Edition Windows 10 Pro

Version 21H2

Installed on ‎3/‎28/‎2022

OS build 19044.1586

Experience Windows Feature Experience Pack 120.2212.4170.0

Graphical user interface, text, application, email

Description automatically generated

Graphical user interface, application

Description automatically generatedGraphical user interface, application

Description automatically generatedI’m trying to generate a mobility library so far I have curated my target peptides and transitions. I also made the following changes shown in the screenshots below before reimporting.

Graphical user interface, application, Word

Description automatically generated

but when I attempt to reimport I run into the following error:

At 1:36 PM:

Failed importing results file 'C:\Users\alan.mckenzie-coe\OneDrive - MOBILion Systems, Inc\Documents\MAF\BATL\20min\Preprocess\Smoothed\NIST Digest 1.d'.

[MidacDataImpl::ccsToDriftTime()] Cannot solve cubic fit, solution not found within bounds [10 ms, 2000 ms].

pwiz.Skyline.Model.Results.ChromCacheBuildException: Failed importing results file 'C:\Users\alan.mckenzie-coe\OneDrive - MOBILion Systems, Inc\Documents\MAF\BATL\20min\Preprocess\Smoothed\NIST Digest 1.d'.

[MidacDataImpl::ccsToDriftTime()] Cannot solve cubic fit, solution not found within bounds [10 ms, 2000 ms]. ---> System.Exception: [MidacDataImpl::ccsToDriftTime()] Cannot solve cubic fit, solution not found within bounds [10 ms, 2000 ms].

at pwiz.CLI.analysis.SpectrumList\_IonMobility.ccsToIonMobility(Double ccs, Double mz, Int32 charge)

at pwiz.ProteowizardWrapper.MsDataFileImpl.IonMobilityFromCCS(Double ccs, Double mz, Int32 charge) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Shared\ProteowizardWrapper\MsDataFileImpl.cs:line 535

at pwiz.Skyline.Model.DocSettings.TransitionIonMobilityFiltering.GetIonMobilityFilter(LibKey ion, Double mz, IIonMobilityFunctionsProvider ionMobilityFunctionsProvider) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\DocSettings\TransitionIonMobilityFiltering.cs:line 143

at pwiz.Skyline.Model.DocSettings.TransitionIonMobilityFiltering.GetIonMobilityFilter(LibKey ion, Double mz, IIonMobilityFunctionsProvider ionMobilityFunctionsProvider, Double ionMobilityRangeMax) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\DocSettings\TransitionIonMobilityFiltering.cs:line 194

at pwiz.Skyline.Model.DocSettings.SrmSettings.GetIonMobilityHelper(PeptideDocNode nodePep, TransitionGroupDocNode nodeGroup, IIonMobilityFunctionsProvider ionMobilityFunctionsProvider, LibraryIonMobilityInfo libraryIonMobilityInfo, Double ionMobilityMax) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\DocSettings\SrmSettings.cs:line 1057

at pwiz.Skyline.Model.DocSettings.SrmSettings.GetIonMobilityFilter(PeptideDocNode nodePep, TransitionGroupDocNode nodeGroup, TransitionDocNode nodeTran, LibraryIonMobilityInfo libraryIonMobilityInfo, IIonMobilityFunctionsProvider instrumentInfo, Double ionMobilityMax) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\DocSettings\SrmSettings.cs:line 1030

at pwiz.Skyline.Model.Results.SpectrumFilter..ctor(SrmDocument document, MsDataFileUri msDataFileUri, IFilterInstrumentInfo instrumentInfo, Nullable`1 maxObservedIonMobilityValue, IRetentionTimePredictor retentionTimePredictor, Boolean firstPass, GlobalChromatogramExtractor gce) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\Results\SpectrumFilter.cs:line 207

at pwiz.Skyline.Model.Results.SpectraChromDataProvider..ctor(MsDataFileImpl dataFile, ChromFileInfo fileInfo, SrmDocument document, IRetentionTimePredictor retentionTimePredictor, String cachePath, IProgressStatus status, Int32 startPercent, Int32 endPercent, IProgressMonitor loader) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\Results\SpectraChromDataProvider.cs:line 121

at pwiz.Skyline.Model.Results.ChromCacheBuilder.CreateSpectraChromProvider(MsDataFileImpl dataFile, ChromFileInfo fileInfo) in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\Results\ChromCacheBuilder.cs:line 1262

at pwiz.Skyline.Model.Results.ChromCacheBuilder.BuildCache() in C:\proj\skyline\_21\_2\_x64\pwiz\_tools\Skyline\Model\Results\ChromCacheBuilder.cs:line 233

--- End of inner exception stack trace ---