

Sparky

**NMR Assignment and Integration
Software**

NMR software

- Placené
 - TopSpin
 - Vyvinut a primárně používán pro obsluhu spektrometrů Bruker
 - Mnoho funkcí pro procesing, zobrazení a analýzu spekter jedno- i vícedimenzionálních
 - Prakticky nemožná analýza vícedimenzionálních spekter
 - Mnova
 - Procesing, analýza a vizualizace 1D a 2D spekter
 - Podpora různých formátů spekter (Bruker, Jeol, Agilent...)
 - Free trial verze
 - ACD/NMR processor
 - Viz Mnova
 - Free verze pro akademické účely s neúplnou funkcionalitou

NMR software

- Freeware
 - NMRPipe
 - Multiplatformní
 - Spracování a analýza jakýchkoli spekter
 - Založeno na UNIX-ových systémech → znalost UNIX-ového prostředí výhodou
 - SpinWorks
 - Pro systém Windows (pro UNIX a Mac jsou zapotřebí emulátory Windows)
 - Procesing analýza 1D a 2D spekter
 - Uživatelsky velice nepříjemné
 - Sparky

Sparky

NMR Assignment and Integration Software

- Vyvinut na University of California, San Francisco
- Multiplatformní
- Volně ke stažení:
<https://www.cgl.ucsf.edu/home/sparky/>
- Napsán v jazyce Python, open source, není dále vyvíjen (poslední verze z roku 2008)
- Rychlý a hardwarově nenáročný software
- Dokáže pracovat pouze s vícedimenzionálními spektry

Sparky - spektra

- Umí spracovat různé formáty spekter, ale práce s nimi je náročná a pomalá (výpočetně)
 - Konverze spekter do formátu *.ucsf
 - Unix: `bruk2ucsf 2rr název_spektra.ucsf`
 - Windows: v příkazovém řádku `bruk2ucsf.exe 2rr název_spektra.ucsf`
 - Spektrum nenesou žádné informace o akvizici, teplotě apod. → nutné řádné pojmenování *.ucsf souborů
(`kolchicine_noesy_800_D2O_25C.ucsf`)
- Vlastní souborová struktura
 - Lists, Projects, Save
- Sparky start
 - Windows: `/sparky/bin/sparky.bat`

Applications ▾ Places ▾ en ▾ Thu Nov 20, 18:01

Sparky 3.110

File View Peak Windows Extensions Help

durec@teslin.ncbr.muni.cz: /home/durec

File Edit View Search Terminal Help

```
durec@teslin ~]$ sparky
```

Pointer Mode

◇ select	F1
◇ center	F2
◇ add grid both	F3
◇ add grid horz	F4
◇ add grid vert	F5
◇ add label	F6
◇ add line	F7
◇ find/add peak	F8
◇ integrate	F10
◆ zoom	F11
◇ duplicate & zoom	F12
◇ assignment copy	sh-F1
◇ assignment guess	sh-F2

hlavní okno

↑

↑

přepínání módu levého tlačítka myši pomocí kláves F1-F12

Trash

durec@teslin.ncbr.muni.cz: /home/... Pointer Mode Sparky 3.110 1 / 4

Sparky - ovládání

- Ovládání pomocí
 - Dvoupísmenných skratek (case-sensitive)
 - Kontextového menu pod pravým tlačítkem myši
 - Menu v hlavním okně
- Otevření spektra/projektu: *fo/jo*
- Uložit spektrum/projekt jako: *fa/ja*
- Uložení spektra/projektu: *fs/js*
- Uložené spektrum: *.save, uložený projekt: *.proj
- Záložné soubory *.bak jsou automaticky vytvářeny při ukládání práce

