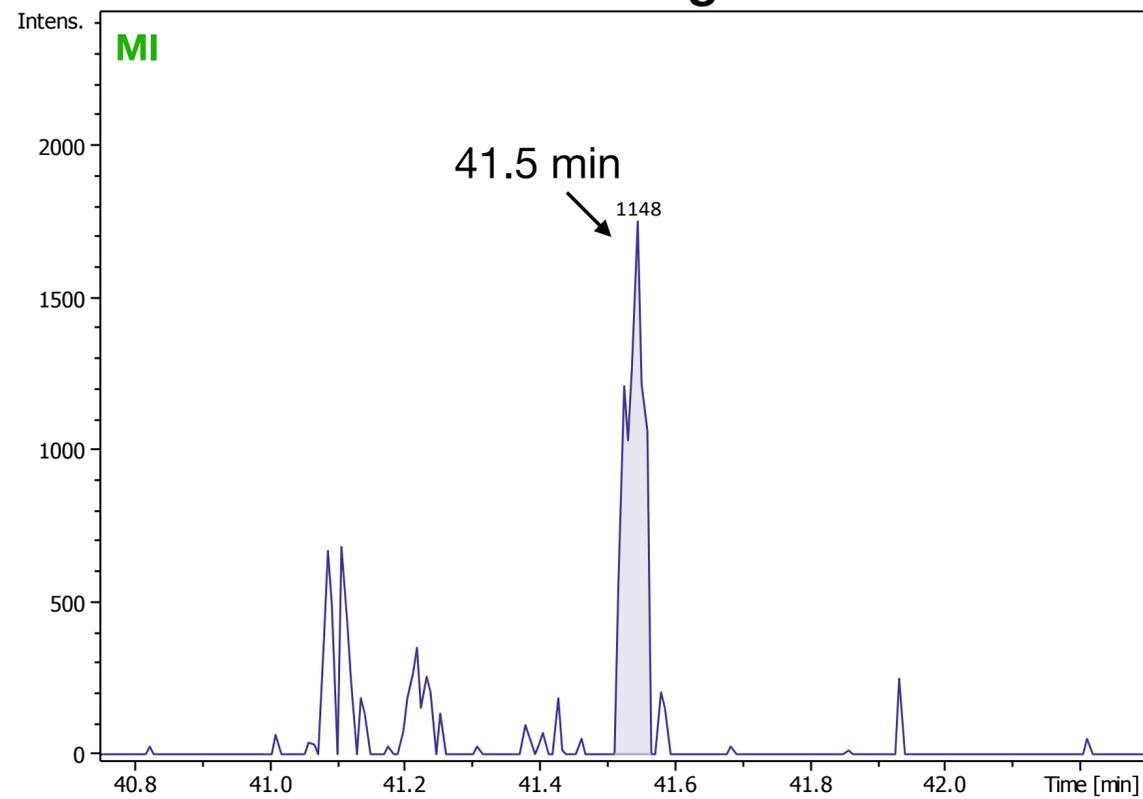
Heatmap



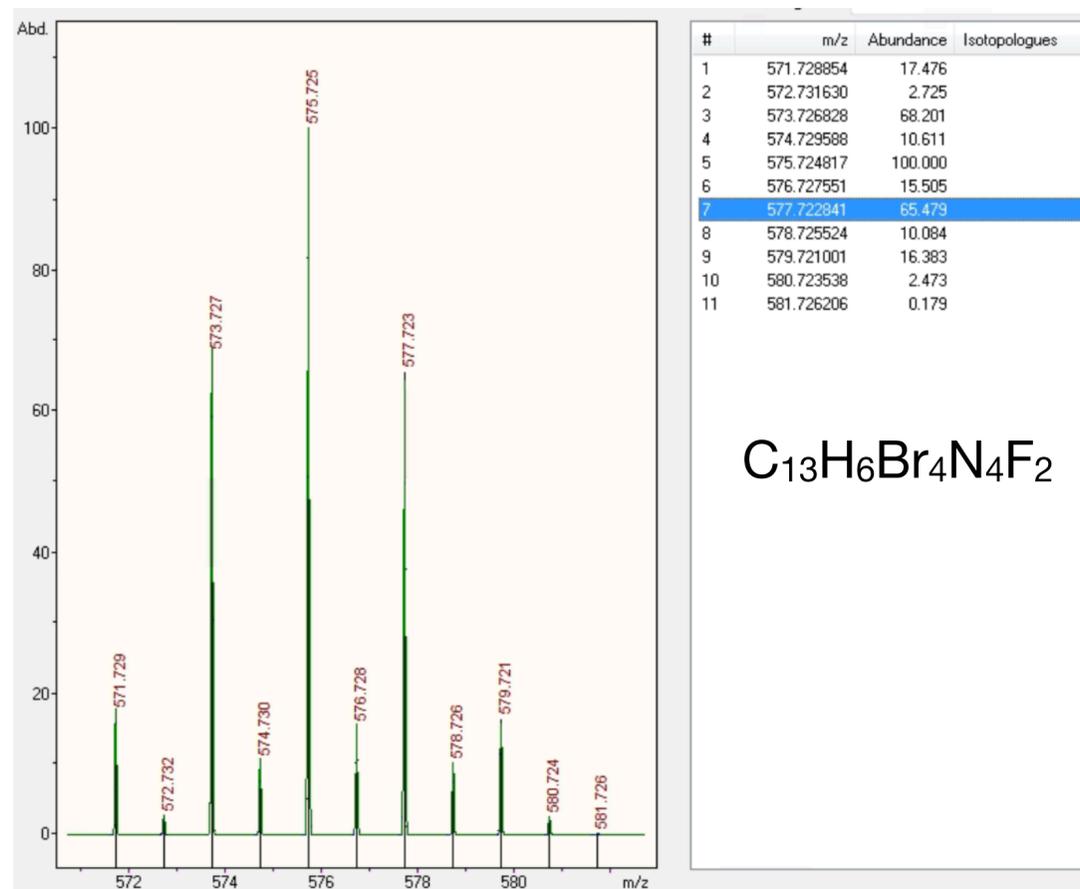
