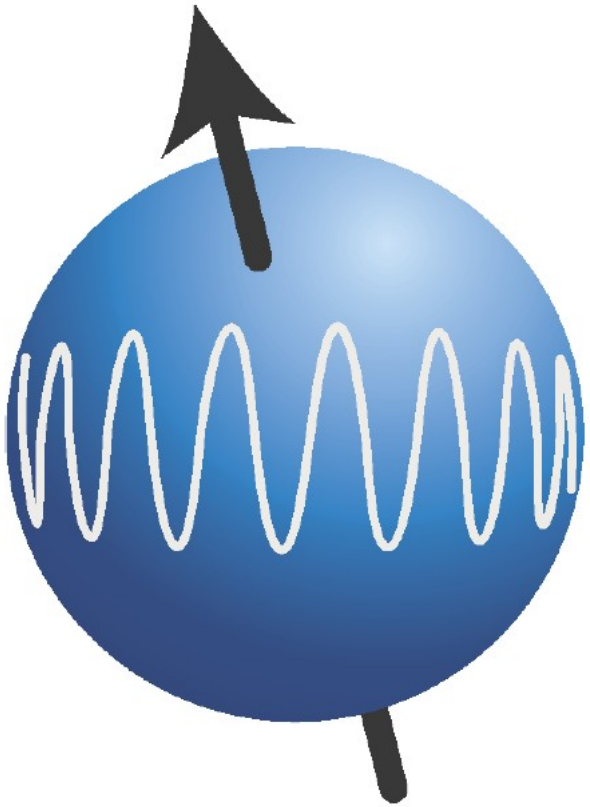


TopSpin

Multiplet Analysis Tutorial

Contents

- 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 ←→ structure correlation

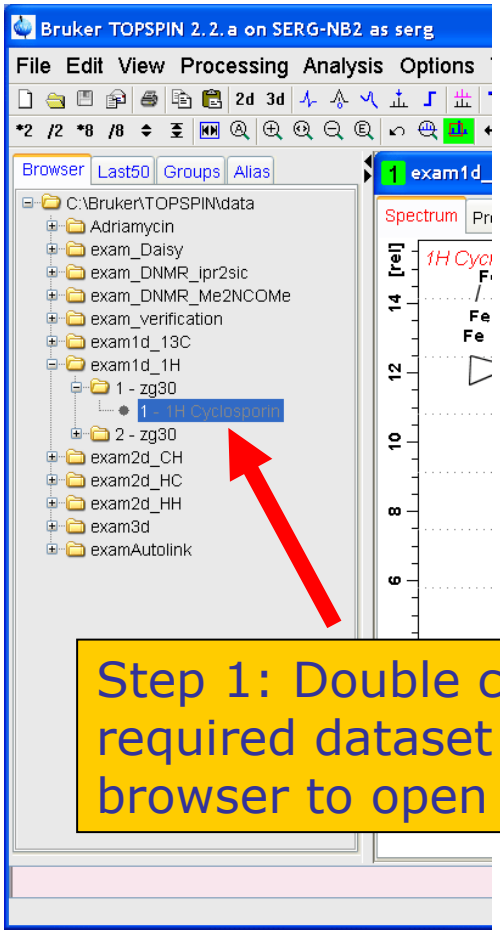
Automatic Multiplet Definition

You may define multiplets automatically:
- in whole displayed region
- in manually selected region

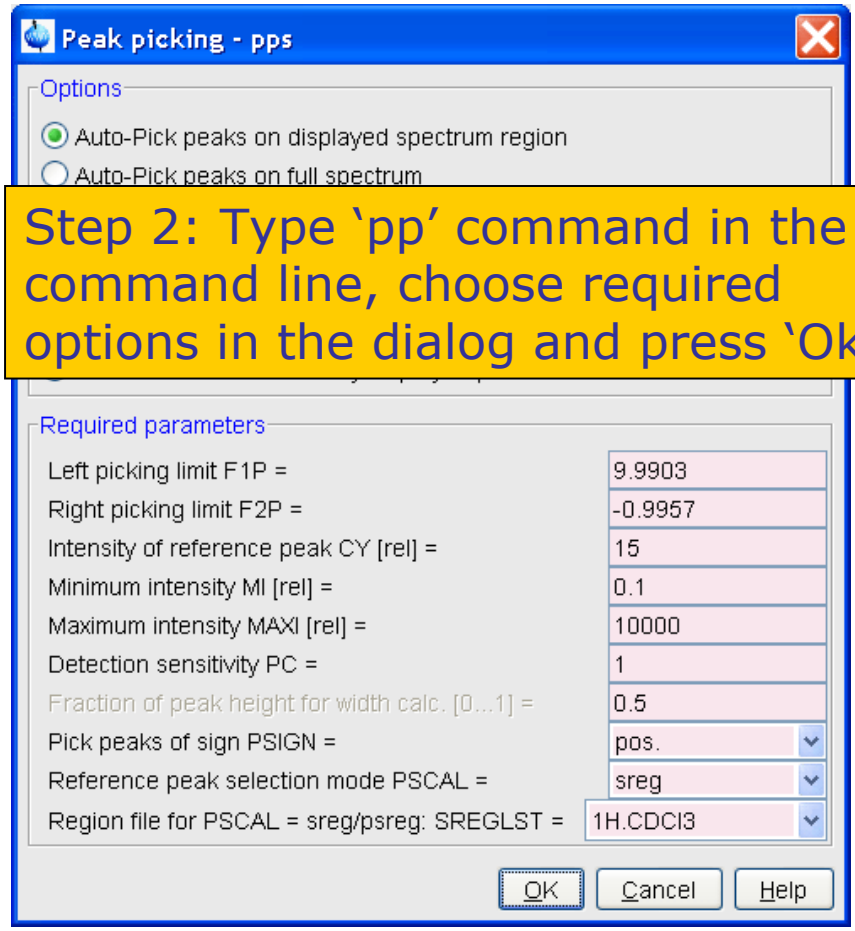
The procedure:
- Open required dataset
- Do Peak Picking first
- Enter Multiplet Analysis
- Use automatic multiplet definition features

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

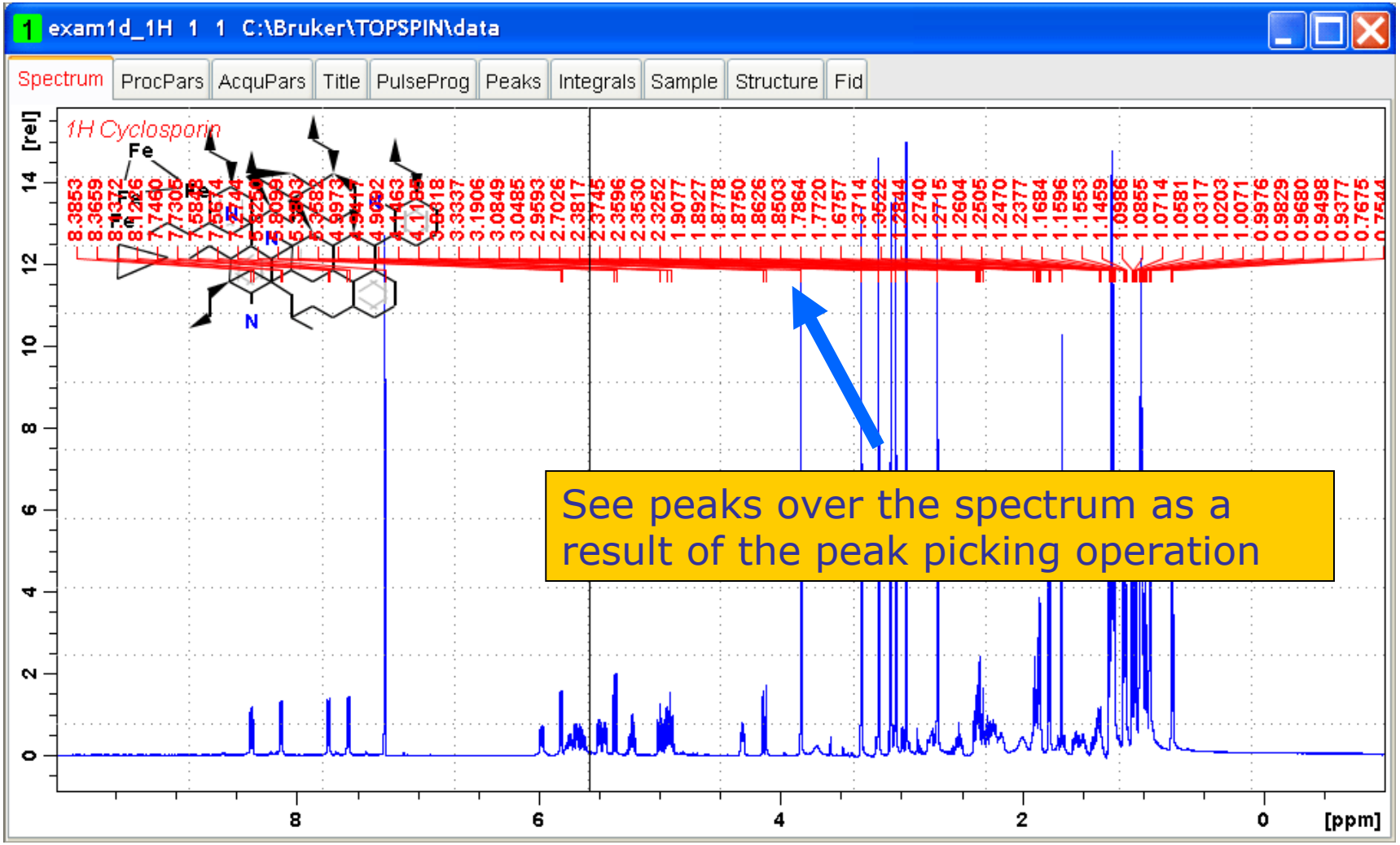


Step 1: Double click required dataset in the browser to open it

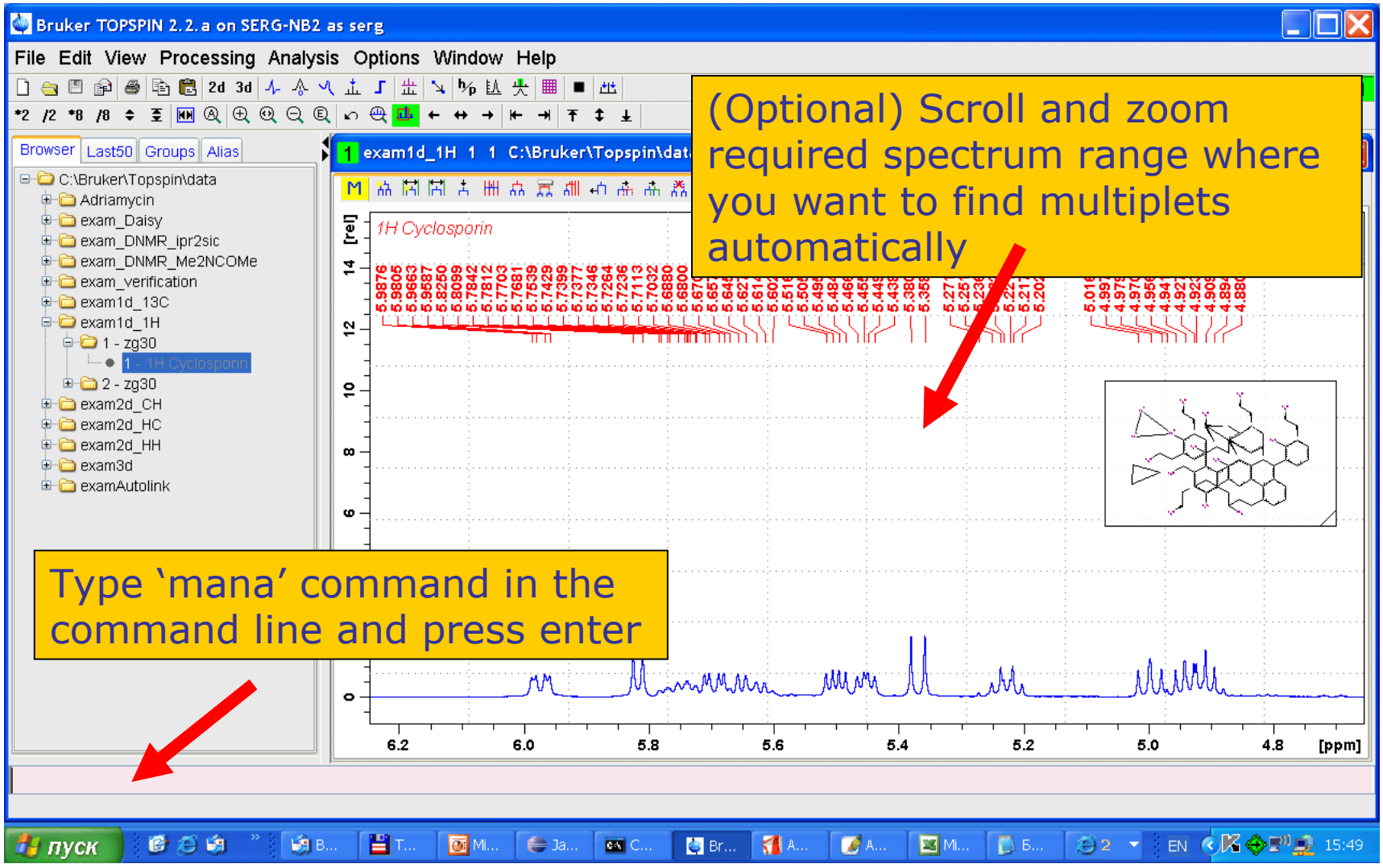


Step 2: Type ‘pp’ command in the command line, choose required options in the dialog and press ‘Ok’