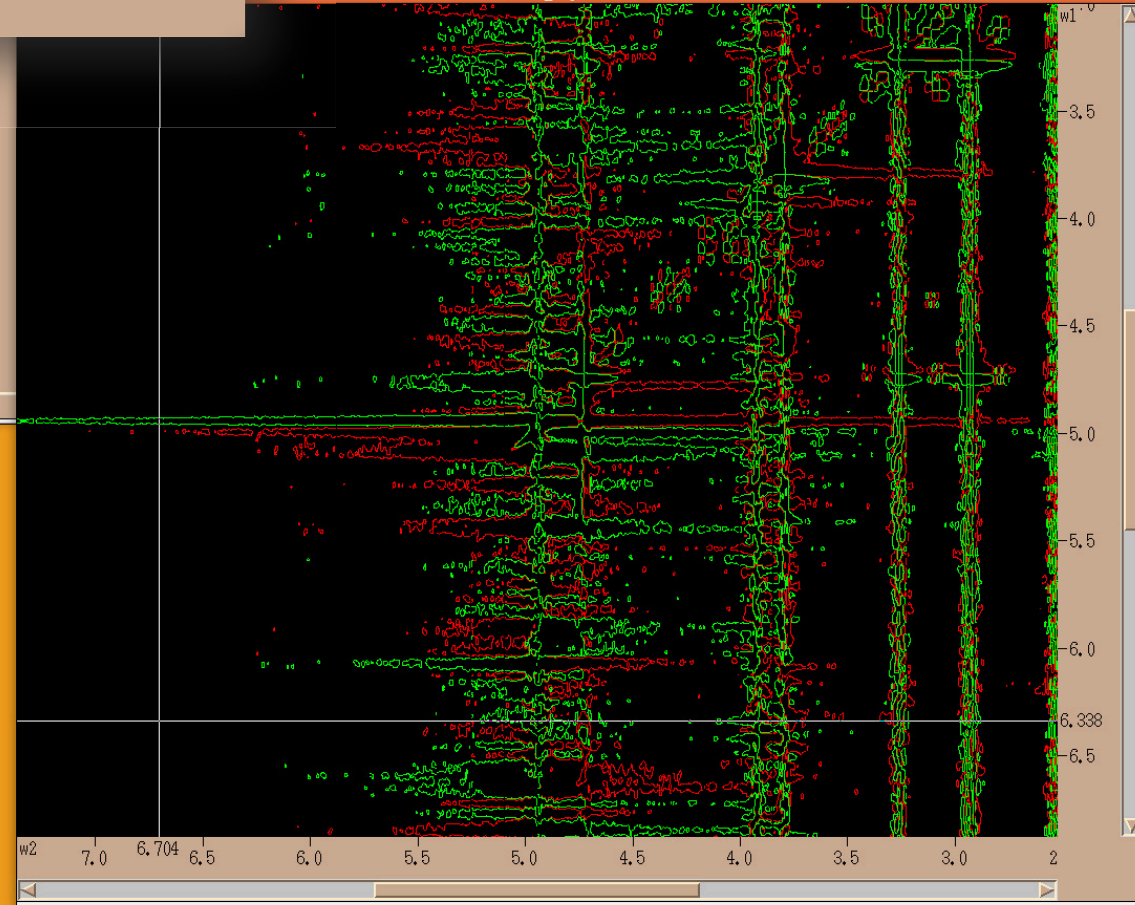
Sparky 3.110

durec@teslin.ncbr.muni.cz: /scratch/durec/FRVS_spektra

File Edit View Search Terminal Help

[durec@teslin FRVS_spektra]\$ sparky

GSSG_DQF-COSY -- selected



- Pointer Mode
- ◇ select F1
 - ◇ center F2
 - ◇ add grid both F3
 - ◇ add grid horz F4
 - ◇ add grid vert F5
 - ◇ add label F6
 - ◇ add line F7
 - ◇ find/add peak F8
 - ◇ integrate F10
 - ◇ zoom F11
 - ◇ duplicate & zoom F12
 - ◇ assignment copy sh-F1
 - ◇ assignment guess sh-F2



zf – full view

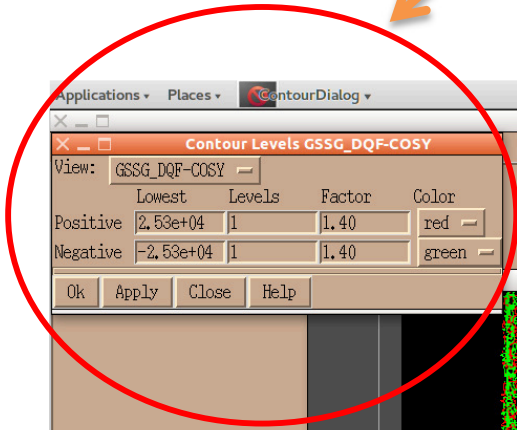
The screenshot displays the Sparky 3.110 NMR software interface. The main window, titled "GSSG_DQF-COSY -- selected", shows a 2D NMR spectrum with a complex pattern of green and red peaks. The horizontal axis (w2) is labeled with values from 10 to -1, and the vertical axis (w1) is labeled from 1 to -9. A mouse cursor is visible over the spectrum. The interface includes a menu bar (File, View, Peak, Windows, Extensions, Help) and a terminal window on the right showing the command "sparky" being executed. A "Pointer Mode" tooltip is visible in the bottom right corner, listing various keyboard shortcuts for navigation and analysis.

Pointer Mode		
◇ select		F1
◇ center		F2
◇ add grid both		F3
◇ add grid horz		F4
◇ add grid vert		F5
◇ add label		F6
◇ add line		F7
◇ find/add peak		F8
◇ integrate		F10
◇ zoom		F11
◇ duplicate & zoom		F12
◇ assignment copy	sh-	F1
◇ assignment guess	sh-	F2

1 / 4

ct – contour levels

vC – contour scale

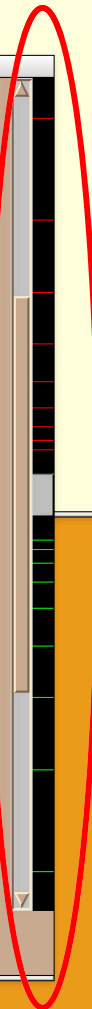
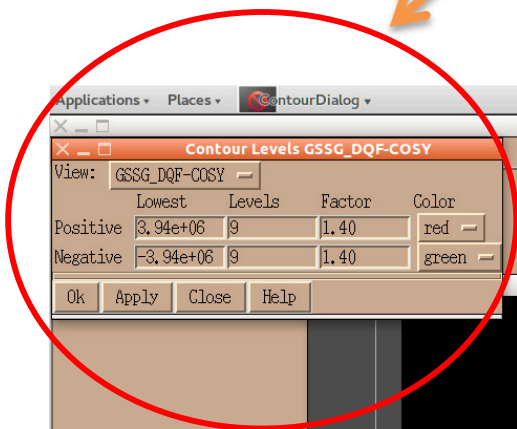


A screenshot of the Sparky 3.110 application interface. The main window displays a 2D contour plot titled 'GSSG_DQF-COSY -- selected'. The plot has a horizontal axis labeled 'w2' with values from 10 to -1 and a vertical axis labeled 'w1' with values from -1 to -9. The plot shows a complex pattern of red and green contours. In the top-left corner, there is a 'Contour Levels GSSG_DQF-COSY' dialog box. In the top-right corner, there is a terminal window with the command '[durec@teslin FRVS_s...@ra]\$ sparky'. In the bottom-right corner, there is a 'Pointer Mode' menu with various keyboard shortcuts. The bottom of the screen shows a taskbar with several open windows and a 'Trash' icon.

