

Folder structure and files of data sets used in the case studies in this manuscript

All files are packed in a zip compressed file and are provided on the homepage:

<http://www.ms.uni-jena.de/en/Software+and+Education.html>

Files DeltaMS	
Case study 1	
CS1.mzXML	11.66 MB
DeltaMS_results_082517-0443AM	
Analysis_settings.html	
EICs CS1.pdf	
Features_Absolute_Intensity CS1.pdf	
Features_Relative_Intensity CS1.pdf	
Mass Spectra CS1.pdf	
Peaktable CS1.csv	
Case study 2	
negative mode	
CS2-neg.mzXML	75.66 MB
DeltaMS_results_082517-0452AM	
Analysis_settings.html	
EICs CS2 neg.pdf	
Features_Absolute_Intensity CSs neg.pdf	
Features_Relative_Intensity CS2 neg.pdf	
Mass Spectra CS2 neg.pdf	
Peaktable CS2 neg.csv	
positive mode	
CS2-pos.mzXML	117.40 MB
DeltaMS_results_082517-0500AM	
Analysis_settings.html	
EICs CS2 pos.pdf	
Features_Absolute_Intensity CS2 pos.pdf	
Features_Relative_Intensity CS2 pos.pdf	
Mass Spectra CS2 pos.pdf	
Peaktable CS2 pos.csv	
DeltaMS_results_082517-0611AM	
Analysis_settings.html	
EICs CS2 pos z2.pdf	
Features_Absolute_Intensity CS2 pos z2.pdf	
Features_Relative_Intensity CS2 pos z2.pdf	
Mass Spectra CS2 pos z2.pdf	
Peaktable CS2 pos z2.csv	
Case study 3	
54Fe 58Fe dataset comparison	
54Fe	
54Fe positive model1.mzXML	16.86 MB
54Fe positive mode2.mzXML	16.71 MB
54Fe positive mode3.mzXML	16.85 MB
54Fe positive mode4.mzXML	17.39 MB
54Fe positive mode5.mzXML	18.13 MB
54Fe positive mode6.mzXML	17.60 MB
54Fe positive mode7.mzXML	17.78 MB
58Fe	
58Fe positive model1.mzXML	16.65 MB
58Fe positive mode2.mzXML	16.57 MB
58Fe positive mode3.mzXML	16.61 MB
58Fe positive mode4.mzXML	17.70 MB
58Fe positive mode5.mzXML	17.38 MB
58Fe positive mode6.mzXML	17.60 MB
58Fe positive mode7.mzXML	17.55 MB
DeltaMS_results_082517-0753AM	

- Analysis_settings.html
 - EICs CS3 Fe dataset comparison.pdf
 - Features_Absolute_Intensity CS3 Fe dataset comparison.pdf
 - Features_Relative_Intensity CS3 Fe dataset comparison.pdf
 - Mass Spectra CS3 dataset Fe comparison.pdf
 - Peaktable CS3 Fe dataset comparison.csv
- 54Fe 58Fe isotope signature**
 - 54Fe 58Fe mixed positive model1.mzXML 15.32 MB
 - 54Fe 58Fe mixed positive mode2.mzXML 14.69 MB
 - 54Fe 58Fe mixed positive mode3.mzXML 14.66 MB
 - 54Fe 58Fe mixed positive mode4.mzXML 14.54 MB
 - DeltaMS_results_082517-1107AM**
 - Analysis_settings.html
 - EICs CS3 54Fe58Fe isotope signature.pdf
 - Features_Absolute_Intensity CS3 54Fe58Fe isotope signature.pdf
 - Features_Relative_Intensity CS3 54Fe58Fe isotope signature.pdf
 - Mass Spectra CS3 54Fe58Fe isotope signature.pdf
 - Peaktable CS3 54Fe58Fe isotope signature.csv
- 95Mo 98Mo isotope signature**
 - 95Mo 98Mo mixed negative model1.mzXML 10.76 MB
 - 95Mo 98Mo mixed negative mode2.mzXML 10.79 MB
 - 95Mo 98Mo mixed negative mode3.mzXML 10.70 MB
 - DeltaMS_results_082517-1120AM**
 - Analysis_settings.html
 - EICs CS3 95Mo98Mo isotope signature.pdf
 - Features_Absolute_Intensity CS3 95Mo98Mo isotope signature.pdf
 - Features_Relative_Intensity CS3 95Mo98Mo isotope signature.pdf
 - Mass Spectra CS3 95Mo98Mo isotope signature.pdf
 - Peaktable CS3 95Mo98Mo isotope signature.csv
- 95Mo 98Mo dataset comparison**
 - 95Mo**
 - 95Mo negative model1.mzXML 11.99 MB
 - 95Mo negative mode2.mzXML 12.12 MB
 - 95Mo negative mode3.mzXML 12.12 MB
 - 95Mo negative mode4.mzXML 12.26 MB
 - 98Mo**
 - 98Mo negative model1.mzXML 12.05 MB
 - 98Mo negative mode2.mzXML 12.22 MB
 - 98Mo negative mode3.mzXML 12.14 MB
 - 98Mo negative mode4.mzXML 12.21 MB
 - DeltaMS_results_082517-1139AM**
 - Analysis_settings.html
 - EICs CS3 95Mo98Mo dataset comparison.pdf
 - Features_Absolute_Intensity CS3 95Mo98Mo dataset comparison.pdf
 - Features_Relative_Intensity CS3 95Mo98Mo dataset comparison.pdf
 - Mass Spectra CS3 95Mo98Mo dataset comparison.pdf
 - Peaktable CS3 95Mo98Mo dataset comparison.csv
- Fe natural**
 - Fe natural positive mode.mzXML 17.71 MB
 - DeltaMS_results_082517-1155AM**
 - Analysis_settings.html
 - EICs CS3 Fe natural.pdf
 - Features_Absolute_Intensity CS3 Fe natural.pdf
 - Features_Relative_Intensity CS3 Fe natural.pdf
 - Mass Spectra CS3 Fe natural.pdf
 - Peaktable CS3 Fe natural.csv
- Mo natural**
 - Mo natural negative model1.mzXML 12.24 MB
 - Mo natural negative mode2.mzXML 12.36 MB
 - DeltaMS_results_082517-#1126AM**
 - Analysis_settings.html
 - EICs CS3 Mo natural.pdf
 - Features_Absolute_Intensity CS3 Mo natural.pdf
 - Features_Relative_Intensity CS3 Mo natural.pdf
 - Mass Spectra CS3 Mo natural.pdf
 - Peaktable CS3 Mo natural.csv