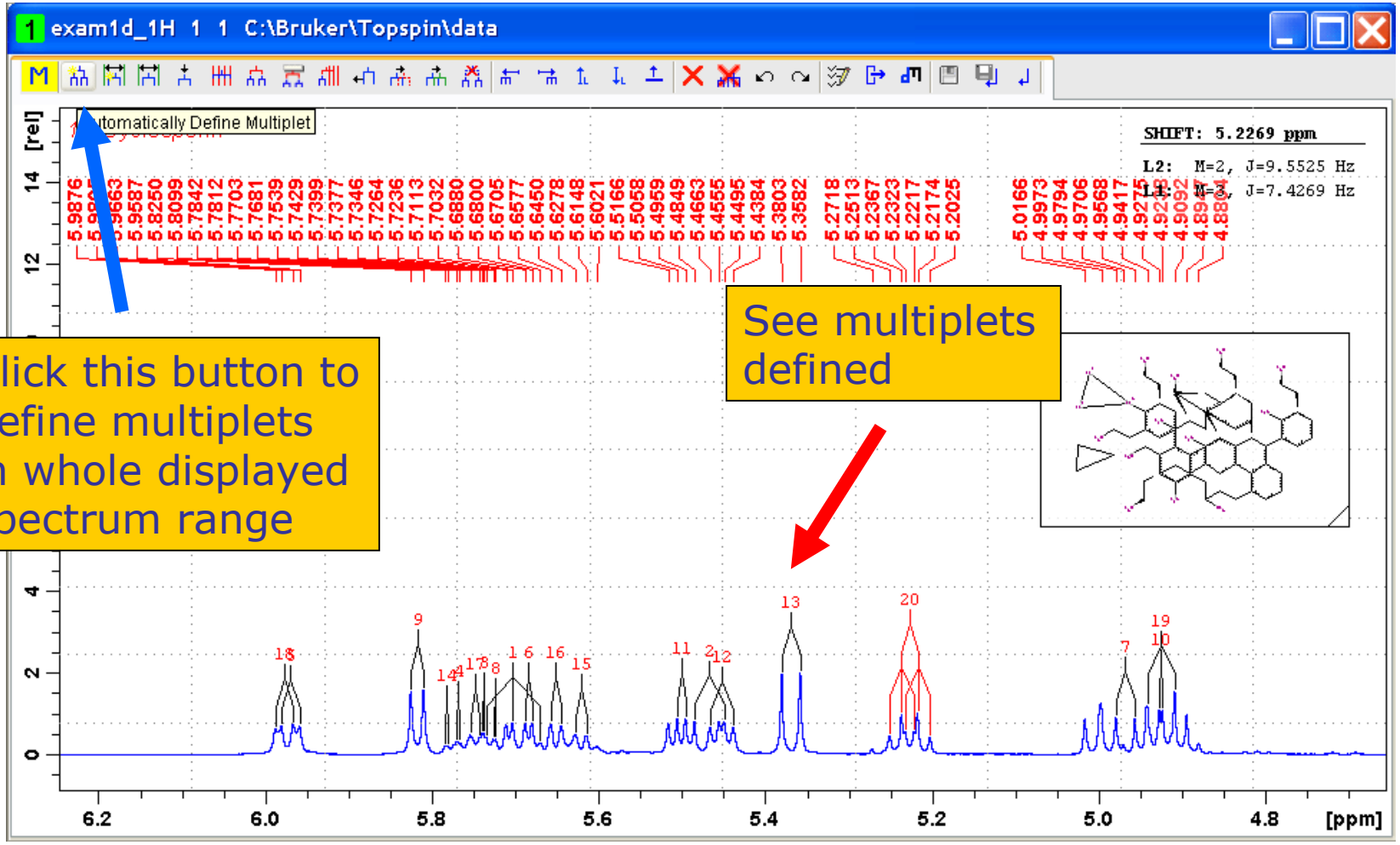
Automatic Multiplet Definition: Peak Picking



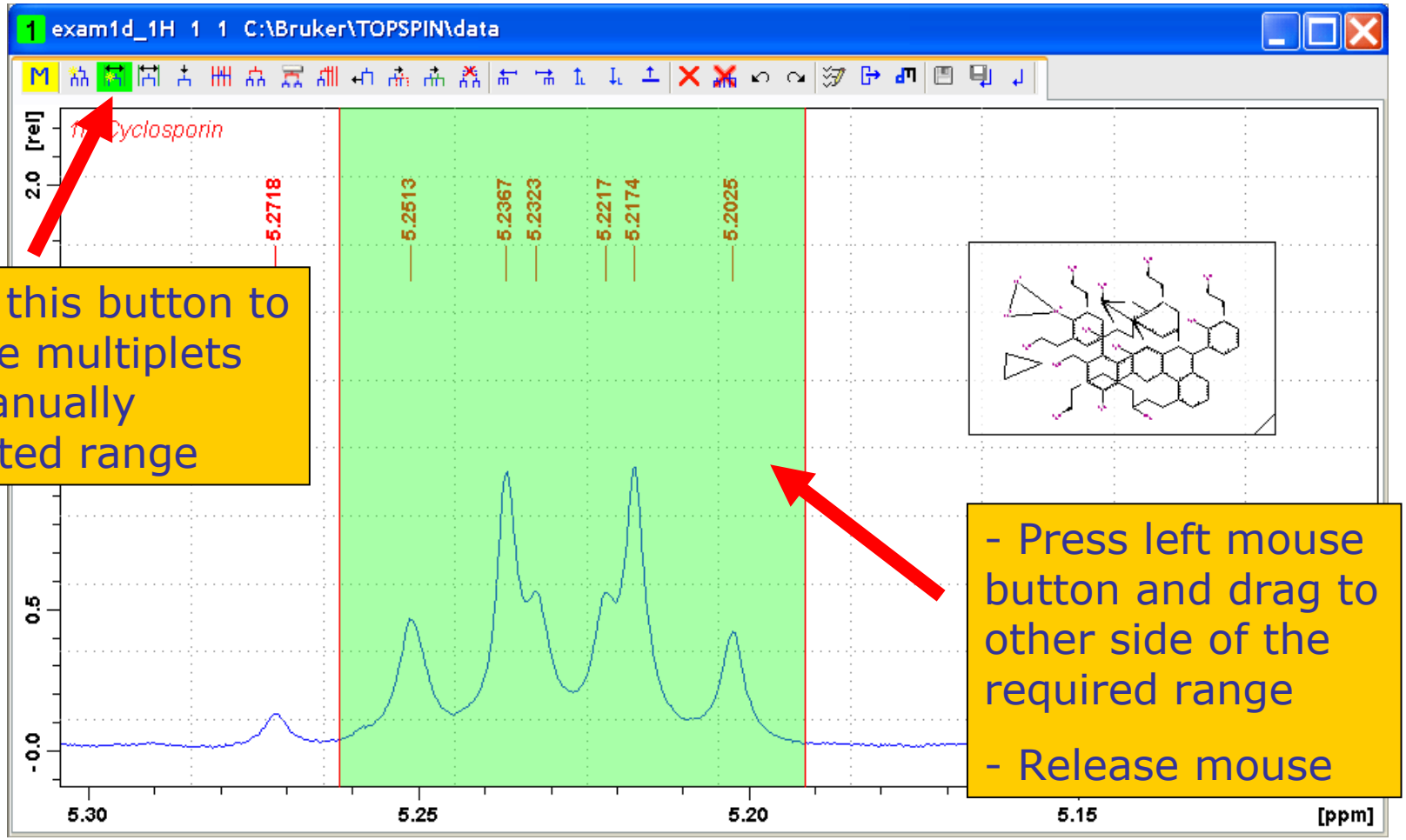
Enter Multiplet Analysis



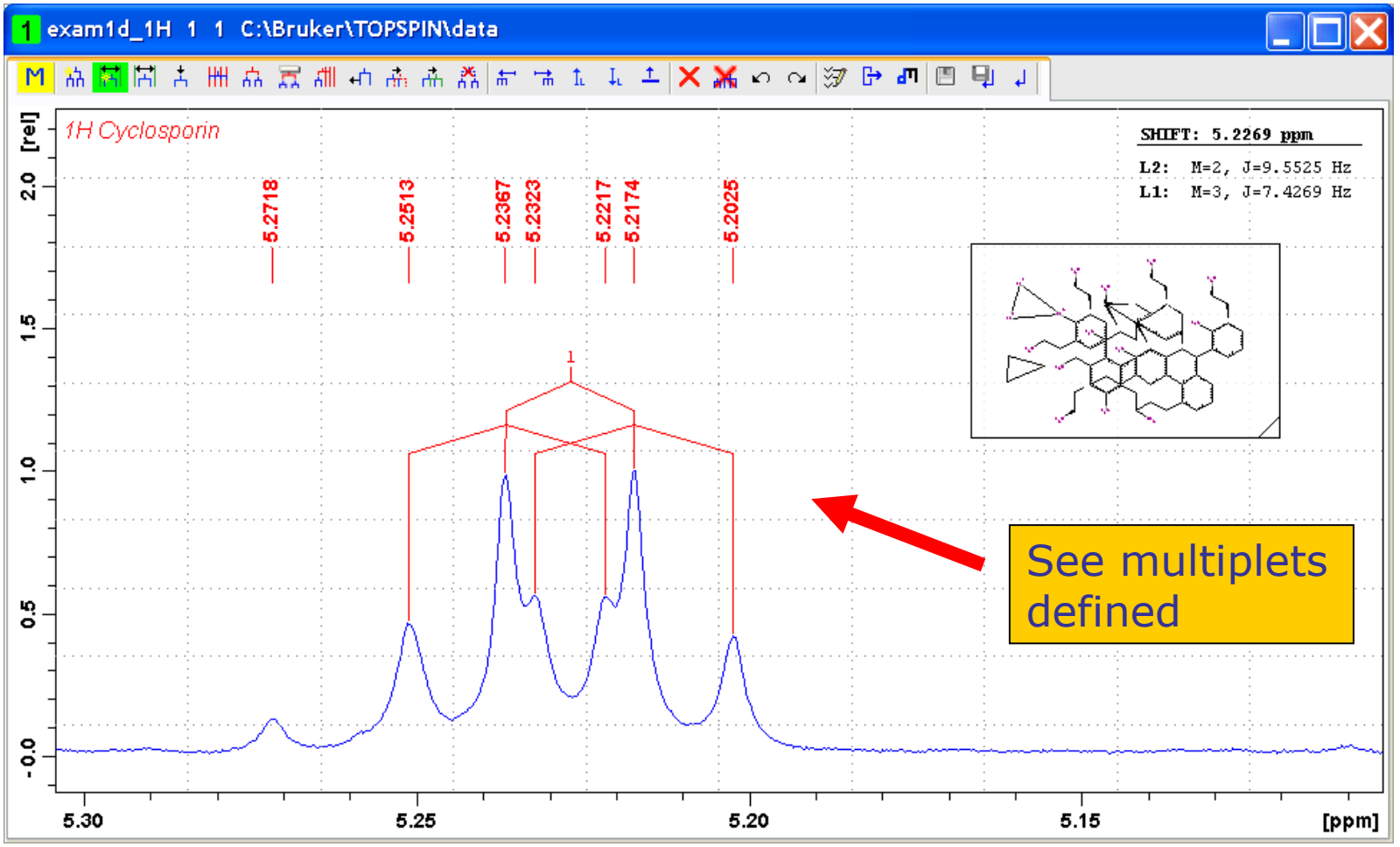
Automatic Definition in Displayed Range



Automatic Definition in Selected Range

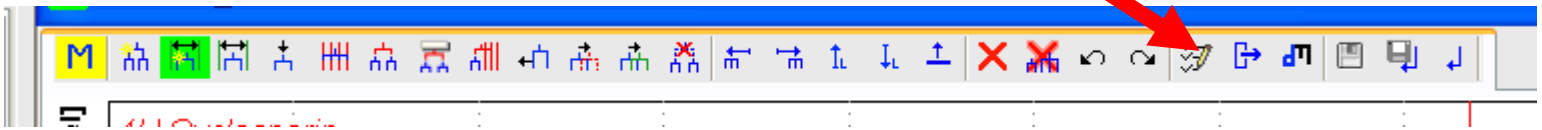


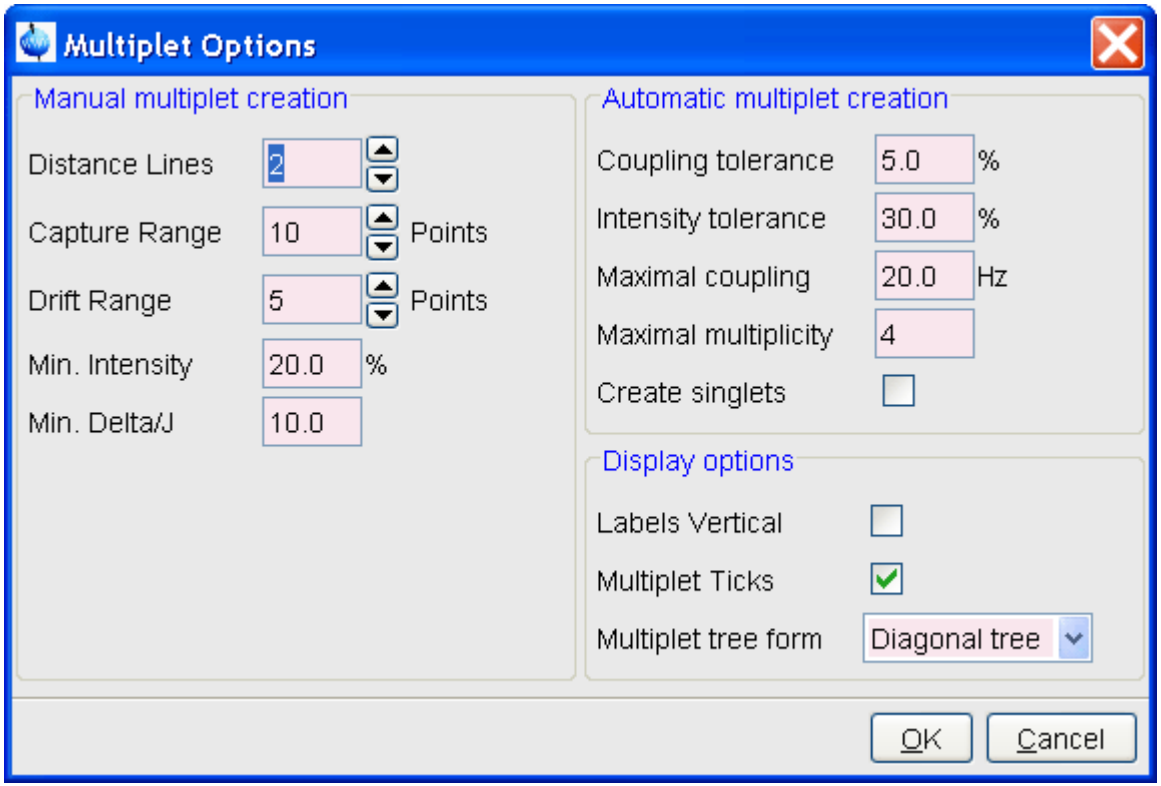
Automatic Definition in Selected Range



Multiplet Options Dialog

Click here to open dialog





Features:

-Define automatic multiplet definition options

-Define manual multiplet definition options

-Define display options

Multiplet 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

Manual Single-Level Multiplet Definition

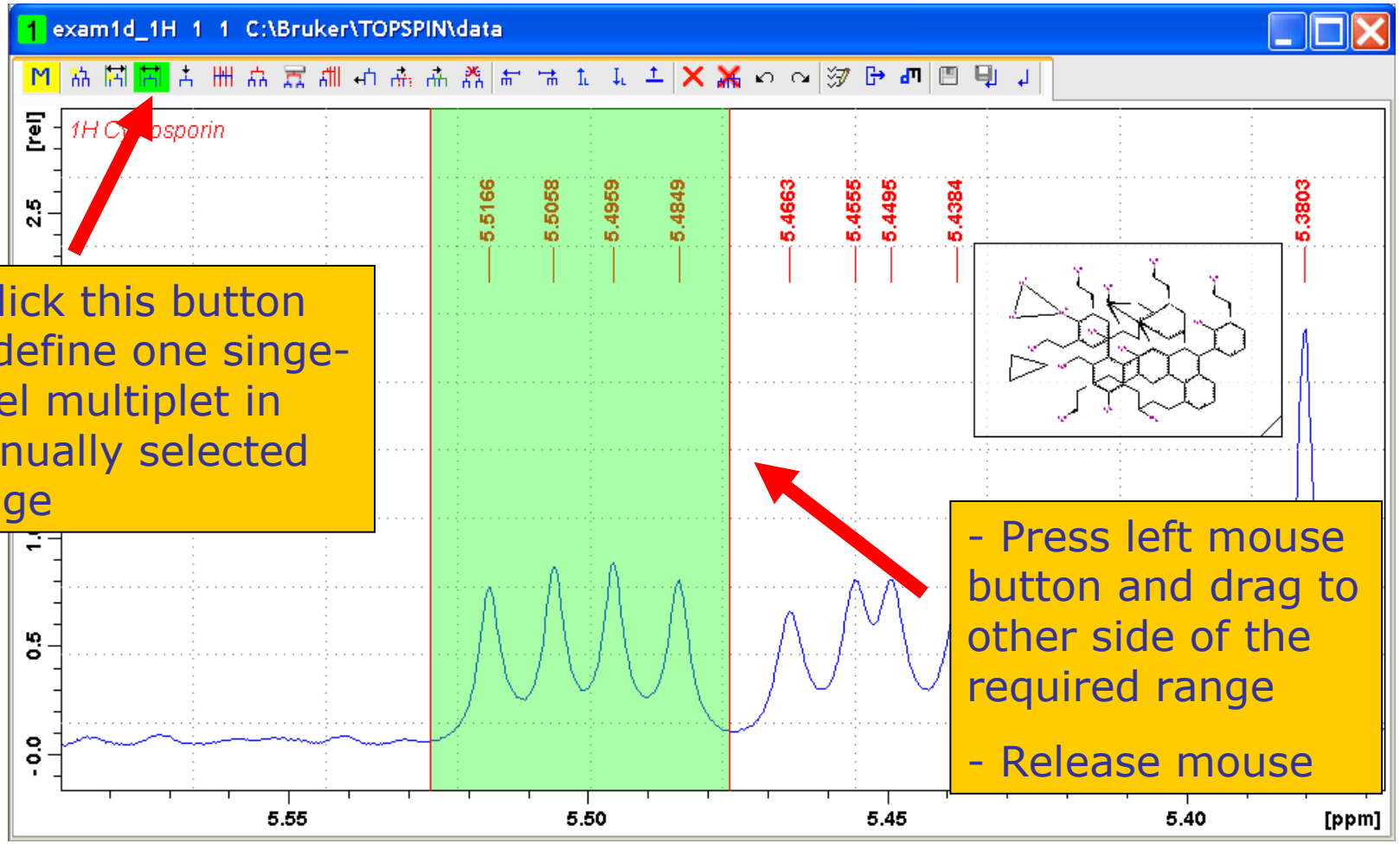
There are three methods to define a singe-level multiplet manually or semi-automatic:

- Define single-level multiplet by region

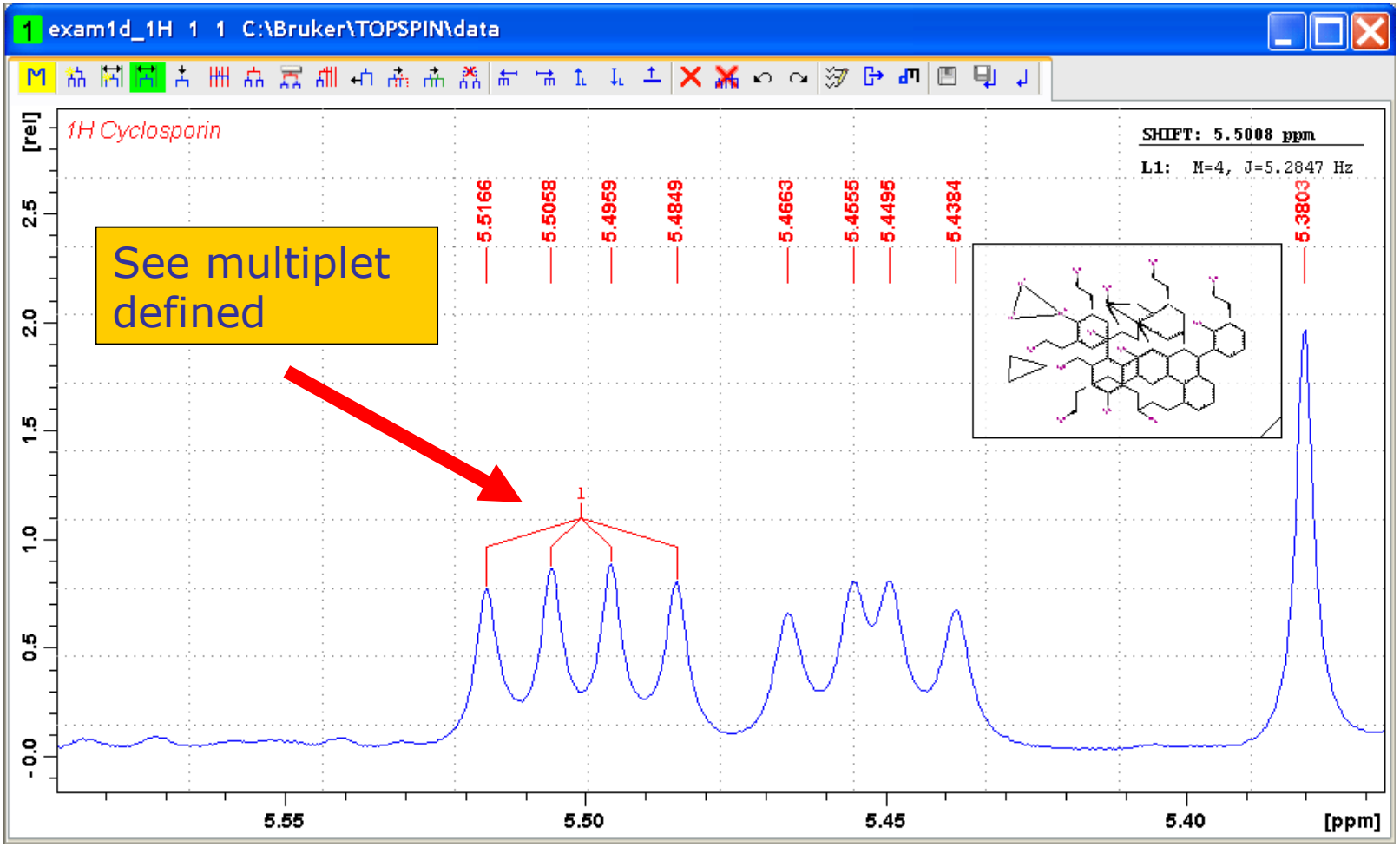
- Define single-level multiplet by selecting peaks manually

