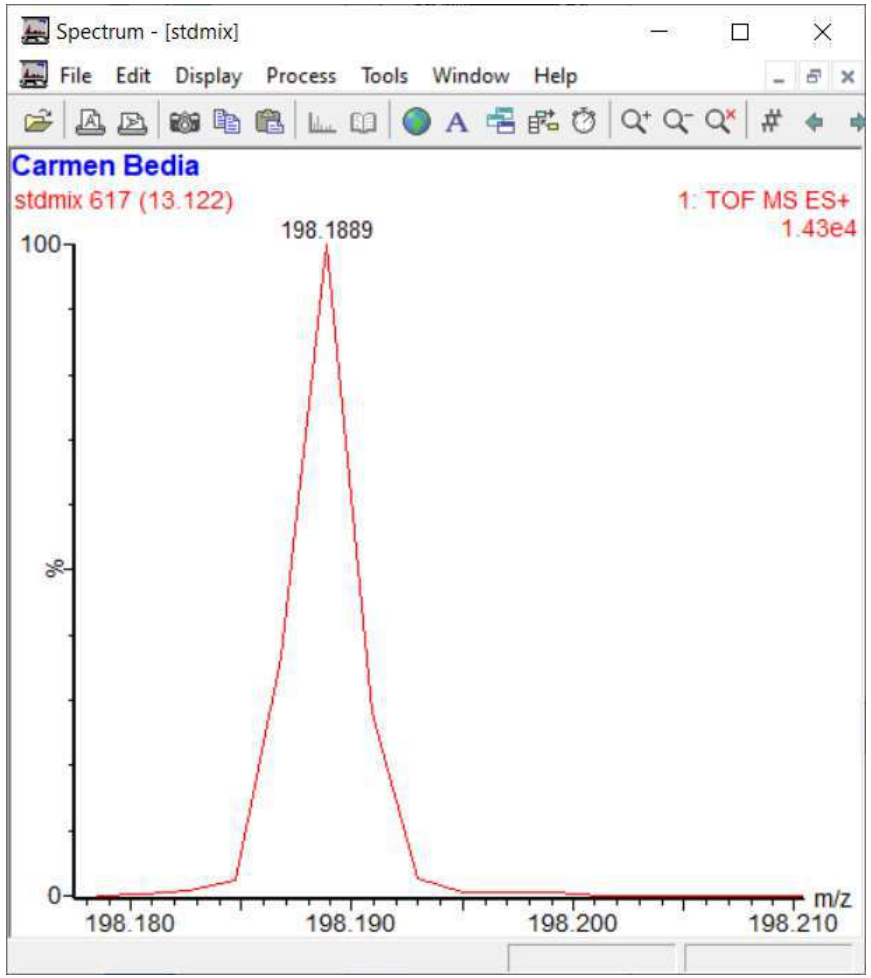
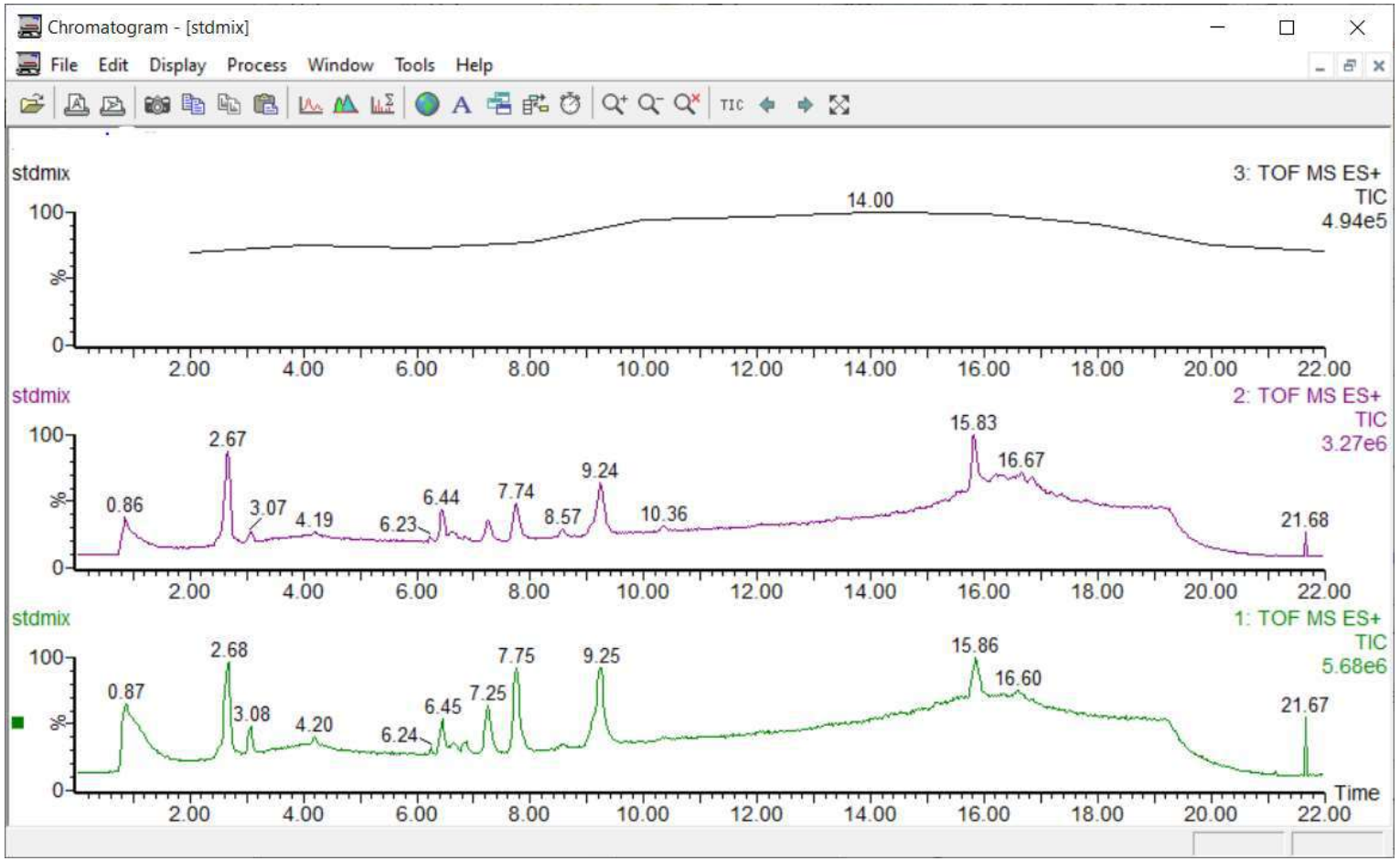


