

11. Januar 2017 / Friederike Pielenz

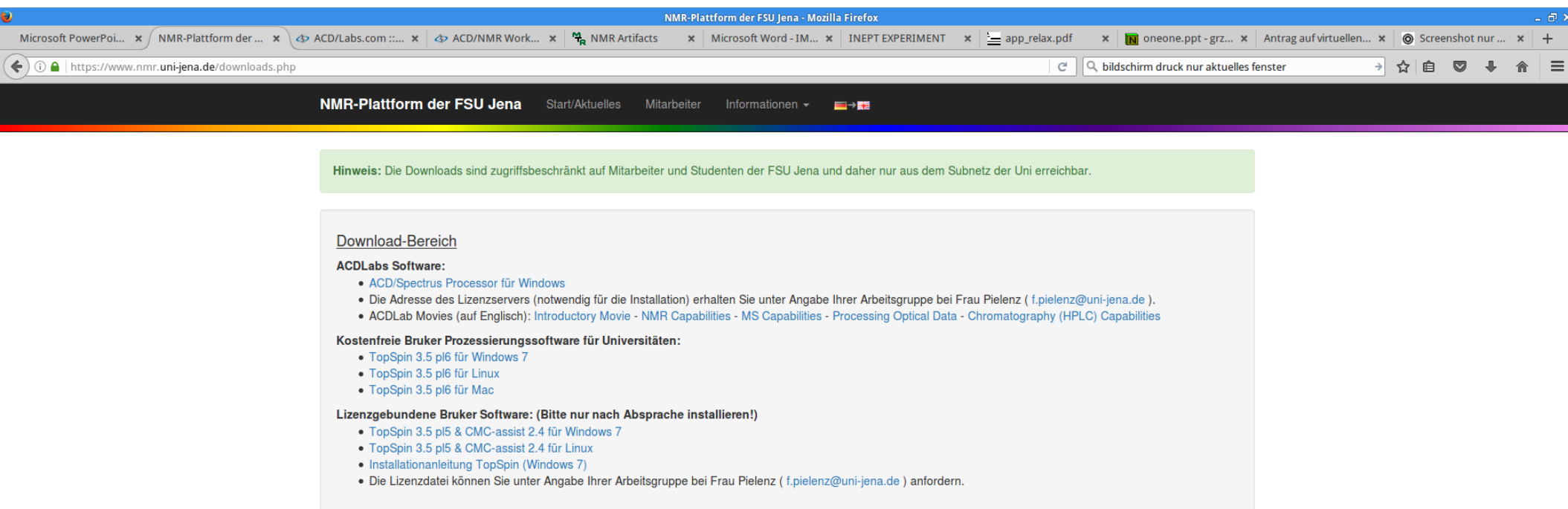
Einführung in ACD-Labs



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
 - 2D-Spektren prozessieren
 - Spektren darstellen und drucken
1. automatisch
2. manuell

Software installieren

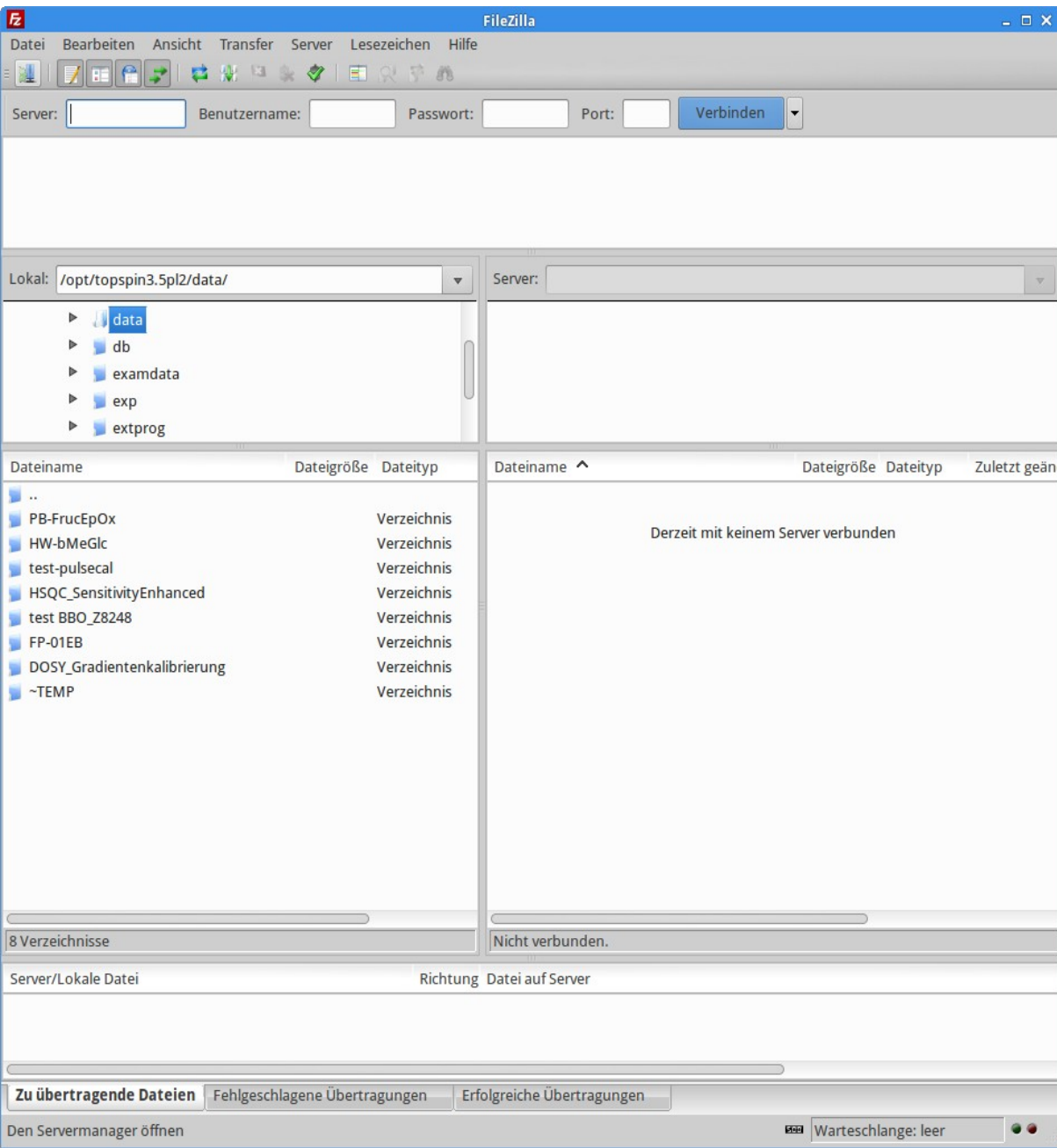


The screenshot shows a web browser window with the URL <https://www.nmr.uni-jena.de/downloads.php>. The page title is "NMR-Plattform der FSU Jena". A green notice box at the top states: "Hinweis: Die Downloads sind zugriffsbeschränkt auf Mitarbeiter und Studenten der FSU Jena und daher nur aus dem Subnetz der Uni erreichbar." Below this, the "Download-Bereich" is divided into three sections:

- ACDLabs Software:**
 - [ACD/Spectrus Processor für Windows](#)
 - Die Adresse des Lizenzservers (notwendig für die Installation) erhalten Sie unter Angabe Ihrer Arbeitsgruppe bei Frau Pielenz (f.pielenz@uni-jena.de).
 - ACDLab Movies (auf Englisch): [Introductory Movie](#) - [NMR Capabilities](#) - [MS Capabilities](#) - [Processing Optical Data](#) - [Chromatography \(HPLC\) Capabilities](#)
- Kostenfreie Bruker Prozessierungssoftware für Universitäten:**
 - [TopSpin 3.5 pl6 für Windows 7](#)
 - [TopSpin 3.5 pl6 für Linux](#)
 - [TopSpin 3.5 pl6 für Mac](#)
- Lizenzgebundene Bruker Software: (Bitte nur nach Absprache installieren!)**
 - [TopSpin 3.5 pl5 & CMC-assist 2.4 für Windows 7](#)
 - [TopSpin 3.5 pl5 & CMC-assist 2.4 für Linux](#)
 - [Installationanleitung TopSpin \(Windows 7\)](#)
 - Die Lizenzdatei können Sie unter Angabe Ihrer Arbeitsgruppe bei Frau Pielenz (f.pielenz@uni-jena.de) anfordern.

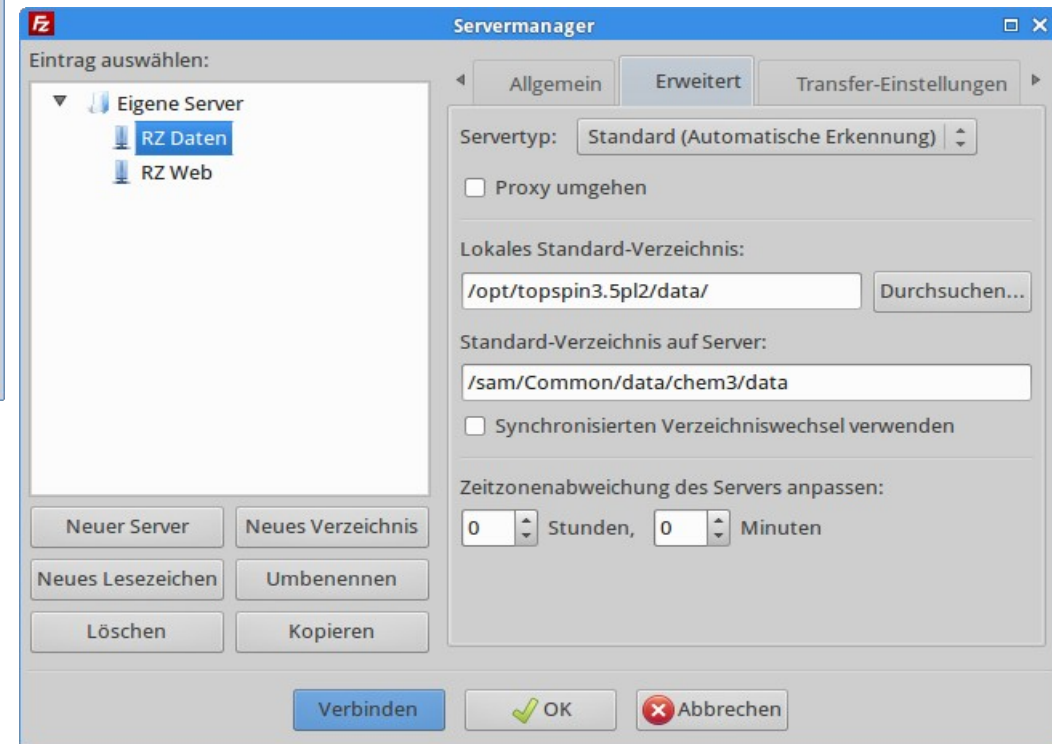
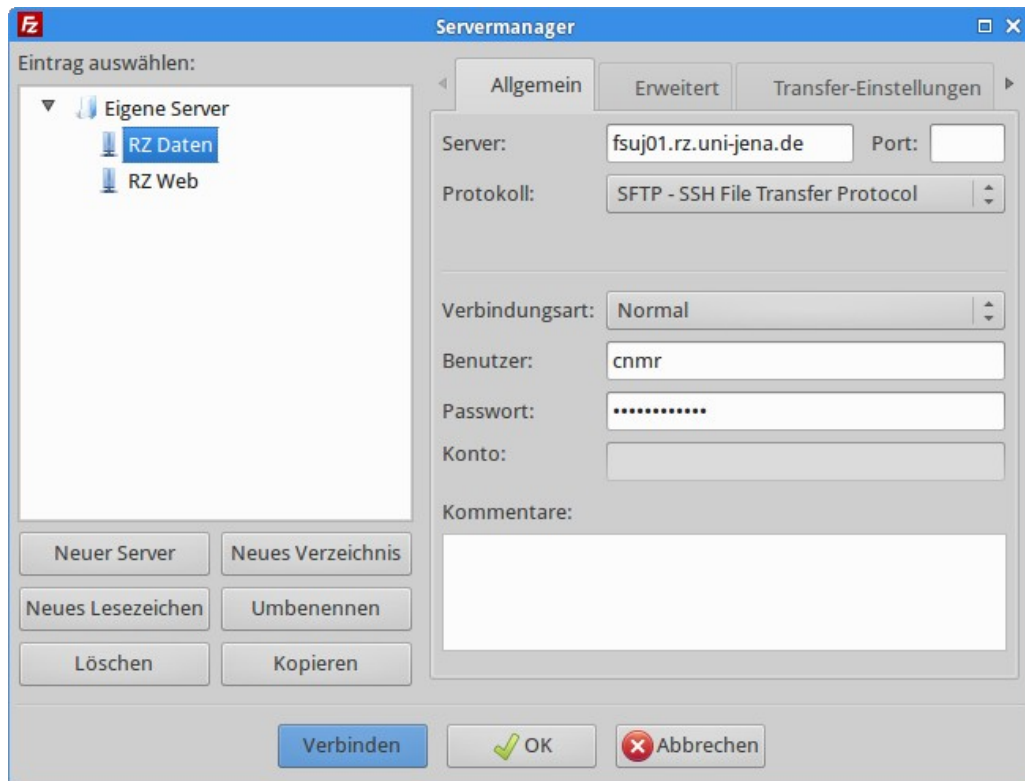
Die Software kann auf der Webseite der NMR-Plattform www.nmr.uni-jena.de heruntergeladen werden. Zur Installation muss der Rechner mit dem Uninetz verbunden sein. Bei Windows10 ist zuvor noch *net framework 3.5* zu installieren.

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

RZ Daten - sftp://cnmr@fsuj01.rz.uni-jena.de - FileZilla

Server: Benutzername: Passwort: Port: Verbinden

Status: Empfangen Verzeichnisstruktur...

Befehl: cd "AG_Arndt"

Antwort: New directory is: "/sam/Common/data/chem3/data/data/AG_Arndt"

Befehl: ls

Status: Listing directory /sam/Common/data/chem3/data/data/AG_Arndt

Status: Anzeigen des Verzeichnisinhalts abgeschlossen

Lokal: /opt/topspin3.5pl2/data/ Server: /sam/Common/data/chem3/data/data/AG_Arndt

Dateiname	Dateigröße	Dateityp	Dateiname	Dateigröße	Dateityp	Zuletzt geändert
..			..			
PB-FrucEpOx		Verzeichnis	Archiv_2015		Verzeichnis	21.01.2016
HW-bMeGlc		Verzeichnis	nmr		Verzeichnis	30.11.2016 10
test-pulsecal		Verzeichnis				
HSQC_SensitivityEnhanced		Verzeichnis				
test BBO_Z8248		Verzeichnis				
FP-01EB		Verzeichnis				
DOSY_Gradientenkalibrierung		Verzeichnis				
~TEMP		Verzeichnis				

8 Verzeichnisse

2 Verzeichnisse

Server/Lokale Datei Richtung Datei auf Server

Zu übertragende Dateien Fehlgeschlagene Übertragungen Erfolgreiche Übertragungen

Warteschlange: leer

RZ Daten - sftp://cnmr@fsuj01.rz.uni-jena.de - FileZilla

Server: Benutzername: Passwort: Port: Verbinden

Status: Empfangen Verzeichnisstruktur...

Befehl: cd "nmr"

Antwort: New directory is: "/sam/Common/data/chem3/data/data/AG_Arndt/nmr"

Befehl: ls

Status: Listing directory /sam/Common/data/chem3/data/data/AG_Arndt/nmr

Status: Anzeigen des Verzeichnisinhalts abgeschlossen

Lokal: /opt/topspin3.5pl2/data/ Server: /sam/Common/data/chem3/data/data/AG_Arndt/nmr

Dateiname	Dateigröße	Dateityp	Dateiname	Dateigröße	Dateityp	Zuletzt geändert
..			..			
PB-FrucEpOx		Verzeichnis	AG-1		Verzeichnis	03.11.2016
HW-bMeGlc		Verzeichnis	AG-10		Verzeichnis	03.11.2016
test-pulsecal		Verzeichnis	AG-11		Verzeichnis	03.11.2016
HSQC_SensitivityEnhanced		Verzeichnis	AG-12		Verzeichnis	03.11.2016
test BBO_Z8248		Verzeichnis	AG-13		Verzeichnis	03.11.2016
FP-01EB		Verzeichnis	AG-14		Verzeichnis	03.11.2016
DOSY_Gradientenkalibrierung		Verzeichnis	AG-15		Verzeichnis	03.11.2016
~TEMP		Verzeichnis	AG-17		Verzeichnis	03.11.2016
			AG-2		Verzeichnis	03.11.2016
			AG-3		Verzeichnis	03.11.2016
			AG-4		Verzeichnis	03.11.2016
			AG-5		Verzeichnis	03.11.2016
			AG-6		Verzeichnis	03.11.2016
			AG-7		Verzeichnis	03.11.2016
			AG-8		Verzeichnis	03.11.2016
			AG-9		Verzeichnis	03.11.2016

8 Verzeichnisse

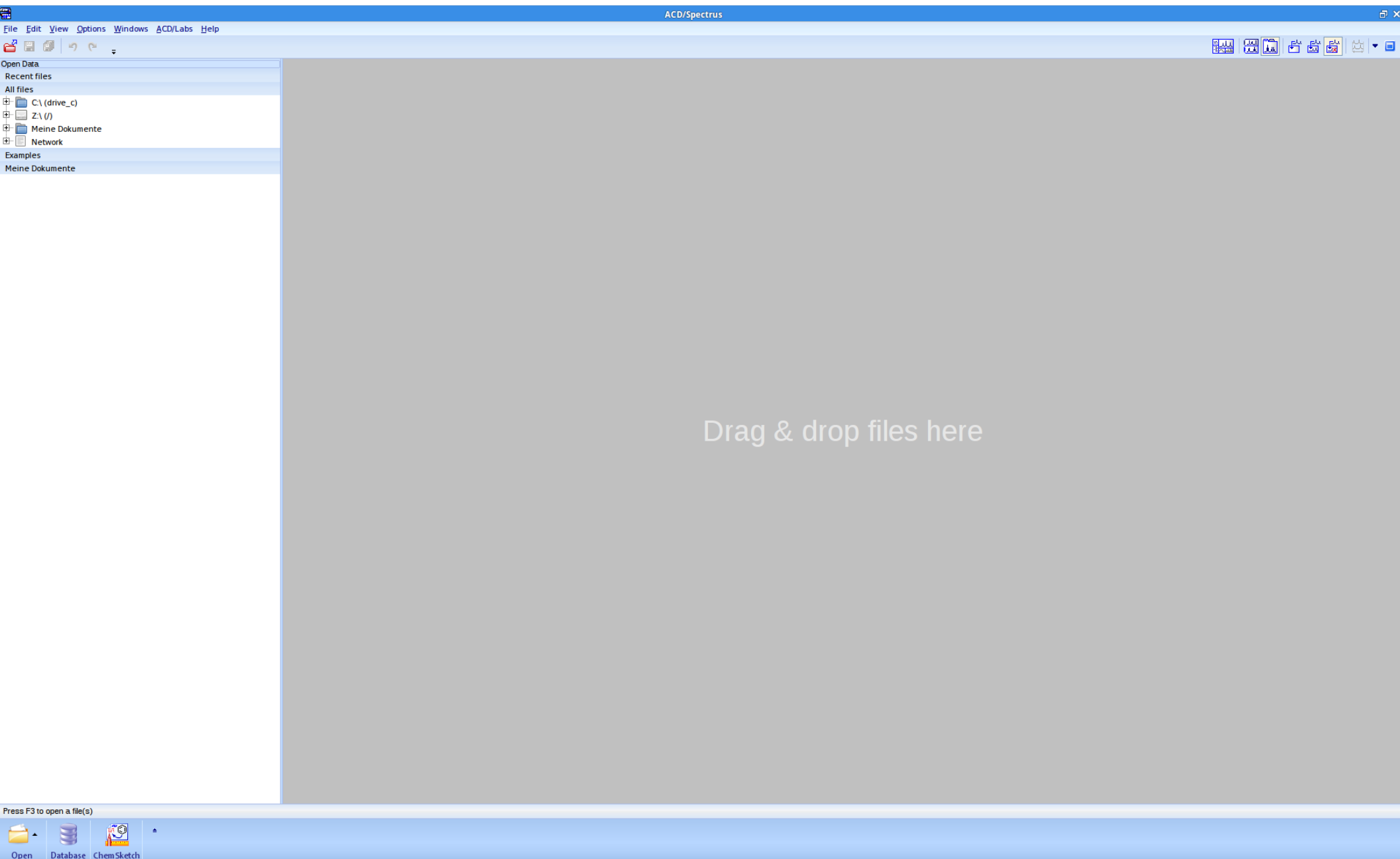
1 Verzeichnis ausgewählt.