- Define single-level multiplet using the 'Free Grid' feature

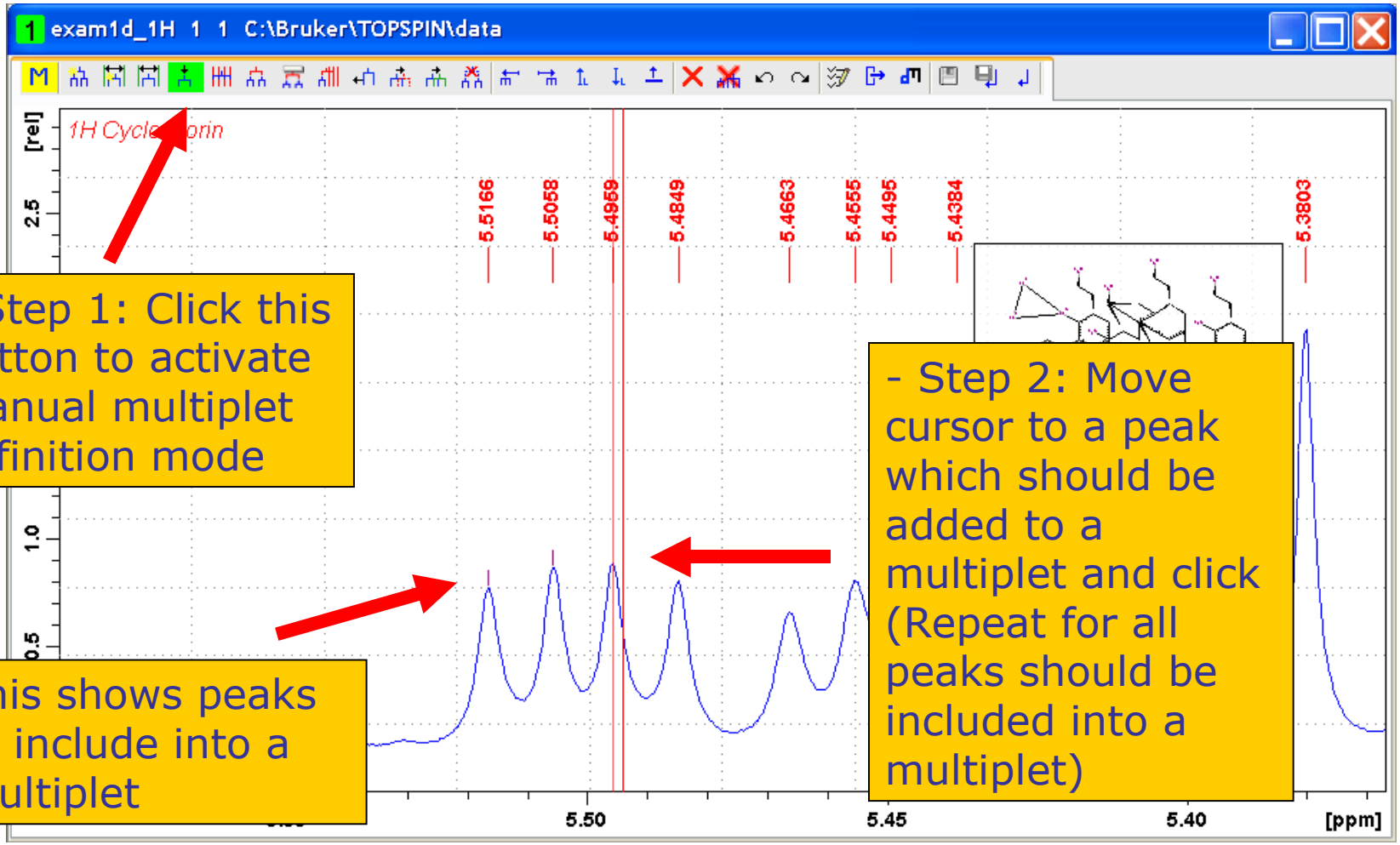
Define single-level multiplet by region



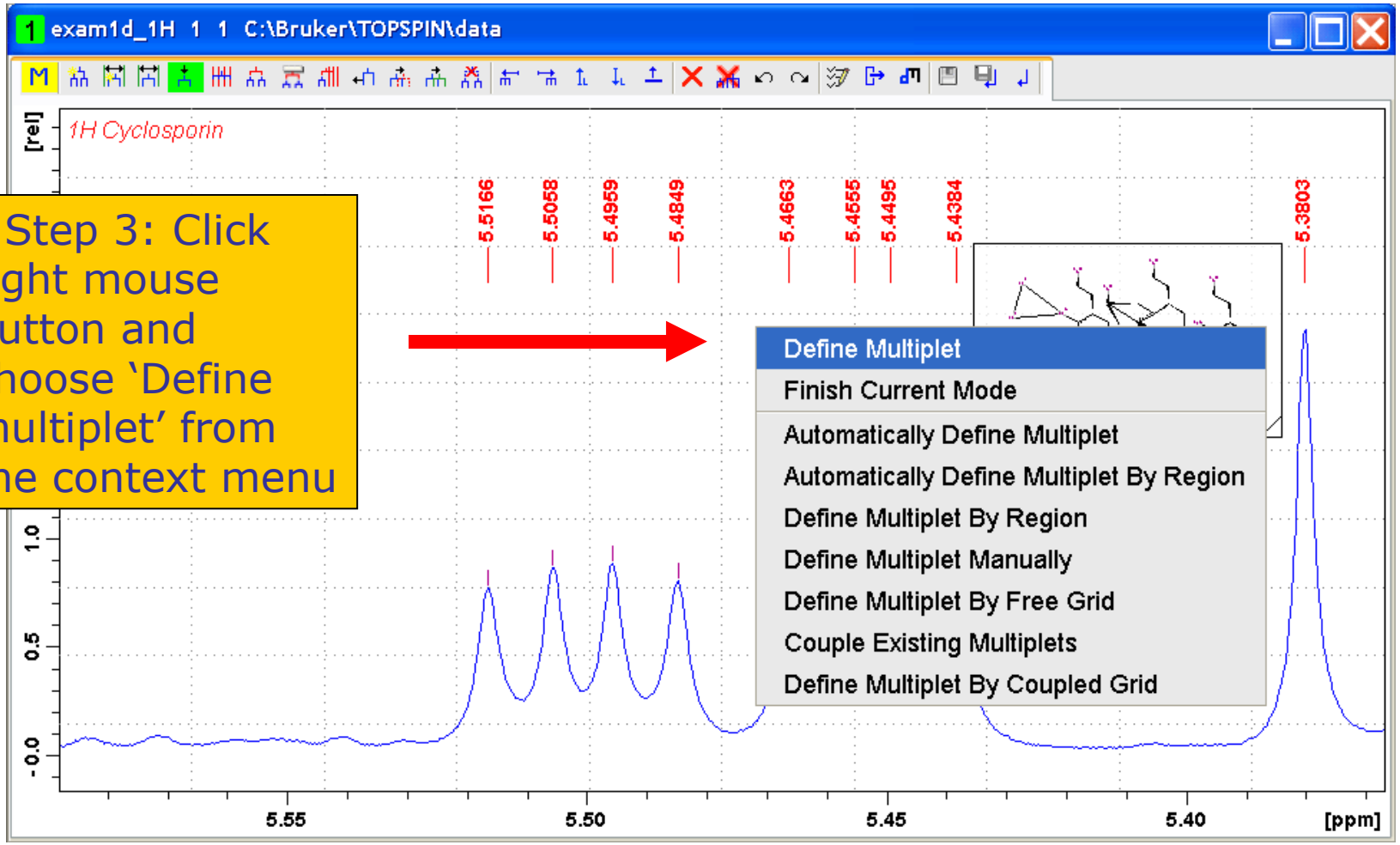
Define single-level multiplet by region



Define single-level multiplet manually

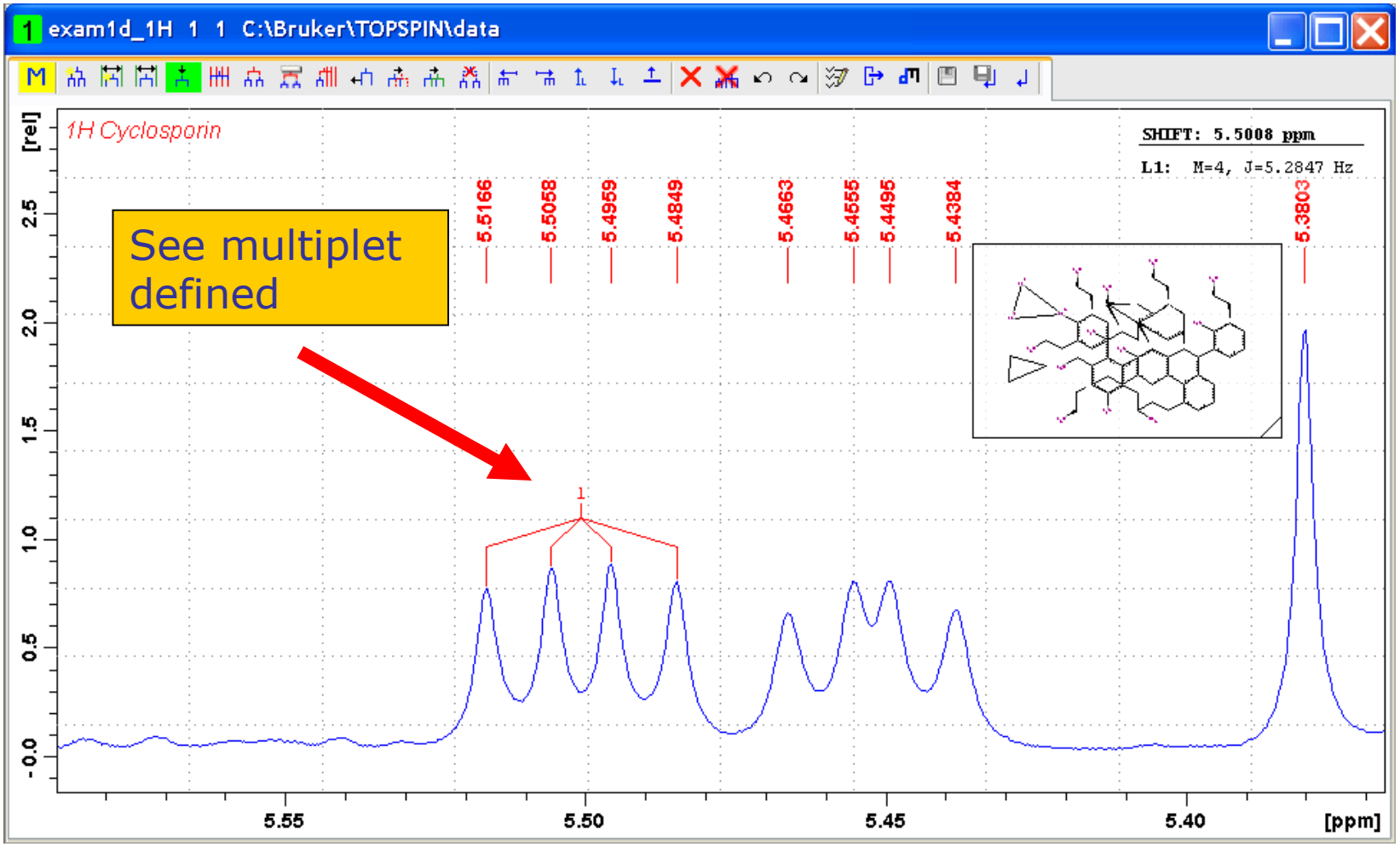


Define single-level multiplet manually

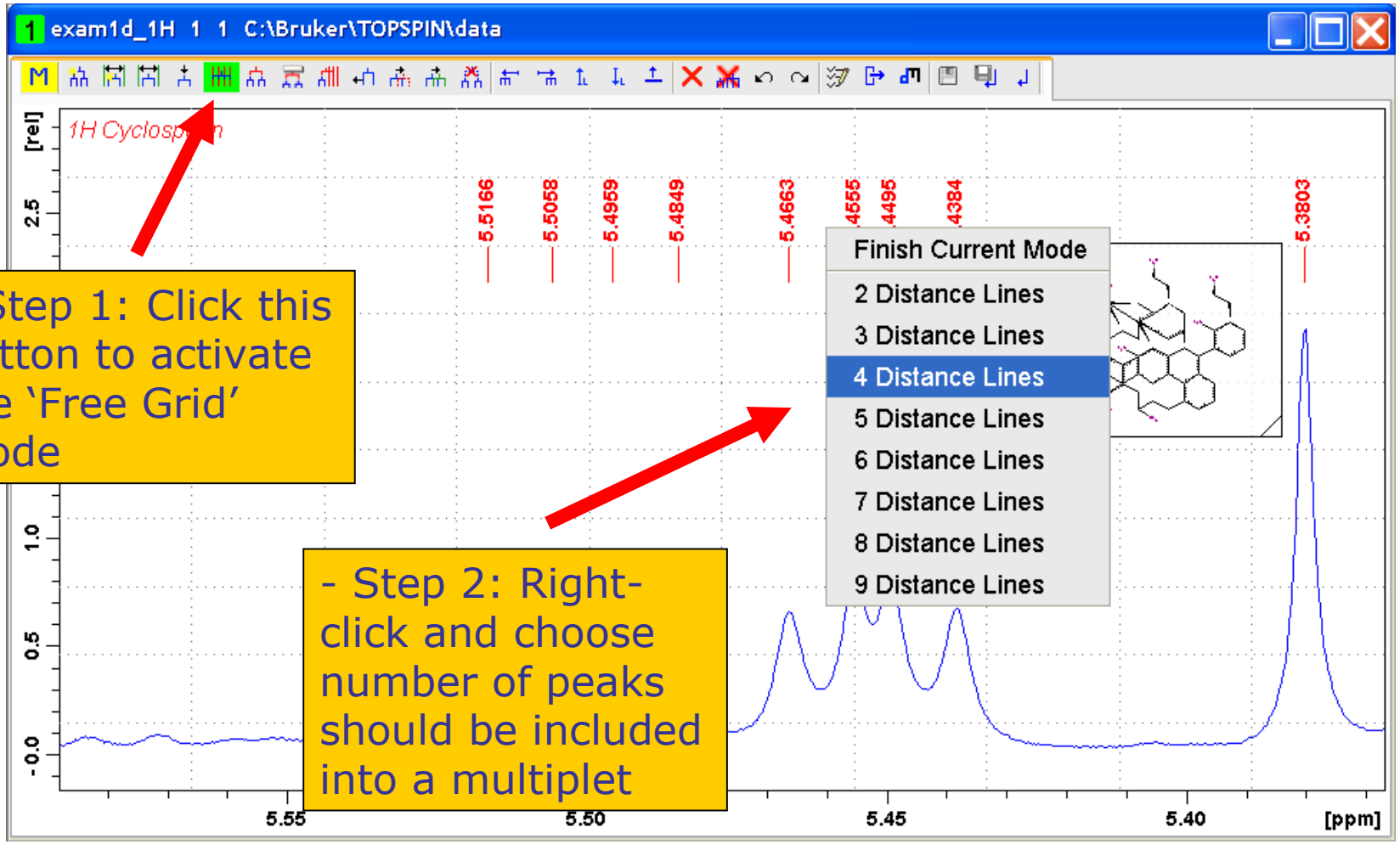


- Step 3: Click right mouse button and choose 'Define multiplet' from the context menu

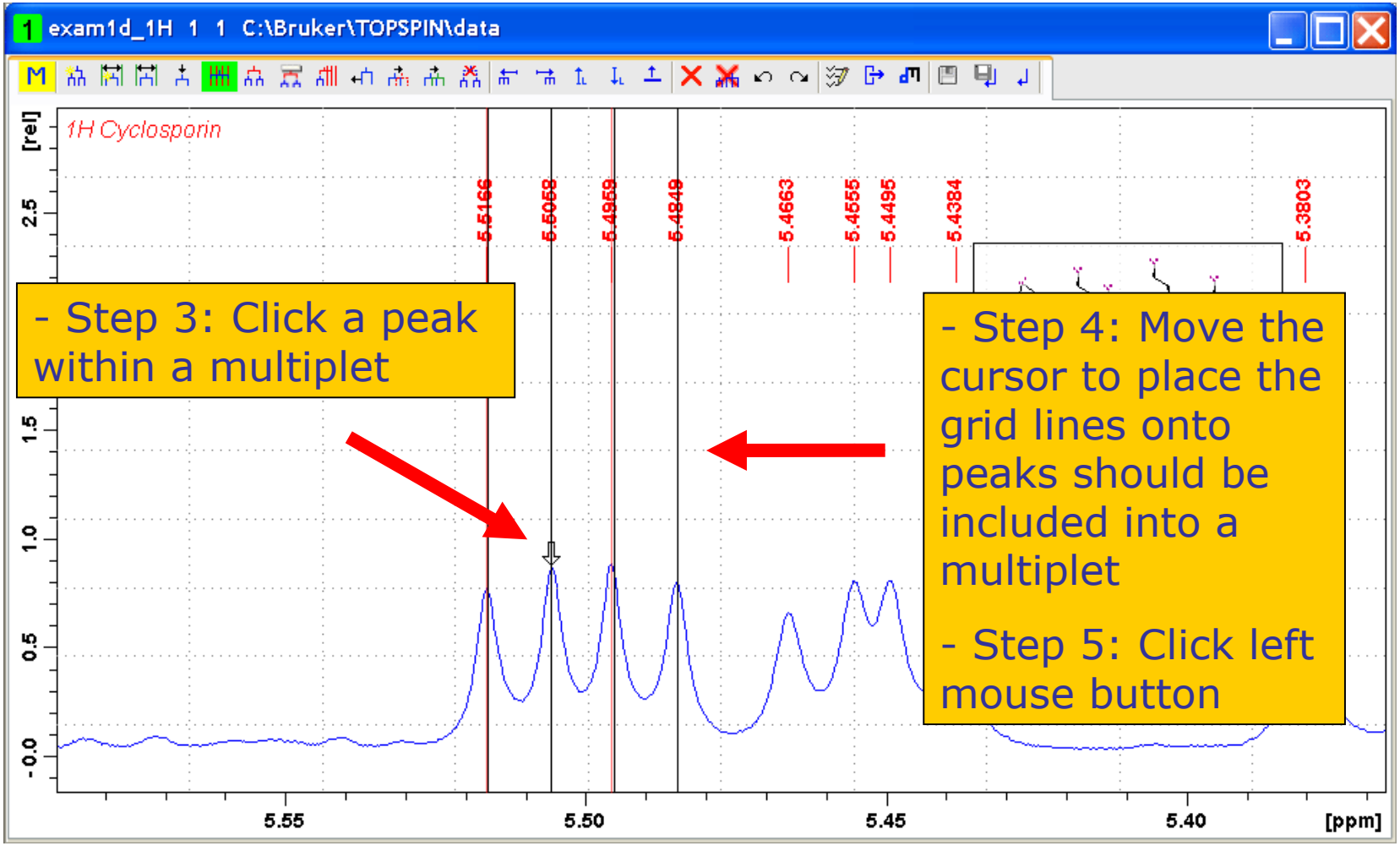
Define single-level multiplet manually



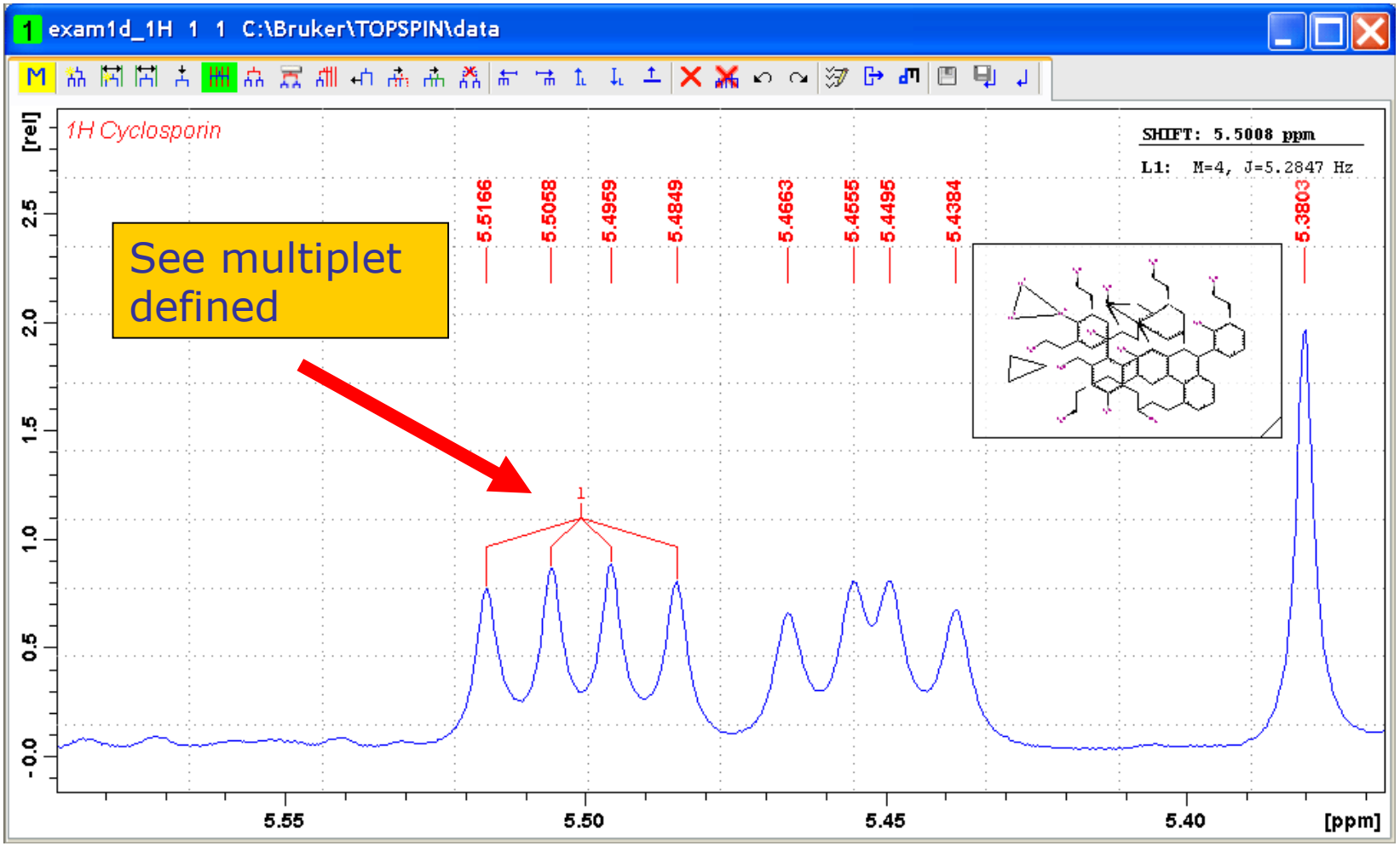
Define single-level multiplet using Free Grid



