

TopSpin

*Multiplet
Analysis
Tutorial*

→ Automatic Multiplet Definition

→ Manual Single-Level Multiplet Definition

→ Manual Multi-Level Multiplet Definition

→ Working with Multiplets

→ Report dialog and export to JMR and Japanese patent format

→ Defining multiplet \leftrightarrow structure correlation

You may define multiplets automatically:

- in whole displayed region
- in manually selected region

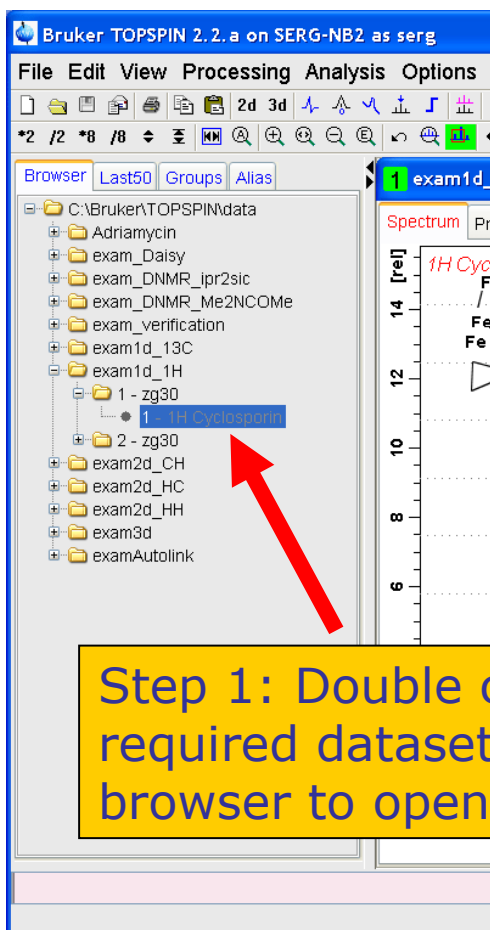
The procedure:

- Open required dataset
- Do Peak Picking first
- Enter Multiplet Analysis
- Use automatic multiplet definition features

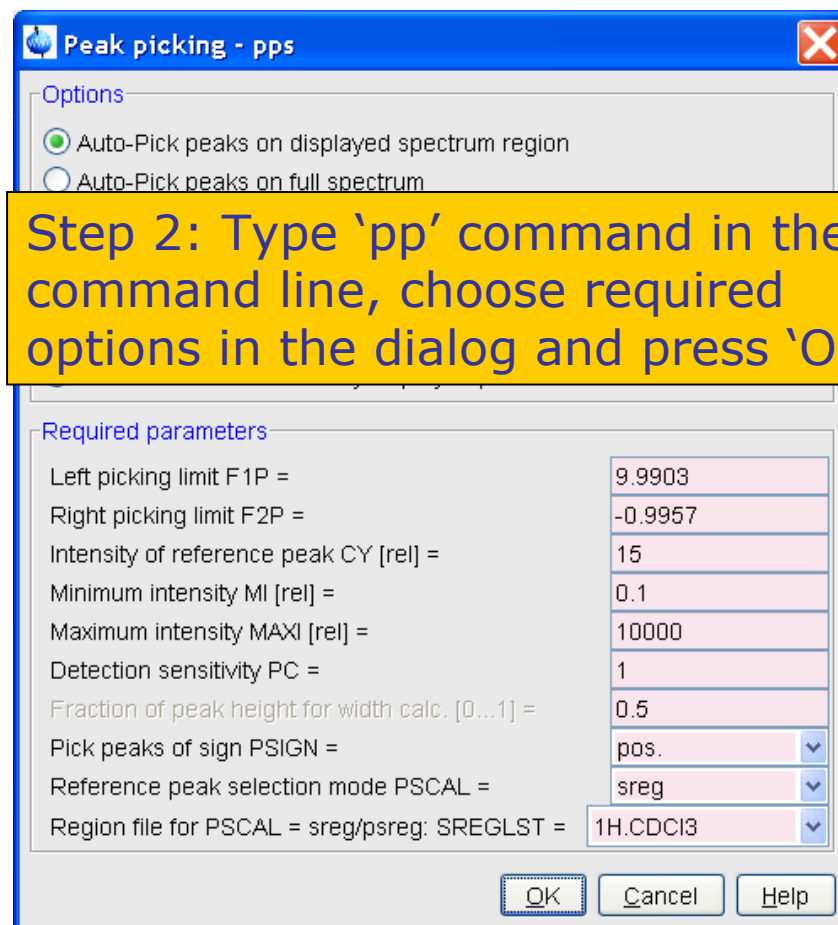
Automatic Multiplet Definition: Peak Picking



Peak Picking must be performed before entering into Multiplet Analysis mode in case of using of automatic multiplet definition feature

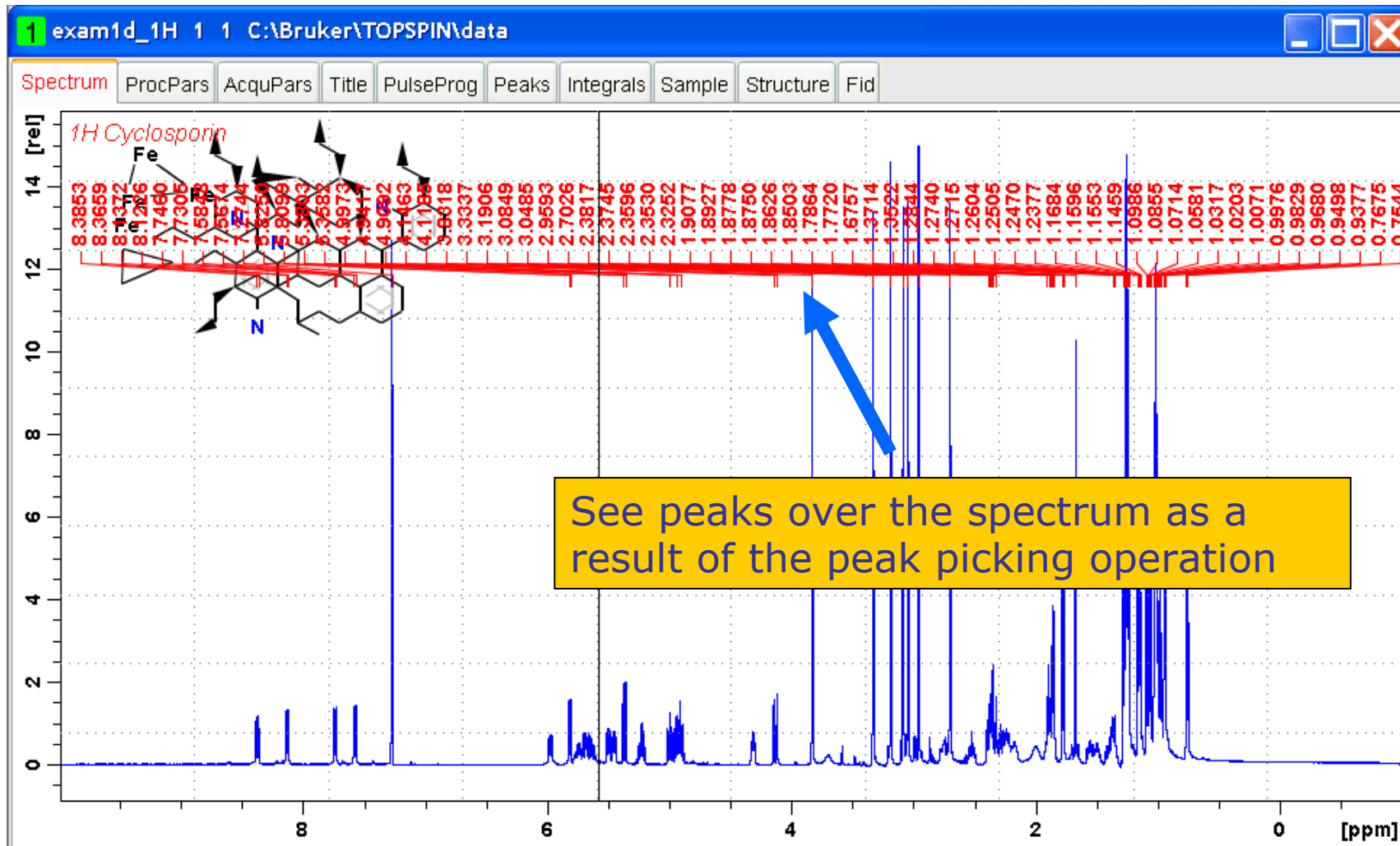


Step 1: Double click required dataset in the browser to open it



Step 2: Type 'pp' command in the command line, choose required options in the dialog and press 'Ok'

Automatic Multiplet Definition: Peak Picking



Enter Multiplet Analysis



1 exam1d_1H 1 1 C:\Bruker\Topspin\data

1H Cyclosporin

(Optional) Scroll and zoom required spectrum range where you want to find multiplets automatically

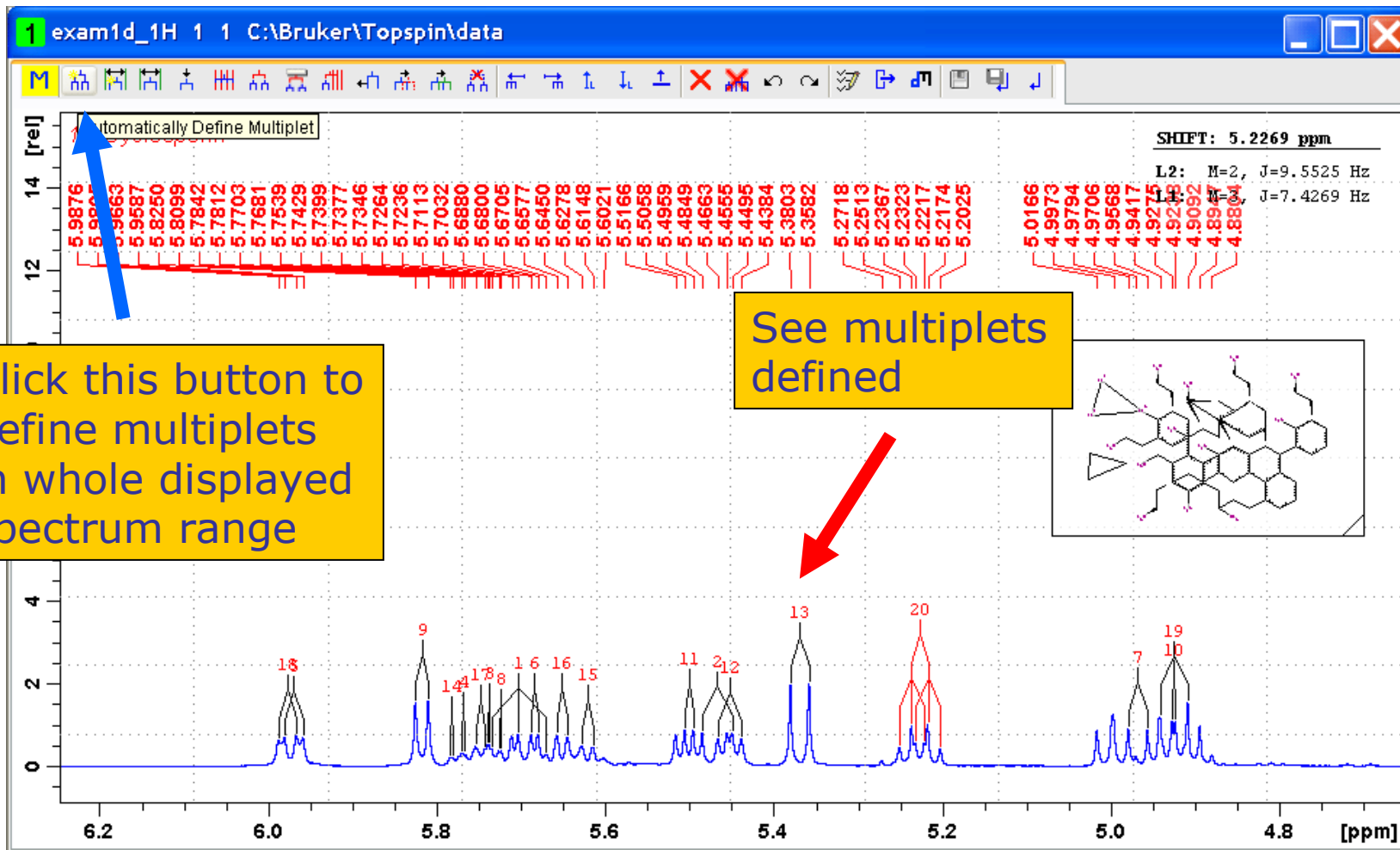
Type 'mana' command in the command line and press enter

Chemical Shift [ppm]
5.9876
5.9805
5.9663
5.9587
5.8250
5.8099
5.7842
5.7703
5.7681
5.7539
5.7429
5.7399
5.7377
5.7346
5.7264
5.7113
5.7032
5.6880
5.6700
5.6570
5.6450
5.6270
5.6170
5.6070
5.5116
5.5050
5.4950
5.4870
5.4660
5.4550
5.4450
5.4380
5.3800
5.3550
5.2700
5.2500
5.2300
5.2100
5.2000
5.0160
4.9970
4.9780
4.9700
4.9560
4.9410
4.9270
4.9230
4.9080
4.8940
4.8800