úprava kontur:

ručně přepsat hodnoty

upravit tažením myši



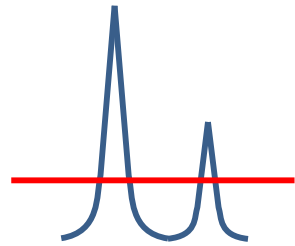
The screenshot shows the Sparky 3.110 interface. At the top, there are window titles: 'Applications', 'Places', 'ContourDialog', 'Sparky 3.110', and a terminal window. The terminal window shows the command 'sparky' being executed. The main window is divided into several panes. The top-left pane is the 'Contour Levels GSSG_DQF-COSY' dialog box. The top-right pane is a terminal window. The bottom-left pane is a 2D plot titled 'GSSG_DQF-COSY -- selected'. The bottom-right pane is a 'Pointer Mode' menu with various actions and their corresponding function keys (F1-F12, sh-F1, sh-F2). The plot shows a 2D NMR spectrum with several peaks highlighted in red and green. The vertical axis is labeled 'w1' and has tick marks from -1 to -9. The horizontal axis is labeled 'w2' and has tick marks from 10.25 to -1. The plot is titled 'GSSG_DQF-COSY -- selected'. The terminal window shows the command 'sparky' being executed. The Pointer Mode menu is open, showing various actions and their corresponding function keys.

- select F1
- center F2
- add grid both F3
- add grid horz F4
- add grid vert F5
- add label F6
- add line F7
- find/add peak F8
- integrate F10
- zoom F11
- duplicate & zoom F12
- assignment copy sh-F1
- assignment guess sh-F2



úprava kontur:

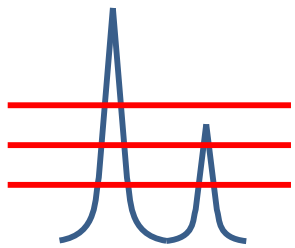
1D



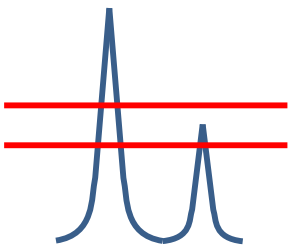
← Lowest positive
Levels = 1



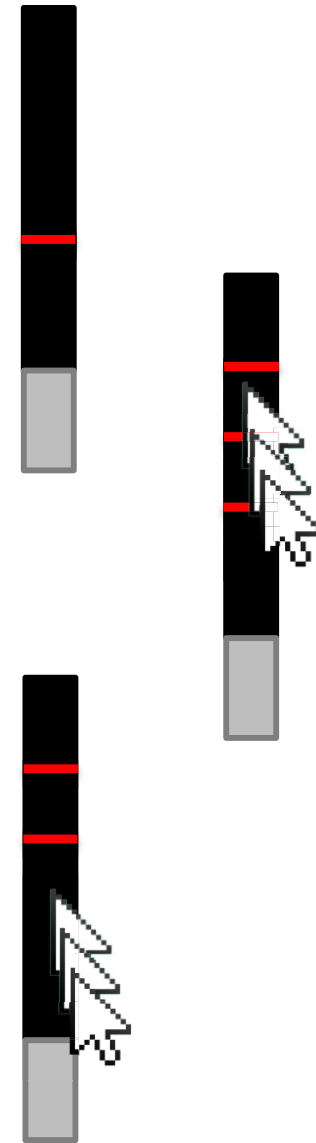
2D



← Lowest positive
Levels = 3



← Lowest positive
Levels = 2



přiblížení spektra:

klávesová skratka: **zi** (zoom in)
přednastavené přiblížení

mód myši – zoom: klávesa F11
kliknutím a tažením myši
se vybraný region zvětší na velikost okna

The screenshot displays the Sparky 3.110 NMR software interface. The main window shows a 2D NMR spectrum titled "GSSG_DQF-COSY -- selected". The x-axis is labeled "w2" and ranges from 10 to 0, with a specific peak at 4.013. The y-axis is labeled "w1" and ranges from -1 to -9, with a specific peak at 4.087. A white box highlights a region of peaks in the upper right quadrant of the spectrum. A mouse cursor is positioned over this region. To the right of the spectrum, a "Pointer Mode" menu is open, listing various actions and their corresponding function keys. The "zoom" option, associated with F11, is circled in red. An orange arrow points from the text above to the "zoom" option in the menu.

Action	Function Key
select	F1
center	F2
add grid both	F3
add grid horz	F4
add grid vert	F5
add label	F6
add line	F7
find/add peak	F8
integrate	F10
zoom	F11
duplicate & zoom	F12
assignment copy sh	F1
assignment guess sh	F2

peak picking:

mód myši – find/add peak: klávesa F8

kliknutím se přidá jeden pík,

označením oblasti se přidají píky všude kde se nachází maximum/minimum

The screenshot displays the Sparky 3.110 software interface. The main window, titled "GSSG_DQF-COSY -- selected", shows a 2D NMR spectrum with several peaks highlighted in red and green. The x-axis is labeled "w2" and ranges from 4.2 to 1.8. The y-axis is labeled "w1.0" and ranges from -2.2 to -4.0. A terminal window in the top right shows the command "durec@teslin ~]S sparky". A "Pointer Mode" menu is open in the bottom right, listing various actions and their corresponding function keys. The "find/add peak" option is circled in red, and an orange arrow points to it from the top right. The bottom status bar shows the current window title "GSSG_DQF-COSY -- selected" and the "Pointer Mode" context menu.

