

# TopSpin

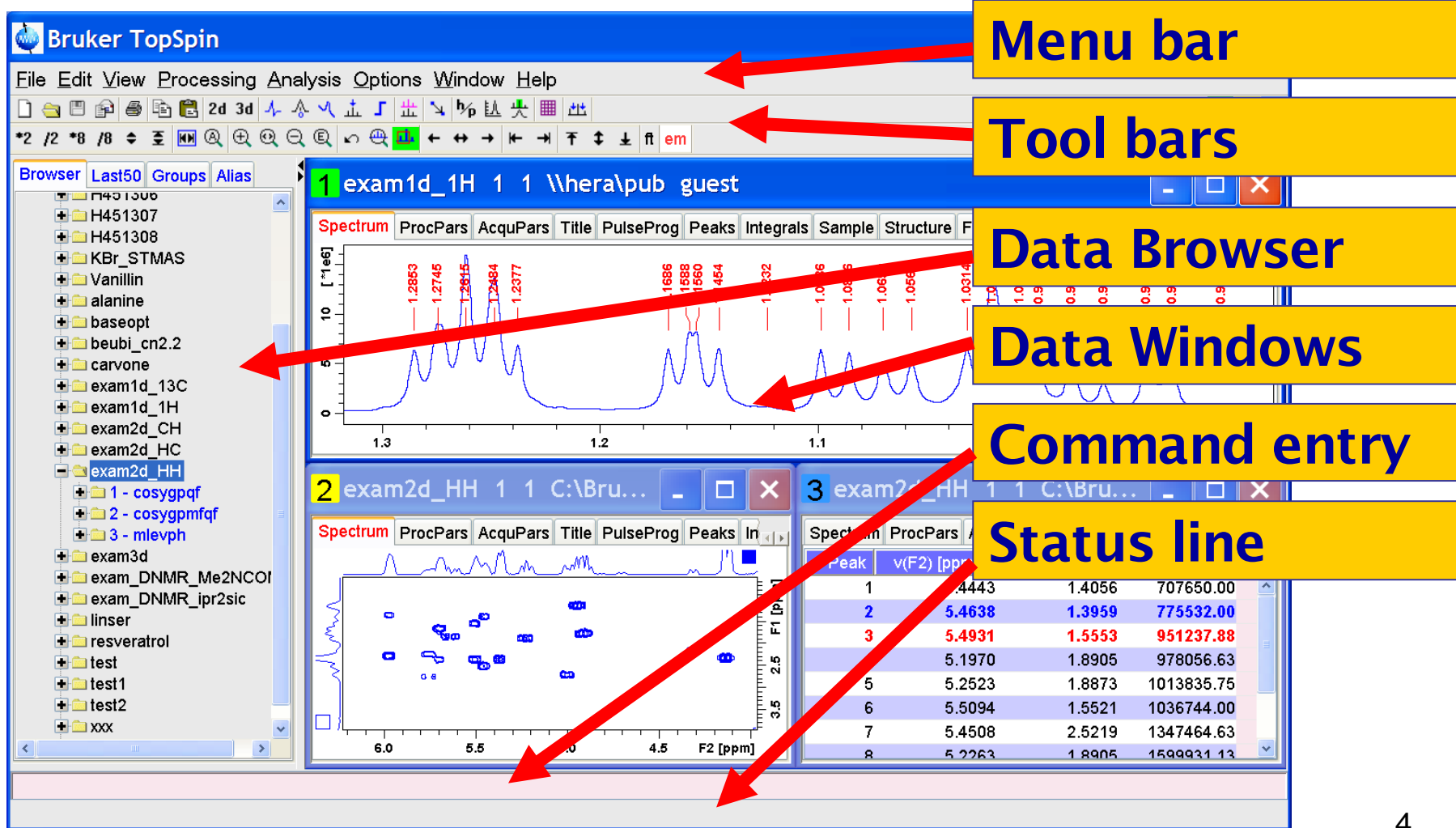
*User Interface Concepts*

- **Basic User Interface Principles**
- **Multiple-Window Interface**
- **Multiple Spectrum Display**
- **Data Browsing**
- **Data Export / Import Formats**
- **Exporting Graphics**
- **User Interface Customization**
- **Command Queuing and Scheduling**

