Friedrich-Schiller-Universität Jena

NMR-Plattform der Chemisch-Geowissenschaftlichen Fakultät

11. Januar 2017 / Friederike Pielenz

Einführung in ACD-Labs

seit 1558

Einführung in ACD-Labs

- Software installieren
  mit Archivserver verbinden
  Daten mit ACD-Labs öffnen

- Phase korrigieren
  „Peak Picking“
  Peaks integrieren
  Peaks u. Achse kalibrieren

  Peaks zuordnen

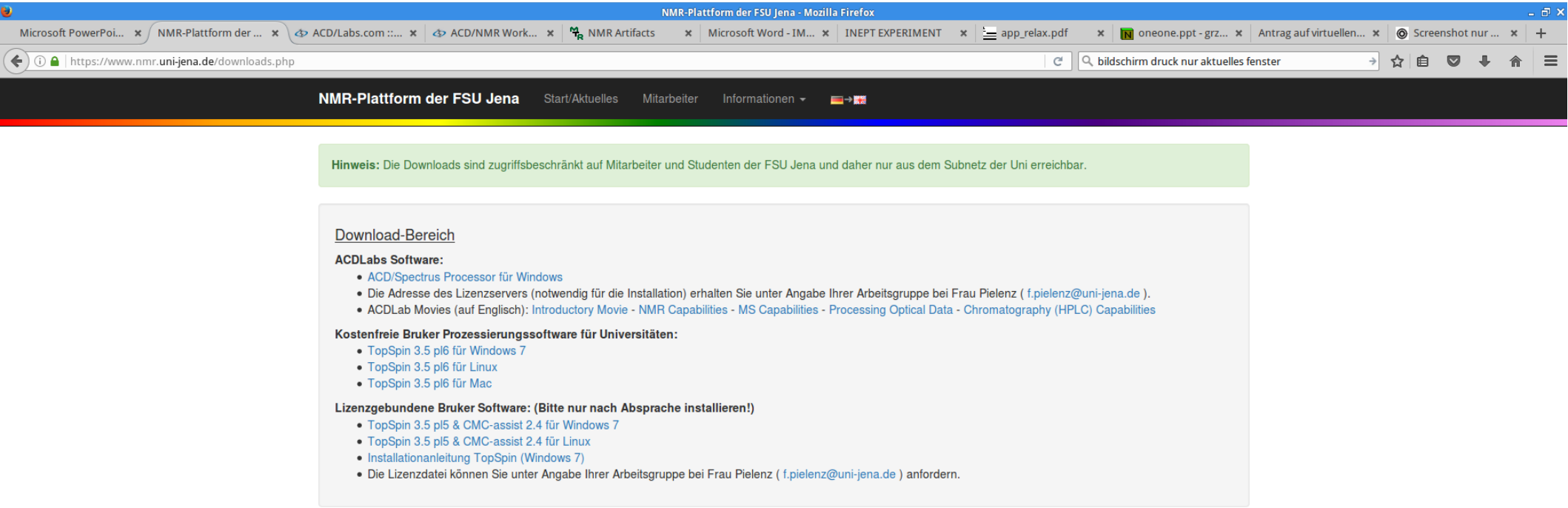
  } 1. automatisch

  } 2. manuell

- 2D-Spektren prozessieren

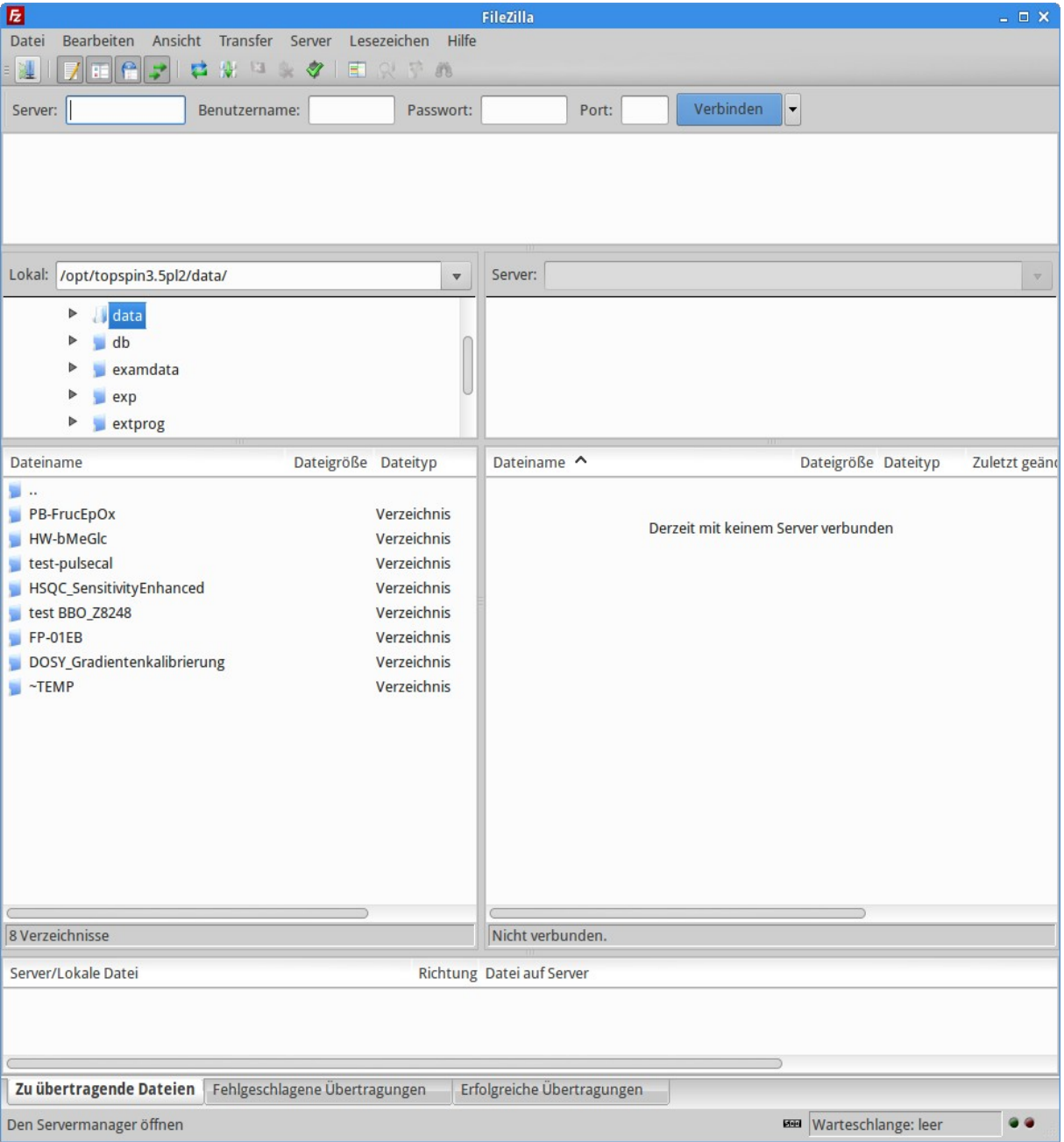
- Spektren darstellen und drucken

Software installieren



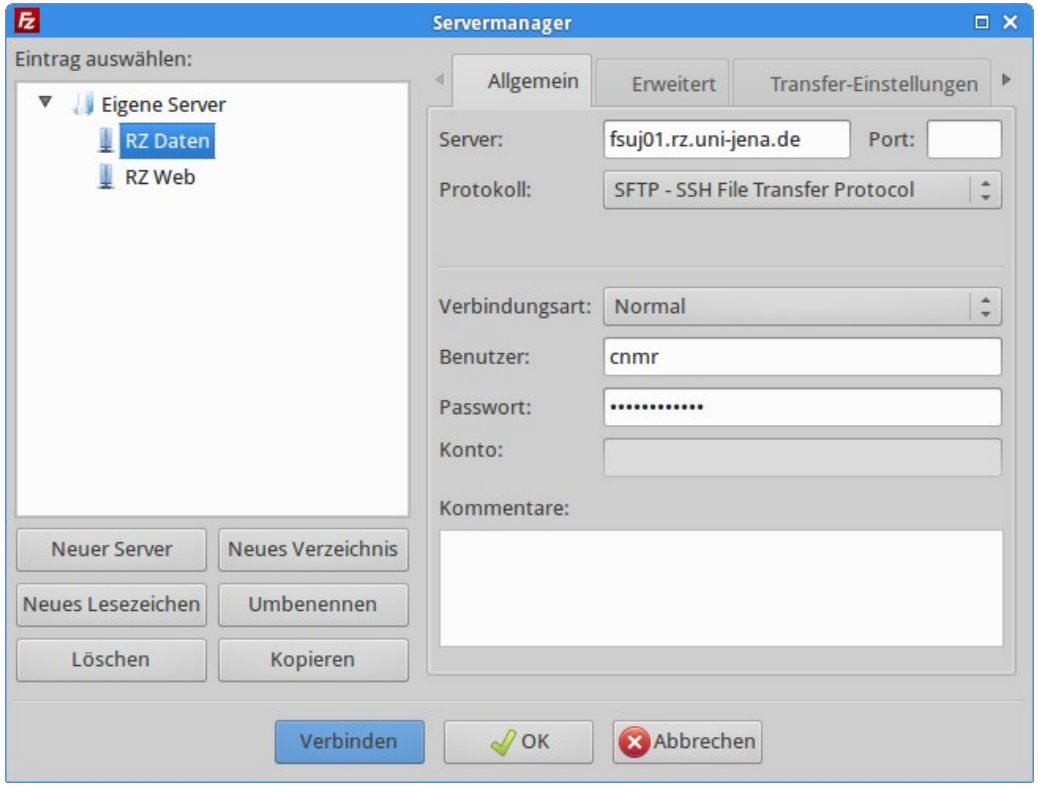
Die Software kann auf der Webseite der NMR-Plattform www.nmr.uni-jena.de heruntergeladen werden.
Zur Installation muss der Rechner mit dem Uninetz verbunden sein.
Bei Windows10 ist zuvor noch *net framework 3.5* zu installieren.

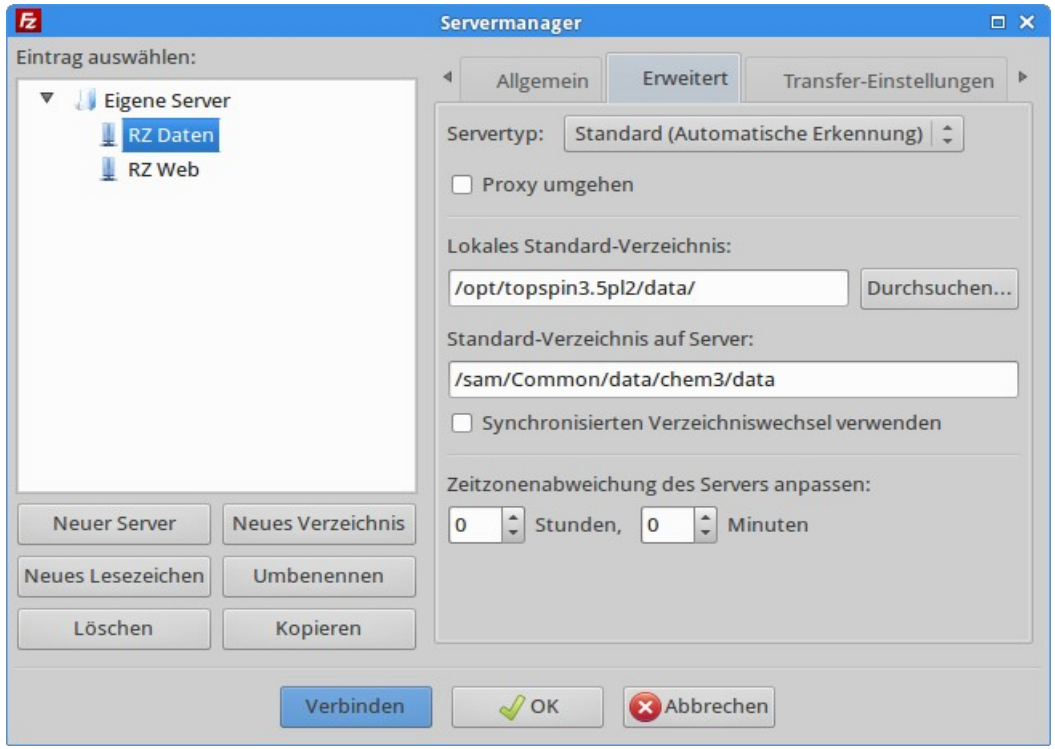
Archivserver



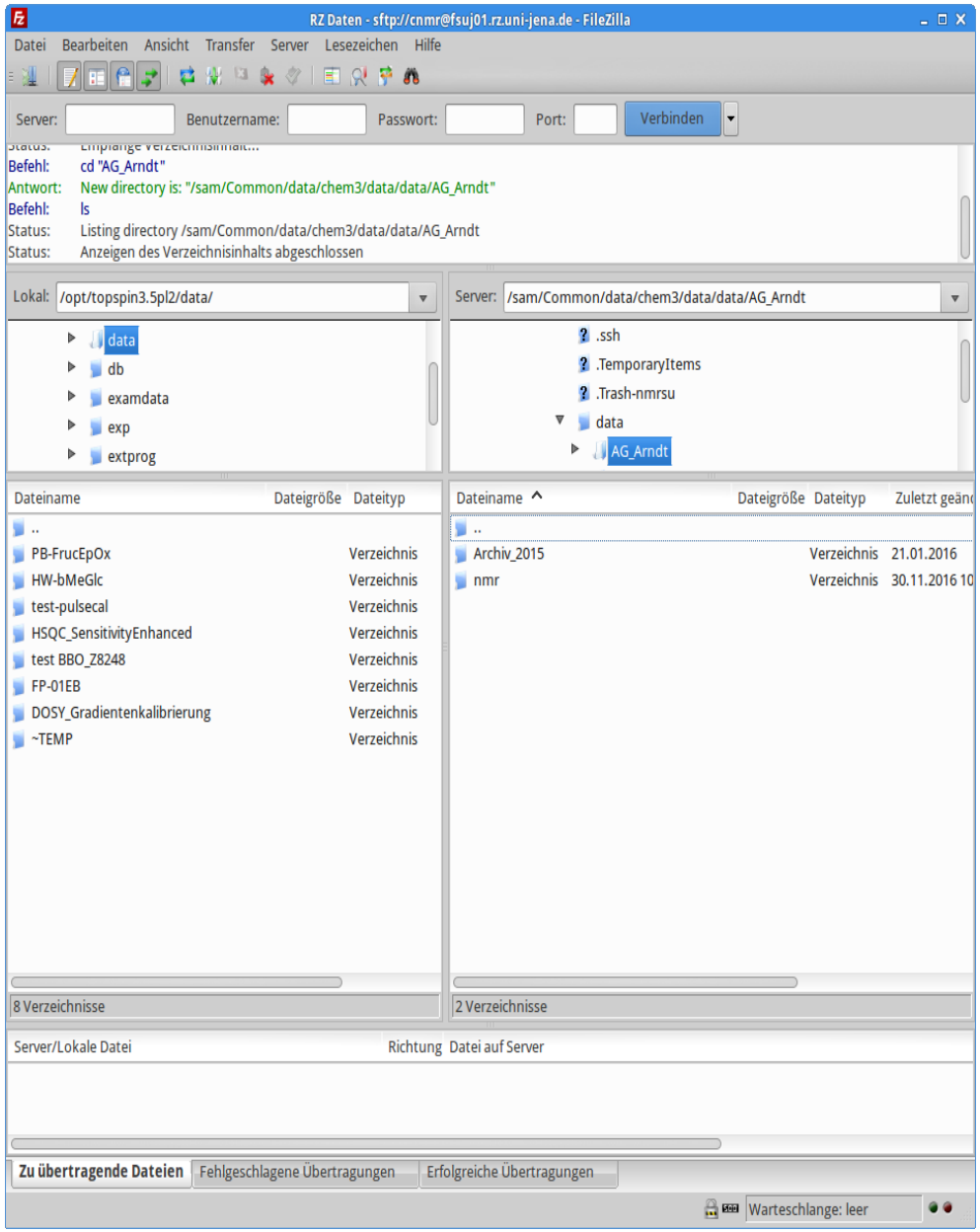
Der Zugriff erfolgt über ein kostenfreies *Secure File Transfer Protocol* (SFTP), z.B. *WinSCP* für Windows oder *FileZilla* für Windows, Linux oder MacOS.

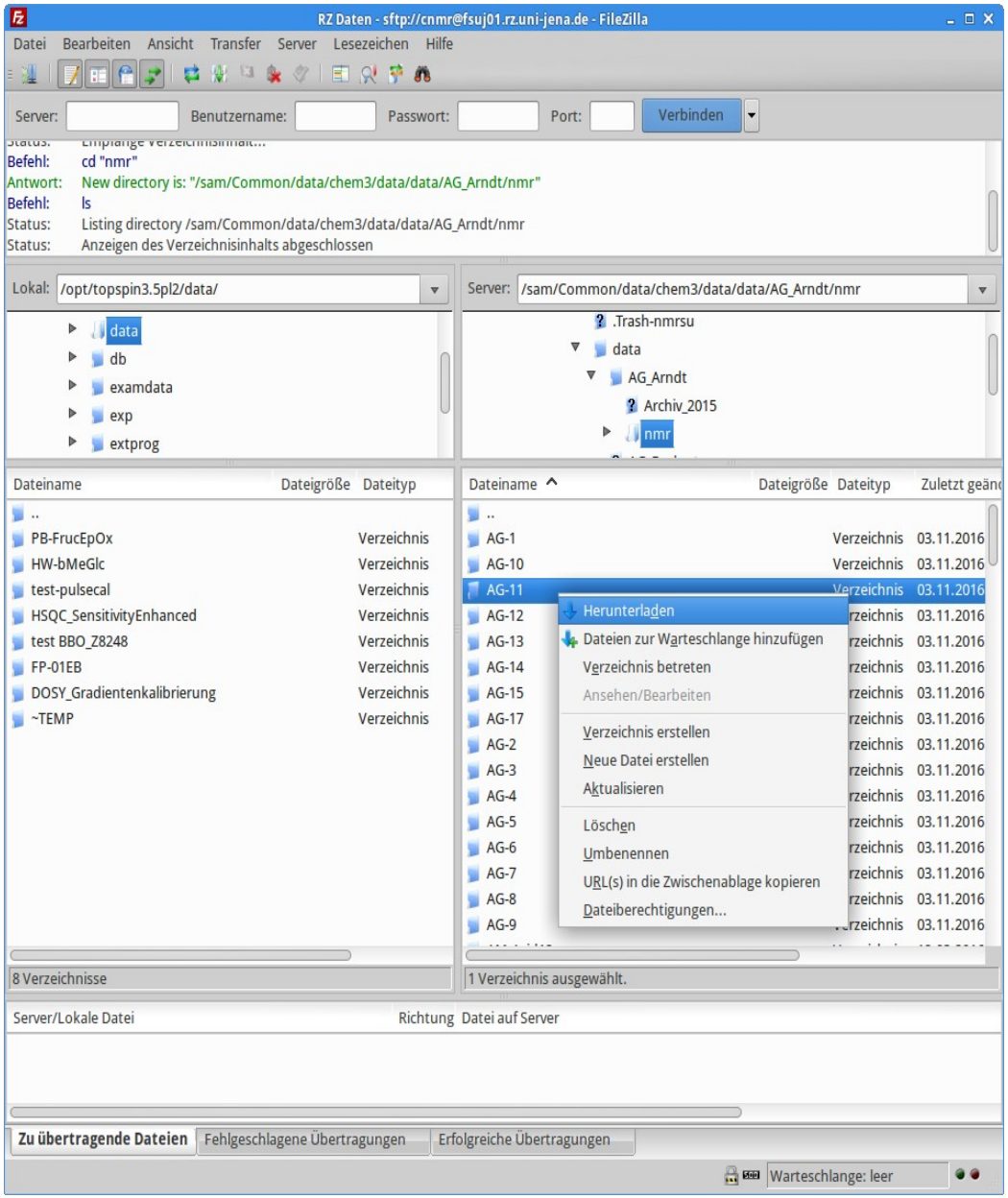
Archivserver



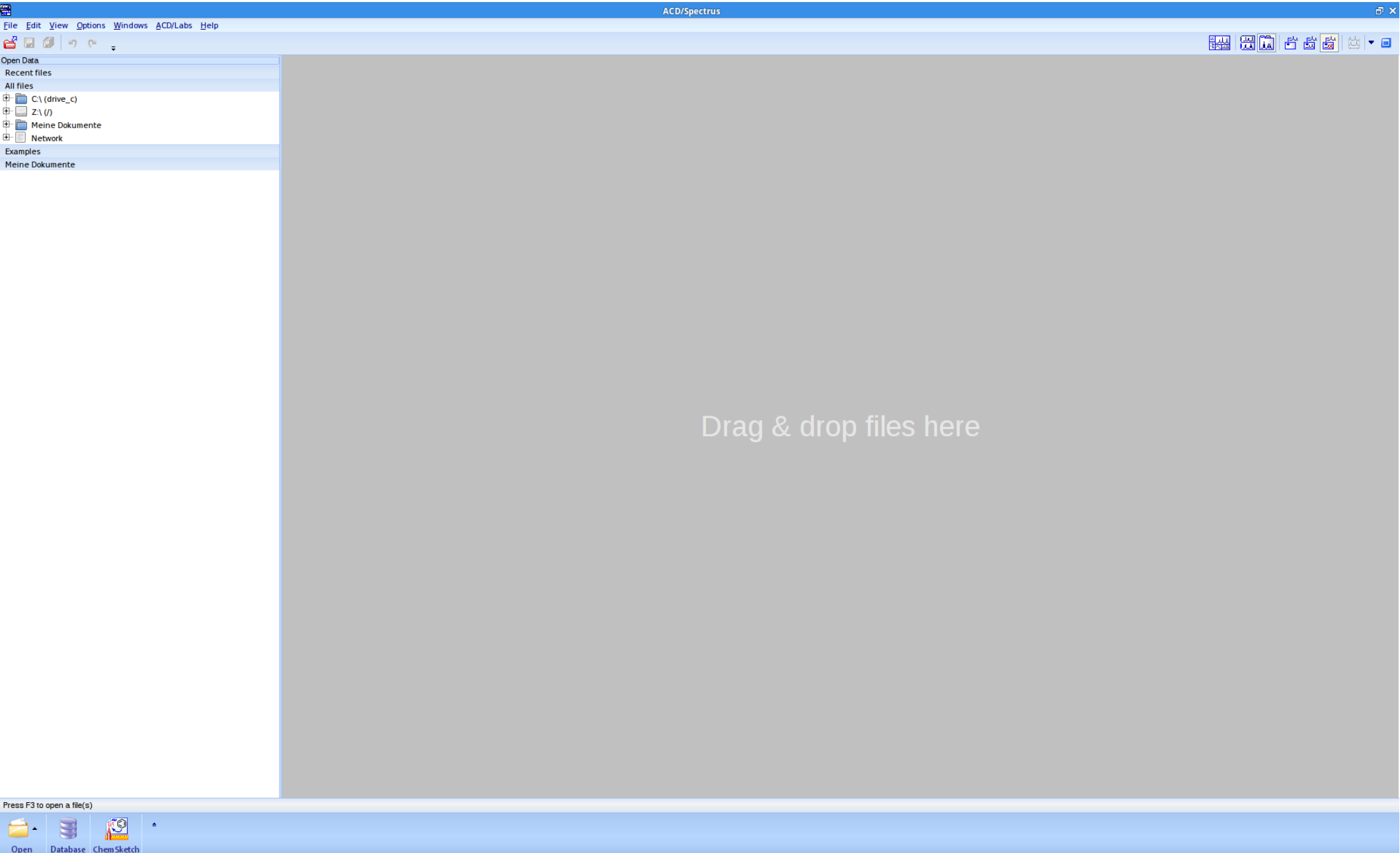


Archivserver





Daten in ACD-Labs öffnen



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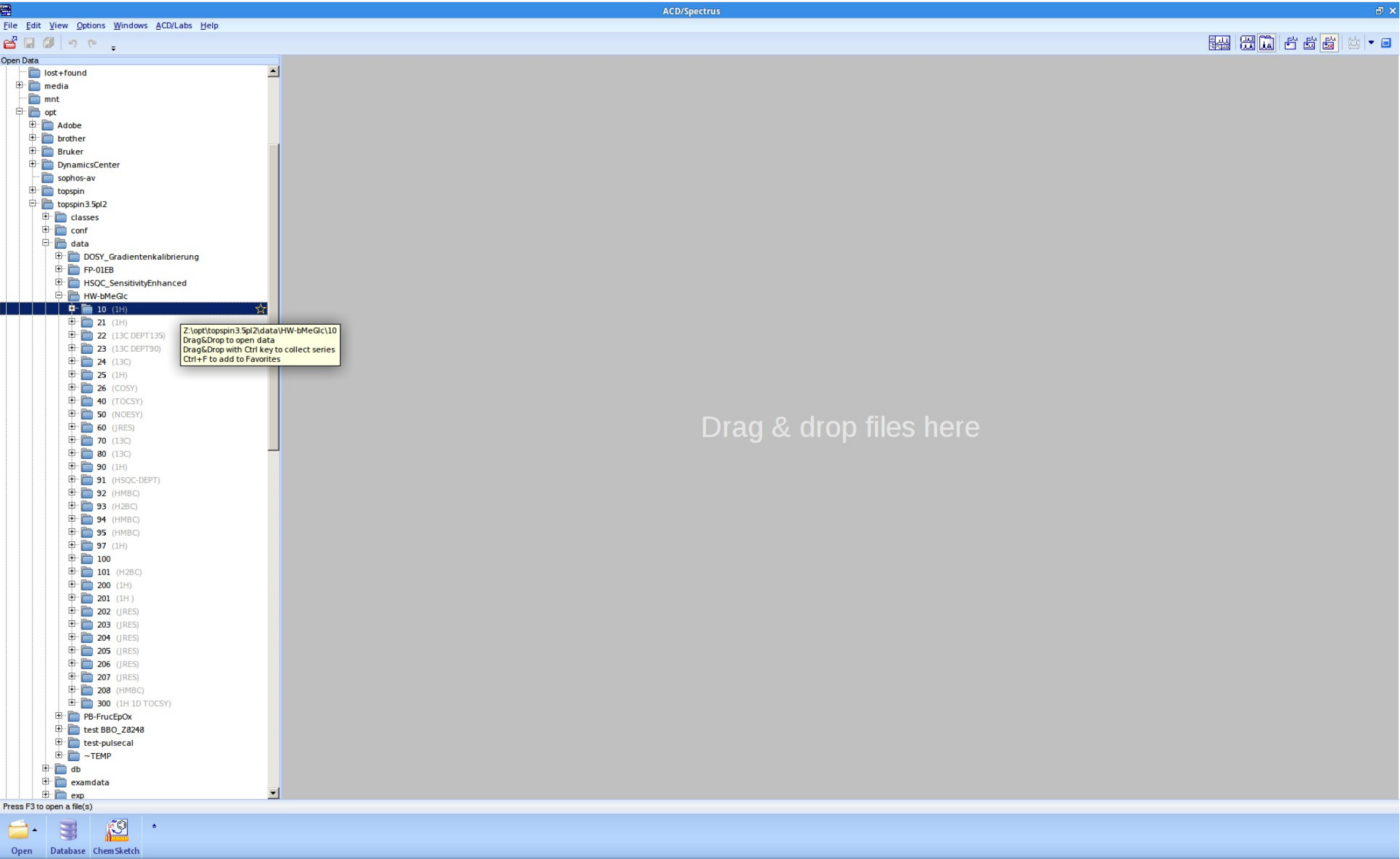

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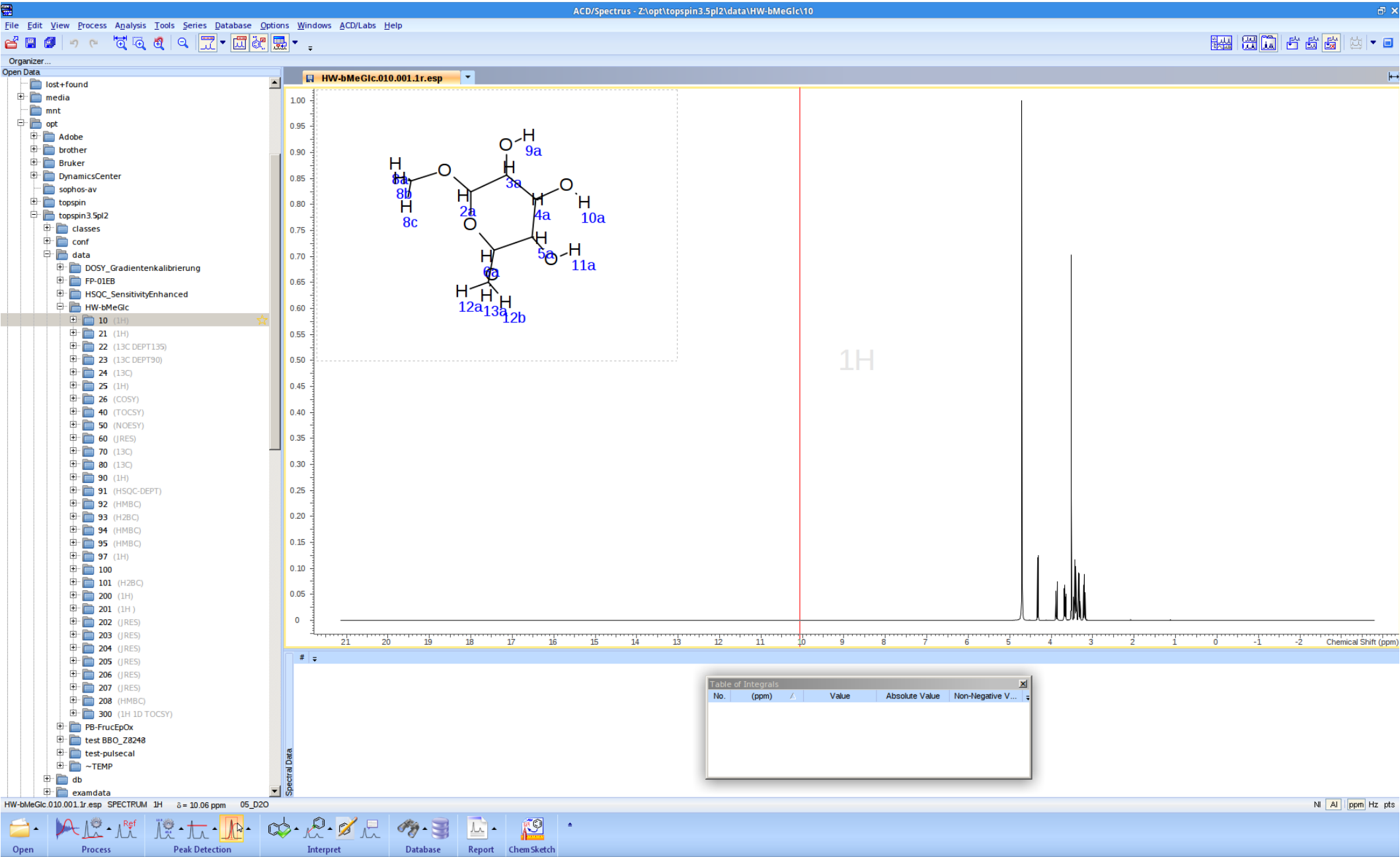

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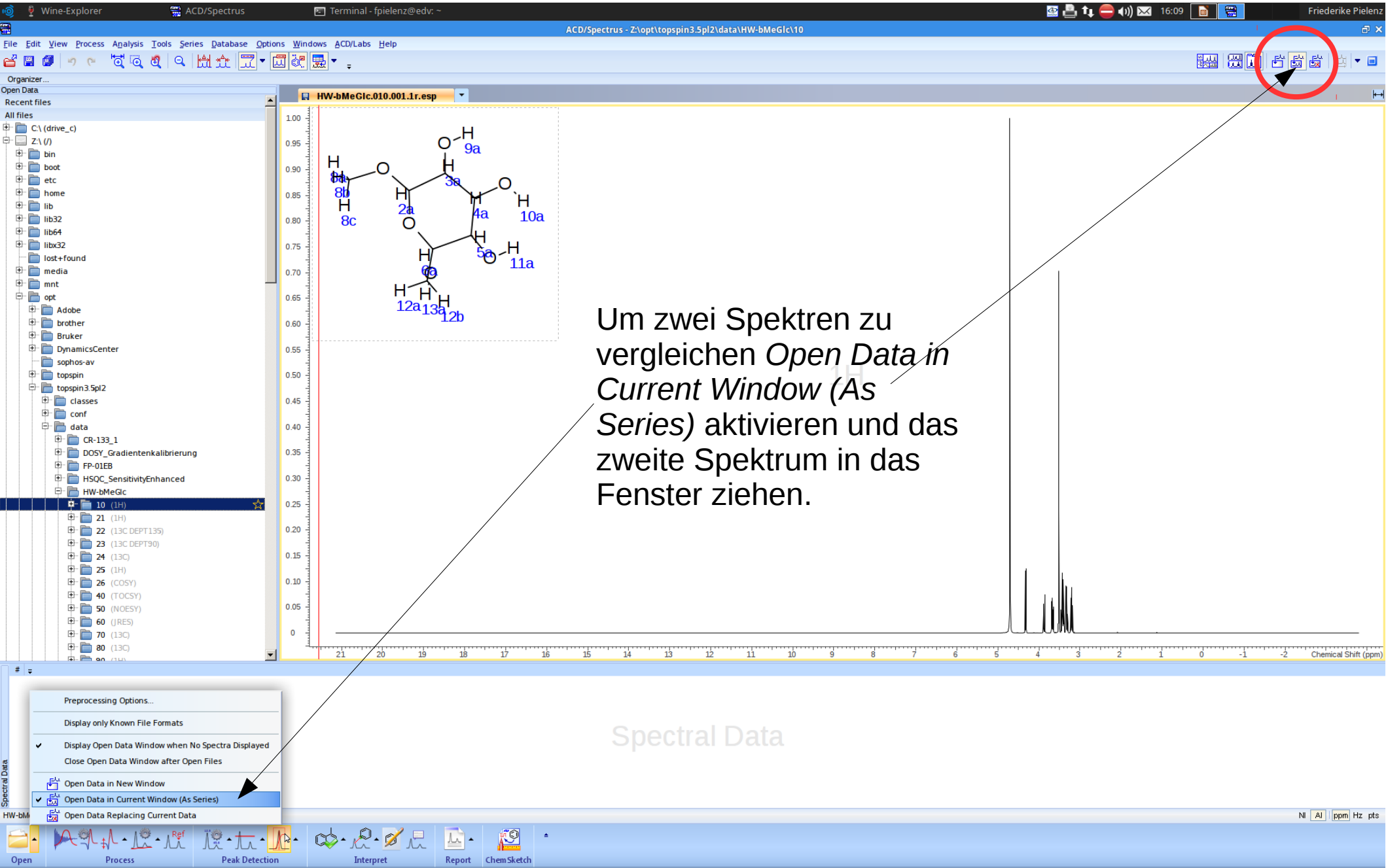