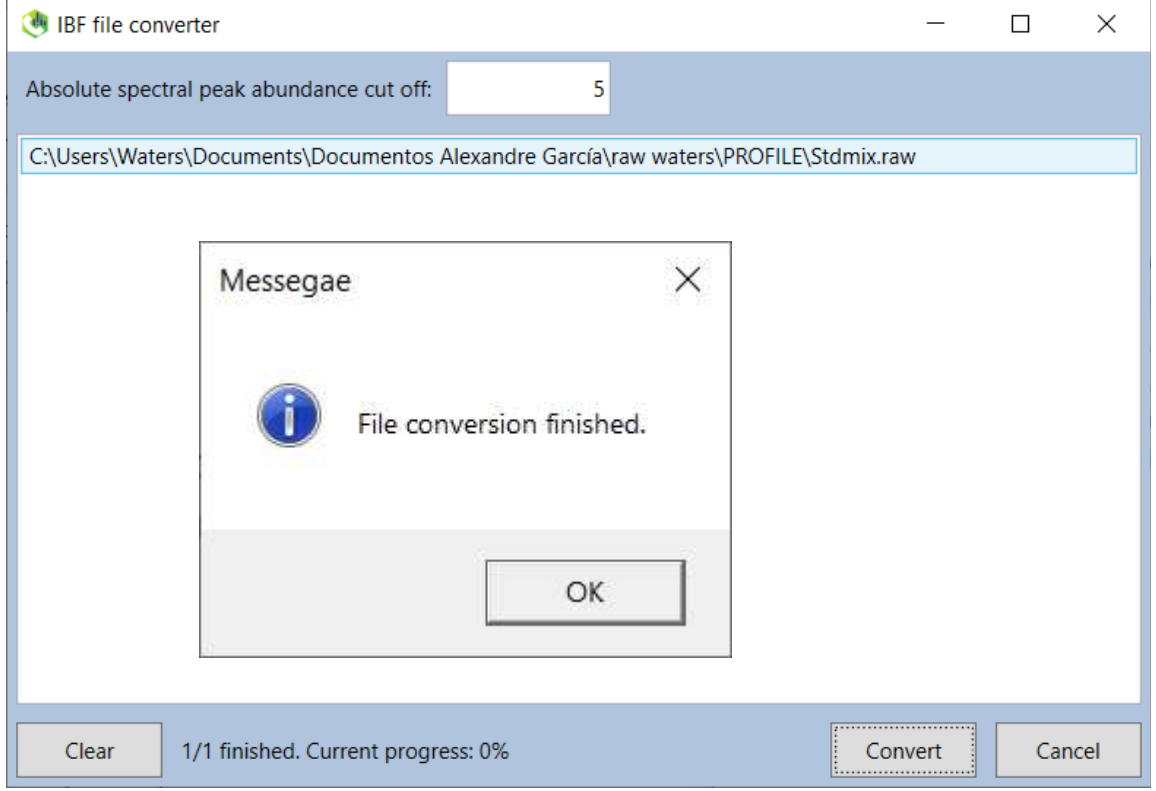


Profile data

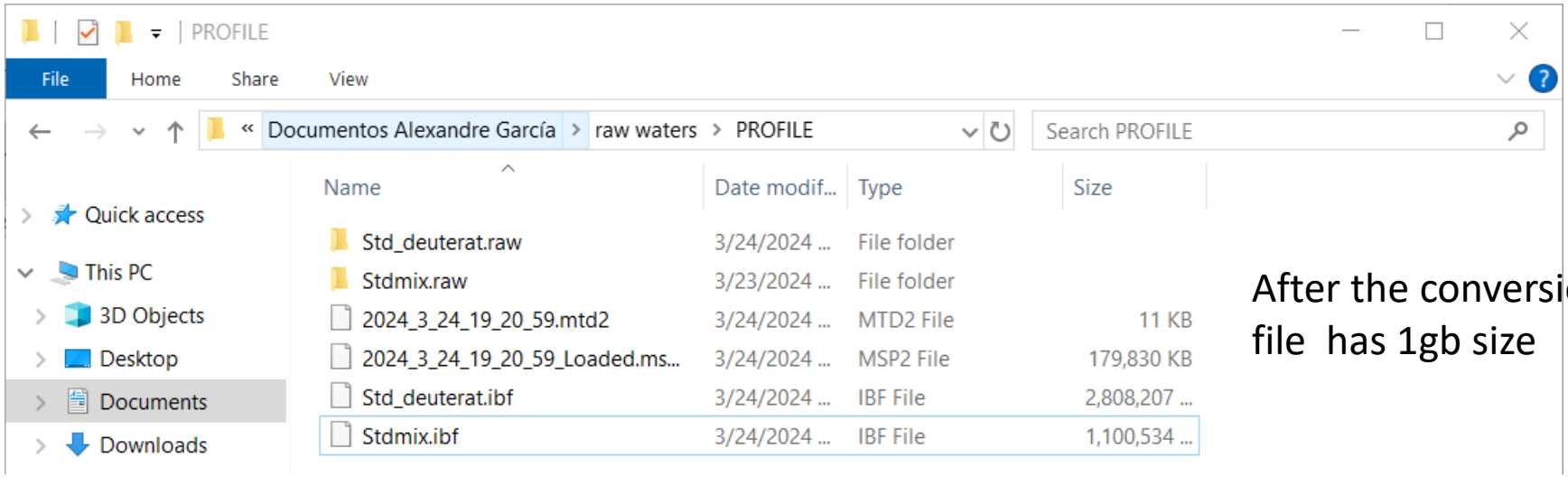
ACQUISITION MODE
HDMSe

Positive polarity

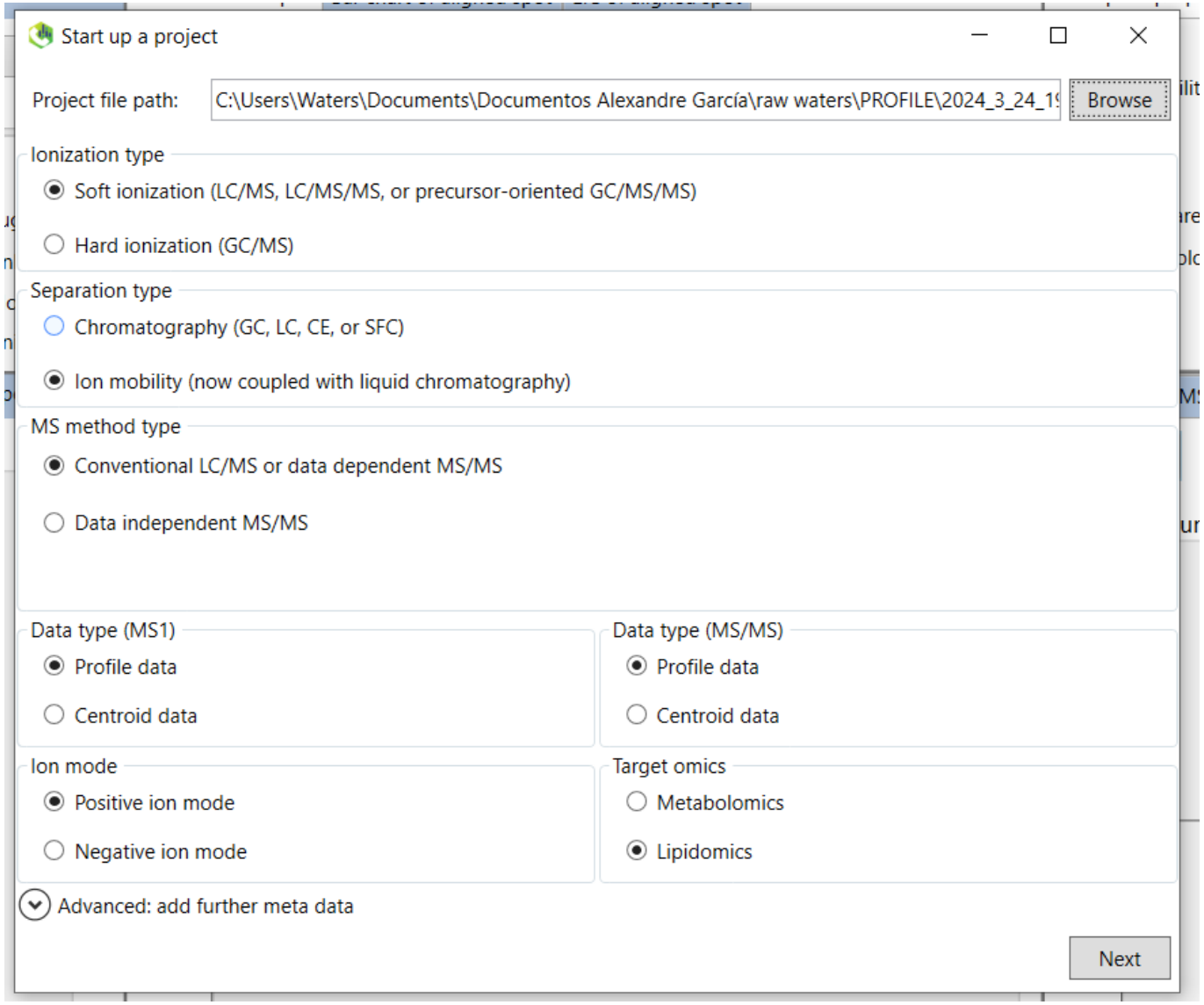
1 Full Scan
2 AIF