Define single-level multiplet using Free Grid



Define single-level multiplet using Free Grid



Manual Multi-Level Multiplet Definition

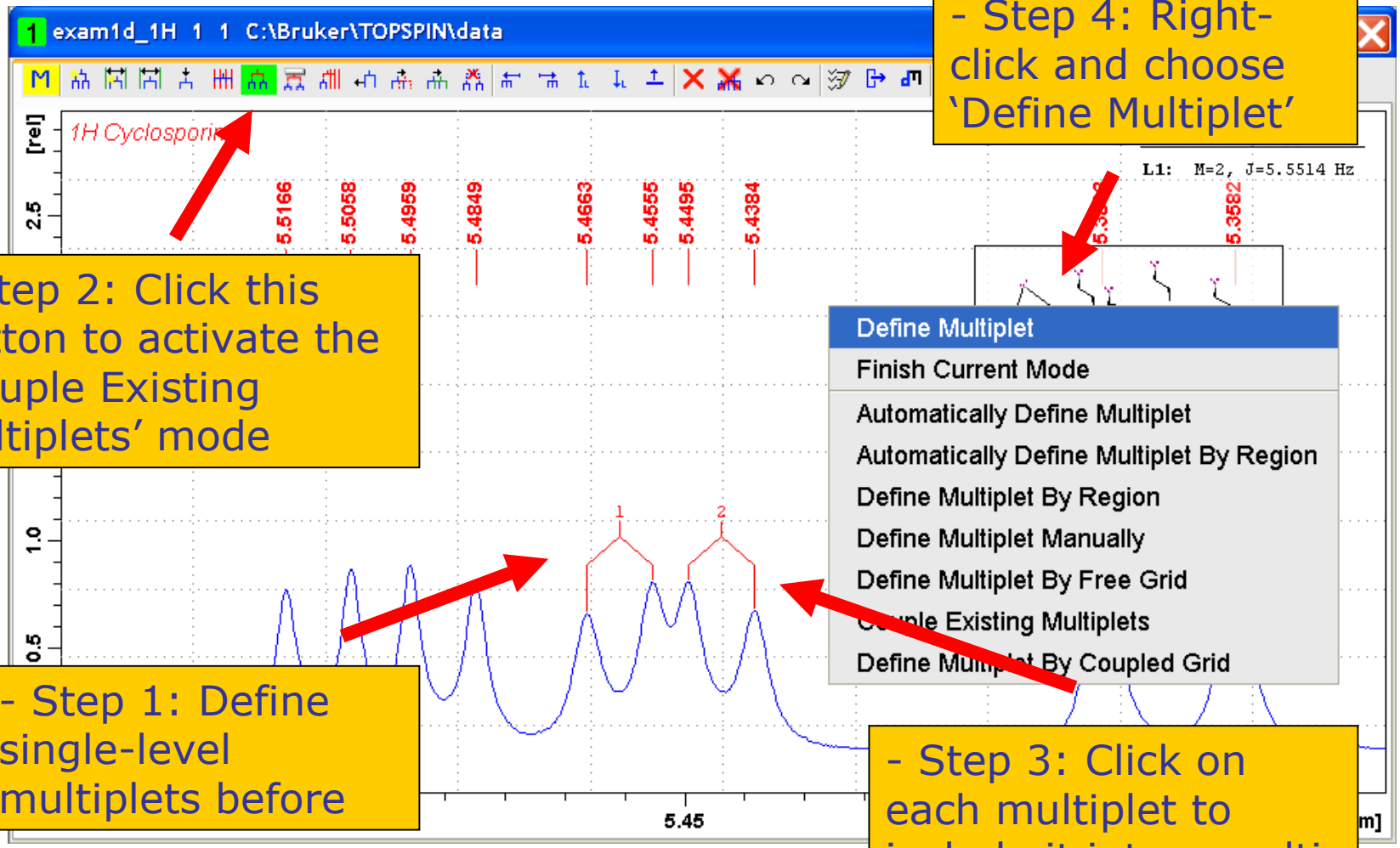
There are three methods to define a multi-level multiplet manually:

- 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



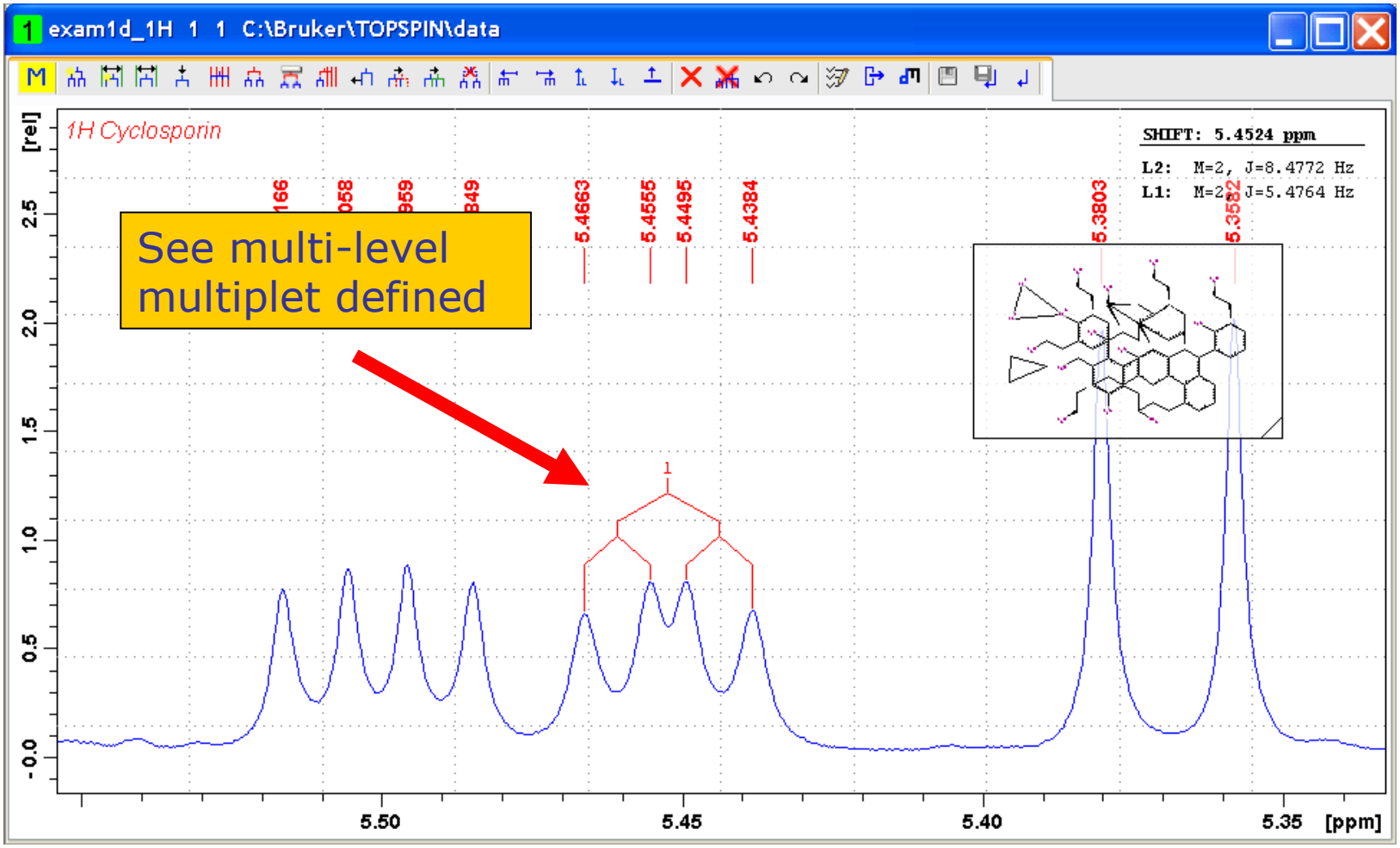
- Step 4: Right-click and choose 'Define Multiplet'

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

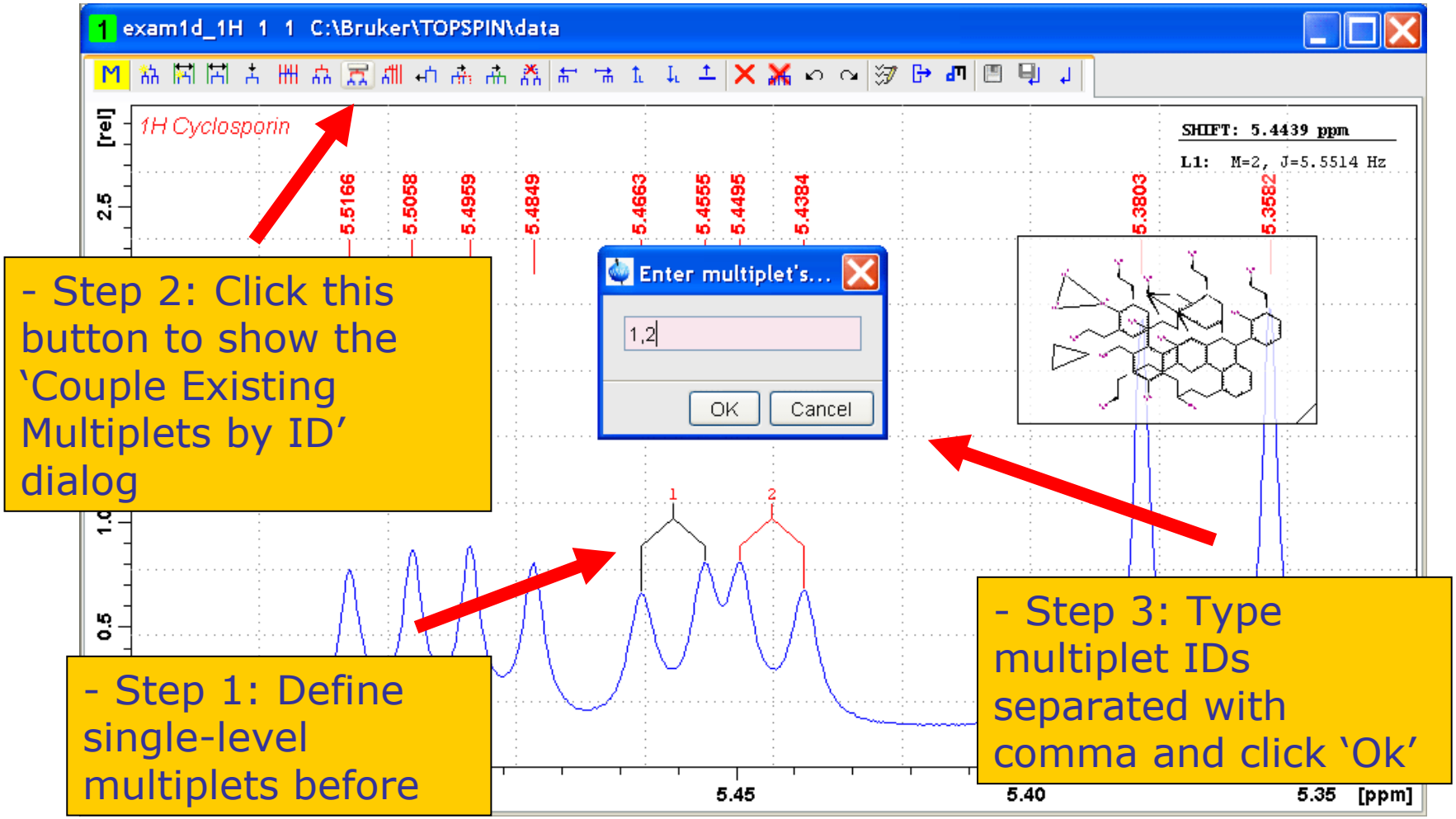
- Step 1: Define single-level multiplets before