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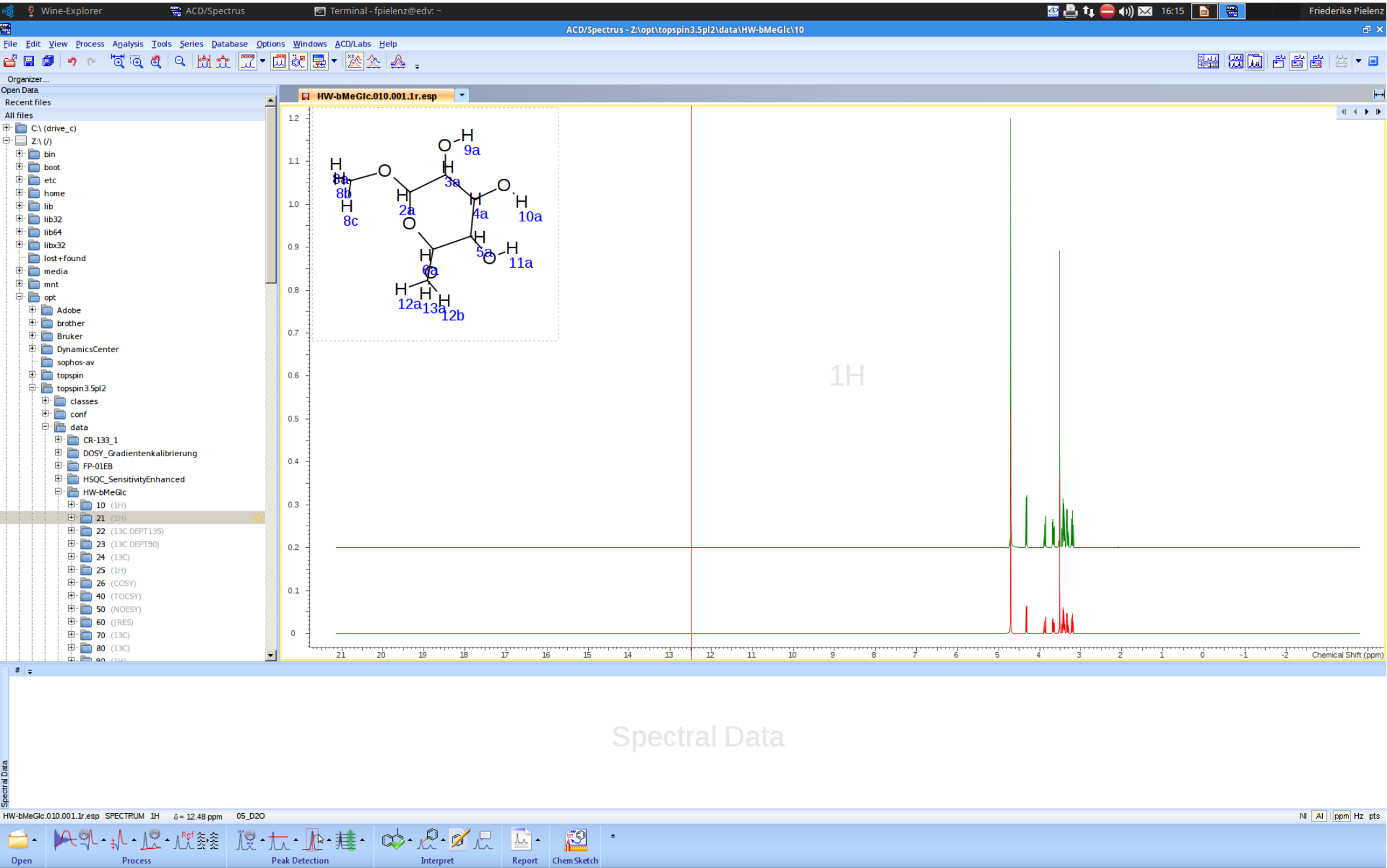

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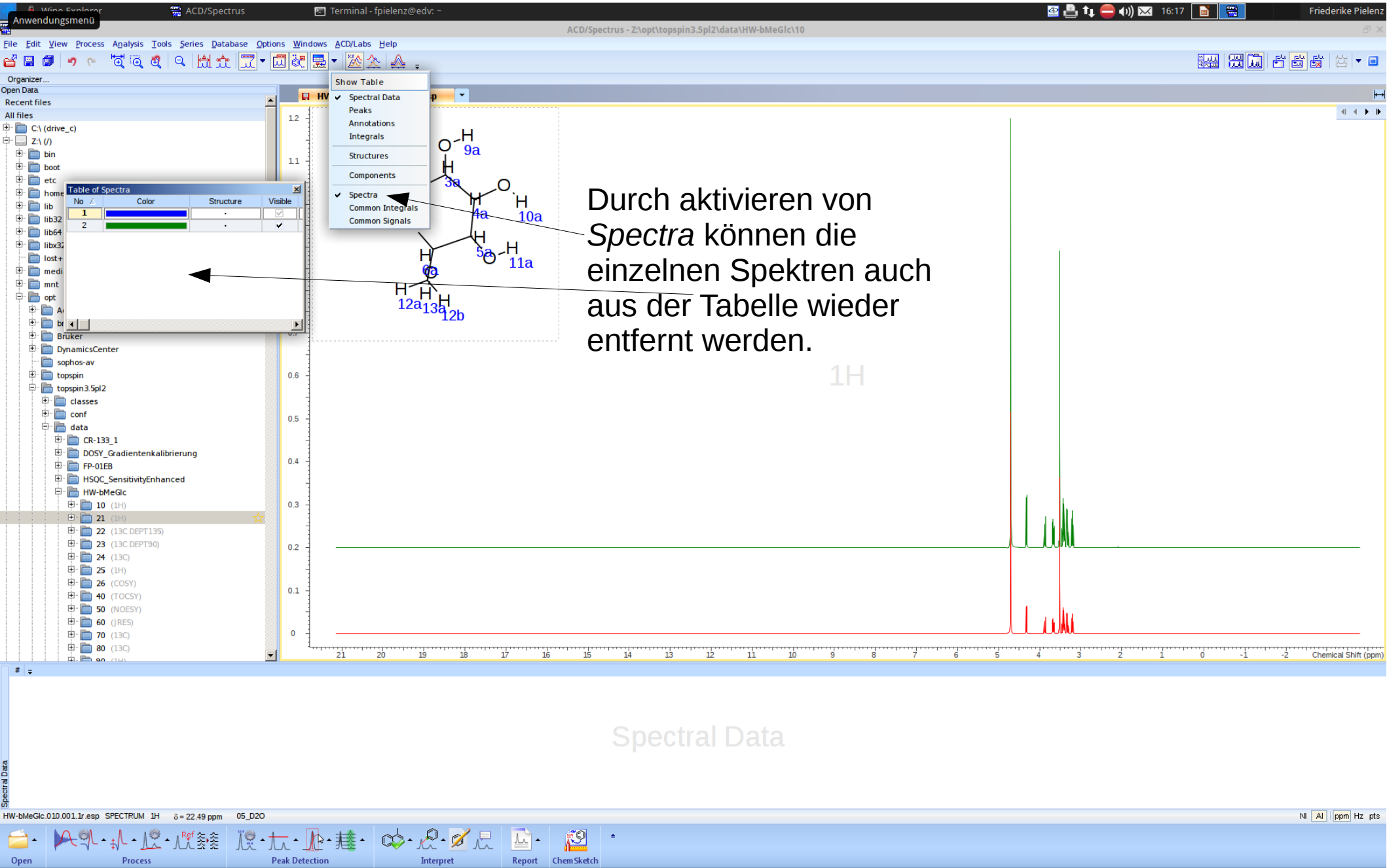

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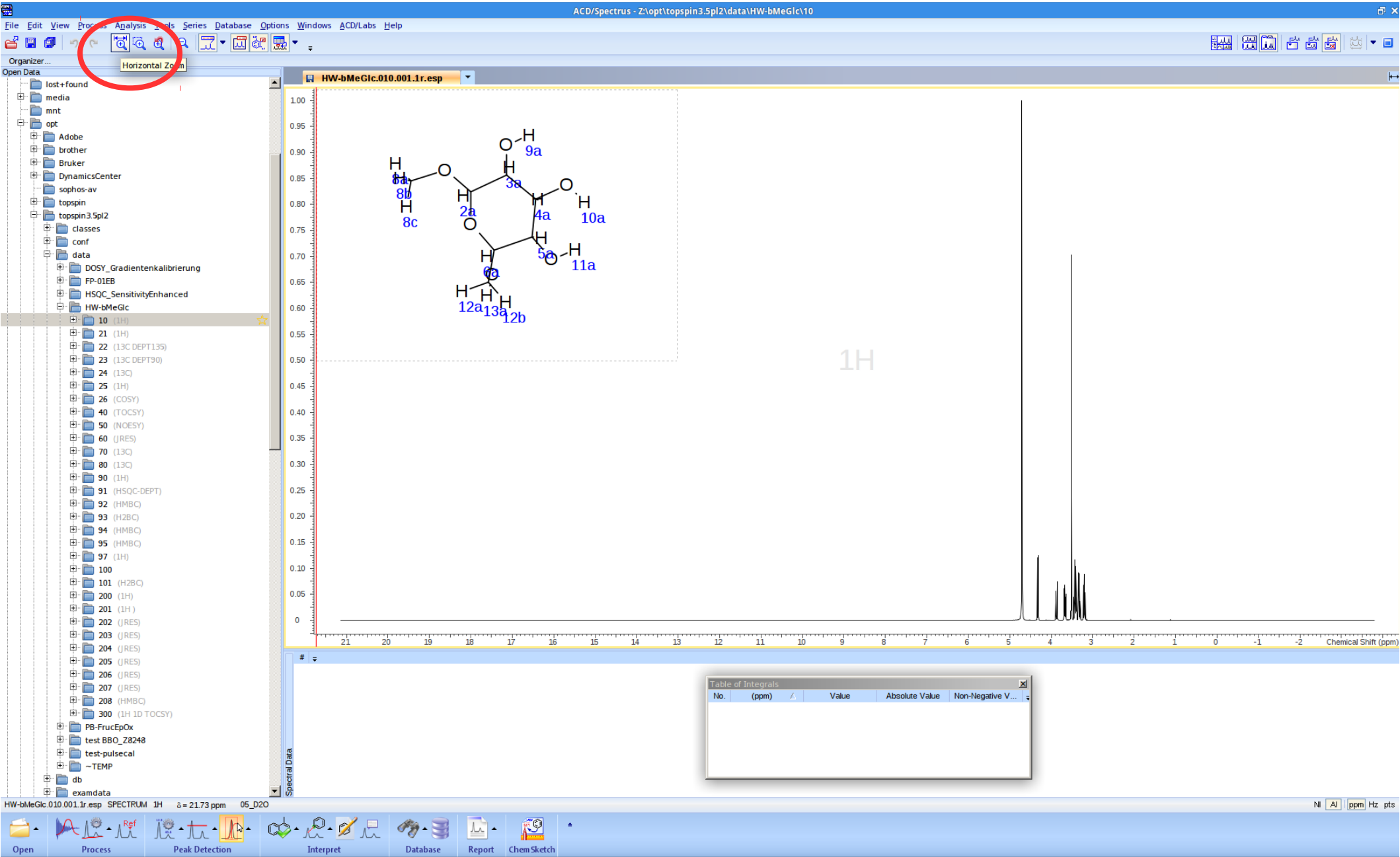
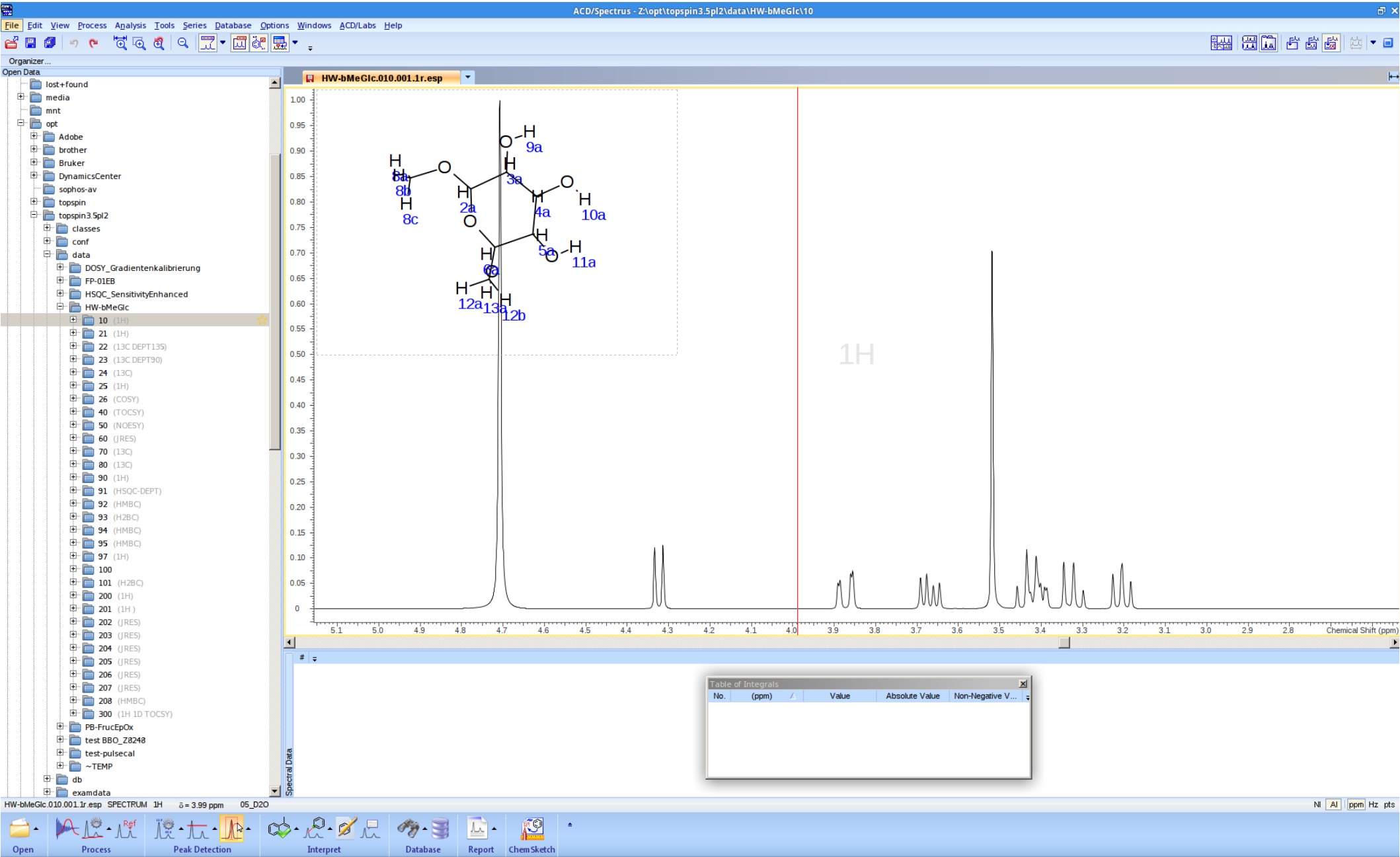


Spektrenausschnitt vergrößern



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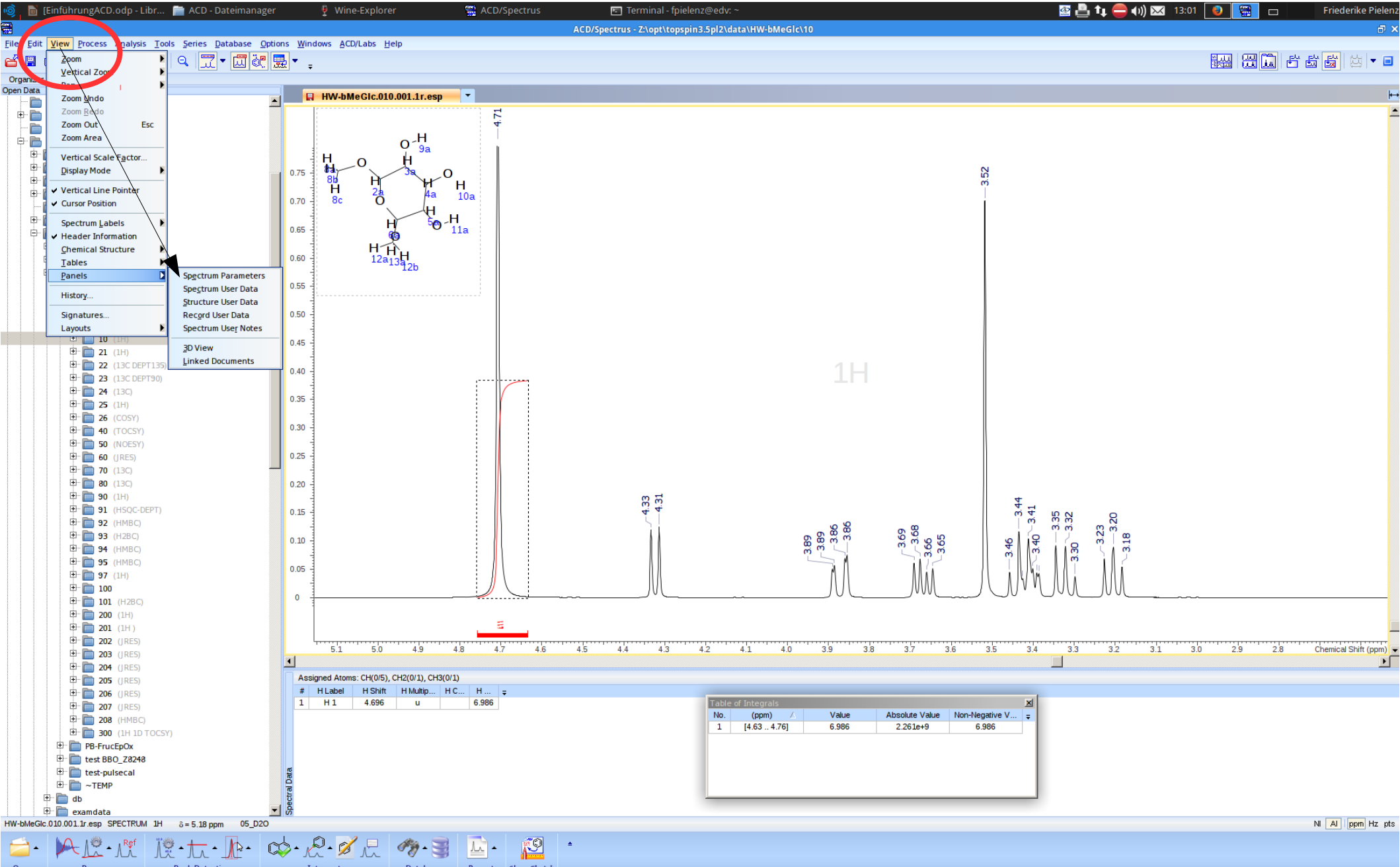
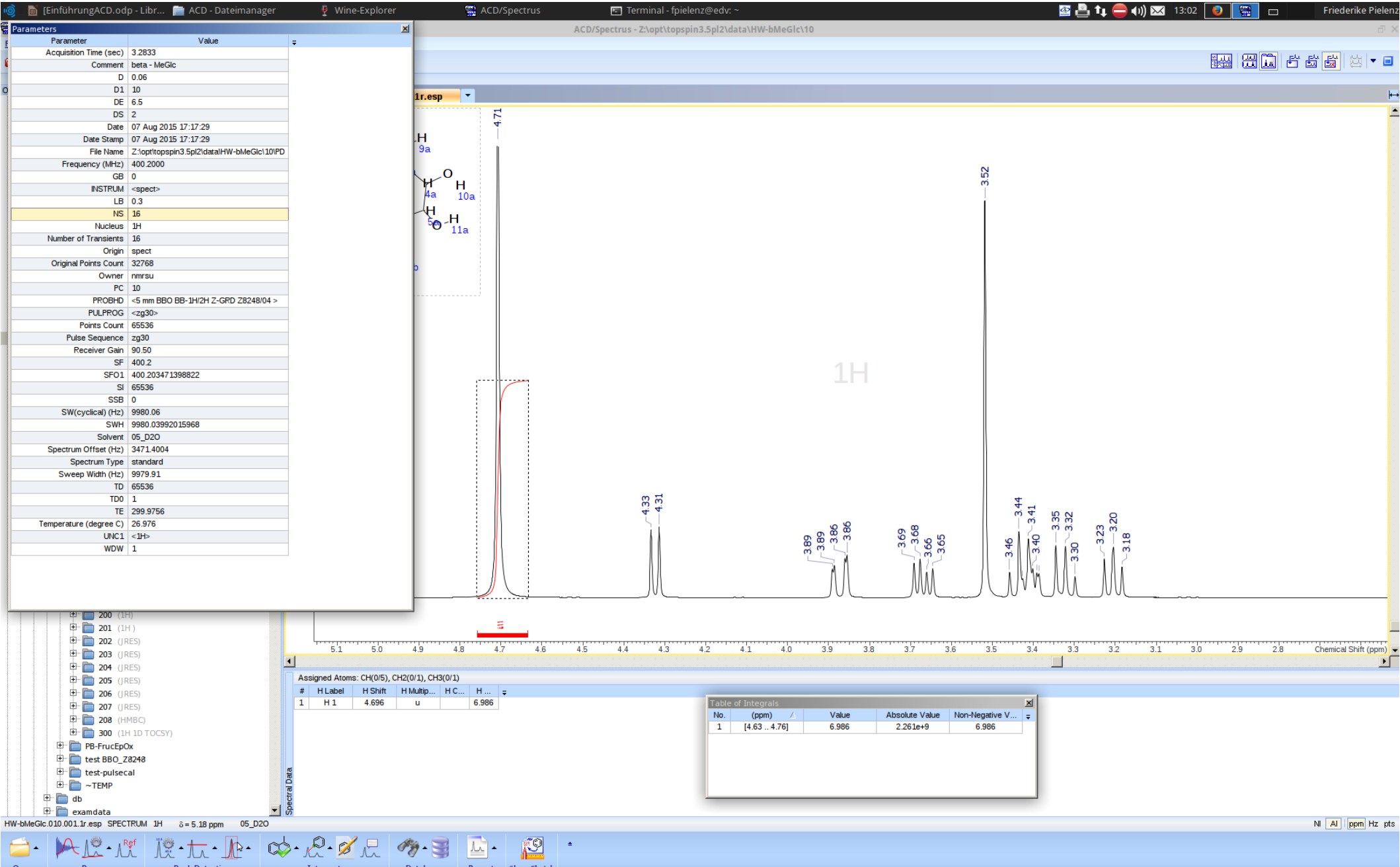
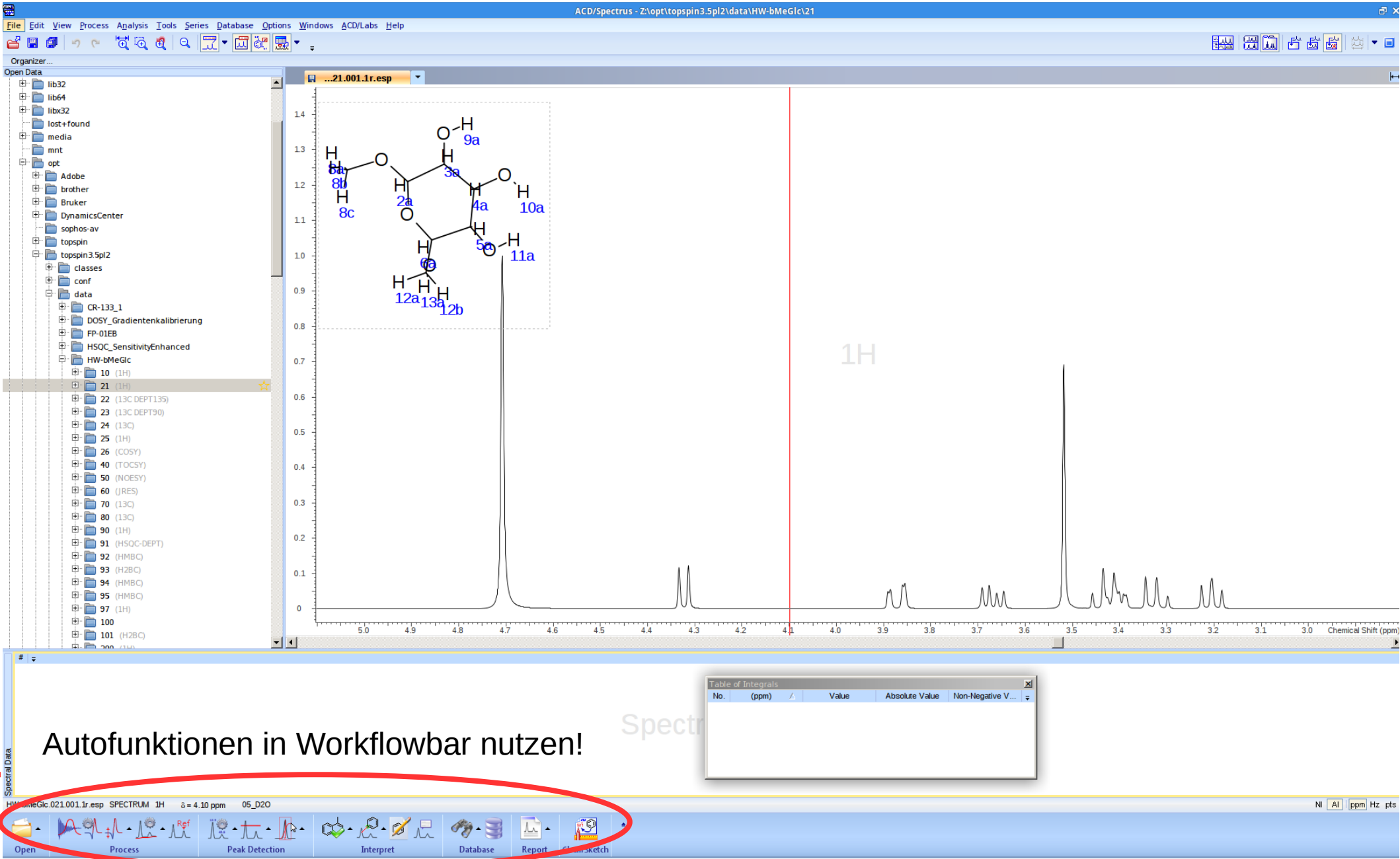


Aufnahmeparameter anzeigen



Idealfall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1H
Chemical Shift (ppm)
Table of Integrals
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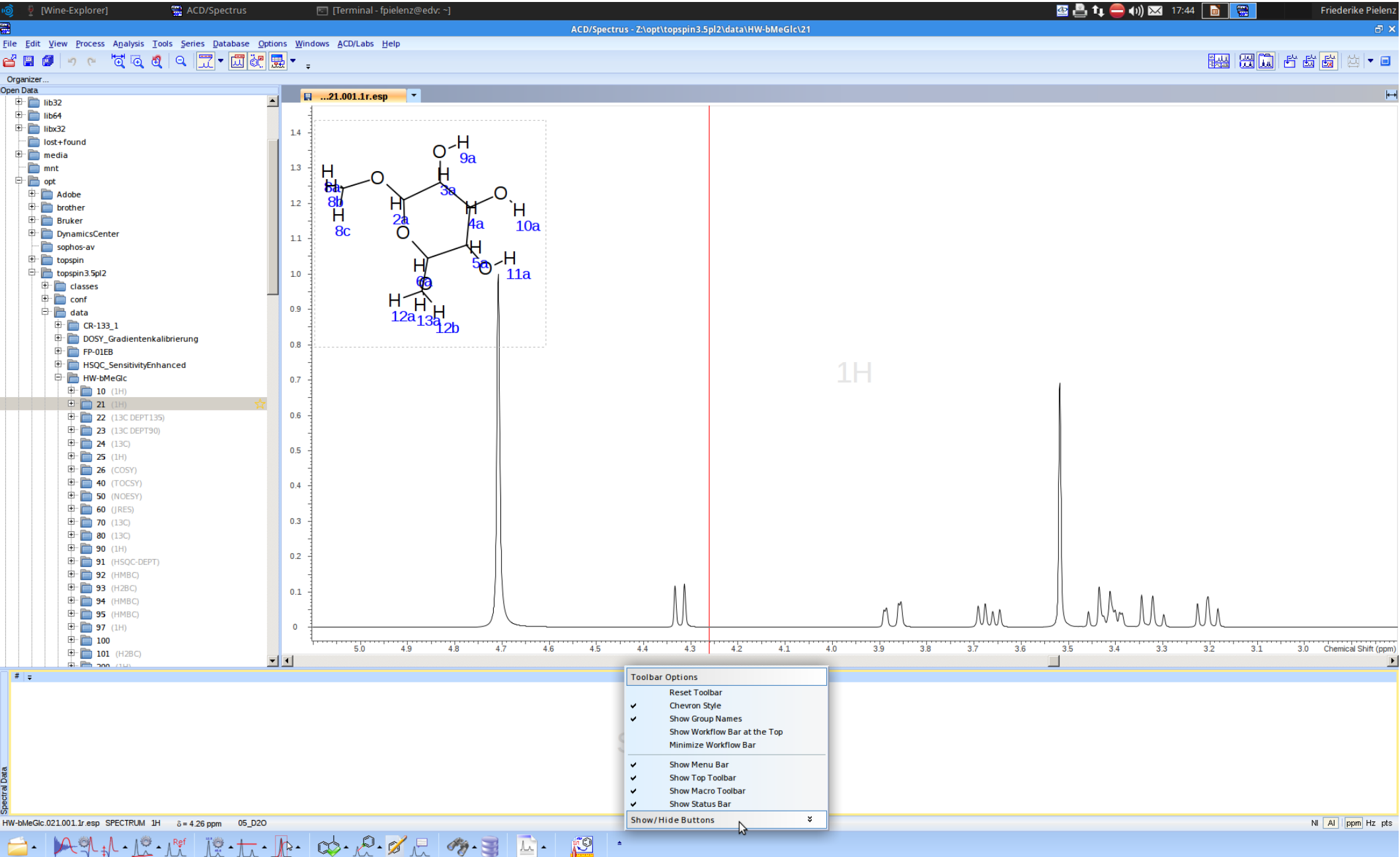
Open
Process
Peak Detection
Interpret
Database
Report

Idealfall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Friederike Pielenz
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Adobe
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Bruker
DynamicsCenter
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DOSY_Gradientenkalibrierung
FP-01EB
HSQC_SensitivityEnhanced
HW-bMeGlc
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21 (1H)
22 (13C DEPT135)
23 (13C DEPT90)
24 (13C)
25 (1H)
26 (COSY)
40 (TOCSY)
50 (NOESY)
60 (JRES)
70 (13C)
80 (13C)
90 (1H)
91 (HSQC-DEPT)
92 (HMBC)
93 (H2BC)
94 (HMBC)
95 (HMBC)
97 (1H)
100
101 (H2BC)
...21.001.1r.esp
1H
Chemical Shift (ppm)
Toolbar Options
Reset Toolbar
Chevron Style
Show Group Names
Show Workflow Bar at the Top
Minimize Workflow Bar
Show Menu Bar
Show Top Toolbar
Show Macro Toolbar
Show Status Bar
Show/Hide Buttons
Spectral Data
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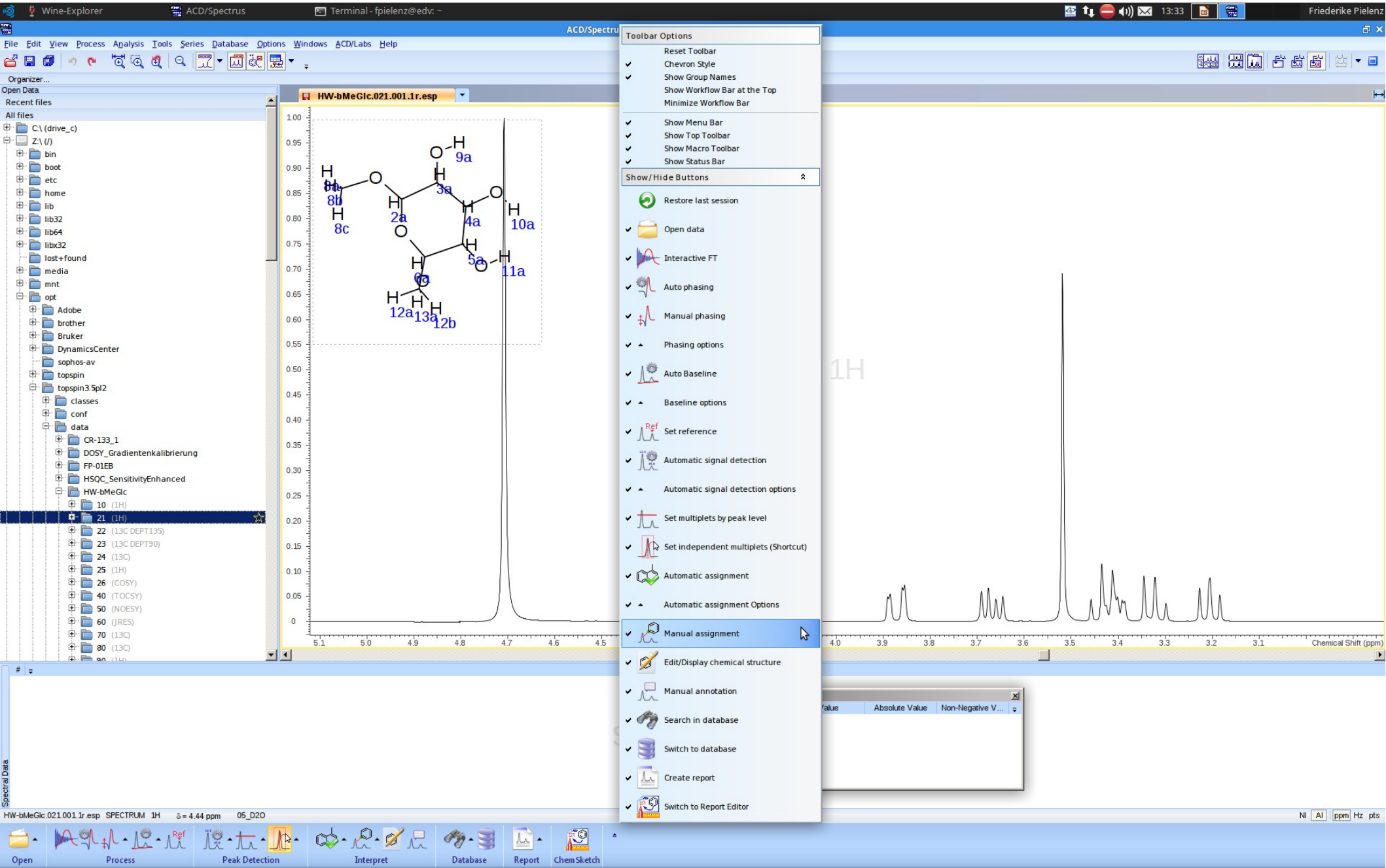
Idealfall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ACD/Spectrus
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All files
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Reset Toolbar
Chevron Style
Show Group Names
Show Workflow Bar at the Top
Minimize Workflow Bar
Show Menu Bar
Show Top Toolbar
Show Macro Toolbar
Show Status Bar
Show/Hide Buttons
Restore last session
Open data
Interactive FT
Auto phasing
Manual phasing
Phasing options
Auto Baseline
Baseline options
Set reference
Automatic signal detection
Automatic signal detection options
Set multiplets by peak level
Set independent multiplets (Shortcut)
Automatic assignment
Automatic assignment Options
Manual assignment
Edit/Display chemical structure
Manual annotation
Search in database
Switch to database
Create report
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Open
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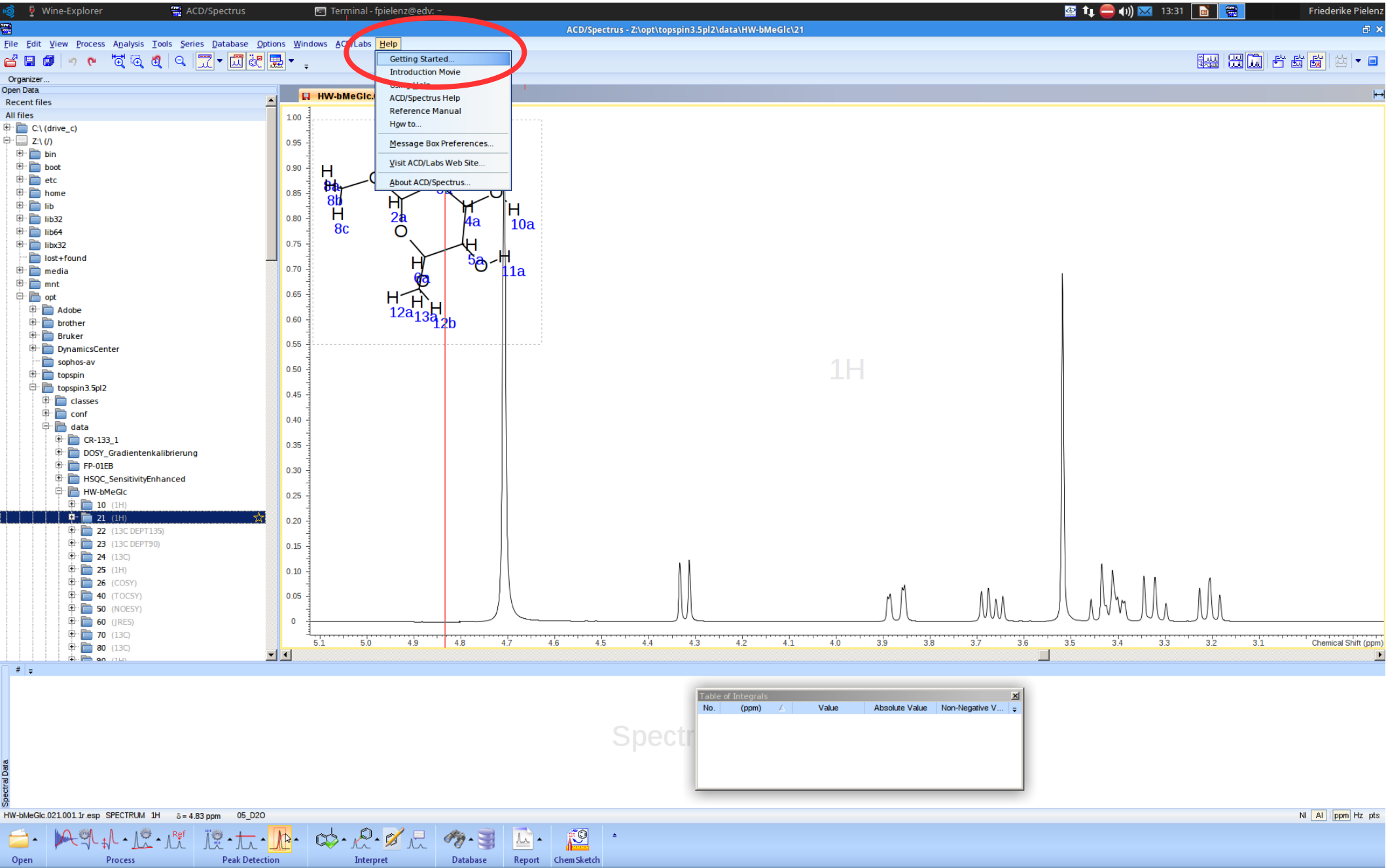
Interpret
Database
Report
ChemSketch