3 Lock mass



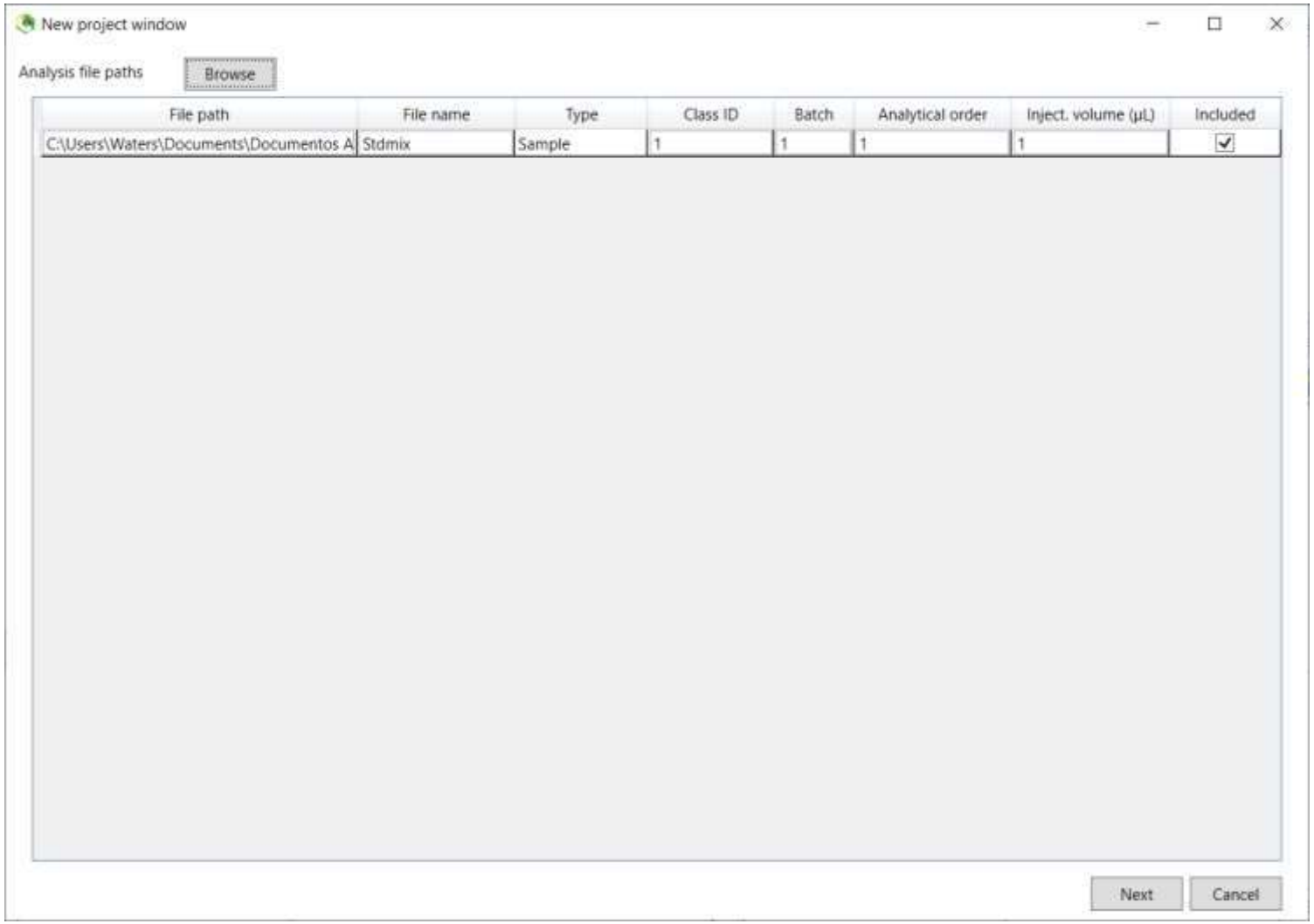
IBF Converter from MS-DIAL Ver 4.70

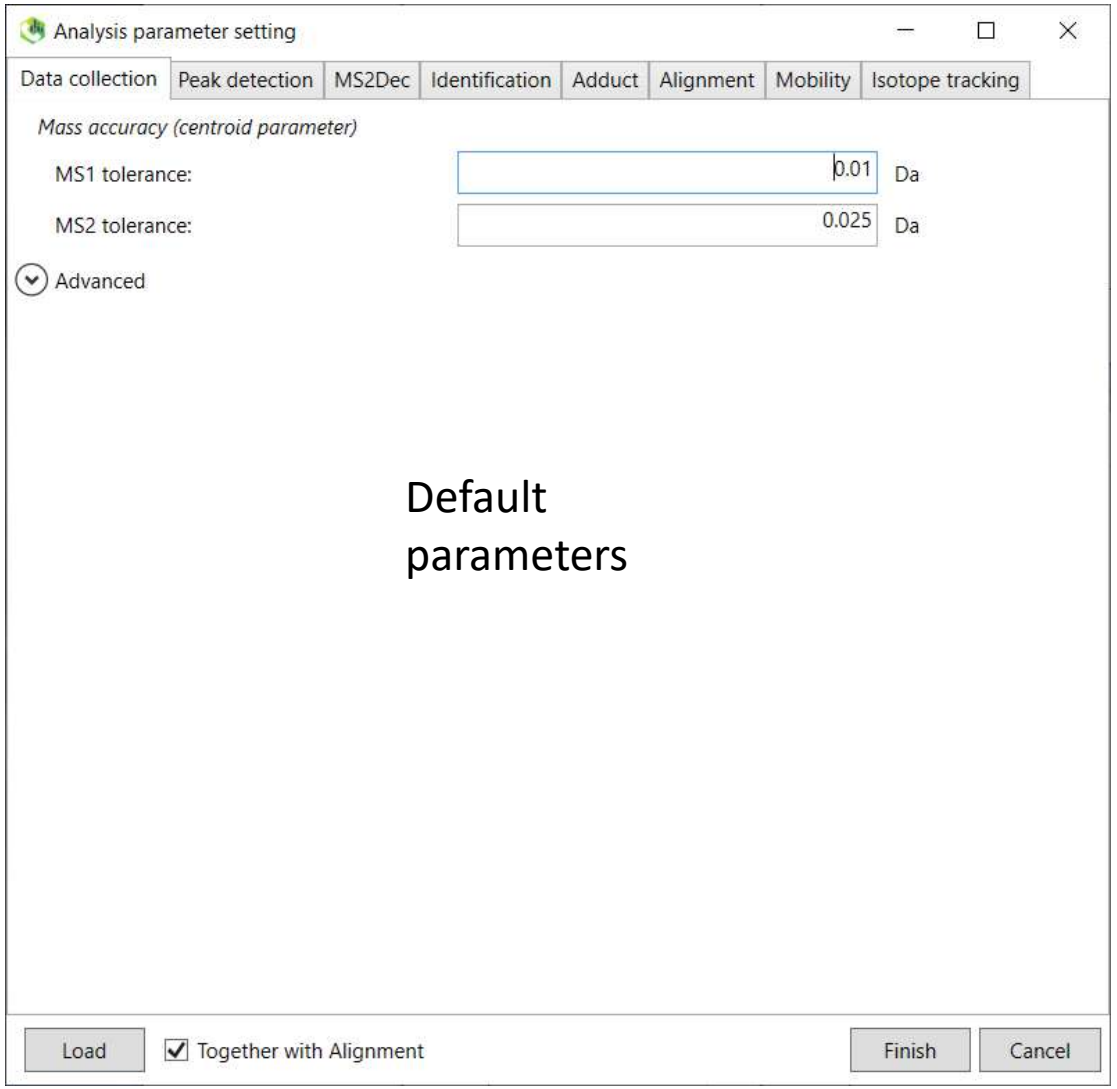


After the conversion, the file has 1gb size

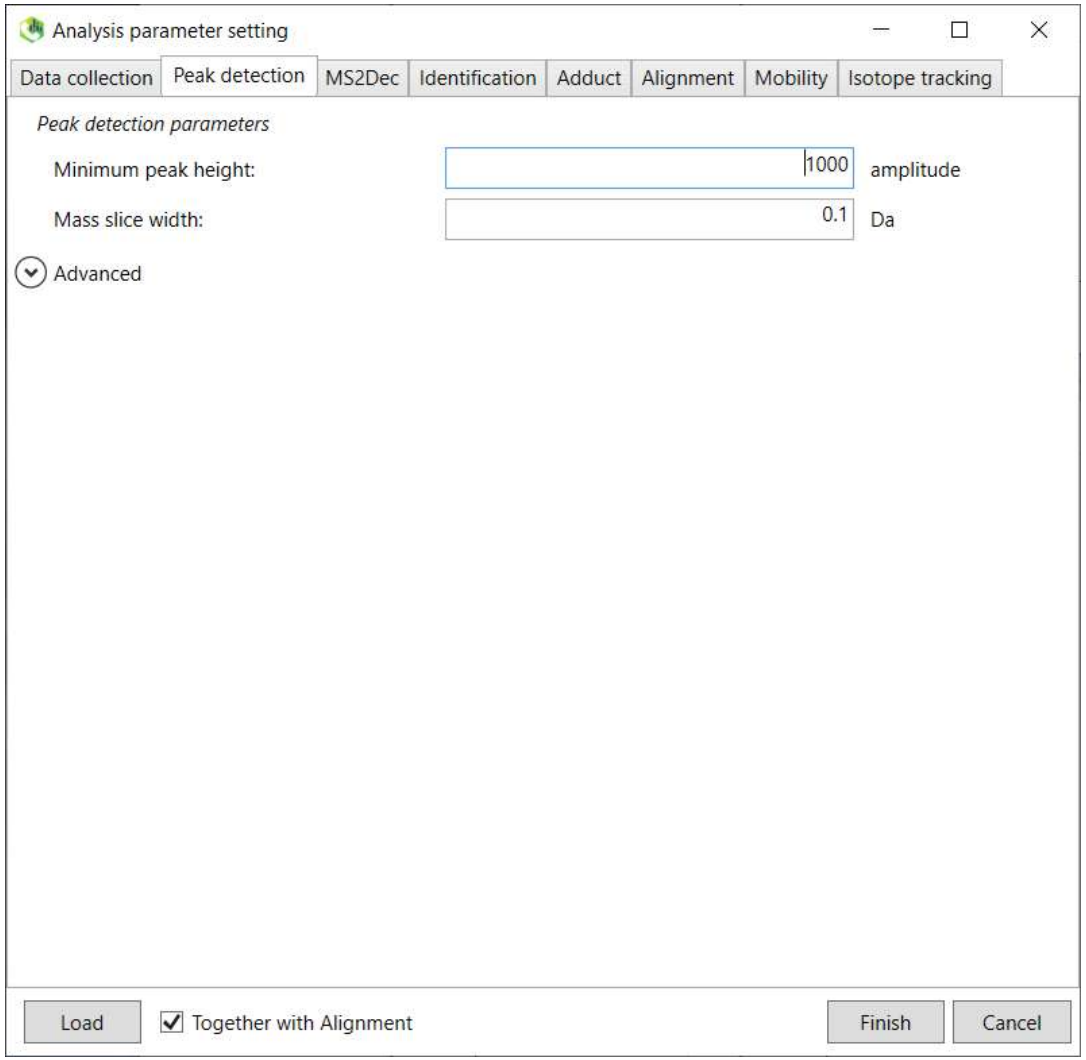


