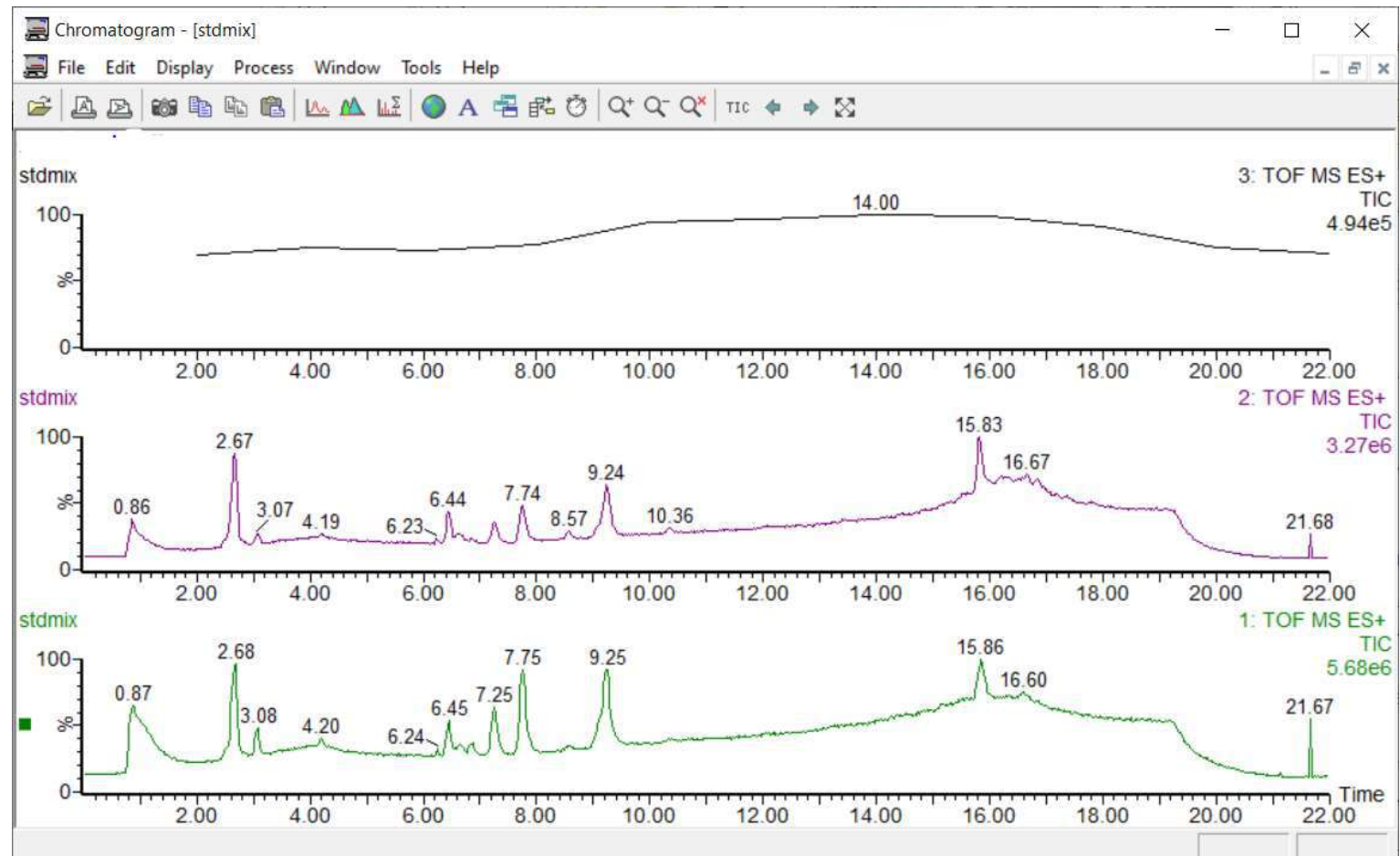


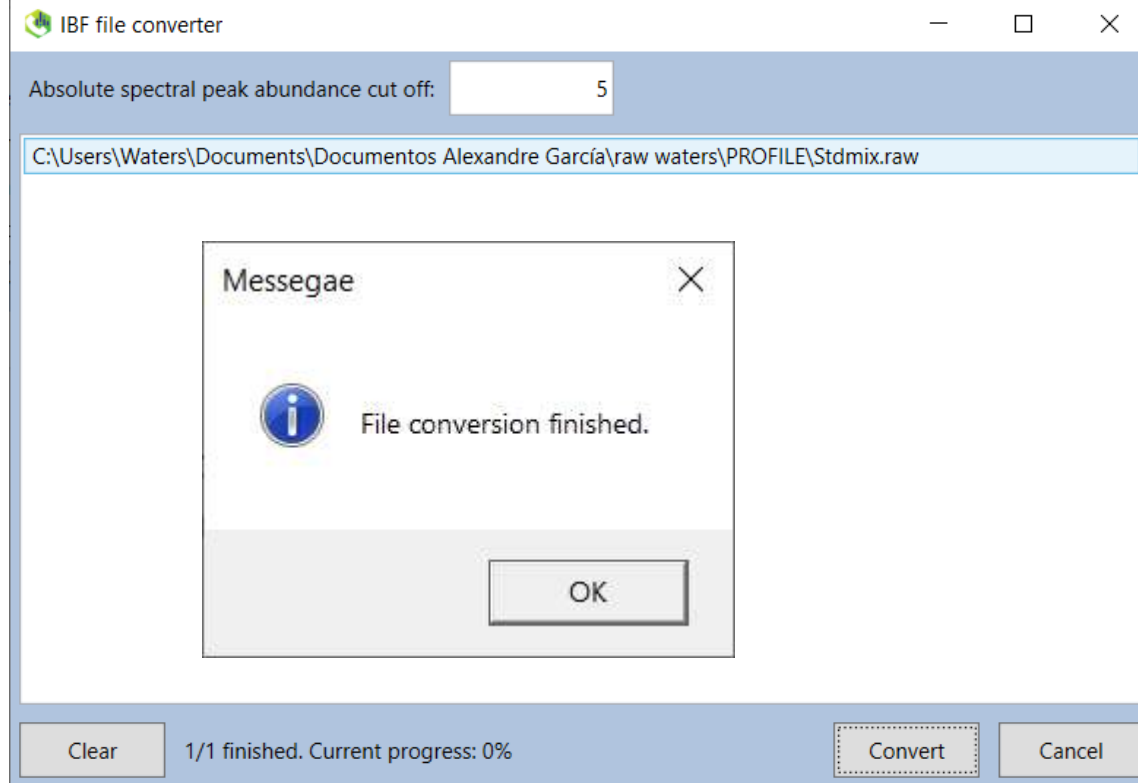
Profile data



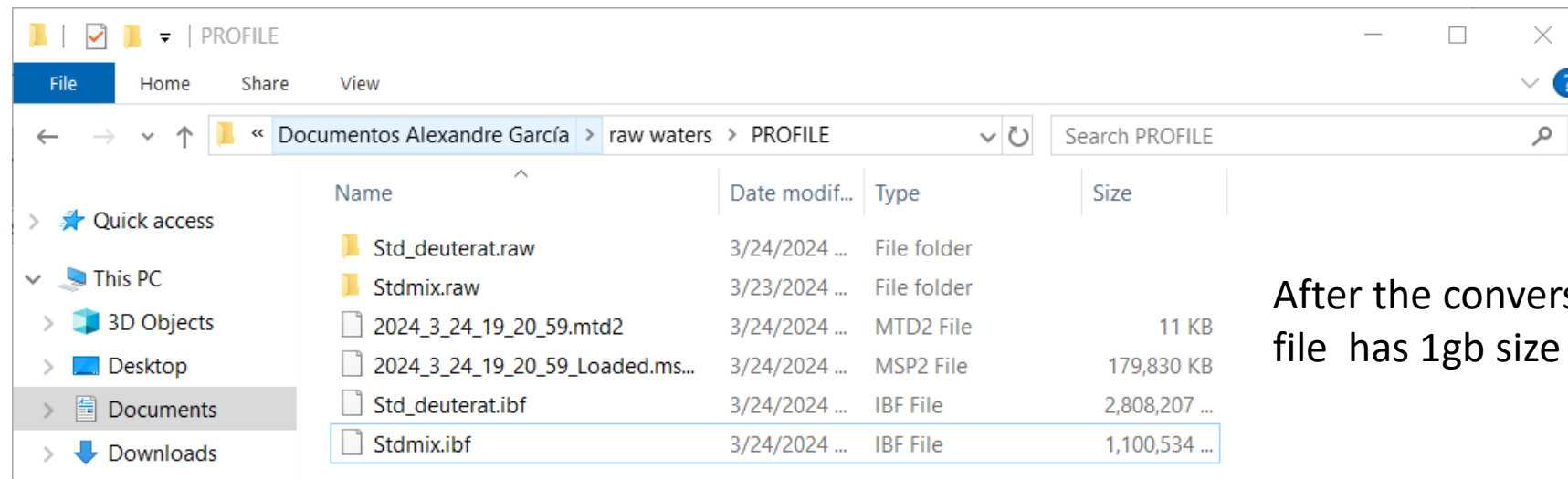
ACQUISITION MODE
HDMSe

Positive
polarity

1 Full Scan
2 AIF
3 Lock mass



IBF Converter from MS-DIAL Ver 4.70



After the conversion, the file has 1gb size

Start up a project

Project file path: C:\Users\Waters\Documents\Documentos Alexandre García\raw waters\PROFILE\2024_3_24_19 Browse

Ionization type

☒ Soft ionization (LC/MS, LC/MS/MS, or precursor-oriented GC/MS/MS)

☐ Hard ionization (GC/MS)

Separation type

☐ Chromatography (GC, LC, CE, or SFC)

☒ Ion mobility (now coupled with liquid chromatography)

MS method type

☒ Conventional LC/MS or data dependent MS/MS

☐ Data independent MS/MS