Idealfall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Getting Started...
Introduction Movie
ACD/Spectrus Help
Reference Manual
How to...
Message Box Preferences...
Visit ACD/Labs Web Site...
About ACD/Spectrus...
Organizer...
Open Data
Recent files
All files
HW-bMeGlc
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Table of Integrals
No.
(ppm)
Value
Absolute Value
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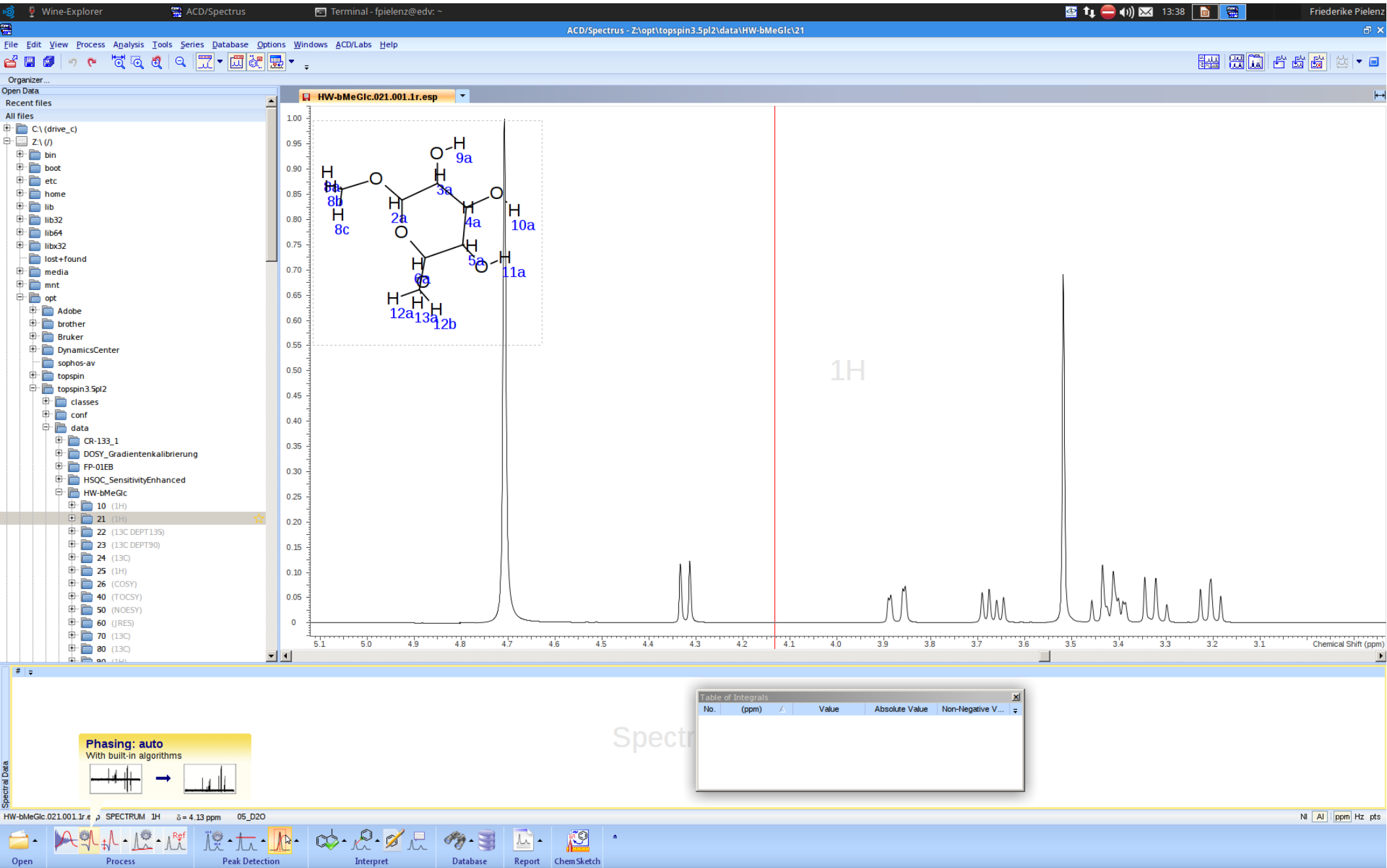
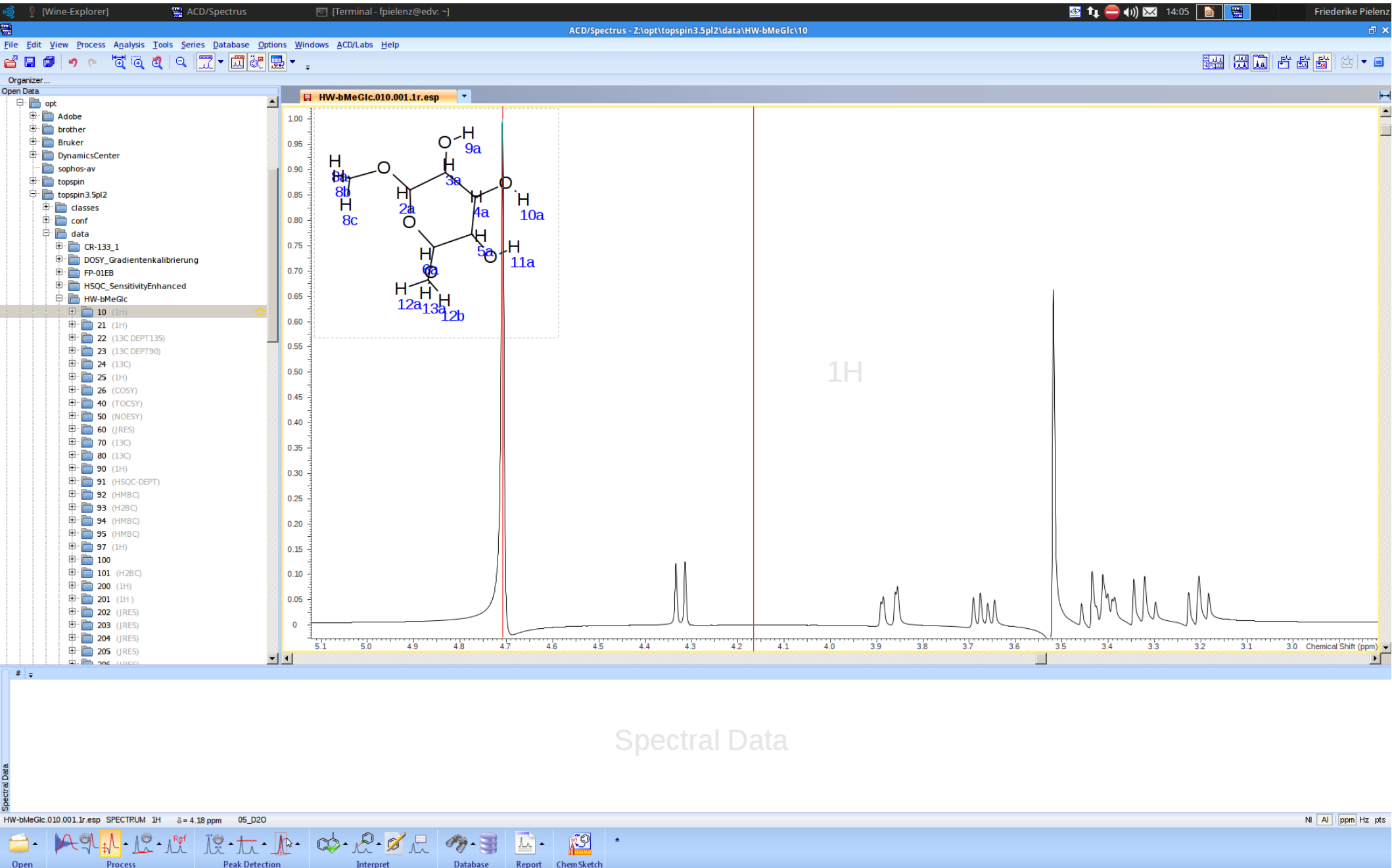
Spectral Data
HW-bMeGlc.021.001.1r.esp SPECTRUM 1H δ = 4.83 ppm 05_D2O
Open
Process
Peak Detection
Interpret
Database
Report
ChemSketch