Action	Function Key
select	F1
center	F2
add grid both	F3
add grid horz	F4
add grid vert	F5
add label	F6
add line	F7
find/add peak	F8
integrate	F10
zoom	F11
duplicate & zoom	F12
assignment copy sh	sh-F1
assignment guess sh	sh-F2

peak picking: úprava velikosti ornamentů (píků, popisků...): **ot** → sizes → upravit velikost podle potřeb (vhodné 0.05) → apply

The screenshot displays the Sparky 3.110 NMR software interface. The main window shows a 2D GSSG_DQF-COSY spectrum with several peaks highlighted in red and green. The x-axis is labeled 'w2' and ranges from 4.2 to 1.8 ppm, with a specific peak at 2.813 ppm. The y-axis is labeled 'w1' and ranges from 1.0 to 4.0 ppm. A terminal window on the right shows the command prompt with the command 'sparky' entered. A 'Pointer Mode' menu is open in the bottom right corner, listing various functions and their corresponding keyboard shortcuts.

Applications ▾ Places ▾ View ▾

Sparky 3.110

durec@teslin.ncbr.muni.cz: /home/durec

File View Peak Windows Extensions Help

File Edit View Search Terminal Help

[durec@teslin ~]\$ sparky

GSSG_DQF-COSY -- selected

w1.0

2.2

2.4

2.6

2.812

3.0

3.2

3.4

3.6

3.8

4.0

w2 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.813 2.6 2.4 2.2 2.0 1.8

Pointer Mode

- select F1
- center F2
- add grid both F3
- add grid horz F4
- add grid vert F5
- add label F6
- add line F7
- find/add peak F8
- integrate F10
- zoom F11
- duplicate & zoom F12
- assignment copy sh-F1
- assignment guess sh-F2

durec@teslin.ncbr.muni.cz: /home/... Pointer Mode

Sparky 3.110

GSSG_DQF-COSY -- selected

1 / 4

peak picking:

výběr: mód myši – select: klávesa F1
kliknutím se přidá označí jeden objekt,
přetažením myši (nebo Shift+klik) se přidá více objektů

The screenshot displays the Sparky 3.110 software interface. The main window, titled "GSSG_DQF-COSY -- selected", shows a 2D NMR spectrum with four quadrants of peaks. The horizontal axis is labeled "w2" and ranges from 3.40 to 2.75. The vertical axis is labeled "w1" and ranges from -2.85 to -3.35. The peaks are colored in red and green, and some are marked with white 'X' symbols. A terminal window in the background shows the command "sparky" being executed. A "Pointer Mode" menu is open in the bottom right corner, listing various actions and their corresponding function keys. The "select" action is highlighted with a red circle, and an orange arrow points to it from the top right of the image.

Action	Function Key
select	F1
center	F2
add grid both	F3
add grid horz	F4
add grid vert	F5
add label	F6
add line	F7
find/add peak	F8
integrate	F10
zoom	F11
duplicate & zoom	F12
assignment copy	sh-F1
assignment guess	sh-F2

peak picking: vytvoření centrálního píku se zvolené skupiny píků – *pg*
(užitečné právě pro multiplety v COSY spektrech)

The screenshot displays the Sparky 3.110 software interface. The main window, titled "GSSG_DQF-COSY -- selected", shows a 2D COSY NMR spectrum with red and green contour lines. The x-axis is labeled "w2" and ranges from 3.40 to 2.75. The y-axis is labeled "w1" and ranges from -2.85 to -3.35. A terminal window on the right shows the command "sparky" being executed. A "Pointer Mode" menu is open in the bottom right corner, listing various functions:

Function	Shortcut
select	F1
center	F2
add grid both	F3
add grid horz	F4
add grid vert	F5
add label	F6
add line	F7
find/add peak	F8
integrate	F10
zoom	F11
duplicate & zoom	F12
assignment copy	sh-F1
assignment guess	sh-F2

The status bar at the bottom shows the current window is "GSSG_DQF-COSY -- selected".

peak picking: seznam píků – *lt*



The screenshot displays the Sparky 3.110 software interface. The main window is titled "GSSG_DQF-COSY -- selected" and shows a 2D NMR spectrum with several peaks highlighted in green and red. The x-axis is labeled "w2" and ranges from 9 to 1. The y-axis is labeled "w1" and ranges from 1 to 8. A "PeakListDialog" window is open in the top-left corner, showing a list of peaks with columns for "Assignment", "w1", and "w2". A terminal window in the top-right corner shows the command "[durec@teslin ~]\$ sparky". A "Pointer Mode" menu is visible in the bottom-right corner, listing various actions and their corresponding function keys.

Assignment	w1	w2
?-?	3.795	3.793
?-?	2.932	2.930
?-?	2.930	3.261
?-?	2.138	2.139
?-?	2.138	3.795
?-?	8.676	8.675
?-?	8.607	8.608
?-?	3.921	8.606
?-?	4.722	8.673
?-?	4.720	4.727
?-?	3.923	3.918
?-?	2.935	4.727
?-?	3.258	4.725
?-?	2.137	2.513
?-?	2.512	2.509
?-?	3.263	3.261

Pointer Mode

- select F1
- center F2
- add grid both F3
- add grid horz F4
- add grid vert F5
- add label F6
- add line F7
- find/add peak F8
- integrate F10
- zoom F11
- duplicate & zoom F12
- assignment copy sh-F1
- assignment guess sh-F2