Server/Lokale Datei Richtung Datei auf Server

Zu übertragende Dateien Fehlgeschlagene Übertragungen Erfolgreiche Übertragungen

Warteschlange: leer

Daten in ACD-Labs öffnen



Daten in ACD-Labs öffnen

ACD/Spectrus

File Edit View Options Windows ACD/Labs Help

Open Data

- lost+found
- media
- mnt
- opt
 - Adobe
 - brother
 - Bruker
 - DynamicsCenter
 - sophos-av
 - topspin
 - topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)

- PB-FrucEpOx
- test BBO_Z0248
- test-pulsecal
- ~TEMP
- db
- examdata
- exp

Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10
Drag&Drop to open data
Drag&Drop with Ctrl key to collect series
Ctrl+F to add to Favorites

Drag & drop files here

Press F3 to open a file(s)

Open Database ChemSketch

Daten in ACD-Labs öffnen

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data...

- lost+found
- media
- mnt
- opt
 - Adobe
 - brother
 - Bruker
 - DynamicsCenter
 - sophos-av
 - topspin
 - topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
 - PB-FrucEpOx
 - test_BBQ_Z8248
 - test-pulsecal
 - ~TEMP
 - db
 - examdata

HW-bMeGlc.010.001.1r.esp

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 10.06$ ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report ChemSketch

Daten in ACD-Labs öffnen

Um zwei Spektren zu vergleichen *Open Data in Current Window (As Series)* aktivieren und das zweite Spektrum in das Fenster ziehen.

Spectral Data

Preprocessing Options...

- Display only Known File Formats
- Display Open Data Window when No Spectra Displayed
- Close Open Data Window after Open Files
- Open Data in New Window
- Open Data in Current Window (As Series)
- Open Data Replacing Current Data

Open Process Peak Detection Interpret Report Chem Sketch

NI | AI | ppm Hz pts

Daten in ACD-Labs öffnen

The screenshot displays the ACD/Labs software interface. On the left, the 'Organizer' pane shows a file tree with 'HW-bMeGlc' selected under 'topspin3 5pl2\data'. The main window shows the chemical structure of HW-bMeGlc (a sugar derivative) with protons labeled 8a, 8b, 8c, 9a, 2a, 3a, 4a, 5a, 10a, 11a, 12a, 13a, and 12b. The 1H NMR spectrum is shown on the right, with peaks corresponding to these labels. The x-axis is 'Chemical Shift (ppm)' ranging from 21 to -2. The y-axis is intensity. A vertical red line is at approximately 12.48 ppm. The spectrum shows a complex multiplet between 3 and 5 ppm and a sharp peak at approximately 10.5 ppm. The text '1H' is visible in the center of the plot area.

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

HW-bMeGlc.010.001.1r.esp

Chemical Shift (ppm)

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 12.48$ ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Report ChemSketch

Daten in ACD-Labs öffnen

Durch aktivieren von *Spectra* können die einzelnen Spektren auch aus der Tabelle wieder entfernt werden.

1H

Spectral Data

No.	Color	Structure	Visible
1	[Blue]	[Structure]	[Checked]
2	[Green]	[Structure]	[Checked]

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H δ = 22.49 ppm 05_D20

NI | AI | ppm Hz pts

Spektrenausschnitt vergrößern

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Horizontal Zoom

HW-bMeGlc.010.001.1r.esp

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)
PB-FrucEpOx
test BBQ_Z8248
test-pulsecal
~TEMP
db
examdata

1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0

21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2

Chemical Shift (ppm)

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 21.73$ ppm 05_D20

Open Process Peak Detection Interpret Database Report ChemSketch

NI AI ppm Hz pts

Spektrenausschnitt vergrößern

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data...

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
 - PB-FrucEpOx
 - test_BBQ_Z8248
 - test-pulsecal
 - ~TEMP
 - db
 - examdata

HW-bMeGlc.010.001.1r.esp

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 3.99$ ppm 05_D20

Open Process Peak Detection Interpret Database Report ChemSketch

NI AI ppm Hz pts

Aufnahmeparameter anzeigen

Screenshot of the ACD/Spectrus software interface showing the process of displaying acquisition parameters for an NMR spectrum.

The main window displays the NMR spectrum of HW-bMeGlc.010.001.1r.esp. The x-axis represents Chemical Shift (ppm) from 5.1 to 2.8. The y-axis represents intensity. A chemical structure of the molecule is shown in the upper left, with protons labeled H1 through H13. A peak at 4.71 ppm is highlighted with a red box and labeled '1H'.

The 'View' menu is open, and the 'Panels' option is selected. The 'Spectrum Parameters' panel is visible, showing the following options:

- Spectrum Parameters
- Spectrum User Data
- Structure User Data
- Recgrd User Data
- Spectrum User Notes

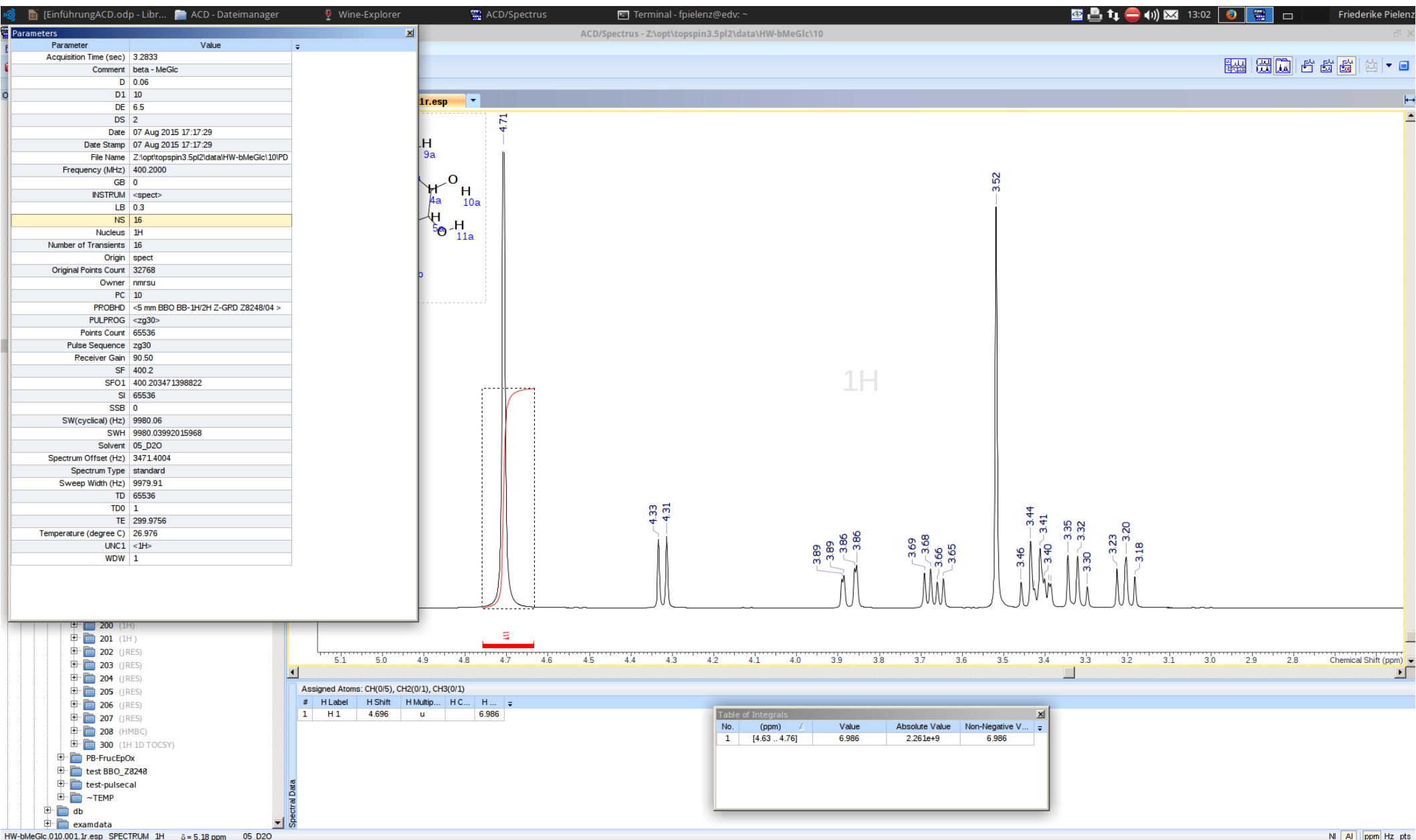
The 'Assigned Atoms' table is shown below the spectrum:

#	H Label	H Shift	H Multip...	H C...	H ...
1	H 1	4.696	u		6.986

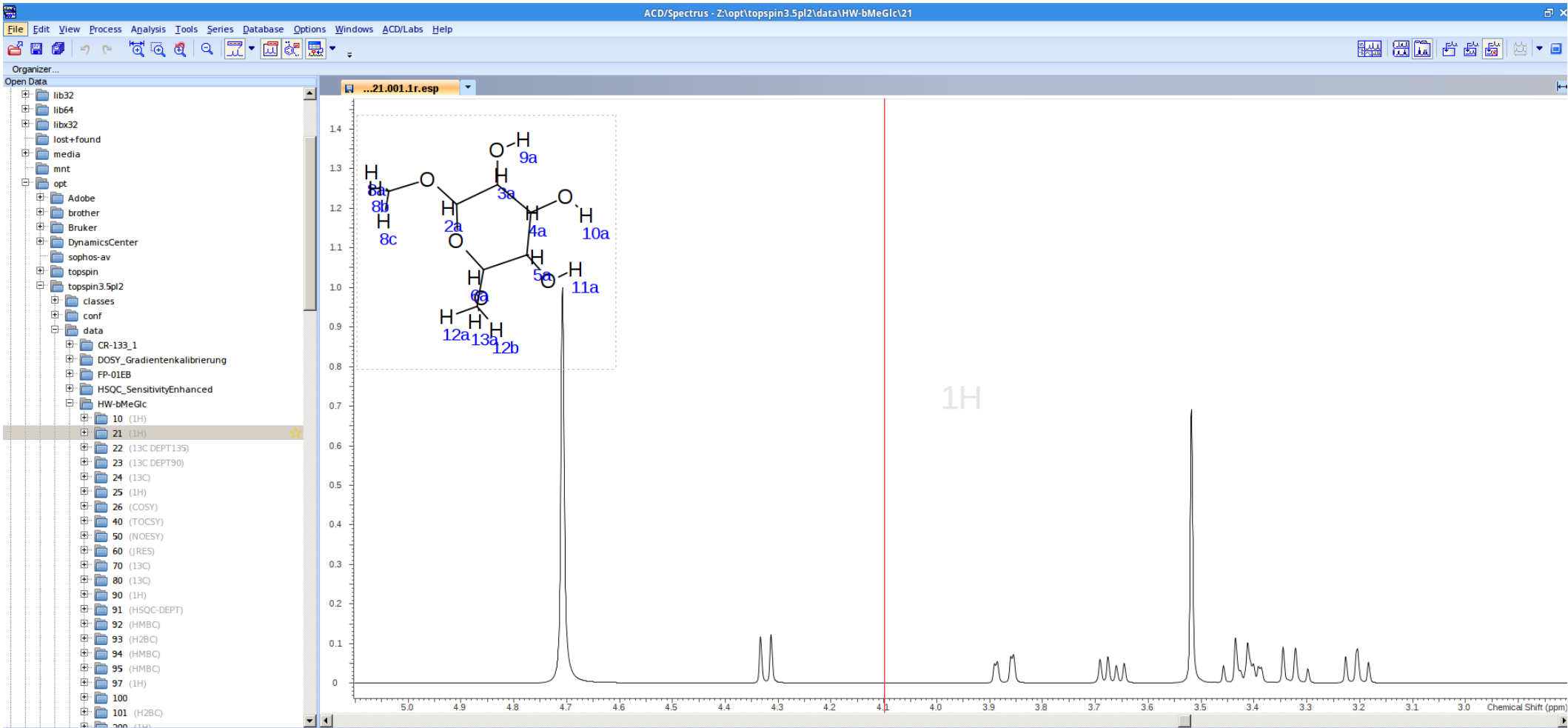
The 'Table of Integrals' window is also open, showing the following data:

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[4.63 .. 4.76]	6.986	2.261e+9	6.986

Aufnahmeparameter anzeigen



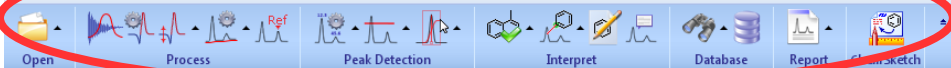
Idealfall



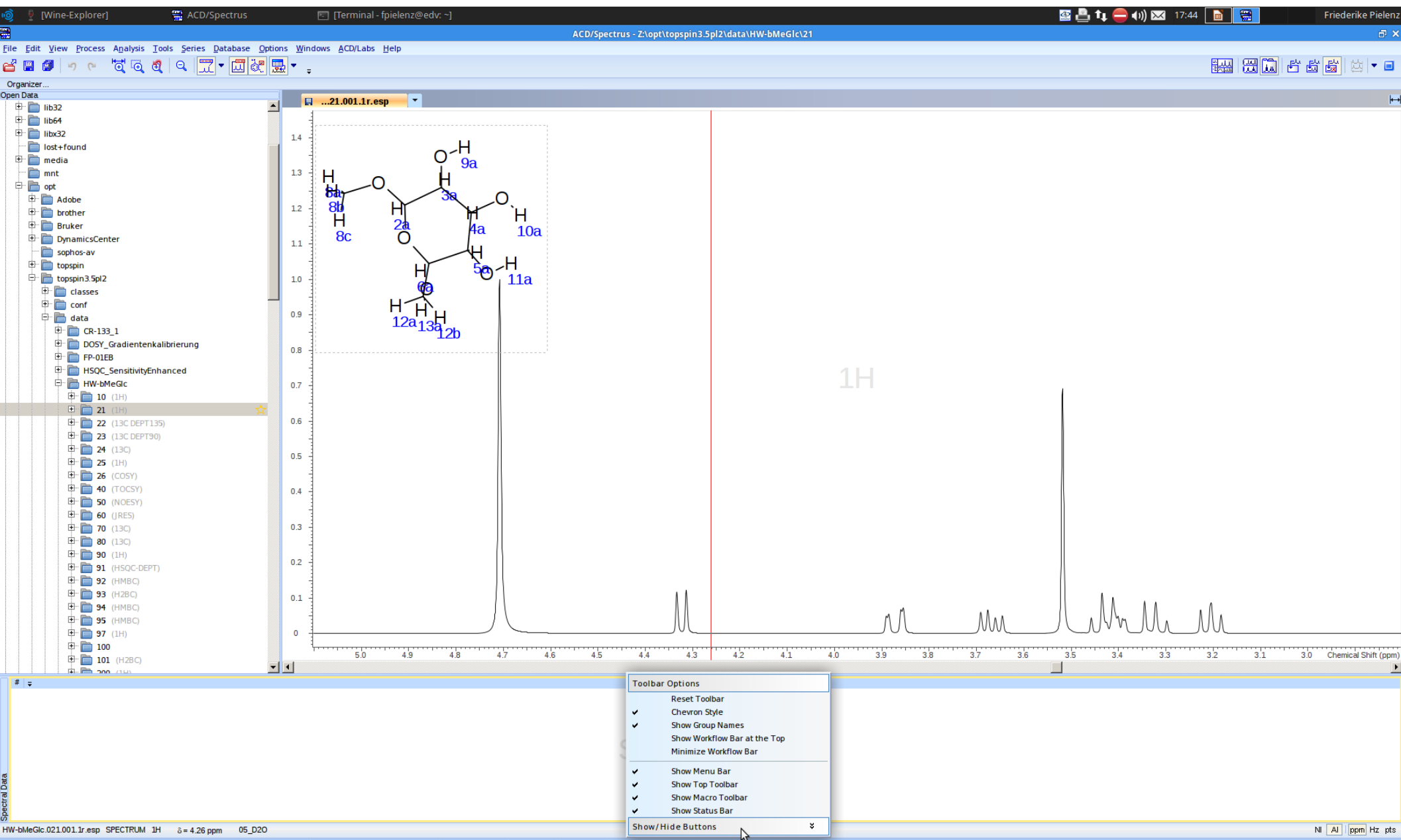
Autofunktionen in Workflowbar nutzen!

HW-bMeGlc.021.001.1r.esp SPECTRUM 1H $\delta = 4.10$ ppm 05_D20

NI AI ppm Hz pts



Idealfall



Idealfall

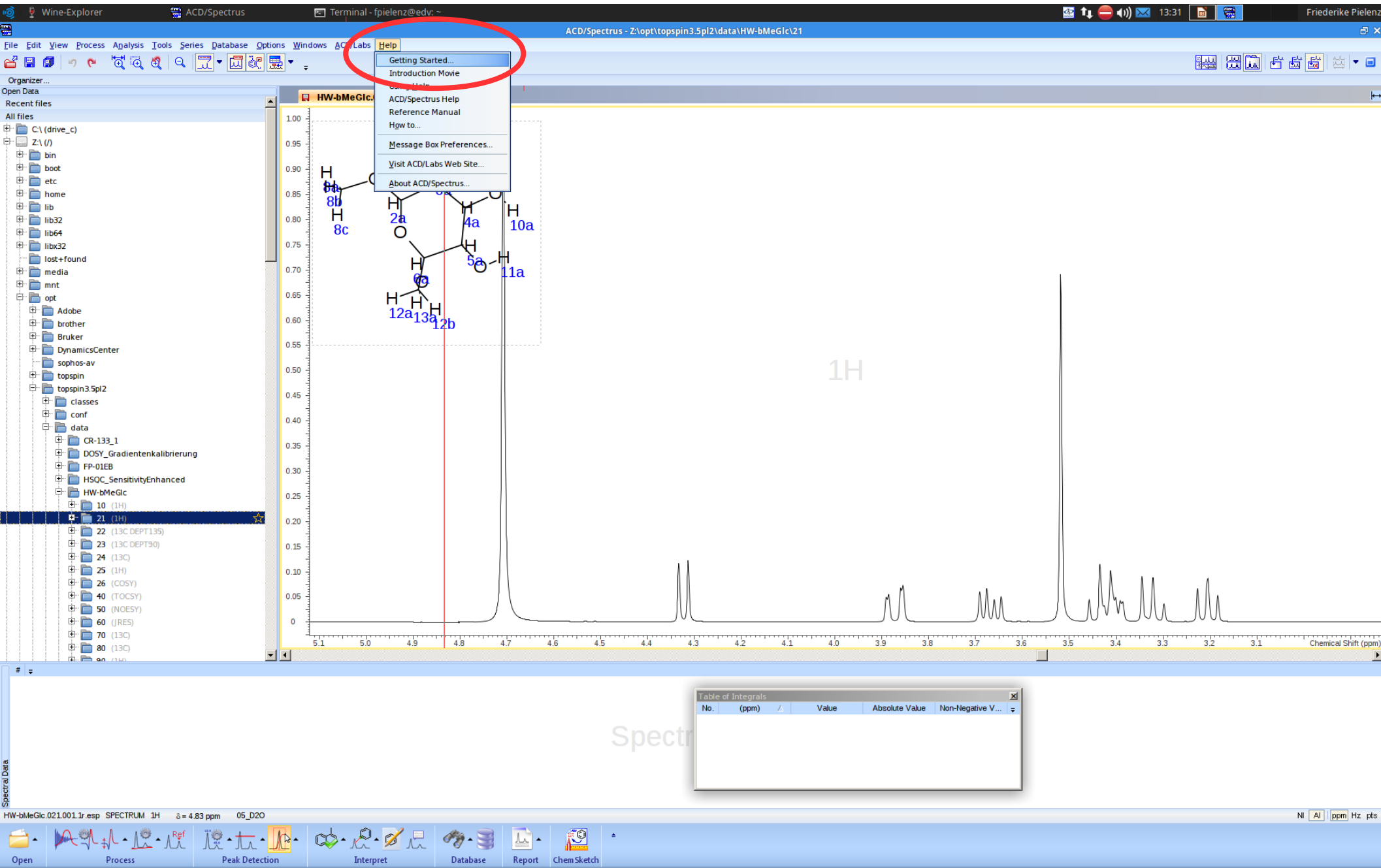
The screenshot displays the ACD/Spectrus software interface. The main window shows a 1H NMR spectrum of HW-bMeGlc (HW-bMethylglucoside) with a chemical structure overlay. The spectrum is centered around 4.7 ppm, with peaks labeled 1a through 13a. The chemical structure is a six-membered ring with various protons labeled: 1a, 2a, 3a, 4a, 5a, 6a, 7a, 8a, 8b, 8c, 9a, 10a, 11a, 12a, 13a, and 13b. The spectrum shows a complex multiplet pattern, with a prominent peak at approximately 4.7 ppm. The x-axis is labeled 'Chemical Shift (ppm)' and ranges from 4.5 to 5.1. The y-axis represents intensity, ranging from 0 to 1.00.