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

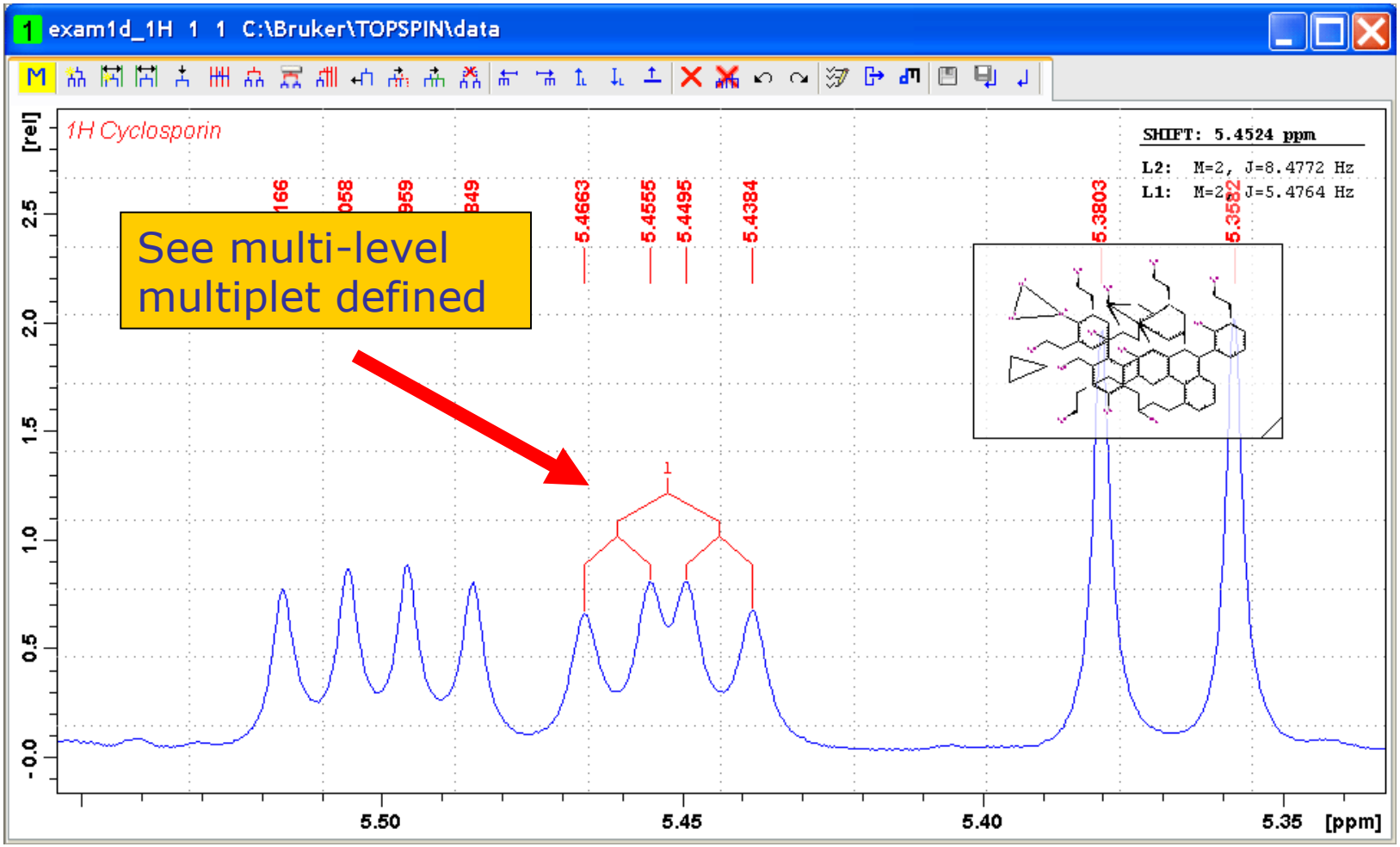
Couple Existing Multiplets



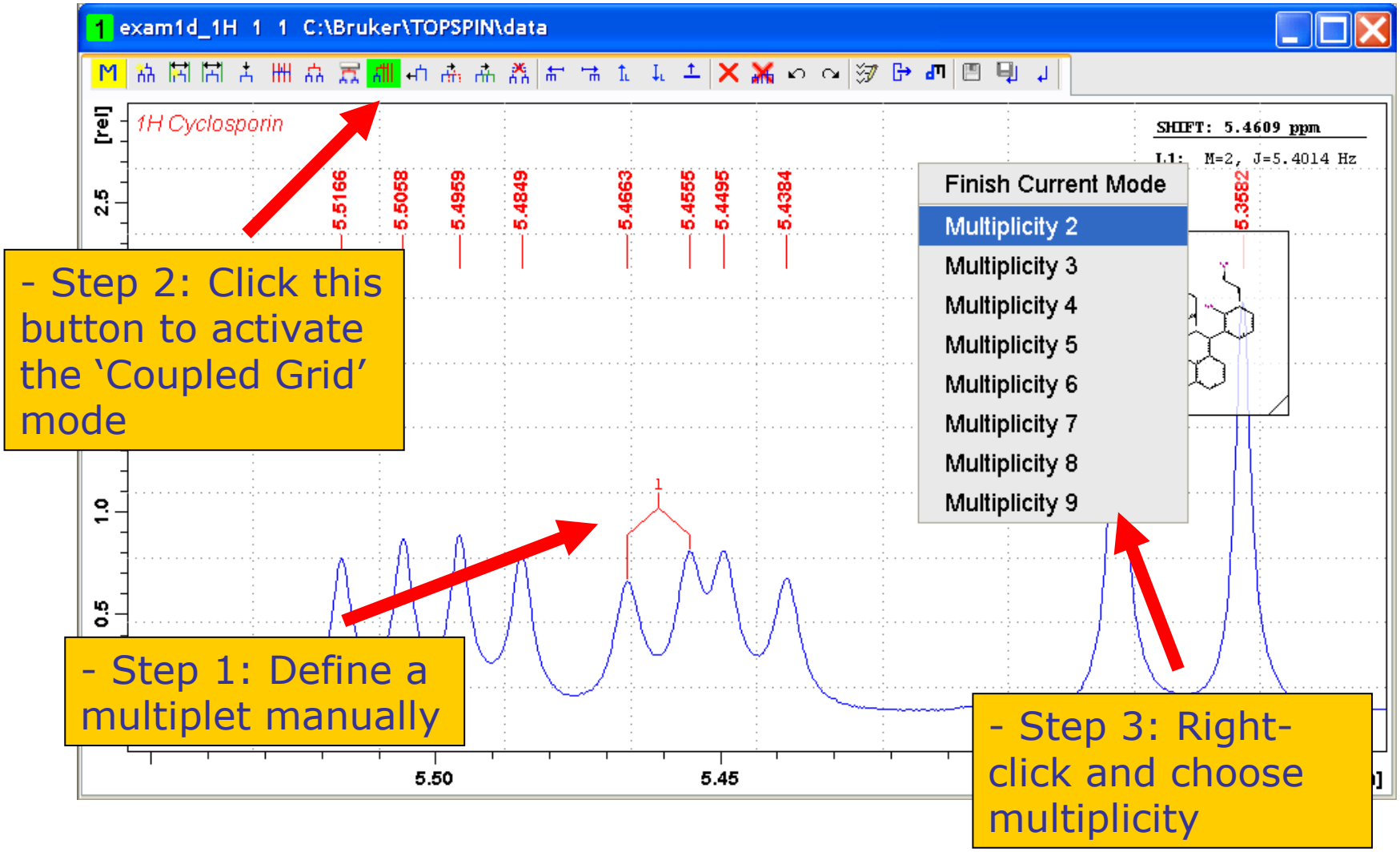
Couple Existing Multiplets by ID



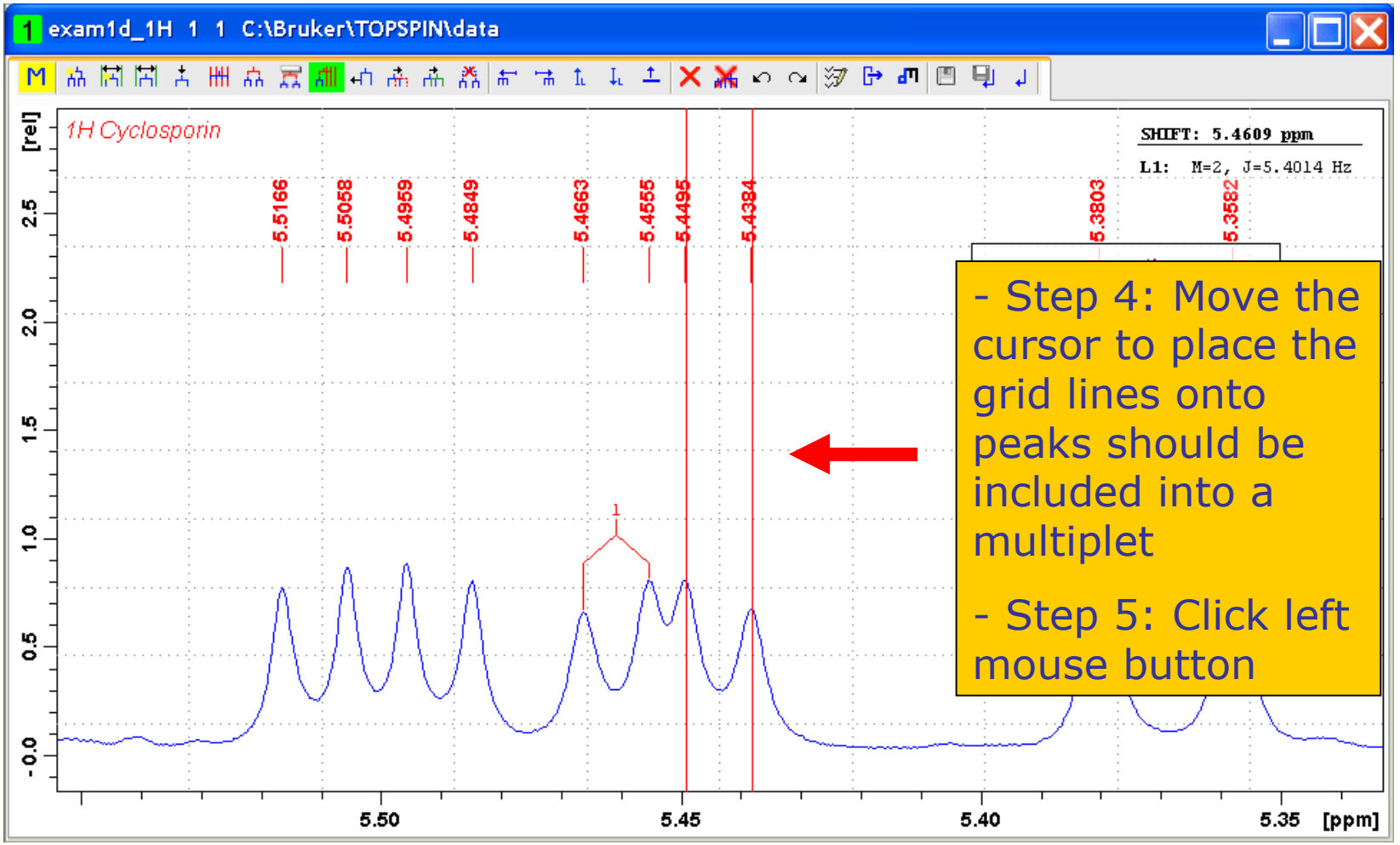
Couple Existing Multiplets by ID



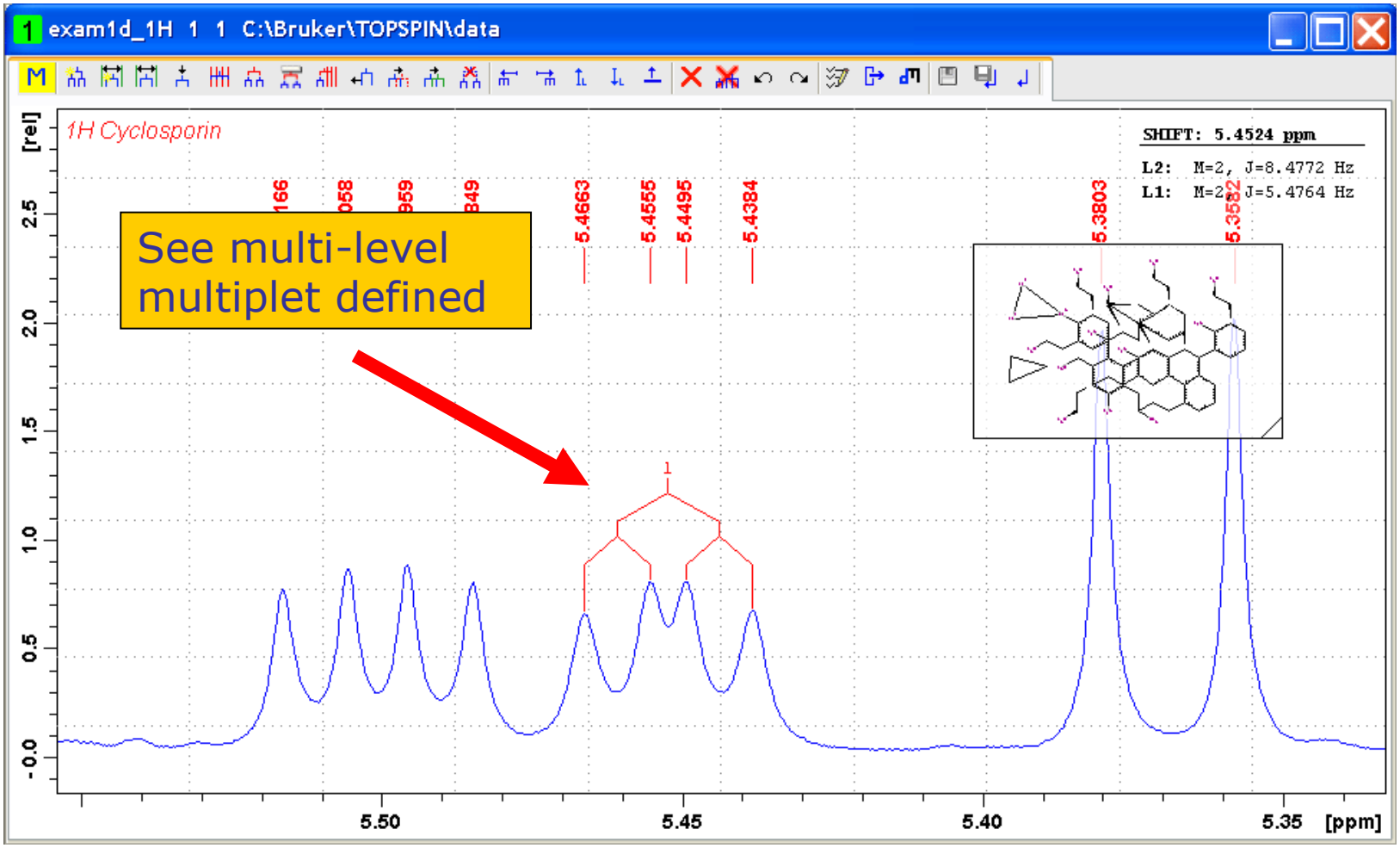
Define multi-level multiplet using Coupled Grid



Define multi-level multiplet using Coupled Grid



Define multi-level multiplet using Coupled Grid

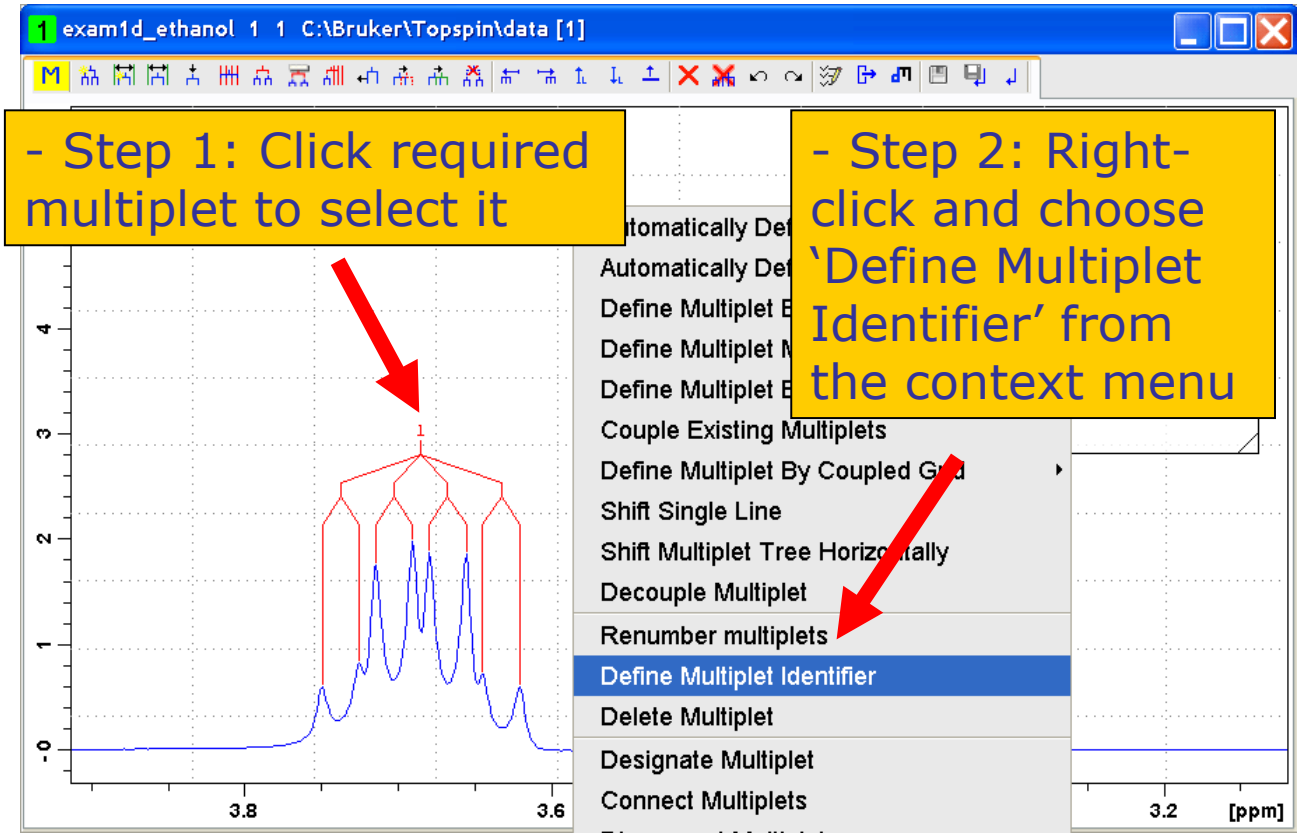


Working with Multiplets

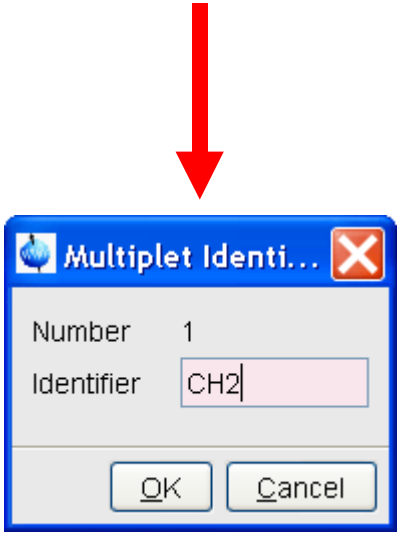
There are several additional operations can be performed with multiplets:

- 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

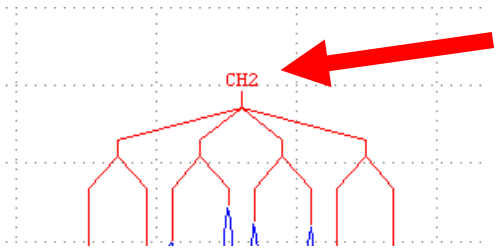
Define Multiplet ID / Label



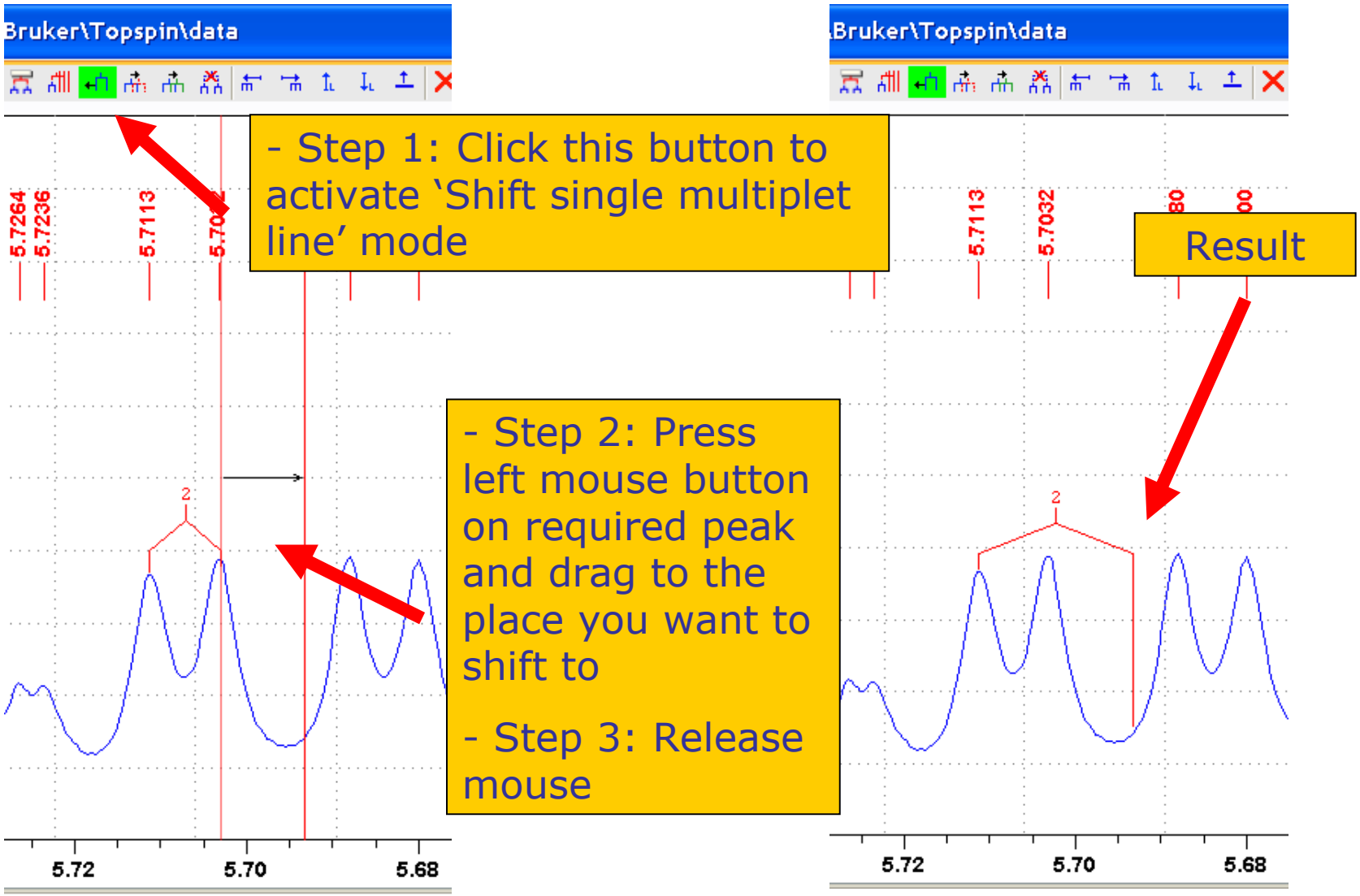
- Step 3: Type new multiplet ID and press 'Ok'



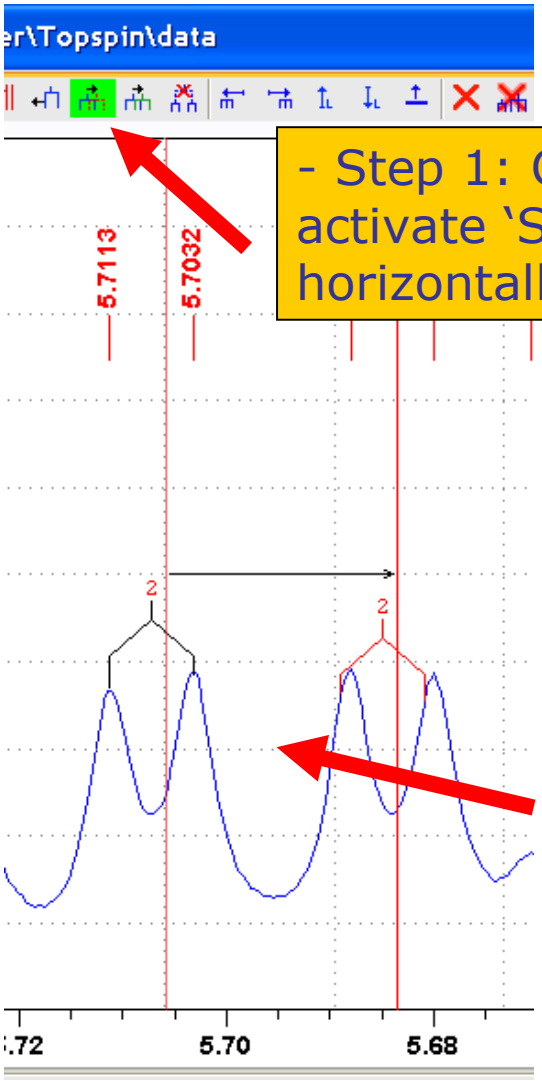
Result



Shift Single Multiplet Line



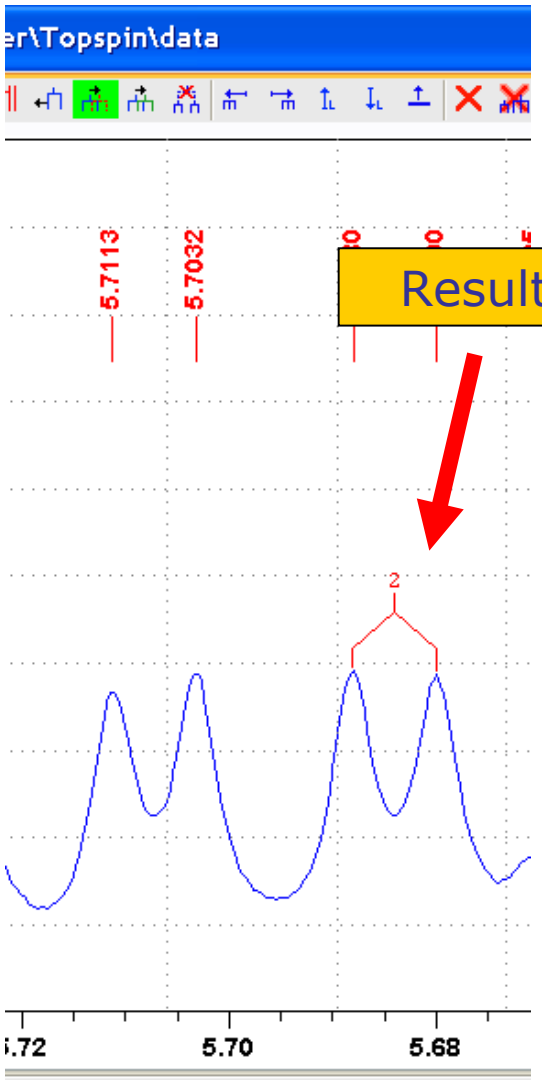
Shift Multiplet Tree Horizontally



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

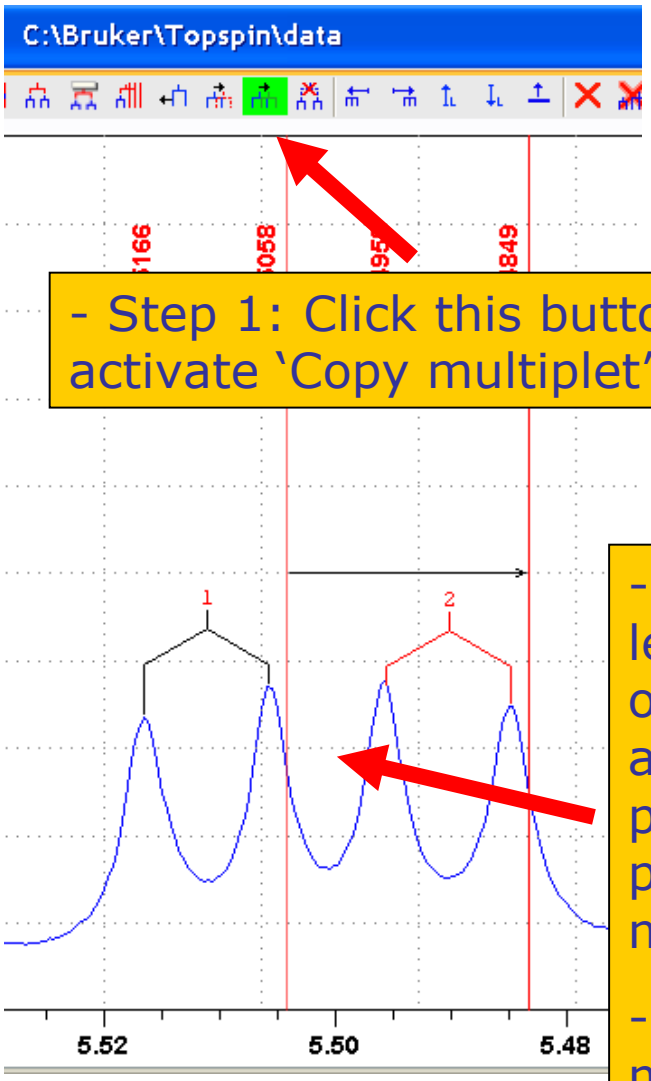
- Step 2: Press left mouse button on the multiplet and drag to the place you want to shift multiplet to

- Step 3: Release mouse



Result

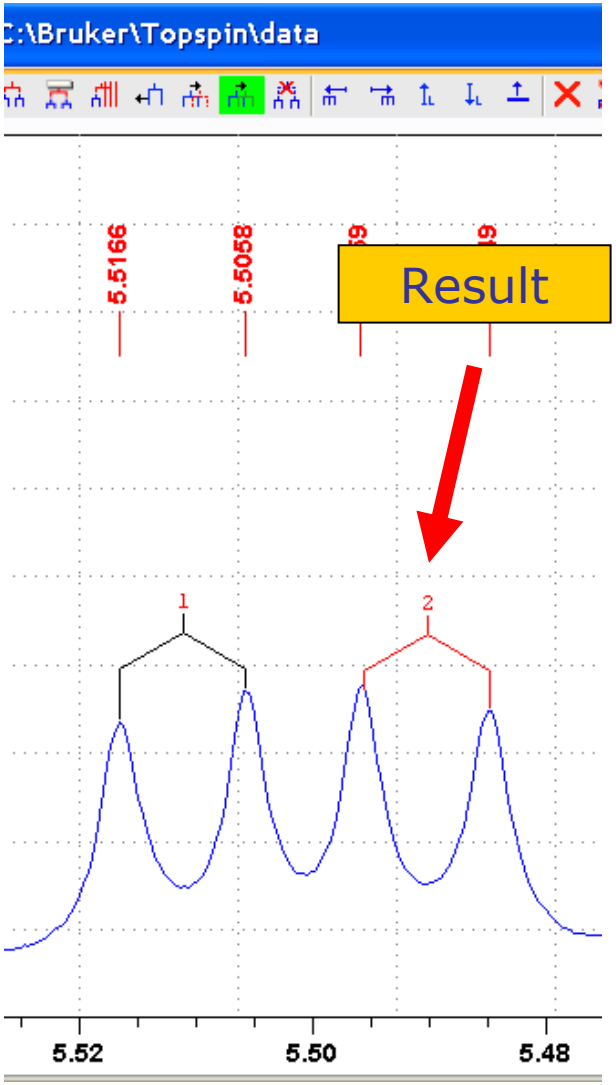
Copy Multiplet



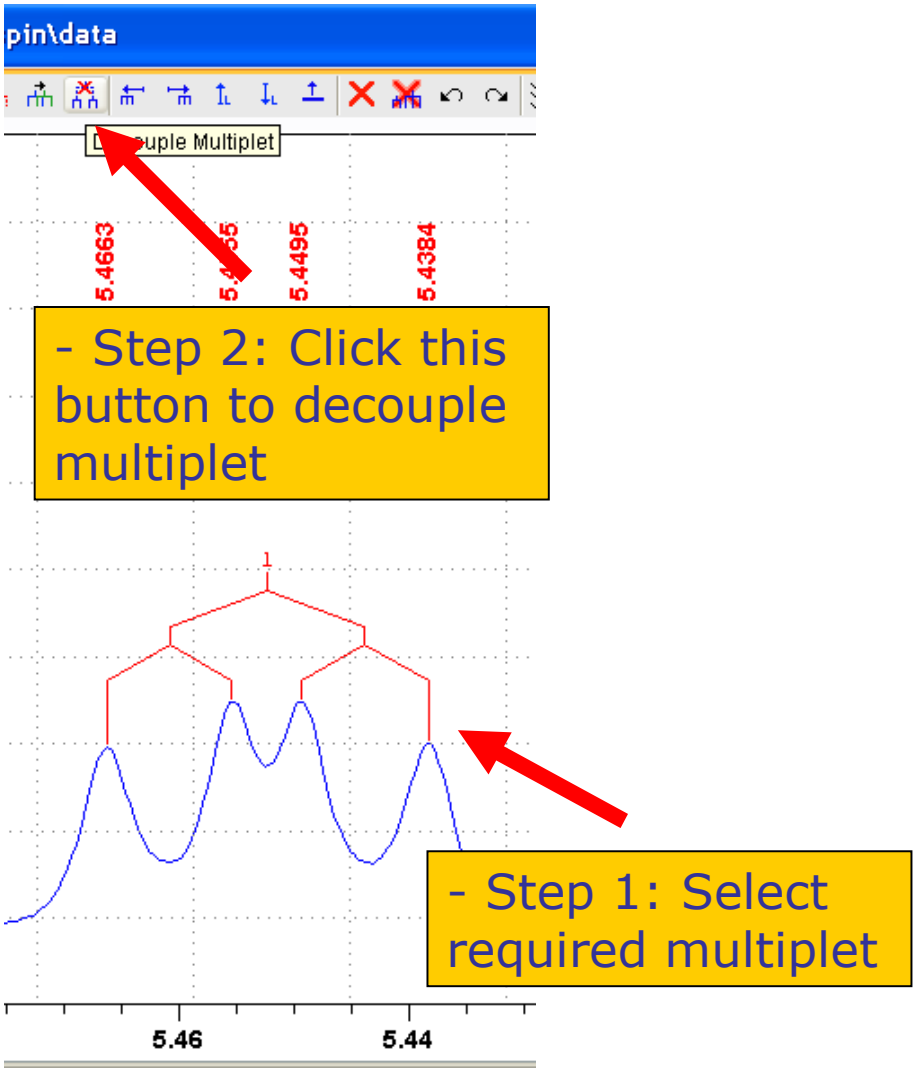
- Step 1: Click this button to activate 'Copy multiplet' mode