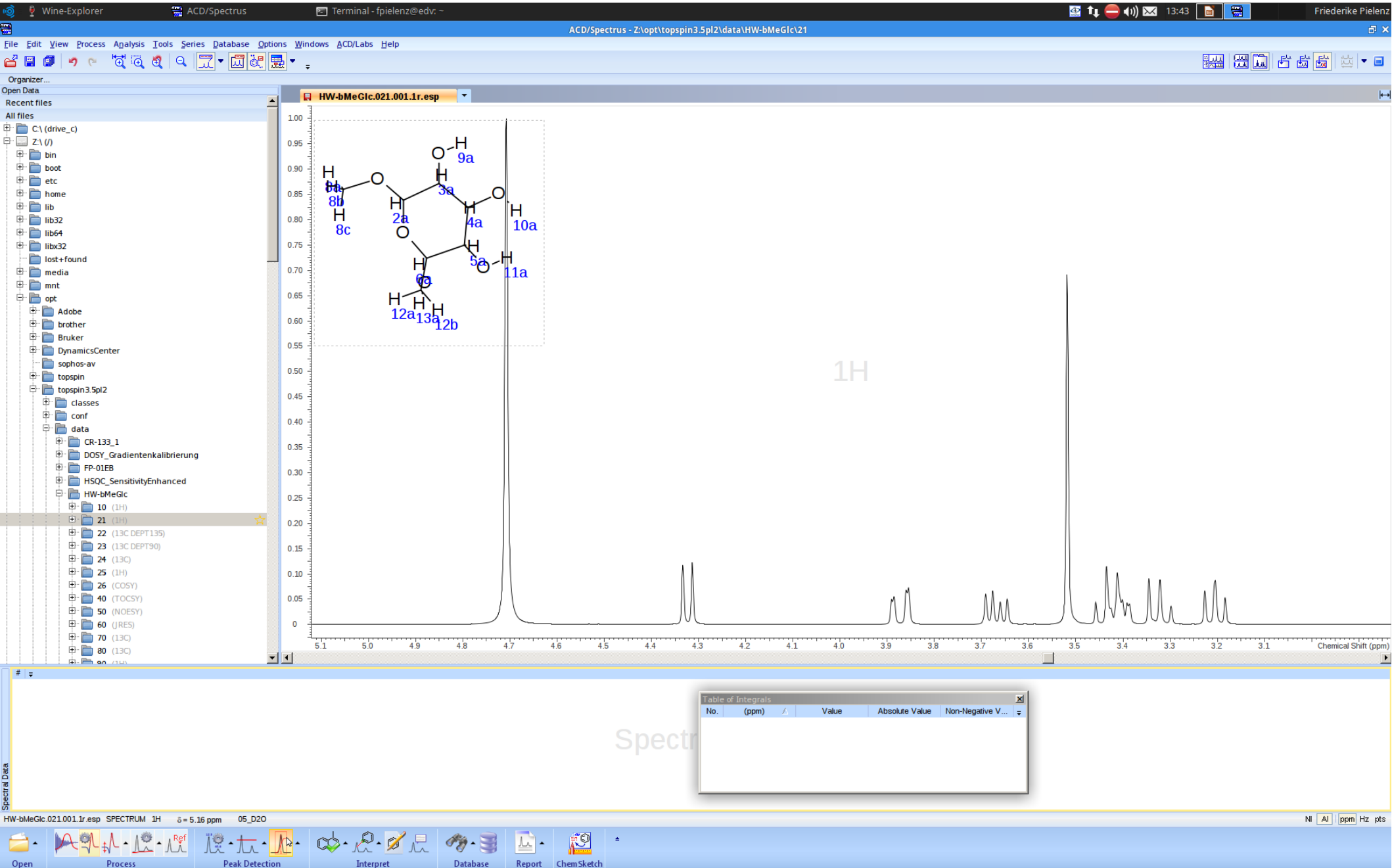
Idealfall – Phase korrigieren



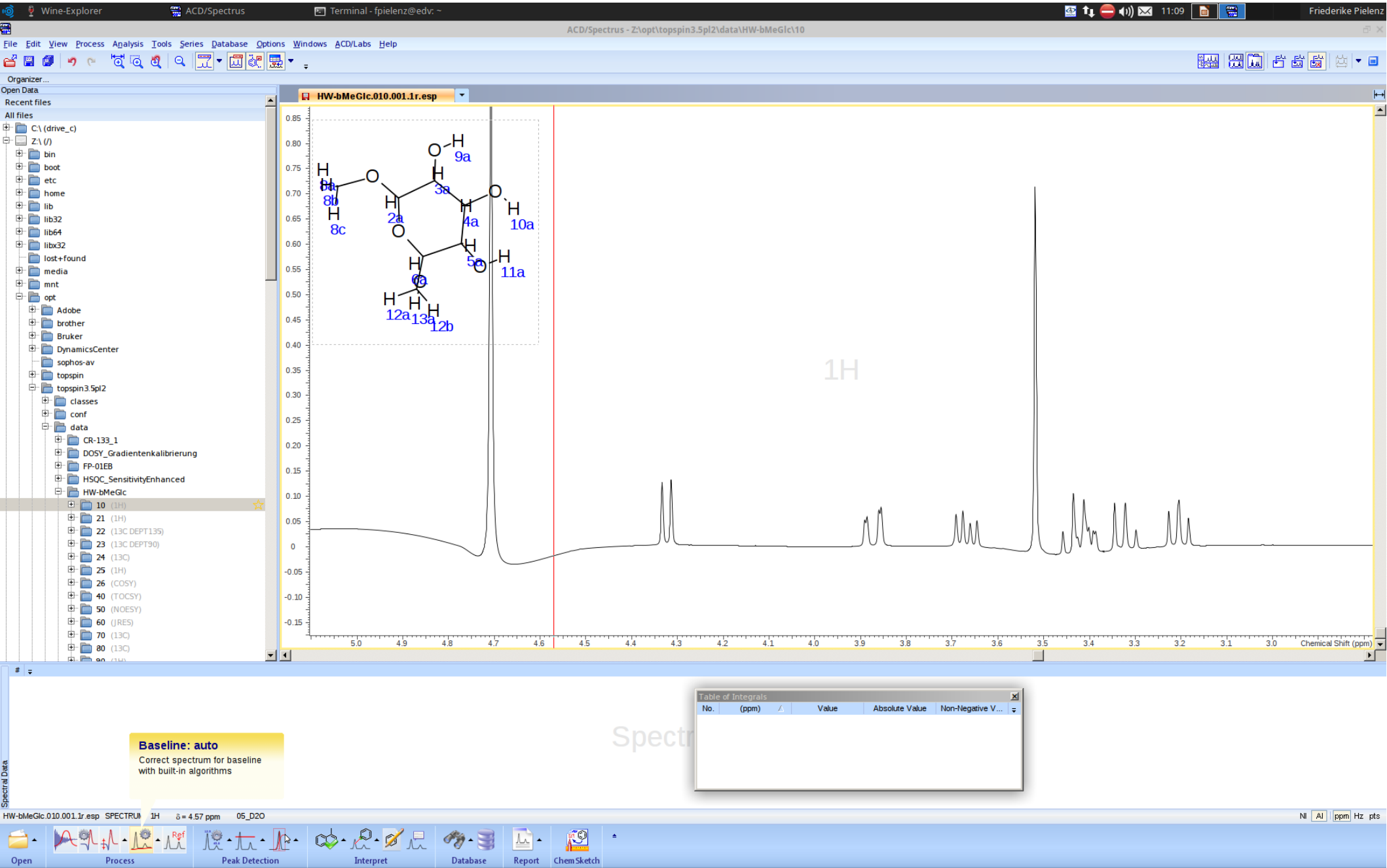
Idealfall – Phase korrigieren



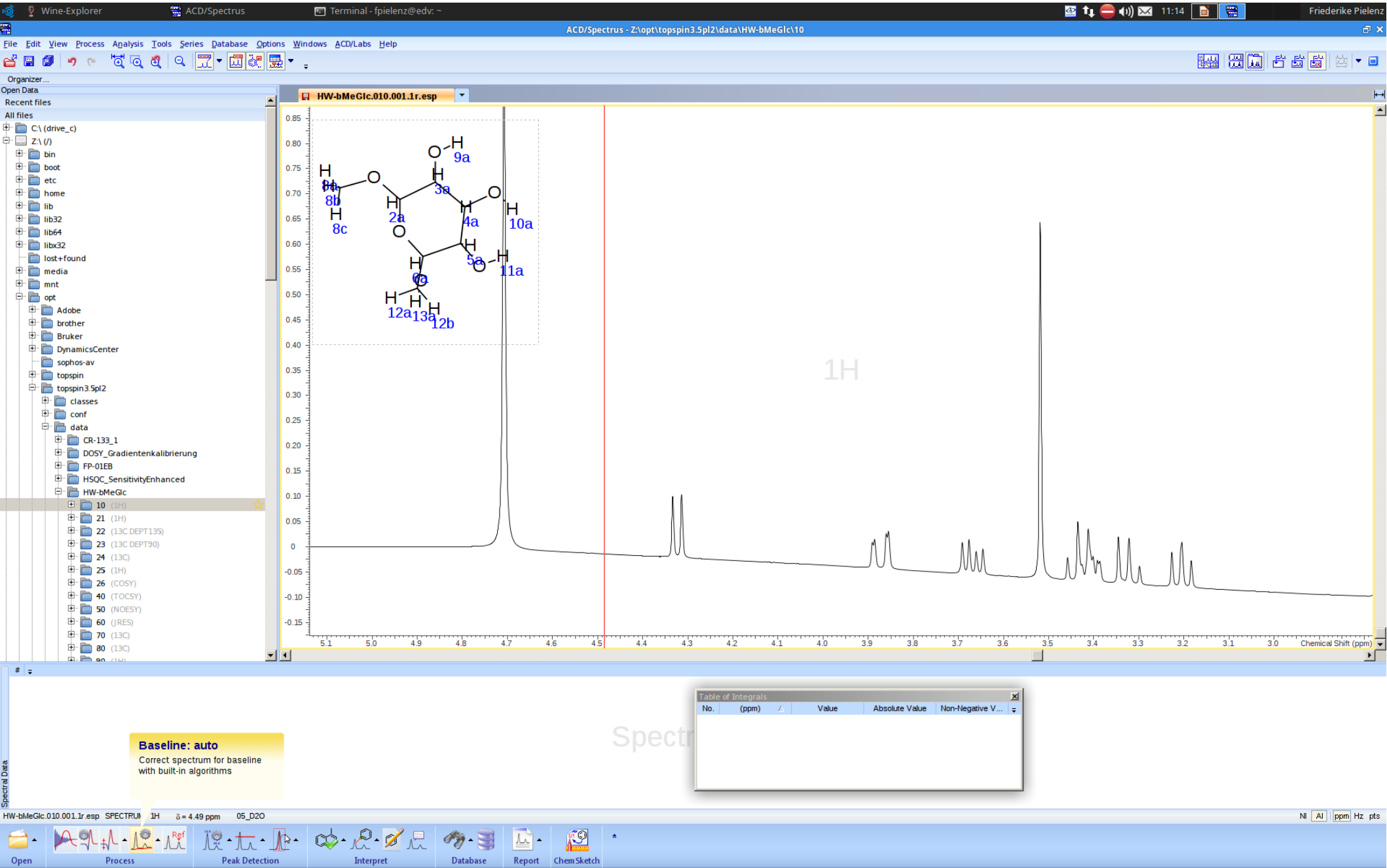
Idealfall – Phase korrigieren



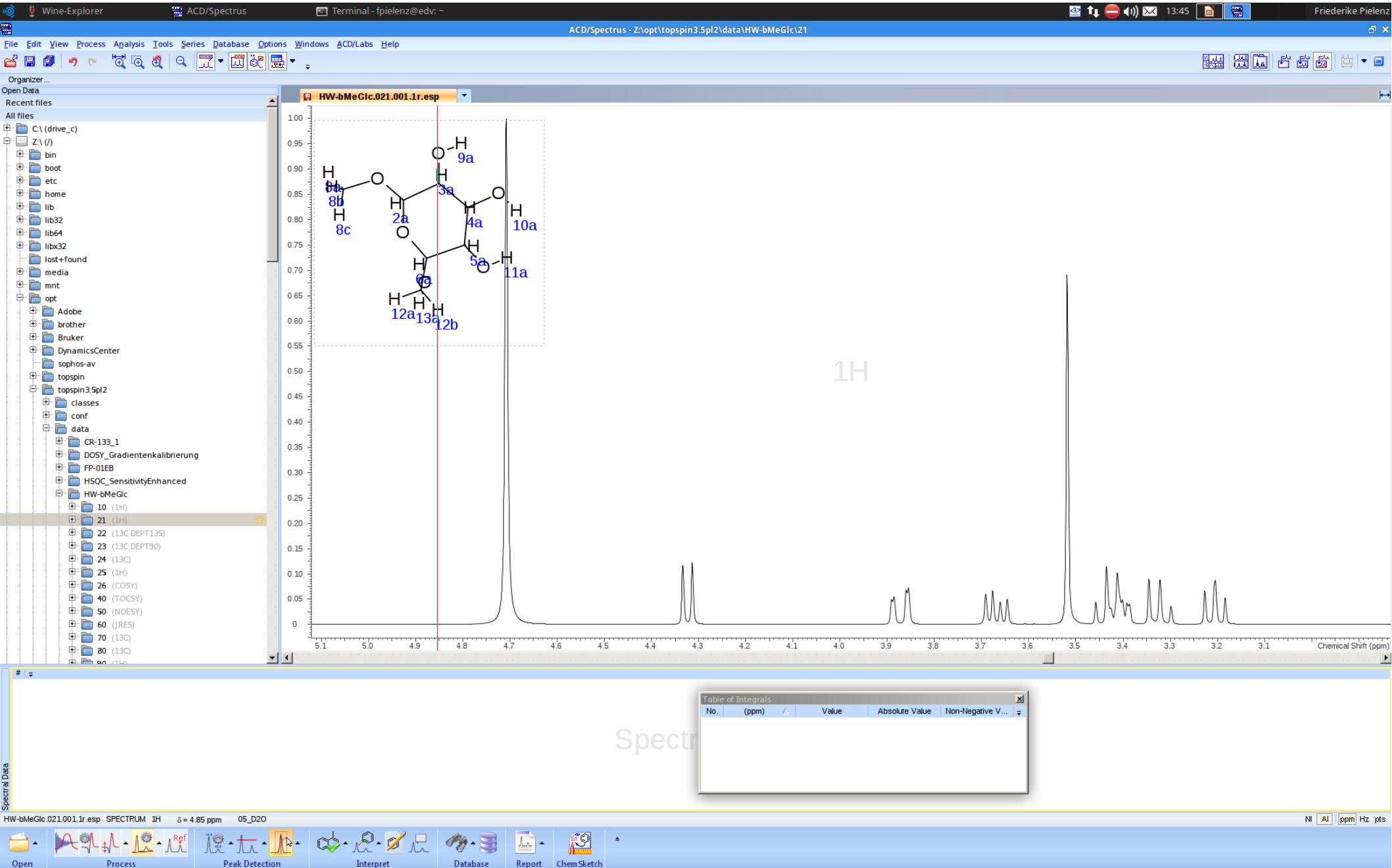
Idealfall – Basislinie korrigieren



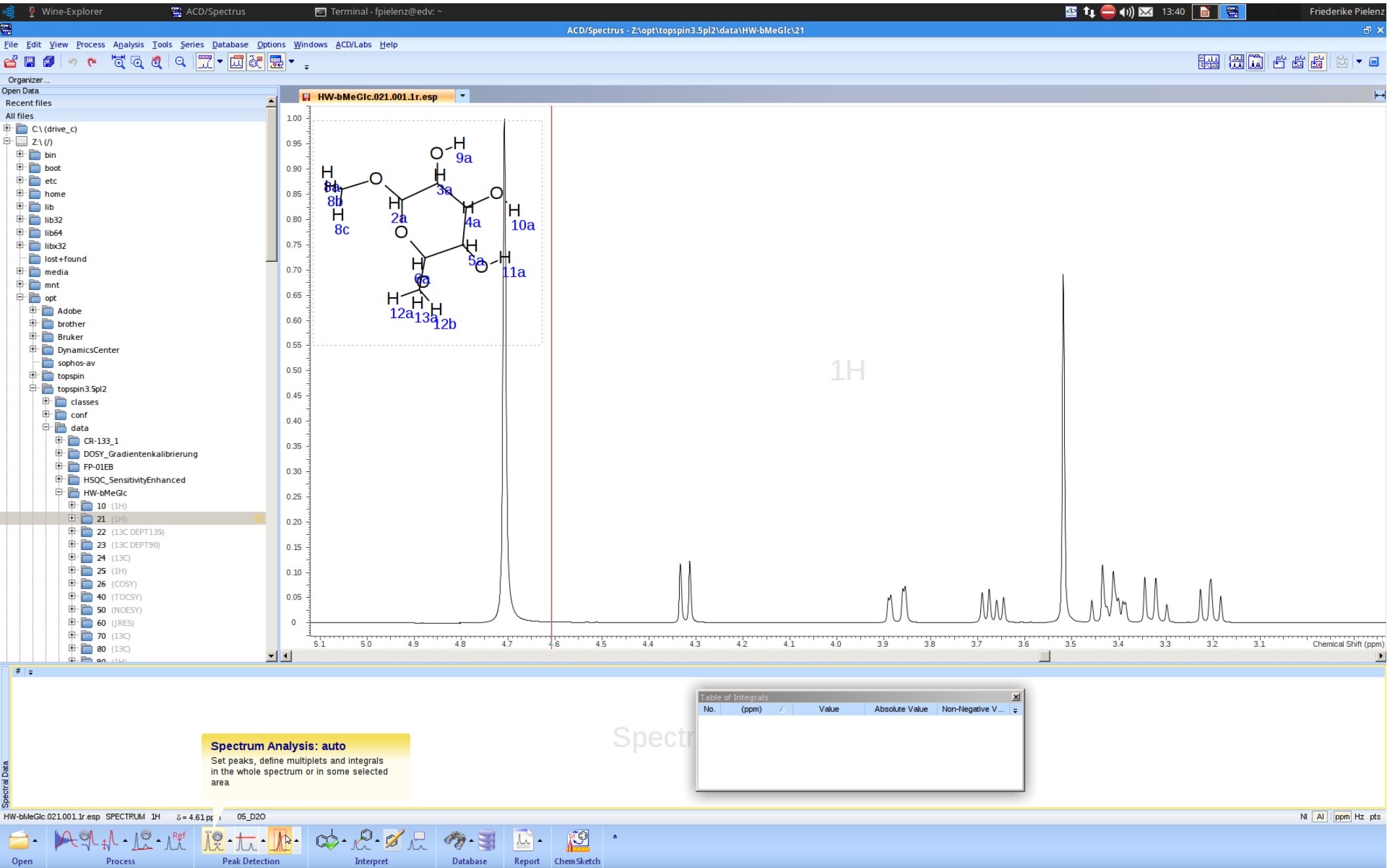
Idealfall – Basislinie korrigieren



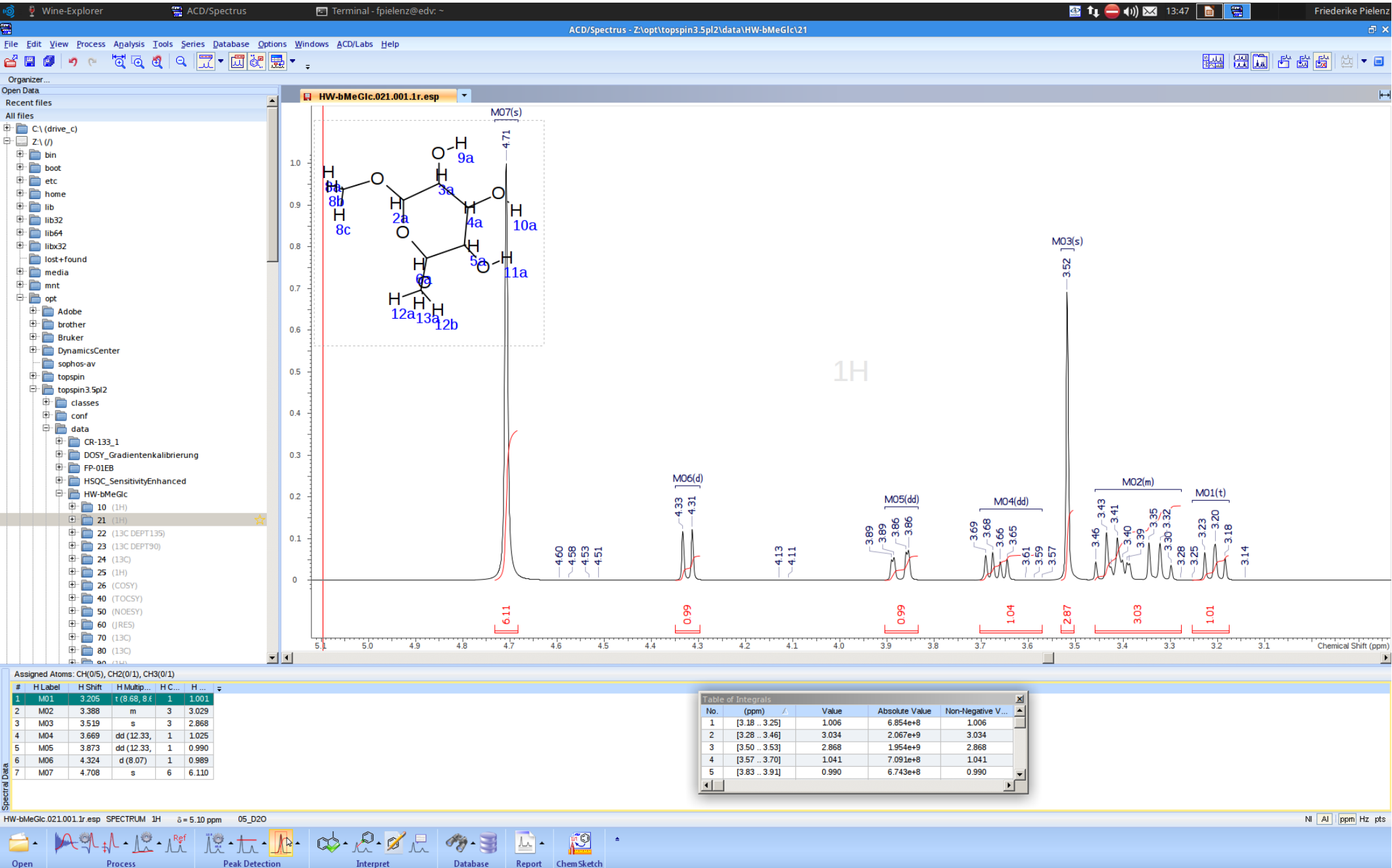
Idealfall – Basislinie korrigieren



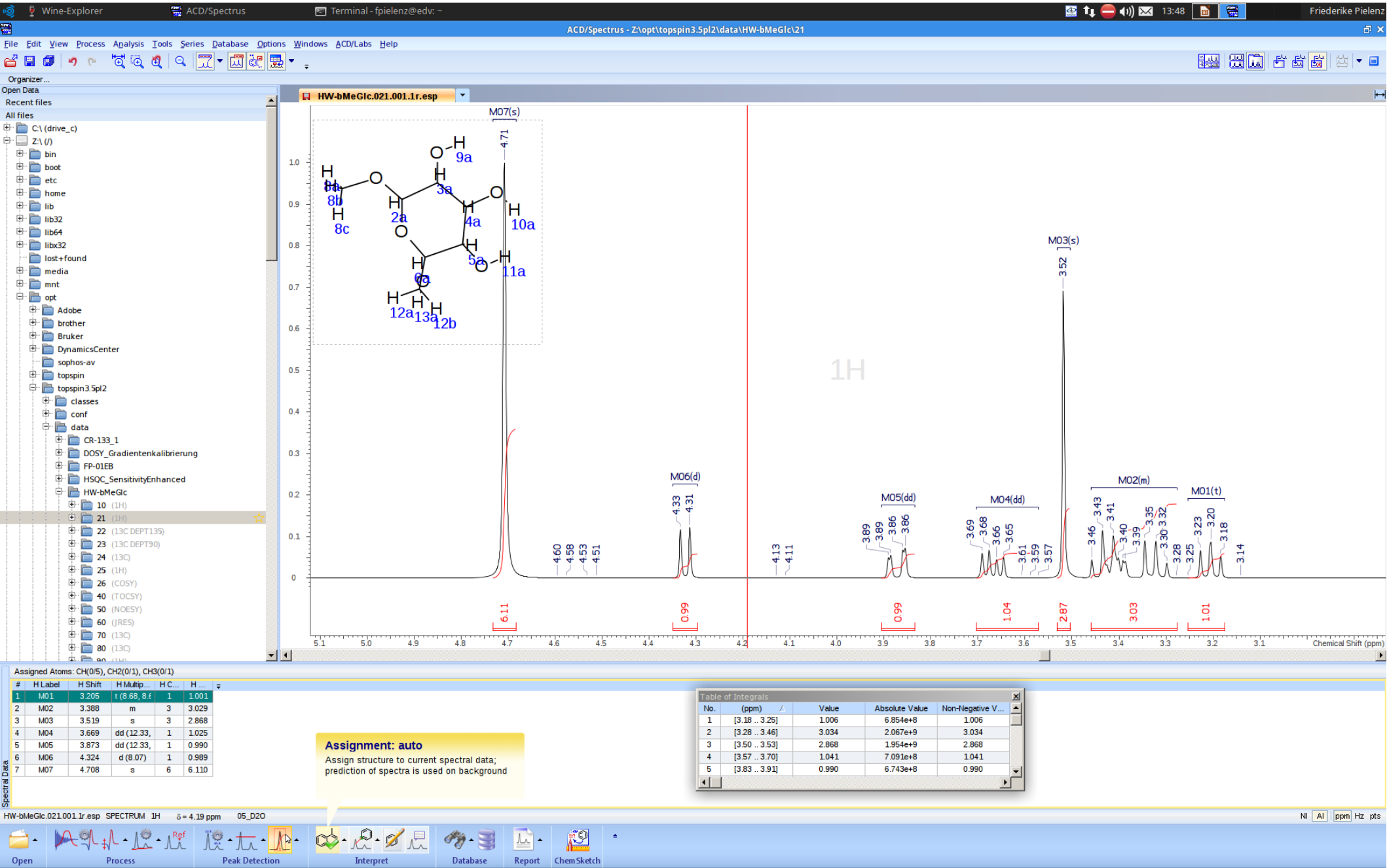
Idealfall - Spektrenanalyse



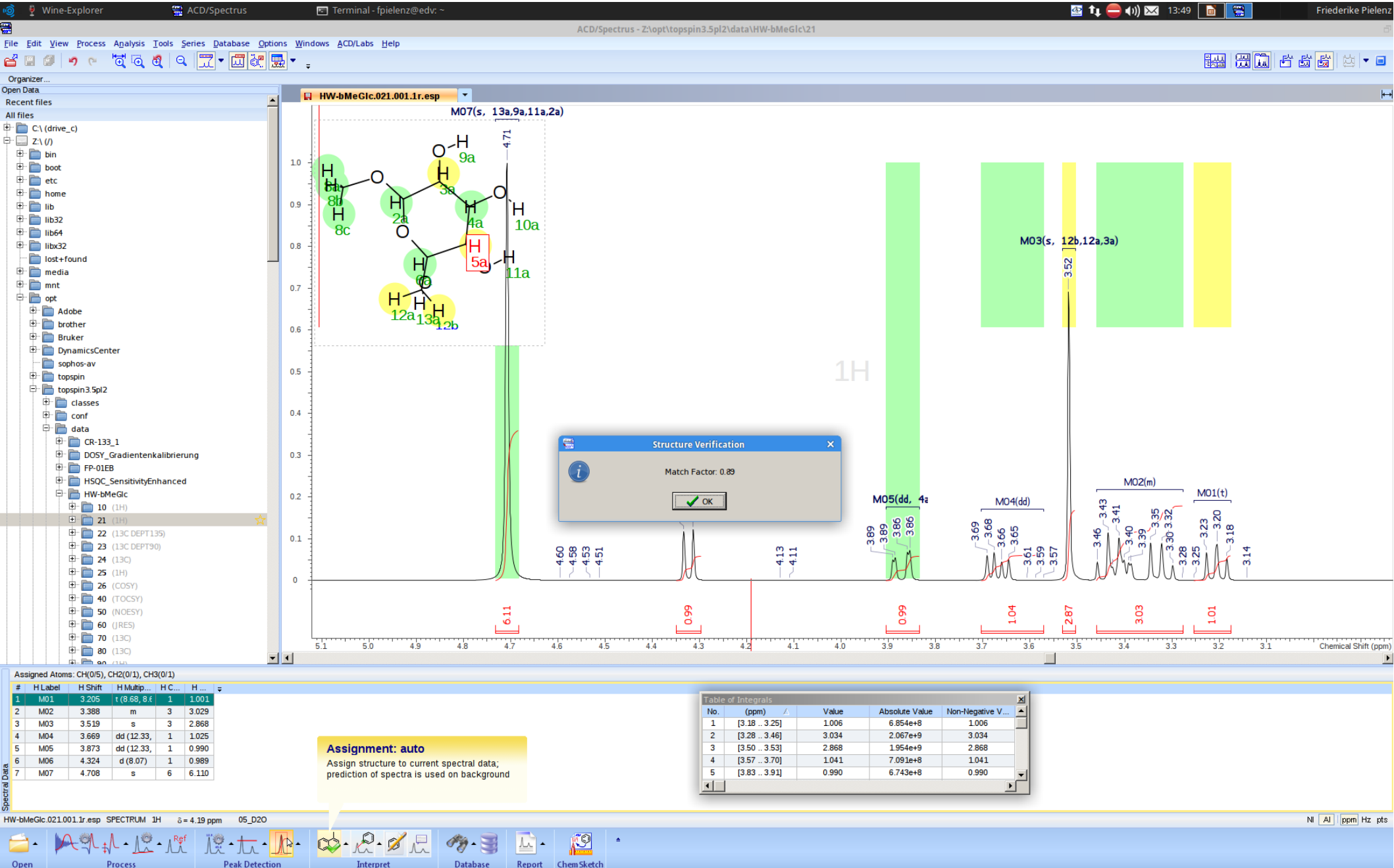
Idealfall - Spektrenanalyse



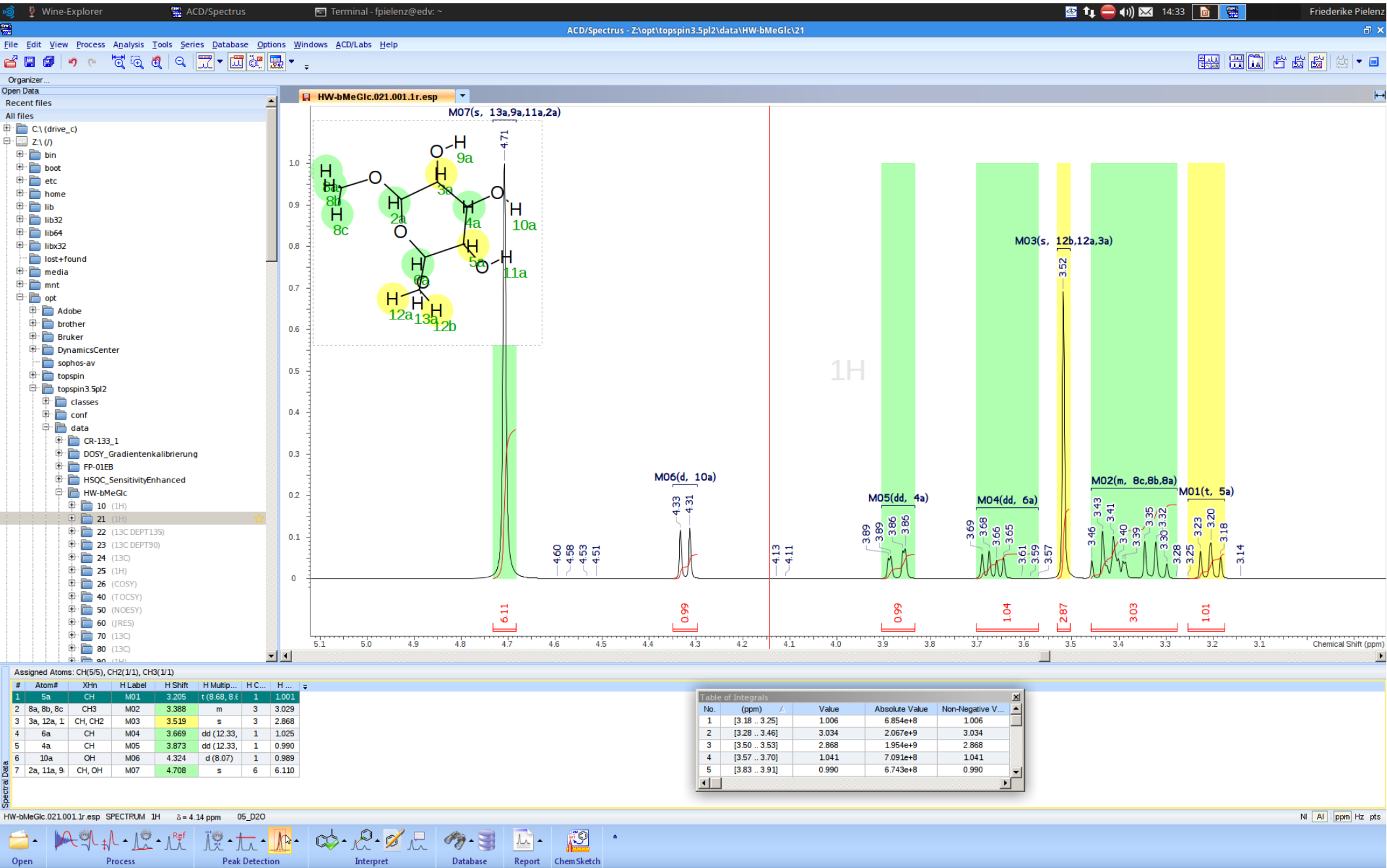
Idealfall - Peakzuordnung



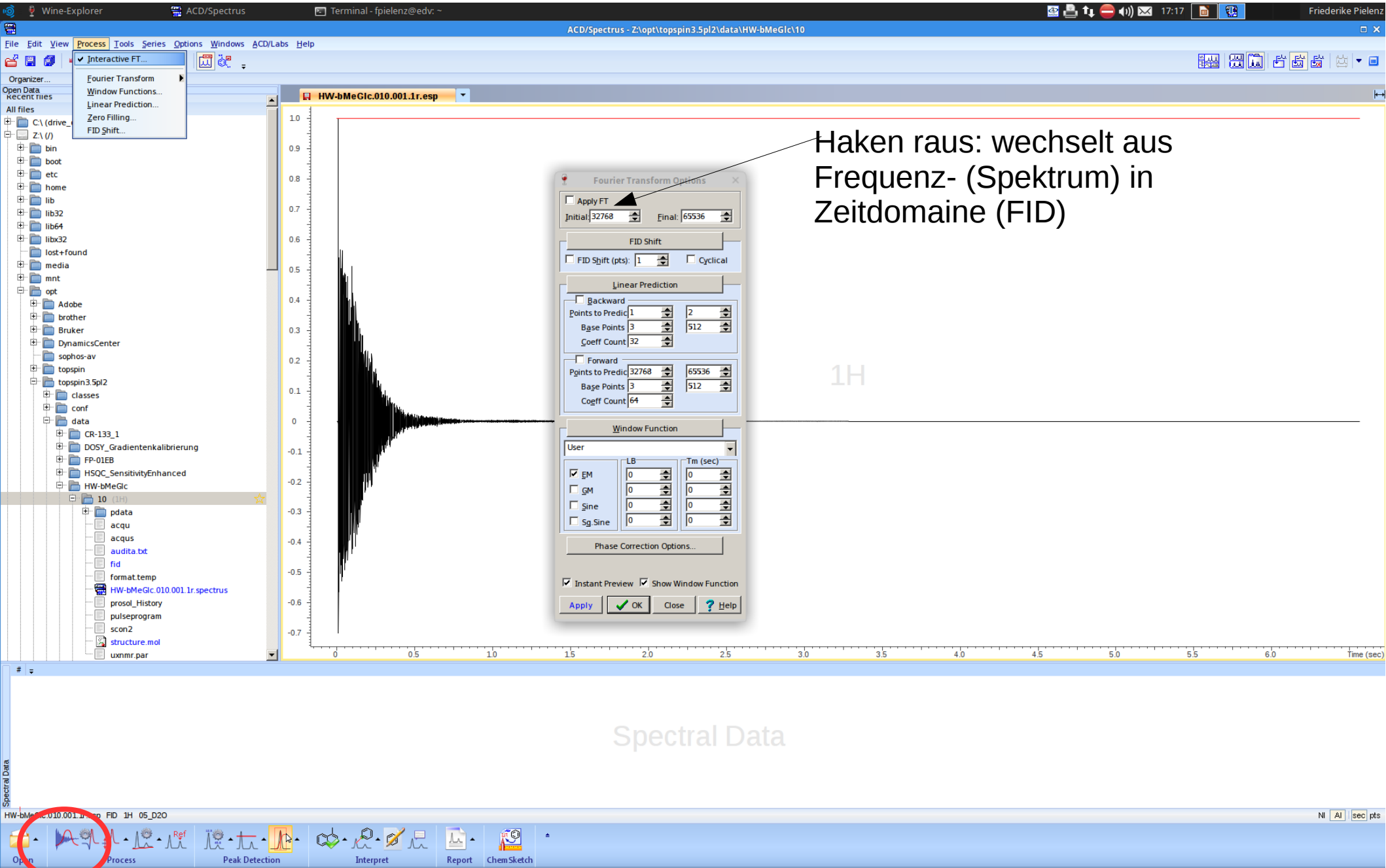
Idealfall – Peakzuordnung prüfen



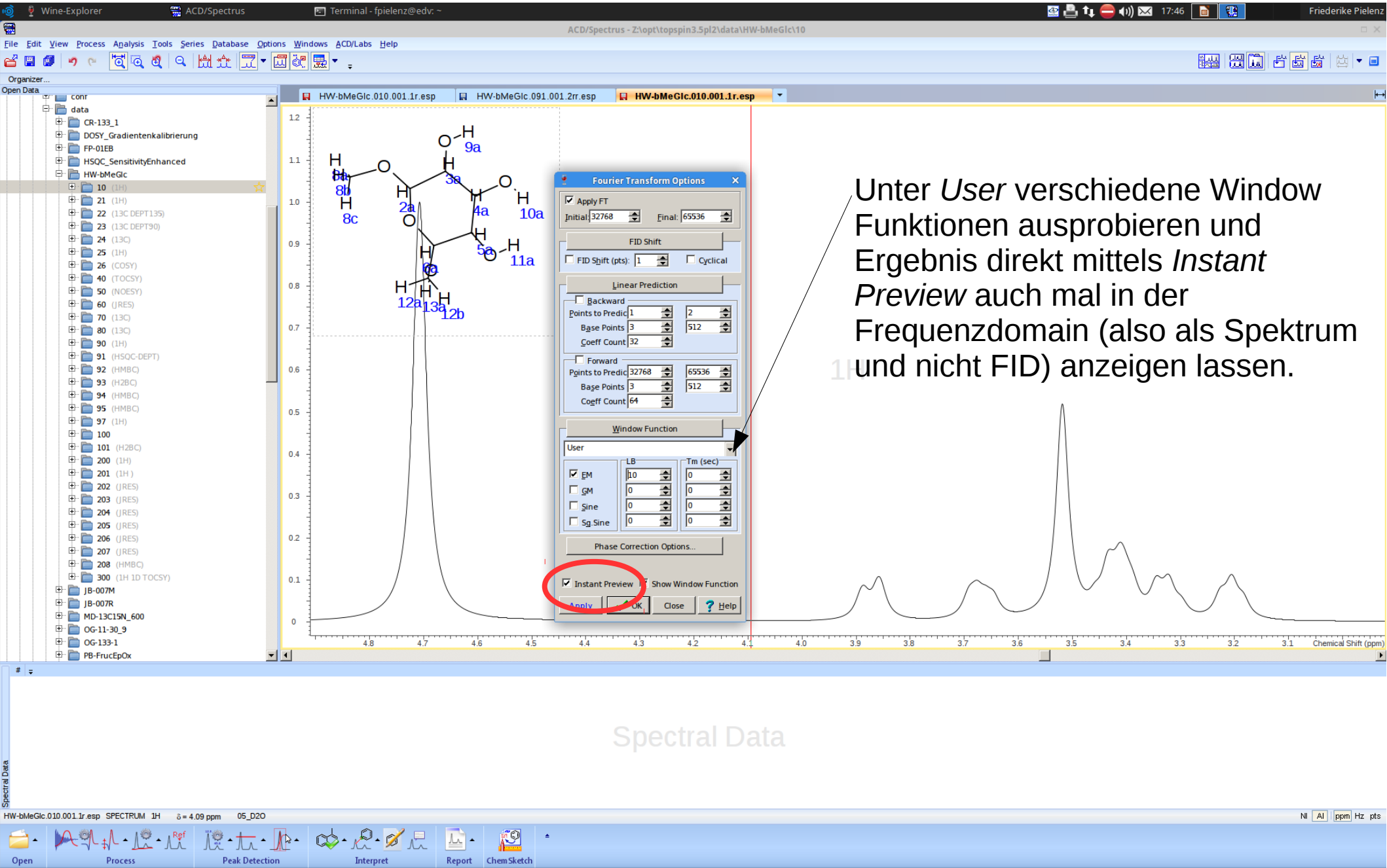
Idealfall – FERTIG!



Vor der FT: Window Funktionen

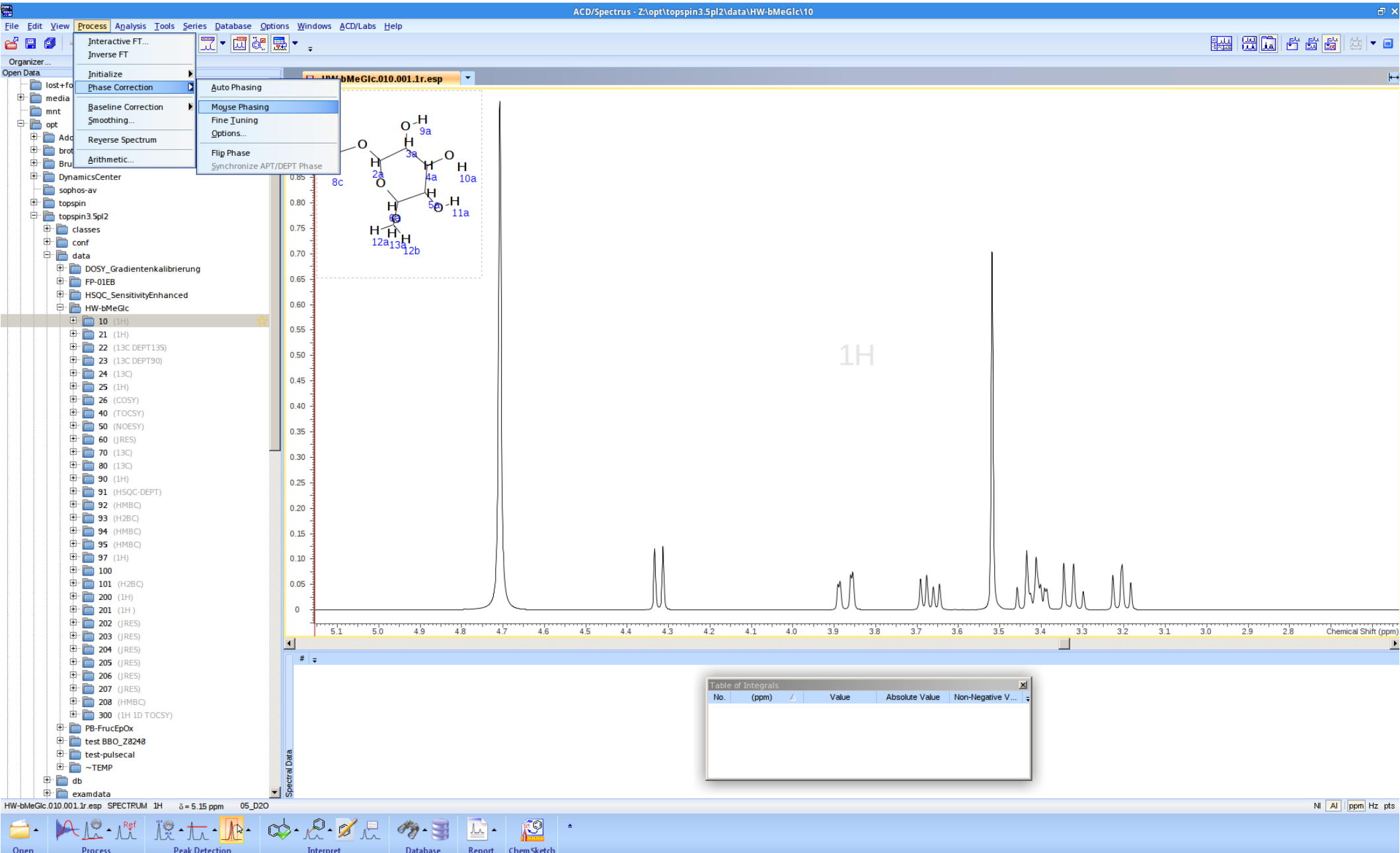


Vor der FT: Window Funktionen

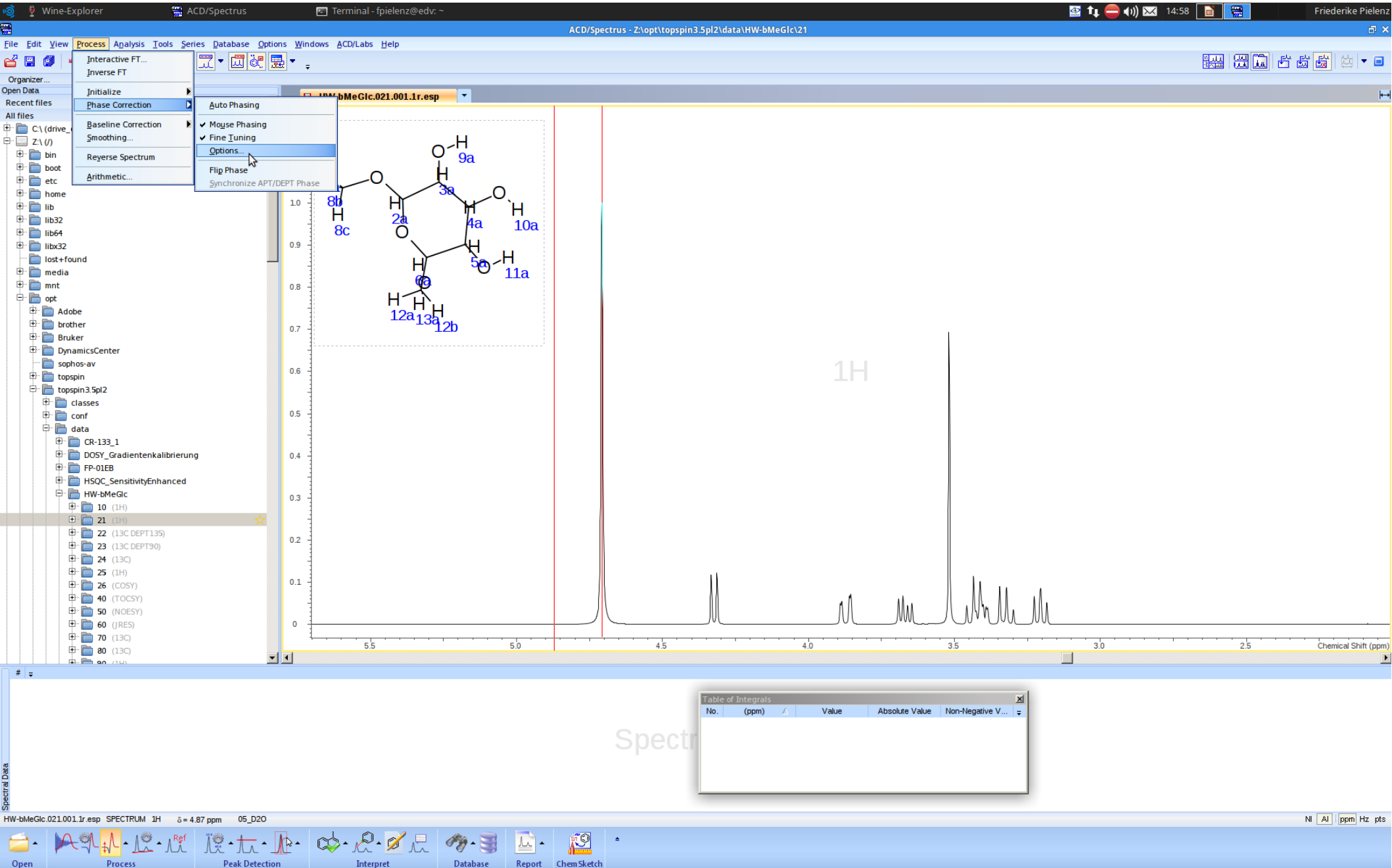


Unter *User* verschiedene Window Funktionen ausprobieren und Ergebnis direkt mittels *Instant Preview* auch mal in der Frequenzdomain (also als Spektrum und nicht FID) anzeigen lassen.

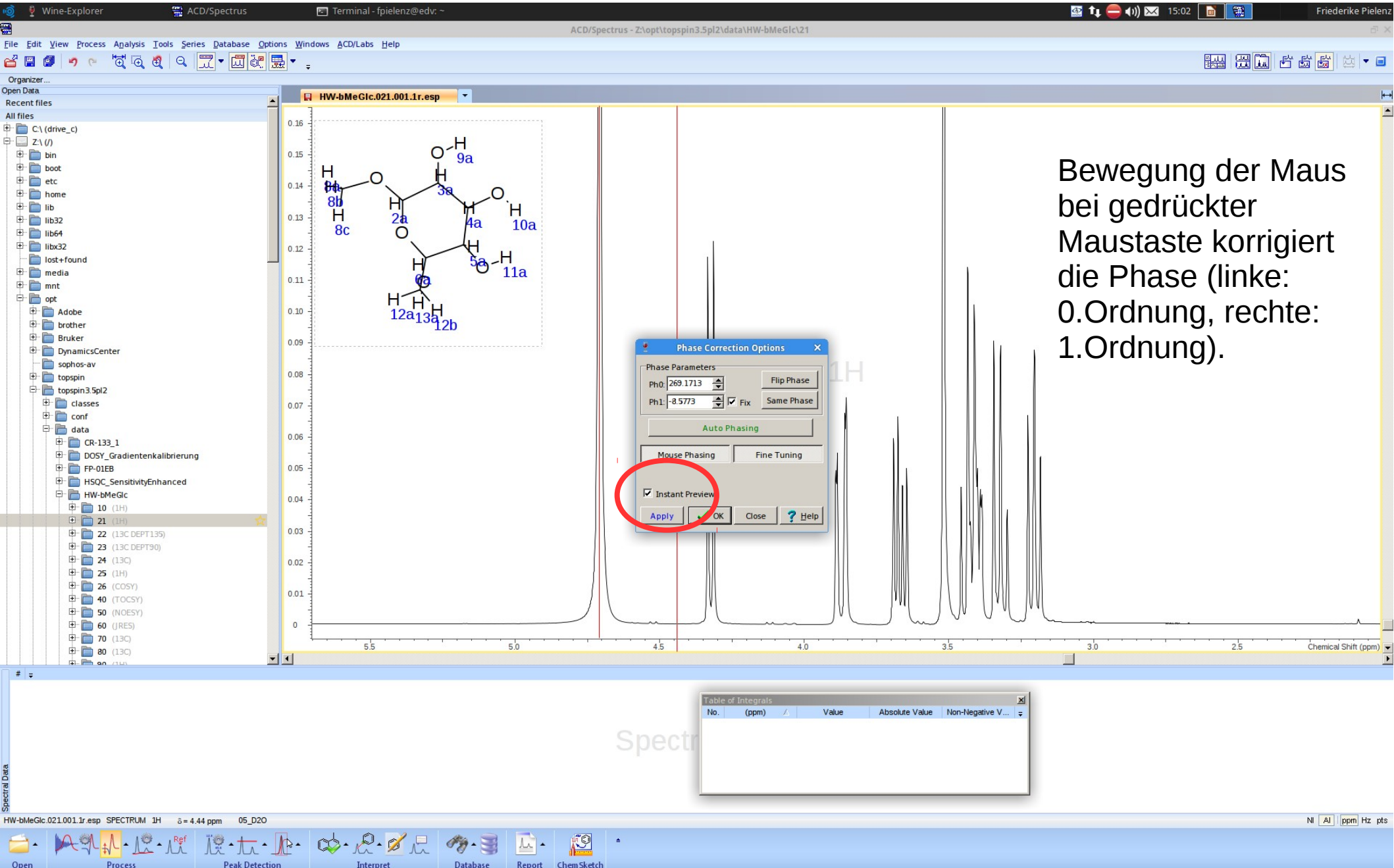
Phase korrigieren



Phase korrigieren

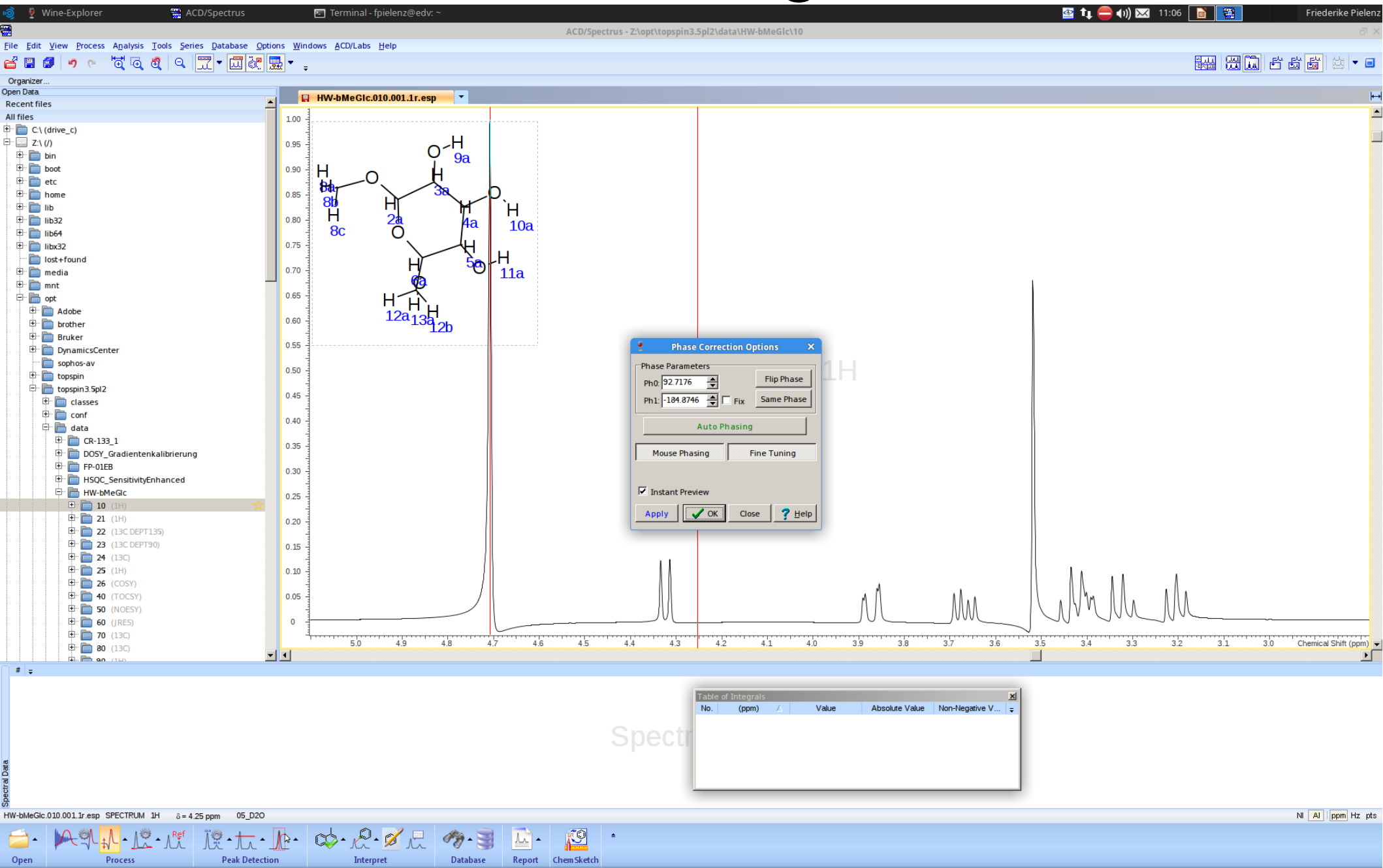


Phase korrigieren

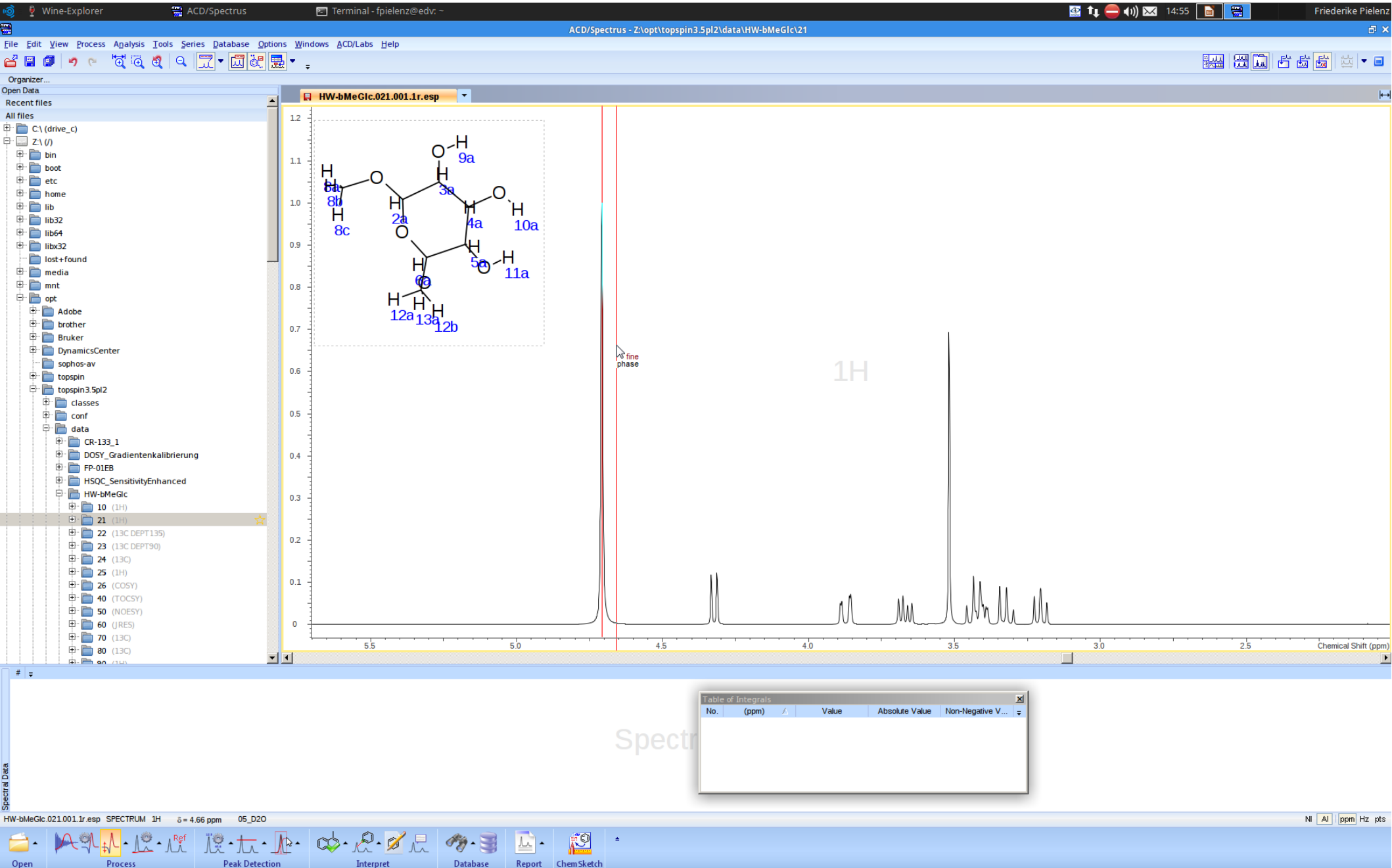


Bewegung der Maus bei gedrückter Maustaste korrigiert die Phase (linke: 0.Ordnung, rechte: 1.Ordnung).