## Features:

- Designed for *Windows and Linux* users with a highly intuitive interface
- Uses most widespread *standards* familiar from word processing, graphics, or presentation programs
- Provides same *look and feel* for your NMR applications

## PC standard user interface elements:



The screenshot shows the Bruker TopSpin software interface. The menu bar at the top includes File, Edit, View, Processing, Analysis, Options, Window, and Help. Below it is a toolbar with various icons for file operations and analysis. On the left is a Data Browser showing a tree view of files and folders. The main area contains three windows: a 1D spectrum window (exam1d\_1H), a 2D spectrum window (exam2d\_HH), and a peak list table (exam2d\_HH). Red arrows point from yellow callout boxes to these elements.

**Menu bar**

**Tool bars**

**Data Browser**

**Data Windows**

**Command entry**

**Status line**

Peak	v(F2) [ppm]	F1 [ppm]	F2 [ppm]
1	4.443	1.4056	707650.00
2	5.4638	1.3959	775532.00
3	5.4931	1.5553	951237.88
	5.1970	1.8905	978056.63
5	5.2523	1.8873	1013835.75
6	5.5094	1.5521	1036744.00
7	5.4508	2.5219	1347464.63
8	5.2263	1.8905	1599931.13

# Basic User Interface Principles



The screenshot displays the Bruker TopSpin software interface. The 'File' menu is open, showing a standard set of options: New... [Ctrl N], Open... [Ctrl O], Reopen, Close [Ctrl W], Close All..., Save... [Ctrl S], Print... [Ctrl P], Export..., Send To..., Run..., and Delete... Below these are several recent files listed with their names and paths. The main window shows an NMR spectrum with peaks labeled with their chemical shifts: 1.2484, 1.2377, 686, 588, 560, 454, 232, and 986. A red arrow points from a yellow callout box to the 'Print...' option in the File menu.

AcquPars	Title	PulseProg	Peaks	Integrals	Sample
1	1	\\hera\pub	guest		
1	exam2d_HH	1	1	C:\Bruker\TOPSPIN	guest
2	resveratrol	1	998	C:\Bruker\TOPSPIN	guest
3	exam1d_1H	1	1	\\hera\pub	guest
4	exam3d	1	1	C:\Bruker\TOPSPIN	guest
5	exam1d_1H	1	3	\\hera\pub	guest
6	exam1d_1H	2	4	\\hera\pub	guest

**Standard type *File menu*:  
No NMR specifics!**

# Basic User Interface Principles



**Right-click context menus everywhere!**

**User-Defined Menu**

- Change Menu Font
- Define Right-Click Action
- Hide Menubar (type SHIFT ESC to reset)

**Reactivate All Invisible/Inactive Buttons**

- Add User-Defined Button
- Change Icon Size
- Change Toolbar Offset
- Hide Toolbars (type SHIFT ESC to reset)

**Display**

- Display In New Window
- Display As 2D Projection
- On/Off: Show PULPROG/Title
- Scroll to active dataset
- Copy
- File Properties
- Delete...
- Files
- Add New Data Dir...
- Remove Selected Data Dirs...

**Display Properties...**

- Save Display Region To...
- Restore Display Region From Params. F1/2
- Set plot height for current position
- File Properties...
- Files

**Command Line History**

- Resize Command Line
- Save As A Macro...

**Acquisition Status Bar On/Off**

The screenshot shows the Bruker TopSpin software interface. The main window displays a spectrum plot for Benzaldehyde. The interface includes a menu bar (File, Edit, View, Processing, Analysis, Options, Window, Help), a toolbar, and a browser pane on the left showing a file tree. A chemical structure of Benzaldehyde is visible in the center. Red arrows point to various UI elements, and callout boxes provide details about right-click context menus and other features.