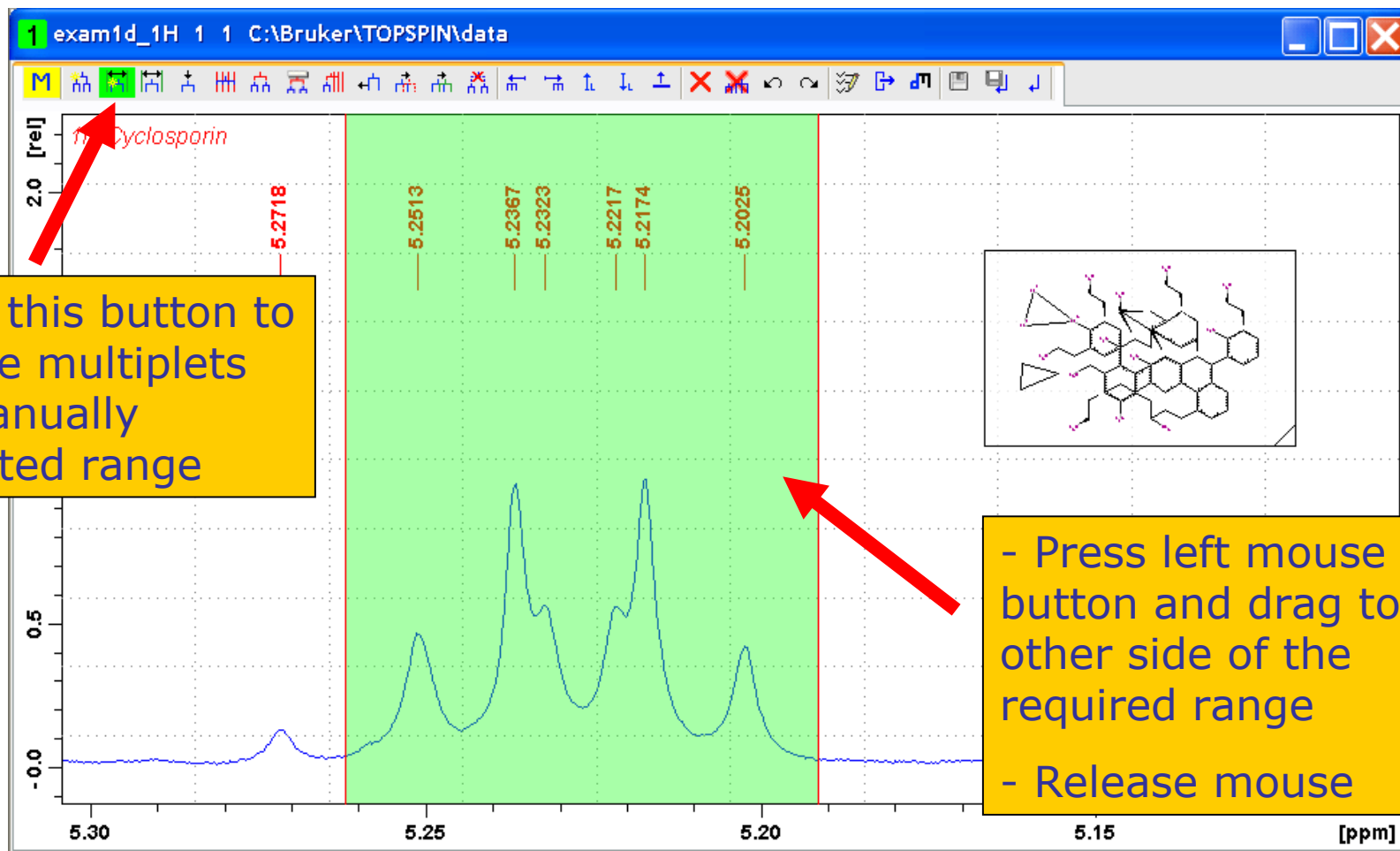
6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 [ppm]

пуск B... T... Mi... Ja... C... Br... A... A... Mi... Б... EN 15:49

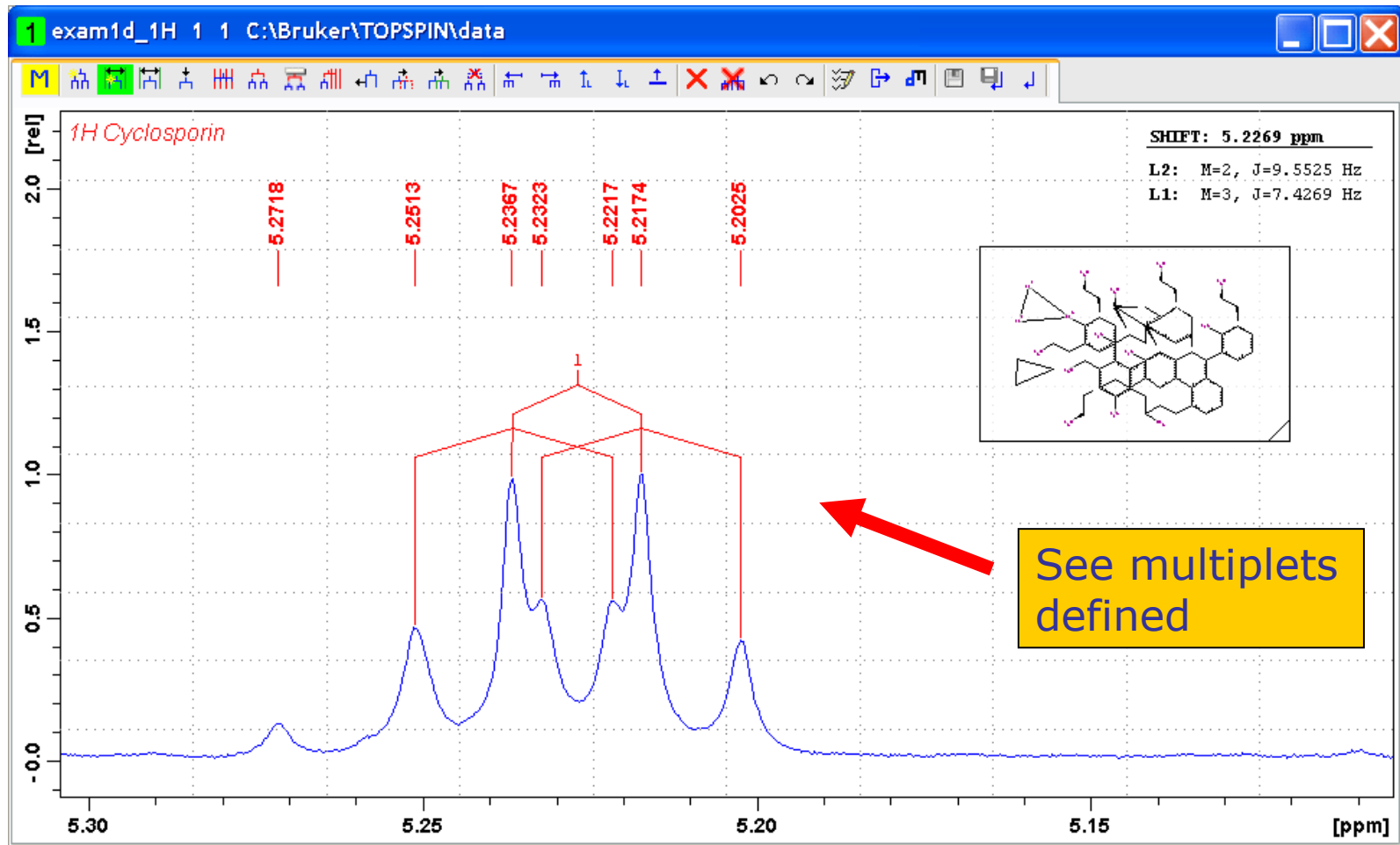
Automatic Definition in Displayed Range



Automatic Definition in Selected Range



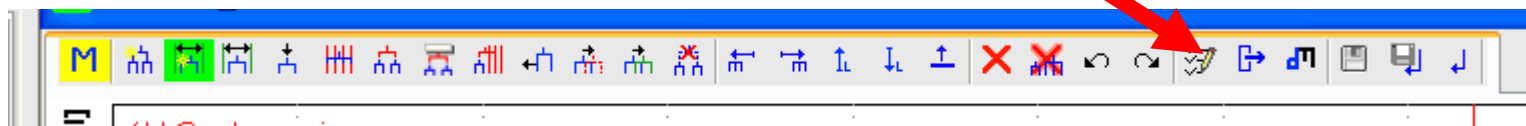
Automatic Definition in Selected Range



Multiplet Options Dialog



Click here to open dialog



Multiplet Options

Manual multiplet creation

Distance Lines: 2

Capture Range: 10 Points

Drift Range: 5 Points

Min. Intensity: 20.0 %

Min. Delta/J: 10.0

Automatic multiplet creation

Coupling tolerance: 5.0 %

Intensity tolerance: 30.0 %

Maximal coupling: 20.0 Hz

Maximal multiplicity: 4

Create singlets:

Display options

Labels Vertical:

Multiplet Ticks:

Multiplet tree form: Diagonal tree

OK Cancel

Features:

- Define automatic multiplet definition options
- Define manual multiplet definition options
- Define display options

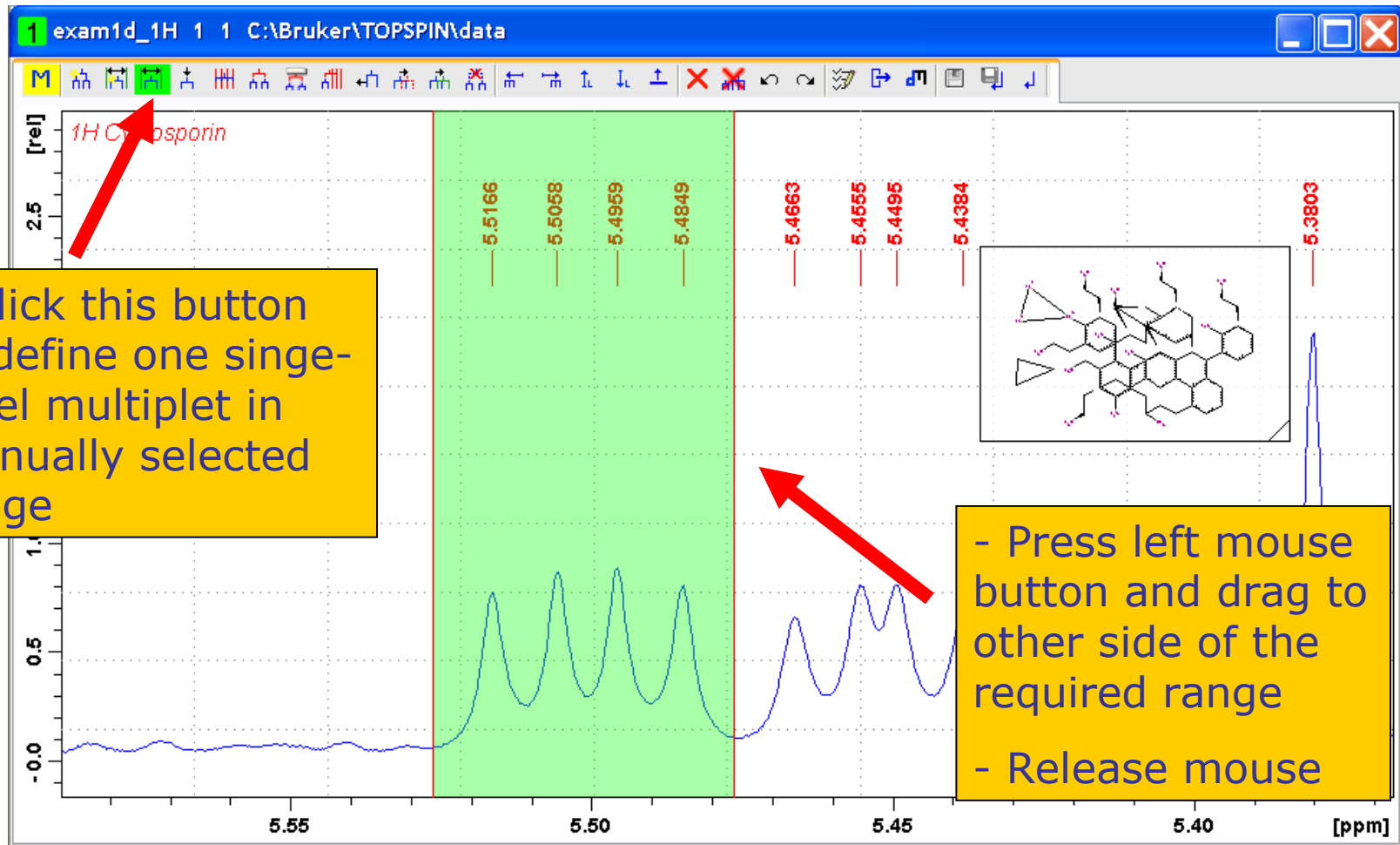
The following options affect automatic multiplet definition algorithm:

- **Coupling tolerance** shows maximal difference between coupling constants J (the distances between peaks) which still allows to add a peak to a multiplet
- **Intensity tolerance** shows maximal difference between peak intensities which still allows to include such peaks into a multiplet
- **Maximal coupling** defines maximal possible coupling constant J
- The algorithm tries to find multiplets of **Maximal multiplicity** or less
- **Create singlets** shows if singlets should be created

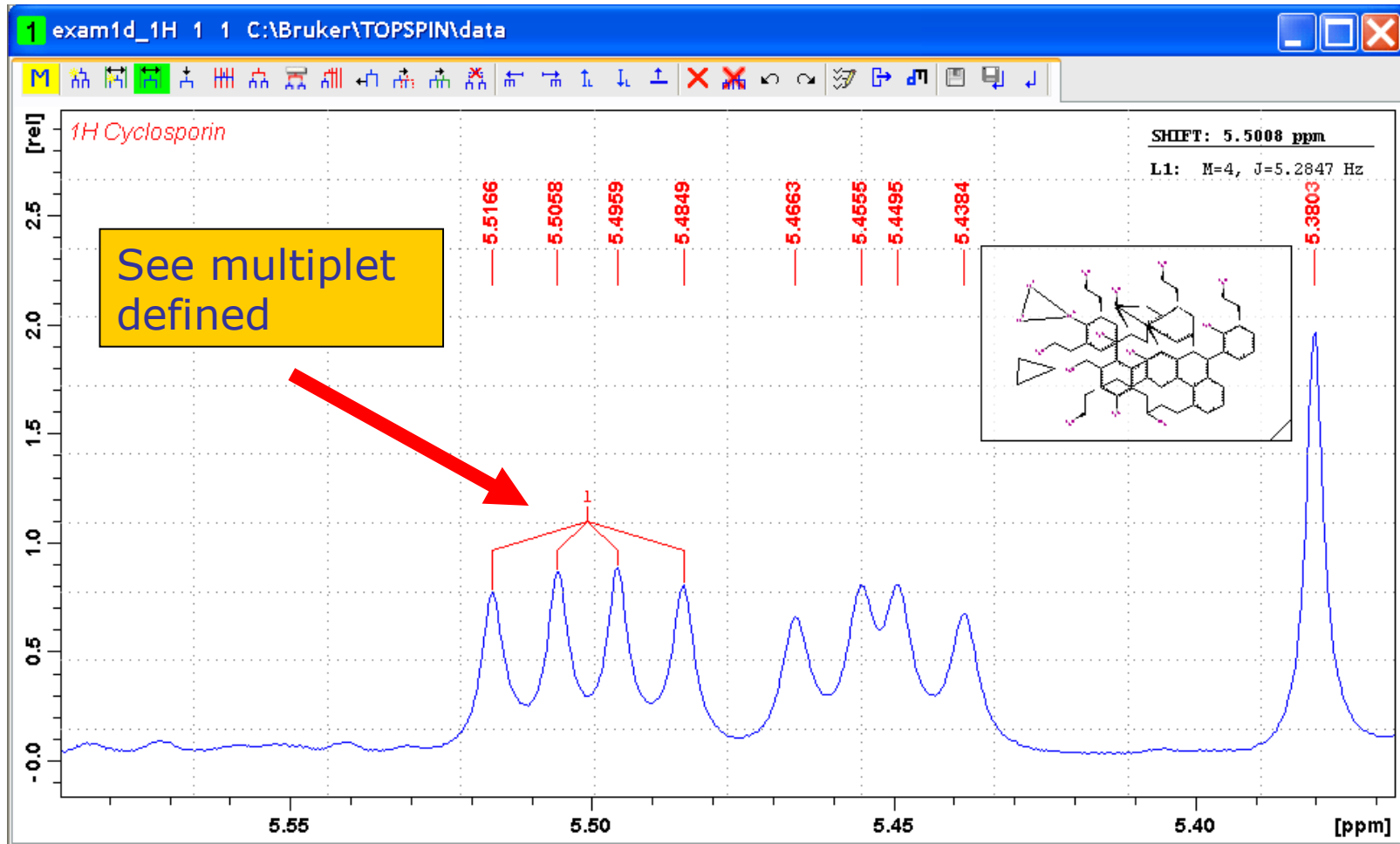
There are three methods to define a single-level multiplet manually or semi-automatic:

- Define single-level multiplet by region
- Define single-level multiplet by selecting peaks manually
- Define single-level multiplet using the 'Free Grid' feature

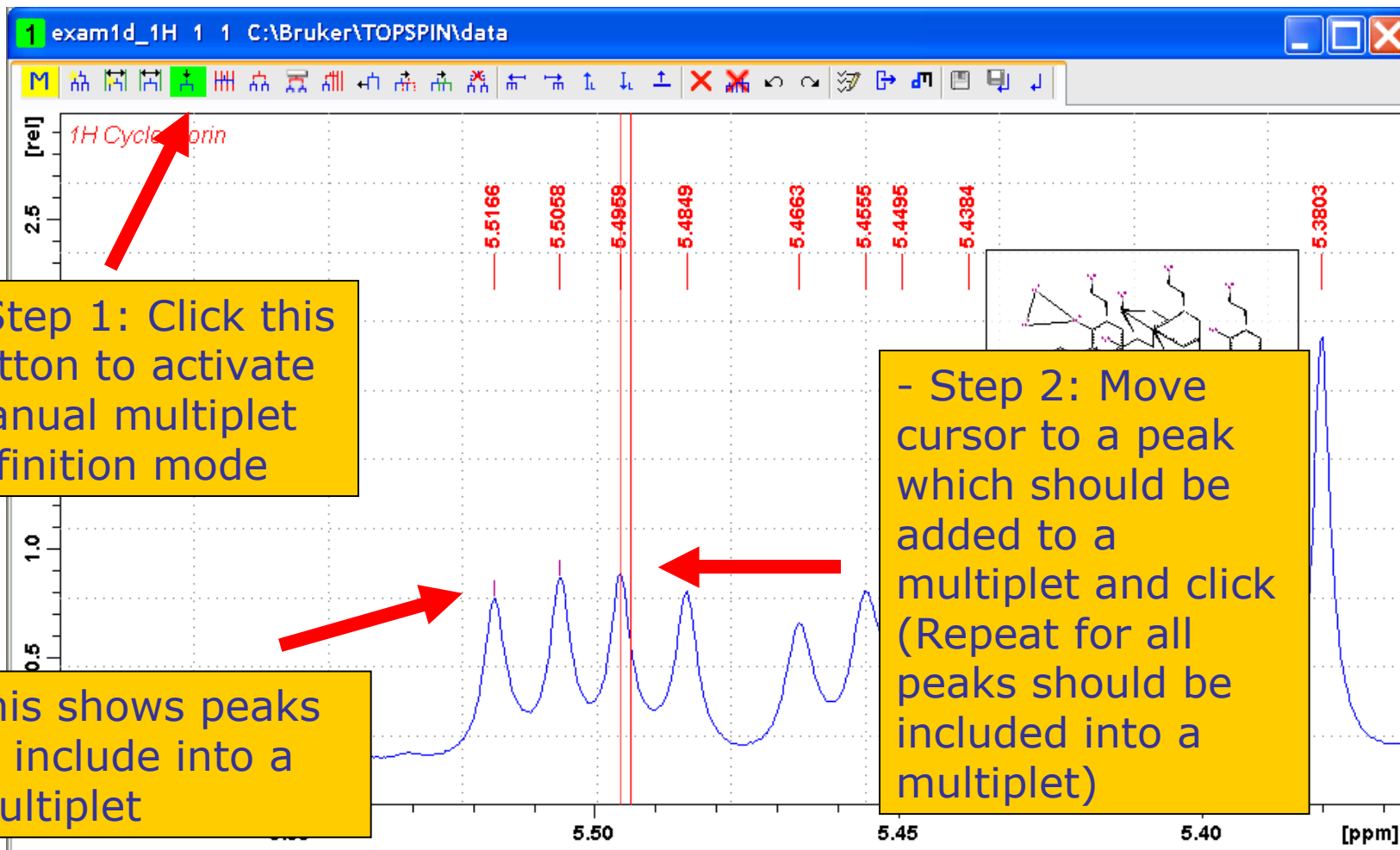
Define single-level multiplet by region



Define single-level multiplet by region



Define single-level multiplet manually



- Step 1: Click this button to activate manual multiplet definition mode

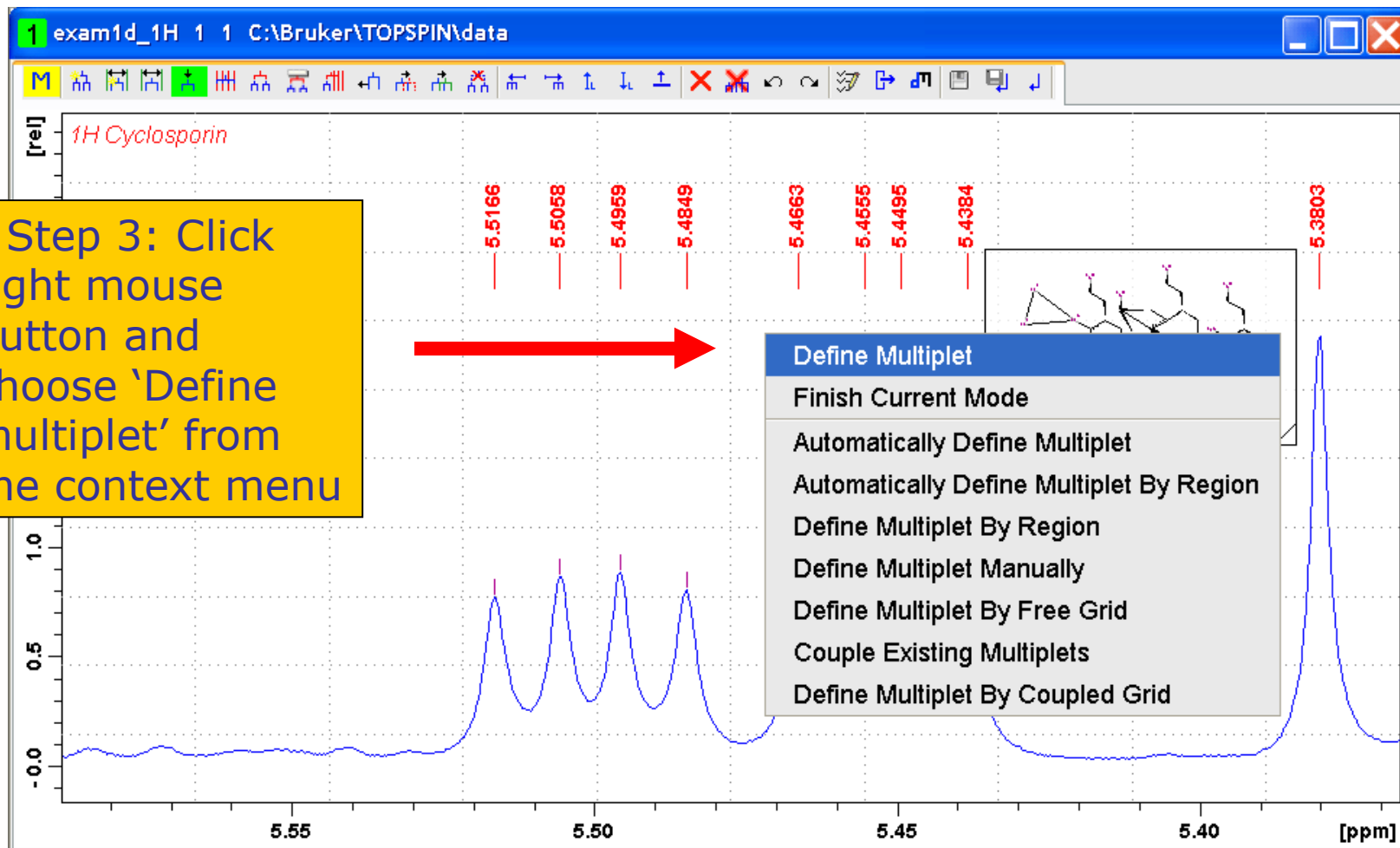
- Step 2: Move cursor to a peak which should be added to a multiplet and click (Repeat for all peaks should be included into a multiplet)