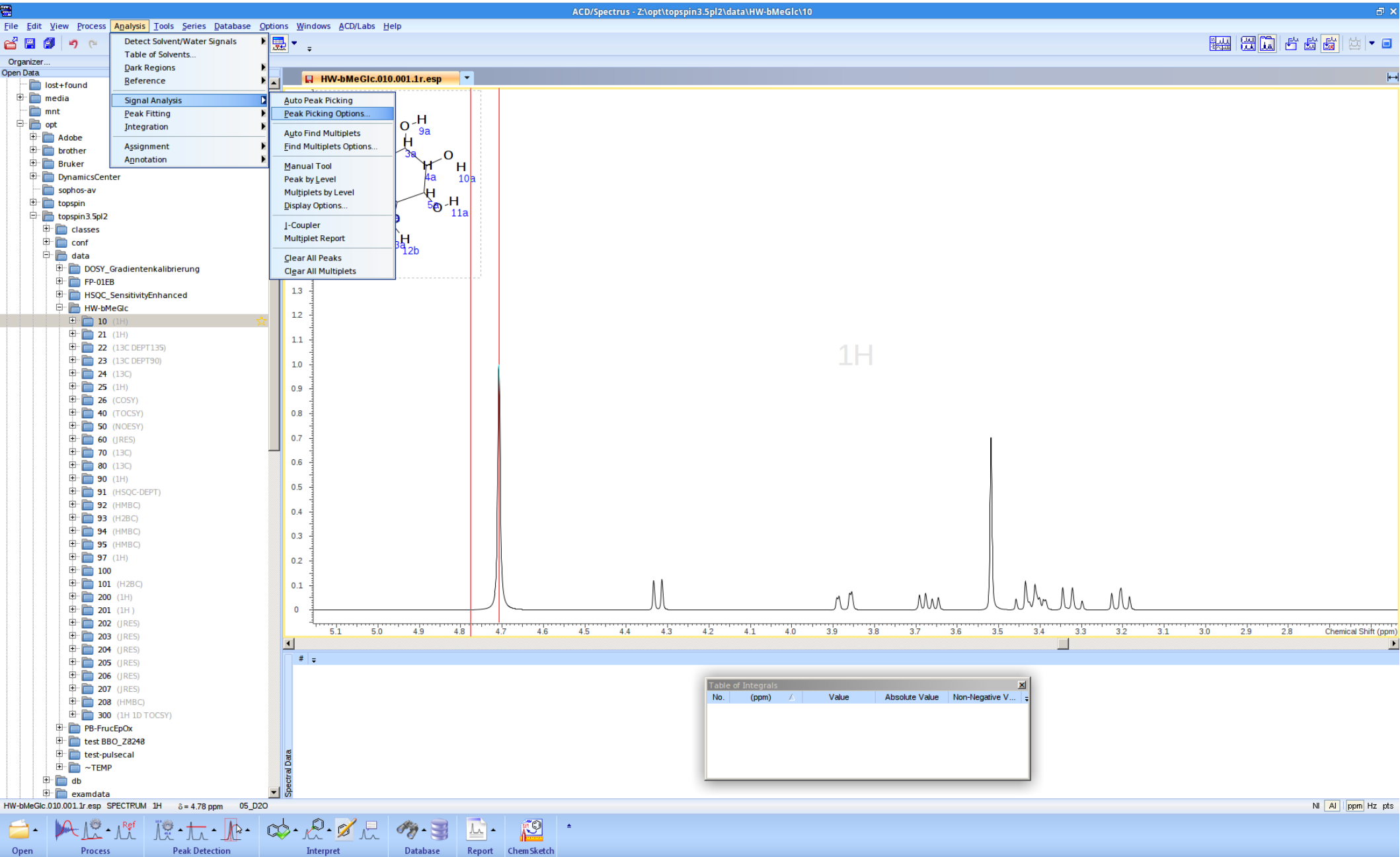
Phase korrigieren



Phase korrigieren



„Peak Picking“



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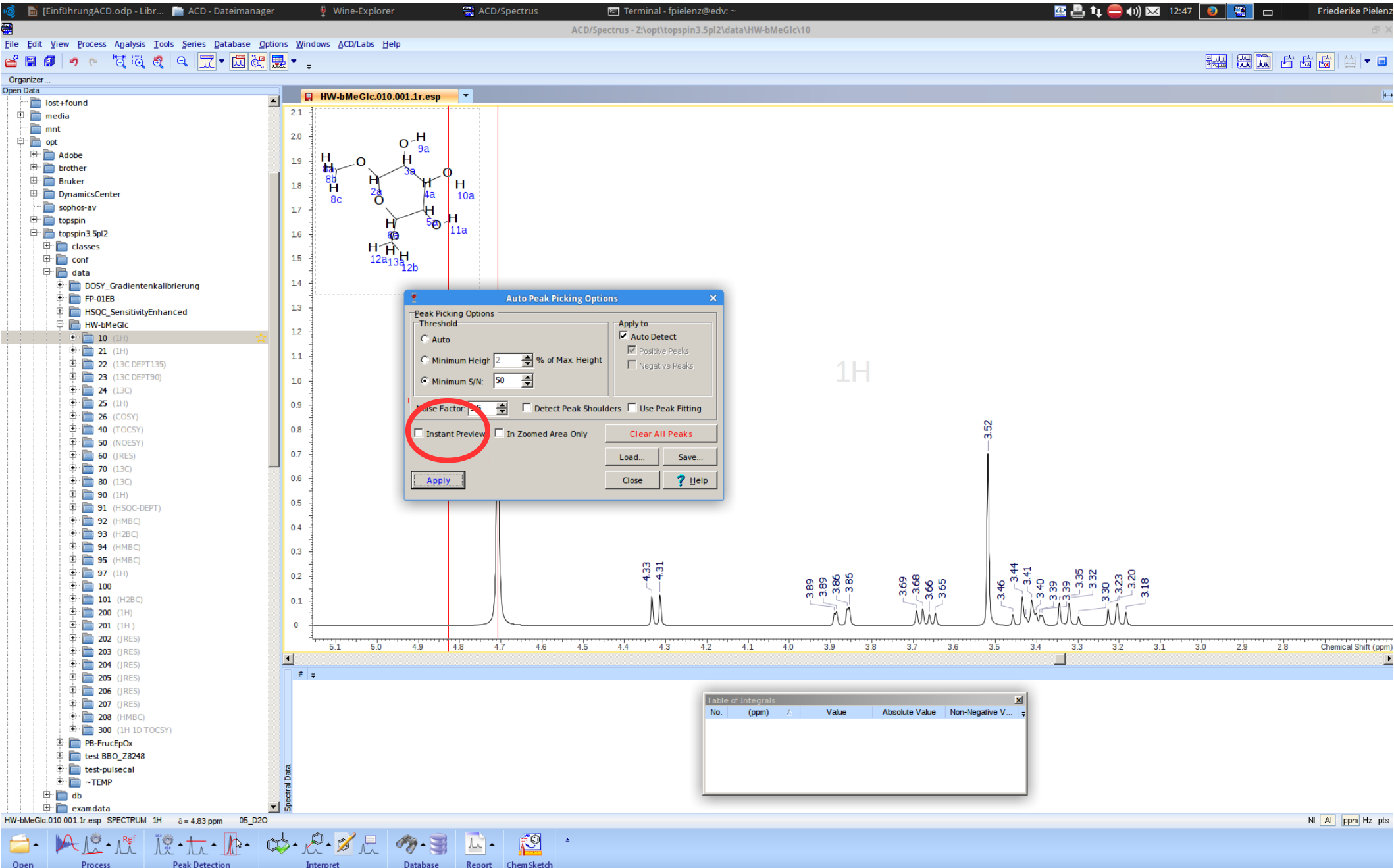
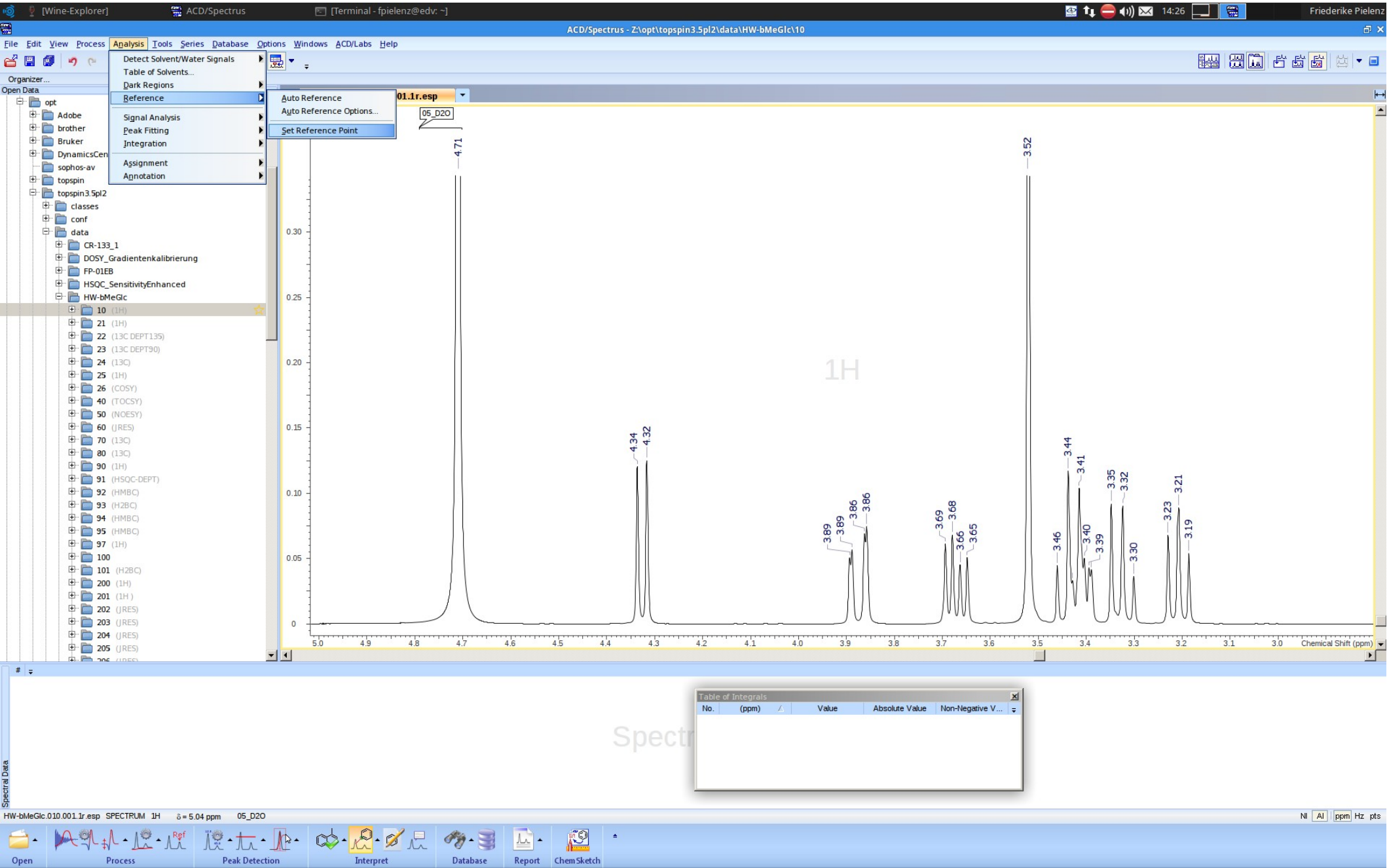
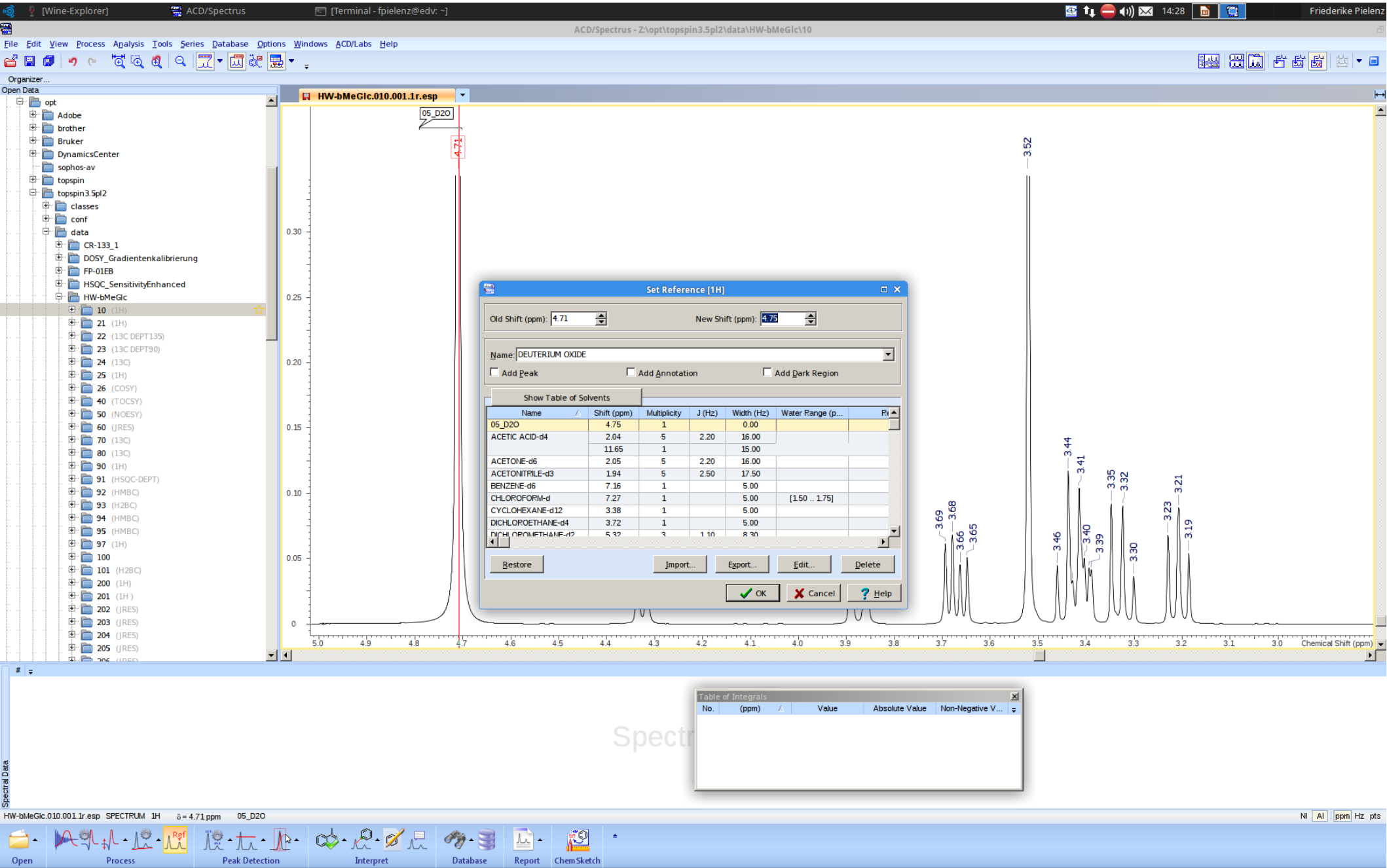


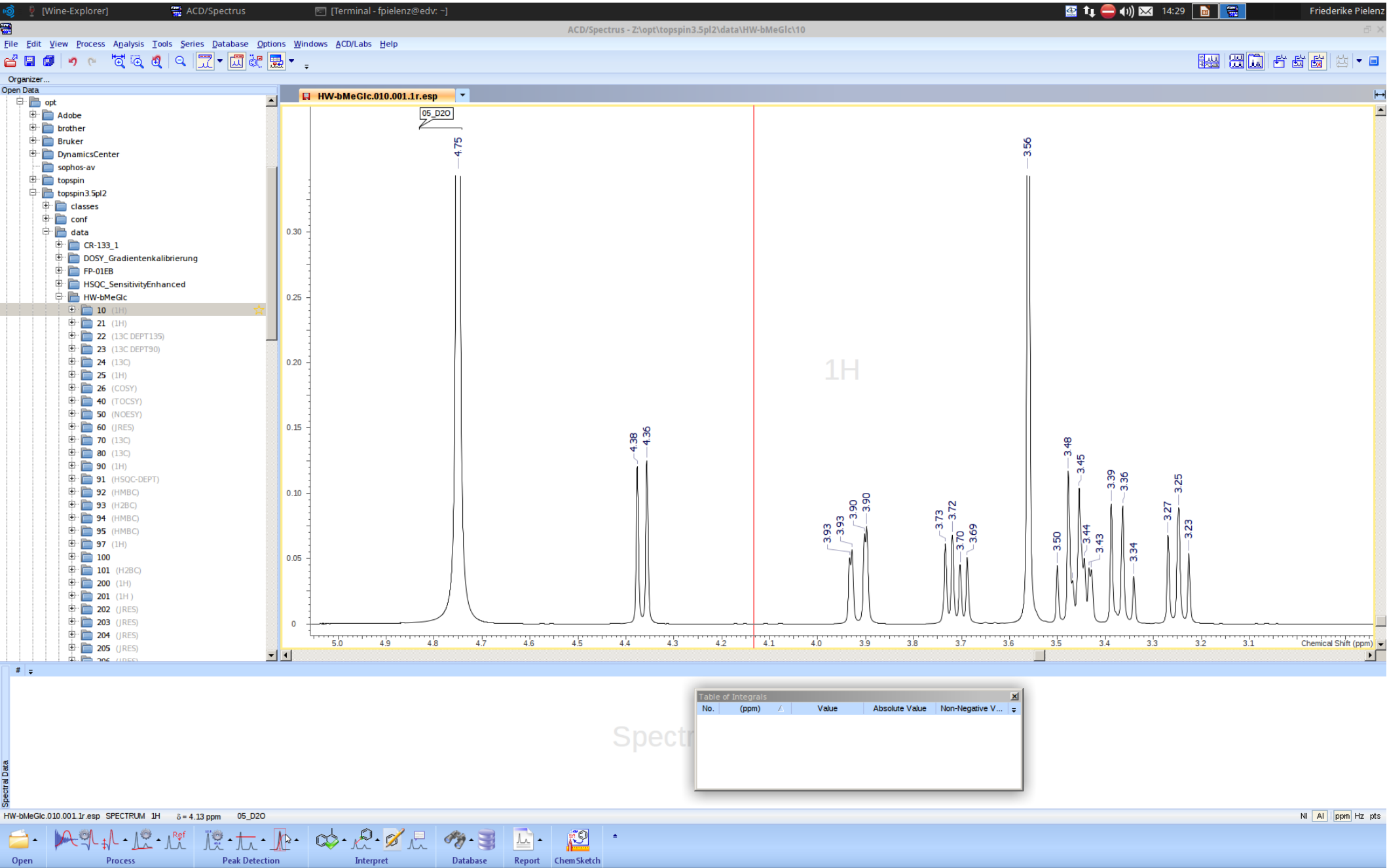
Peakshift kalibrieren



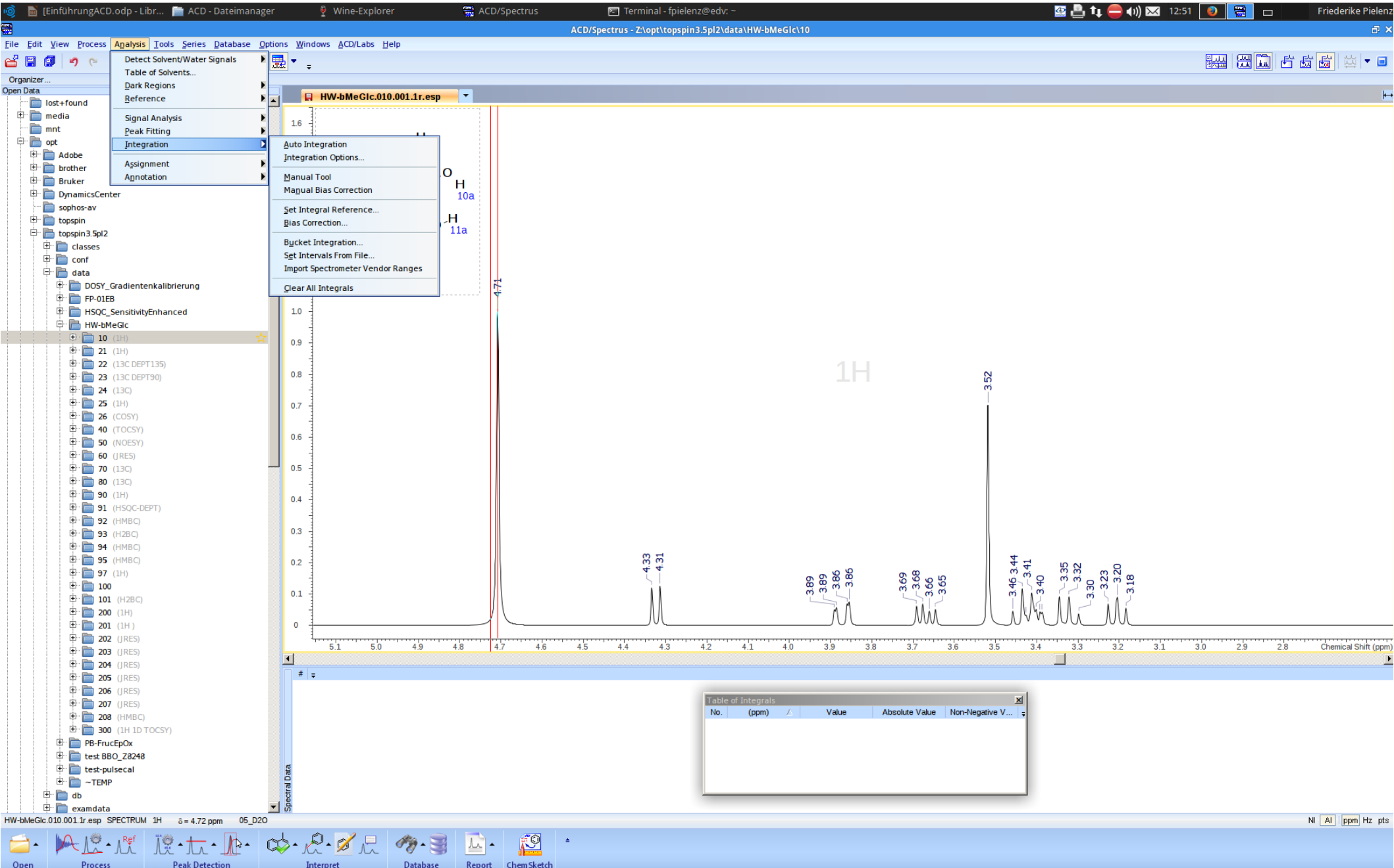
Peakshift kalibrieren



Peakshift kalibrieren



Peaks integrieren



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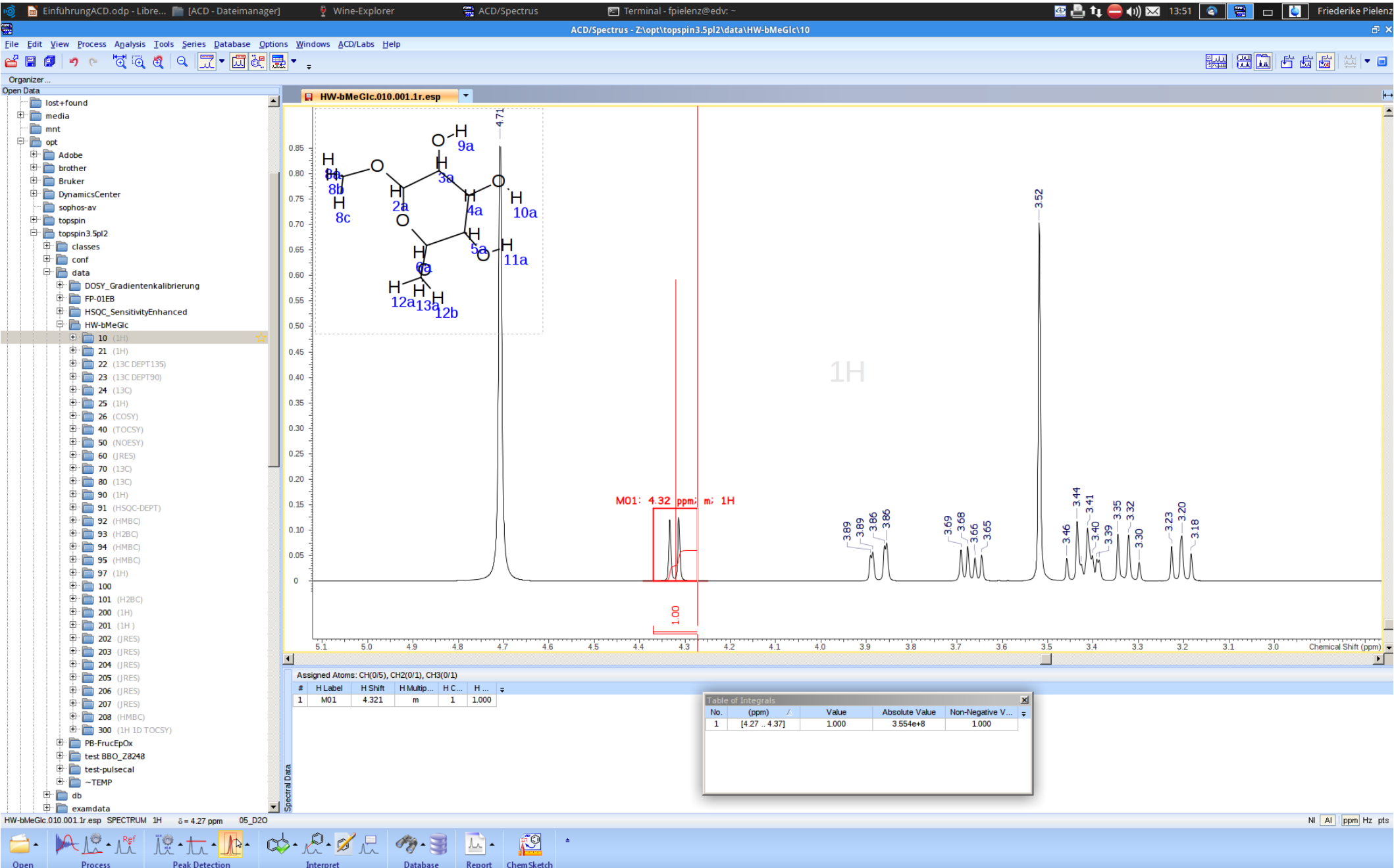

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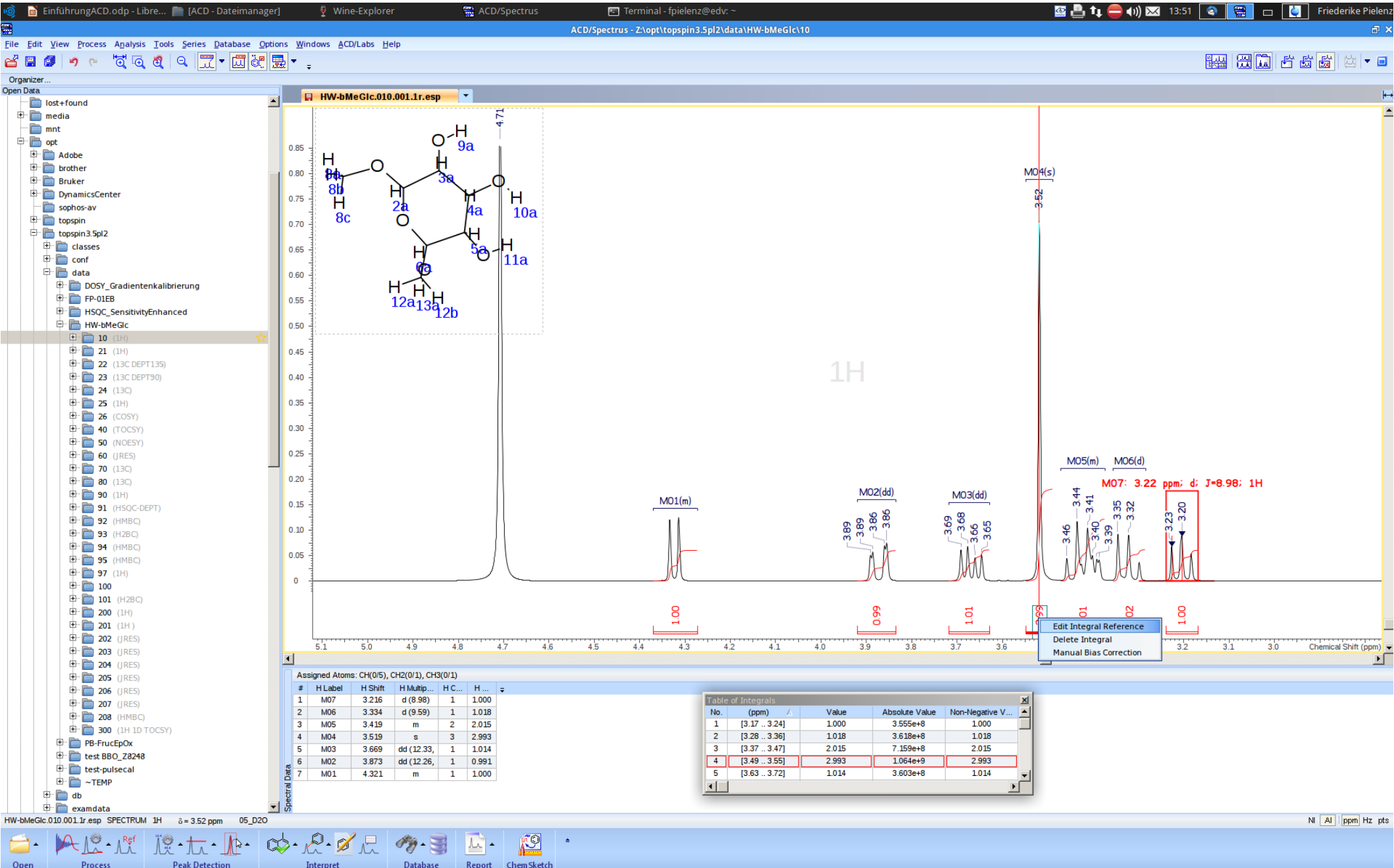
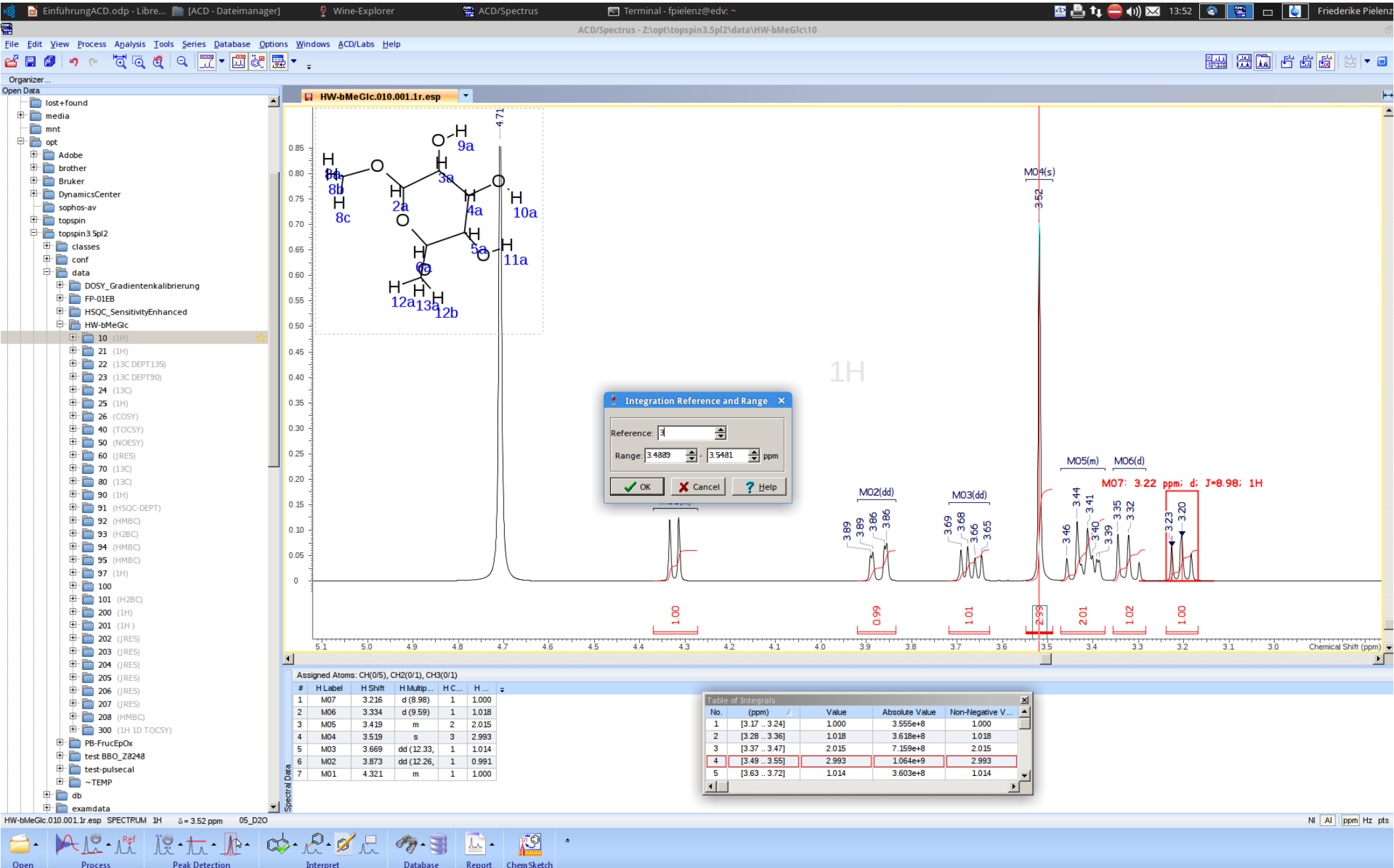
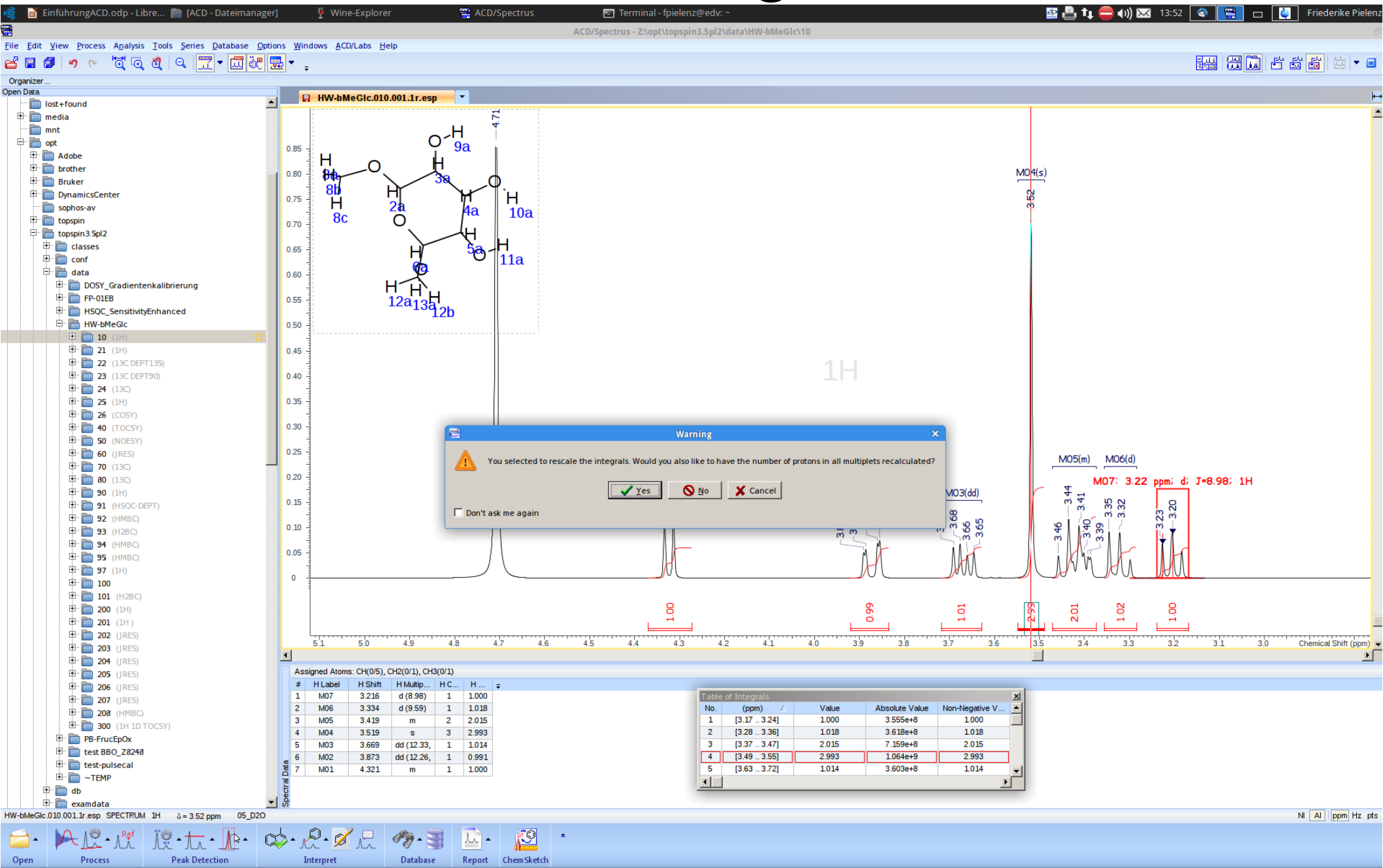