# Multiple-Window Interface



Display and process several datasets simultaneously

**Bruker TopSpin**

File Edit View Processing Analysis Options Window Help

1 2 3

\*2 /2 \*8 /8

Browser Last50 Groups Alias

- H451306
- H451307
- H451308
- KBr\_STMAS
- Vanillin
- alanine
- baseopt
- beubi\_cn2.2
- carvone
- exam1d\_13C
- exam1d\_1H
- exam2d\_CH
- exam2d\_HC
- exam2d\_HH
  - 1 - cosygpfq
  - 2 - cosygpmfq
  - 3 - mlevph
- exam3d
- exam\_DNMR\_Me2NCOI
- exam\_DNMR\_ipr2sic
- linser
- resveratrol
- test
- test1
- test2
- xxx

**1 exam1d\_1H 1 1 \\hera\pub guest**

Spectrum ProcPars AcqPars Title PulseProg Peaks Integrals Sample Structure Fid

**2 exam2d\_HH 1 1 C:\Bru...**

Spectrum ProcPars AcqPars Title PulseProg Peaks In

**3 exam2d\_HH 1 1 C:\Bru...**

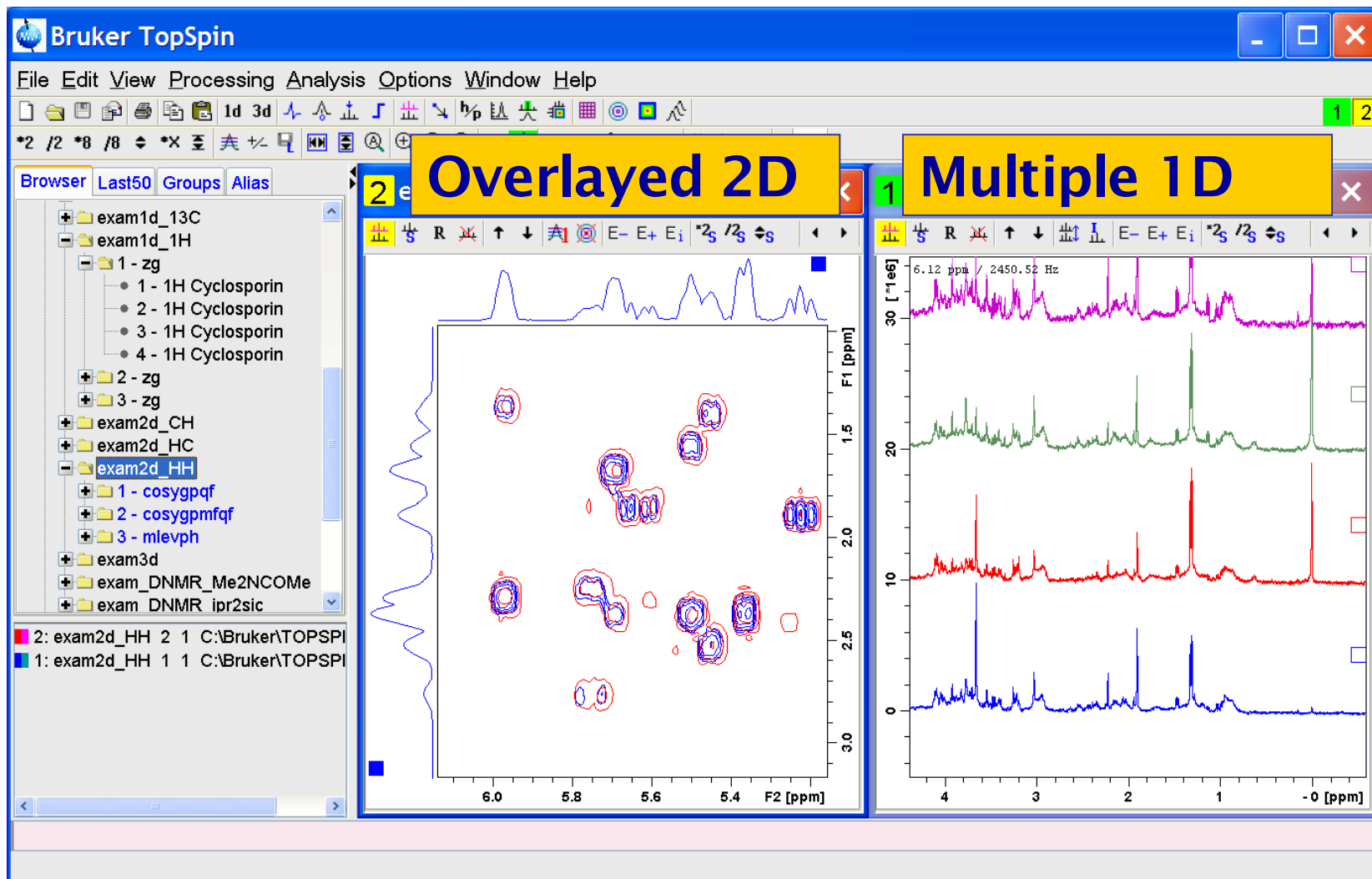
Spectrum ProcPars AcqPars Title PulseProg Peaks In