This shows peaks to include into a multiplet

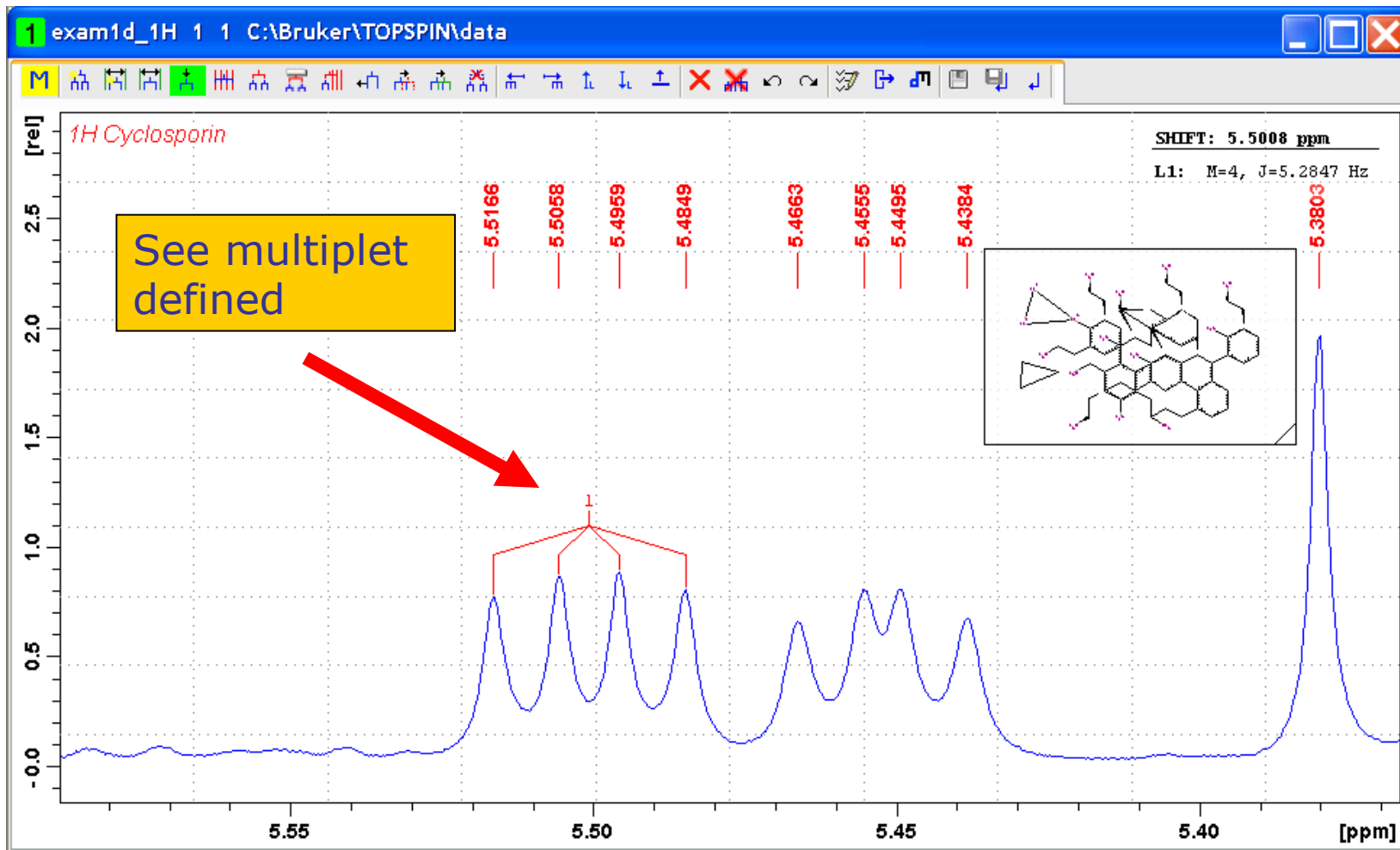
Define single-level multiplet manually



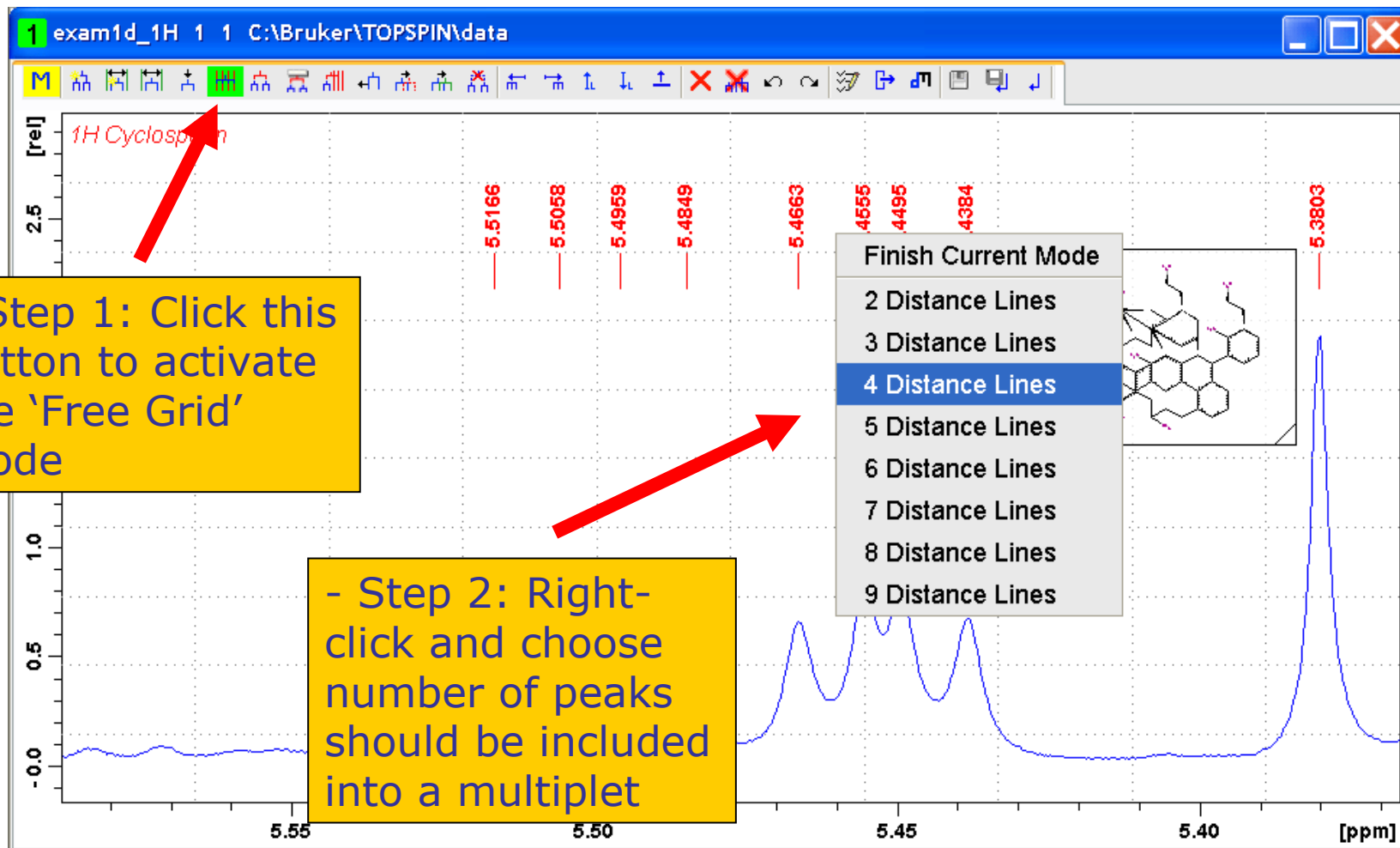
- Step 3: Click right mouse button and choose 'Define multiplet' from the context menu



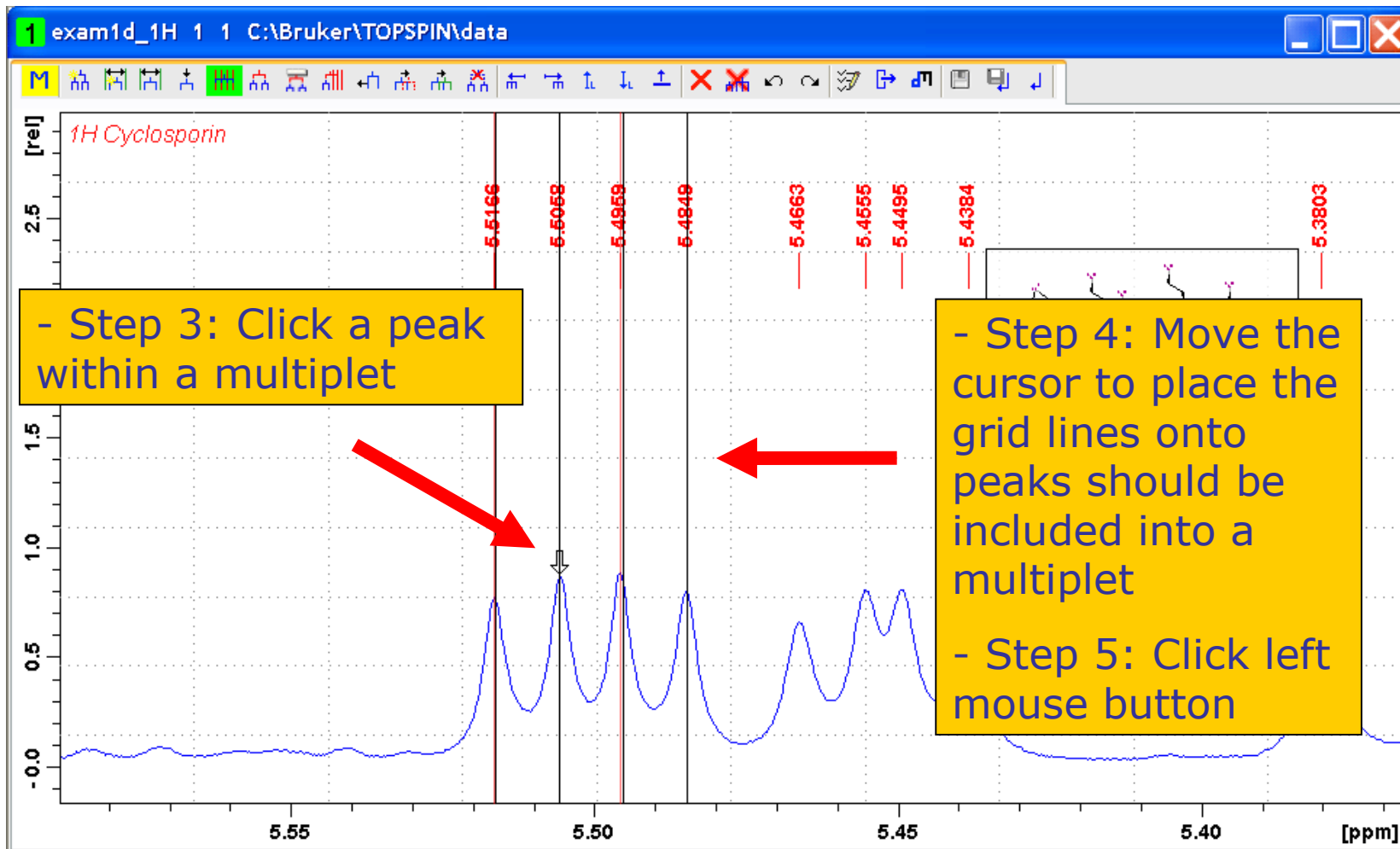
Define single-level multiplet manually



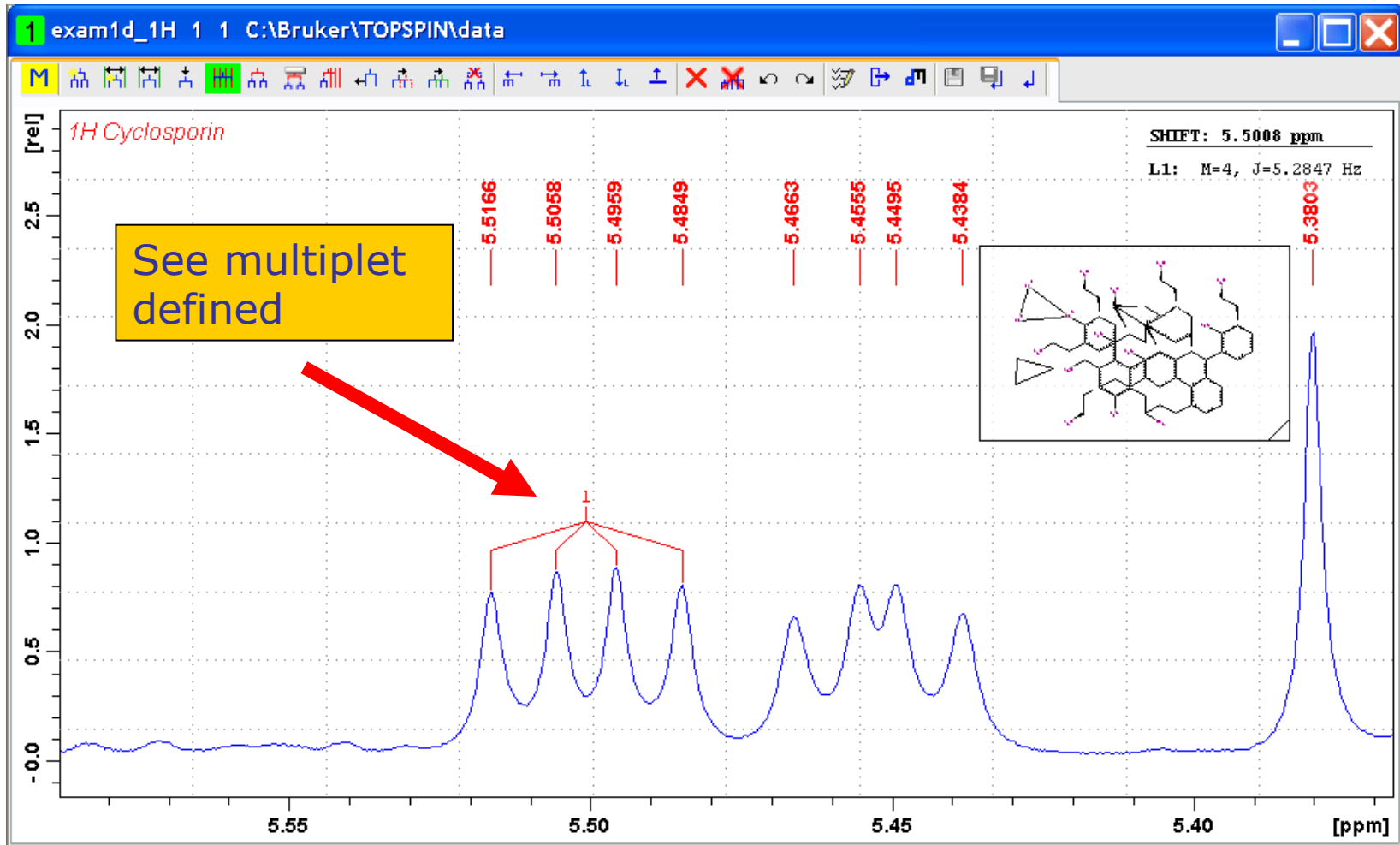
Define single-level multiplet using Free Grid



Define single-level multiplet using Free Grid



Define single-level multiplet using Free Grid



There are three methods to define a multi-level multiplet manually:

- Define multi-level multiplet by coupling existing multiplets of the same structure
- Define multi-level multiplet by coupling existing multiplets by ID
- Define multi-level multiplet using the 'Coupled Grid' feature

Couple Existing Multiplets

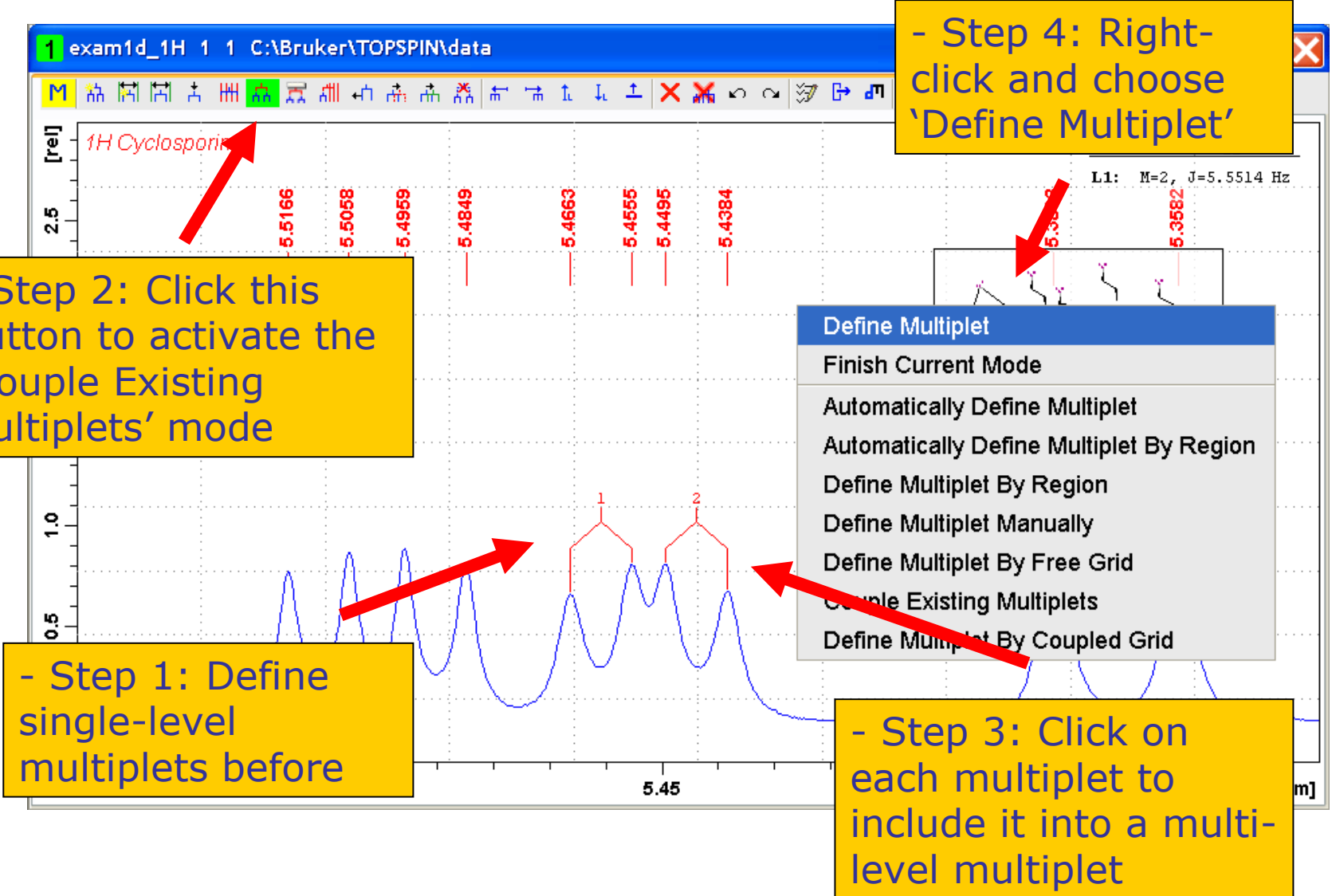


- Step 4: Right-click and choose 'Define Multiplet'