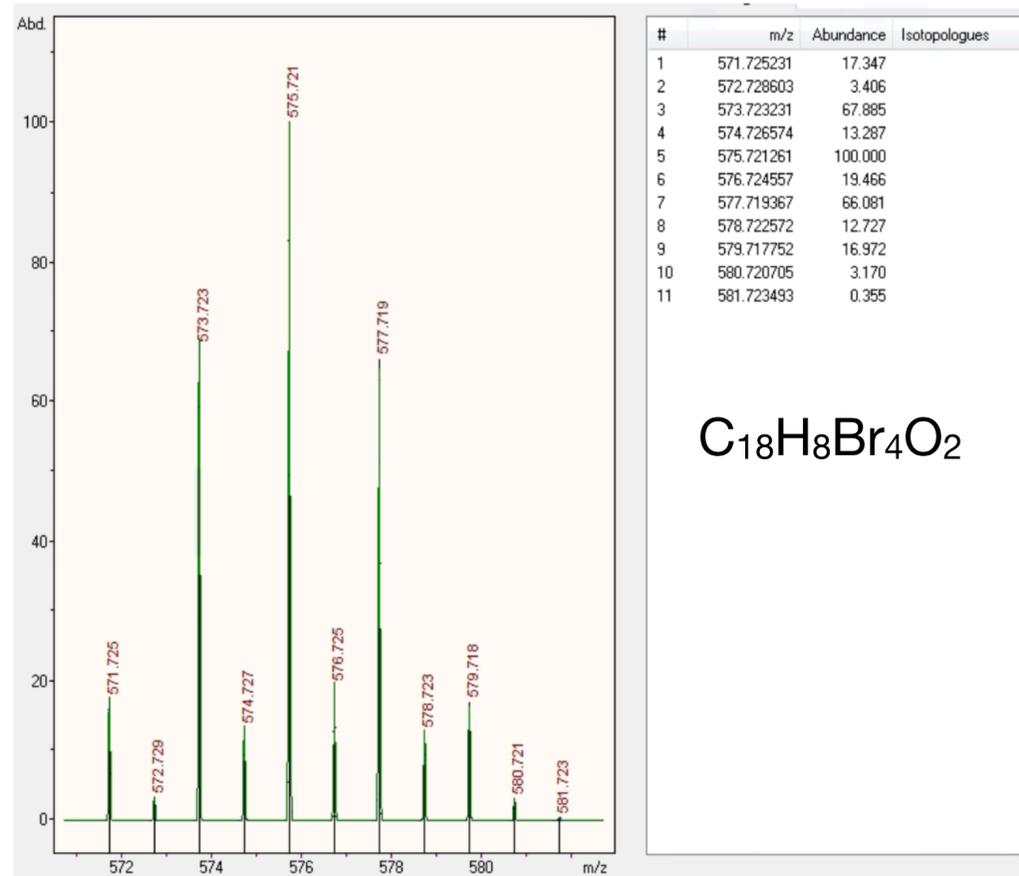
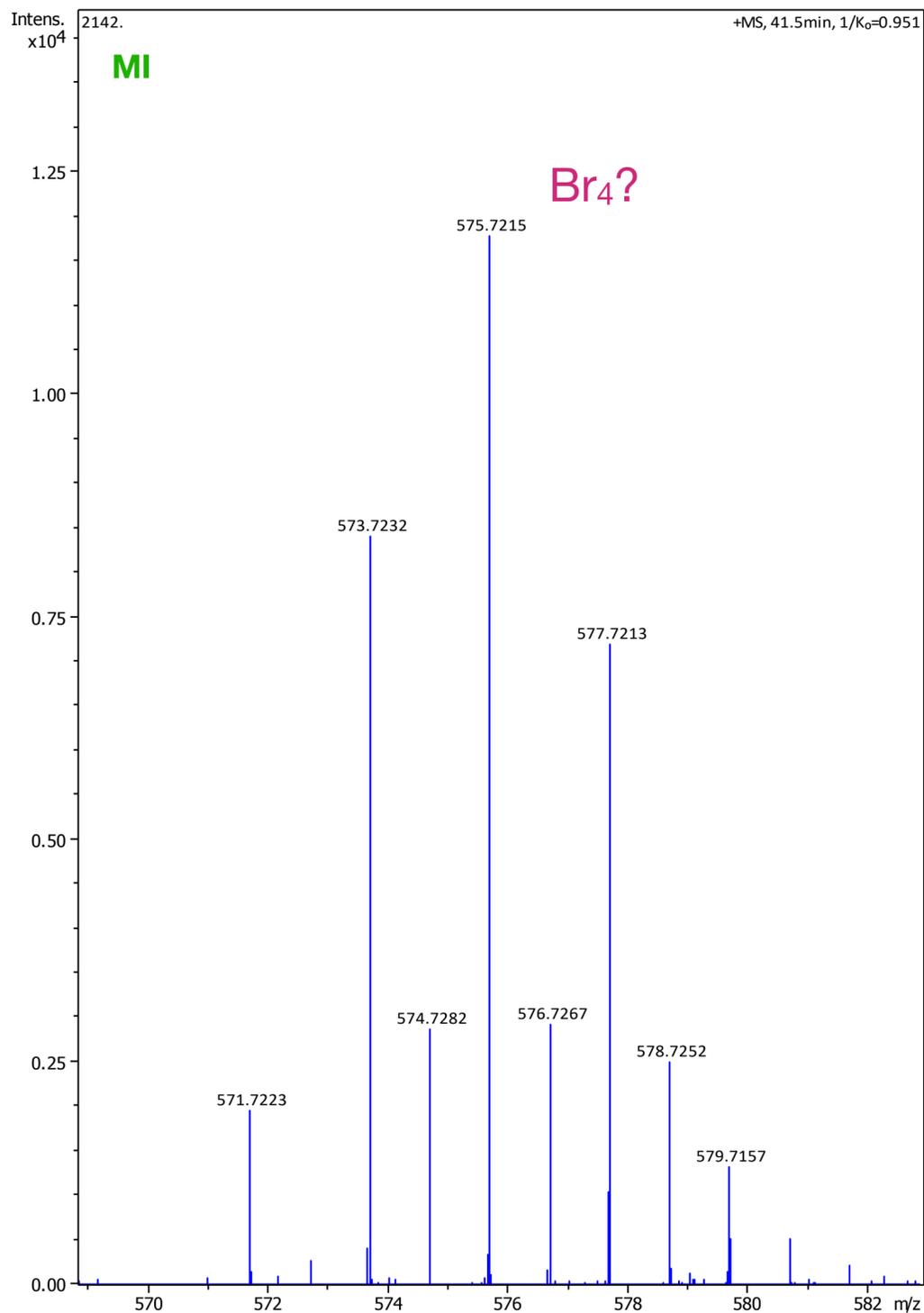
Ion mobility spectrum