Peak	v(F2) [ppm]	v(F1) [ppm]	Intensity
1	5.4443	1.4056	707650.00
2	5.4638	1.3959	775532.00
3	5.4931	1.5553	951237.88
4	5.1970	1.8905	978056.63
5	5.2523	1.8873	1013835.75
6	5.5094	1.5521	1036744.00
7	5.4508	2.5219	1347464.63
8	5.2263	1.8905	1599931.13

# Multiple-Spectrum Display



Display and compare several spectra simultaneously in the same window





# Data Browsing



**Bruker TopSpin** **Browse dataset *hierarchy***

File Edit View Processing Analysis Options Window Help

\*2 /2 \*8 /8

**View the *50 last used* datasets**

Browser **Last50** Groups Alias

- carvorie
  - exam1d\_13C
  - exam1d\_1H
    - 1 - zg
      - 1 - 1H Cyclosporin
      - 2 - 1H Cyclosporin
      - 3 - 1H Cyclosporin
      - 4 - 1H Cyclosporin
    - 2 - zg
    - 3 - zg
  - exam2d\_CH
  - exam2d\_HC
  - exam2d\_HH
  - 1 - cosyg
  - 2 - cosyg
  - 3 - mlevp
- exam3d
- exam\_DNM
- exam\_DNM
- linser
- resveratrol
- test
- test1
- test2
- xxx
- ~TEMP
- saft

**Define and view *alias names* for datasets**

**Define and view *groups of datasets* ("projects")**

# Data Browsing



**Bruker TopSpin**

File Edit View Processing Analysis Options Window Help

Browser Last50 Groups Alias

- carvorie
  - exam1d\_13C
  - exam1d\_1H
    - 1 - zg
      - 1 - 1H Cyclosporin
      - 2 - 1H Cyclosporin
      - 3 - 1H Cyclosporin
      - 4 - 1H Cyclosporin
    - 2 - zg
    - 3 - zg
  - exam2d\_13C
  - exam2d\_1H
  - exam2d\_HH
    - 1 - cosygpqf
    - 2 - cosygpmfqf
    - 3 - mlevph
  - exam3d
  - exam\_DNMR\_Me2NCOMe
  - exam\_DNMR\_ipr2sic
  - linser
  - resveratrol
  - test
  - test1
  - test2
  - xxx
  - ~TEMP
- saft

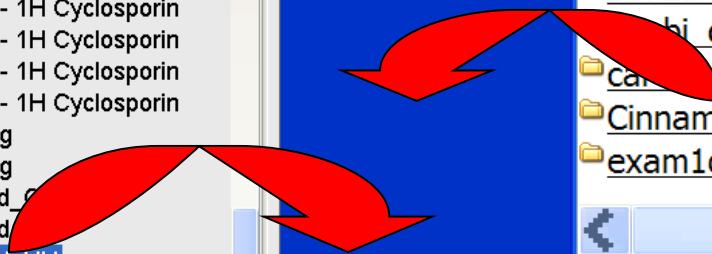
C:\Bruker\TOPSPIN\data\guest\nmr

Datei Bearbeiten Ansicht Favoriten Extras ?