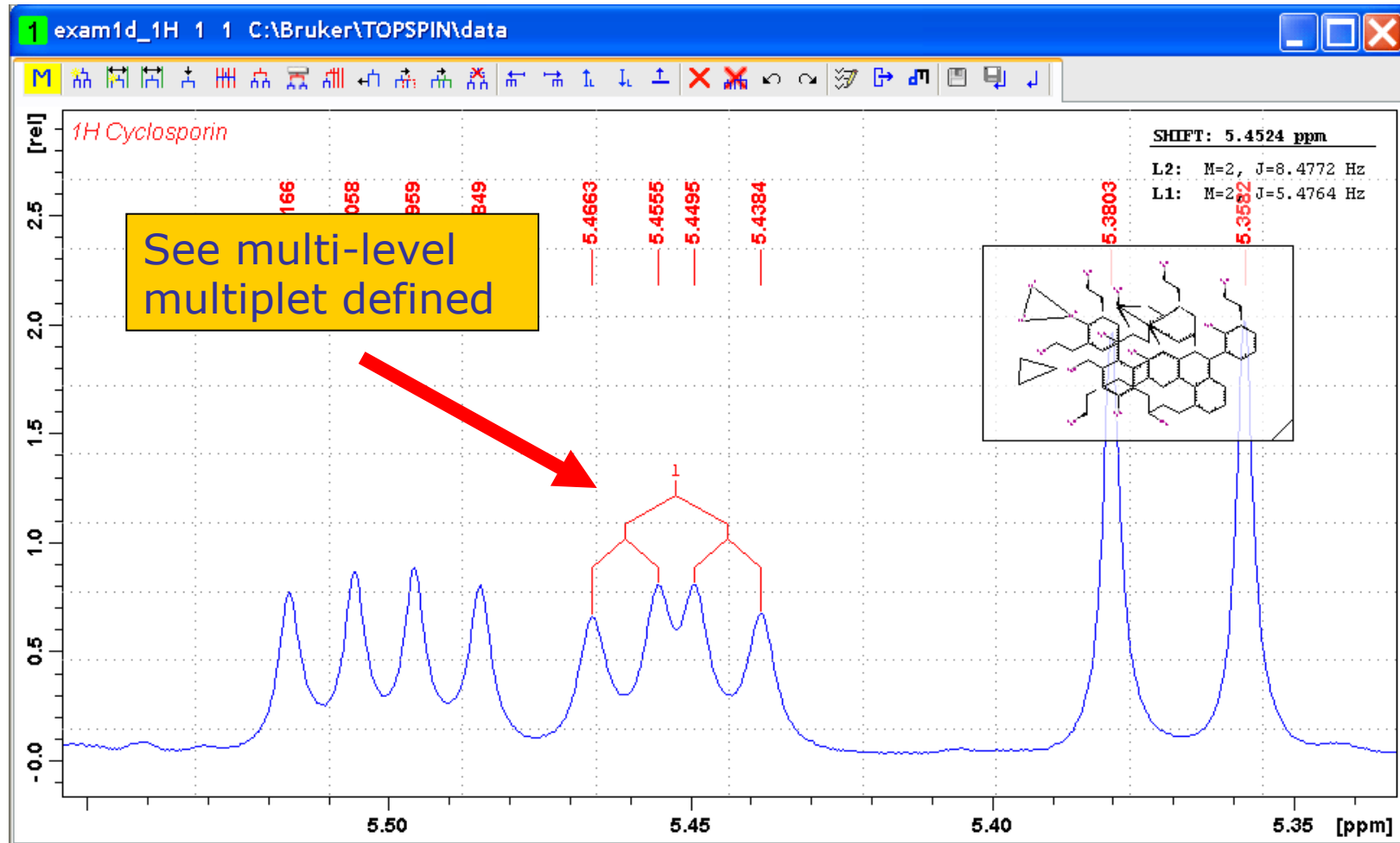
- Step 2: Click this button to activate the 'Couple Existing Multiplets' mode

- Step 1: Define single-level multiplets before

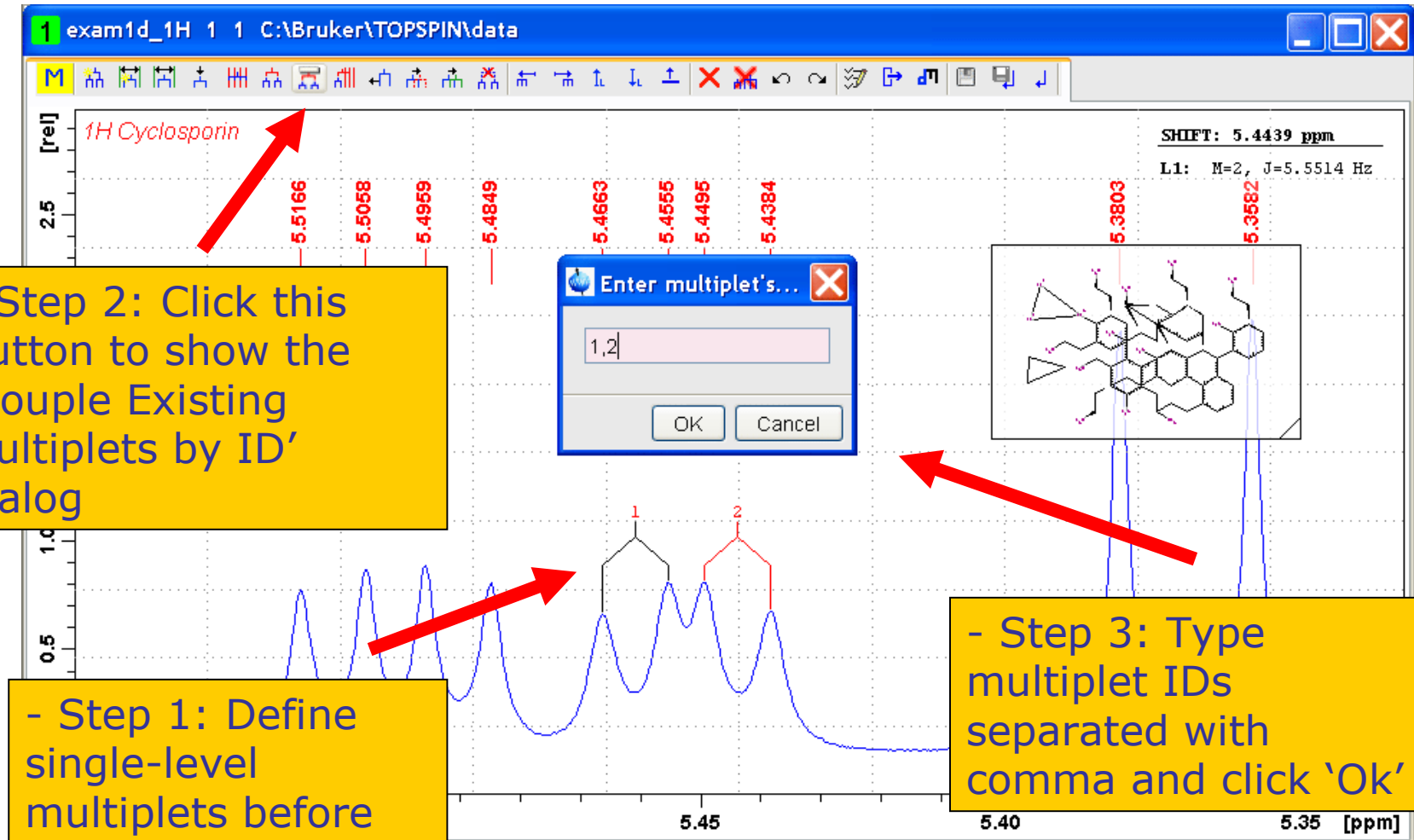
- Step 3: Click on each multiplet to include it into a multi-level multiplet



