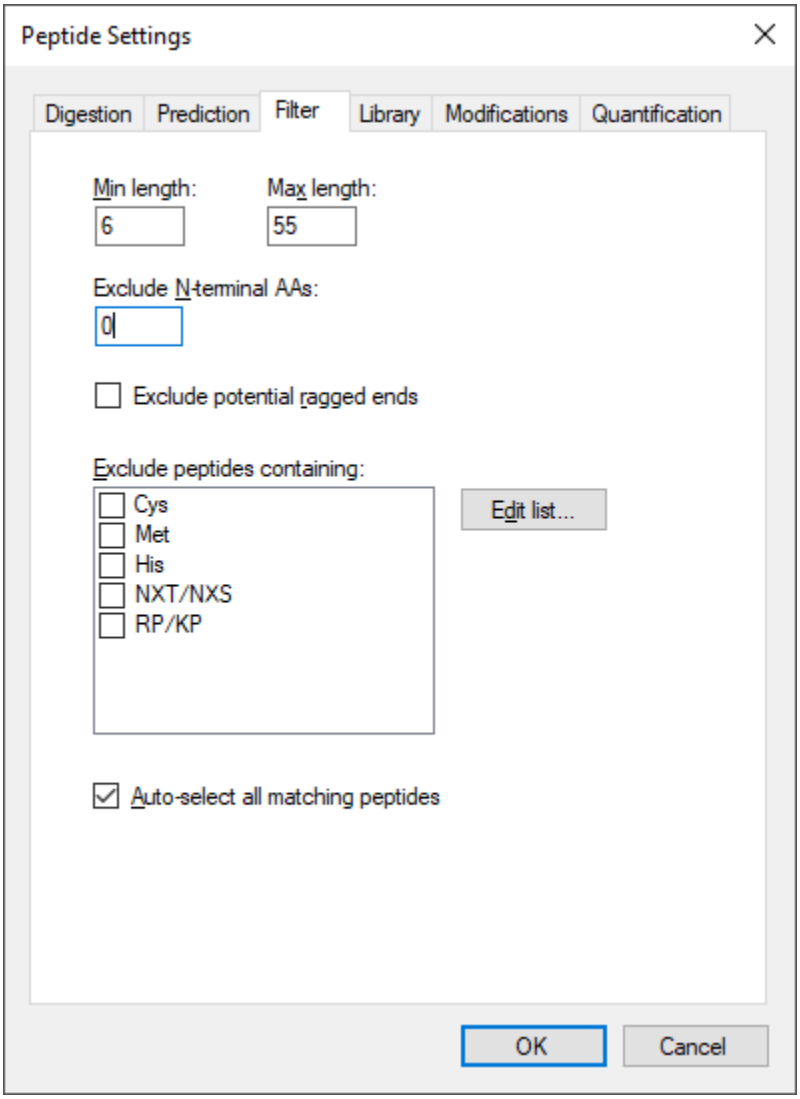
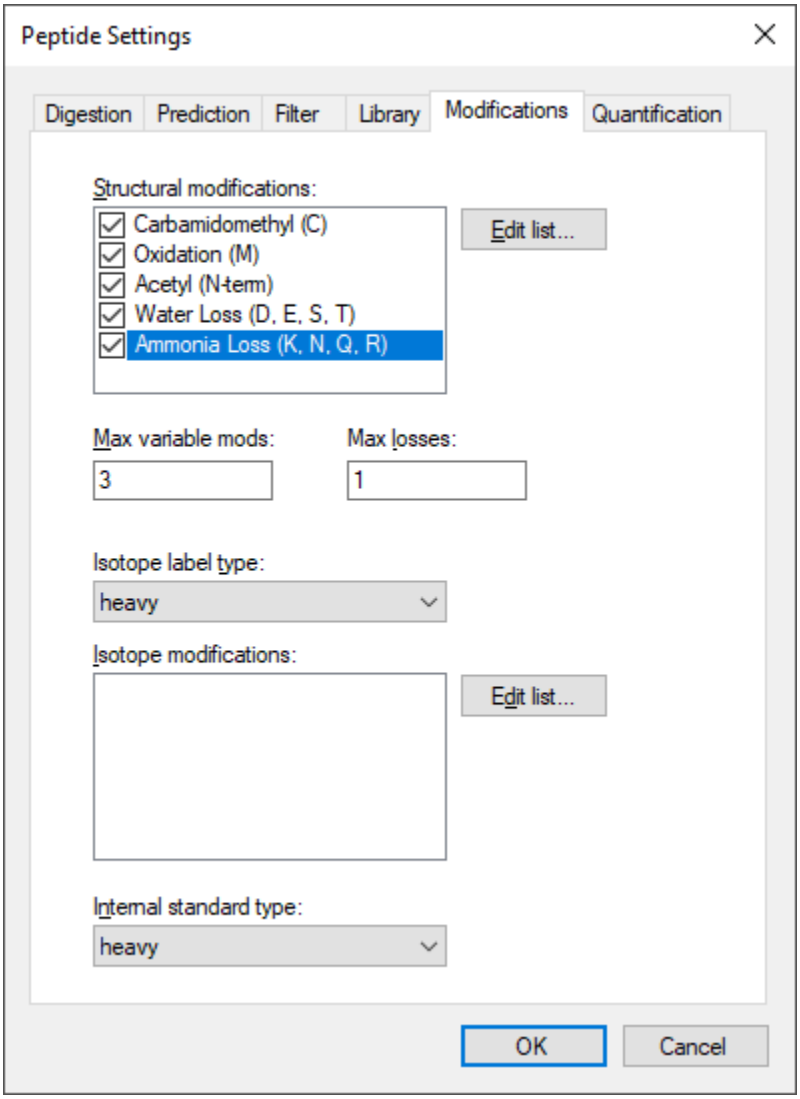
Bruderer Data Settings