A 'Manual assignment' menu is open, showing various options for peak assignment and analysis. The menu items are:

- 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
 - Switch to Report Editor

The status bar at the bottom indicates the current file is 'HW-bMeGlc.021.001.1r.esp', the spectrum is 'SPECTRUM 1H', and the chemical shift is $\delta = 4.44$ ppm. The date is '05_D20'. The bottom toolbar includes buttons for 'Open', 'Process', 'Peak Detection', 'Interpret', 'Database', 'Report', and 'Chem Sketch'.

Idealfall



Idealfall – Phase korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv: - 13:38 Friederike Pielenz

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\21

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data Recent files All files C:\(drive_c) Z:\(l) bin boot etc home lib lib32 lib64 libx32 lost+found media mnt opt Adobe brother Bruker DynamicsCenter sophos-av topspin topspin3.5pl2 classes conf data CR-133_1 DOSY_Gradientenkalibrierung FP-01EB HSQC_SensitivityEnhanced 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)

HW-bMeGlc.021.001.1r.esp

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

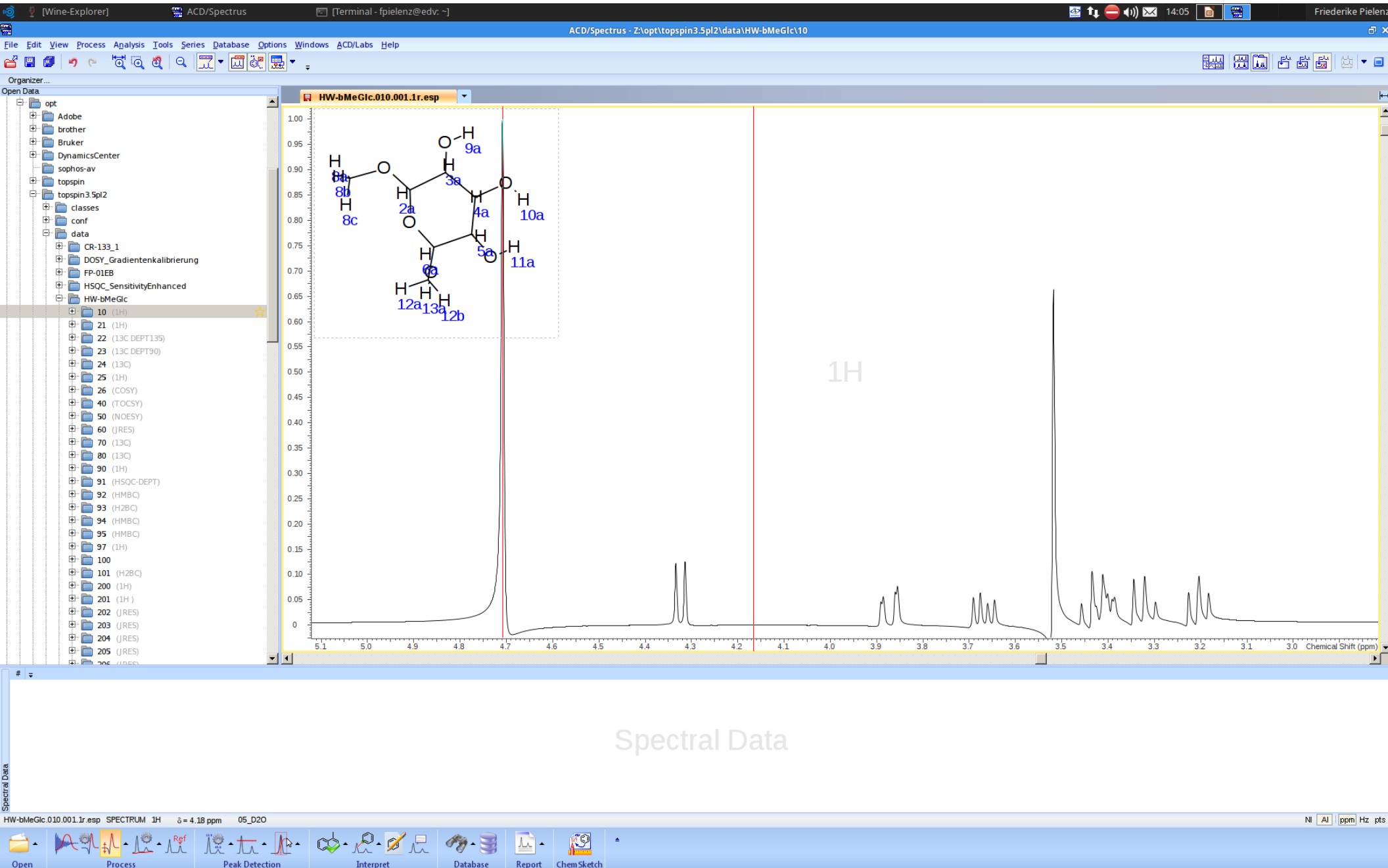
Phasing: auto
With built-in algorithms

HW-bMeGlc.021.001.1r.e SPECTRUM 1H $\delta = 4.13$ ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report Chem Sketch

Idealfall – Phase korrigieren



Spectral Data

Idealfall – Phase korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv. - 13:43 Friederike Pielenz

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\21

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data Recent files All files C:\ (drive_c) Z:\ (f) bin boot etc home lib lib32 lib64 libx32 lost+found media mnt opt Adobe brother Bruker DynamicsCenter sophos-av topspin topspin3.5pl2 classes conf data CR-133_1 DOSY_Gradientenkalibrierung FP-01EB HSQC_SensitivityEnhanced 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) 80 (1H)

HW-bMeGlc.021.001.1r.esp

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectr

HW-bMeGlc.021.001.1r.esp SPECTRUM 1H δ = 5.16 ppm 05_D20

Open Process Peak Detection Interpret Database Report ChemSketch

NI Al ppm Hz pts

Idealfall – Basislinie korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv: ~

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data

Recent files

All files

C:\(drive_c)

Z:\(I)

bin

boot

etc

home

lib

lib32

lib64

libx32

lost+found

media

mnt

opt

Adobe

brother

Bruker

DynamicsCenter

sophos-av

topspin

topspin3.5pl2

classes

conf

data

CR-133_1

DOSY_Gradientenkalibrierung

FP-01EB

HSQC_SensitivityEnhanced

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 (13C)

HW-bMeGlc.010.001.1r.esp

0.85

0.80

0.75

0.70

0.65

0.60

0.55

0.50

0.45

0.40

0.35

0.30

0.25

0.20

0.15

0.10

0.05

0

-0.05

-0.10

-0.15

5.0

4.9

4.8

4.7

4.6

4.5

4.4

4.3

4.2

4.1

4.0

3.9

3.8

3.7

3.6

3.5

3.4

3.3

3.2

3.1

3.0

Chemical Shift (ppm)

1H

9a

3a

2a

4a

5a

10a

11a

8a

8b

8c

12a

13a

12b

Table of Integrals

No.	(ppm)	Δ	Value	Absolute Value	Non-Negative V...

Baseline: auto
Correct spectrum for baseline with built-in algorithms

Spectr

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H δ = 4.57 ppm 05_D20

NI | AI | ppm Hz pts

Open Process Peak Detection Interpret Database Report Chem Sketch

Idealfall – Basislinie korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv: ~

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data

Recent files

All files

C:\(drive_c)

Z:\(j)

bin

boot

etc

home

lib

lib32

lib64

libx32

lost+found

media

mnt

opt

Adobe

brother

Bruker

DynamicsCenter

sophos-av

topspin

topspin3.5pl2

classes

conf

data

CR-133_1

DOSY_Gradientenkalibrierung

FP-01EB

HSQC_SensitivityEnhanced

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 (13C)

HW-bMeGlc.010.001.1r.esp

Chemical Shift (ppm)

1H

Table of Integrals

No.	(ppm)	Δ	Value	Absolute Value	Non-Negative V...

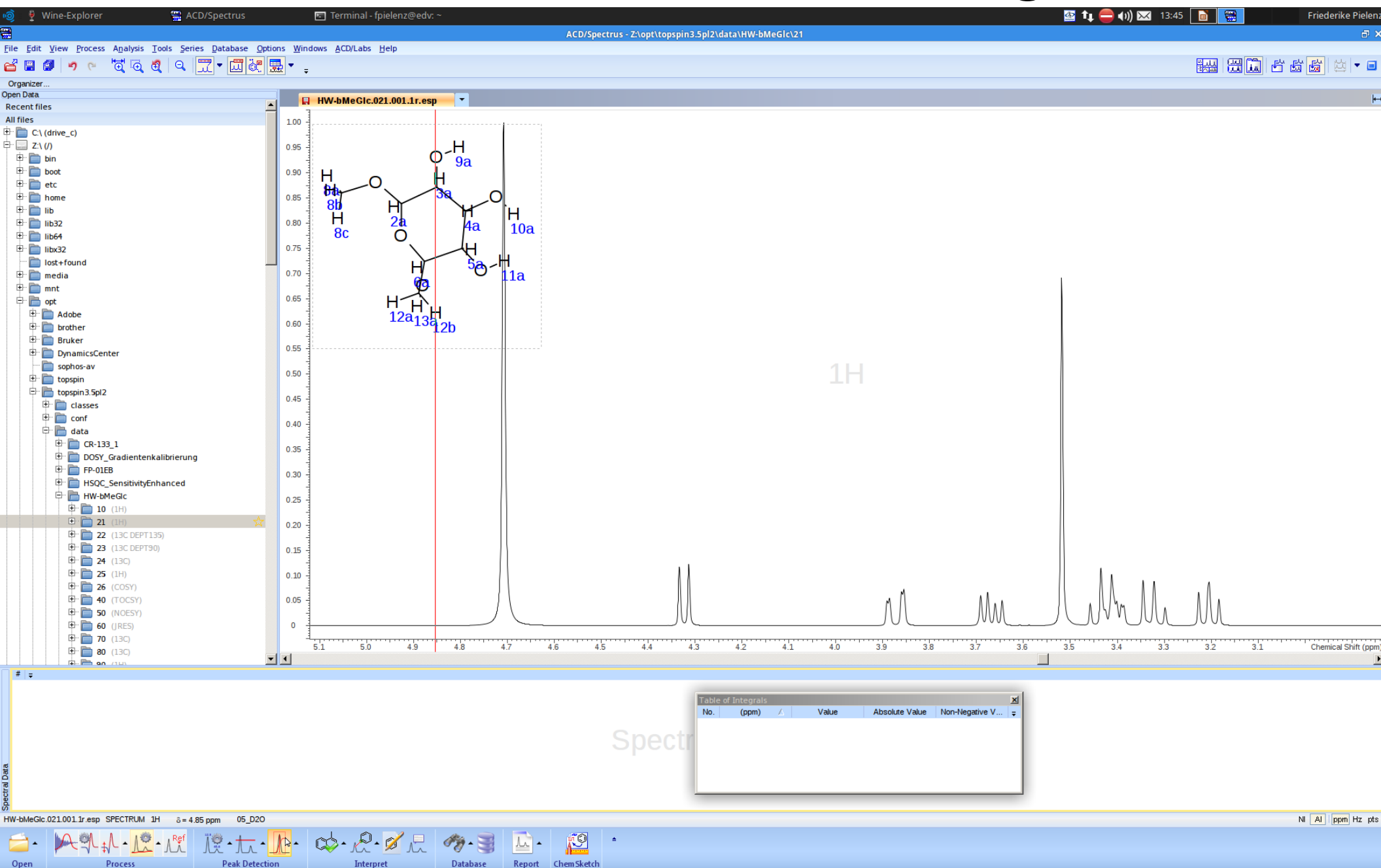
Baseline: auto
Correct spectrum for baseline with built-in algorithms

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H δ = 4.49 ppm 05_D20

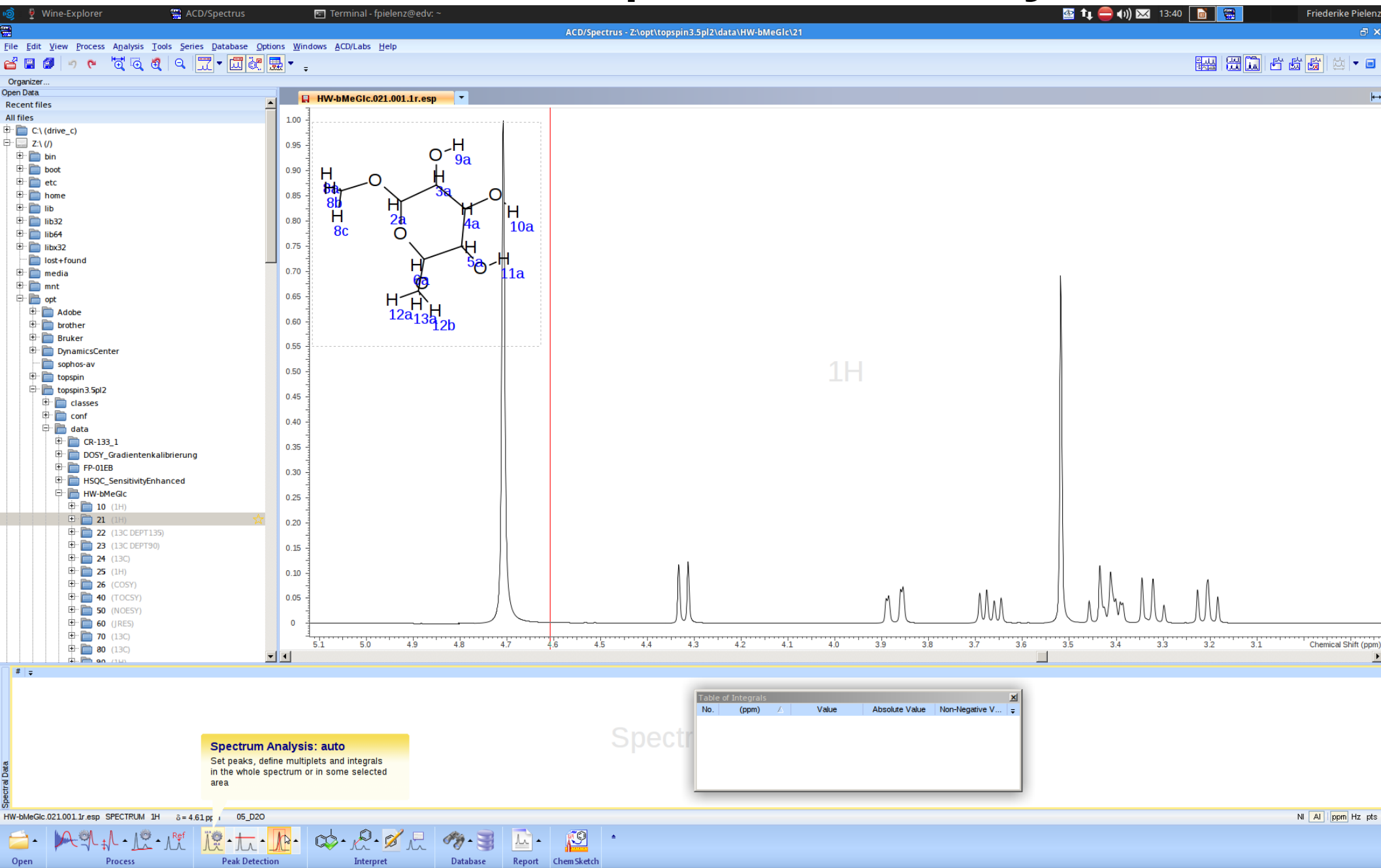
Open Process Peak Detection Interpret Database Report Chem Sketch