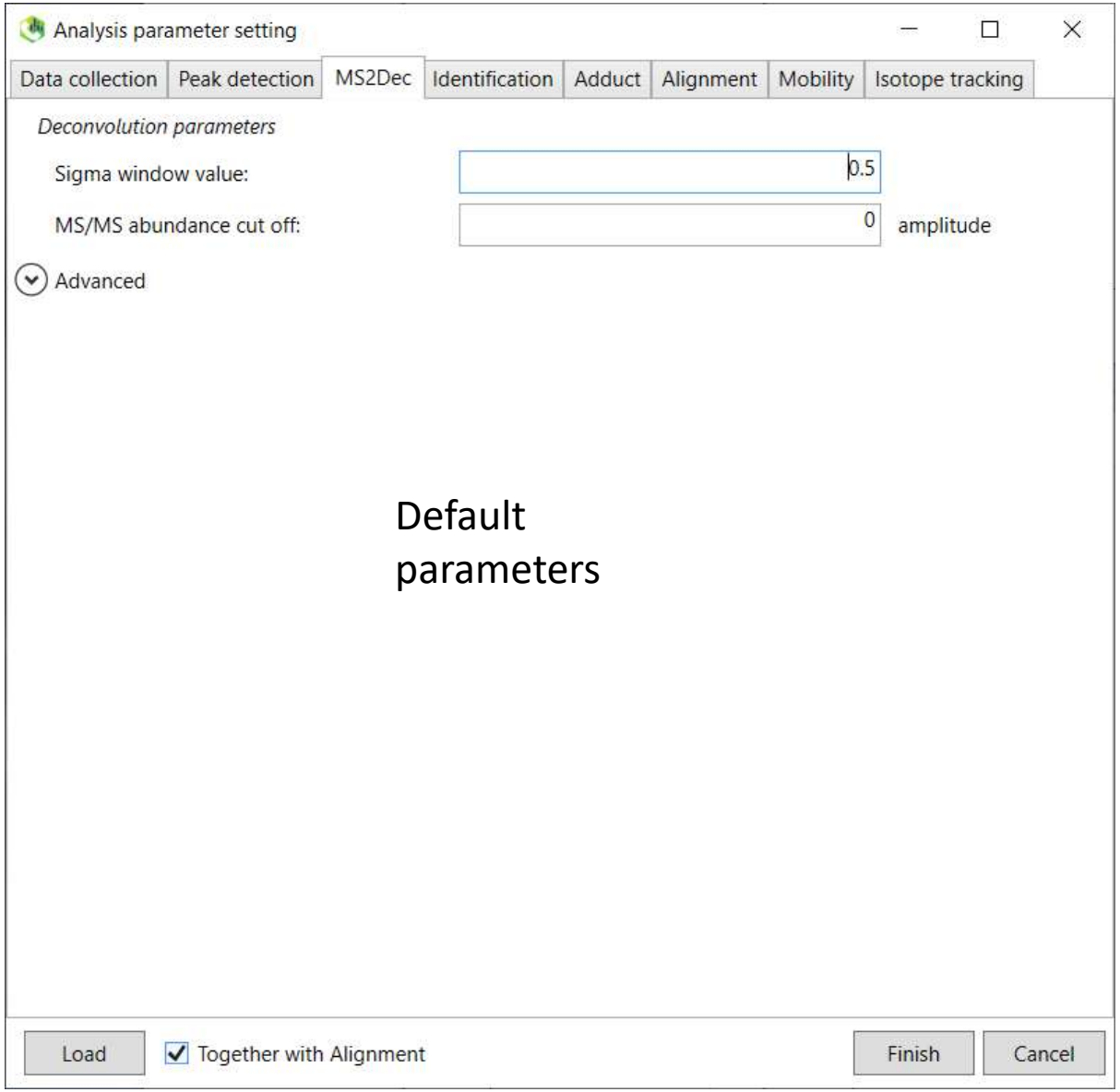
MSDIAL ver.4.9.221218
Windowsx64


New project window
Analysis file paths
Browse
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
Next
Cancel