Chromatogram



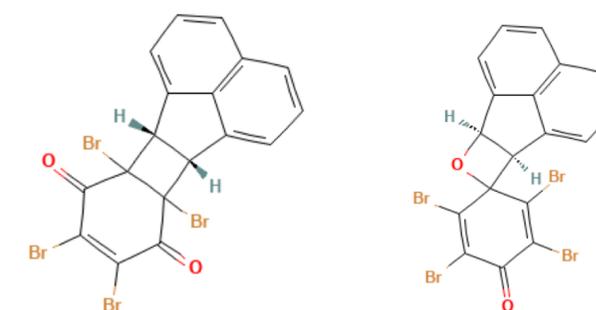
Mass spectrum & isotopic profile



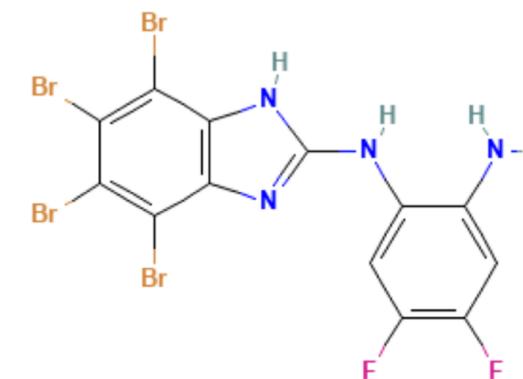
Tandem spectrum

Tentative candidate(s)

PubChem



C₁₈H₈Br₄O₂



C₁₃H₆Br₄N₄F₂

Confidence level

5