NI | AI | ppm Hz pts

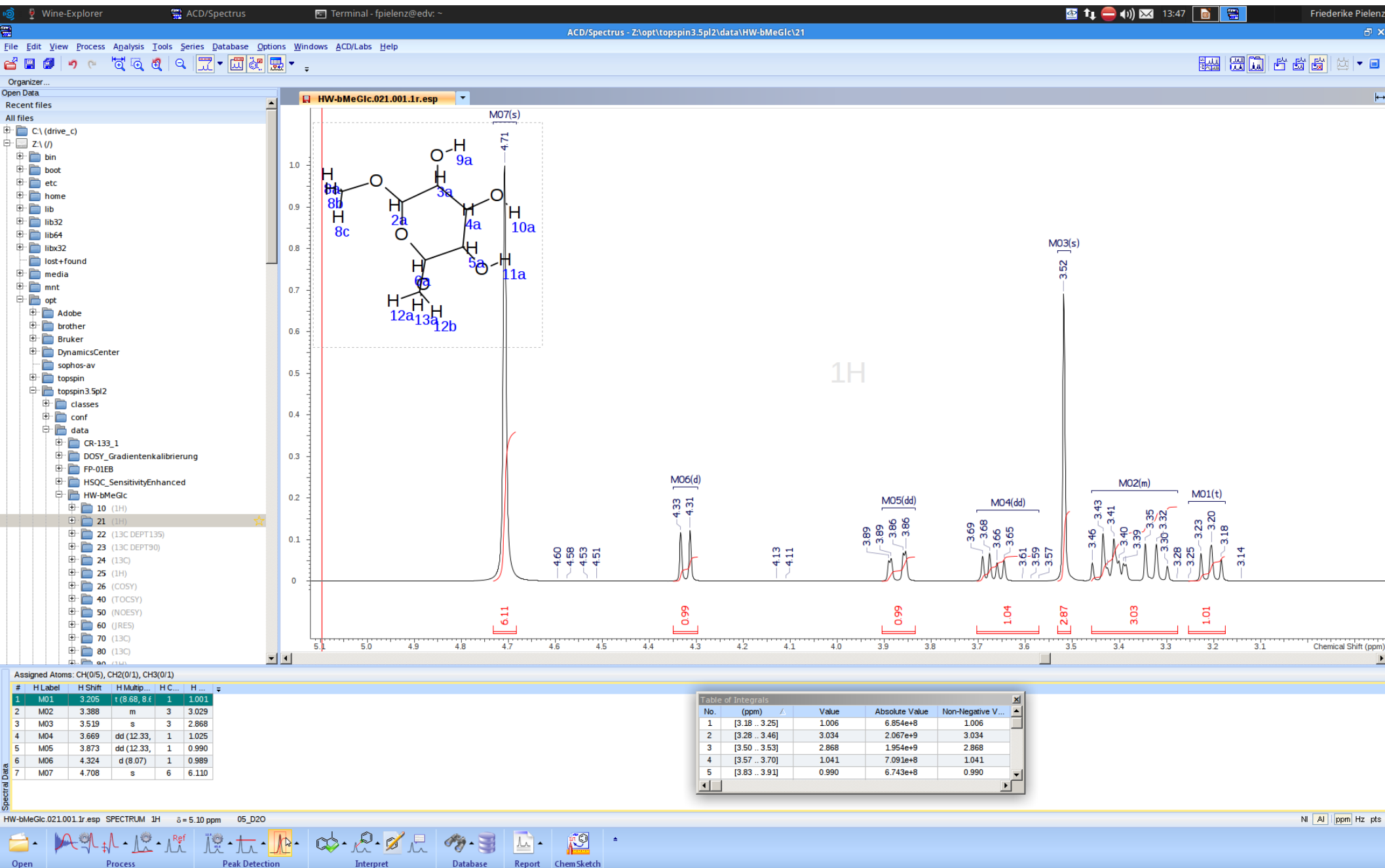
Idealfall – Basislinie korrigieren



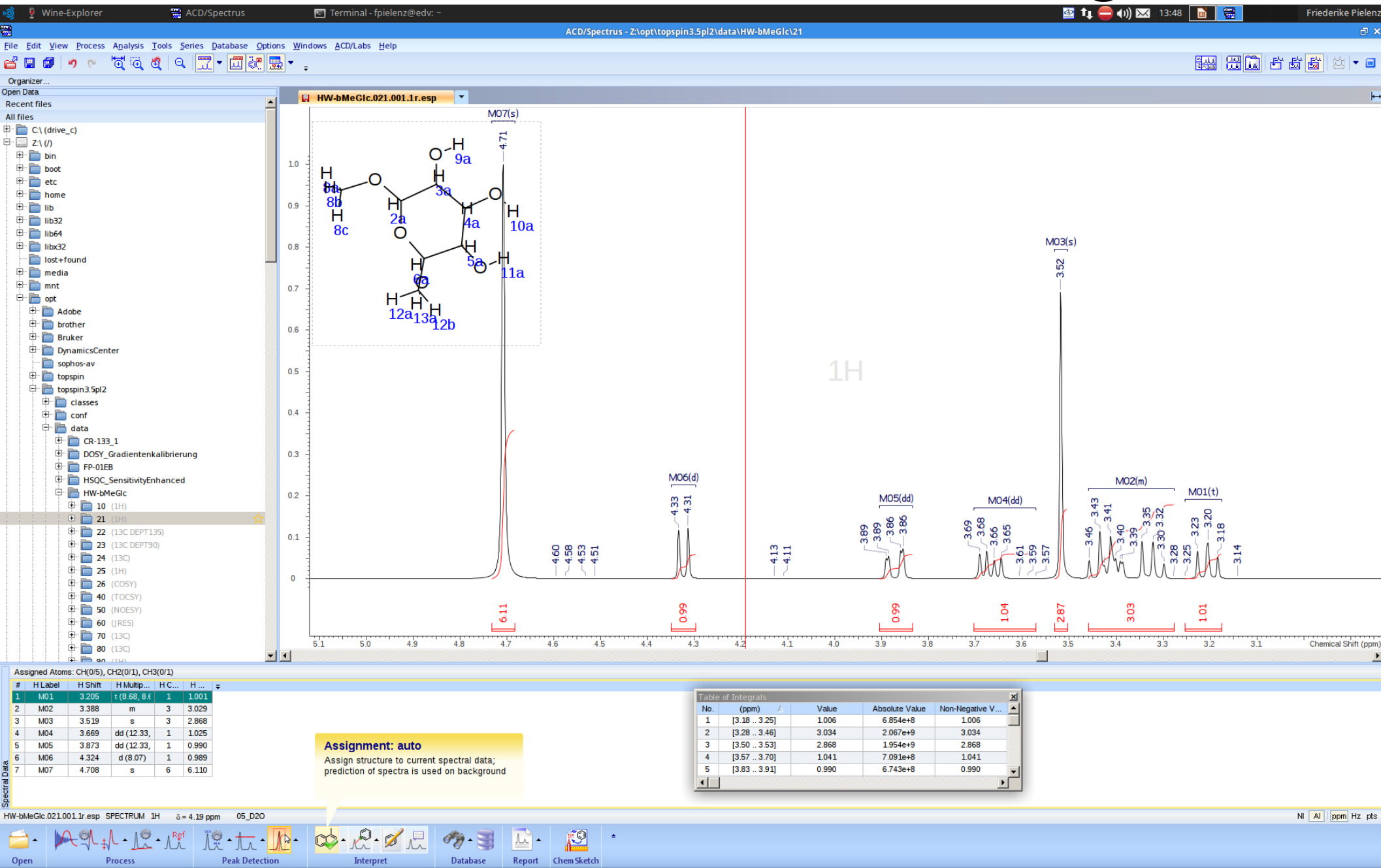
Idealfall - Spektrenanalyse



Idealfall - Spektrenanalyse



Idealfall - Peakzuordnung



Idealfall – Peakzuordnung prüfen

Wine-Explorer ACD/Spectrus Terminal - fpieienz@edv. - ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\21

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data Recent files All files

HW-bMeGlc.021.001.1r.esp

M07(s, 13a,9a,11a,2a)

M03(s, 12b,12a,3a)

M05(dd, 4a)

M04(dd)

M02(m)

M01(t)

Structure Verification
Match Factor: 0.89
OK

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M01	3.205	t (8.68, 8.6)	1	1.001
2	M02	3.388	m	3	3.029
3	M03	3.519	s	3	2.868
4	M04	3.669	dd (12.33, 1)	1	1.025
5	M05	3.873	dd (12.33, 1)	1	0.990
6	M06	4.324	d (8.07)	1	0.989
7	M07	4.708	s	6	6.110

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.18 .. 3.25]	1.006	6.854e+8	1.006
2	[3.28 .. 3.46]	3.034	2.067e+9	3.034
3	[3.50 .. 3.53]	2.868	1.954e+9	2.868
4	[3.57 .. 3.70]	1.041	7.091e+8	1.041
5	[3.83 .. 3.91]	0.990	6.743e+8	0.990

Assignment: auto
Assign structure to current spectral data;
prediction of spectra is used on background

HW-bMeGlc.021.001.1r.esp SPECTRUM 1H δ = 4.19 ppm 05_D20

NI | All | ppm | Hz | pts

Idealfall – FERTIG!



Vor der FT: Window Funktionen

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Tools Series Options Windows ACD/Labs Help

Interactive FT...

- Fourier Transform
- Window Functions...
- Linear Prediction...
- Zero Filling...
- FID Shift...

HW-bMeGlc.010.001.1r.esp

Fourier Transform Options

Apply FT

Initial: 32768 Final: 65536

FID Shift

FID Shift (pts): 1 Cyclical

Linear Prediction

Backward

Points to Predic: 1 2

Base Points: 3 512

Coeff Count: 32

Forward

Points to Predic: 32768 65536

Base Points: 3 512

Coeff Count: 64

Window Function

User

	LB	Tm (sec)
<input checked="" type="checkbox"/> EM	0	0
<input type="checkbox"/> GM	0	0
<input type="checkbox"/> Sine	0	0
<input type="checkbox"/> Sq Sine	0	0

Phase Correction Options...

Instant Preview Show Window Function

Apply OK Close Help

1H

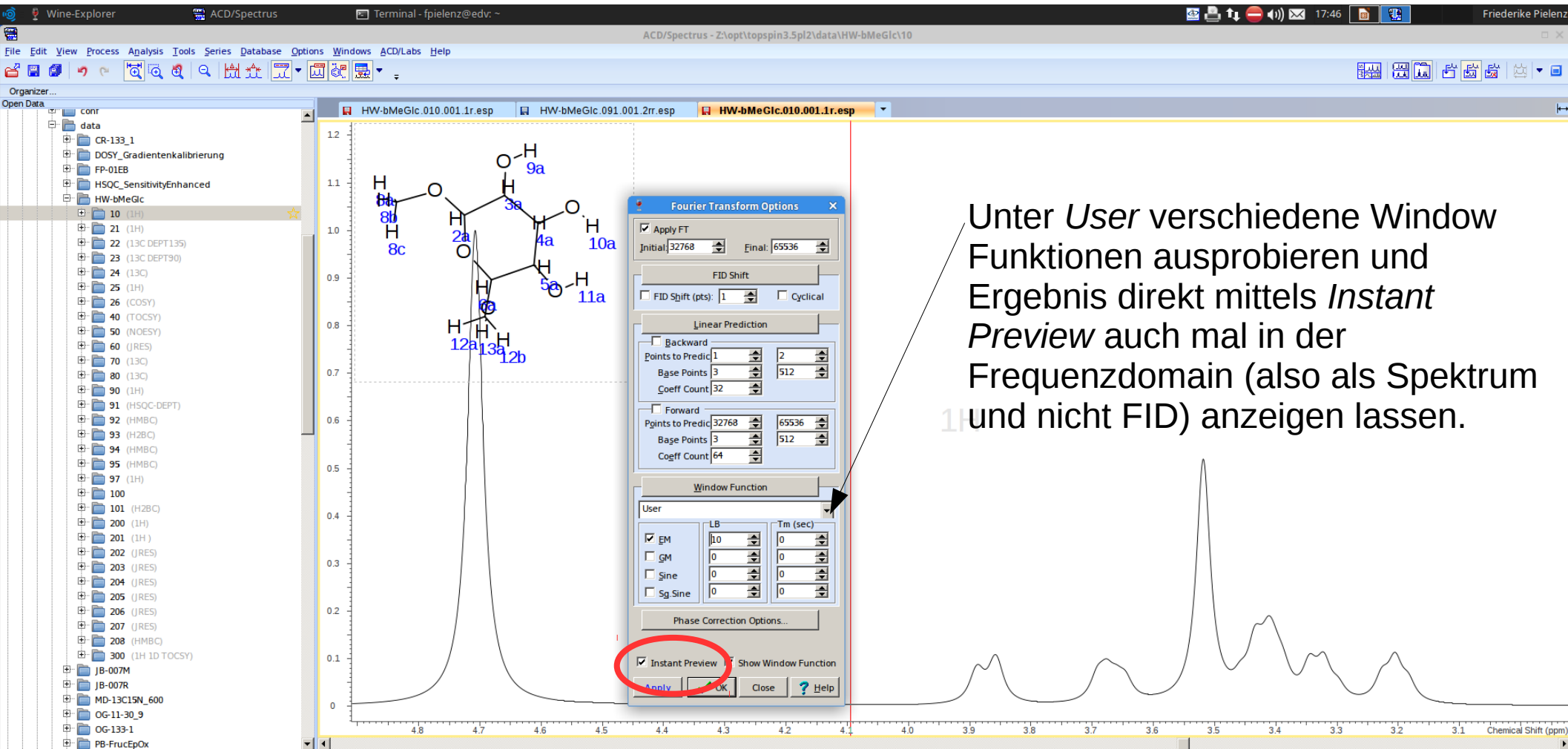
Spectral Data

HW-bMeGlc.010.001.1r.esp FID 1H 05_D20

Open Process Peak Detection Interpret Report ChemSketch

Ni Alt sec pts

Vor der FT: Window Funktionen



Spectral Data

Phase korrigieren

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View **Process** Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data

Process menu:

- Interactive FT...
- Inverse FT
- Initialize
- Phase Correction
 - Auto Phasing
 - Mouse Phasing
 - Fine Tuning
 - Options...
 - Flip Phase
 - Synchronize APT/DEPT Phase
- Baseline Correction
- Smoothing...
- Reverse Spectrum
- Arithmetic...

HW-bMeGlc.010.001.1r.esp

Chemical structure: COC1OC(O)C(O)C(O)O1 (Methyl-beta-D-glucopyranoside)

Peak labels: 8c, 9a, 3a, 4a, 10a, 5a, 11a, 12a, 13a, 12b

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 5.15$ ppm 05_D20

NI AI ppm Hz pts

Phase korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv. - ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\21

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data Recent files All files C:\(drive_ Z:\(/ bin boot etc home lib lib32 lib64 libx32 lost+found media mnt opt Adobe brother Bruker DynamicsCenter sophos-av topspin topspin3.5pl2 classes conf data CR-133_1 DOSY_Gradientenkalibrierung FP-01EB HSQC_SensitivityEnhanced 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) 80 (1H)

Process Analysis Tools Series Database Options Windows ACD/Labs Help

Interactive FT... Inverse FT Initialize Phase Correction Baseline Correction Smoothing... Reverse Spectrum Arithmetic... Auto Phasing Mouse Phasing Fine Tuning Options... Flip Phase Synchronize APT/DEPT Phase

HW-bMeGlc.021.001.1r.esp

Chemical Shift (ppm)

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectr

HW-bMeGlc.021.001.1r.esp SPECTRUM 1H δ = 4.87 ppm 05_D20 NI Al ppm Hz pts

Open Process Peak Detection Interpret Database Report ChemSketch

Phase korrigieren

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

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Phase korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv: - ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data

Recent files

All files

C:\(drive_c)

Z:\(l)

bin

boot

etc

home

lib

lib32

lib64

libx32

lost+found

media

mnt

opt

Adobe

brother

Bruker

DynamicsCenter

sophos-av

topspin

topspin3.5pl2

classes

conf

data

CR-133_1

DOSY_Gradientenkalibrierung

FP-01EB

HSQC_SensitivityEnhanced

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)

80 (1H)

HW-bMeGlc.010.001.1r.esp

1.00

0.95

0.90

0.85

0.80

0.75

0.70

0.65

0.60

0.55

0.50

0.45

0.40

0.35

0.30

0.25

0.20

0.15

0.10

0.05

0

5.0

4.9

4.8

4.7

4.6

4.5

4.4

4.3

4.2

4.1

4.0

3.9

3.8

3.7

3.6

3.5

3.4

3.3

3.2

3.1

3.0

Chemical Shift (ppm)

9a

8a

8b

8c

2a

3a

4a

5a

10a

11a

12a

13a

12b

Phase Correction Options

Phase Parameters

Ph0: 92.7176 Flip Phase

Ph1: -104.0746 Fix Same Phase

Auto Phasing

Mouse Phasing Fine Tuning

Instant Preview

Apply OK Close Help

Table of Integrals

No.	(ppm)	Δ	Value	Absolute Value	Non-Negative V...

Spectr

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H δ = 4.25 ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report ChemSketch

Phase korrigieren

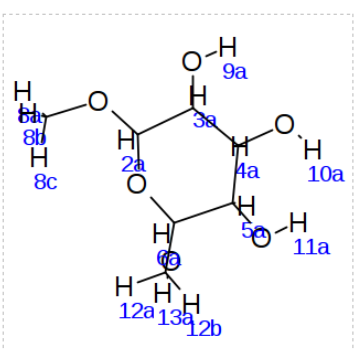
Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv. - 14:55 Friederike Pielenz

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\21

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data Recent files All files C:\ (drive_c) Z:\ (f) bin boot etc home lib lib32 lib64 libx32 lost+found media mnt opt Adobe brother Bruker DynamicsCenter sophos-av topspin topspin3.5pl2 classes conf data CR-133_1 DOSY_Gradientenkalibrierung FP-01EB HSQC_SensitivityEnhanced 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) 80 (1H)

HW-bMeGlc.021.001.1r.esp



1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

5.5 5.0 4.5 4.0 3.5 3.0 2.5

Chemical Shift (ppm)

fine phase

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectr

HW-bMeGlc.021.001.1r.esp SPECTRUM 1H $\delta = 4.66$ ppm 05_D2O

Open Process Peak Detection Interpret Database Report ChemSketch

NI Al ppm Hz pts

„Peak Picking“

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
 - PB-FrucEpOx
 - test BBO_Z8248
 - test-pulsecal
 - ~TEMP
 - db
 - examdata

Signal Analysis

- Detect Solvent/Water Signals
- Table of Solvents...
- Dark Regions
- Reference
- Signal Analysis
 - Auto Peak Picking
 - Peak Picking Options...
 - Auto Find Multiplets
 - Find Multiplets Options...
 - Manual Tool
 - Peak by Level
 - Multiplets by Level
 - Display Options...
 - J-Coupler
 - Multiplet Report
 - Clear All Peaks
 - Clear All Multiplets

HW-bMeGlc.010.001.1r.esp

Chemical structure diagram showing proton assignments: 9a, 10a, 11a, 12b, 5a, 6a, 7a, 8a, 9b, 10b, 11b, 12a.

1H

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 4.78$ ppm 05_D20

Open Process Ref Peak Detection Interpret Database Report Chem Sketch

NI AI ppm Hz pts

Peakshift kalibrieren

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data...

HW-bMeGlc.010.001.1r.esp

05_D2O

4.71

3.52

3.69 3.68 3.65 3.46 3.44 3.41 3.40 3.39 3.35 3.32 3.30 3.23 3.21 3.19

Set Reference [1H]

Old Shift (ppm): 4.71 New Shift (ppm): 4.75

Name: DEUTERIUM OXIDE

Add Peak Add Annotation Add Dark Region

Show Table of Solvents

Name	Shift (ppm)	Multiplicity	J (Hz)	Width (Hz)	Water Range (p...	R1
05_D2O	4.75	1		0.00		
ACETIC ACID-d4	2.04	5	2.20	16.00		
	11.65	1		15.00		
ACETONE-d6	2.05	5	2.20	16.00		
ACETONITRILE-d3	1.94	5	2.50	17.50		
BENZENE-d6	7.16	1		5.00		
CHLOROFORM-d	7.27	1		5.00	[150 .. 175]	
CYCLOHEXANE-d12	3.38	1		5.00		
DICHLOROETHANE-d4	3.72	1		5.00		
DICHLOROMETHANE-d2	5.32	3	1.10	8.30		

Restore Import... Export... Edit... Delete

OK Cancel Help

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 4.71$ ppm 05_D2O

Open Process Peak Detection Interpret Database Report Chem Sketch

NI | AI | ppm Hz pts

Peaks integrieren

The screenshot displays the ACD/Spectrus software interface. The main window shows an NMR spectrum with a peak at 4.71 ppm labeled '1H'. A context menu is open over the spectrum, listing various integration options such as 'Auto Integration', 'Integration Options...', 'Manual Tool', and 'Magual Bias Correction'. The 'Table of Integrals' window is also visible, showing a table with columns for 'No.', '(ppm)', 'Value', 'Absolute Value', and 'Non-Negative V...'. The table is currently empty.

No.	(ppm)	Value	Absolute Value	Non-Negative V...

The spectrum shows several peaks with their chemical shifts (ppm) labeled: 4.33, 4.31, 3.89, 3.86, 3.66, 3.65, 3.69, 3.68, 3.52, 3.46, 3.44, 3.41, 3.40, 3.35, 3.32, 3.30, 3.23, 3.20, 3.18. The x-axis is labeled 'Chemical Shift (ppm)' and ranges from 5.1 to 2.8. The y-axis is labeled 'Spectral Data' and ranges from 0 to 1.0.