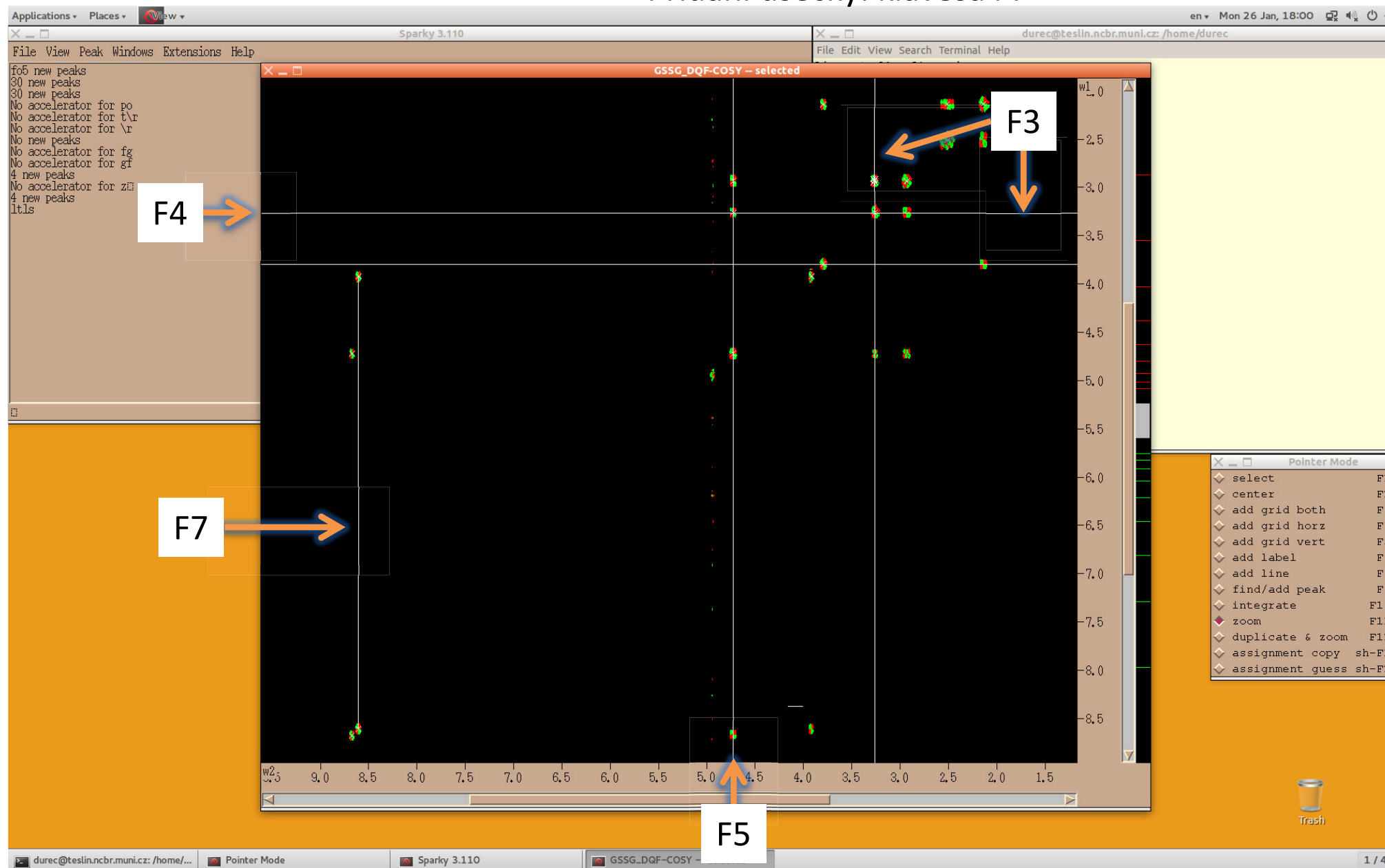
vyznačení spinových systémů:

Přidání vertikální i horizontální linie: klávesa F3

Přidání horizontální linie: klávesa F4

Přidání vertikální linie: klávesa F5

Přidání úsečky: klávesa F7



vyznačení spinových systémů:

úprava farby ornamentů (čar, popisků...): **ot** → color →
označit objekt/y → zvolit barvu dle libosti → apply

The screenshot displays the Sparky 3.110 NMR software interface. The main window shows a 2D NMR spectrum titled 'GSSG_DQF-COSY -- selected'. The x-axis is labeled 'w2' and ranges from 9.0 to 1.5 ppm. The y-axis is labeled 'w1' and ranges from 0 to -8.5 ppm. The spectrum shows several cross-peaks connected by colored lines (ornaments). A red circle highlights the 'Ornament Properties' dialog box, which is open over the spectrum. The dialog box has a 'Color ...' button and an 'Apply' button. Below the dialog box, a color selection palette is visible, listing various colors such as black, white, gray, red, green, blue, yellow, magenta, cyan, light blue, light green, light yellow, gold, orange, pink, beige, turquoise, coral, maroon, purple, and tomato. A 'Pointer Mode' menu is also visible in the bottom right corner, listing various actions and their corresponding function keys (F1-F12).

Applications ▾ Places ▾

en ▾ Mon 26 Jan, 18:11

Sparky 3.110

durec@teslin.ncbr.muni.cz: /home/durec

File View Peak Windows Extensions Help

File Edit View Search Terminal Help

GSSG_DQF-COSY -- selected

Ornament Properties

Description: 1 line

Lock position

Color ... Note ... Sizes ... Visibility ..

Apply Close Help

ot

Ornan

- black
- white
- gray
- red
- green
- blue
- yellow
- magenta
- cyan
- light blue
- light green
- light yellow
- gold
- orange
- pink
- beige
- turquoise
- coral
- maroon
- purple
- tomato

Close

Pointer Mode

- select F1
- center F2
- add grid both F3
- add grid horz F4
- add grid vert F5
- add label F6
- add line F7
- find/add peak F8
- integrate F10
- zoom F11
- duplicate & zoom F12
- assignment copy sh-F1
- assignment guess sh-F2

Trash

durec@teslin.ncbr.muni.cz: /home/... Pointer Mode Sparky 3.110 GSSG_DQF-COSY -- selected Ornament Properties Ornament Color

1 / 4

přiřazování signálů:

označit pík: mód myši – select: klávesa F1 → klávesová zkratka **at** – assignment → vepsat označení skupiny (např. zkratka rezidua) a označení atomu (např. NH) podle rezonance v osi w1 a w2 → apply

The screenshot displays the Sparky 3.110 NMR software interface. The main window shows a 2D COSY spectrum with two cross-peaks. The left peak is highlighted with a red box and a white arrow pointing to the text "CysNH-NH". The right peak is highlighted with a green box. The x-axis is labeled "w2" and the y-axis is labeled "w1".