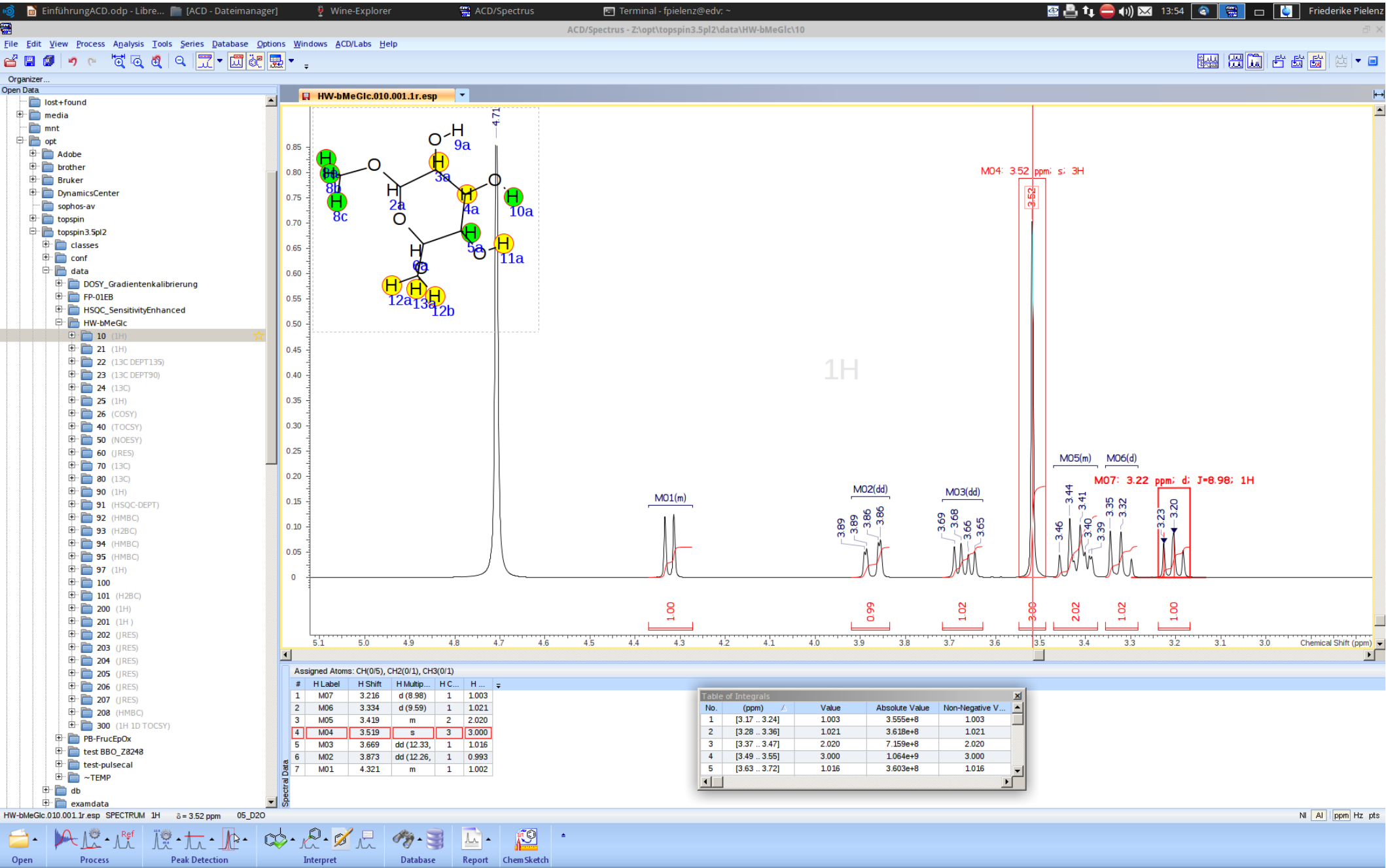
Peaks integrieren



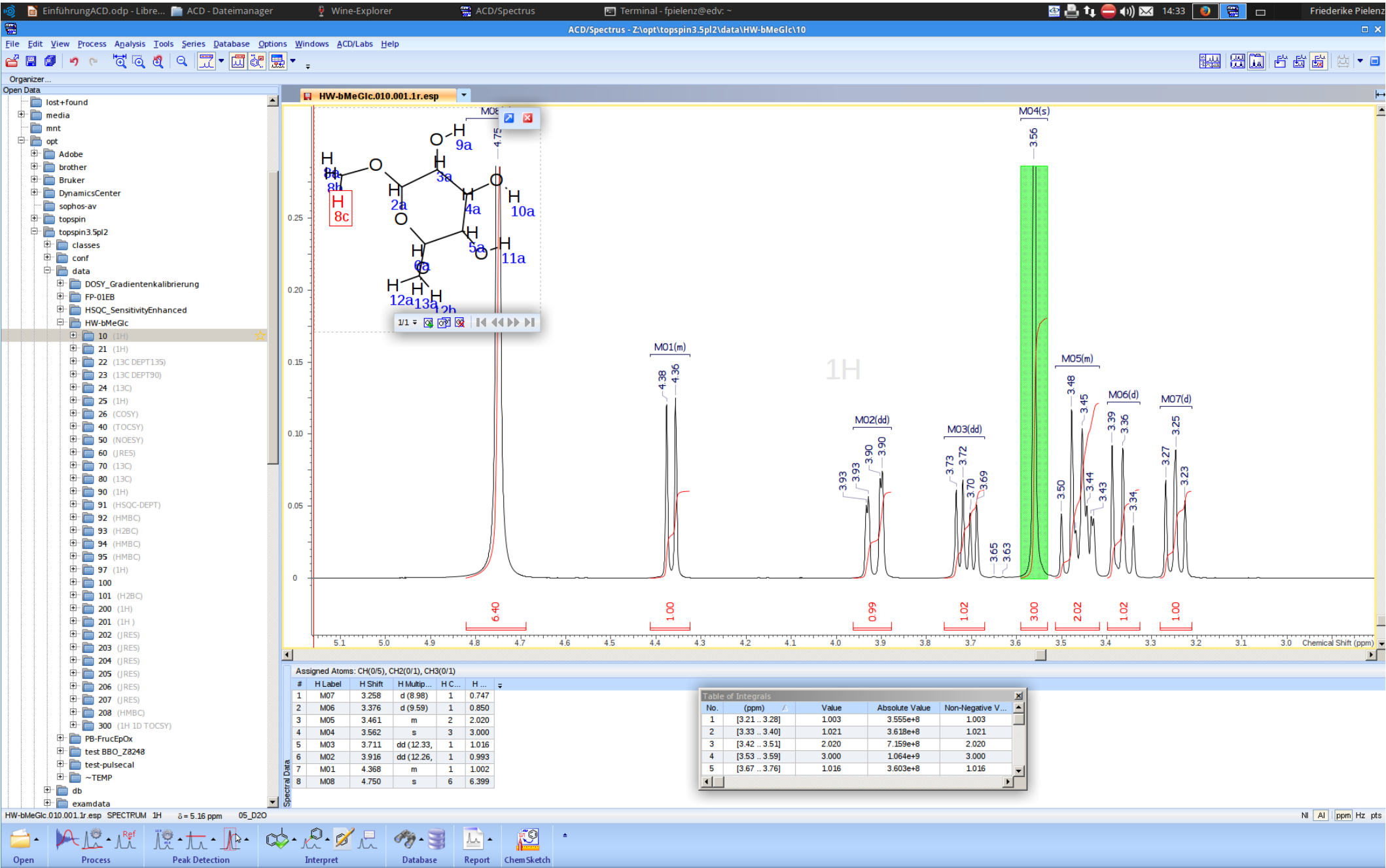
Peaks integrieren



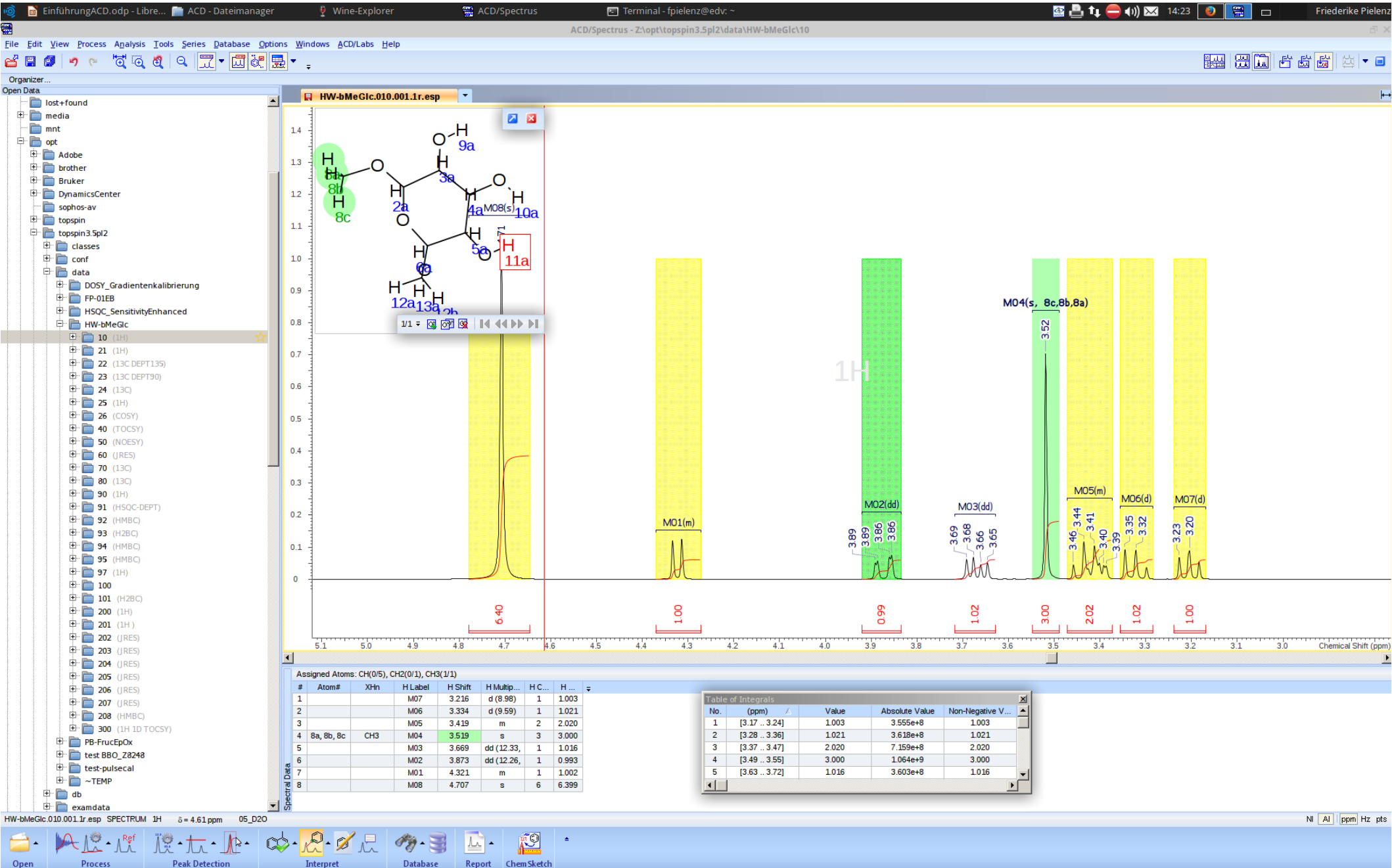
Peaks zuordnen



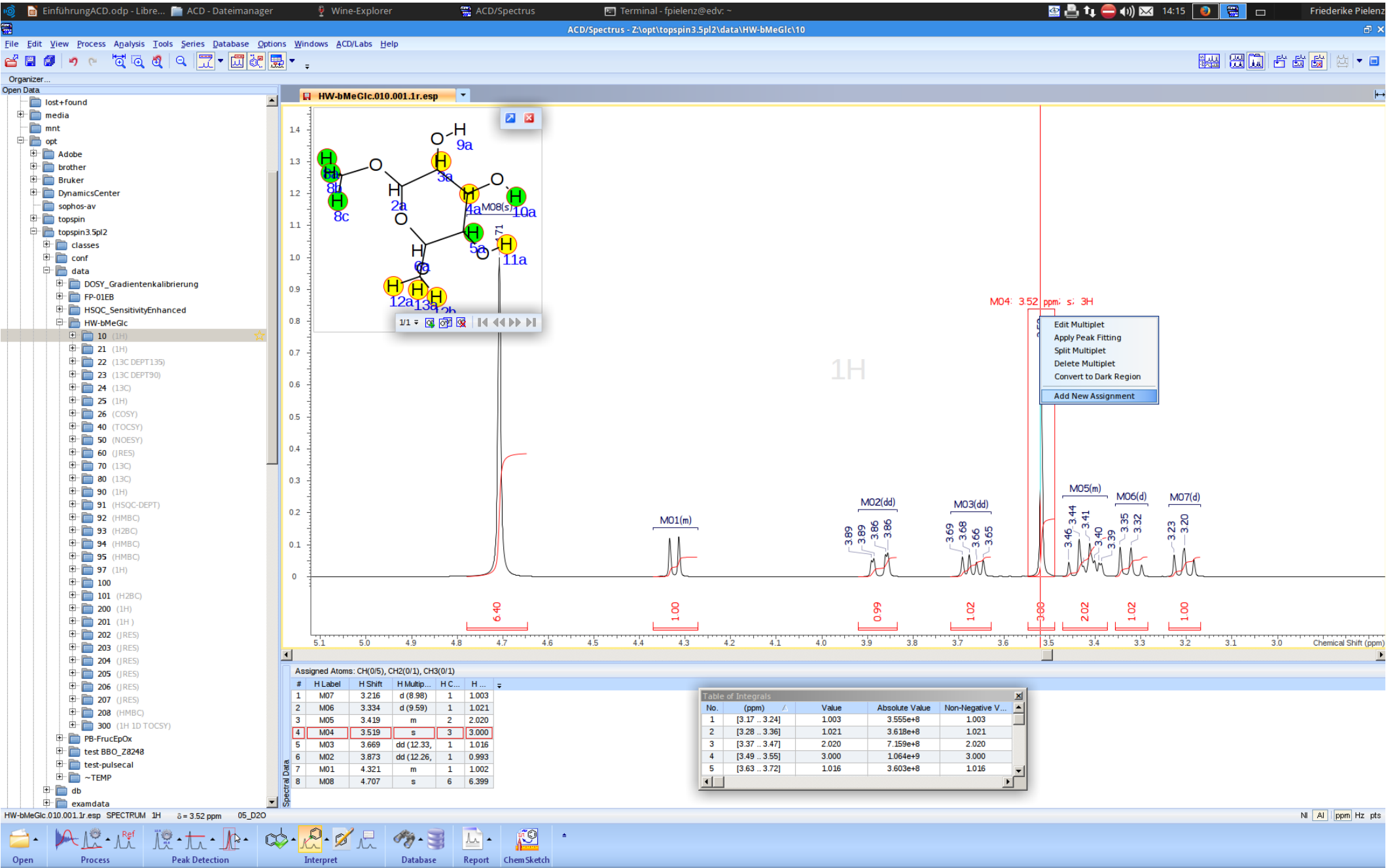
Peaks zuordnen



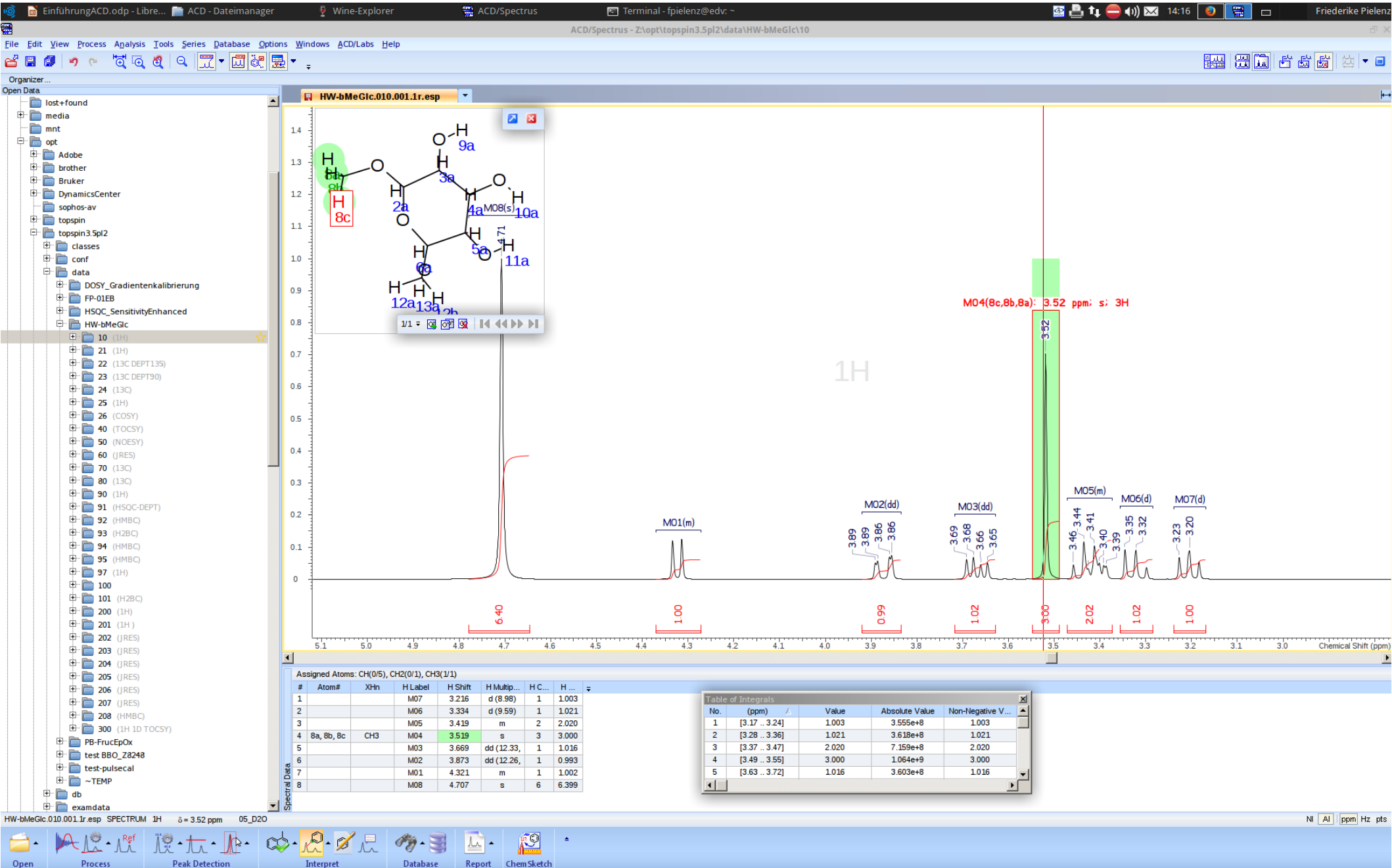
Peaks zuordnen



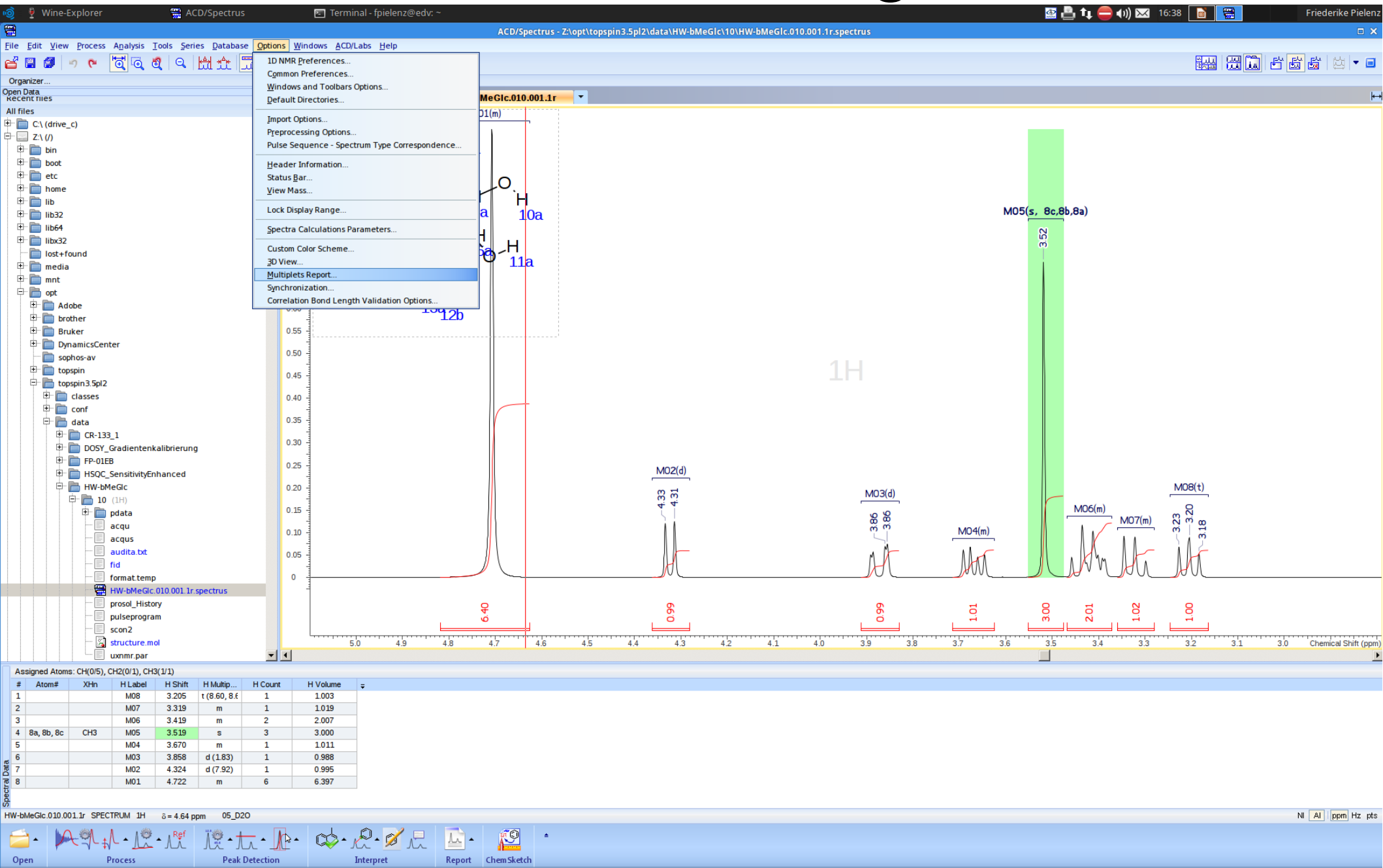
Peaks zuordnen



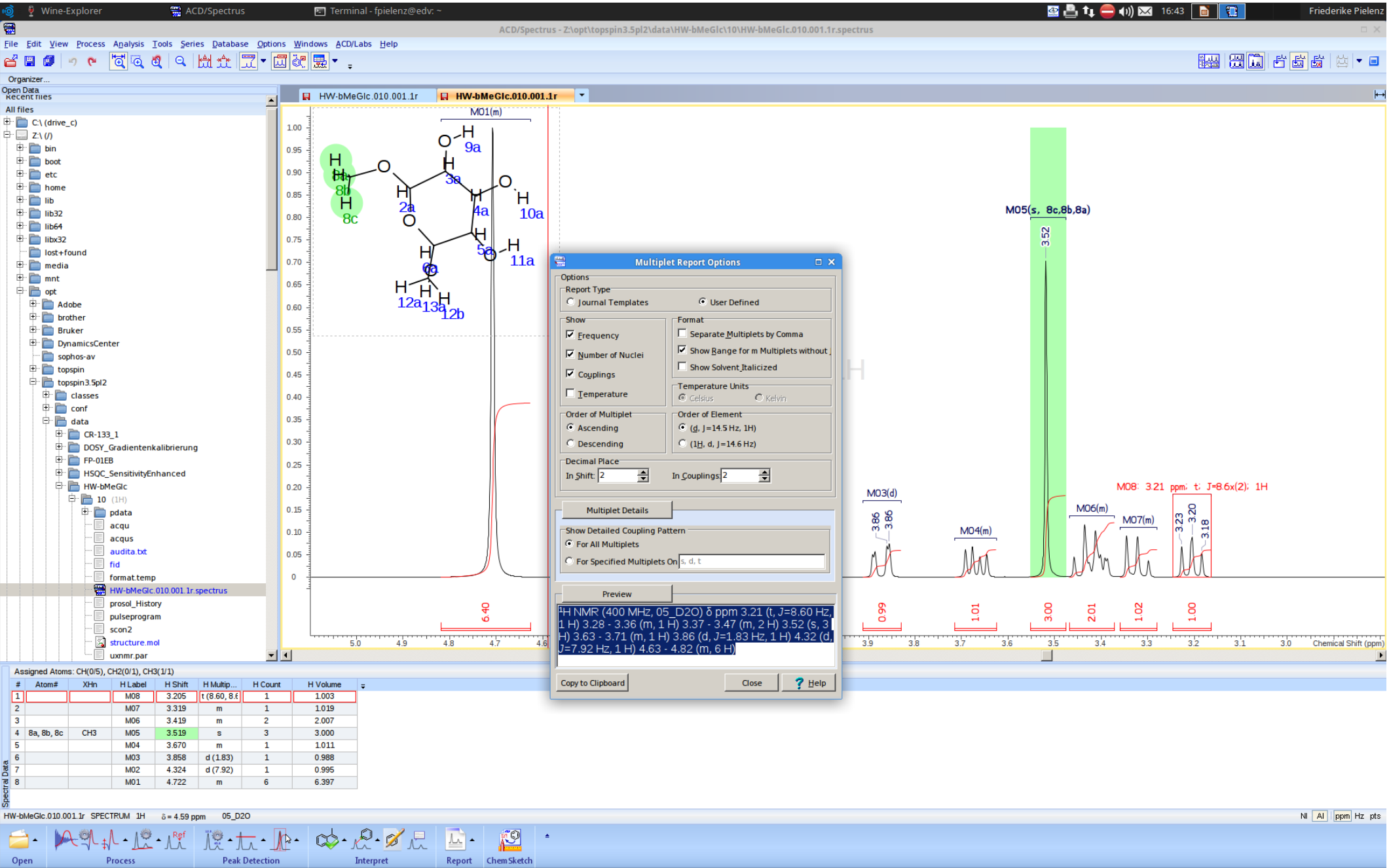
Peaks zuordnen



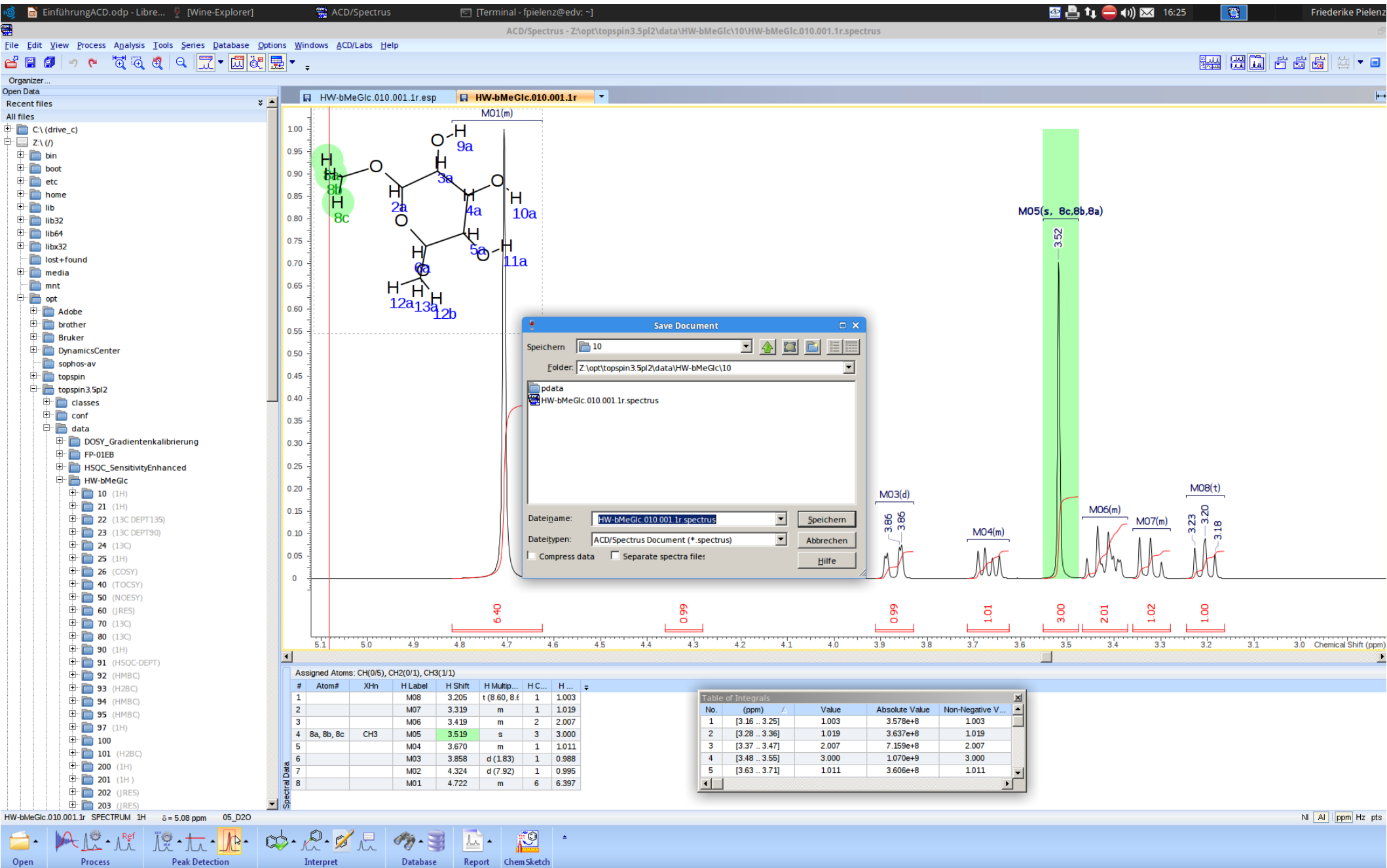
Patent String



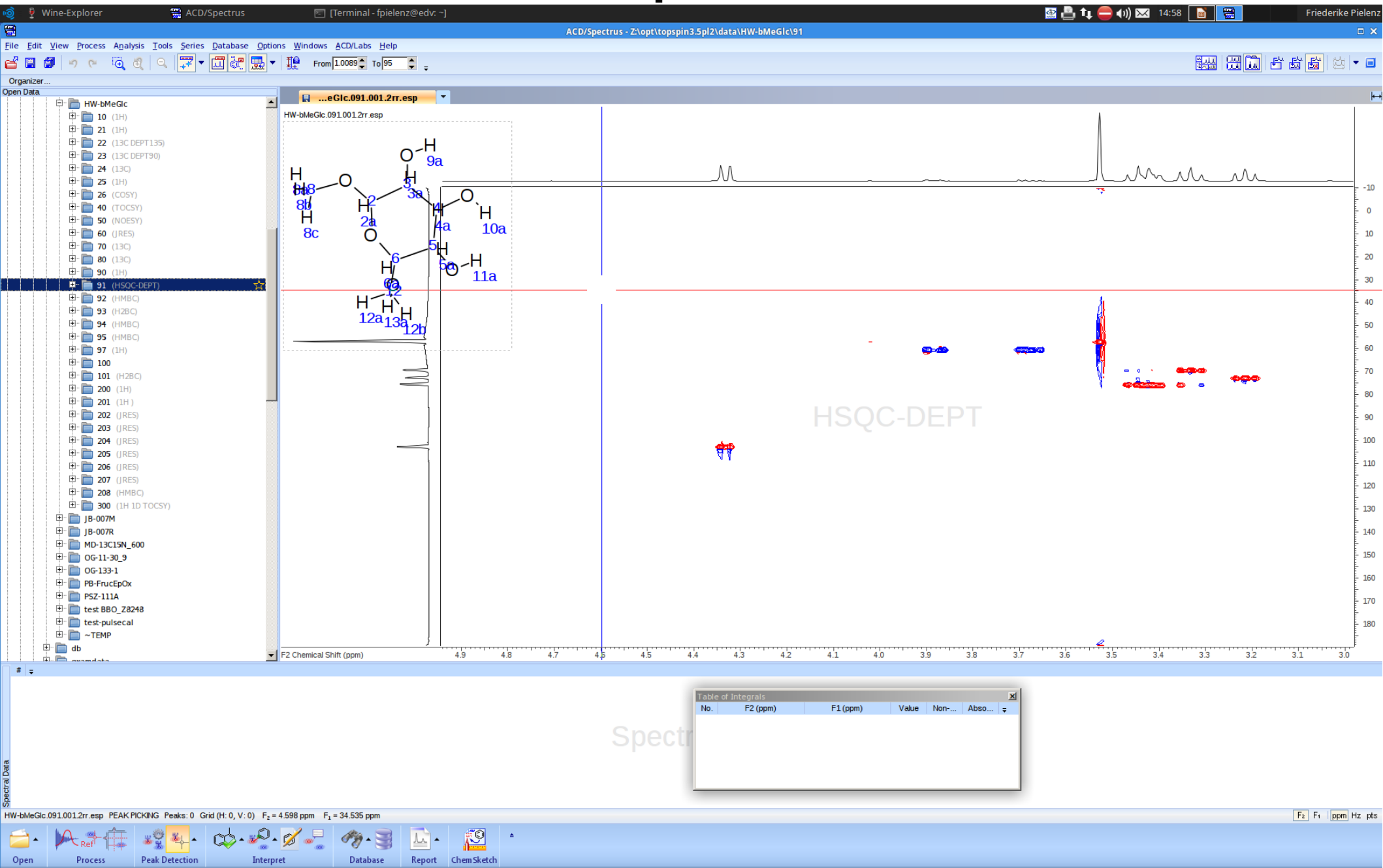
Patent String



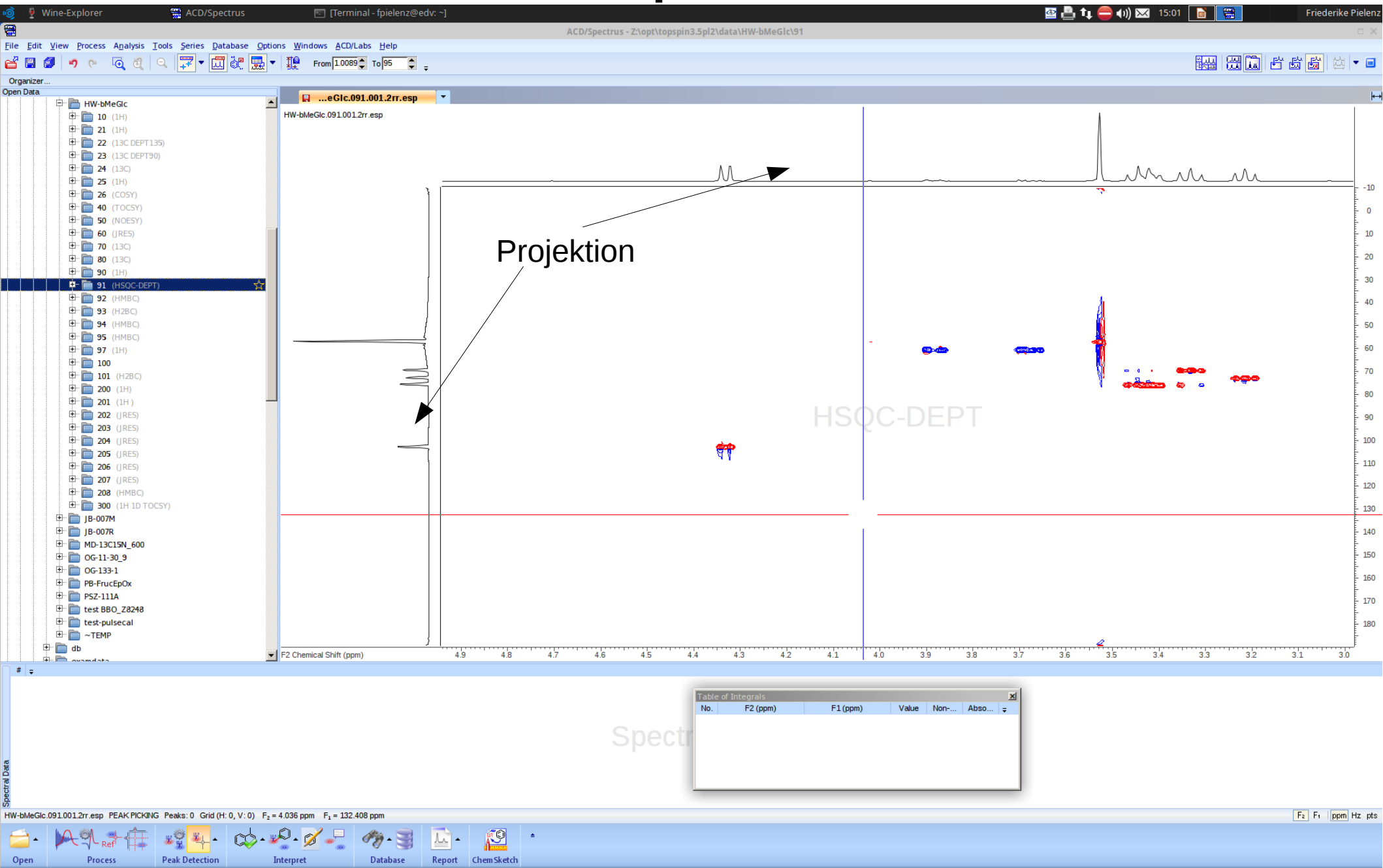
Datei speichern!