Peaks integrieren

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
- classes
- conf
- data
- DOSY_Gradientenkalibrierung
- FP-01EB
- HSQC_SensitivityEnhanced
- 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)
- PB-FrucEpOx
- test BBO_28248
- test-pulsecal
- ~TEMP
- db
- examdata

HW-bMeGlc.010.001.1r.esp

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M01	4.321	m	1	1000

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[4.27 .. 4.37]	1.000	3.554e+8	1.000

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 4.27$ ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report Chem Sketch

Peaks integrieren

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data

- lost-found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
 - PB-FrucEpOx
 - test BBO_Z8248
 - test-pulsecal
 - ~TEMP
 - db
 - examdata

HW-bMeGlc.010.001.1r.esp

1H

M01(m) M02(dd) M03(dd) M04(s) M05(m) M06(d) M07: 3.22 ppm; d; J=8.98; 1H

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M07	3.216	d (8.98)	1	1.000
2	M06	3.334	d (9.59)	1	1.018
3	M05	3.419	m	2	2.015
4	M04	3.519	s	3	2.993
5	M03	3.669	dd (12.33,	1	1.014
6	M02	3.873	dd (12.26,	1	0.991
7	M01	4.321	m	1	1.000

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.17 .. 3.24]	1.000	3.555e+8	1.000
2	[3.28 .. 3.36]	1.018	3.618e+8	1.018
3	[3.37 .. 3.47]	2.015	7.159e+8	2.015
4	[3.49 .. 3.55]	2.993	1.064e+9	2.993
5	[3.63 .. 3.72]	1.014	3.603e+8	1.014

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H δ = 3.52 ppm 05_D20

NI AI ppm Hz pts

Peaks integrieren

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...
Open Data

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
- PB-FrucEpOx
- test BBO_Z8248
- test-pulsecal
- ~TEMP
- db
- examdata

HW-bMeGlc.010.001.1r.esp

Integration Reference and Range

Reference: 3

Range: 3.4889 - 3.5481 ppm

OK Cancel Help

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M07	3.216	d (8.98)	1	1.000
2	M06	3.334	d (9.59)	1	1.018
3	M05	3.419	m	2	2.015
4	M04	3.519	s	3	2.993
5	M03	3.669	dd (12.33,	1	1.014
6	M02	3.873	dd (12.26,	1	0.991
7	M01	4.321	m	1	1.000

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.17 .. 3.24]	1.000	3.555e+8	1.000
2	[3.28 .. 3.36]	1.018	3.618e+8	1.018
3	[3.37 .. 3.47]	2.015	7.159e+8	2.015
4	[3.49 .. 3.55]	2.993	1.064e+9	2.993
5	[3.63 .. 3.72]	1.014	3.603e+8	1.014

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 3.52$ ppm 05_D20

NI AI ppm Hz pts

Peaks integrieren

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
 - PB-FrucEpOx
 - test BBQ_Z8248
 - test-pulsescal
 - ~TEMP
 - db
 - examdata

HW-bMeGlc.010.001.1r.esp

Warning

You selected to rescale the integrals. Would you also like to have the number of protons in all multiplets recalculated?

Yes No Cancel

Don't ask me again

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.17 .. 3.24]	1.000	3.555e+8	1.000
2	[3.28 .. 3.36]	1.018	3.618e+8	1.018
3	[3.37 .. 3.47]	2.015	7.159e+8	2.015
4	[3.49 .. 3.55]	2.993	1.064e+9	2.993
5	[3.63 .. 3.72]	1.014	3.603e+8	1.014

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M07	3.216	d (8.98)	1	1.000
2	M06	3.334	d (9.59)	1	1.018
3	M05	3.419	m	2	2.015
4	M04	3.519	s	3	2.993
5	M03	3.669	dd (12.33,	1	1.014
6	M02	3.873	dd (12.26,	1	0.991
7	M01	4.321	m	1	1.000

Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 3.52$ ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report ChemSketch

Peaks zuordnen

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data...

lost+found
media
mnt
opt
Adobe
brother
Bruker
DynamicsCenter
sophos-av
topspin
topspin3.5pl2
classes
conf
data
DOSY_Gradientenkalibrierung
FP-01EB
HSQC_SensitivityEnhanced
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)
PB-FrucEpOx
test BBO_28248
test-pulsescal
~TEMP
db
examdata

HW-bMeGlc.010.001.1r.esp

4.71

9a
3a
4a
10a
11a
8b
8c
2a
5a
6a
12a
13a
12b

1H

M04: 3.52 ppm; s; 3H

M07: 3.22 ppm; d; J=8.98; 1H

M01(m)
M02(dd)
M03(dd)

3.69
3.69
3.86
3.86

3.69
3.68
3.66
3.65

3.46
3.44
3.41
3.40
3.39
3.35
3.32

3.23
3.20

1.00
0.99
1.02
3.00
2.02
1.02
1.00

5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0

Chemical Shift (ppm)

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M07	3.216	d (8.98)	1	1.003
2	M06	3.334	d (9.59)	1	1.021
3	M05	3.419	m	2	2.020
4	M04	3.519	s	3	3.000
5	M03	3.669	dd (12.33,	1	1.016
6	M02	3.873	dd (12.26,	1	0.993
7	M01	4.321	m	1	1.002

Spectral Data

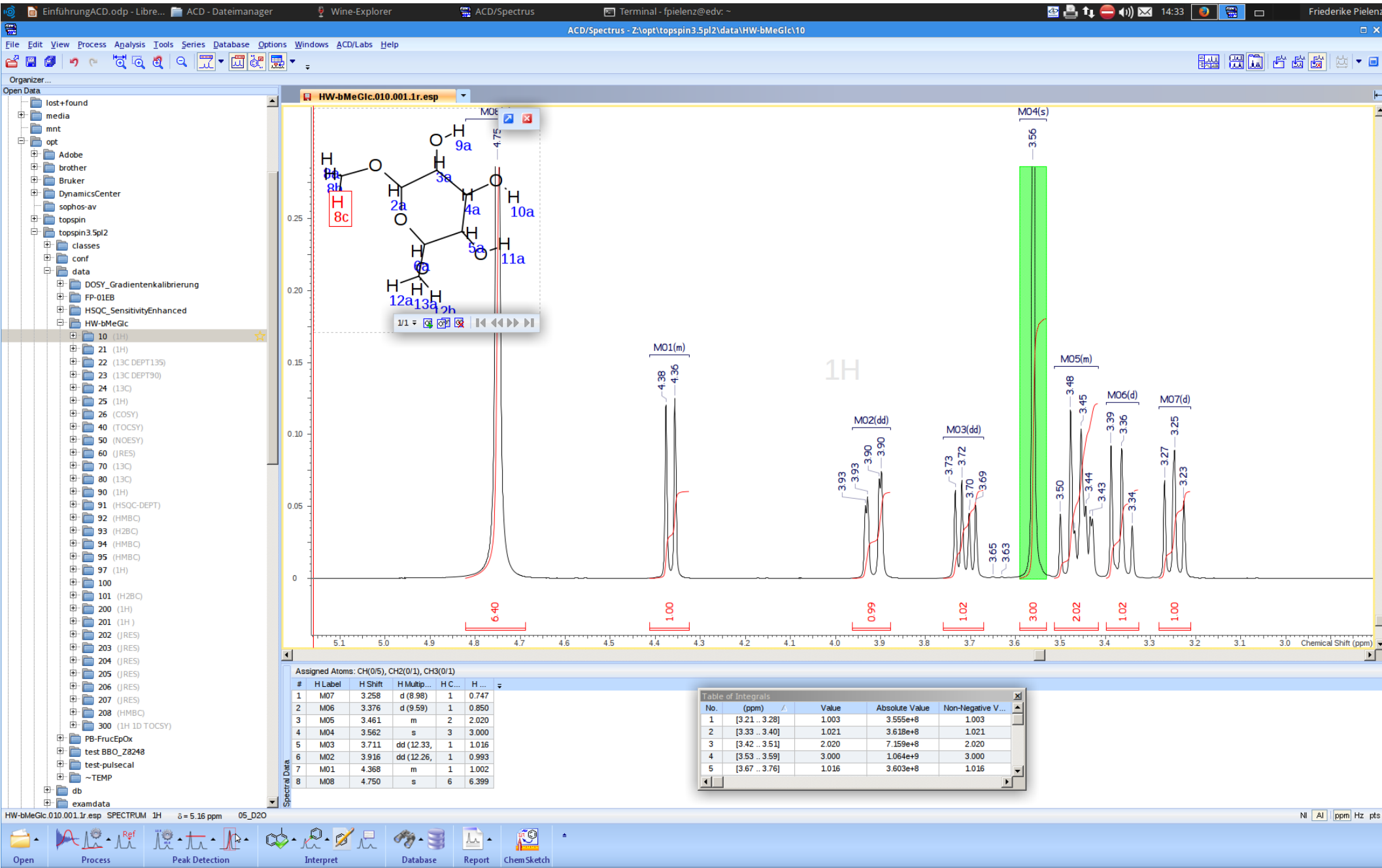
No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.17 .. 3.24]	1.003	3.555e+8	1.003
2	[3.28 .. 3.36]	1.021	3.618e+8	1.021
3	[3.37 .. 3.47]	2.020	7.159e+8	2.020
4	[3.49 .. 3.55]	3.000	1.064e+9	3.000
5	[3.63 .. 3.72]	1.016	3.603e+8	1.016

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 3.52$ ppm 05_D20

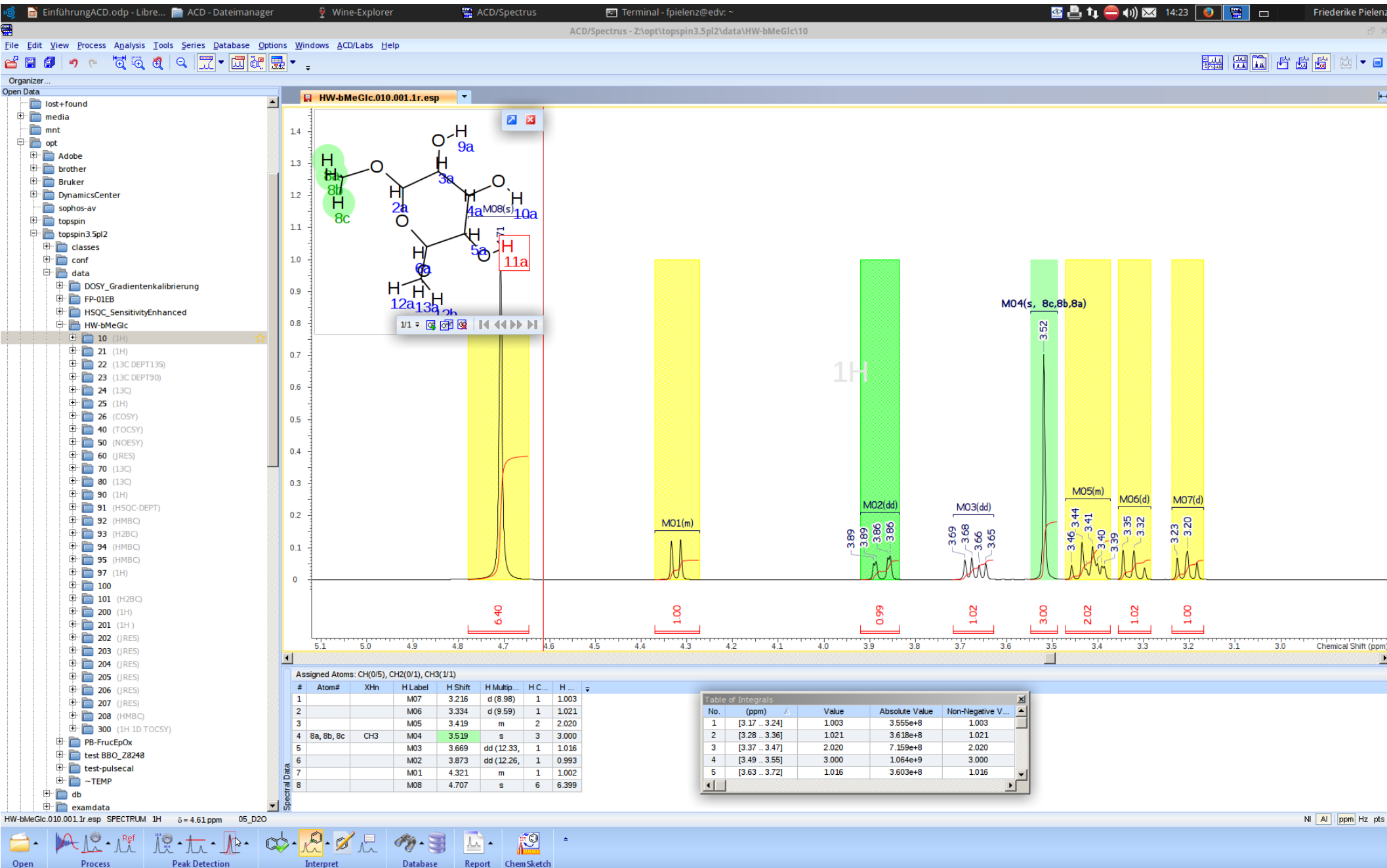
NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report Chem Sketch

Peaks zuordnen



Peaks zuordnen



Peaks zuordnen

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5pl2
 - classes
 - conf
 - data
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)
 - PB-FrucEpOx
 - test BBQ_Z8248
 - test-pulsecal
 - ~TEMP
 - db
 - examdata

HW-bMeGlc.010.001.1r.esp

1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 Chemical Shift (ppm)

M04: 3.52 ppm: s: 3H

Edit Multiplet
Apply Peak Fitting
Split Multiplet
Delete Multiplet
Convert to Dark Region
Add New Assignment

M07(d) 3.23 3.20
M06(d) 3.35 3.32
M05(m) 3.46 3.44 3.41
M03(dd) 3.69 3.68 3.66 3.65
M02(dd) 3.89 3.86 3.86
M01(m) 4.321
6.40
1.00
0.99
1.02
3.00
2.02
1.02
1.00

Assigned Atoms: CH(0/5), CH2(0/1), CH3(0/1)

#	H Label	H Shift	H Multip...	H C...	H ...
1	M07	3.216	d (8.98)	1	1.003
2	M06	3.334	d (9.59)	1	1.021
3	M05	3.419	m	2	2.020
4	M04	3.519	s	3	3.000
5	M03	3.669	dd (12.33,	1	1.016
6	M02	3.873	dd (12.26,	1	0.993
7	M01	4.321	m	1	1.002
8	M08	4.707	s	6	6.399

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.17 .. 3.24]	1.003	3.555e+8	1.003
2	[3.28 .. 3.36]	1.021	3.618e+8	1.021
3	[3.37 .. 3.47]	2.020	7.159e+8	2.020
4	[3.49 .. 3.55]	3.000	1.064e+9	3.000
5	[3.63 .. 3.72]	1.016	3.603e+8	1.016

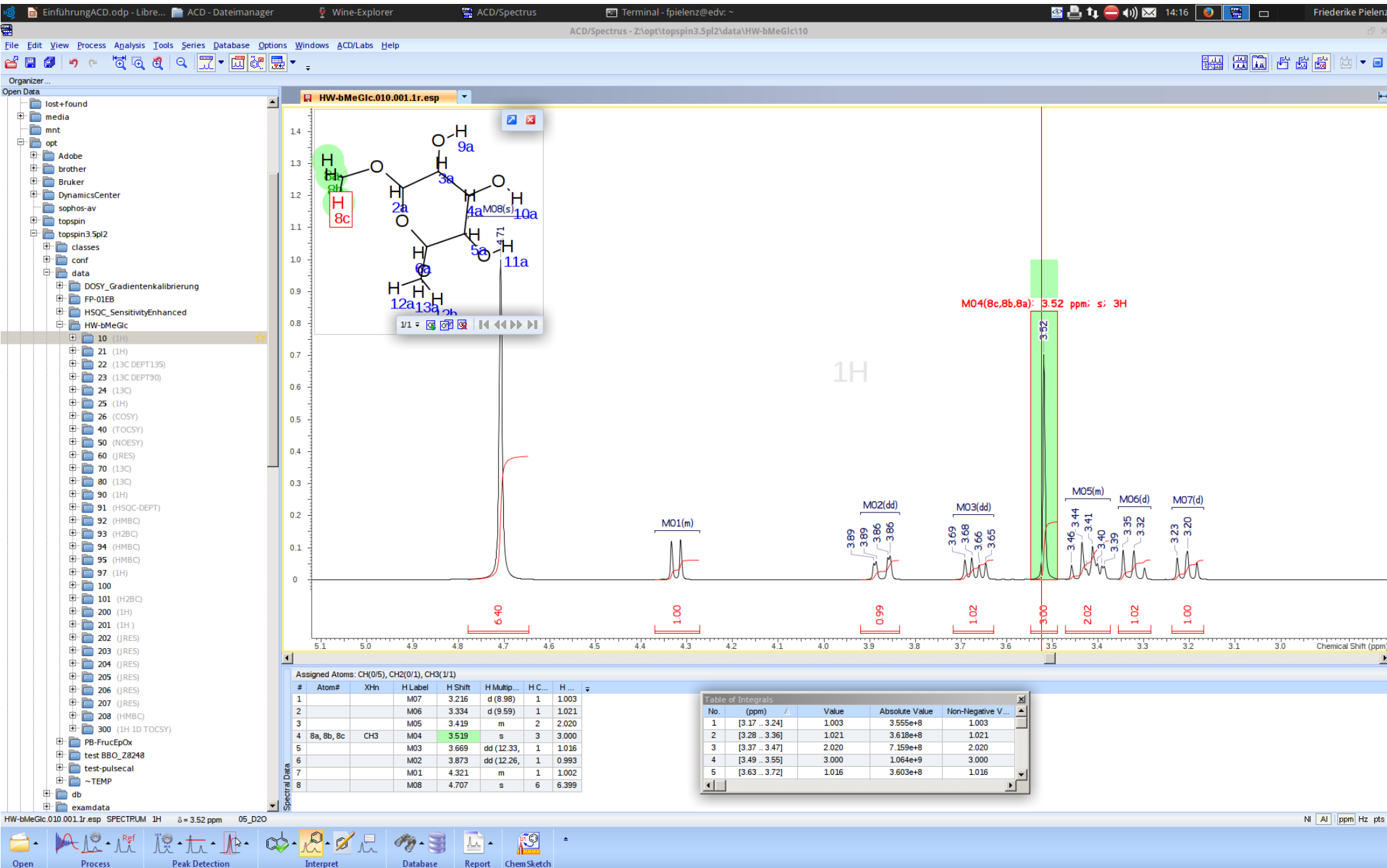
Spectral Data

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 3.52$ ppm 05_D20

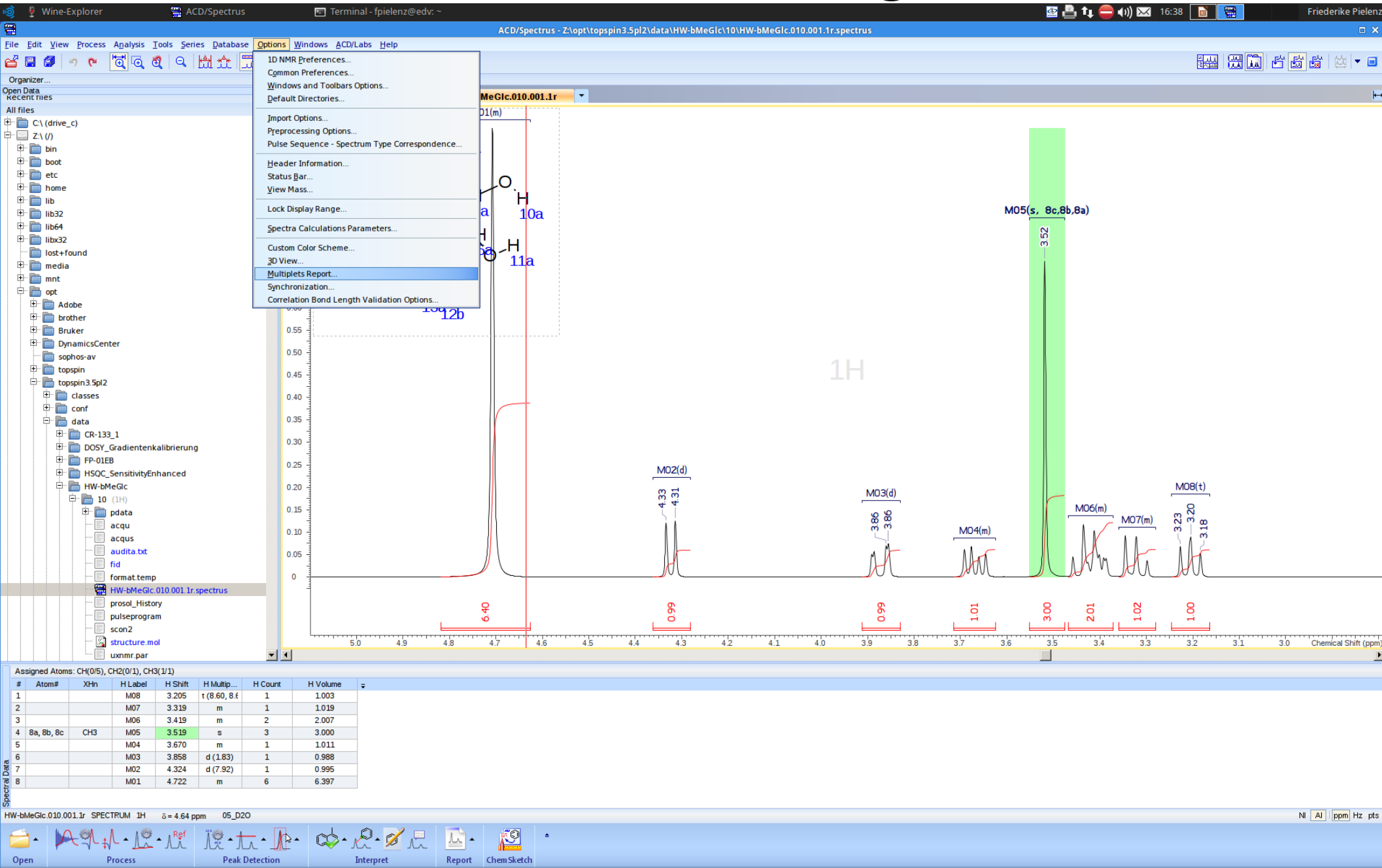
Open Process Peak Detection Interpret Database Report ChemSketch