An "Assignment GSSG_DQF-COSY" dialog box is open on the left, with a red circle around its table. The table contains the following data:

Axis	Group	Atom	Resonance	Peak	
w1	1H	Cys	NH	8.675	8.676
w2	1H	Cys	NH	8.675	8.675

Below the table, the "Resonances" section shows "Cys" and "NH" with a resonance value of "8.675". The dialog box has buttons for "Resonance Peaks...", "Guessing...", "Ok", "Apply", "Close", and "Help".

A "Pointer Mode" menu is open on the right, listing various mouse and keyboard shortcuts:

- select F1
- center F2
- add grid both F3
- add grid horz F4
- add grid vert F5
- add label F6
- add line F7
- find/add peak F8
- integrate F10
- zoom F11
- duplicate & zoom F12
- assignment copy sh-F1
- assignment guess sh-F2

The bottom status bar shows the current window is "GSSG_DQF-COSY -- selected" and the assignment dialog is "Assignment GSSG_DQF-COSY". The system tray includes a "Trash" icon and the page number "1 / 4".

přiřazování signálů:

kliknutím na označení osy se ze seznamu přiřazených frekvencí vybere přiřazení, které je nejbliž k frekvenci aktuálně vybraného píku v dané osy (nemusí být nutně správně!!), dvojklikem na řádek seznamu se pak název skupiny a atomu doplní k aktuálnímu píku

The screenshot displays the Sparky 3.110 software interface. The main window is titled "Assignment GSSG_DQF-COSY". On the left, there is a table for assigning peaks to axes. The table has columns for Axis, Group, Atom, Resonance, and Peak. The "w2" axis is selected, and the "Cys NH" resonance at 8.675 is highlighted. Below the table are buttons for "Resonance Peaks ...", "Guessing ...", "Ok", "Apply", "Close", and "Help".

Axis	Group	Atom	Resonance	Peak
<input type="checkbox"/> w1	1H			4.722
<input checked="" type="checkbox"/> w2	1H	Cys	NH	8.675

Below the table, the "Resonances" list shows:

Resonance	Atom	Peak
Gly	NH	8.607
Cys	NH	8.675

The main plot area shows a 2D NMR spectrum with a red and green contour plot. A red circle highlights the peak at approximately (8.675, 4.722). A vertical red line connects this peak to the "w2" axis label at the bottom left, which is also circled in red. A "Pointer Mode" menu is visible on the right side of the plot area, listing various actions like "select", "center", "add grid both", etc., with their corresponding function keys (F1-F12).

přirázování signálů:

zkratka **tb** – tabulka přiřazení
rezidua vs. atomy,
možnost zobrazení statistiky

možnost exportu do
textového souboru
(→ Save)

zkratka **lt** – seznam píků již s
přiřazením, příp. s dalšími daty
(→ Options)

Assignment Table

	Ha	Hb	Hb'	Hb''	Hc	NH
Cys	4.724	-	2.932	3.261	-	8.675
Glu	3.794	2.138	-	-	2.511	-
Gly	3.921	-	-	-	-	8.607

Spectrum Peaks GSSG_DQF-COSY

Assignment	w1	w2
CysHa-Ha	4.720	4.727
CysHa-NH	4.722	8.673
CysHb'-Ha	2.935	4.727
CysHb'-Hb'	2.932	2.930
CysHb'-Hb''	2.930	3.261
CysHb''-Ha	3.258	4.725
CysHb''-Hb''	3.263	3.261
CysNH-NH	8.676	8.675
GluHa-Ha	3.795	3.793
GluHb-Ha	2.138	3.795
GluHb-Hb	2.138	2.139
GluHb-Hc	2.137	2.513
GluHc-Hc	2.512	2.509
GlyHa-Ha	3.923	3.918
GlyHa-NH	3.921	8.606
GlyNH-NH	8.607	8.608