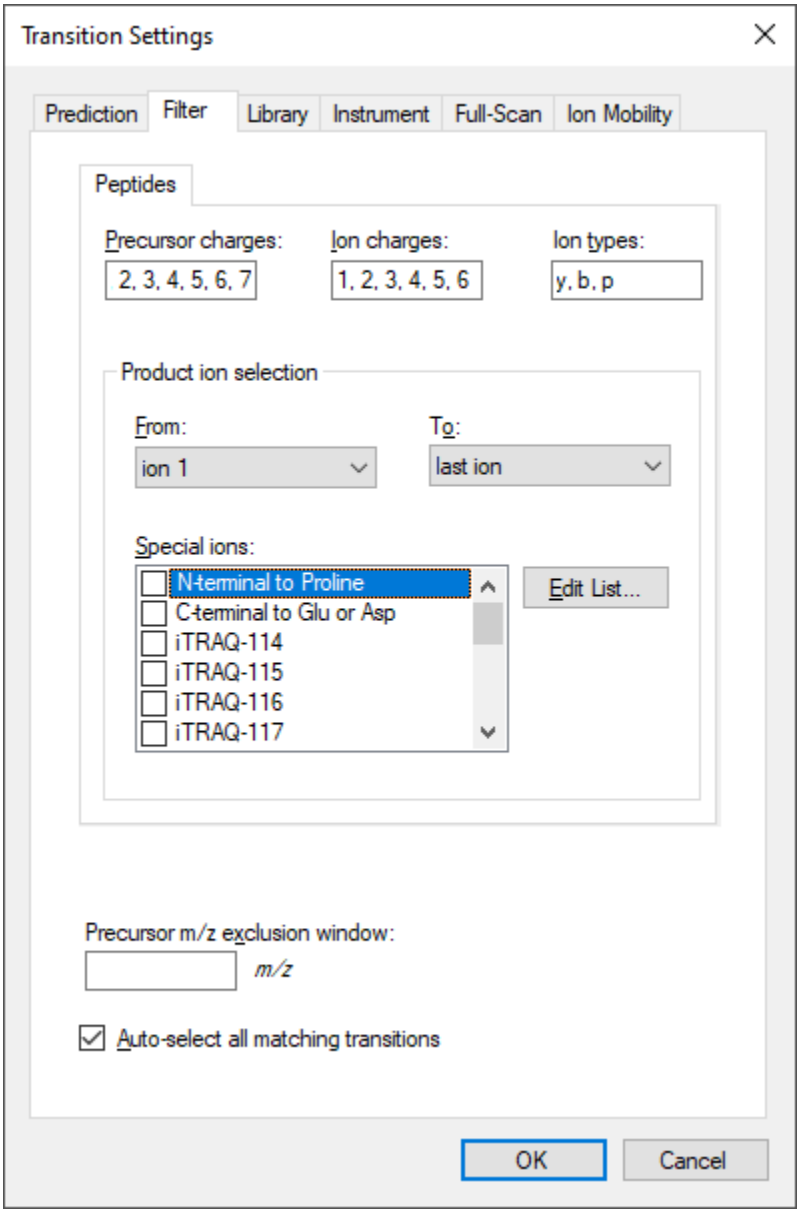
- Open reports\MSstats_annotations.sky
- New document – Settings > Default – No (New document again to clear Audit Log)
- Save as Bruderer.sky
- Peptide Filter – Length 6 to 55, Exclude 0