NI AU ppm Hz pts

Peaks zuordnen



Patent String



Patent String

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv: ~

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10\HW-bMeGlc.010.001.1r.spectrus

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... Open Data Recent Files

All files

C:\ (drive_c)

Z:\ (j)

bin

boot

etc

home

lib

lib32

lib64

libx32

lost+found

media

mnt

opt

Adobe

brother

Bruker

DynamicsCenter

sophos-av

topspin

topspin3.5pl2

classes

conf

data

CR-133_1

DOSY_Gradientenkalibrierung

FP-01EB

HSQC_SensitivityEnhanced

HW-bMeGlc

10 (1H)

pdata

acqu

acqus

audita.txt

fid

format.temp

HW-bMeGlc.010.001.1r.spectrus

prosol_History

pulseprogram

scon2

structure.mol

uxnmr.par

HW-bMeGlc.010.001.1r HW-bMeGlc.010.001.1r

1.00

0.95

0.90

0.85

0.80

0.75

0.70

0.65

0.60

0.55

0.50

0.45

0.40

0.35

0.30

0.25

0.20

0.15

0.10

0.05

0

5.0

4.9

4.8

4.7

4.6

6.40

M01(m)

9a

3a

2a

4a

10a

11a

8b

8c

12a

13a

12b

Multiplet Report Options

Options

Report Type

Journal Templates User Defined

Show

Frequency

Number of Nuclei

Couplings

Temperature

Format

Separate Multiplets by Comma

Show Range for m Multiplets without

Show Solvent_Italicized

Temperature Units

Celsius Kelvin

Order of Element

(d, J=14.5 Hz, 1H)

(1H, d, J=14.6 Hz)

Decimal Place

In Shift: 2

In Couplings: 2

Multiplet Details

Show Detailed Coupling Pattern

For All Multiplets

For Specified Multiplets On: s, d, t

Preview

^1H NMR (400 MHz, 05_D2O) δ ppm 3.21 (t, J=8.60 Hz, 1 H) 3.28 - 3.36 (m, 1 H) 3.37 - 3.47 (m, 2 H) 3.52 (s, 3 H) 3.63 - 3.71 (m, 1 H) 3.86 (d, J=1.83 Hz, 1 H) 4.32 (d, J=7.92 Hz, 1 H) 4.63 - 4.82 (m, 6 H)

M03(d)

3.86

3.86

0.99

M04(m)

1.01

M05(s, 8c,8b,8a)

3.52

3.00

M06(m)

2.01

M07(m)

1.02

M08: 3.21 ppm: t: J=8.6x(2): 1H

3.23

3.20

3.18

1.00

Chemical Shift (ppm)

Assigned Atoms: CH(0/5), CH2(0/1), CH3(1/1)

#	Atom#	XHn	H Label	H Shift	H Mult...	H Count	H Volume
1			M08	3.205	t (8.60, 8.6)	1	1.003
2			M07	3.319	m	1	1.019
3			M06	3.419	m	2	2.007
4	8a, 8b, 8c	CH3	M05	3.519	s	3	3.000
5			M04	3.670	m	1	1.011
6			M03	3.858	d (1.83)	1	0.988
7			M02	4.324	d (7.92)	1	0.995
8			M01	4.722	m	6	6.397

Spectral Data

HW-bMeGlc.010.001.1r SPECTRUM 1H δ = 4.59 ppm 05_D2O

NI | Al | ppm | Hz | pts

Open Process Peak Detection Interpret Report Chem Sketch

Datei speichern!

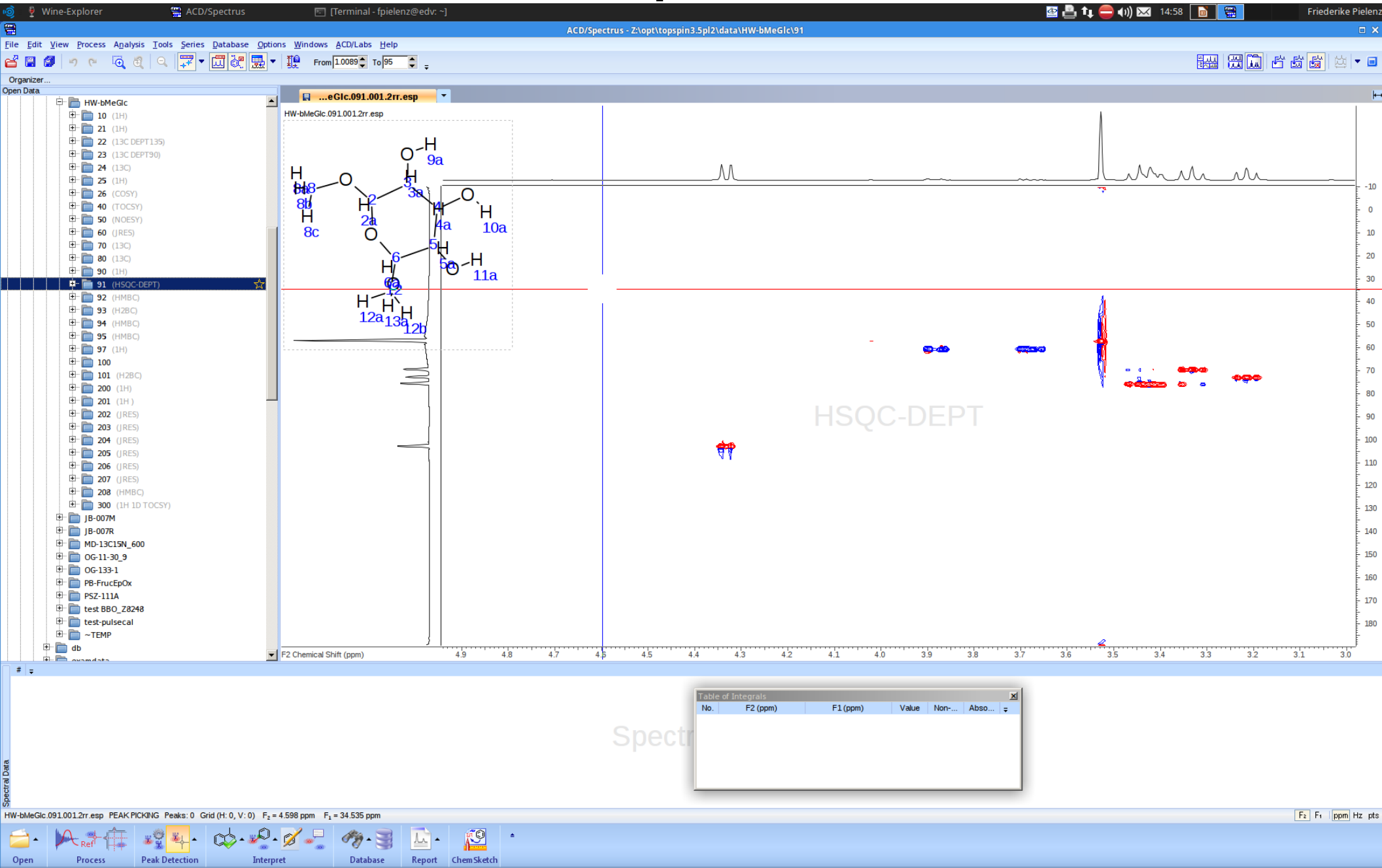
The screenshot displays the ACD/Labs software interface. The main window shows a 1H NMR spectrum of HW-bMeGlc. The x-axis represents the chemical shift in ppm, ranging from 5.1 to 3.0. The y-axis represents the intensity. The spectrum shows several peaks, with the most prominent one at 3.52 ppm, labeled M05(s, 8c,8b,8a). Other peaks are labeled M03(d), M04(m), M06(m), M07(m), and M08(t). The chemical structure of HW-bMeGlc is shown in the background, with protons labeled 1a through 13a. A 'Save Document' dialog box is open, showing the file name 'HW-bMeGlc.010.001.1r.spectrus' and the folder path 'Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10'. A 'Table of Integrals' window is also visible, showing integration values for various peaks.

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.16 .. 3.25]	1.003	3.578e+8	1.003
2	[3.28 .. 3.36]	1.019	3.637e+8	1.019
3	[3.37 .. 3.47]	2.007	7.159e+8	2.007
4	[3.48 .. 3.55]	3.000	1.070e+9	3.000
5	[3.63 .. 3.71]	1.011	3.606e+8	1.011

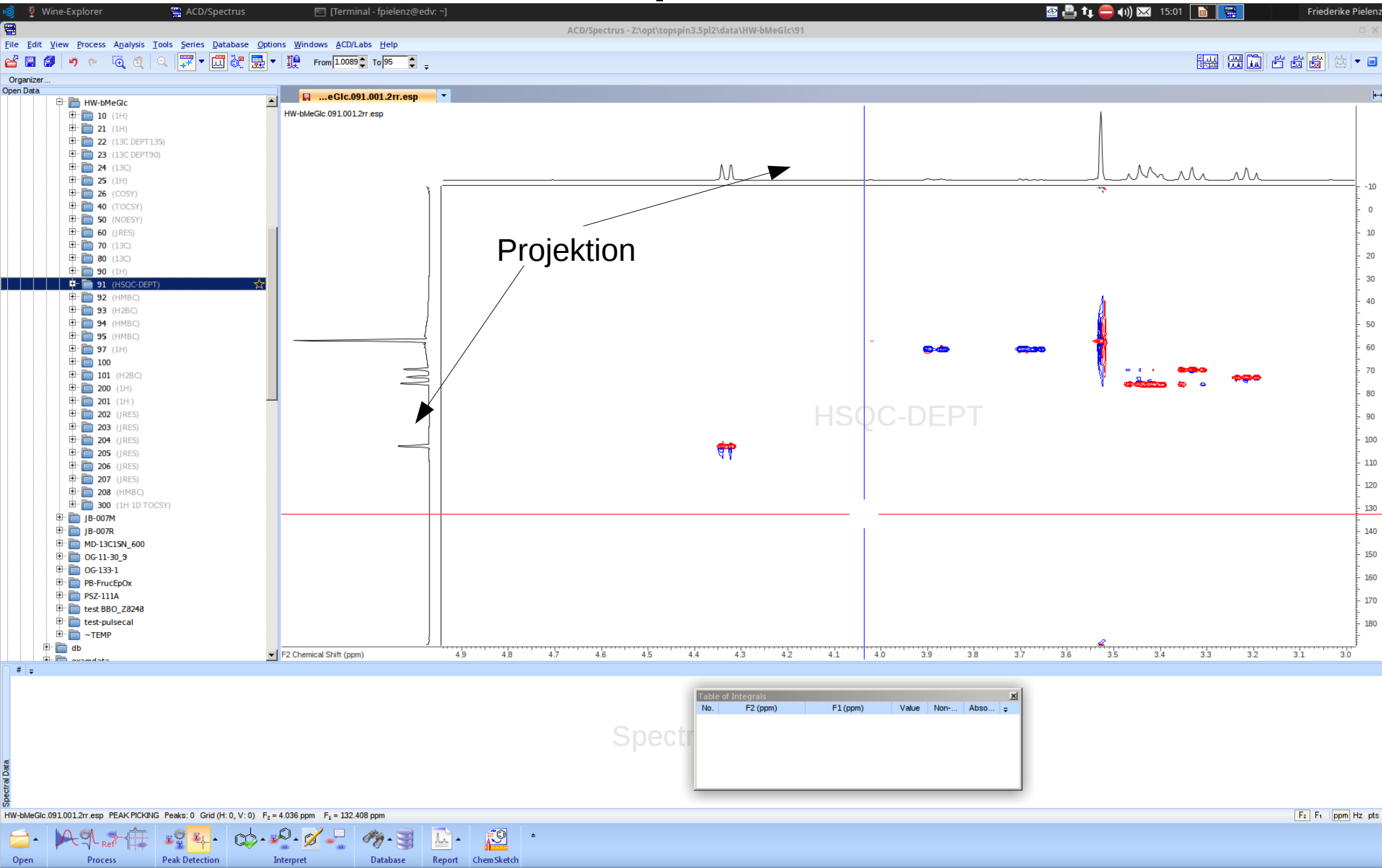
Assigned Atoms: CH(0/5), CH2(0/1), CH3(1/1)

#	Atom#	XHn	H Label	H Shift	H Multip...	H C...	H ...
1			M08	3.205	t (8.60, 8.6)	1	1.003
2			M07	3.319	m	1	1.019
3			M06	3.419	m	2	2.007
4	8a, 8b, 8c	CH3	M05	3.519	s	3	3.000
5			M04	3.670	m	1	1.011
6			M03	3.858	d (1.83)	1	0.988
7			M02	4.324	d (7.92)	1	0.995
8			M01	4.722	m	6	6.397

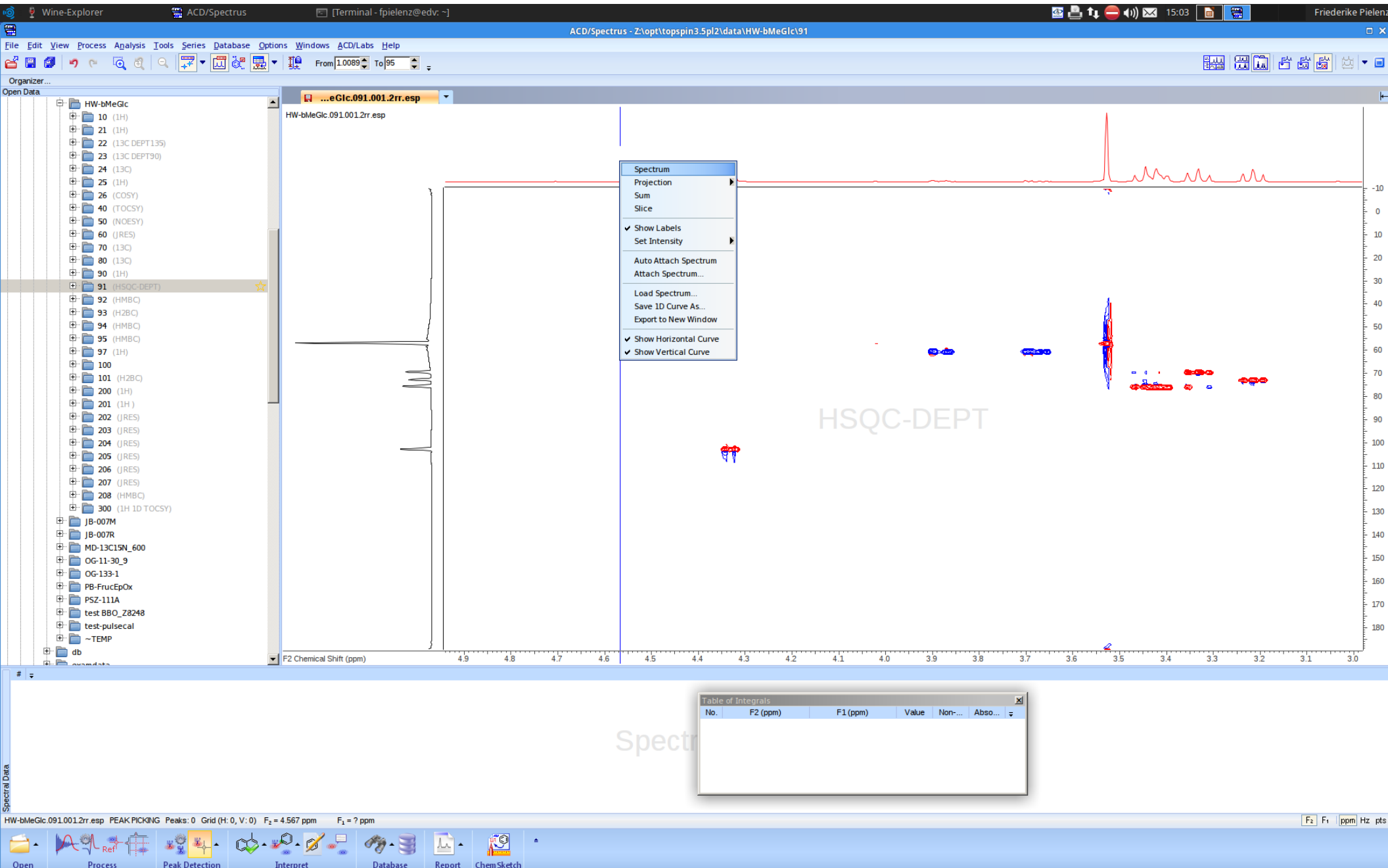
2D-Spektren



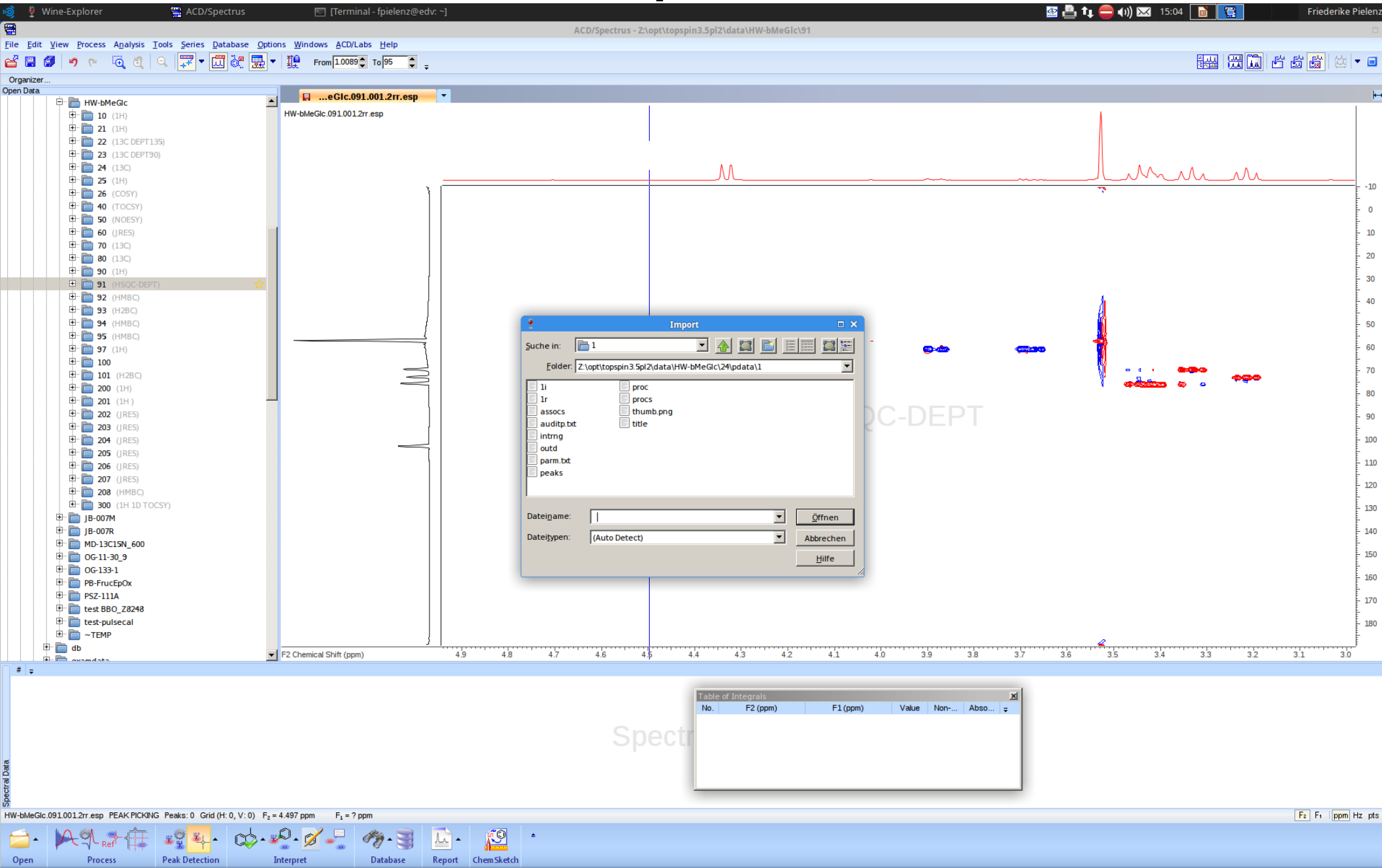
2D-Spektren



2D-Spektren



2D-Spektren



2D-Spektren

Wine-Explorer ACD/Spectrus [Terminal - fpielenz@edv: ~]

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\1

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_28248
 - test-pulsecal
 - ~TEMP
 - db

HW-bMeGlc.091.001.2rr.esp

HW-bMeGlc.091.001.2rr.esp

Import

Suche in: 10

Folder: Z:\opt\topspin3.5pl2\data\HW-bMeGlc\10

- pdata
- acq
- 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

HSQC-DEPT

F2 Chemical Shift (ppm)

Table of Integrals

No.	F2 (ppm)	F1 (ppm)	Value	Non-...	Abso-...