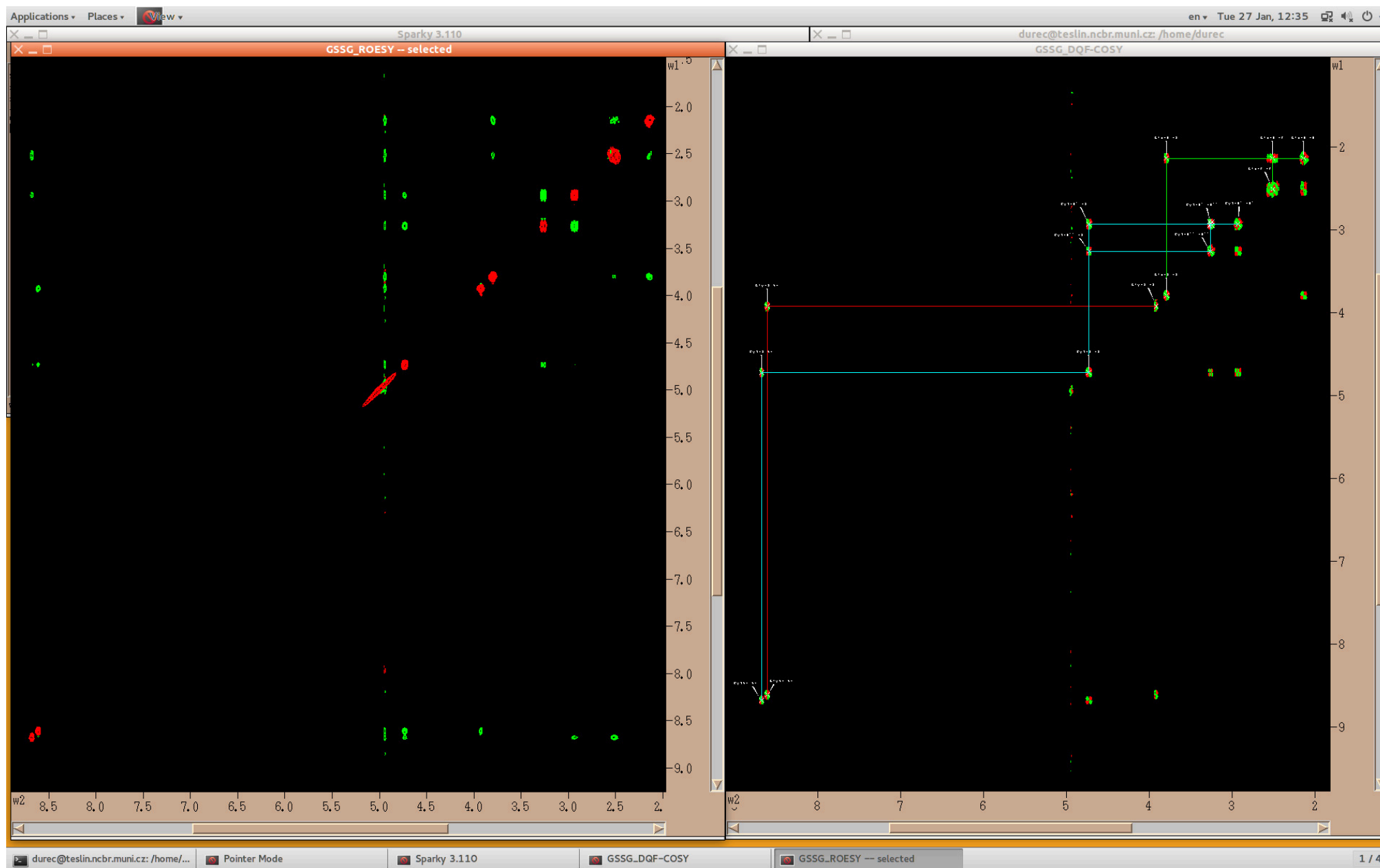
Pointer Mode

Action	Shortcut
select	F1
center	F2
add grid both	F3
add grid horz	F4
add grid vert	F5
add label	F6
add line	F7
find/add peak	F8
integrate	F10
zoom	F11
duplicate & zoom	F12
assignment copy	sh-F1
assignment guess	sh-F2

práce s vícero spektry:

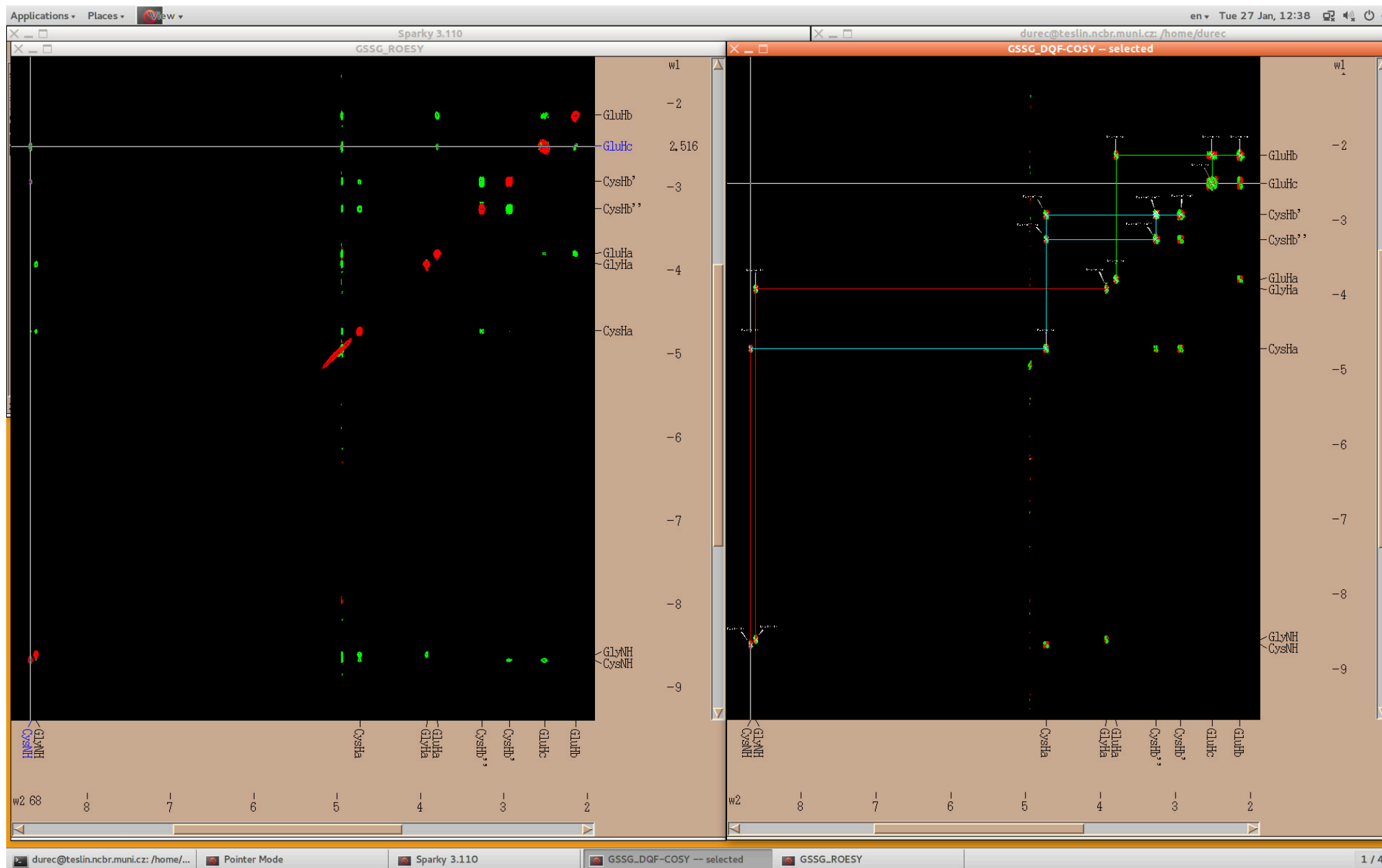
přiřazení z jednoho spektra je k dispozici i pro další spektra