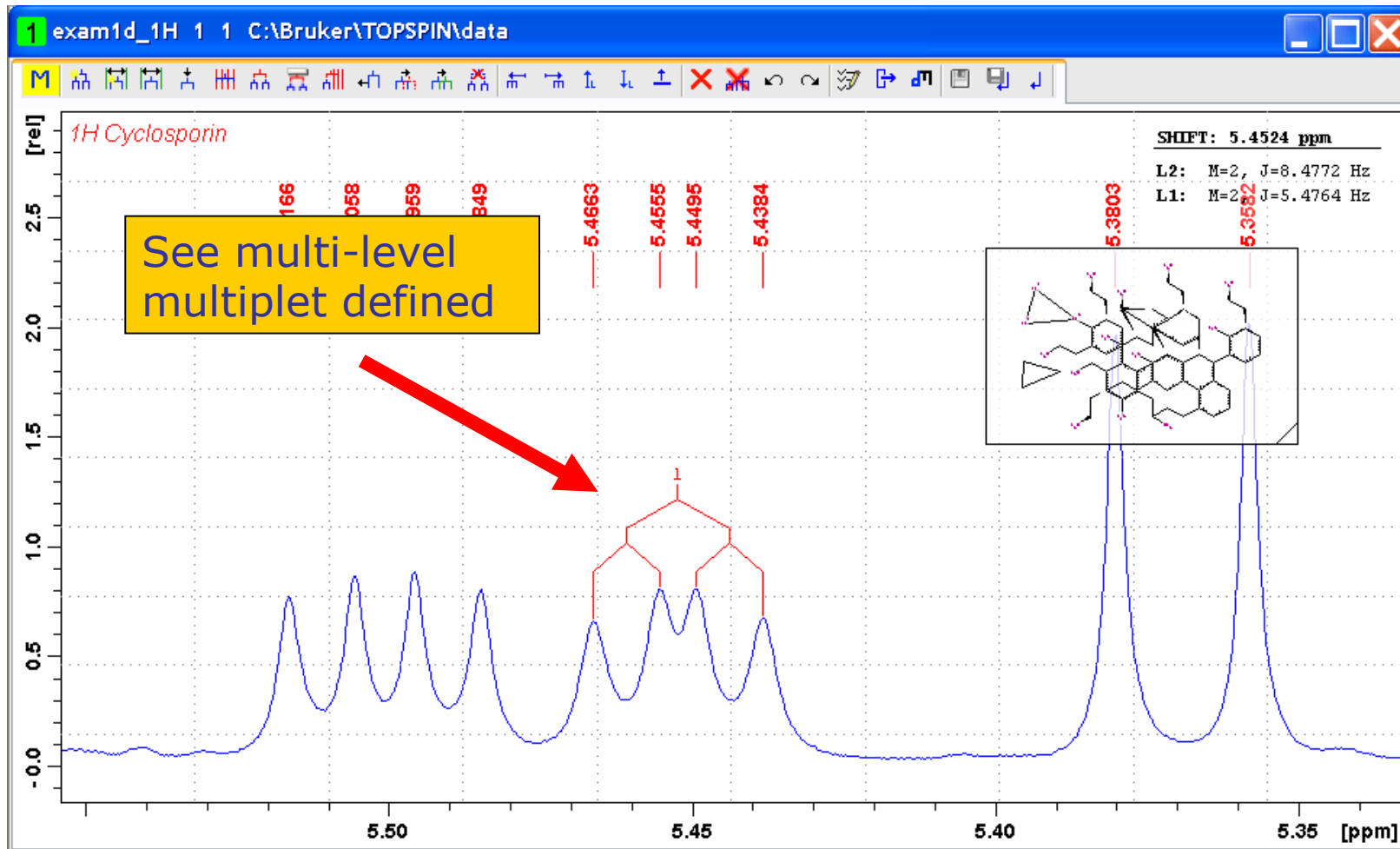
Couple Existing Multiplets



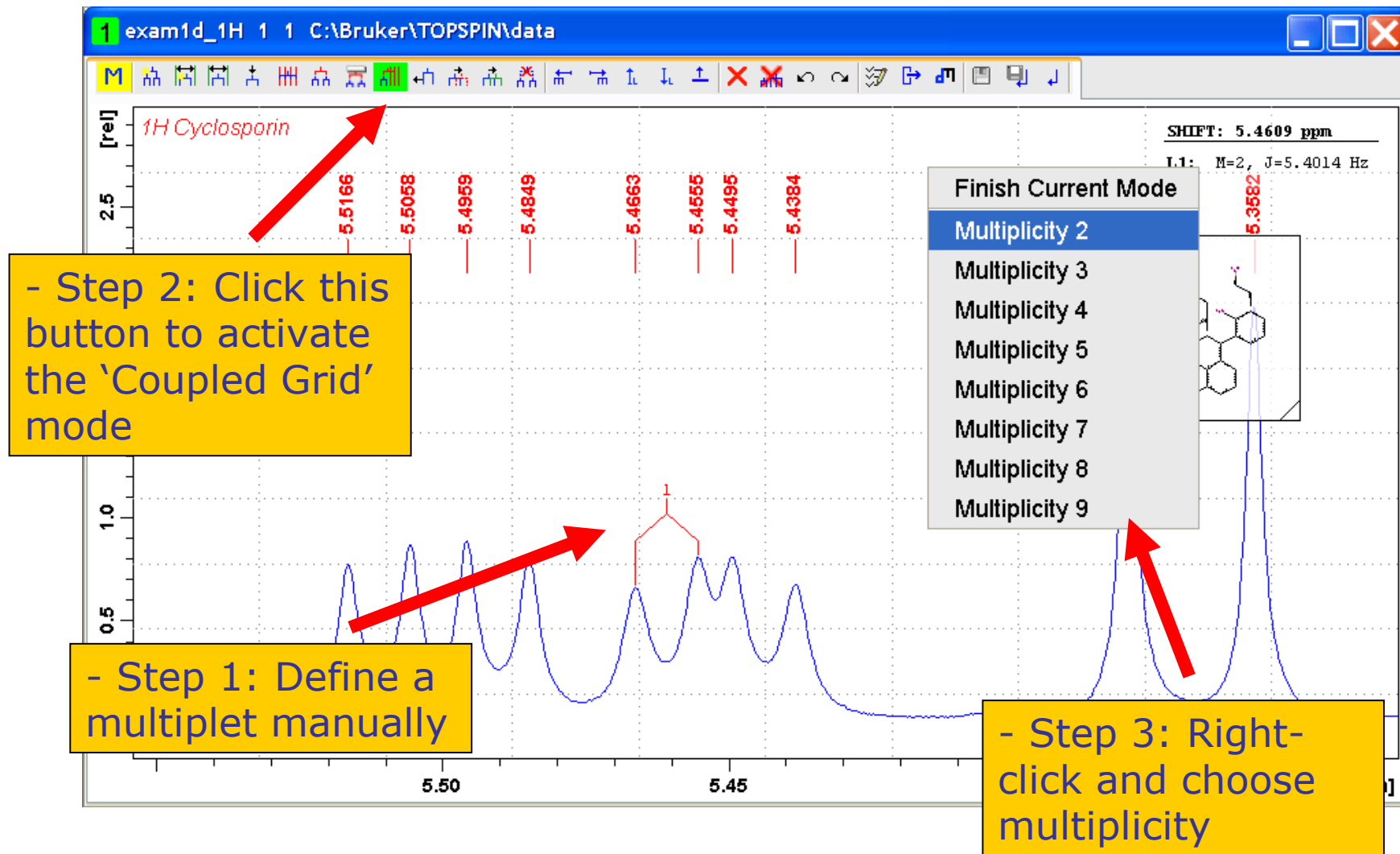
Couple Existing Multiplets by ID



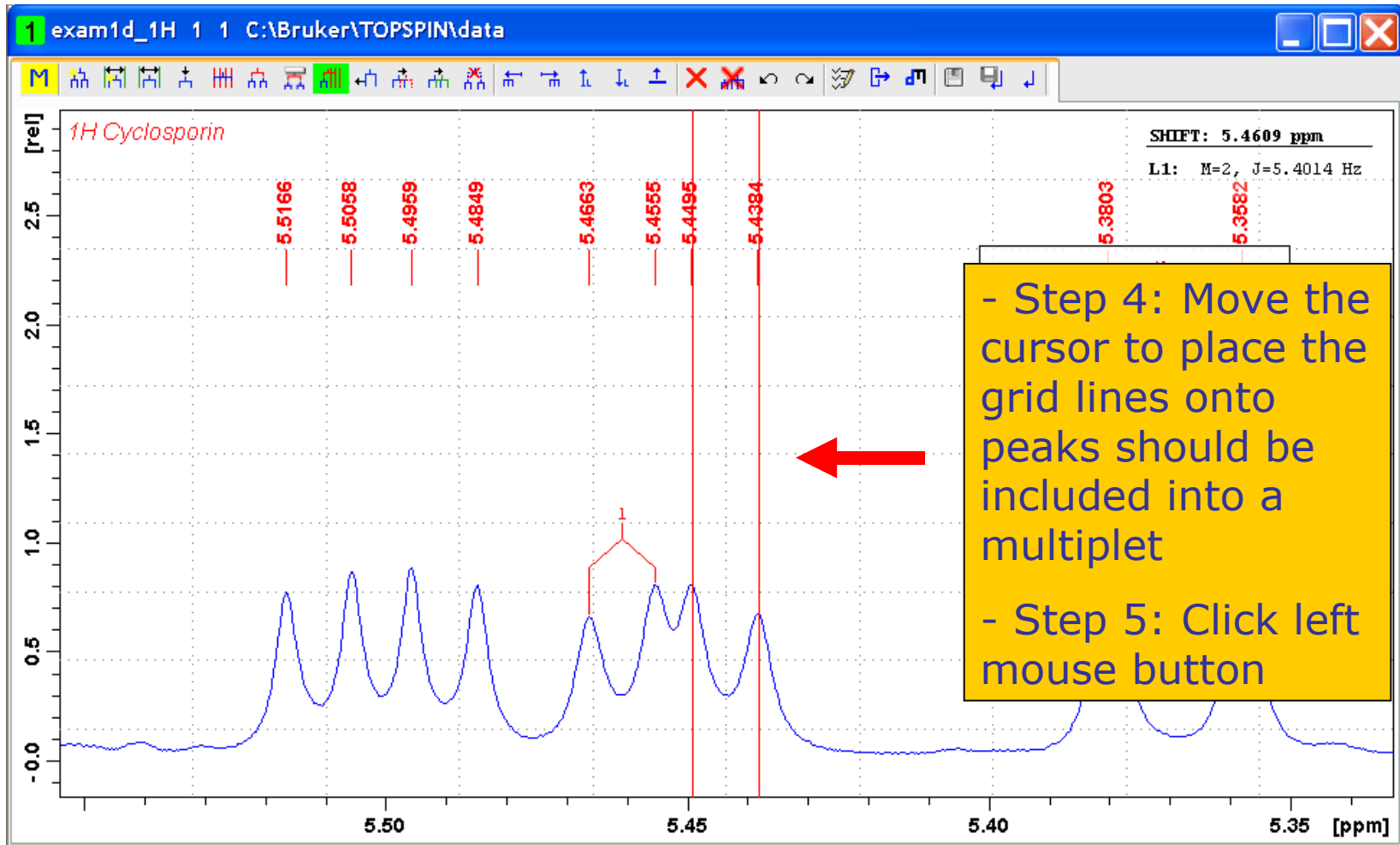
Couple Existing Multiplets by ID



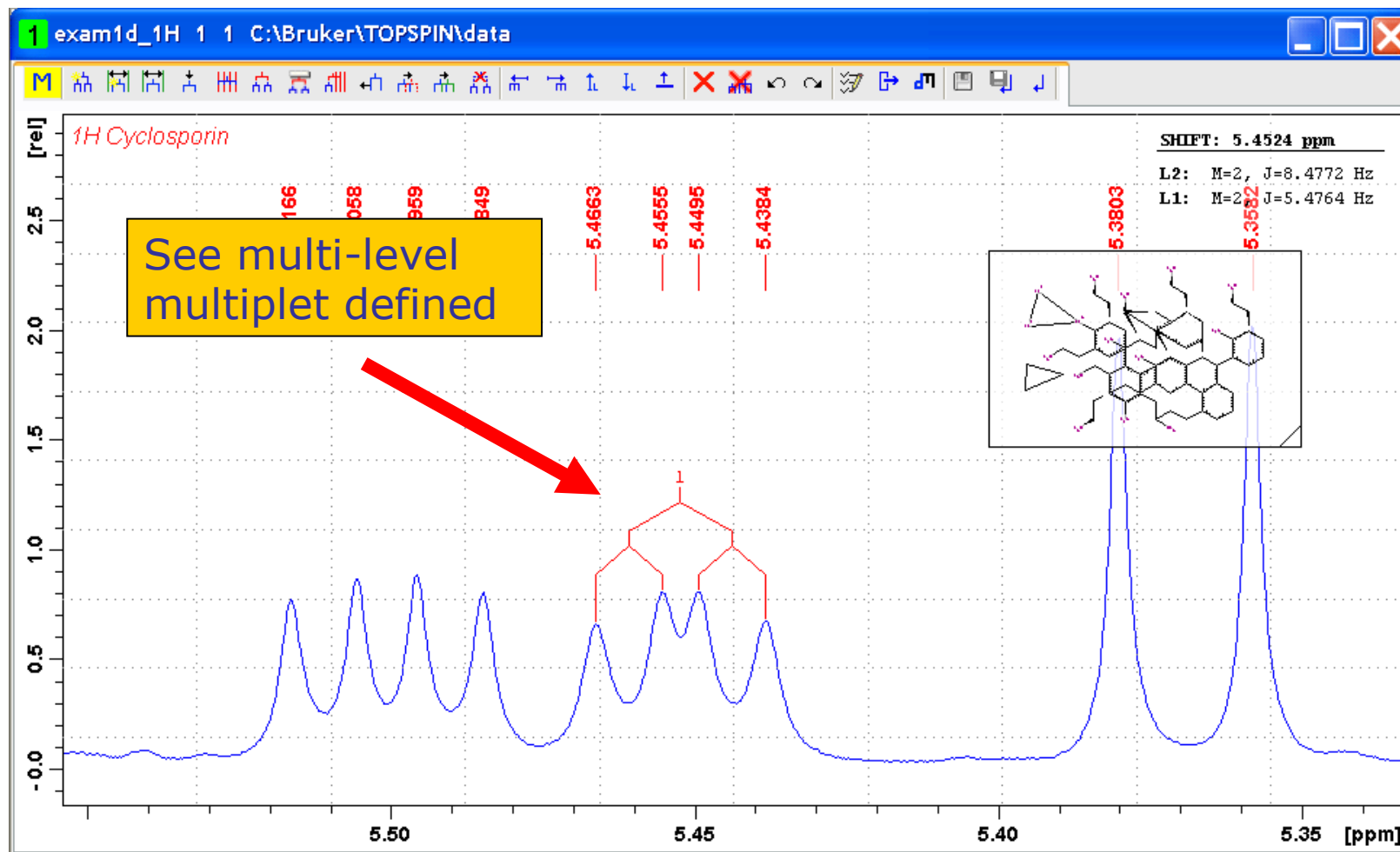
Define multi-level multiplet using Coupled Grid



Define multi-level multiplet using Coupled Grid



Define multi-level multiplet using Coupled Grid



There are several additional operations can be performed with multiplets:

- Changing multiplet ID / Label
- Shift single multiplet line
- Shift multiplet tree horizontally
- Copy multiplet
- Decouple multiplet
- Select next/previous multiplet
- Shift multiplet tree vertically
- Delete selected multiplet
- Delete all multiplets

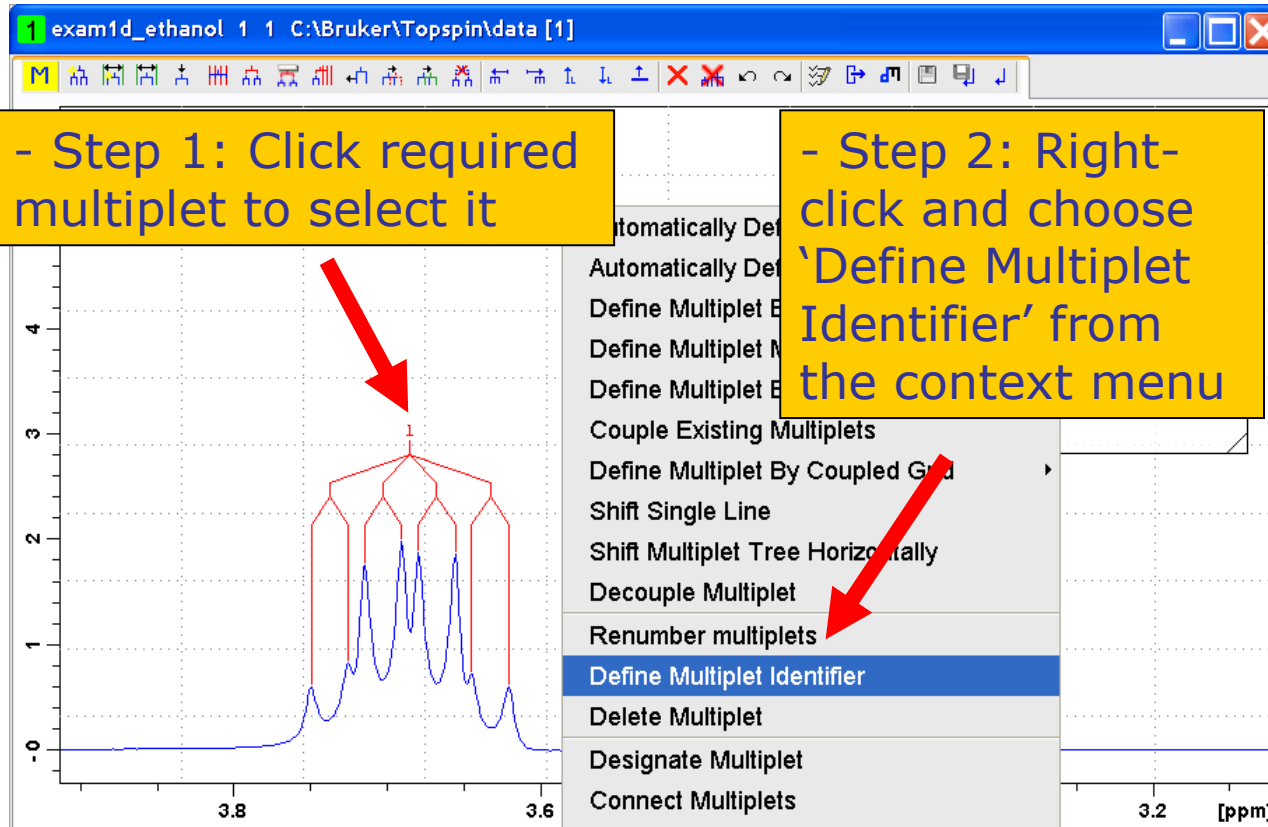
Define Multiplet ID / Label



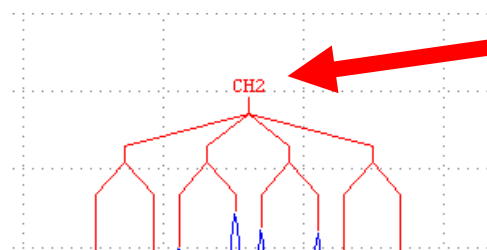
- Step 1: Click required multiplet to select it

- Step 2: Right-click and choose 'Define Multiplet Identifier' from the context menu

- Step 3: Type new multiplet ID and press 'Ok'

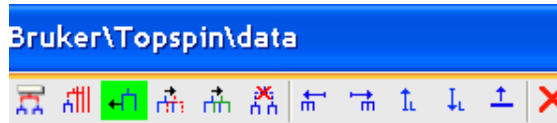


The 'Multiplet Identifier' dialog box is shown. The 'Number' field is set to 1, and the 'Identifier' field contains 'CH2'. The 'OK' button is highlighted.