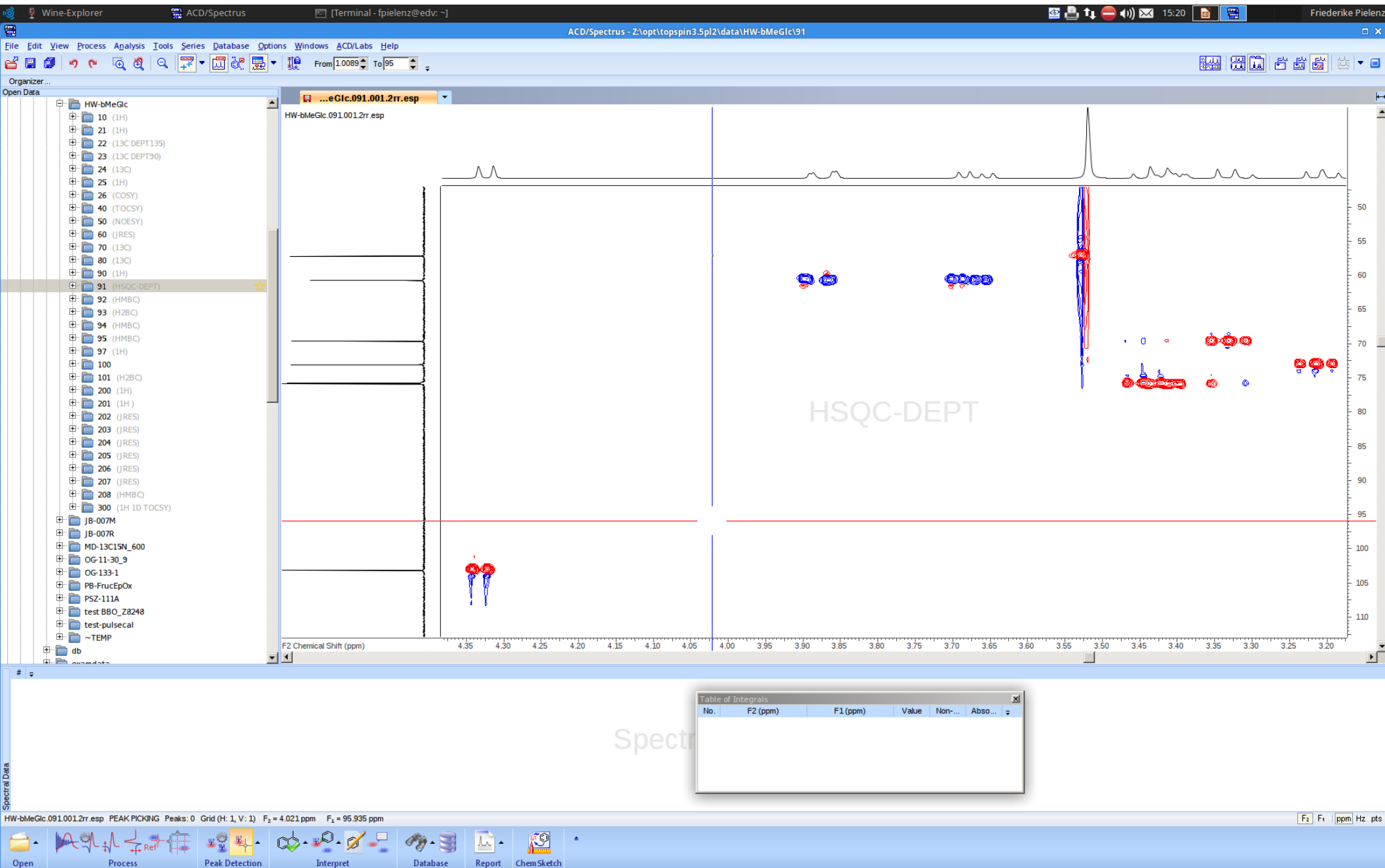
Spectr

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 Chem Sketch

F₂ F₁ ppm Hz pts

2D-Spektren



2D-Spektren Phase korrigieren

Wine-Explorer ACD/Spectrus Terminal - fpielenz@edv: ~

ACD/Spectrus - Z:\opt\topspin3.5pl2\data\HW-bMeGlc\91

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer... From 2.8536 To 95

Open Data

- opt
 - Adobe
 - brother
 - Bruker
 - DynamicsCenter
 - sophos-av
 - topspin
 - topspin3.5pl2
 - classes
 - conf
 - data
 - CR-133_1
 - DOSY_Gradientenkalibrierung
 - FP-01EB
 - HSQC_SensitivityEnhanced
 - 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)

HW-bMeGlc.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-...	Abs-...

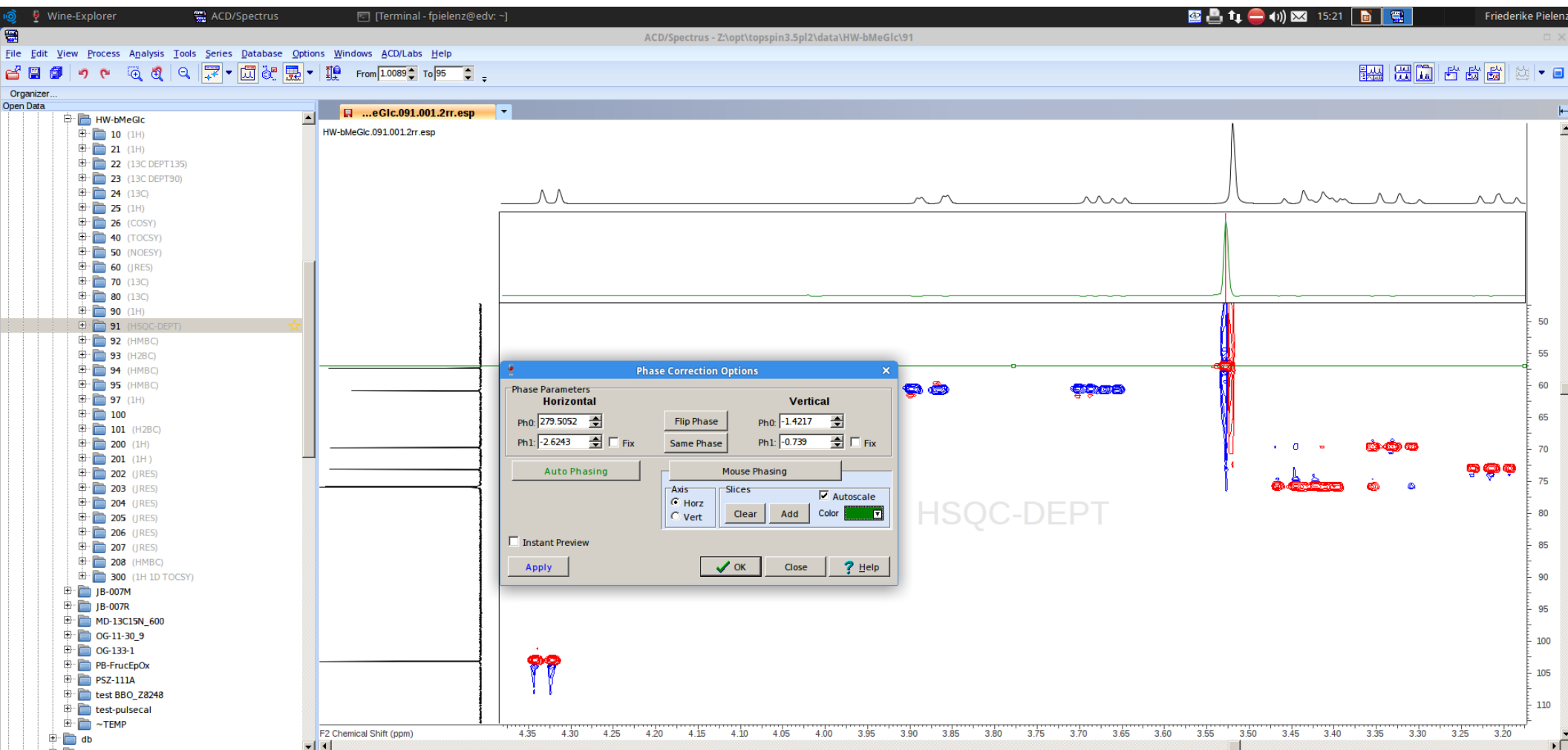
Spectral Data

HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F₂ = 4.089 ppm F₁ = 74.042 ppm

Open Process Peak Detection Interpret Database Report ChemSketch

F₂ F₁ ppm Hz pts

2D-Spektren Phase korrigieren



No.	F2 (ppm)	F1 (ppm)	Value	Non...	Abs...

2D-Spektren Phase korrigieren

Wine-Explorer ACD/Spectrus [Terminal - fpielenz@edv: ~]

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

HW-bMeGlc.091.001.2rr.esp

HW-bMeGlc.091.001.2rr.esp

Phase Correction Options

Phase Parameters

Horizontal		Vertical	
Ph0:	282.7318	Flip Phase	Ph0: -1.4217
Ph1:	-10.6243	Same Phase	Ph1: -0.739

Auto Phasing

Mouse Phasing

Axis

Horz Vert

Slices

Autoscale

Clear Add Color

Instant Preview

Apply OK Close Help

HSQC-DEPT

F2 Chemical Shift (ppm)

Table of Integrals

No.	F2 (ppm)	F1 (ppm)	Value	Non-...	Abso...

Spectr

HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F₂ = 4.074 ppm F₁ = ? ppm

Open Process Peak Detection Interpret Database Report Chem Sketch

F₂ F₁ ppm Hz pts

2D-Spektren Phase korrigieren

The screenshot displays the ACD/Spectrus interface with an HSQC-DEPT 2D NMR spectrum. The 'Phase Correction Options' dialog box is open, showing the following parameters:

Phase Parameters	
Horizontal	Vertical
Ph0: 282.7318	Ph0: -1.4217
Ph1: -10.6243	Ph1: -0.739

The 'Instant Preview' checkbox is highlighted with a red circle. The 'Apply' button is also visible. The background shows the 2D spectrum with various peaks and a 1D projection at the top.

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

No.	F2 (ppm)	F1 (ppm)	Value	Non...	Abso...

2D-Spektren Phase korrigieren

Wine-Explorer ACD/Spectrus [Terminal - fpielenz@edv: ~] 15:29 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... From 1.0089 To 95

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

HW-bMeGlc.091.001.2rr.esp

Phase Correction Options

Phase Parameters

Horizontal		Vertical	
Ph0:	282.7318	Flip Phase	Ph0: 359.9181
Ph1:	-10.6243	Same Phase	Ph1: -4.739

Auto Phasing

Mouse Phasing

Axis: Horz Vert

Slices: Autoscale

Color: [Dropdown]

Instant Preview

Apply OK Close Help

HSQC-DEPT

F2 Chemical Shift (ppm)

Table of Integrals

No.	F2 (ppm)	F1 (ppm)	Value	Non...	Absc...

Spectr

HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F₂ = 4.036 ppm F₁ = ? ppm

Open Process Peak Detection Interpret Database Report ChemSketch

F₂ F₁ ppm Hz pts

2D-Spektren Phase korrigieren

HSQC-DEPT

Schnittebene durch drehen des Mausrades anpassen.

No.	F2 (ppm)	F1 (ppm)	Value	Non-...	Abs-...

HW-bMeGlc.091.001.2rr.esp PEAK PICKING Peaks: 0 Grid (H: 0, V: 0) F₂ = 4.332 ppm F₁ = 103.125 ppm

Report erstellen

ACD/Spectrus - Z:\home\fpielenz\Schreibtisch\HW-bMeGlc.010.001.1r.esp

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data...

lost+found
media
mnt
opt
Adobe
brother
Bruker
DynamicsCenter
sophos-av
topspin
topspin3.5pi2
classes
conf
data
DOSY_Gradientenkalibrierung
FP-01EB
HSQC_SensitivityEnhanced
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)
PB-FrucEpoX
test BBO_28248
test-pulsecal
~TEMP
db
examdata

HW-bMeGlc.010.001.1r.esp

MOB(s)

1H

M01: 4.37 ppm; m; 1H

M02(dd)

M03(dd)

M04(s; 8c,8b,8a)

M05(m)

M06(d)

M07(d)

Chemical Shift (ppm)

Assigned Atoms: CH(0/5), CH2(0/1), CH3(1/1)

#	Atom#	X1h	H Label	H Shift
1			M07	3.258
2			M06	3.376
3			M05	3.461
4	8a, 8b, 8c	CH3	M04	3.562
5			M03	3.711
6			M02	3.916
7			M01	4.368
8			M08	4.750

Report

- Standard
- By Template
- All Visible Documents
- Report Setup...
- Template
- 1dnmr
- bruker1hnmrreporttemplate
- Set Template...

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.21 .. 3.28]	1.003	3.555e+8	1.003
2	[3.33 .. 3.40]	1.021	3.618e+8	1.021
3	[3.42 .. 3.51]	2.020	7.159e+8	2.020
4	[3.53 .. 3.59]	3.000	1.064e+9	3.000
5	[3.67 .. 3.76]	1.016	3.603e+8	1.016
6	[3.88 .. 3.96]	0.993	3.521e+8	0.993

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 4.31$ ppm 05_D20

Open Process Peak Detection Interpret Database Report Chem Sketch

Report erstellen

ACD/Spectrus - Z:\home\fpiehlz\Schreibtisch\HW-bMeGlc.010.001.1r.esp

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data...

- lost+found
- media
- mnt
- opt
- Adobe
- brother
- Bruker
- DynamicsCenter
- sophos-av
- topspin
- topspin3.5p12
- classes
- conf
- data
- DOSY_Gradientenkalibrierung
- FP-01EB
- HSQC_SensitivityEnhanced
- 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)
 - PB-FrucEpoX
 - test BBO_28248
 - test-pulsecal
 - ~TEMP
 - db
 - examdata

HW-bMeGlc.010.001.1r.esp

MOB(s)

1H

Report Page Setup

Spectrum Structure Tables View Text

Spectrum Regic

Whole Spectrum

Zoom Region

Fixed

%: -1.339 - 9.3348

%: -0.0467 - 1.3798

Current

Units

ppm

Hz

Points

Display Mode

Absolute Intensity

Normalized Intensity

Show Last Calculated Spectrum

Show All Series on One Page

Show Each Spectrum on One Page

Always Landscape Orientation

OK Cancel Help

MO4(s, 8c,8b,8a)

MO2(dd)

MO3(dd)

MO5(m)

MO6(d)

MO7(d)

3.93 3.93 3.90 3.90

3.73 3.72 3.70 3.69

3.50 3.48 3.45 3.44 3.43 3.39 3.36 3.34

3.27 3.25 3.23

6.40 1.00 0.99 1.02 3.00 2.02 1.02 1.00

Chemical Shift (ppm)

Assigned Atoms: CH(0/5), CH2(0/1), CH3(1/1)

#	Atom#	X1h	H Label	H Shift	H Multip...	H C...	H ...
1			M07	3.258	d (8.98)	1	0.747
2			M06	3.376	d (9.59)	1	0.850
3			M05	3.461	m	2	2.020
4	8a, 8b, 8c	CH3	M04	3.562	s	3	3.000
5			M03	3.711	dd (12.33,	1	1.016
6			M02	3.916	dd (12.26,	1	0.993
7			M01	4.368	m	1	1.002
8			M08	4.750	s	6	6.399

Spectral Data

Table of Integrals

No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.21 .. 3.28]	1.003	3.555e+8	1.003
2	[3.33 .. 3.40]	1.021	3.618e+8	1.021
3	[3.42 .. 3.51]	2.020	7.159e+8	2.020
4	[3.53 .. 3.59]	3.000	1.064e+9	3.000
5	[3.67 .. 3.76]	1.016	3.603e+8	1.016
6	[3.88 .. 3.96]	0.993	3.521e+8	0.993

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 4.31$ ppm 05_D20

NI AI ppm Hz pts

Open Process Peak Detection Interpret Database Report ChemSketch

Report erstellen

ACD/Spectrum - How to... ACD/Spectrum [Terminal - fpielenz@edv: ~]

ACD/Spectrum - Z:\home\fpierenz\Schreibtisch\HW-bMeGlc.010.001.1r.esp

File Edit View Process Analysis Tools Series Database Options Windows ACD/Labs Help

Organizer...