Zurück Suchen Ordner Wechseln zu

Adresse C:\Bruker\TOPSPIN\data\guest\nmr

~TEMP	exam1d_13C	H451305
alanine	exam2d_CH	H451306
baseopt	exam2d_HC	H451307
Benzaldehyde	exam2d_HH	H451308
bi_cn2.2	exam3d	KBr STMAS
carvorie	exam_DNMR_ipr2sic	linser
Cinnamaldehyde	exam_DNMR_Me2NCOMe	resveratrol
exam1d_1H	H451304	test



**Open dataset by *Drag & Drop***  
- from TopSpin browser  
- Windows/Linux file explorer

# Data Browsing

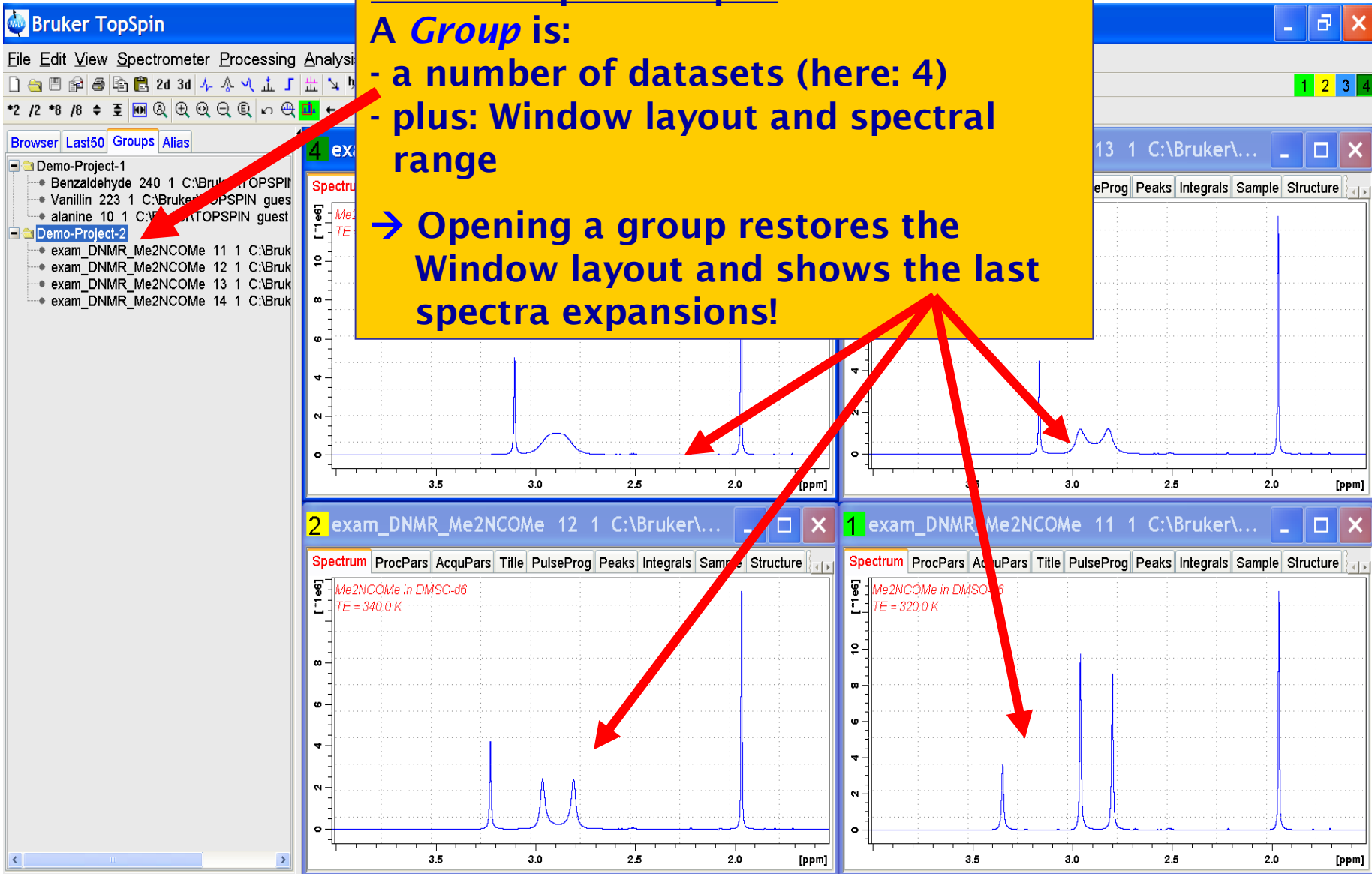


## Data Groups Example:

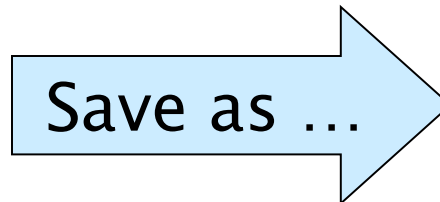
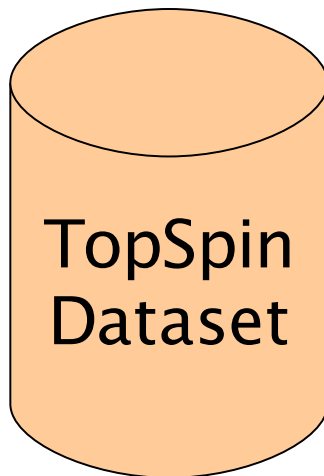
A *Group* is:

- a number of datasets (here: 4)
- plus: Window layout and spectral range

→ Opening a group restores the Window layout and shows the last spectra expansions!