Data type (MS1)

☒ Profile data

☐ Centroid data

Data type (MS/MS)

☒ Profile data

☐ Centroid data

Ion mode

☒ Positive ion mode

☐ Negative ion mode

Target omics

☐ Metabolomics

☒ Lipidomics

☒ Advanced: add further meta data

Next

MSDIAL ver.4.9.221218
Windowsx64

New project window

Analysis file paths

File path	File name	Type	Class ID	Batch	Analytical order	Inject. volume (μL)	Included
C:\Users\Waters\Documents\Documentos A	Stdmix	Sample	1	1	1	1	<input checked="" type="checkbox"/>

Analysis parameter setting

Data collection Peak detection MS2Dec Identification Adduct Alignment Mobility Isotope tracking

Mass accuracy (centroid parameter)

MS1 tolerance: 0.01 Da

MS2 tolerance: 0.025 Da

Advanced

Default parameters

Load ☒ Together with Alignment Finish Cancel

Analysis parameter setting

Data collection Peak detection MS2Dec Identification Adduct Alignment Mobility Isotope tracking

Peak detection parameters

Minimum peak height: 1000 amplitude

Mass slice width: 0.1 Da

Advanced

Load ☒ Together with Alignment Finish Cancel

Analysis parameter setting

Data collection Peak detection MS2Dec Identification Adduct Alignment Mobility Isotope tracking

Deconvolution parameters

Sigma window value:

MS/MS abundance cut off: amplitude

▼ Advanced

Default parameters

Load ☒ Together with Alignment Finish Cancel

Analysis parameter setting

Data collection Peak detection MS2Dec Identification Adduct Alignment Mobility Isotope tracking

MSP file and MS/MS identification setting

MSP file:

Retention time tolerance: min

Accurate mass tolerance (MS1): Da

Accurate mass tolerance (MS2): Da

Identification score cut off: %

Use retention time for scoring: ☐

Use retention time for filtering: ☐

▼ Advanced

Load ☒ Together with Alignment Finish Cancel

Analysis parameter setting

Data collection

Peak detection

MS2Dec

Identification

Adduct

Alignment

Mobility

Isotope tracking

Adduct ion setting

User-defined adduct

Molecular species	Charge	Accurate mass [Da]	Included
[M+H] ⁺	1	1.007276	<input checked="" type="checkbox"/>
[M+NH ₄] ⁺	1	18.033823	<input checked="" type="checkbox"/>
[M+Na] ⁺	1	22.989218	<input type="checkbox"/>
[M+CH ₃ OH+H] ⁺	1	33.033489	<input type="checkbox"/>
[M+K] ⁺	1	38.963158	<input checked="" type="checkbox"/>
[M+Li] ⁺	1	7.01600455	<input type="checkbox"/>
[M+ACN+H] ⁺	1	42.033823	<input type="checkbox"/>
[M+H-H ₂ O] ⁺	1	-17.002191	<input type="checkbox"/>
[M+H-2H ₂ O] ⁺	1	-30.012756	<input type="checkbox"/>
[M+2Na-H] ⁺	1	44.97116	<input type="checkbox"/>
[M+IsoProp+H] ⁺	1	61.06534	<input type="checkbox"/>
[M+ACN+Na] ⁺	1	64.015765	<input type="checkbox"/>
[M+2K-H] ⁺	1	76.91904	<input type="checkbox"/>
[M+DMSO+H] ⁺	1	79.02122	<input type="checkbox"/>
[M+2ACN+H] ⁺	1	83.06037	<input type="checkbox"/>
[M+IsoProp+Na+H] ⁺	1	84.05511	<input type="checkbox"/>
[M-C ₆ H ₁₀ O ₄ +H] ⁺	1	-145.050085	<input type="checkbox"/>
[M-C ₆ H ₁₀ O ₅ +H] ⁺	1	-161.045	<input type="checkbox"/>
[M-C ₆ H ₈ O ₆ +H] ⁺	1	-175.024265	<input type="checkbox"/>
[2M+H] ⁺	1	1.007276	<input type="checkbox"/>
[2M+NH ₄] ⁺	1	18.033823	<input type="checkbox"/>
[2M+Na] ⁺	1	22.989218	<input type="checkbox"/>
[2M+3H ₂ O+2H] ⁺	1	28.02312	<input type="checkbox"/>
[2M+K] ⁺	1	38.963158	<input type="checkbox"/>
[2M+ACN+H] ⁺	1	42.033823	<input type="checkbox"/>

Load

☒ Together with Alignment

Finish

Cancel

Analysis parameter setting

Data collection

Peak detection

MS2Dec

Identification

Adduct

Alignment

Mobility

Isotope tracking

Alignment parameters setting

Result name:

alignmentResult_2024_3_24_19_30_36

Reference file:

Stdmix

Retention time tolerance:

0.05

min

MS1 tolerance:

0.015

Da

Advanced

Load

☒ Together with Alignment

Finish

Cancel

Default
parameters

Analysis parameter setting

Data collection Peak detection MS2Dec Identification Adduct Alignment Mobility Isotope tracking

Mobility type

☐ TIMS (Bruker) ☐ DTIMS (Agilent) ☒ TWIMS (Waters)

CCS calibration data: Status: imported

Peak picking

Accumulated RT range: min

Identification

CCS tolerance: Ao²

Use CCS for scoring: ☐

Use CCS for filtering metabolites: ☒

Alignment

Mobility tolerance: msec

☒ Together with Alignment

Waters CCS calibration data setting

File name	Coefficient	T0	Exponent
Stdmix	454.891998291016	0.876062989234924	0.52123898267746

Ion mobility calibration is loaded

Analysis parameter setting

Data collection Peak detection MS2Dec Identification Adduct Alignment Mobility Isotope tracking

Tracking of isotope labels ☐

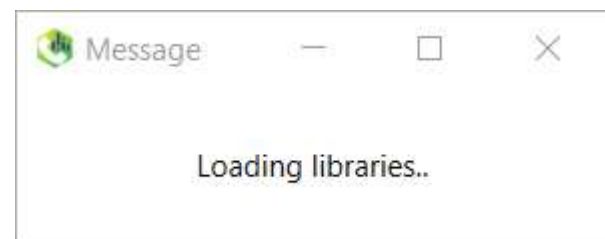
Labeled element: 13C

Non-labeled reference file: Stdmix

☐ Use target formula library:

☐ Set fully-labeled reference file: Stdmix

☒ Together with Alignment



Error



There is no peak information in Std_deuterat. So please select other files or check ion mode for it and re-analyze it with the ion mode setting.

OK