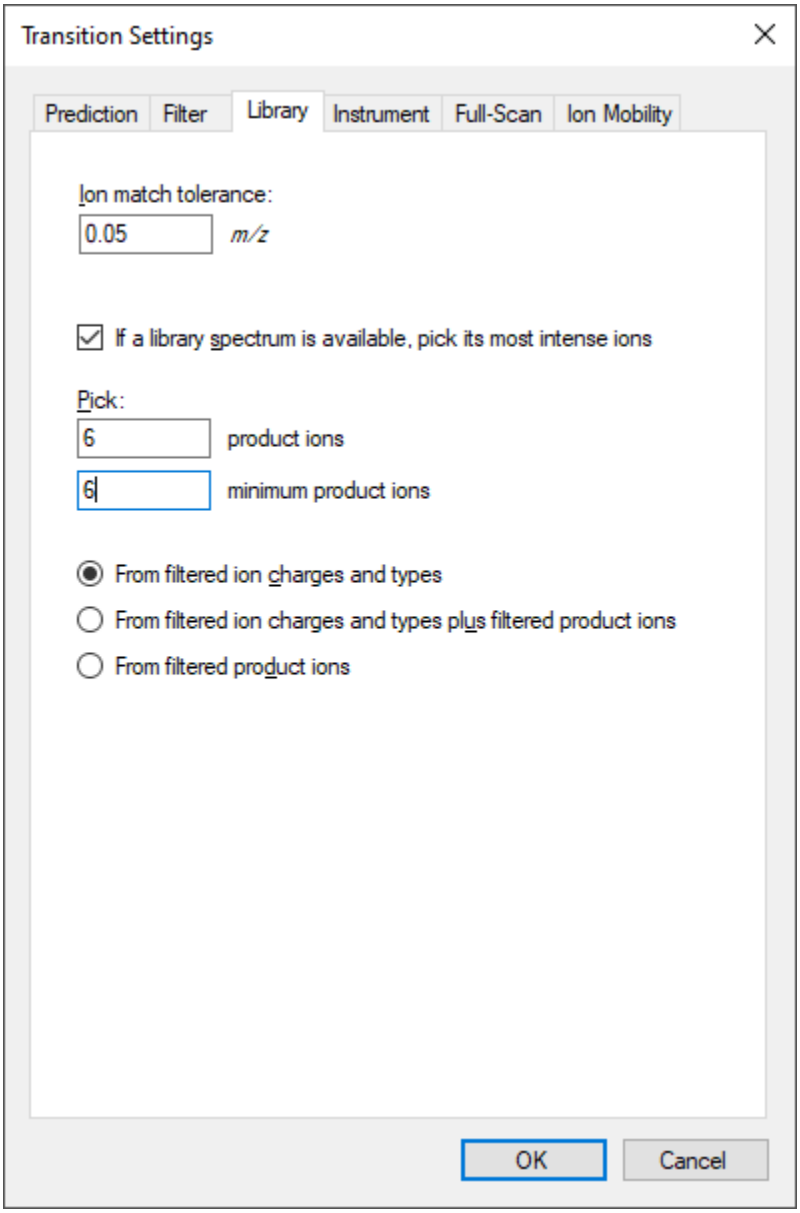
- Peptide Modifications – Carb (C), Oxy (M), Acetyl (N-term), Water Loss, Ammonia Loss



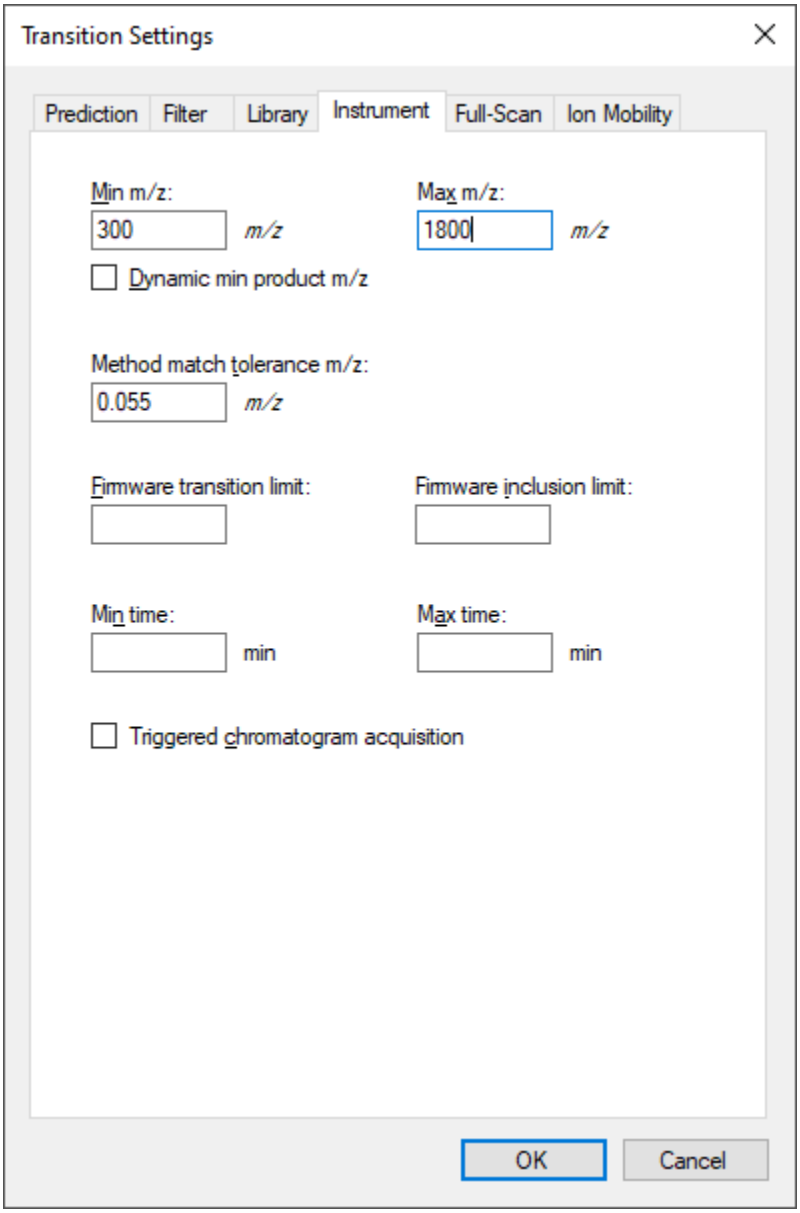
- Transition Filter – Pre charge: 1-7, Ion charge: 1-6, Ion types: y, b, p (1 through last)