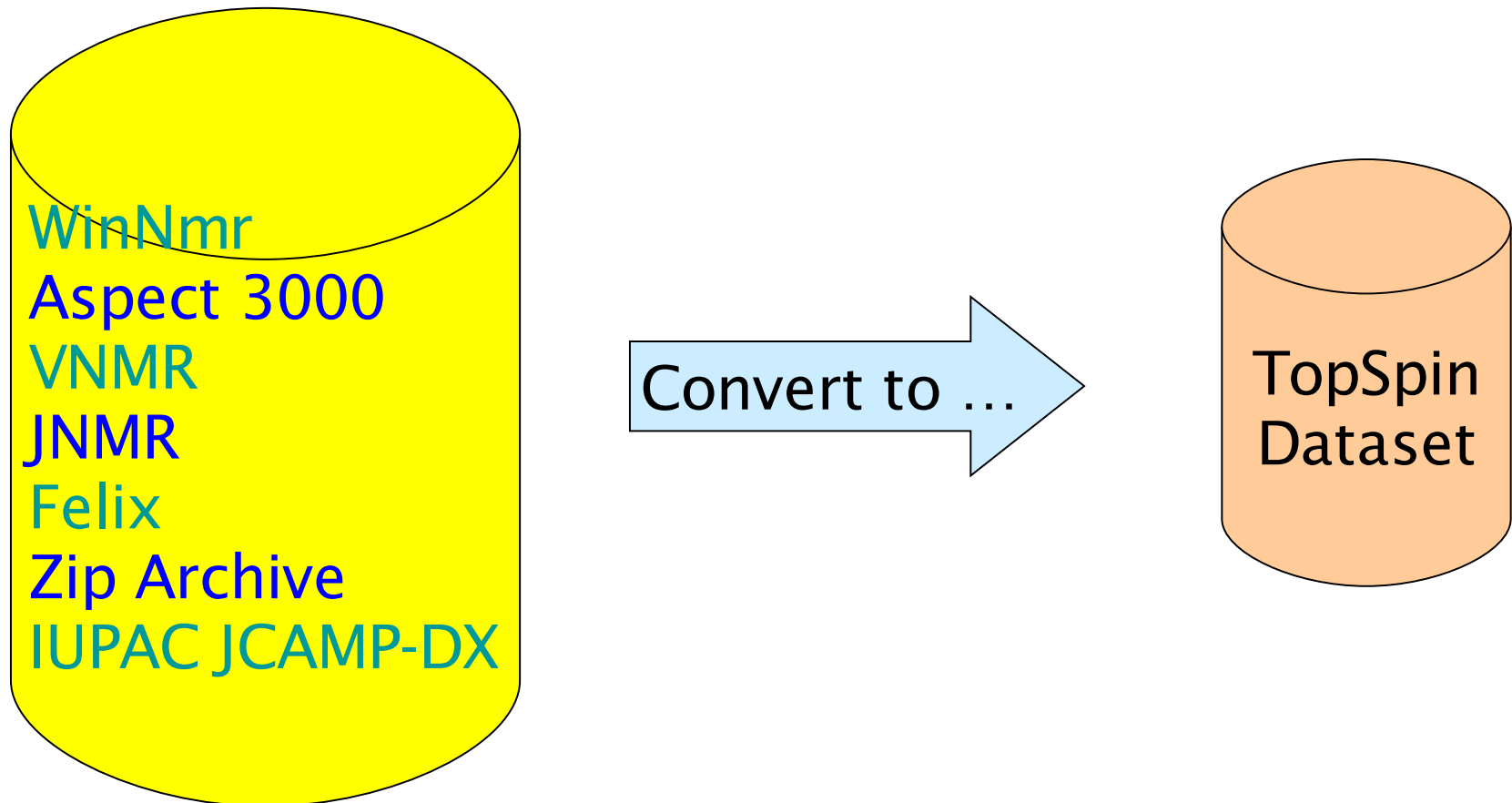


## Export TopSpin data in various formats



\* Collaborative Computing Project for NMR (<http://www.ccpn.ac.uk>)

## Import data from various formats into TopSpin



# Exporting Graphics

Export the contents of a window into a file or other programs using a desired *graphics format*



**Formats**  
clipboard, .png,  
.jpg, .wmf, .emf

Word  
OpenOffice  
PowerPoint  
etc.



## Adjust the TopSpin appearance according to your preferences

- Font sizes and colors
- Size of Icons
- Spectra colors and line thickness
- Background colors
- Menu Contents
- Tool buttons
- Functions keys
- Command names

Define your own user interface panels to launch commands, AU programs, etc.

**Basic NMR Experiments**

Close Selective →  Tips

X Nucleus = 13C

Lock	Tune Match	Auto Shim
1H	X{1H} with NOE	X Nuc. no dec
X{1H} no NOE	X{1H} DEPT90	X{1H} DEPT135
1H-1H Gr.COSY	1H-X Gr.HSQC	1H-X Gr.HMBC
1H-1H NOESY	1H-1H TOCSY	1H-1H ROESY
1H-1H COSY	1H-X HSQC	1H-X HMBC

**Selective NMR Experiments**

Close Basic →  Tips

Lock	Tune Match	Auto Shim
1H		Sel.Pulse Calibr.
Sel. Exc		Sel.Grad. Exc.
Sel. COSY		Sel.Gr. COSY
Sel. NOESY		Sel.Gr. NOESY
Sel. TOCSY		Sel.Gr. TOCSY
Sel. ROESY		Sel.Gr. ROESY