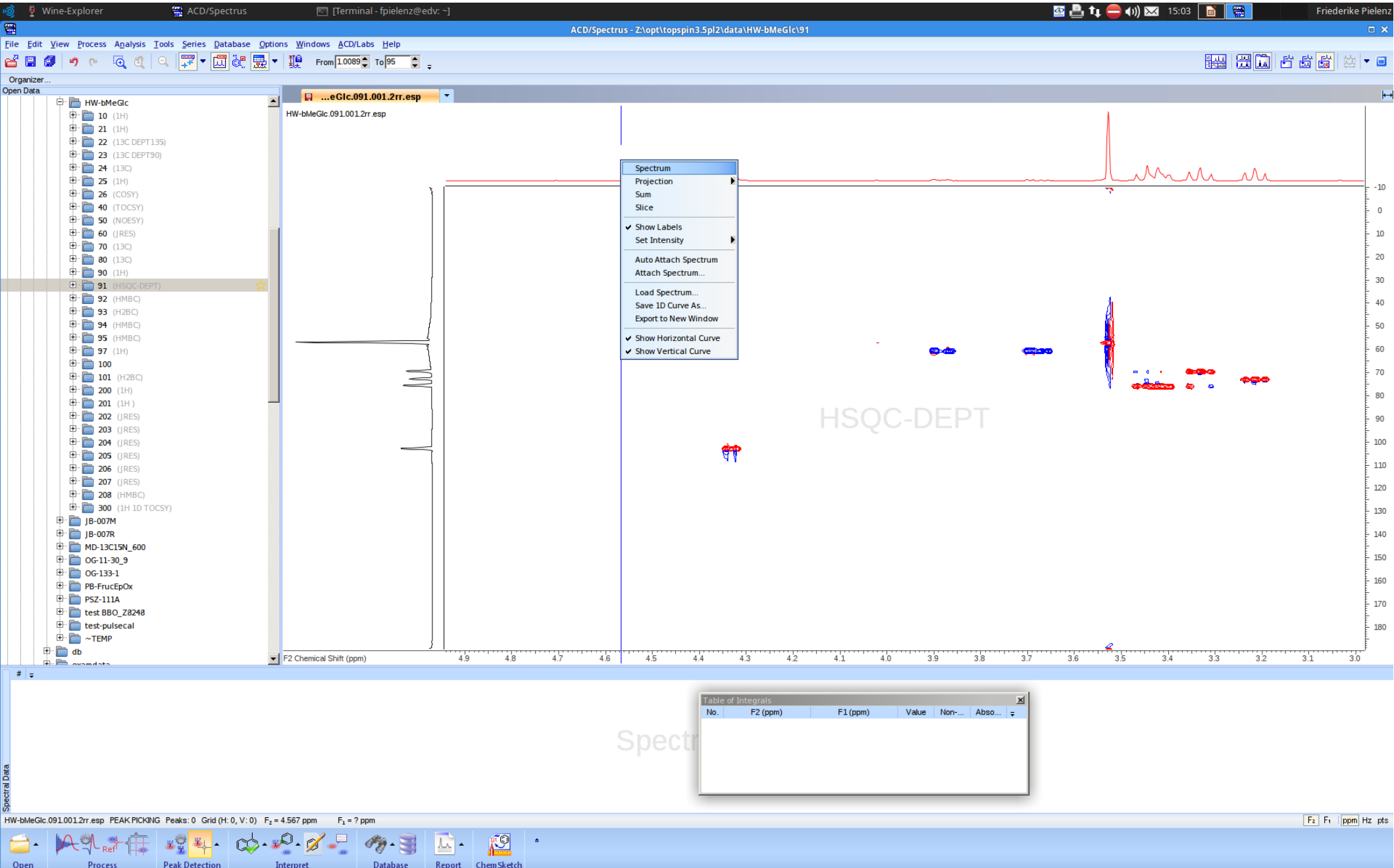
2D-Spektren


Wine-Explorer
ACD/Spectrus
[Terminal - fpielenz@edv: ~]
14:58
Friederike Pielenz
ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\91
File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help
From 1.0089 To 95
Organizer...
Open Data
HW-bMeGlc
10 (1H)
21 (1H)
22 (13C DEPT135)
23 (13C DEPT90)
24 (13C)
25 (1H)
26 (COSY)
40 (TOCSY)
50 (NOESY)
60 (JRES)
70 (13C)
80 (13C)
90 (1H)
91 (HSQC-DEPT)
92 (HMBC)
93 (H2BC)
94 (HMBC)
95 (HMBC)
97 (1H)
100
101 (H2BC)
200 (1H)
201 (1H)
202 (JRES)
203 (JRES)
204 (JRES)
205 (JRES)
206 (JRES)
207 (JRES)
208 (HMBC)
300 (1H 1D TOCSY)
JB-007M
JB-007R
MD-13C15N_600
OG-11-30_9
OG-133-1
PB-FrucEpOx
PSZ-111A
test BBO_Z8248
test-pulsecal
~TEMP
db
...eGlc.091.001.2rr.esp
HW-bMeGlc.091.001.2rr.esp
HSQC-DEPT
F2 Chemical Shift (ppm)
Table of Integrals
No. F2 (ppm) F1 (ppm) Value Non-... Abso...
Spectral Data
HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F2 = 4.598 ppm F1 = 34.535 ppm
Open Process Peak Detection Interpret Database Report ChemSketch

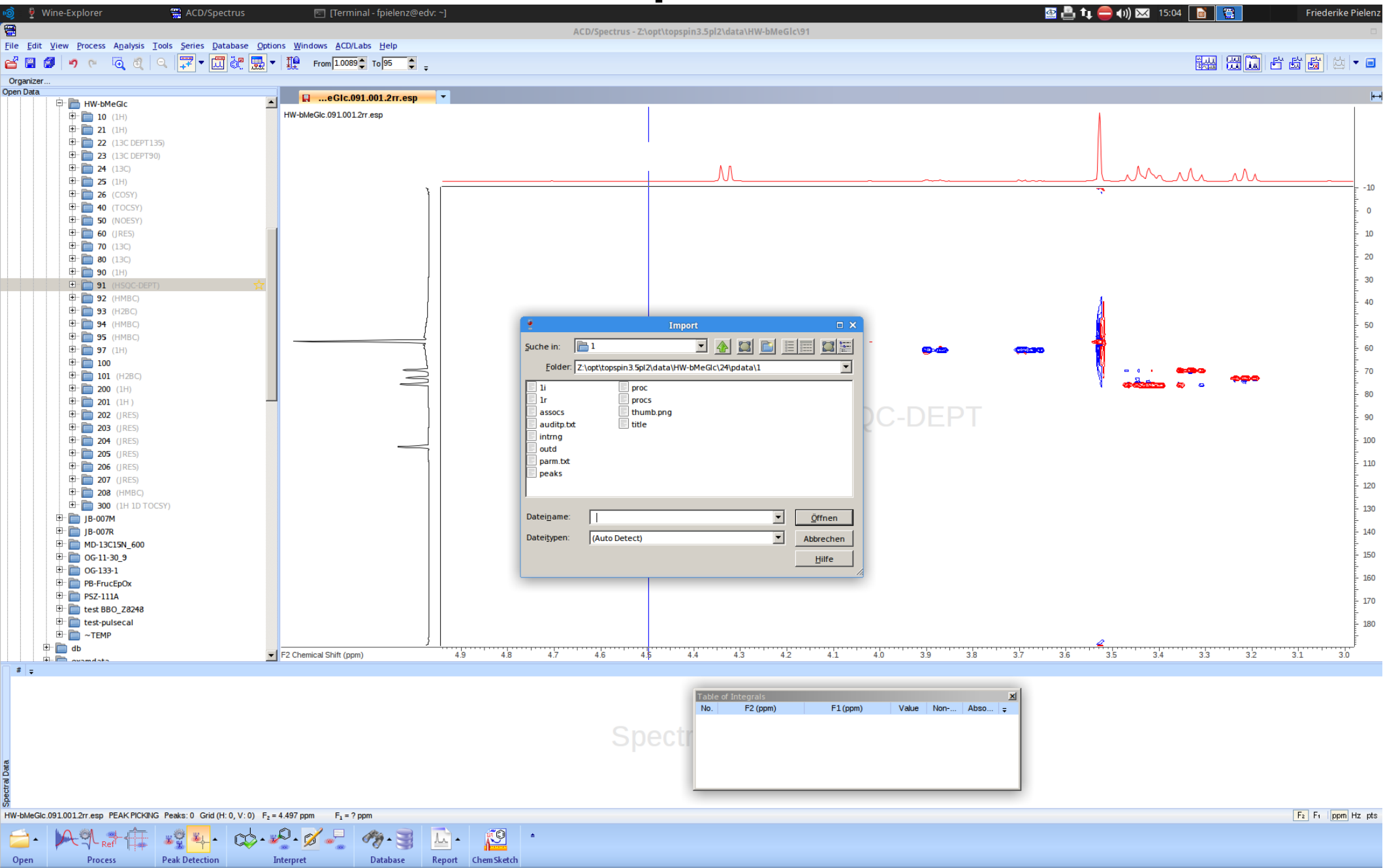
2D-Spektren


Projektion
HSQC-DEPT
HW-bMeGlc.091.001.2rr.esp
F2 Chemical Shift (ppm)

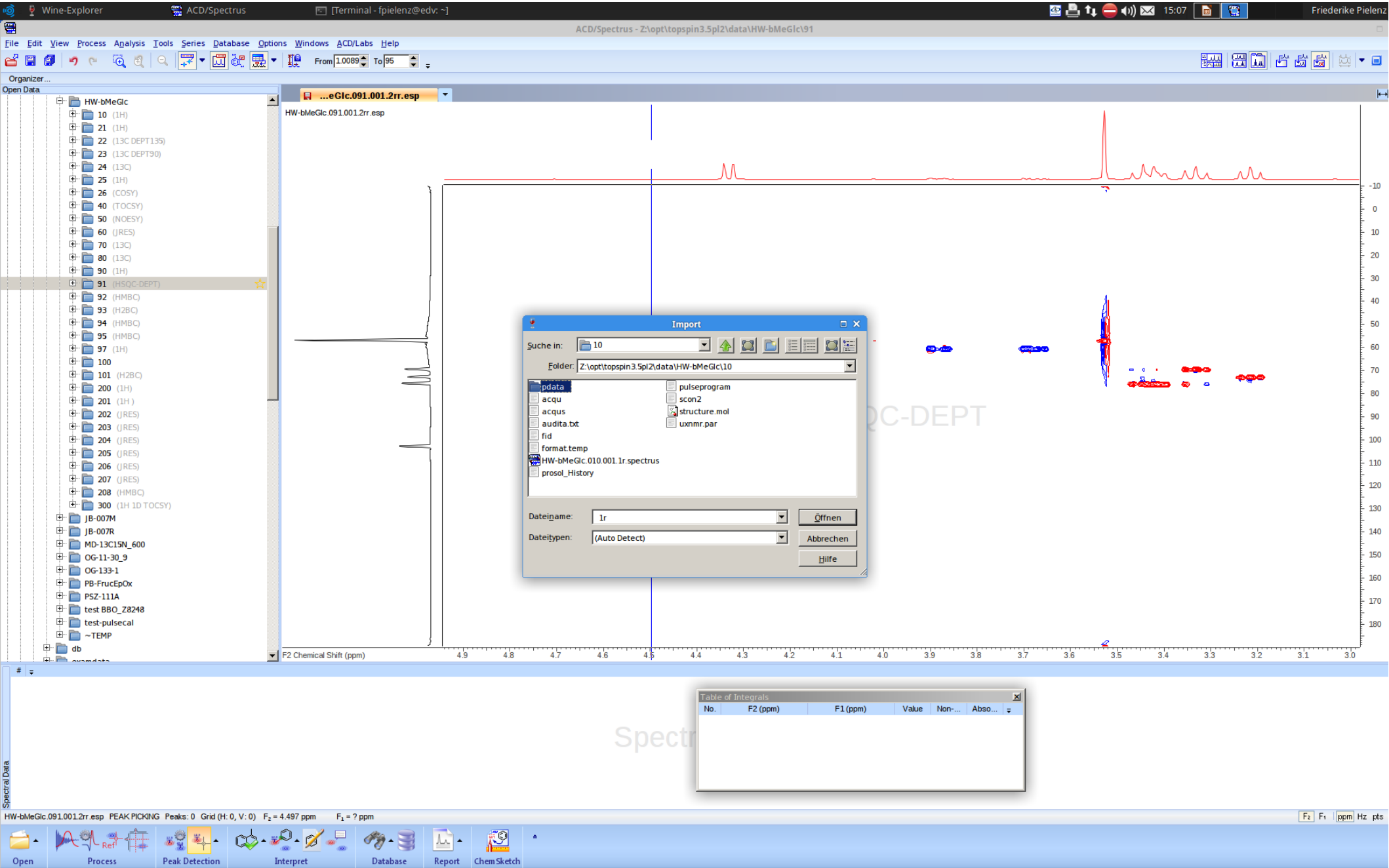
2D-Spektren


Wine-Explorer
ACD/Spectrus
[Terminal - fpielenz@edv: ~]
15:03
Friederike Pielenz
ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\91
File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help
From 1.0089 To 95
Organizer...
Open Data
HW-bMeGlc
10 (1H)
21 (1H)
22 (13C DEPT135)
23 (13C DEPT90)
24 (13C)
25 (1H)
26 (COSY)
40 (TOCSY)
50 (NOESY)
60 (JRES)
70 (13C)
80 (13C)
90 (1H)
91 (HSQC-DEPT)
92 (HMBC)
93 (H2BC)
94 (HMBC)
95 (HMBC)
97 (1H)
100
101 (H2BC)
200 (1H)
201 (1H)
202 (JRES)
203 (JRES)
204 (JRES)
205 (JRES)
206 (JRES)
207 (JRES)
208 (HMBC)
300 (1H 1D TOCSY)
JB-007M
JB-007R
MD-13C15N_600
OG-11-30_9
OG-133-1
PB-FrucEpOx
PSZ-111A
test BBO_Z8248
test-pulsecal
~TEMP
db
...eGlc.091.001.2rr.esp
HW-bMeGlc.091.001.2rr.esp
Spectrum
Projection
Sum
Slice
Show Labels
Set Intensity
Auto Attach Spectrum
Attach Spectrum...
Load Spectrum...
Save 1D Curve As...
Export to New Window
Show Horizontal Curve
Show Vertical Curve
HSQC-DEPT
F2 Chemical Shift (ppm)
Table of Integrals
No. F2 (ppm) F1 (ppm) Value Non-... Abso...
Spectral Data
HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F2 = 4.567 ppm F1 = ? ppm
Open Process Peak Detection Interpret Database Report ChemSketch

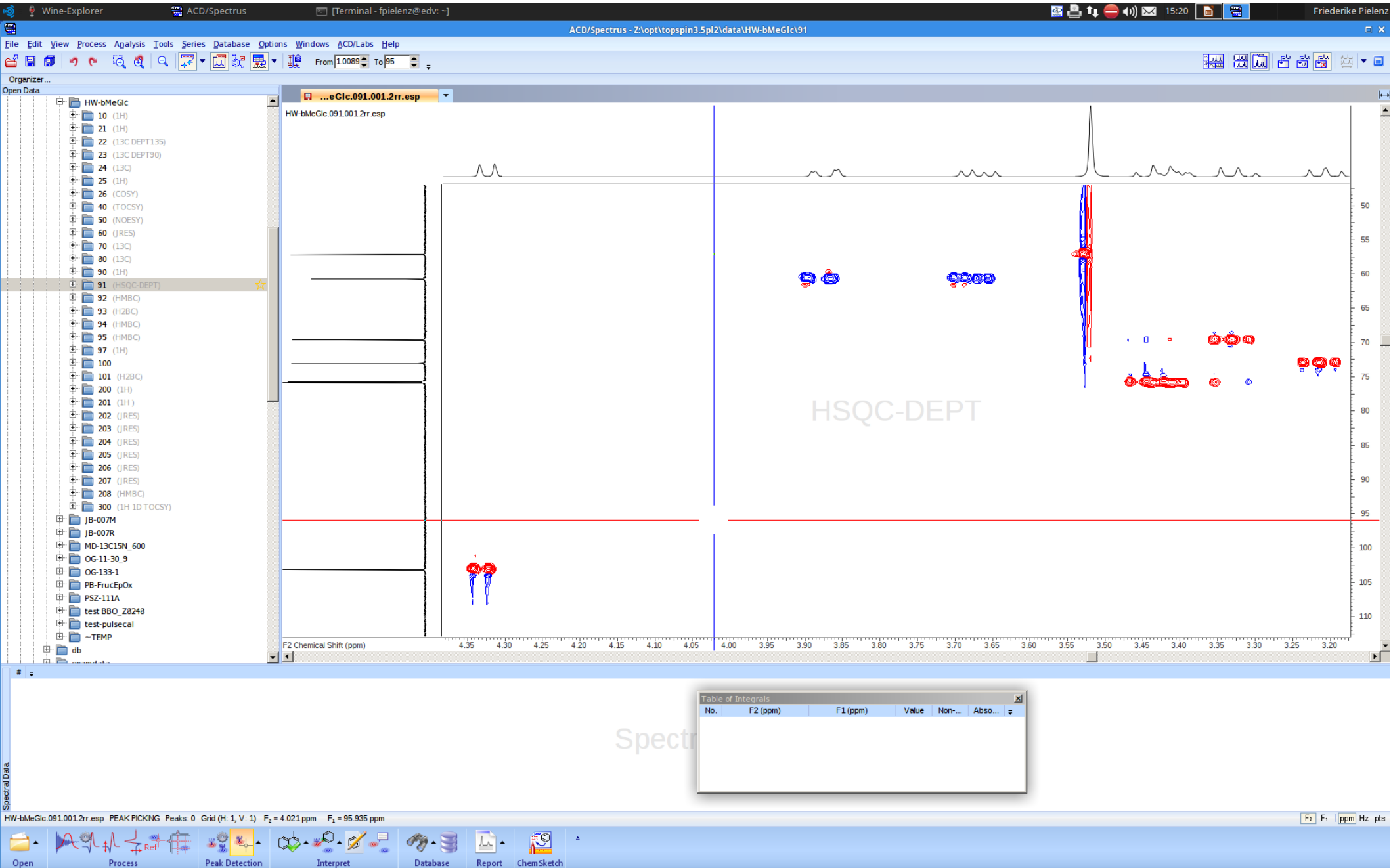
2D-Spektren


Wine-Explorer
ACD/Spectrus
[Terminal - fpielenz@edv: ~]
15:04
Friederike Pielenz
ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\91
File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help
Organizer...
Open Data
HW-bMeGlc
10 (1H)
21 (1H)
22 (13C DEPT135)
23 (13C DEPT90)
24 (13C)
25 (1H)
26 (COSY)
40 (TOCSY)
50 (NOESY)
60 (JRES)
70 (13C)
80 (13C)
90 (1H)
91 (HSQC-DEPT)
92 (HMBC)
93 (H2BC)
94 (HMBC)
95 (HMBC)
97 (1H)
100
101 (H2BC)
200 (1H)
201 (1H)
202 (JRES)
203 (JRES)
204 (JRES)
205 (JRES)
206 (JRES)
207 (JRES)
208 (HMBC)
300 (1H 1D TOCSY)
JB-007M
JB-007R
MD-13C15N_600
OG-11-30_9
OG-133-1
PB-FrucEpOx
PSZ-111A
test BBO_Z8248
test-pulsecal
~TEMP
db
...eGlc.091.001.2rr.esp
HW-bMeGlc.091.001.2rr.esp
Import
Suche in: 1
Folder: Z:\opt\topspin3.5pl2\data\HW-bMeGlc\24\pdata\1
1i
1r
assocs
auditp.txt
intrng
outd
parm.txt
peaks
proc
procs
thumb.png
title
Dateiname:
Dateitypen: (Auto Detect)
Öffnen
Abbrechen
Hilfe
F2 Chemical Shift (ppm)
Table of Integrals
No. F2 (ppm) F1 (ppm) Value Non-... Abso...
Spectral Data
HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F2 = 4.497 ppm F1 = ? ppm
Open
Process
Peak Detection
Interpret
Database
Report
ChemSketch

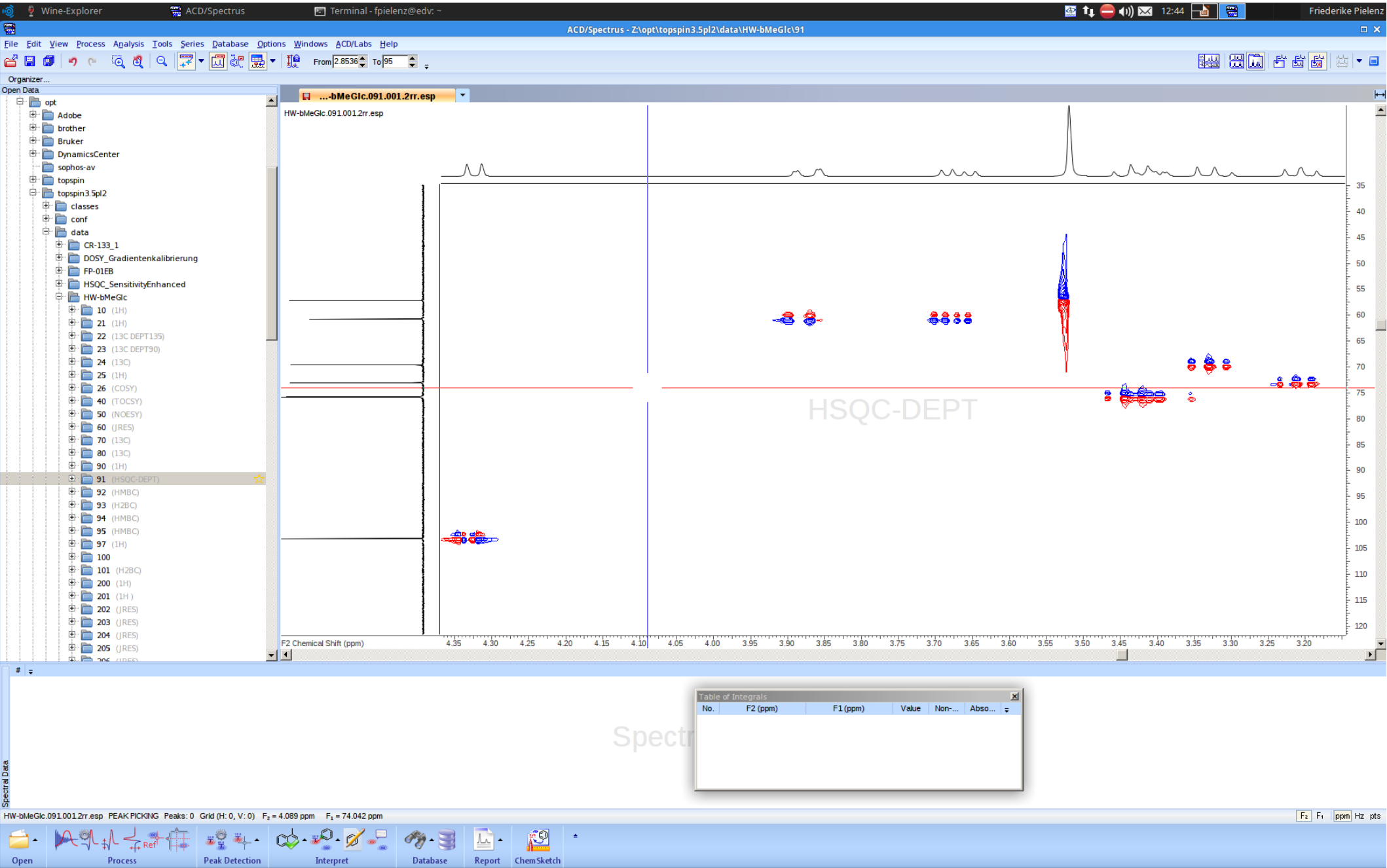
2D-Spektren


Wine-Explorer
ACD/Spectrus
[Terminal - fpielenz@edv: ~]
15:07
Friederike Pielenz
ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\91
File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help
From 1.0089 To 95
Organizer...
Open Data
HW-bMeGlc
10 (1H)
21 (1H)
22 (13C DEPT135)
23 (13C DEPT90)
24 (13C)
25 (1H)
26 (COSY)
40 (TOCSY)
50 (NOESY)
60 (JRES)
70 (13C)
80 (13C)
90 (1H)
91 (HSQC-DEPT)
92 (HMBC)
93 (H2BC)
94 (HMBC)
95 (HMBC)
97 (1H)
100
101 (H2BC)
200 (1H)
201 (1H)
202 (JRES)
203 (JRES)
204 (JRES)
205 (JRES)
206 (JRES)
207 (JRES)
208 (HMBC)
300 (1H 1D TOCSY)
JB-007M
JB-007R
MD-13C15N_600
OG-11-30_9
OG-133-1
PB-FrucEpOx
PSZ-111A
test BBO_Z8248
test-pulsecal
~TEMP
db
...eGlc.091.001.2rr.esp
HW-bMeGlc.091.001.2rr.esp
Import
Suche in: 10
Folder: Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10
pdata
acqu
acqus
audita.txt
fid
format.temp
HW-bMeGlc.010.001.1r.spectrus
prosol_History
pulseprogram
scon2
structure.mol
uxnmr.par
Dateiname: 1r
Dateitypen: (Auto Detect)
Öffnen
Abbrechen
Hilfe
F2 Chemical Shift (ppm)
Table of Integrals
No. F2 (ppm) F1 (ppm) Value Non-... Abso...
Spectral Data
HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F2 = 4.497 ppm F1 = ? ppm
Open
Process
Peak Detection
Interpret
Database
Report
ChemSketch

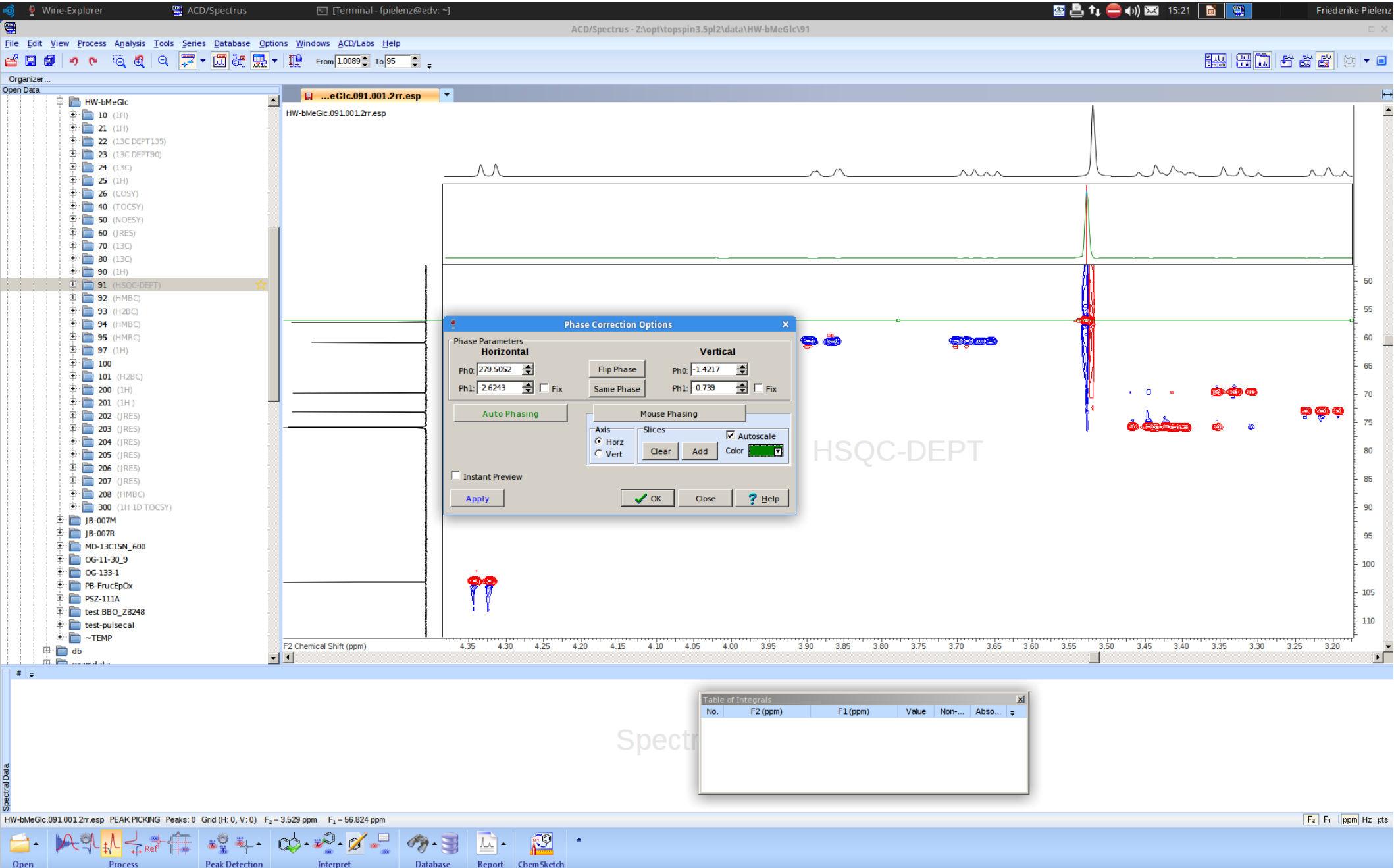
2D-Spektren


Wine-Explorer
ACD/Spectrus
[Terminal - fpielenz@edv: ~]
15:20
Friederike Pielenz
ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\91
File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help
From 1.0089 To 95
Organizer...
Open Data
HW-bMeGlc
10 (1H)
21 (1H)
22 (13C DEPT135)
23 (13C DEPT90)
24 (13C)
25 (1H)
26 (COSY)
40 (TOCSY)
50 (NOESY)
60 (JRES)
70 (13C)
80 (13C)
90 (1H)
91 (HSQC-DEPT)
92 (HMBC)
93 (H2BC)
94 (HMBC)
95 (HMBC)
97 (1H)
100
101 (H2BC)
200 (1H)
201 (1H)
202 (JRES)
203 (JRES)
204 (JRES)
205 (JRES)
206 (JRES)
207 (JRES)
208 (HMBC)
300 (1H 1D TOCSY)
JB-007M
JB-007R
MD-13C15N_600
OG-11-30_9
OG-133-1
PB-FrucEpOx
PSZ-111A
test BBO_Z8248
test-pulsecal
~TEMP
db
...eGlc.091.001.2rr.esp
HW-bMeGlc.091.001.2rr.esp
HSQC-DEPT
F2 Chemical Shift (ppm)
4.35 4.30 4.25 4.20 4.15 4.10 4.05 4.00 3.95 3.90 3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25 3.20
50 55 60 65 70 75 80 85 90 95 100 105 110
Table of Integrals
No. F2 (ppm) F1 (ppm) Value Non-... Abso...
Spectral Data
HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 1, V: 1) F2 = 4.021 ppm F1 = 95.935 ppm
F2 F1 ppm Hz pts
Open
Process
Peak Detection
Interpret
Database
Report
ChemSketch