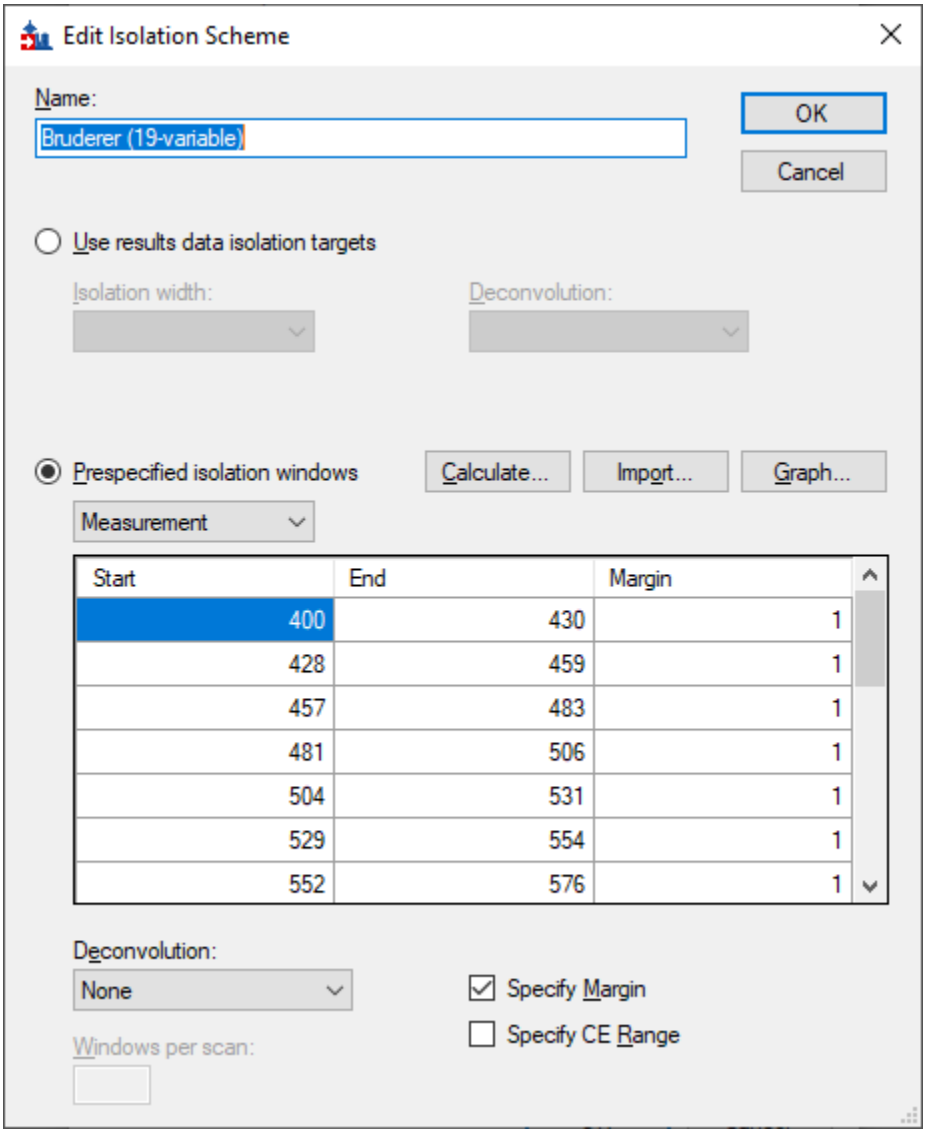
- Transition Library – Pick 6 with 6 min, charges and types