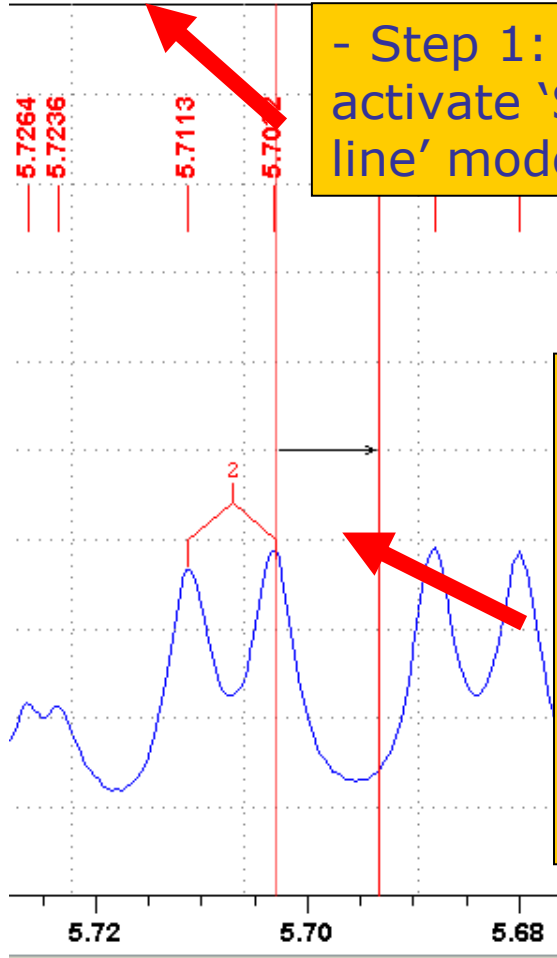


Result

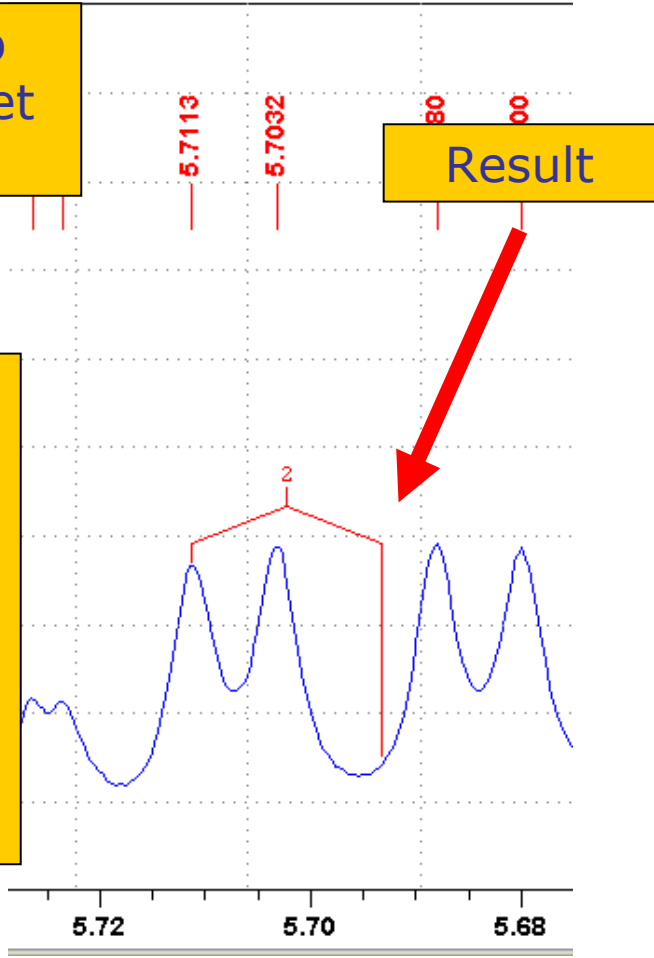
Shift Single Multiplet Line



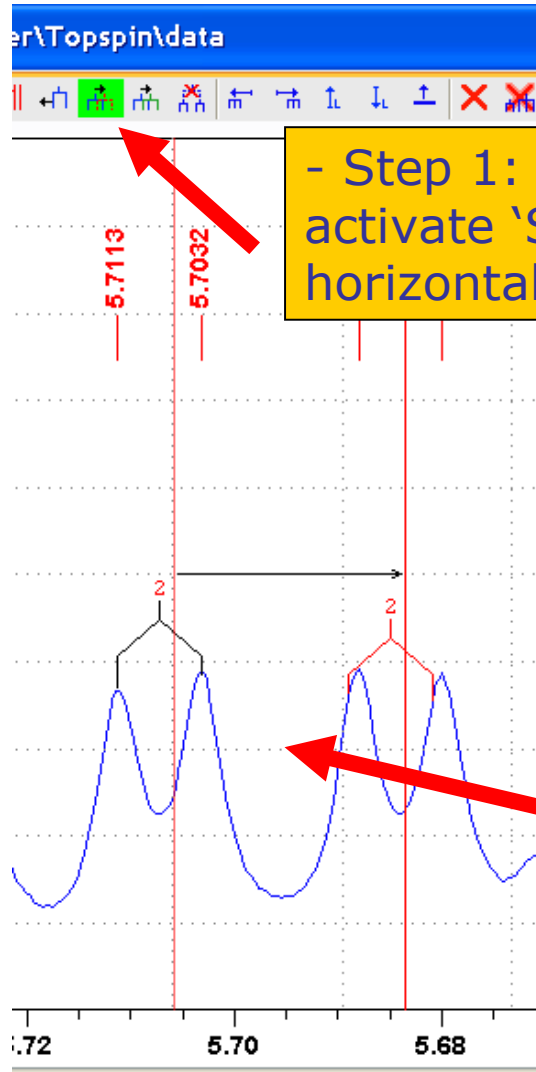
- Step 1: Click this button to activate 'Shift single multiplet line' mode



- Step 2: Press left mouse button on required peak and drag to the place you want to shift to
- Step 3: Release mouse

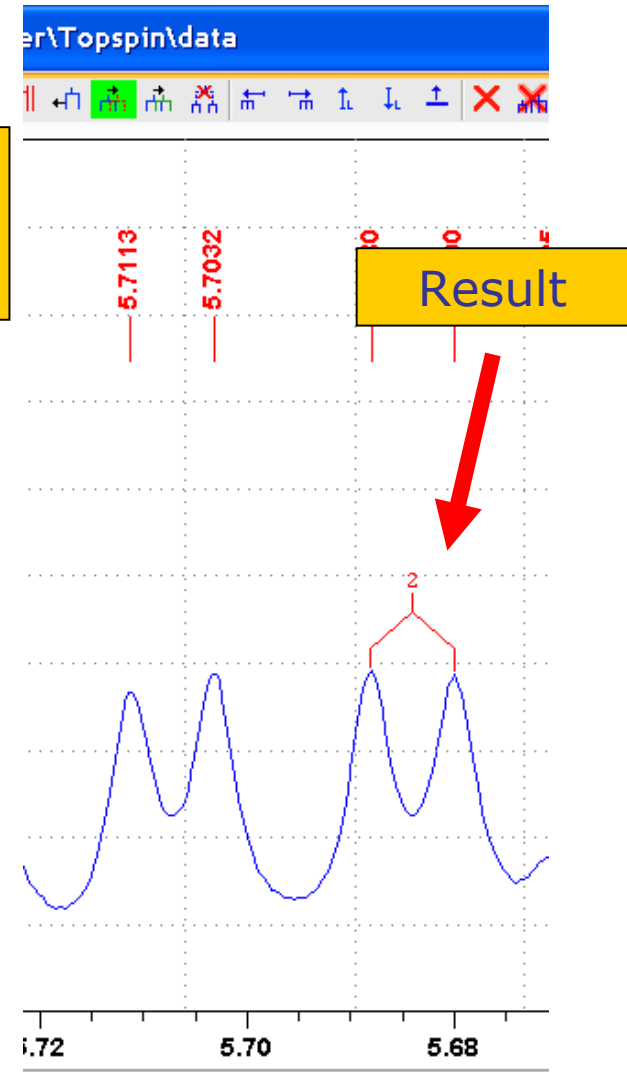


Shift Multiplet Tree Horizontally

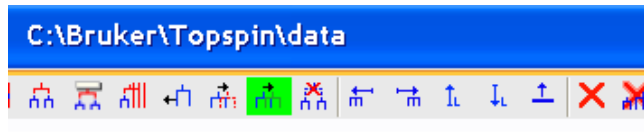


- Step 1: Click this button to activate 'Shift multiplet tree horizontally' mode

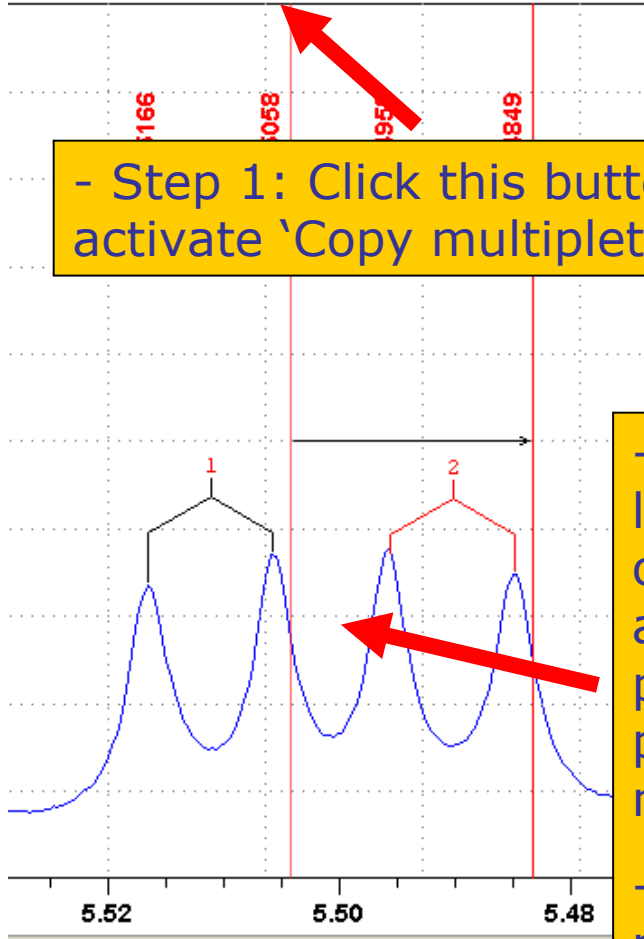
- Step 2: Press left mouse button on the multiplet and drag to the place you want to shift multiplet to
- Step 3: Release mouse



Copy Multiplet

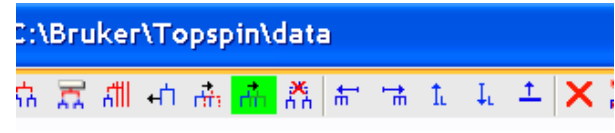


- Step 1: Click this button to activate 'Copy multiplet' mode

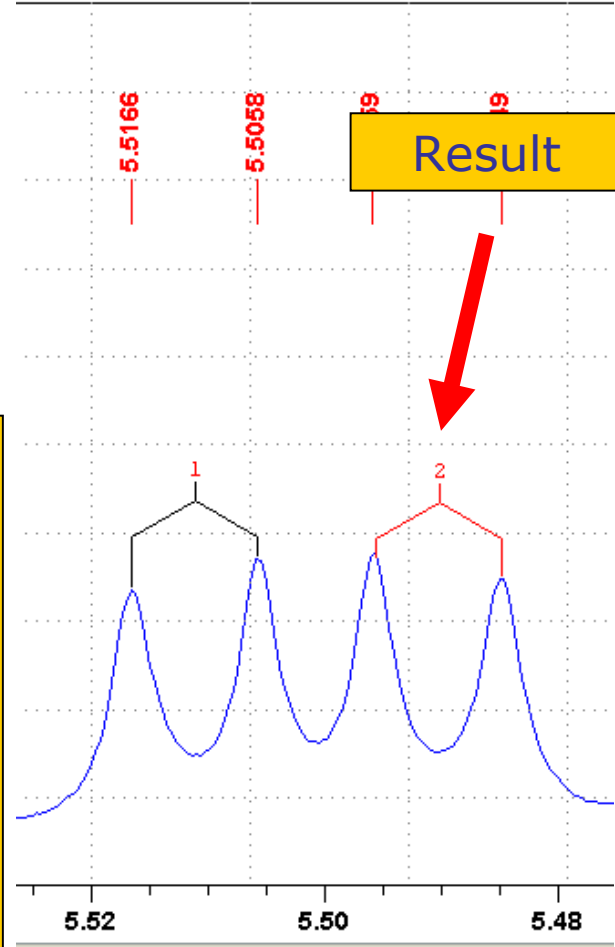


- Step 2: Press left mouse button on the multiplet and drag to the place you want to place copy of the multiplet

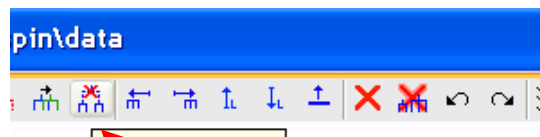
- Step 3: Release mouse



Result



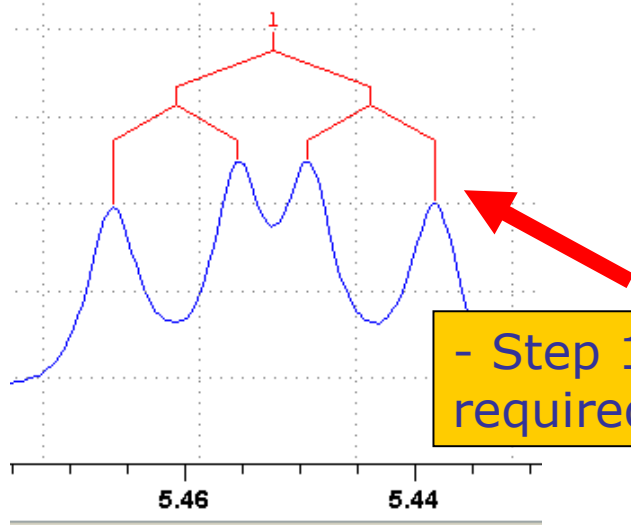
Decouple Multiplet



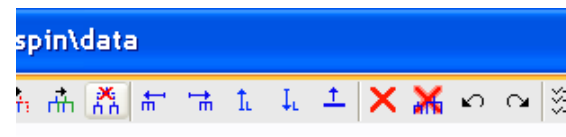
Decouple Multiplet

5.4663
5.4555
5.4495
5.4384

- Step 2: Click this button to decouple multiplet

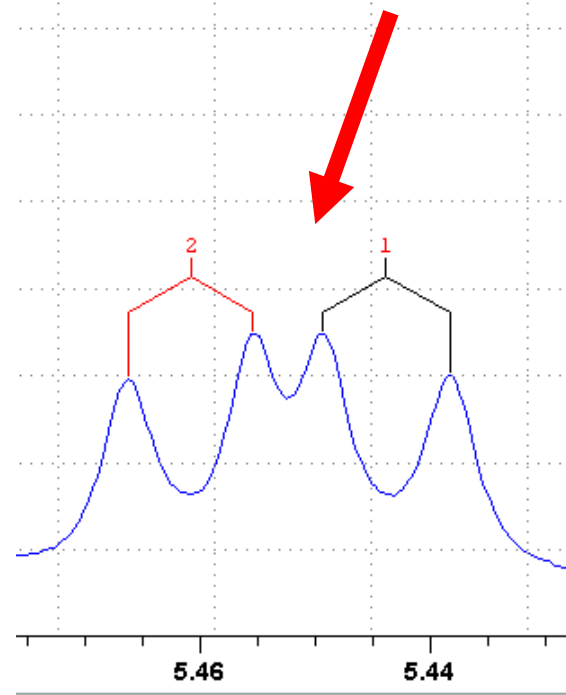


- Step 1: Select required multiplet



5.4663
5.4555
5.4495
5.4384

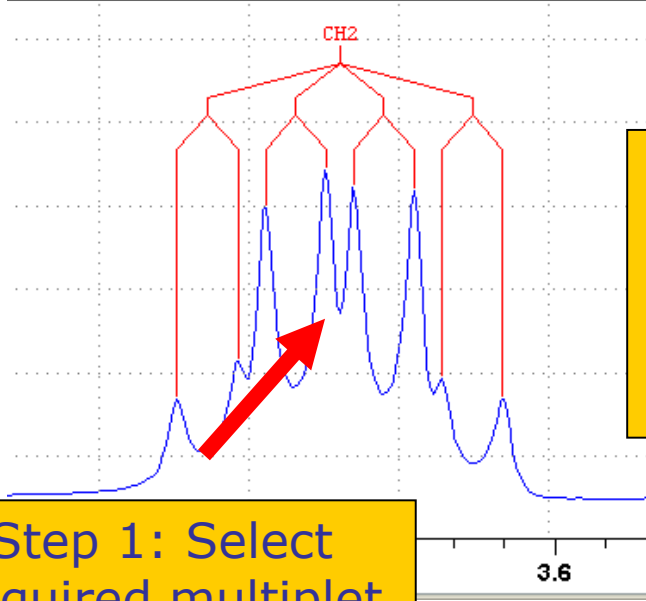
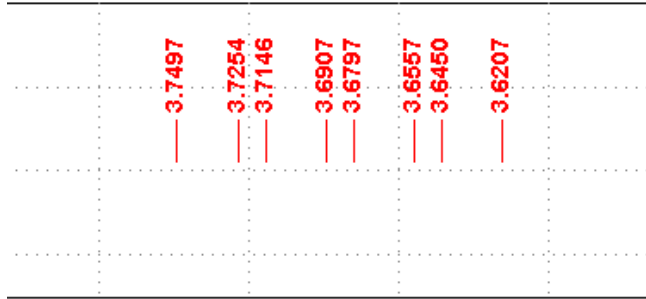
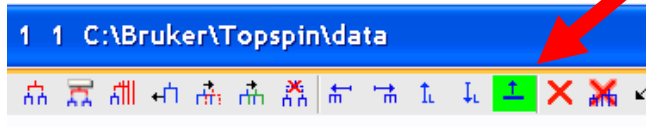
Result