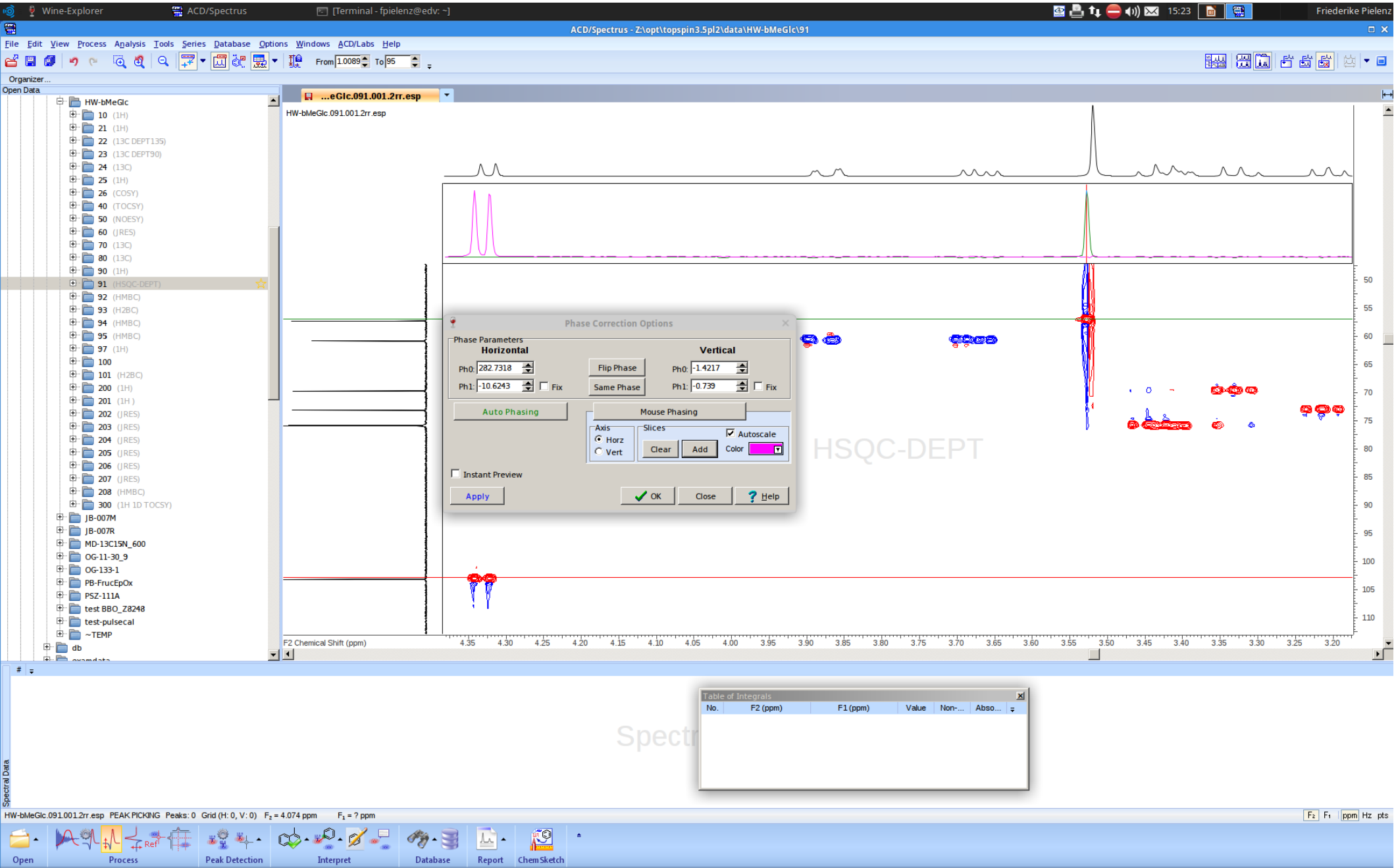
2D-Spektren Phase korrigieren



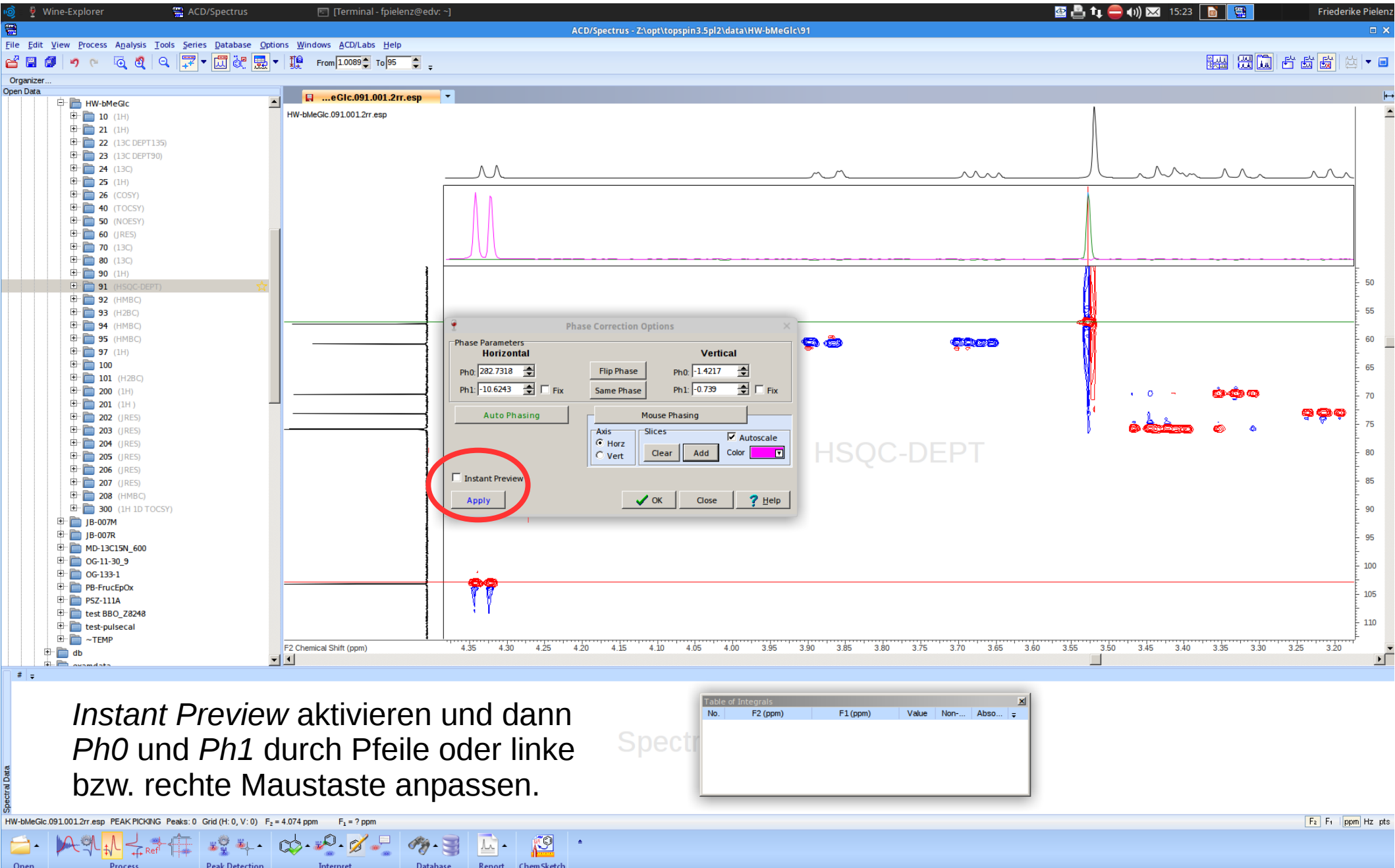
2D-Spektren Phase korrigieren



2D-Spektren Phase korrigieren

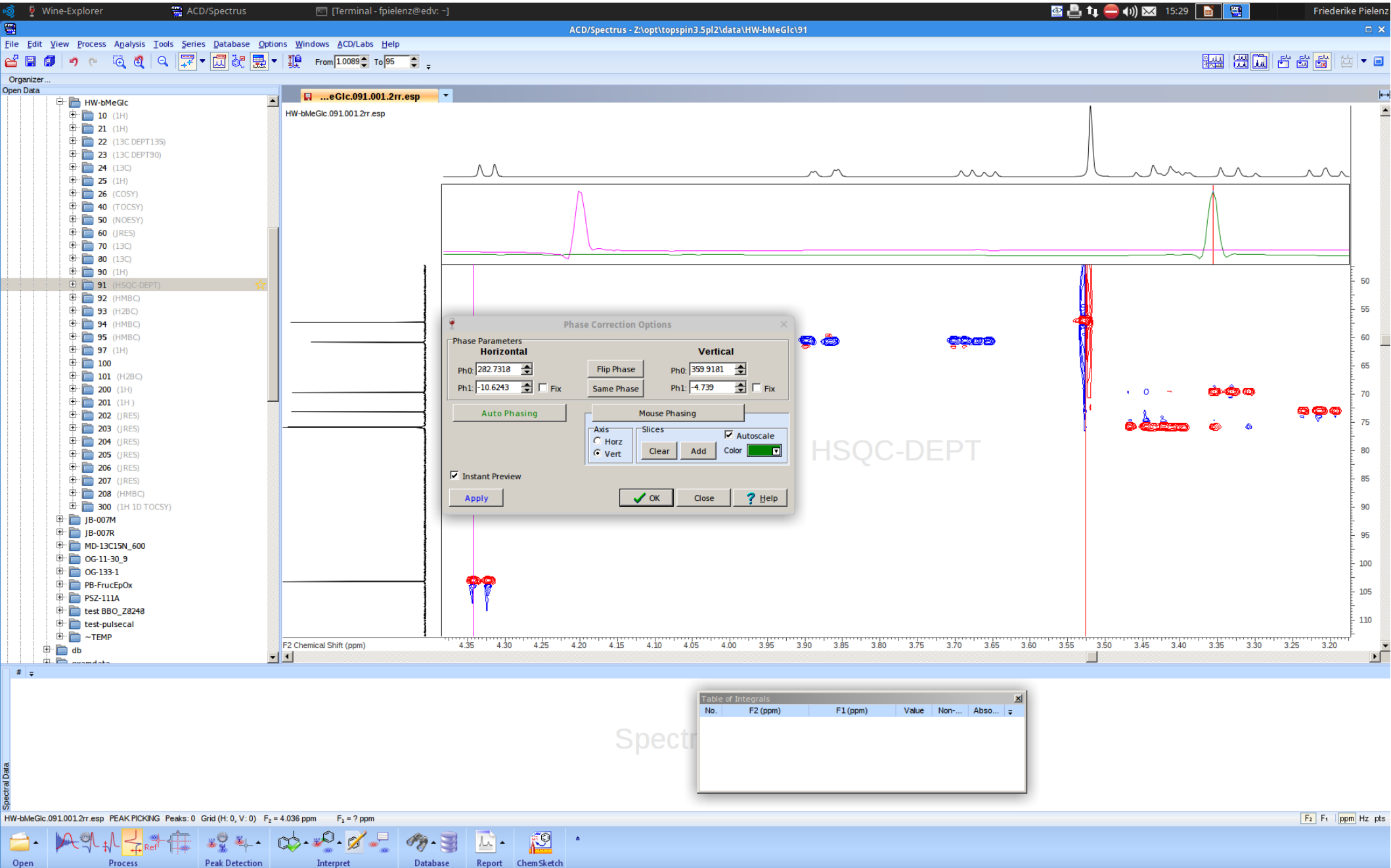


2D-Spektren Phase korrigieren

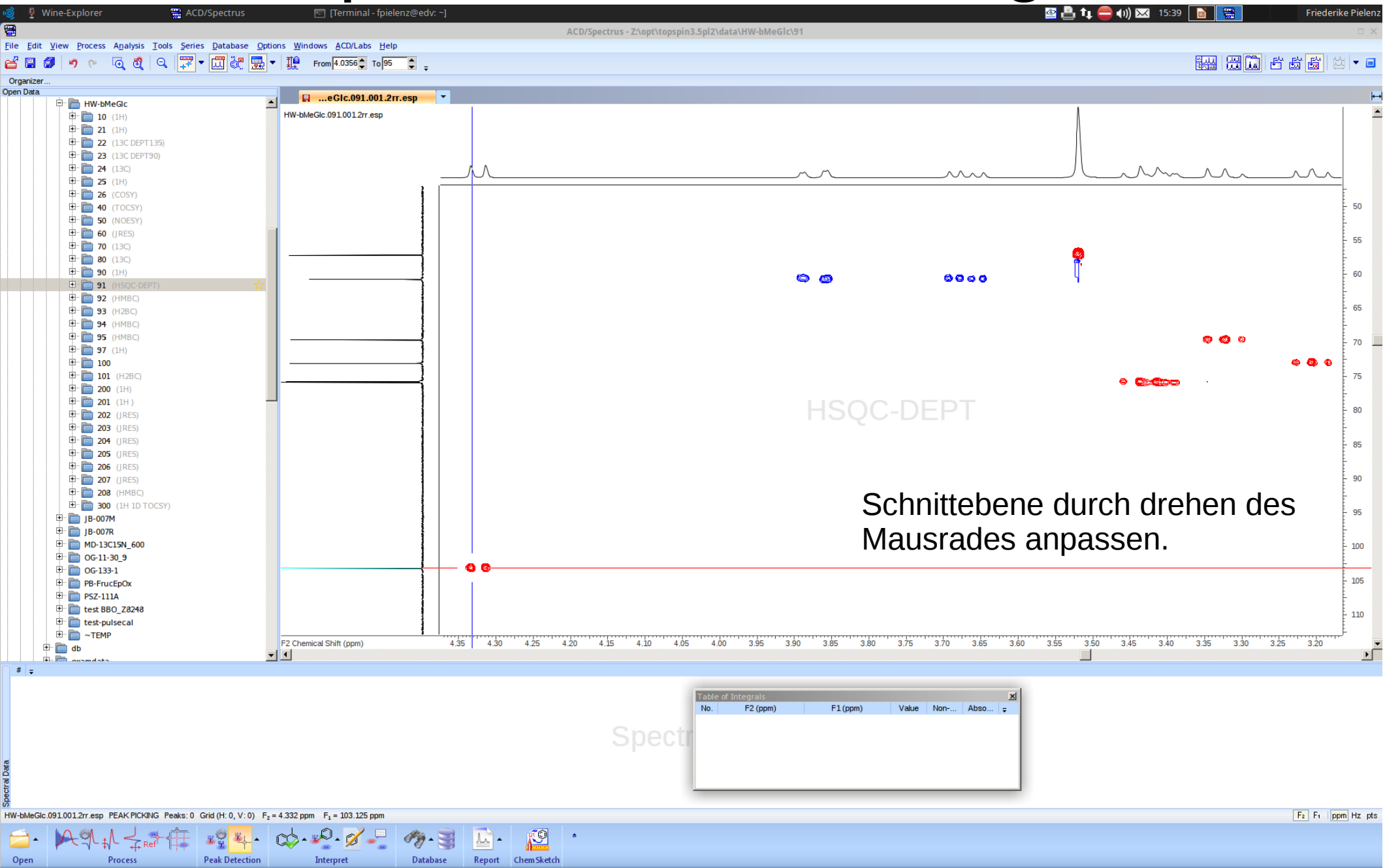


Instant Preview aktivieren und dann *Ph0* und *Ph1* durch Pfeile oder linke bzw. rechte Maustaste anpassen.

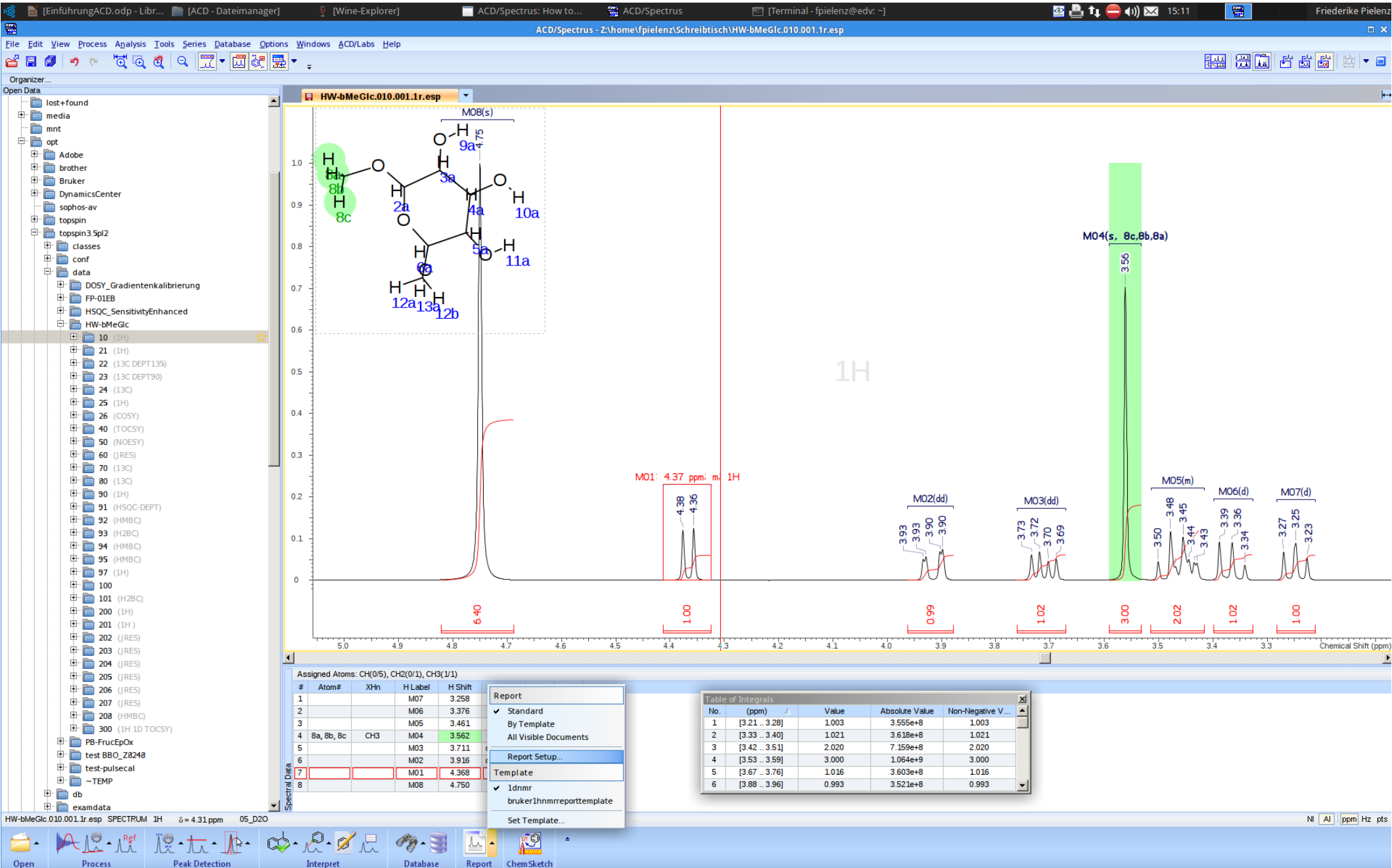
2D-Spektren Phase korrigieren



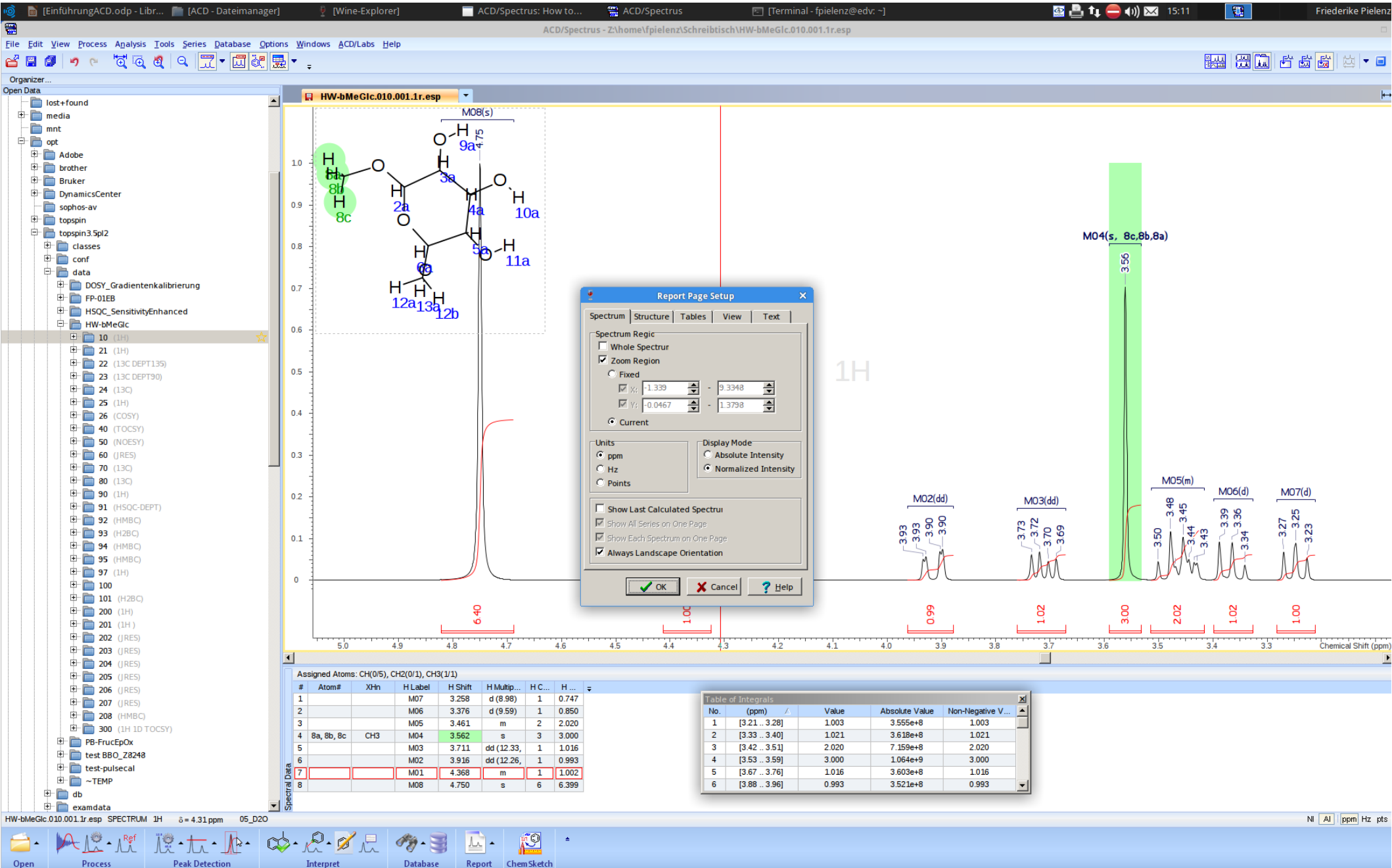
2D-Spektren Phase korrigieren



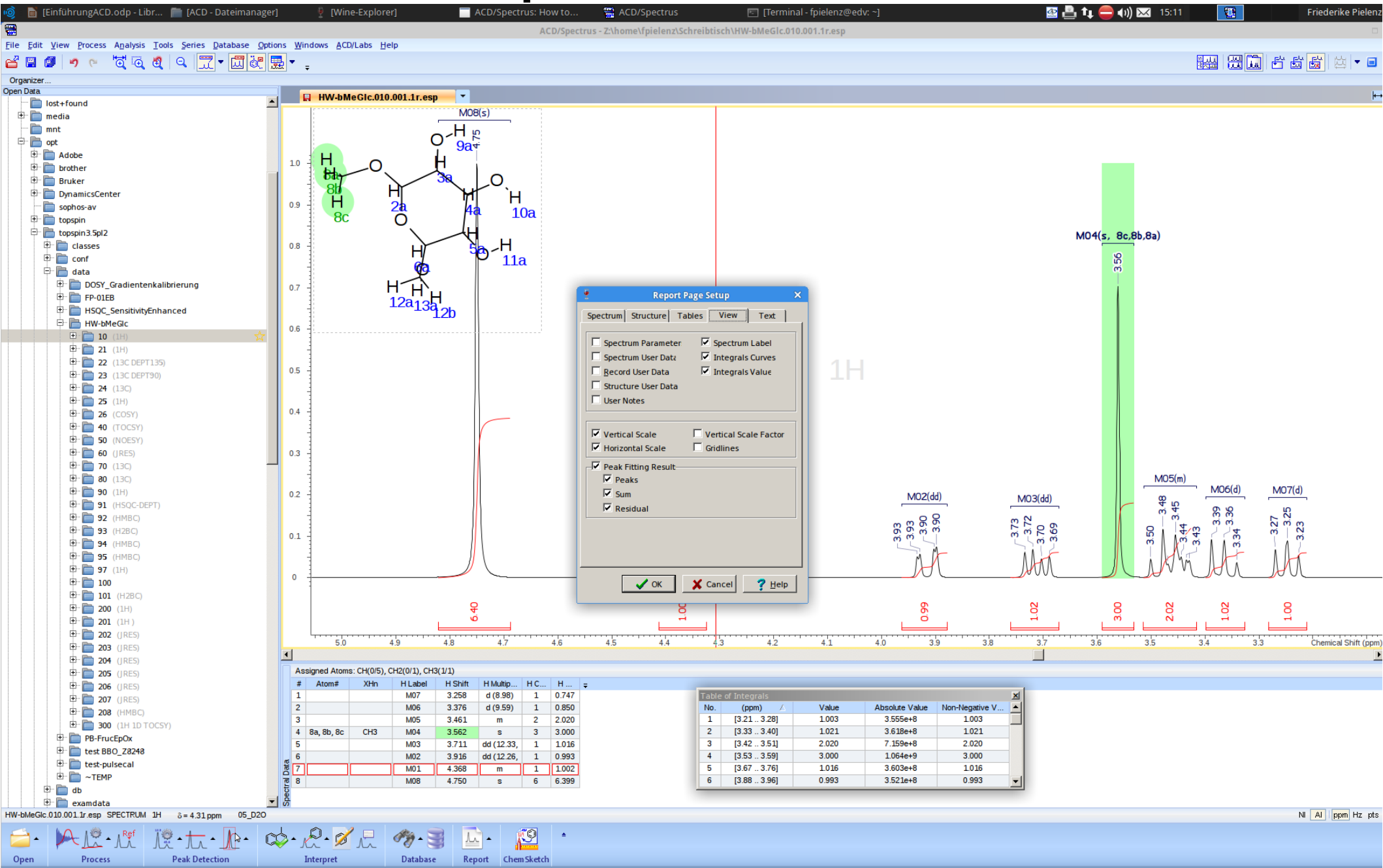
Report erstellen



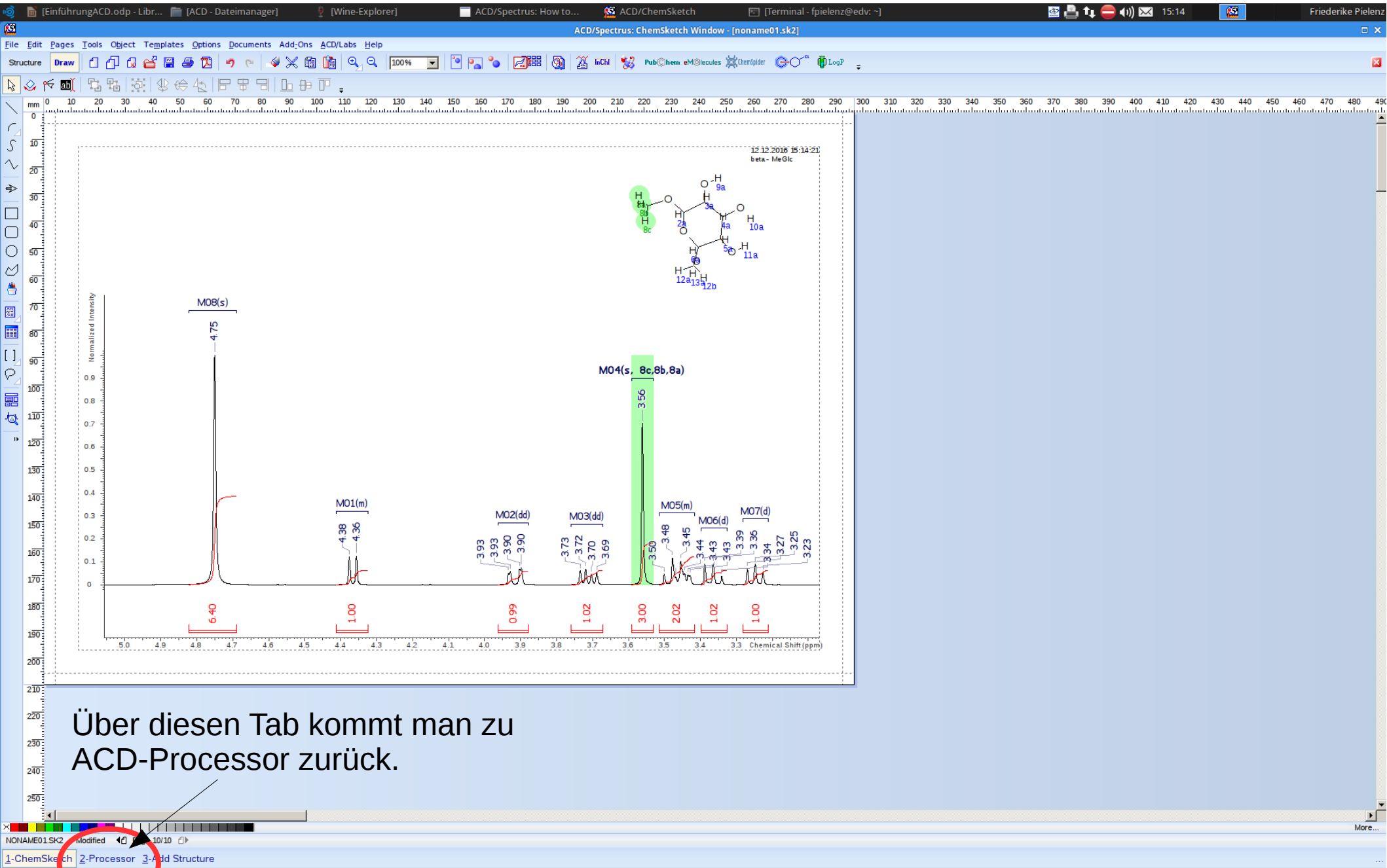
Report erstellen



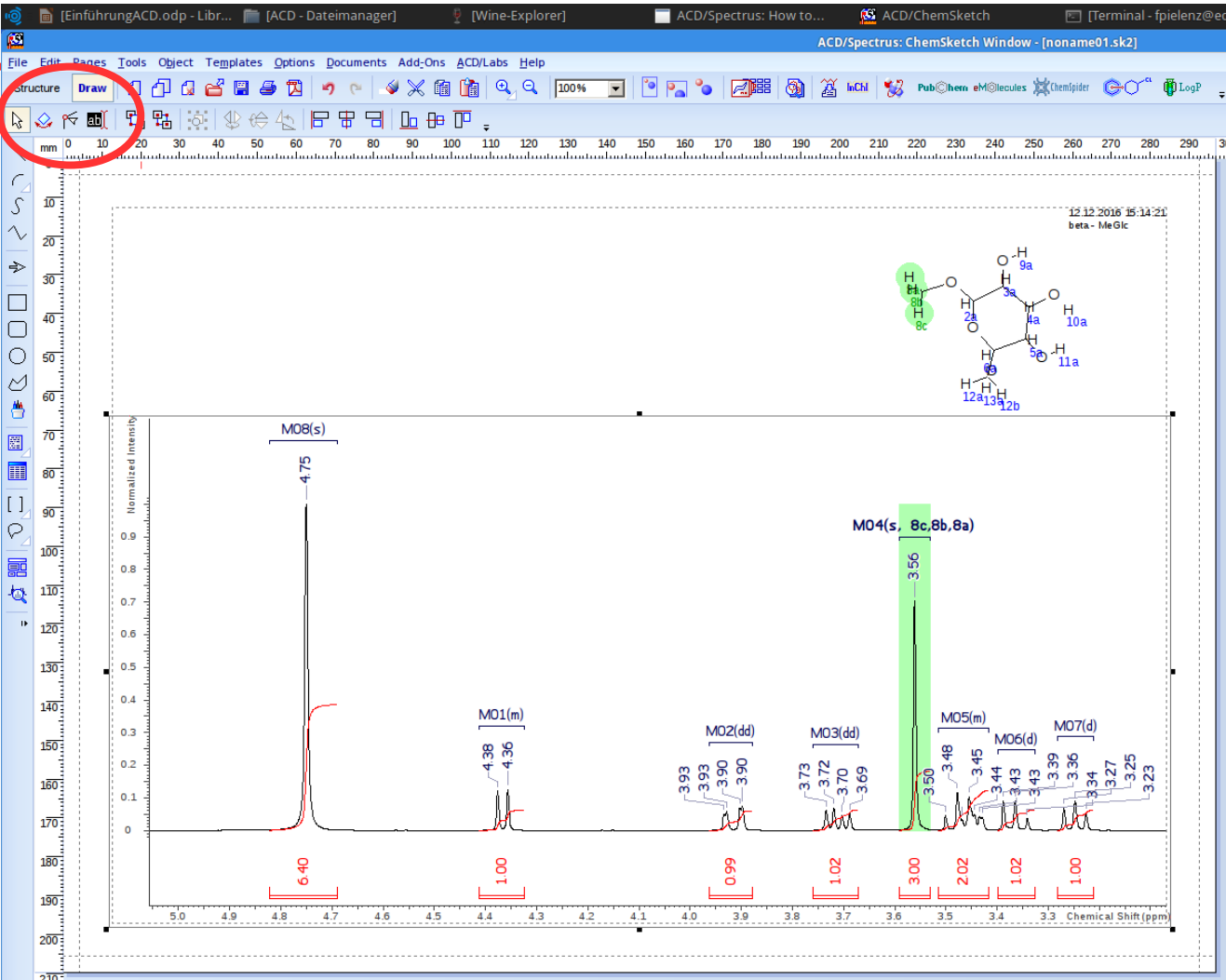
Report erstellen



Report erstellen



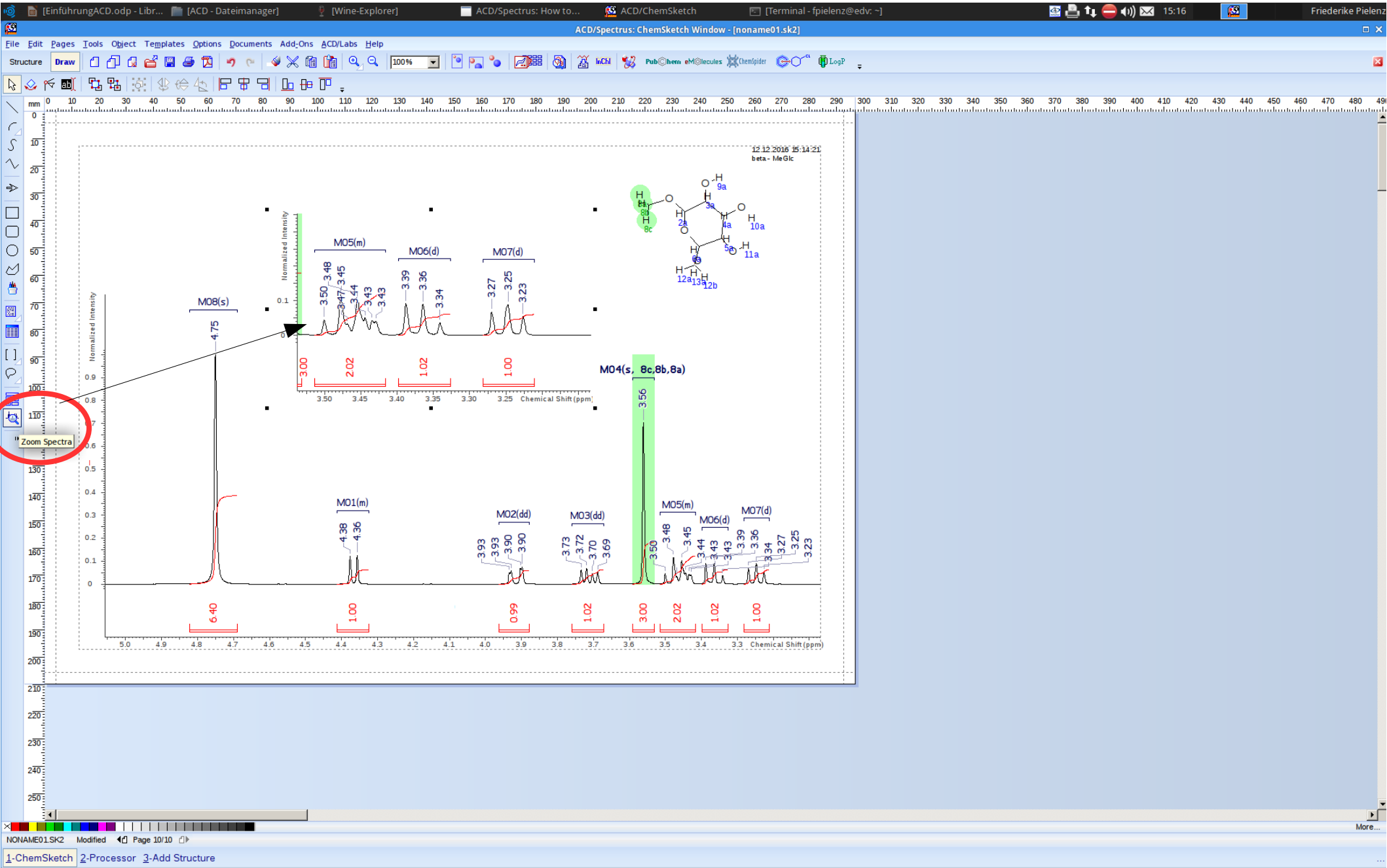
Report erstellen



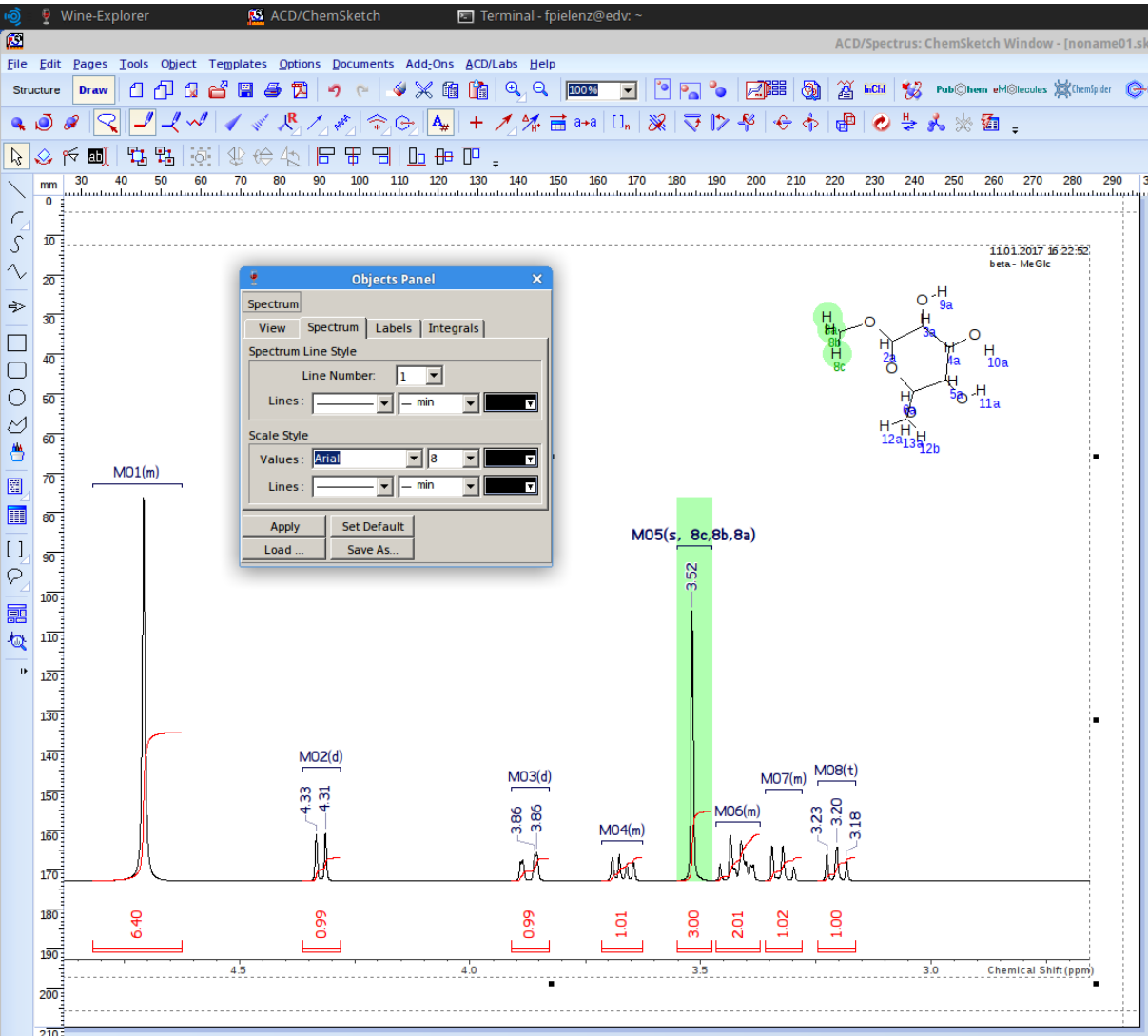
Objekt muss zuvor markiert und kann dann ggf. verschoben oder gelöscht werden.

Das Spektrum kann mittels *copy+paste* zum Beispiel in Office verwendet werden.

Report erstellen

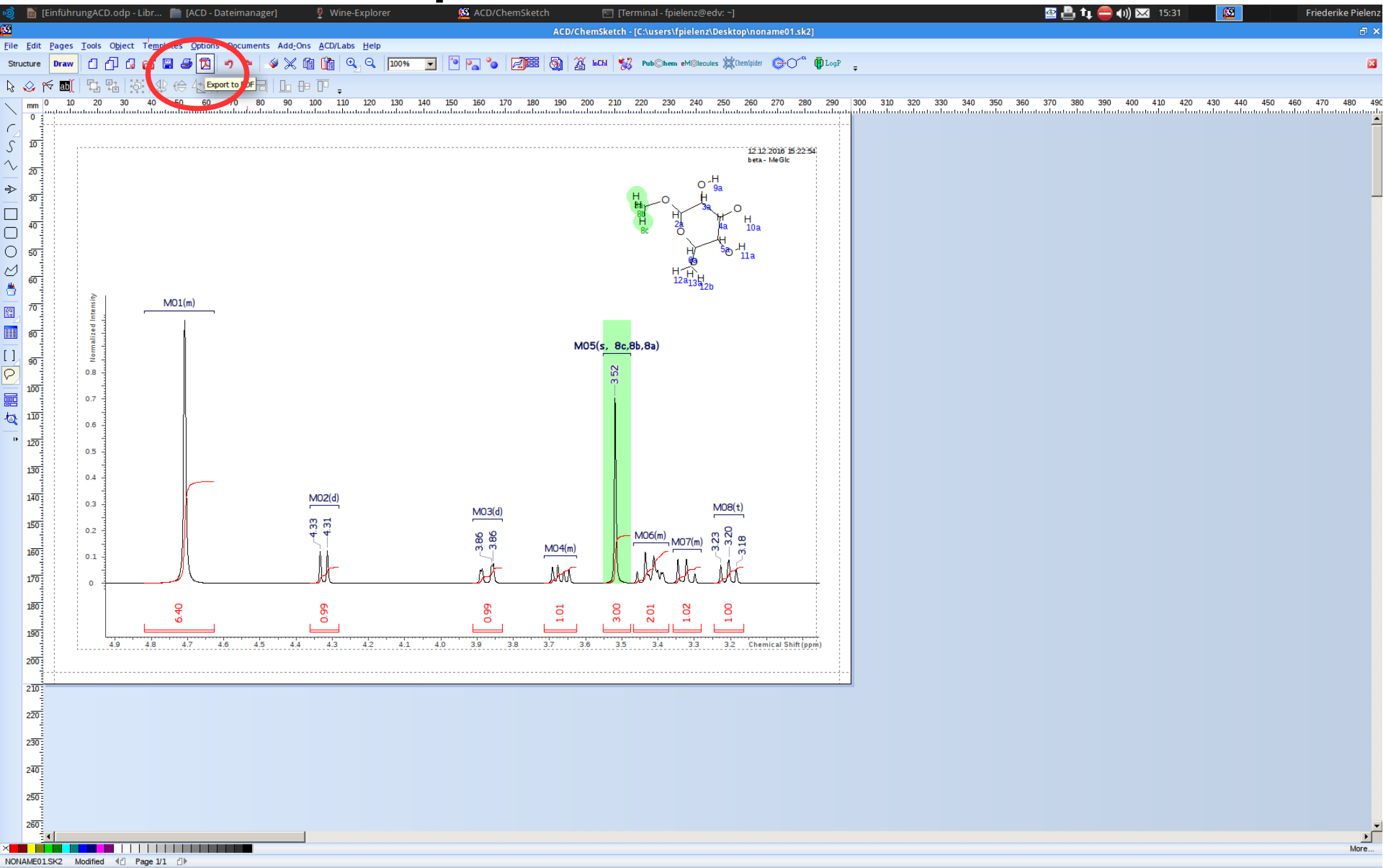


Report erstellen



Durch Doppelklick auf das Objekt öffnet sich ein Fenster um das Layout anzupassen und zu speichern.

Spektrum drucken



Fragen?