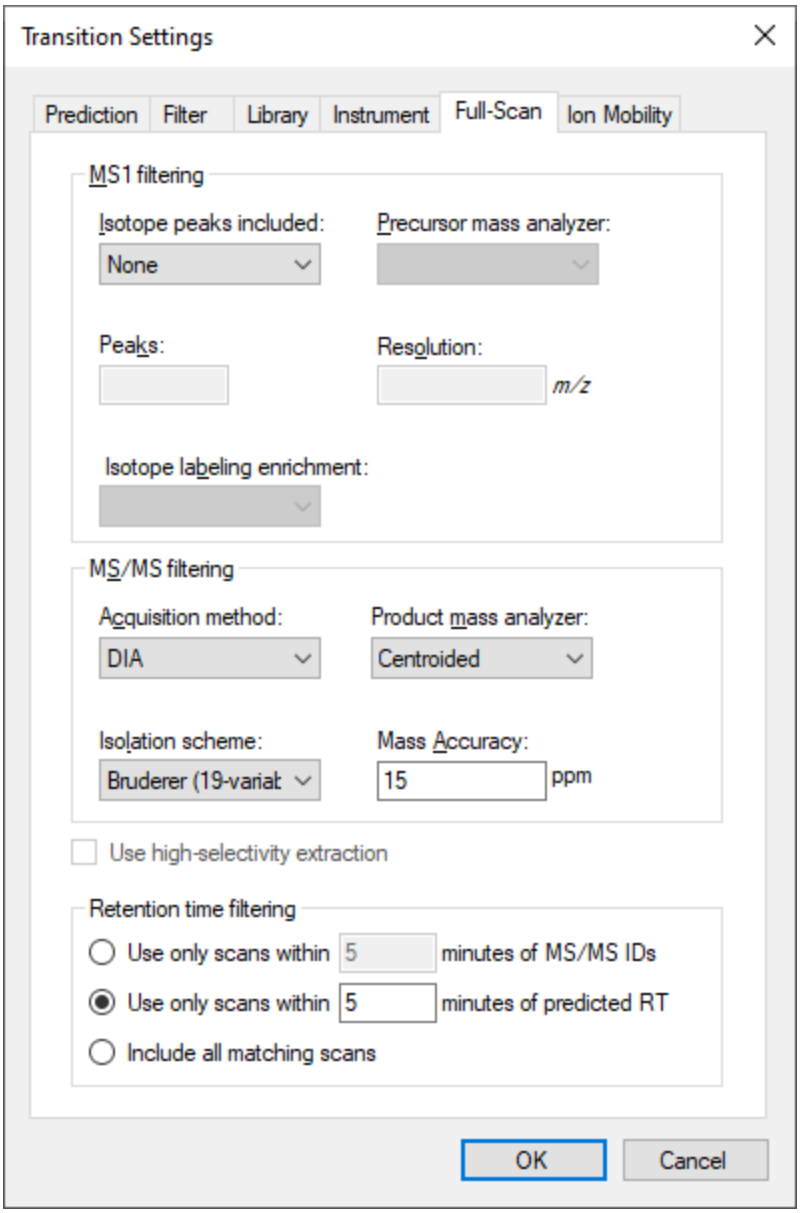


- Transition Instrument – 300 to 1800 m/z

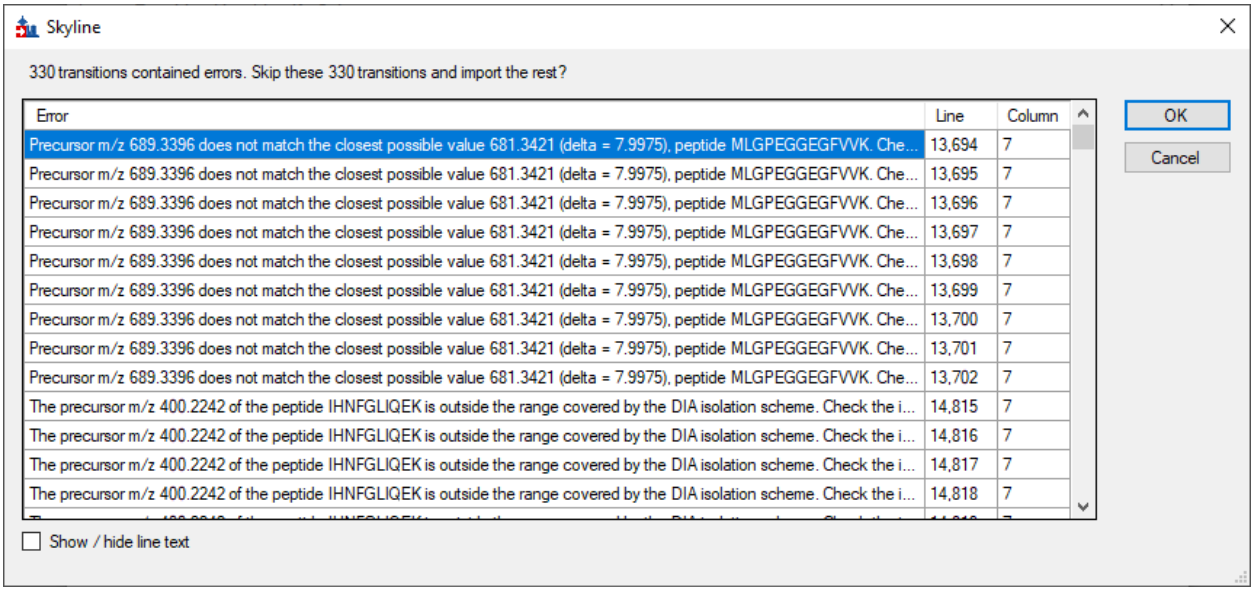


- Transition Full-Scan – DIA Centroided 15 ppm (import scans/mzML file) – Predicted RT

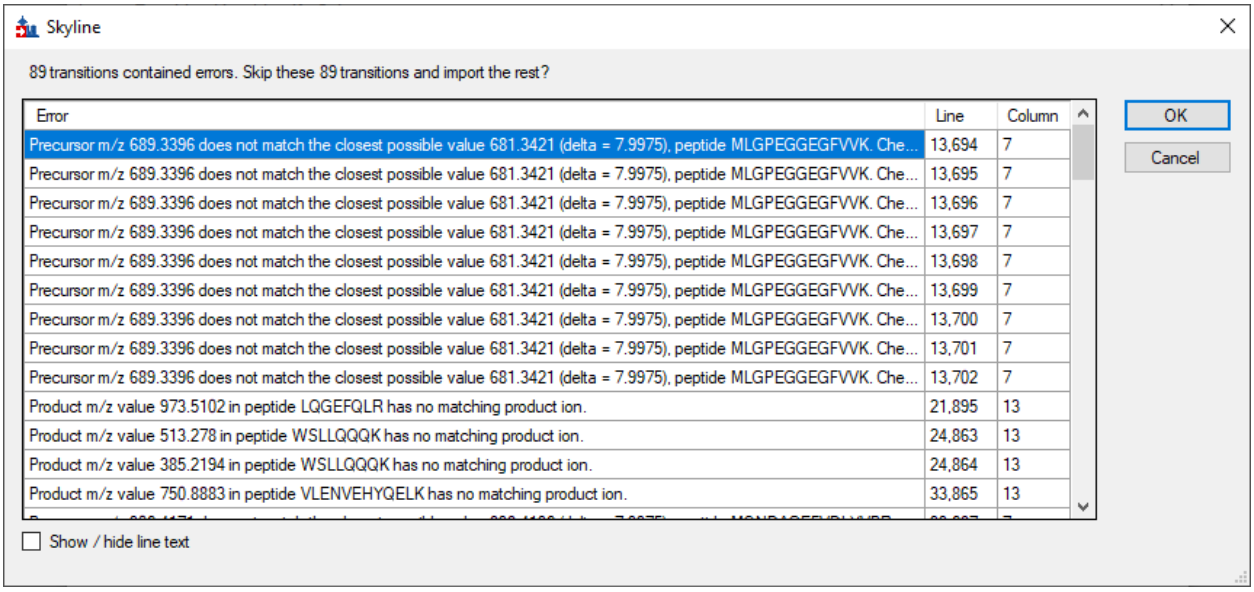



Transition Settings
Prediction
Filter
Library
Instrument
Full-Scan
Ion Mobility
MS1 filtering
Isotope peaks included:
None
Precursor mass analyzer:
Peaks:
Resolution:
m/z
Isotope labeling enrichment:
MS/MS filtering
Acquisition method:
DIA
Product mass analyzer:
Centroided
Isolation scheme:
Bruderer (19-variat
Mass Accuracy:
15
ppm
Use high-selectivity extraction
Retention time filtering
Use only scans within 5 minutes of MS/MS IDs
Use only scans within 5 minutes of predicted RT
Include all matching scans
OK
Cancel

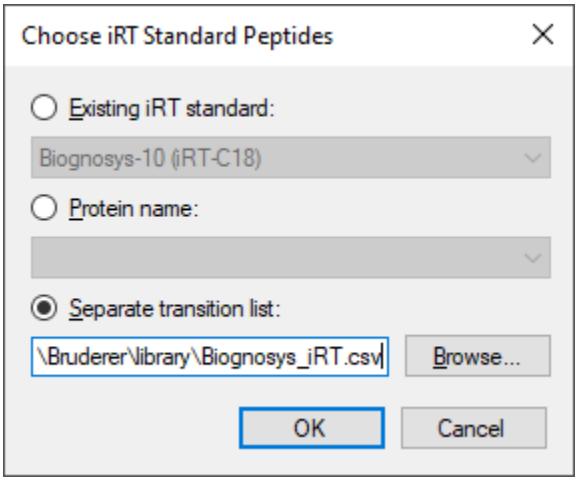
- Import Assay Library “mcp.M114.044305-2-Profiling.csv” (330 lines of errors)