- otevřít ROESY spektrum: **fo** → načíst GSSG_ROESY.ucsf → přizpůsobit vzhled (kontury, barvy, velikosti...)



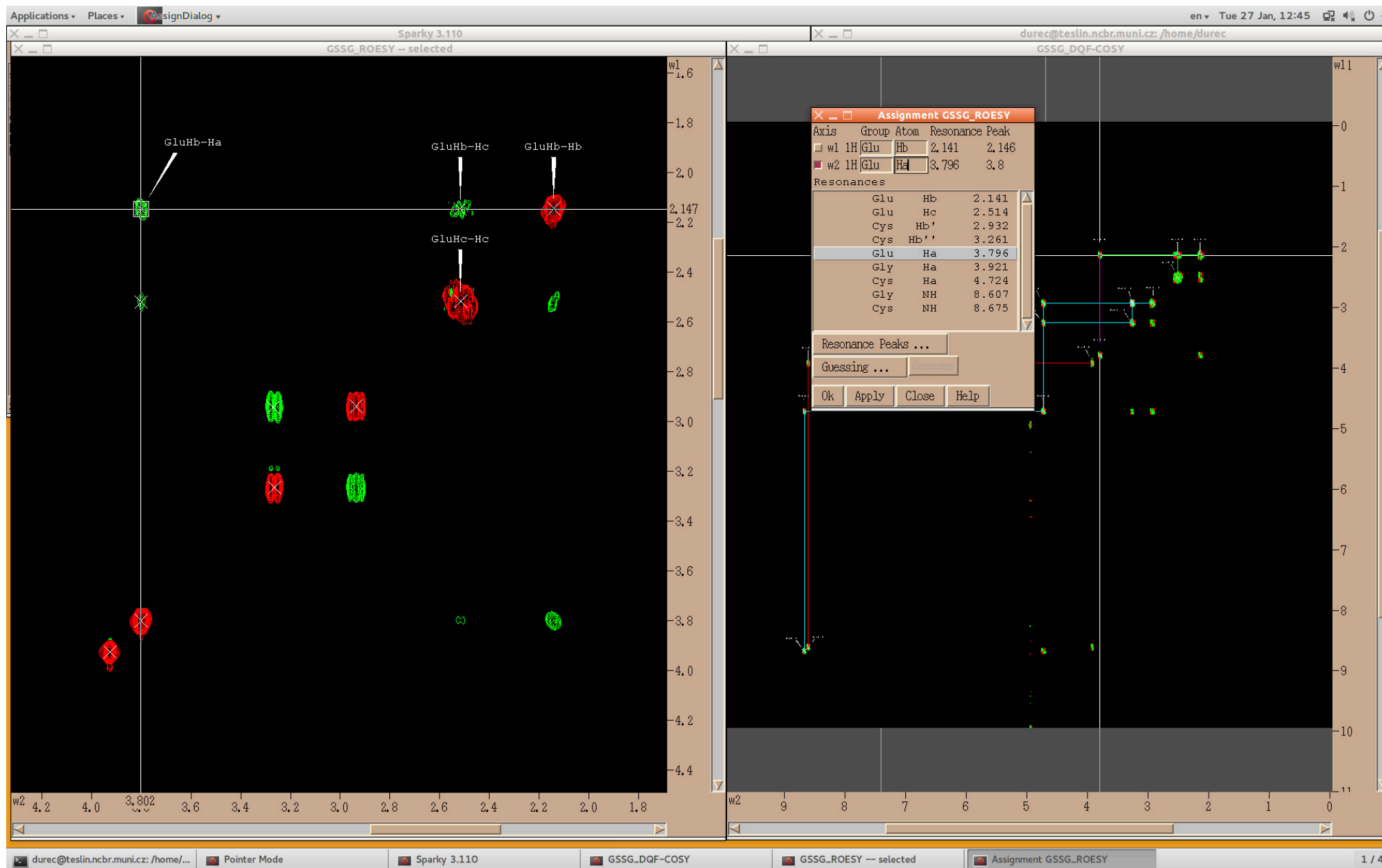
práce s vícero spektry:

zobrazení přiřazených (průměrných) rezonancí na okraji spekter - **vR**



práce s vícero spektry:

přiřazení ROESY pomocí *at*:



práce s vícero spektry:

synchronizace zobrazení spekter: zkratka **yt** – umožní současně posouvat zesynchronizované osy vícero spekter když se posouváme v jednom z nich, zakliknout osy a spektra, které chceme vzájemně zesynchronizovat → Synchronize