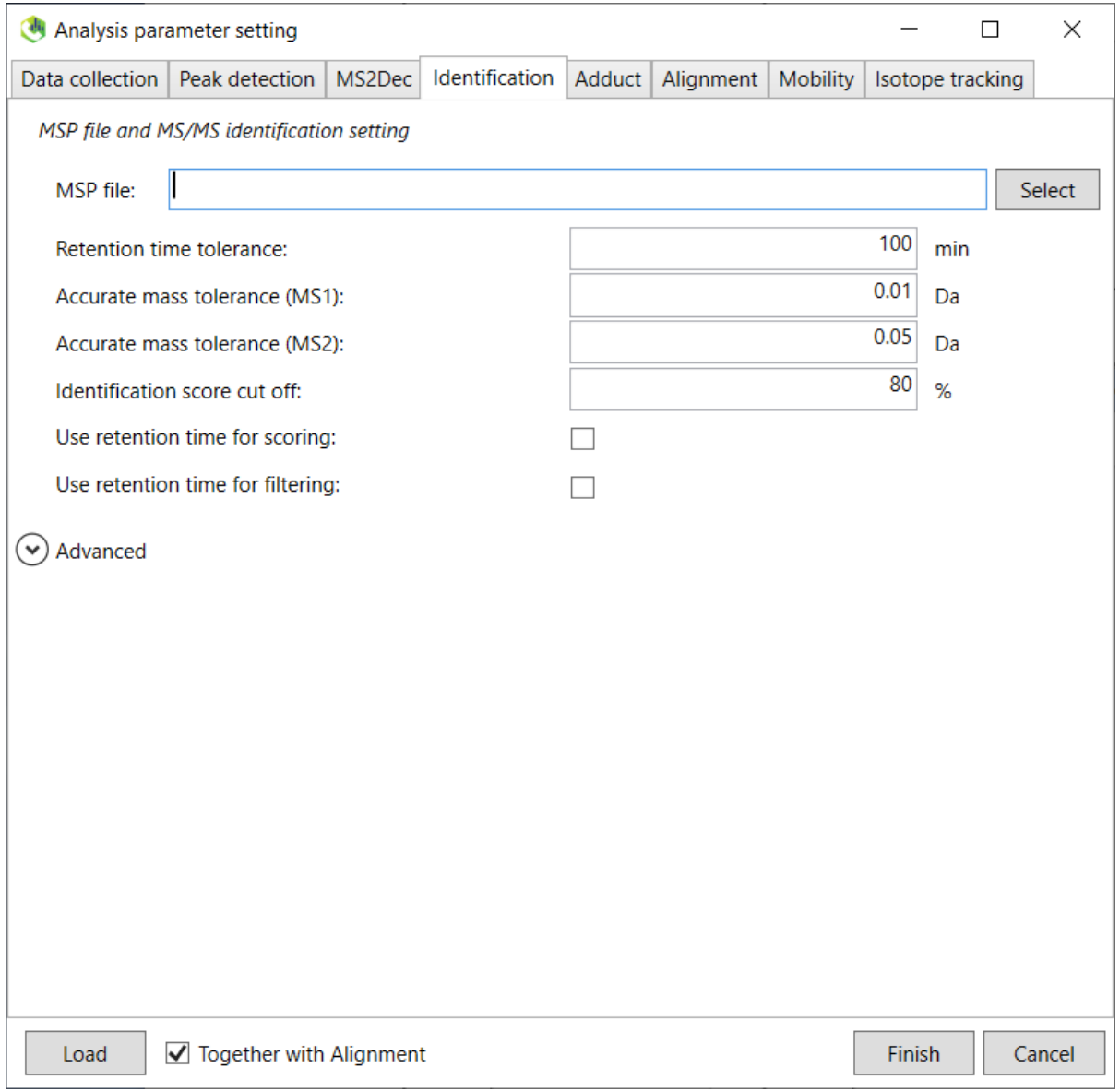


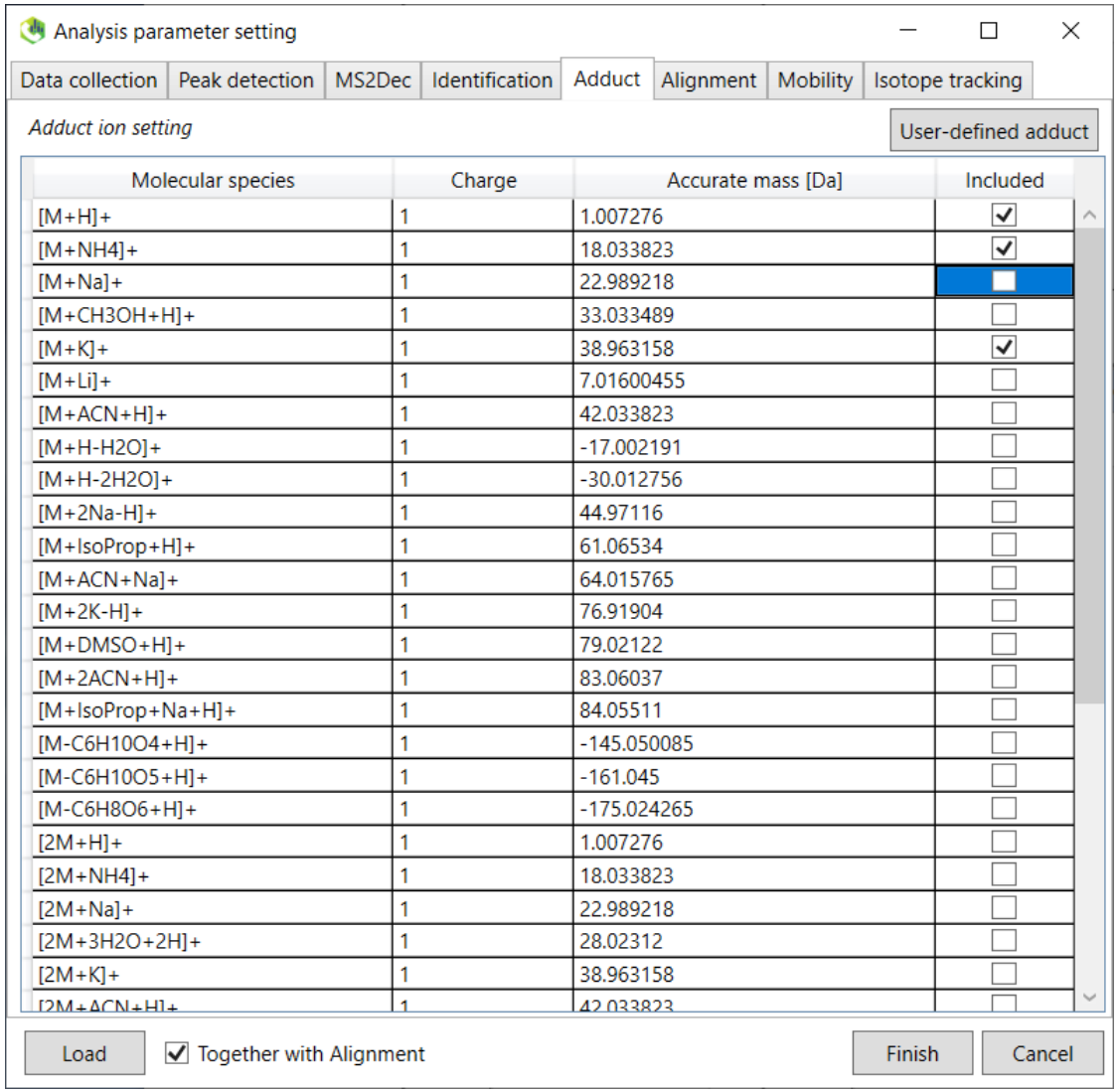
Default parameters

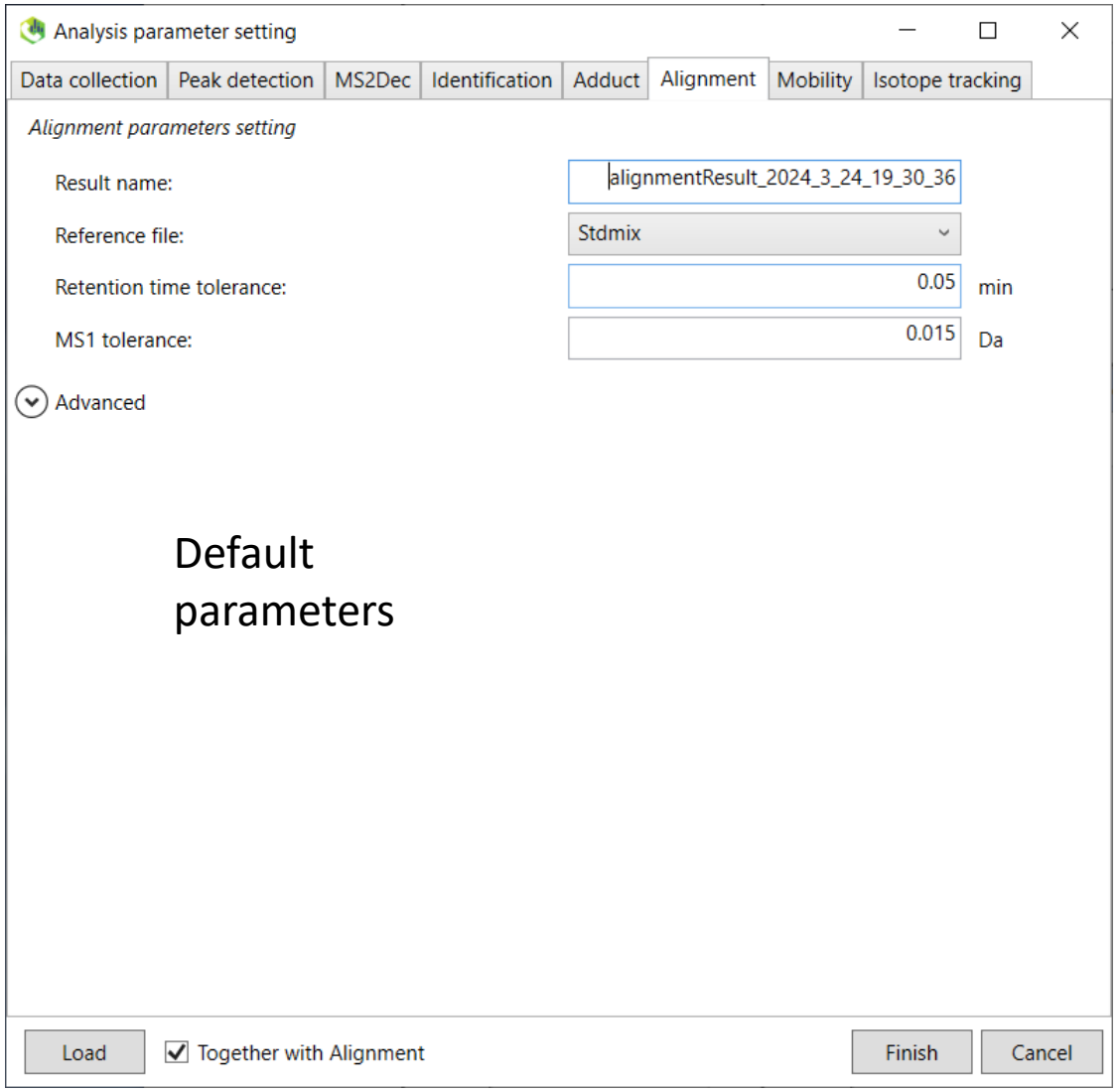


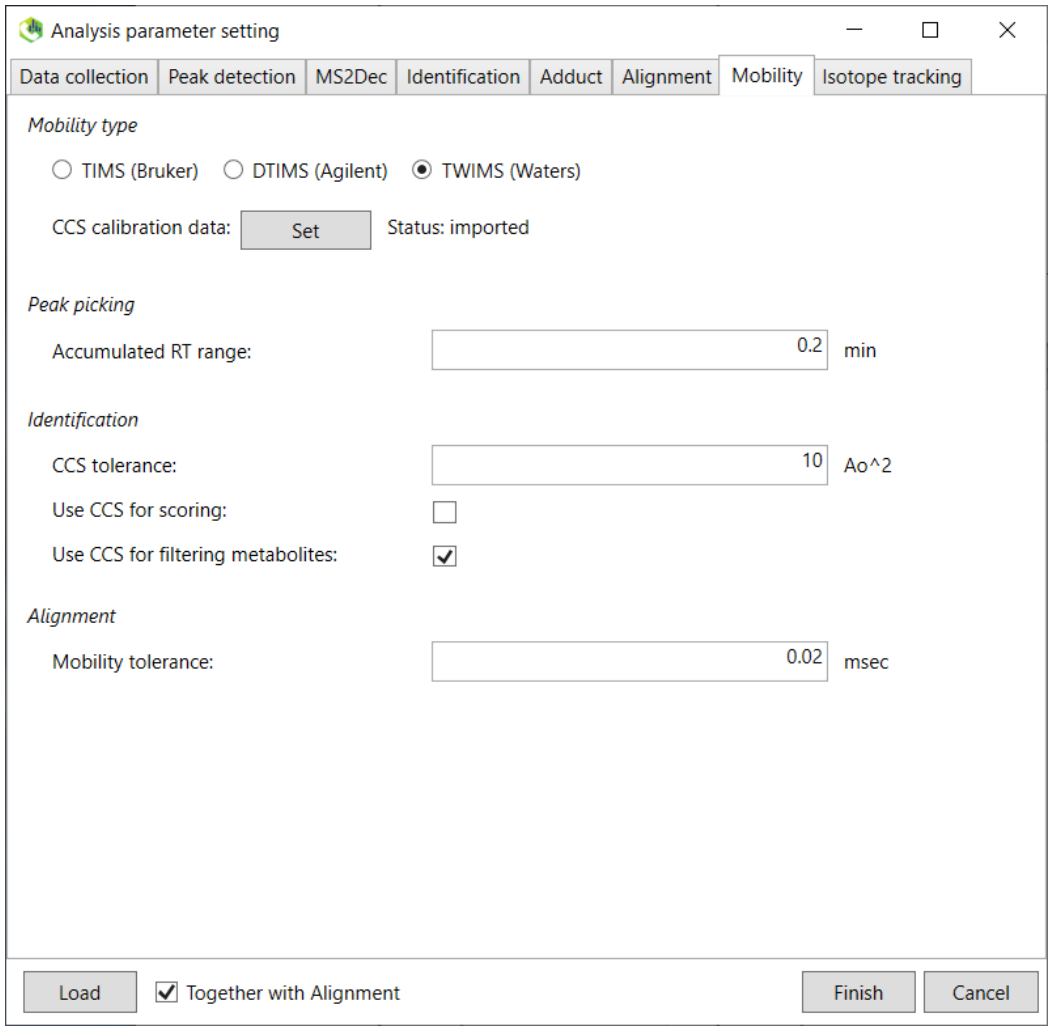


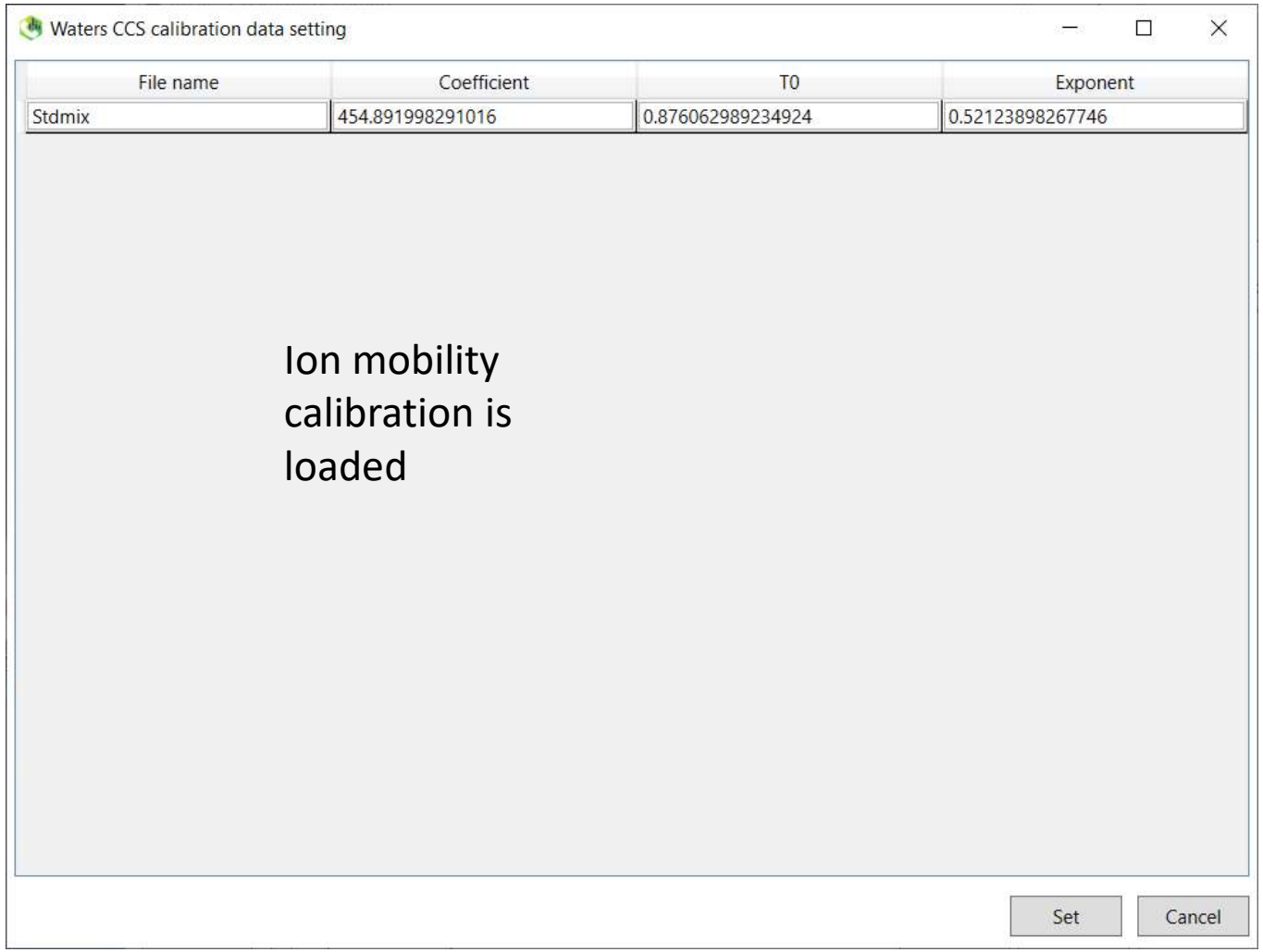
Default parameters

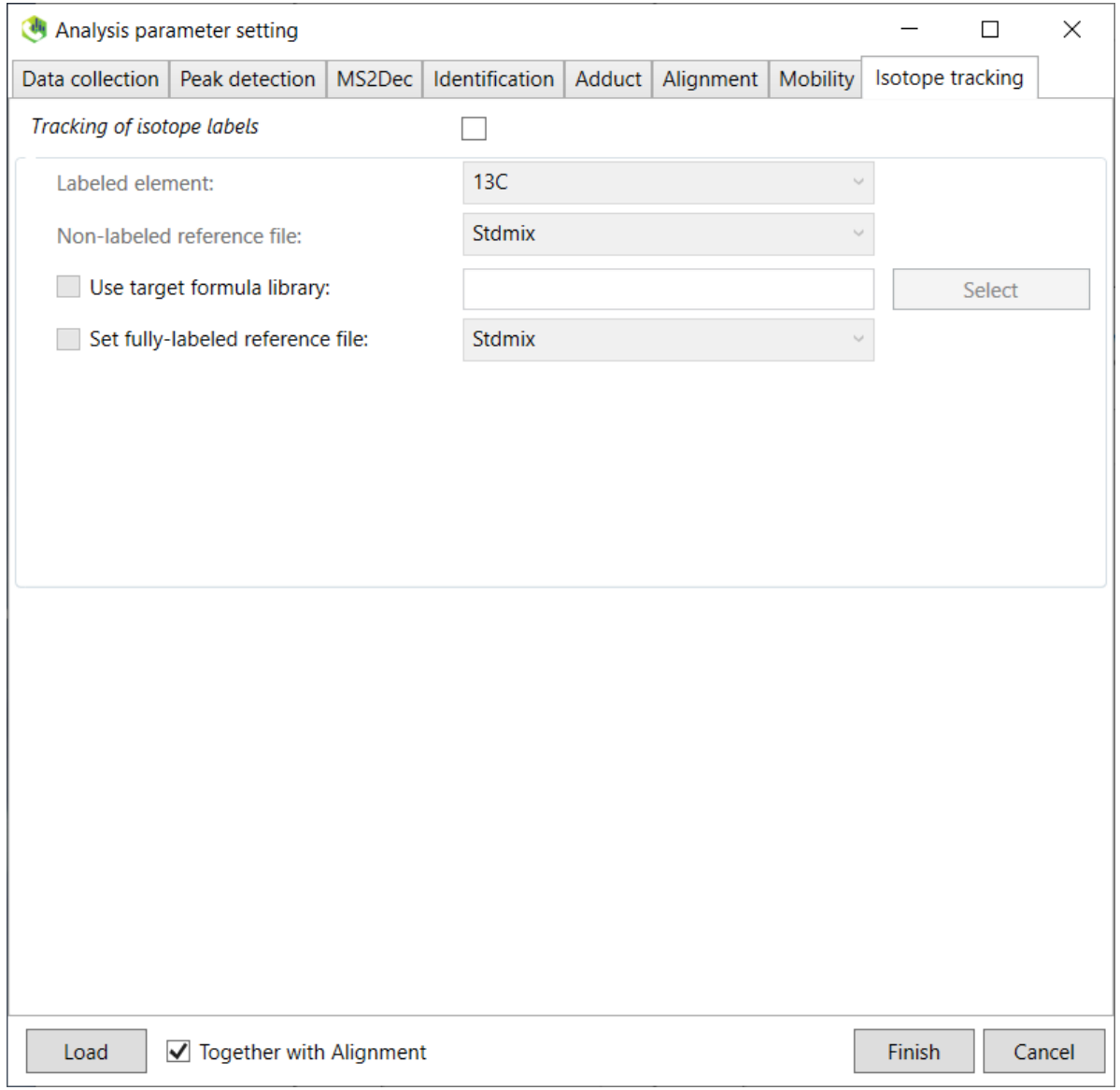


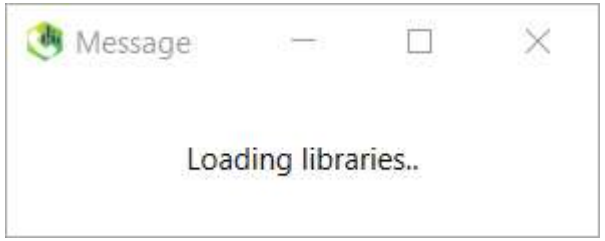

Analysis parameter setting
Data collection
Peak detection
MS2Dec
Identification
Adduct
Alignment
Mobility
Isotope tracking
Adduct ion setting
User-defined adduct
Molecular species
Charge
Accurate mass [Da]
Included
[M+H]+ 1 1.007276