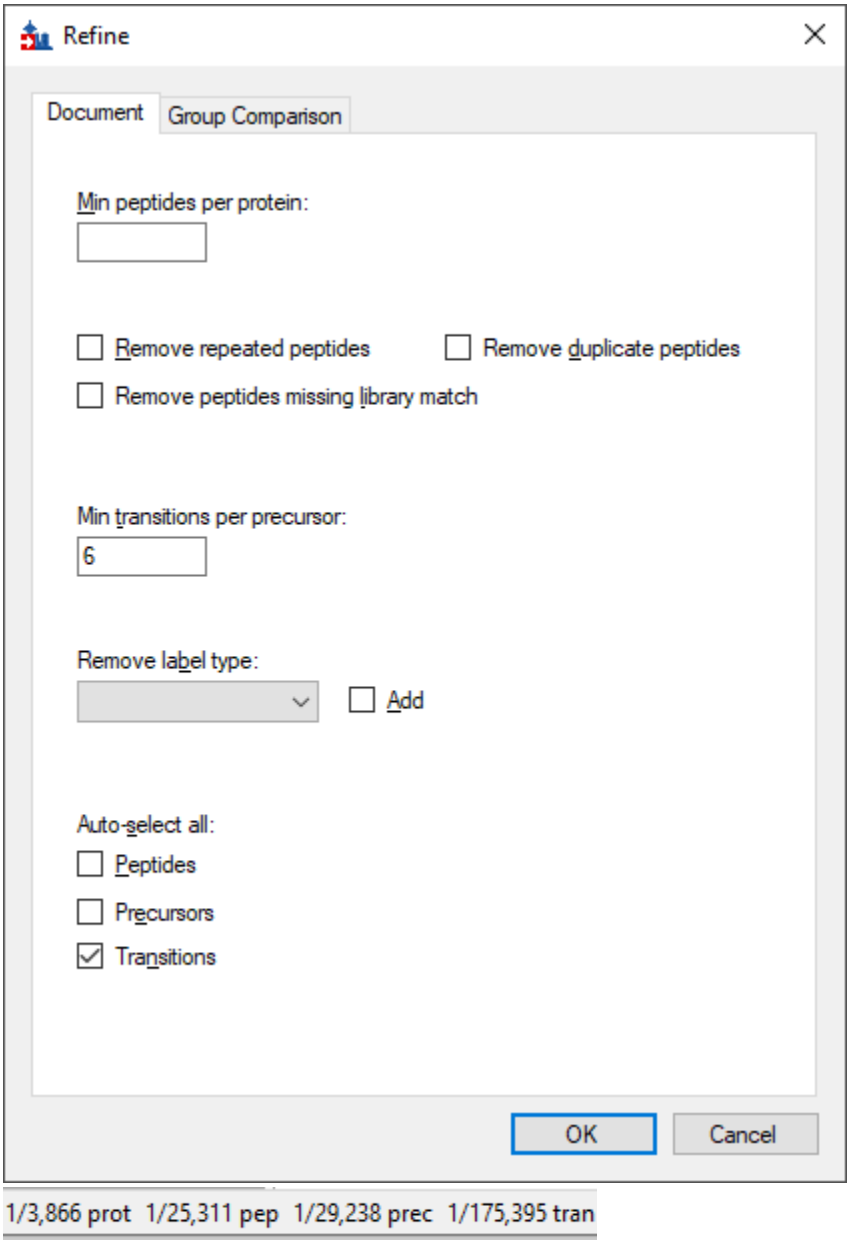
- Explain precursors between 400 and 401 and adjust Transition Settings
- Import Assay Library (89 lines of errors – explain Oxi (M) and Acetyl (N-term) and move on)