Open Data

lost+found
media
mnt
opt
Adobe
brother
Bruker
DynamicsCenter
sophos-av
topspin
topspin3.5pl2
classes
conf
data
DOSY_Gradientenkalibrierung
FP-01EB
HSQC_SensitivityEnhanced
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)
PB-FrucEpOx
test BBO_Z8248
test-pulsescal
~TEMP
db
examdata

HW-bMeGlc.010.001.1r.esp

M08(s)

9a^{7.75}
9a^{4.75}
10a
11a
5a
4a
3a
2a
12a, 13a, 12b
8c
8b
8a

M04(s, 8c, 8b, 8a) 3.56

M02(dd) 3.93, 3.93, 3.90, 3.90
M03(dd) 3.73, 3.72, 3.70, 3.69
M05(m) 3.50, 3.48, 3.45, 3.44, 3.43
M06(d) 3.39, 3.36, 3.34
M07(d) 3.27, 3.25, 3.23

6.40
1.00
0.99
1.02
3.00
2.02
1.02
1.00

1H

Report Page Setup

Spectrum Structure Tables View Text

Spectrum Parameter Spectrum Label
 Spectrum User Data Integrals Curves
 Record User Data Integrals Value
 Structure User Data
 User Notes

Vertical Scale Vertical Scale Factor
 Horizontal Scale Gridlines

Peak Fitting Result
 Peaks
 Sum
 Residual

OK Cancel Help

Assigned Atoms: CH(0/5), CH2(0/1), CH3(1/1)

#	Atom#	XIn	H Label	H Shift	H Multip...	H C...	H ...
1			M07	3.258	d (8.98)	1	0.747
2			M06	3.376	d (9.59)	1	0.850
3			M05	3.461	m	2	2.020
4	8a, 8b, 8c	CH3	M04	3.562	s	3	3.000
5			M03	3.711	dd (12.33,	1	1.016
6			M02	3.916	dd (12.26,	1	0.993
7			M01	4.368	m	1	1.002
8			M08	4.750	s	6	6.399

Spectral Data

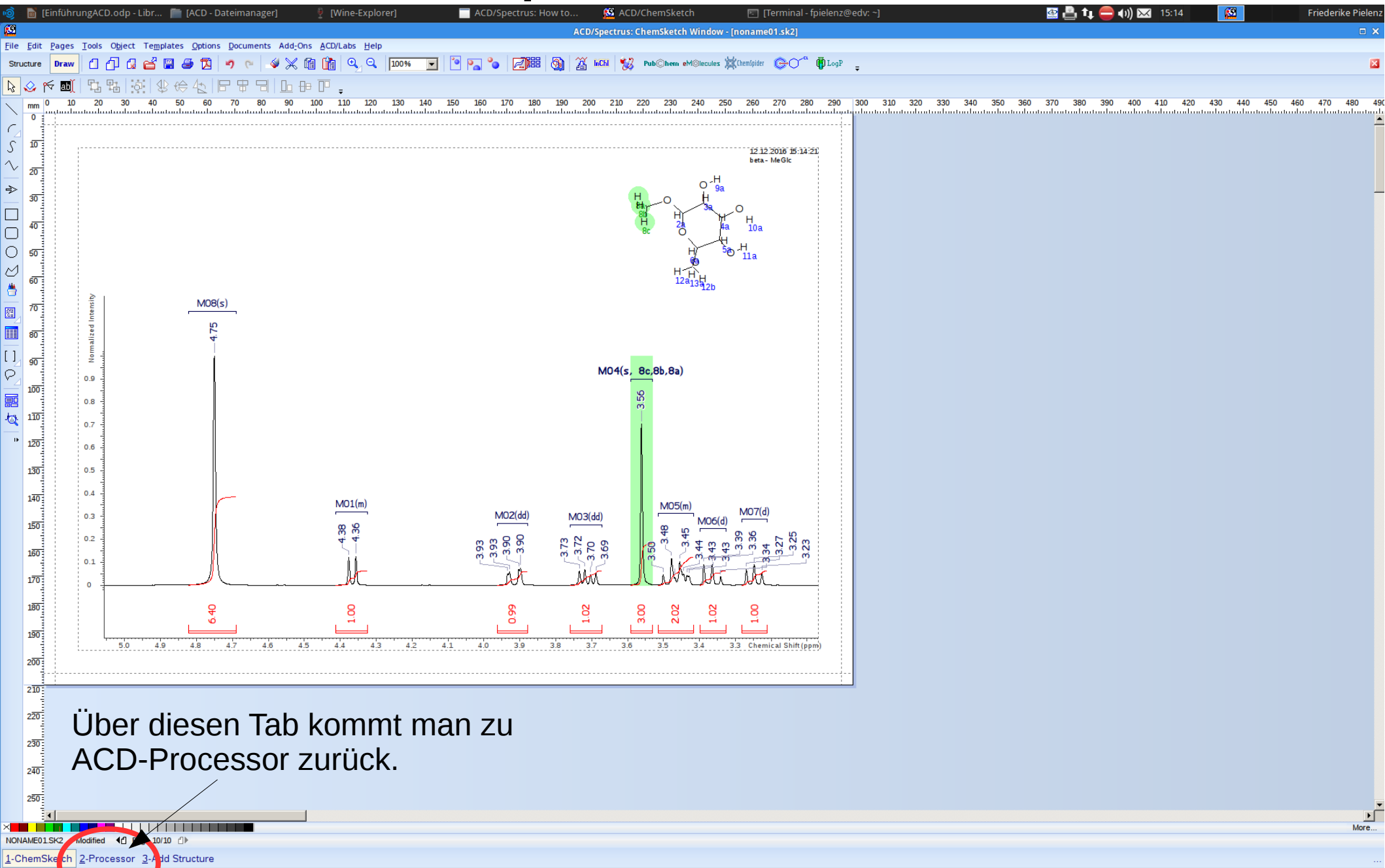
No.	(ppm)	Value	Absolute Value	Non-Negative V...
1	[3.21 .. 3.28]	1.003	3.555e+8	1.003
2	[3.33 .. 3.40]	1.021	3.618e+8	1.021
3	[3.42 .. 3.51]	2.020	7.159e+8	2.020
4	[3.53 .. 3.59]	3.000	1.064e+9	3.000
5	[3.67 .. 3.76]	1.016	3.603e+8	1.016
6	[3.88 .. 3.96]	0.993	3.521e+8	0.993

HW-bMeGlc.010.001.1r.esp SPECTRUM 1H $\delta = 4.31$ ppm 05_D20

Open Process Peak Detection Interpret Database Report ChemSketch

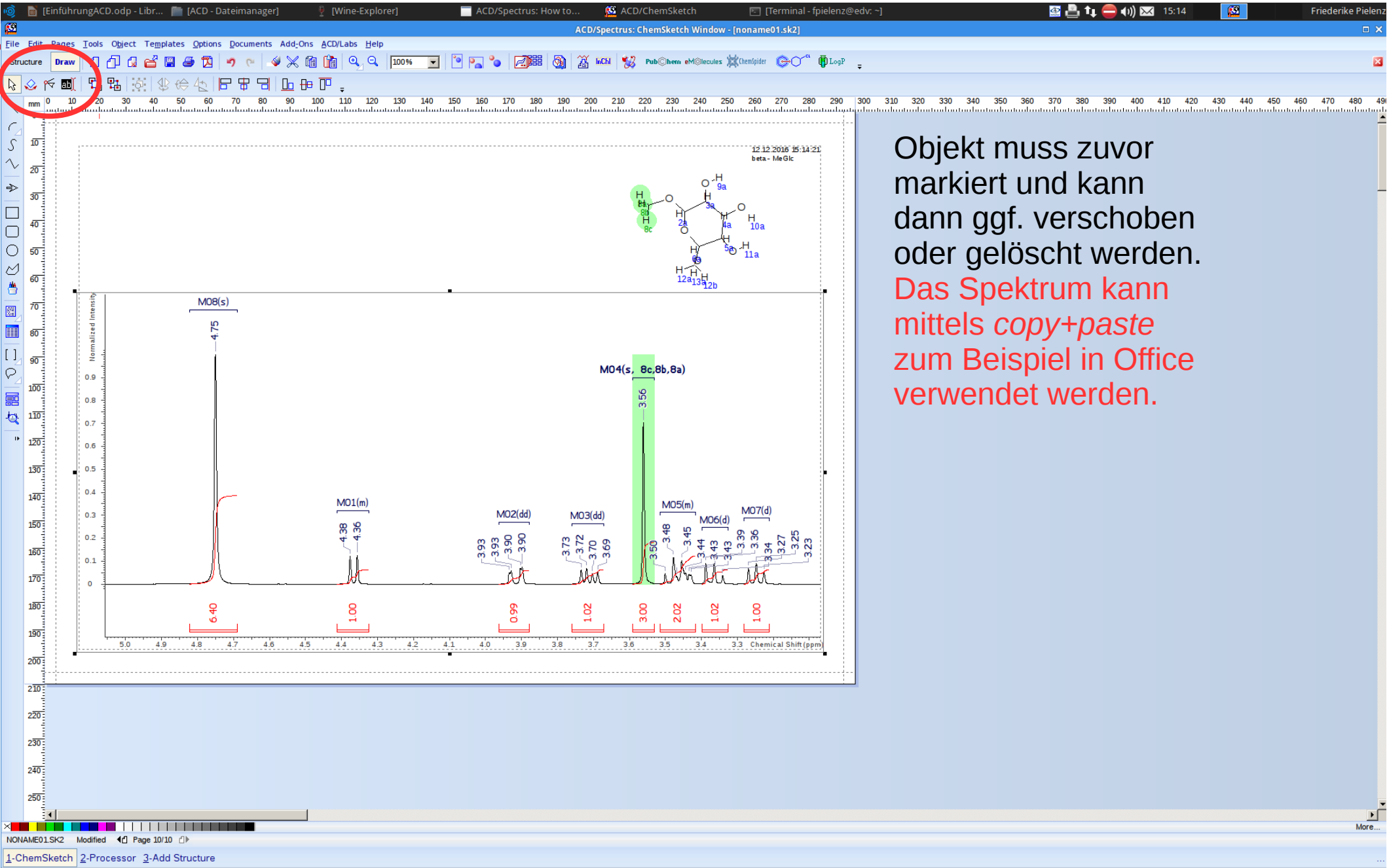
NI AI ppm Hz pts

Report erstellen



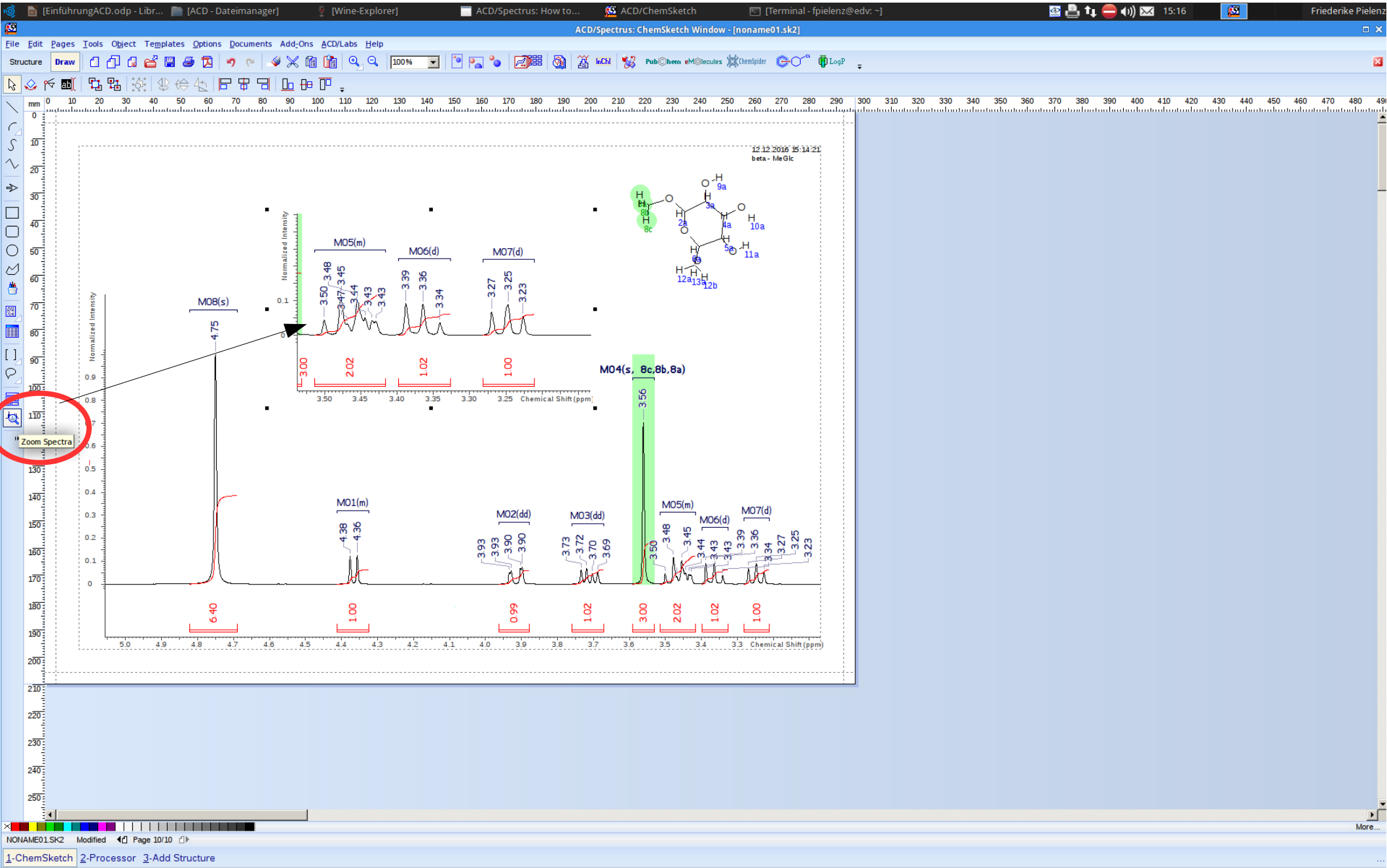
Über diesen Tab kommt man zu ACD-Processor zurück.

Report erstellen

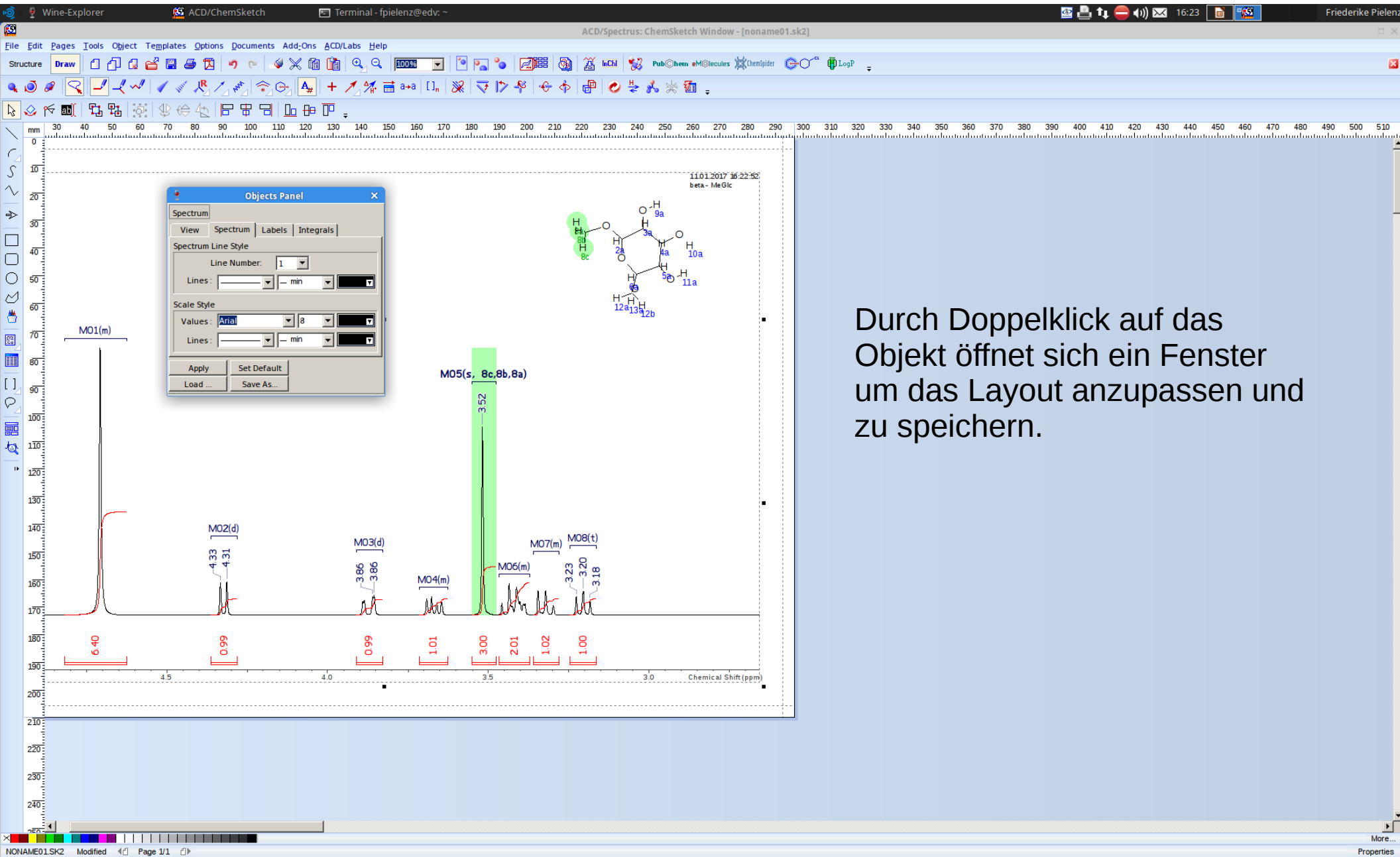


Objekt muss zuvor markiert und kann dann ggf. verschoben oder gelöscht werden. Das Spektrum kann mittels *copy+paste* zum Beispiel in Office verwendet werden.

Report erstellen

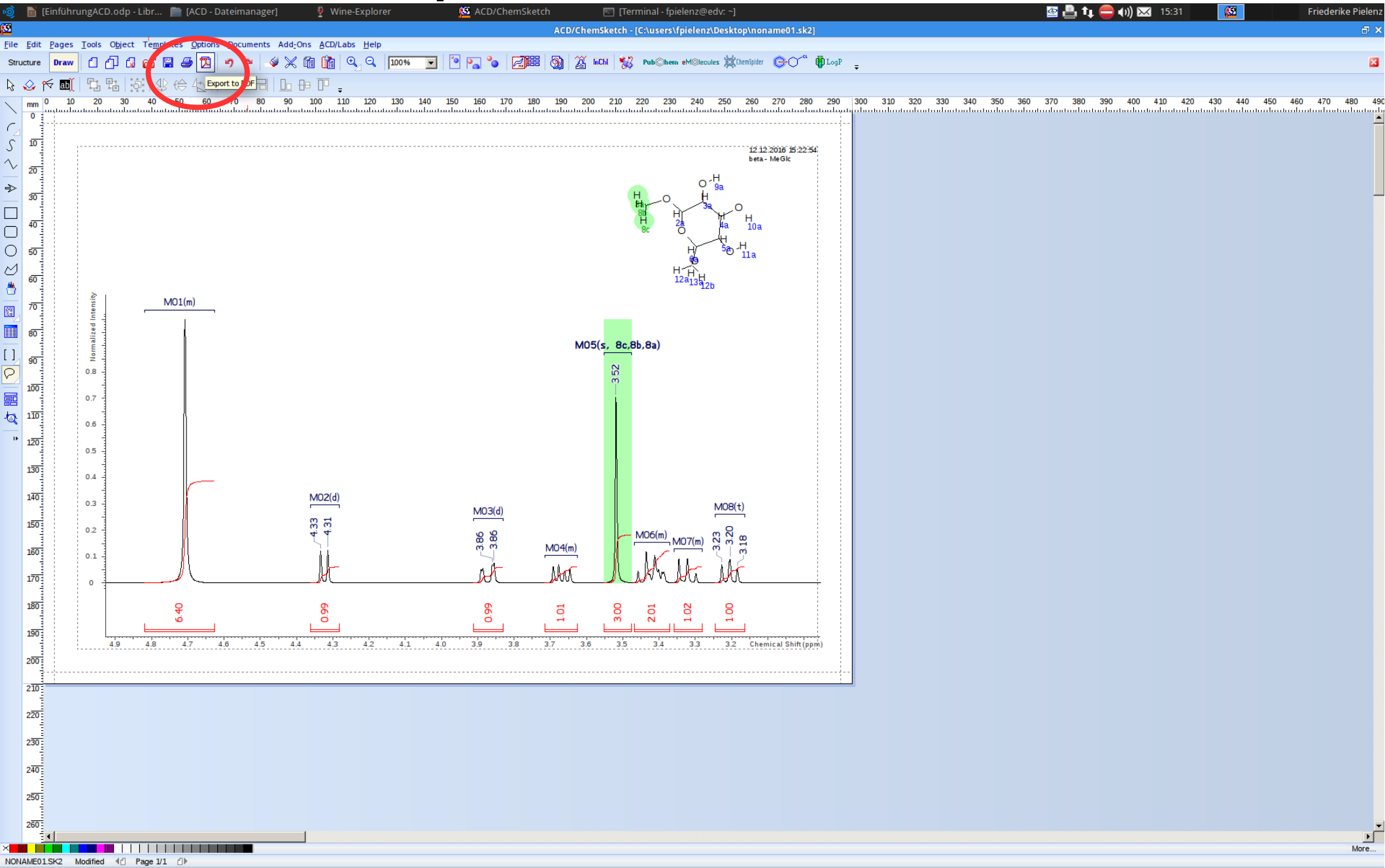


Report erstellen



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

Spektrum drucken



Fragen?