[M+NH4]+ 1 18.033823
[M+Na]+ 1 22.989218
[M+CH3OH+H]+ 1 33.033489
[M+K]+ 1 38.963158
[M+Li]+ 1 7.01600455
[M+ACN+H]+ 1 42.033823
[M+H-H2O]+ 1 -17.002191
[M+H-2H2O]+ 1 -30.012756
[M+2Na-H]+ 1 44.97116
[M+IsoProp+H]+ 1 61.06534
[M+ACN+Na]+ 1 64.015765
[M+2K-H]+ 1 76.91904
[M+DMSO+H]+ 1 79.02122
[M+2ACN+H]+ 1 83.06037
[M+IsoProp+Na+H]+ 1 84.05511
[M-C6H10O4+H]+ 1 -145.050085
[M-C6H10O5+H]+ 1 -161.045
[M-C6H8O6+H]+ 1 -175.024265
[2M+H]+ 1 1.007276
[2M+NH4]+ 1 18.033823
[2M+Na]+ 1 22.989218
[2M+3H2O+2H]+ 1 28.02312
[2M+K]+ 1 38.963158
Load
Together with Alignment
Finish
Cancel

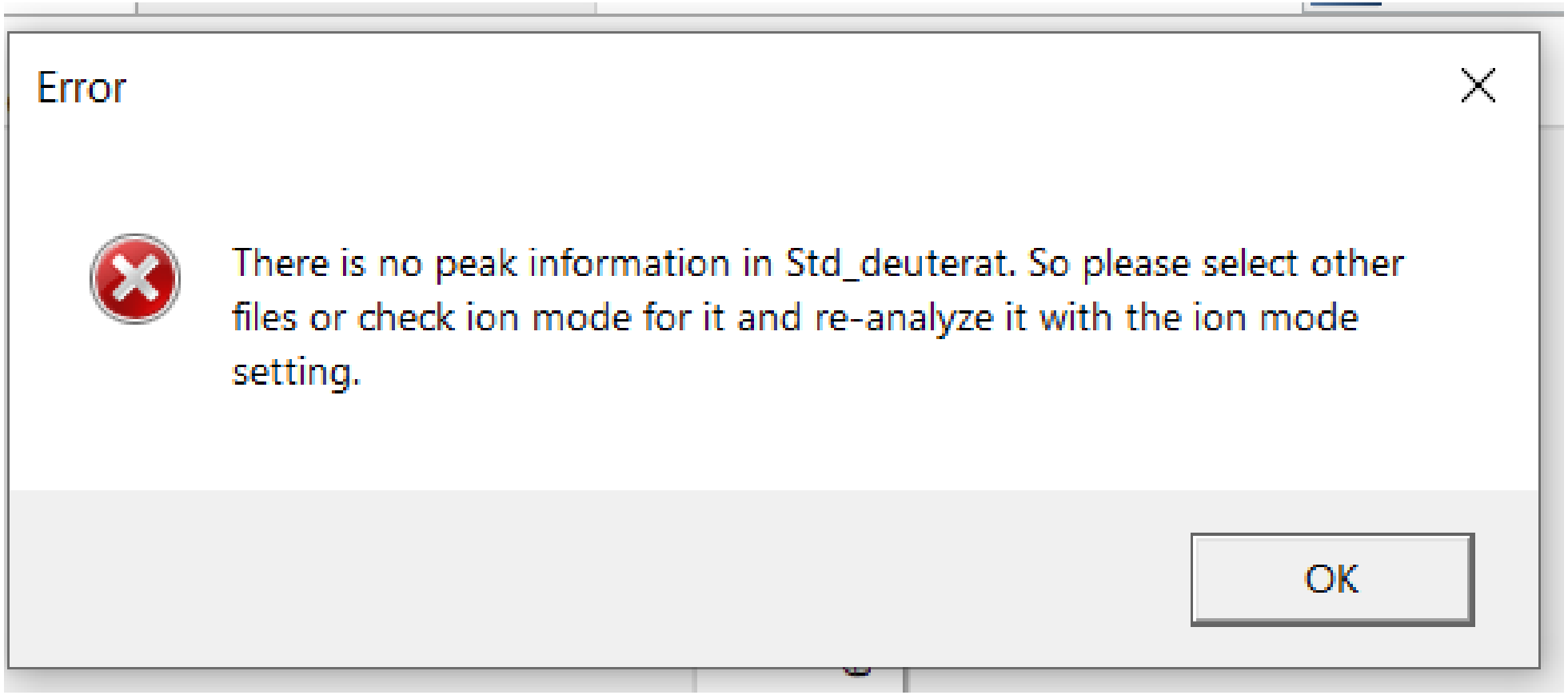

Analysis parameter setting
Data collection
Peak detection
MS2Dec
Identification
Adduct
Alignment
Mobility
Isotope tracking
Alignment parameters setting
Result name:
alignmentResult_2024_3_24_19_30_36
Reference file:
Stdmix
Retention time tolerance:
0.05
min
MS1 tolerance:
0.015
Da
Advanced
Default parameters
Load
Together with Alignment
Finish
Cancel


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:
Set
Status: imported
Peak picking
Accumulated RT range:
0.2
min
Identification
CCS tolerance:
10
Ao^2
Use CCS for scoring:
Use CCS for filtering metabolites:
Alignment
Mobility tolerance:
0.02
msec
Load
Together with Alignment
Finish
Cancel


Waters CCS calibration data setting
File name
Coefficient
T0
Exponent
Stdmix
454.891998291016
0.876062989234924
0.52123898267746
Ion mobility calibration is loaded
Set
Cancel


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:
Select
Set fully-labeled reference file:
Stdmix
Load
Together with Alignment
Finish
Cancel


Message
Loading libraries..


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