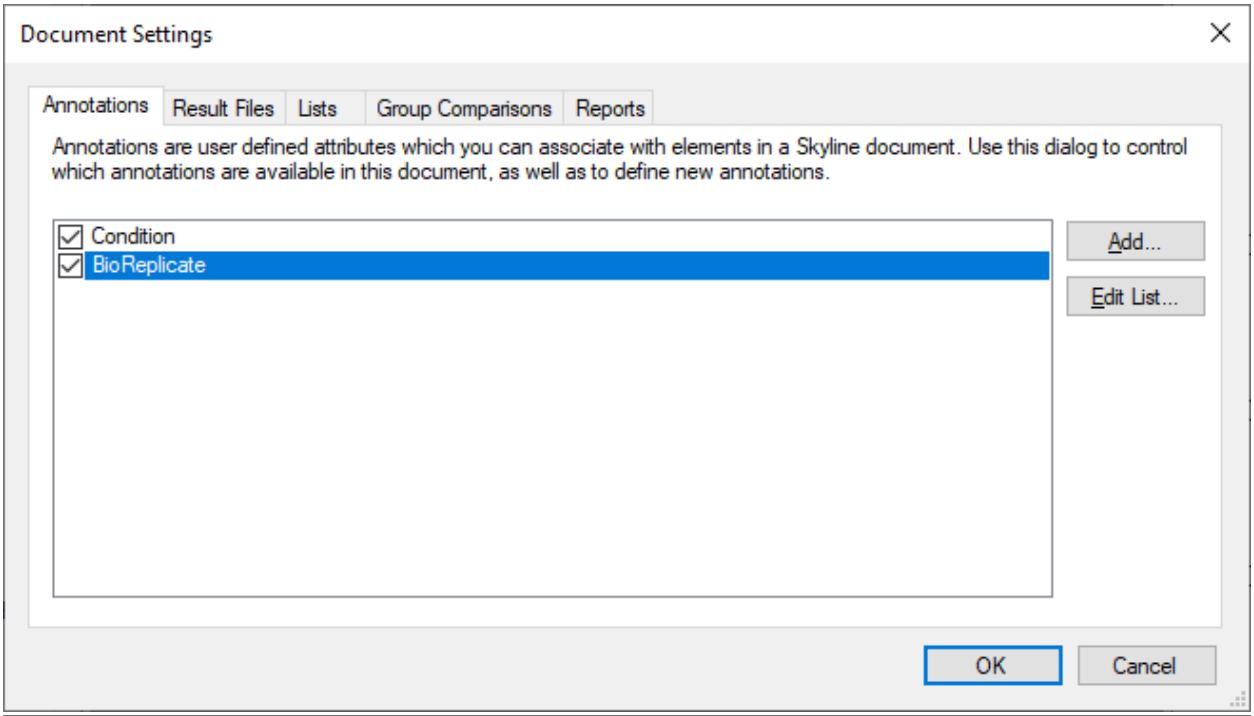
- Separate transition list “Biognosys_iRT.csv”

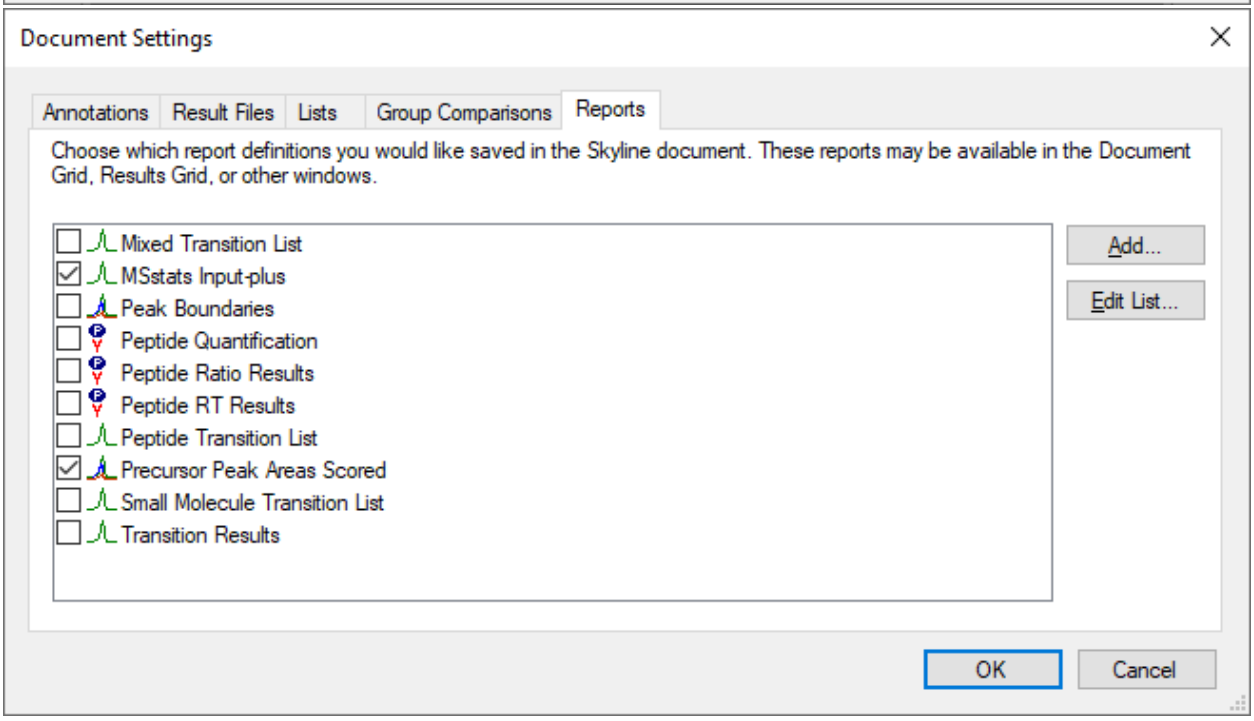


- Refine > Advanced – min trans 6, auto-select trans



- Settings > Document – add MSstats annotations and reports





- Save and exit