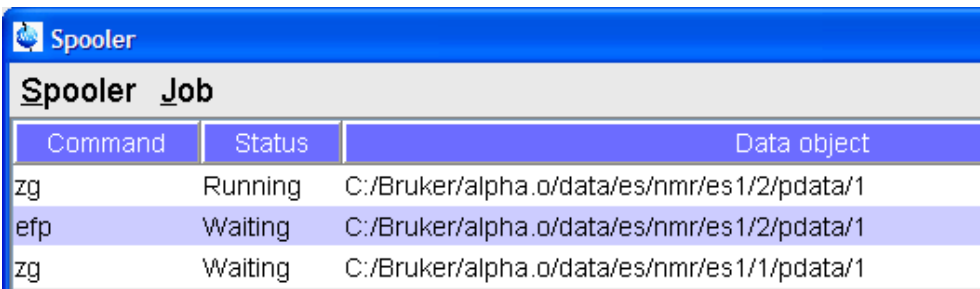
**1D Processing Panel**

Close To 2D  Tips

EM	FT	PK
Print	EXPORT	SEND TO

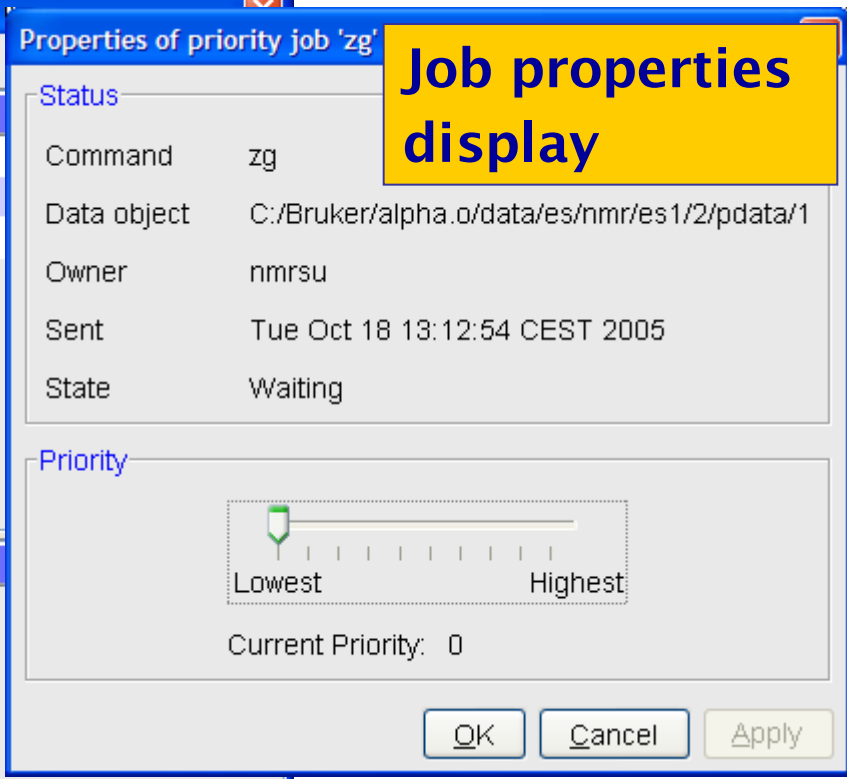


**TopSpin allows you to queue or schedule acquisition or processing tasks**



Command	Status	Data object
zg	Running	C:/Bruker/alpha.o/data/es/nmr/es1/2/pdata/1
efp	Waiting	C:/Bruker/alpha.o/data/es/nmr/es1/2/pdata/1
zg	Waiting	C:/Bruker/alpha.o/data/es/nmr/es1/1/pdata/1

**Spooler display with queued commands**



**Job properties display**

Status

Command zg

Data object C:/Bruker/alpha.o/data/es/nmr/es1/2/pdata/1

Owner nmrsu

Sent Tue Oct 18 13:12:54 CEST 2005

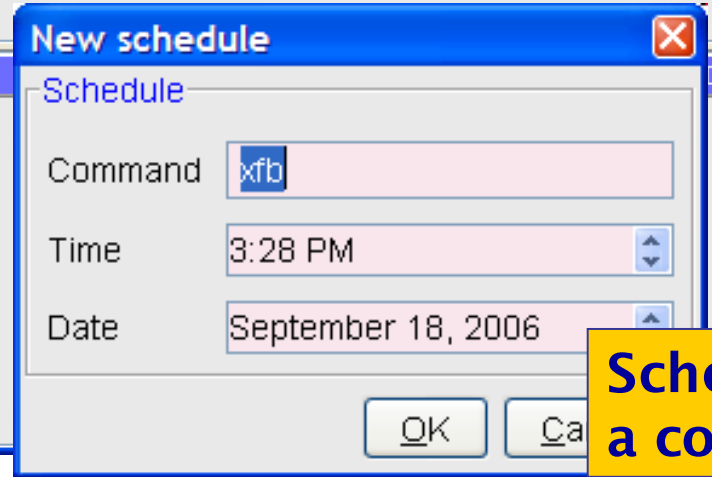
State Waiting

Priority

Lowest Highest

Current Priority: 0

OK Cancel Apply



**New schedule**

Schedule

Command xfb

Time 3:28 PM

Date September 18, 2006

OK Cancel

**Scheduling a command**