Shift Multiplet Tree Vertically

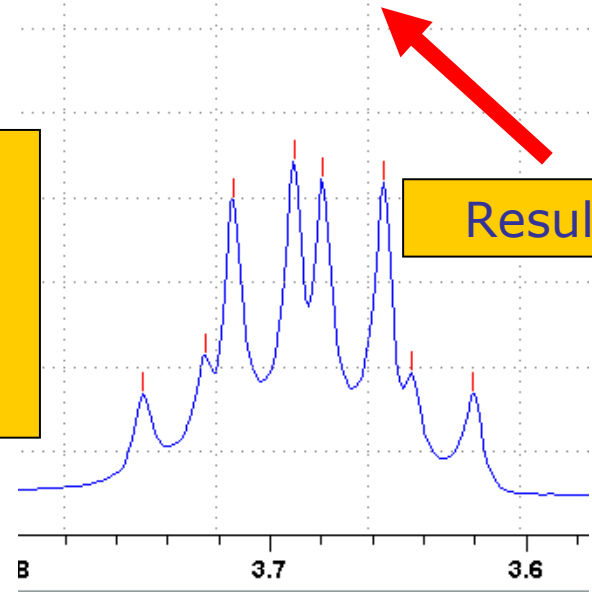
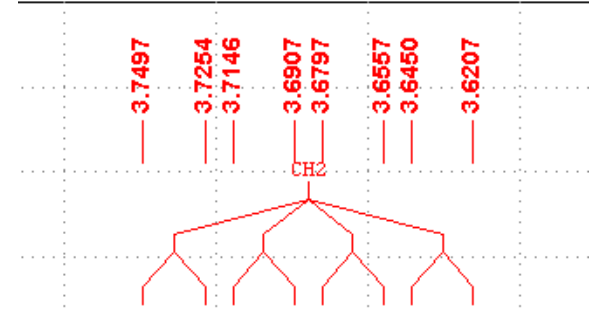
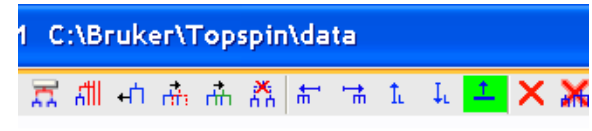


- Step 2: Click this button to activate mode



- Step 1: Select required multiplet

- Step 3: Move mouse cursor where you want to place multiplet tree and click

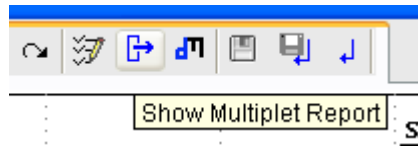


Result

Report Dialog



To activate dialog



Multiplet table:

- Multiplet IDs
- J constants
- Multiplicities
- Connections

Assign Connections / Report

ID	Shift [p...]	J [Hz]	M	Connection
CH2	3.6852	6.9846	4	J(CH2, CH3)
		4.8282	2	J(CH2, OH)
OH	2.8738	4.8532	3	J(OH, CH2)
CH3	1.2220	7.0547	3	J(CH3, CH2)

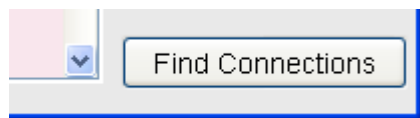
Export in text format

Export multiplet information to JMR and JPF formats

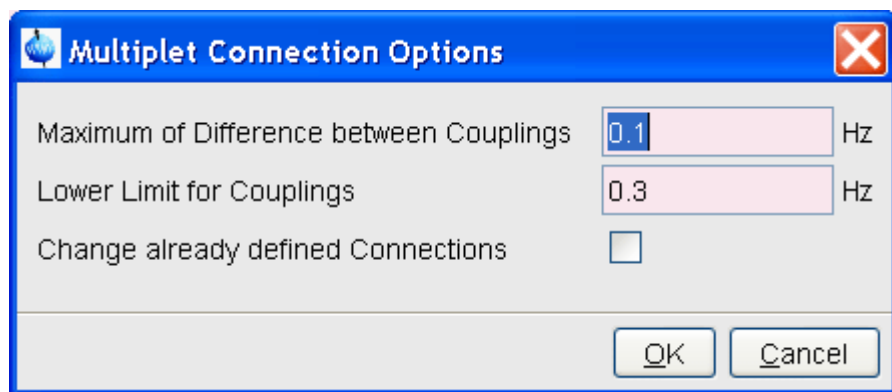
Finding connections (required only if you use manual multiplet definition)

Buttons: Ok, Print, Copy, Save..., Start editor, JMR, JPF, Find Connections

Finding Connections



- Step 1: Press 'Find Connection' button in the Report dialog



Assign Connections / Report

Before

	Shift [p...	J [Hz]	M	Connection
	3.6852	6.9846	4	J(CH2, O)
		4.8282	2	J(CH2, O)
OH	2.8738	4.8532	3	J(OH, O)
CH3	1.2220	7.0547	3	J(CH3, O)

- Step 2: Choose connection options and press 'Ok'

Assign Connections / Report

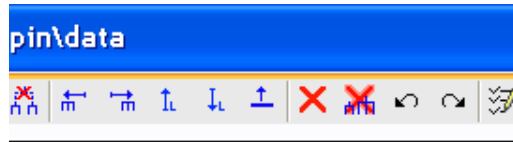
After

ID	Shift [p...	J [Hz]	M	Connection
CH2	3.6852	6.9846	4	J(CH2, CH3)
		4.8282	2	J(CH2, OH)
OH	2.8738	4.8532	3	J(OH, CH2)
CH3	1.2220	7.0547	3	J(CH3, CH2)

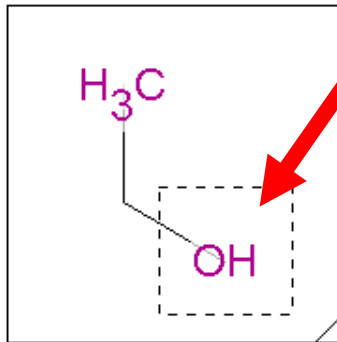
Features:

- *Multiplet Analysis allows to define atoms-to-multiplet correlations if you have molecule structure defined for the dataset*
- *It is possible to view such correlation inside and outside of Multiplet Analysis module*

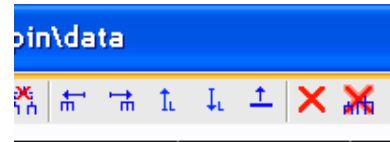
Define Structure Correlations



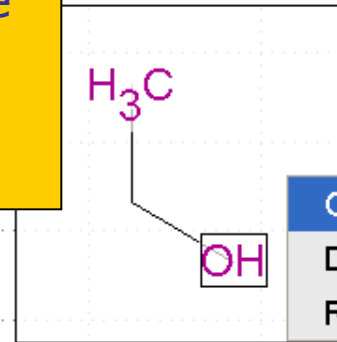
2.8981
2.8738
2.8496



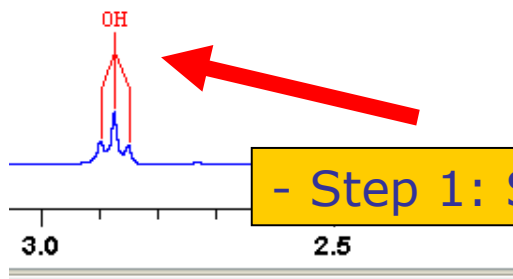
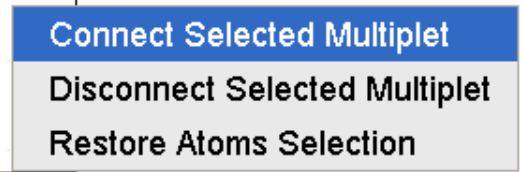
- Step 2: Select required part of molecule to be connected to the selected multiplet



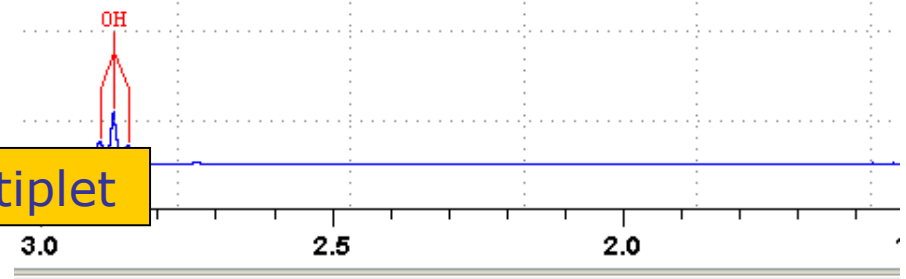
2.8981



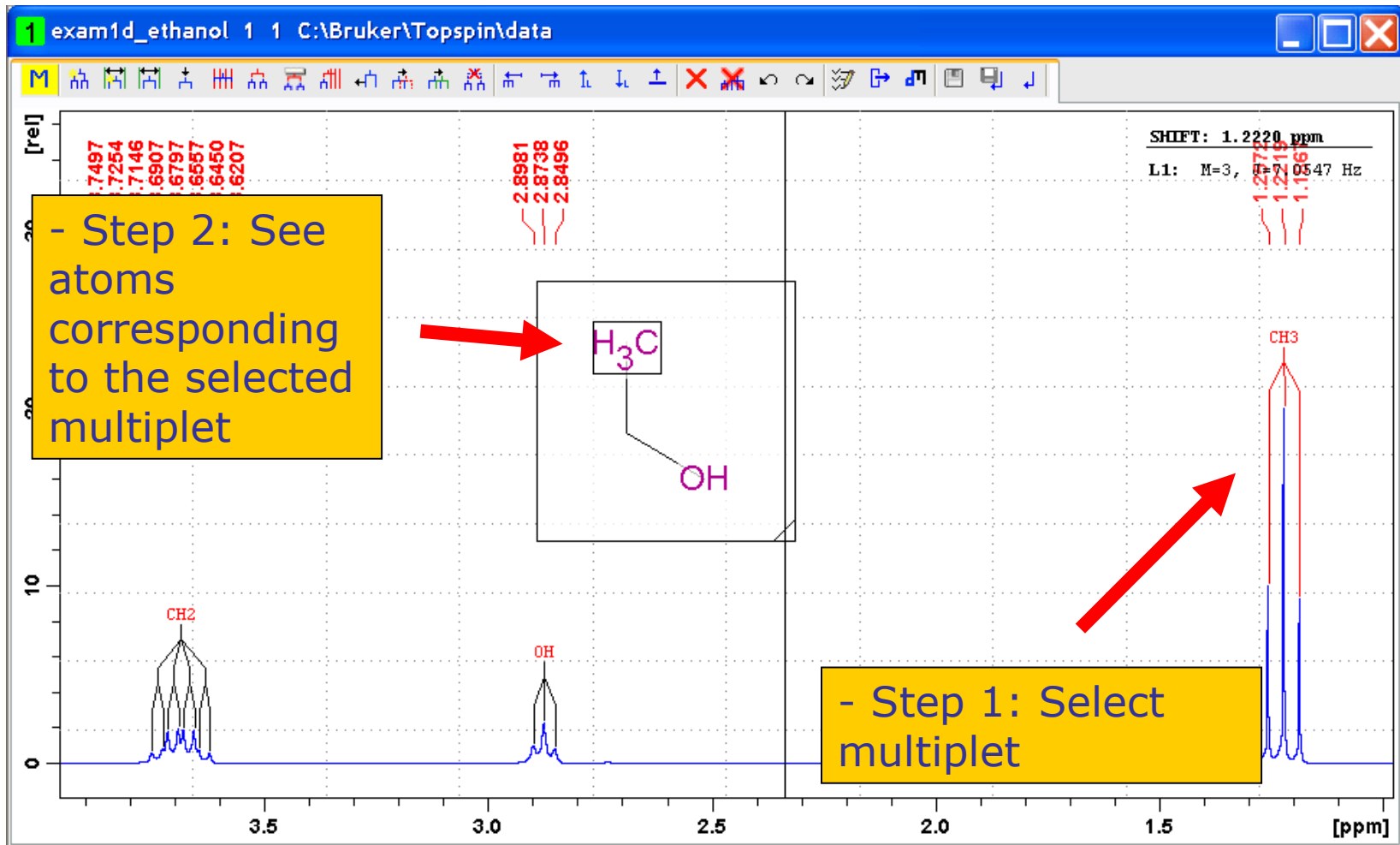
- Step 3: Right click on the molecule and choose 'Connect Selected Multiplet'



- Step 1: Select multiplet



View Structure Correlations



View Structure Correlations Outside Multiplet Analysis