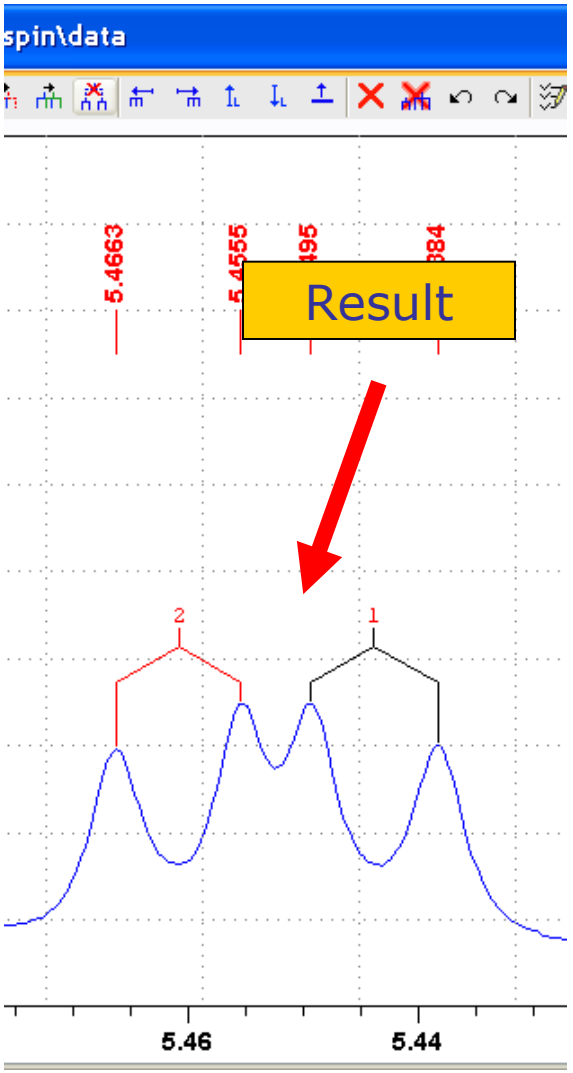
- Step 2: Press left mouse button on the multiplet and drag to the place you want to place copy of the multiplet

- Step 3: Release mouse



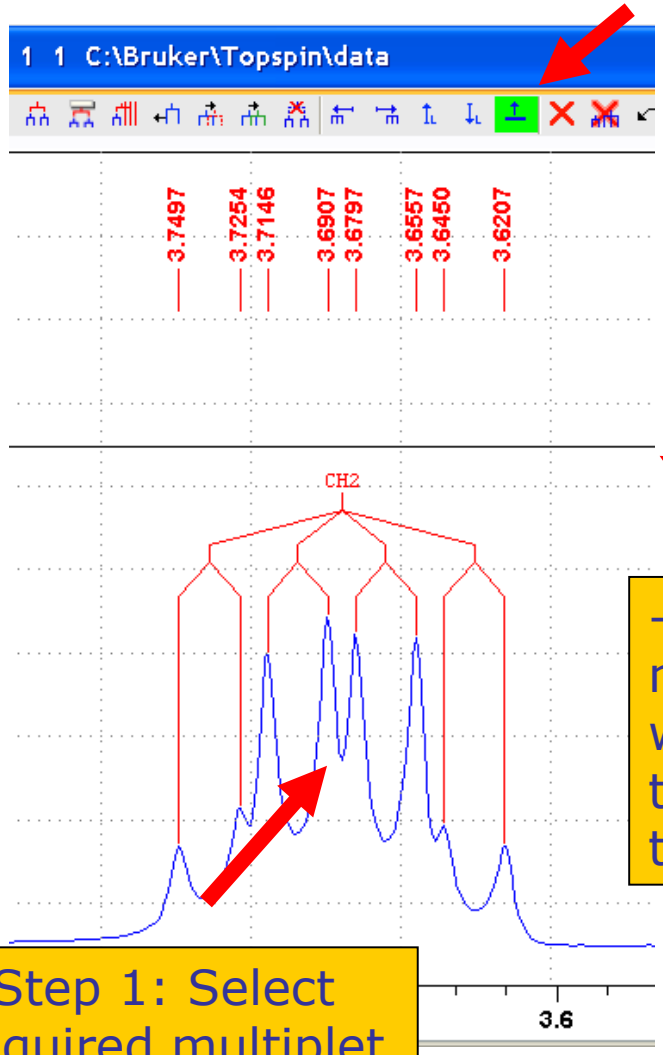
Decouple Multiplet



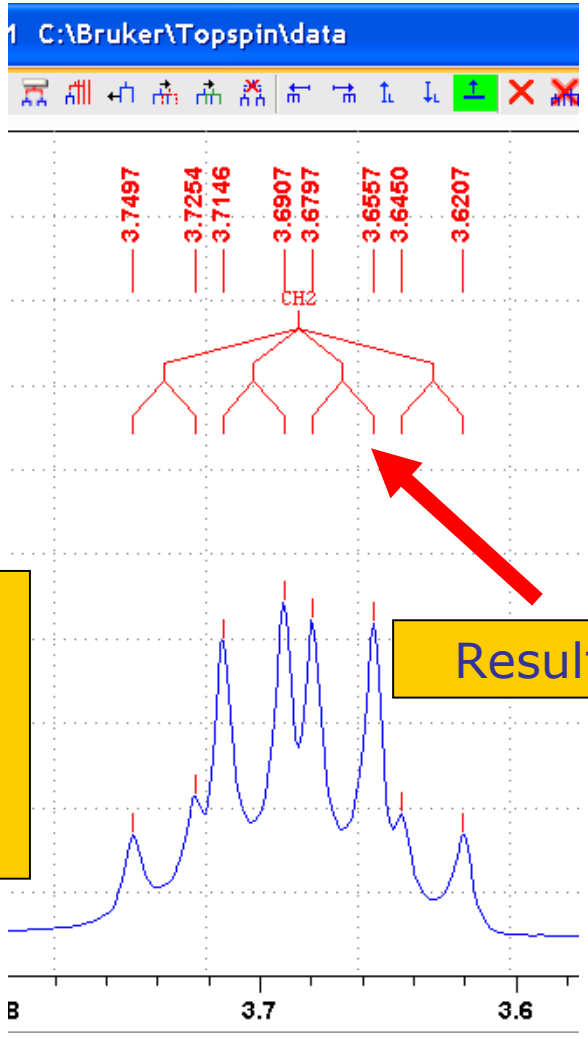


Shift Multiplet Tree Vertically

- Step 2: Click this button to activate mode



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

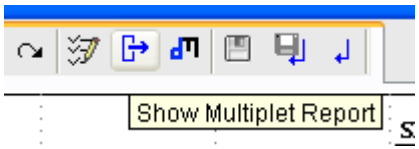


Result

- Step 1: Select required multiplet

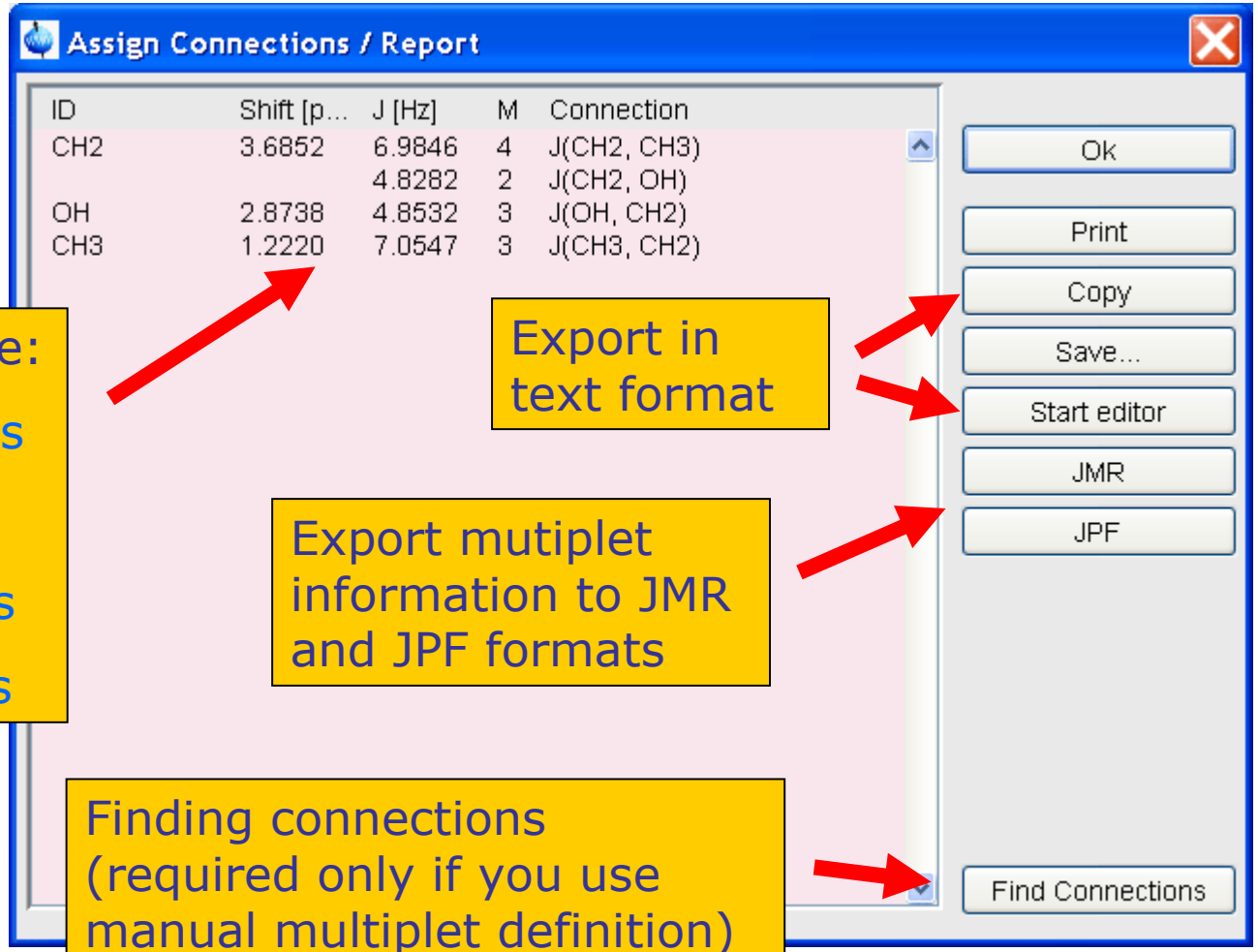
Report Dialog

To activate dialog



Multiplet table:

- Multiplet IDs
- J constants
- Multiplicities
- Connections

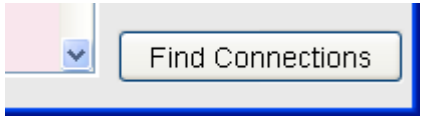


Export in text format

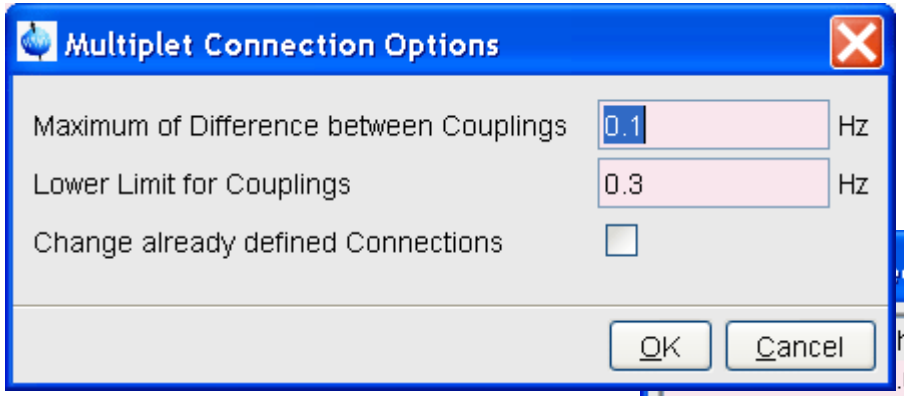
Export mutiplet information to JMR and JPF formats

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

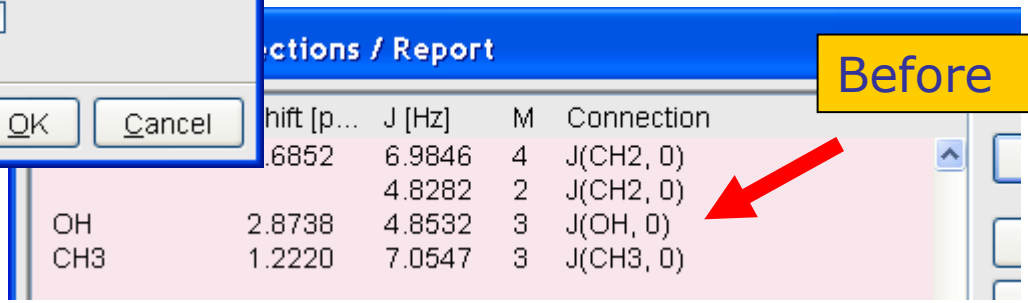
Finding Connections

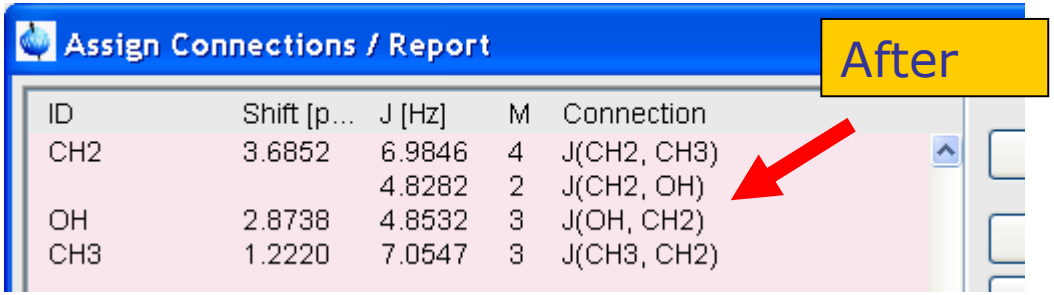


- Step 1: Press 'Find Connection' button in the Report dialog



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





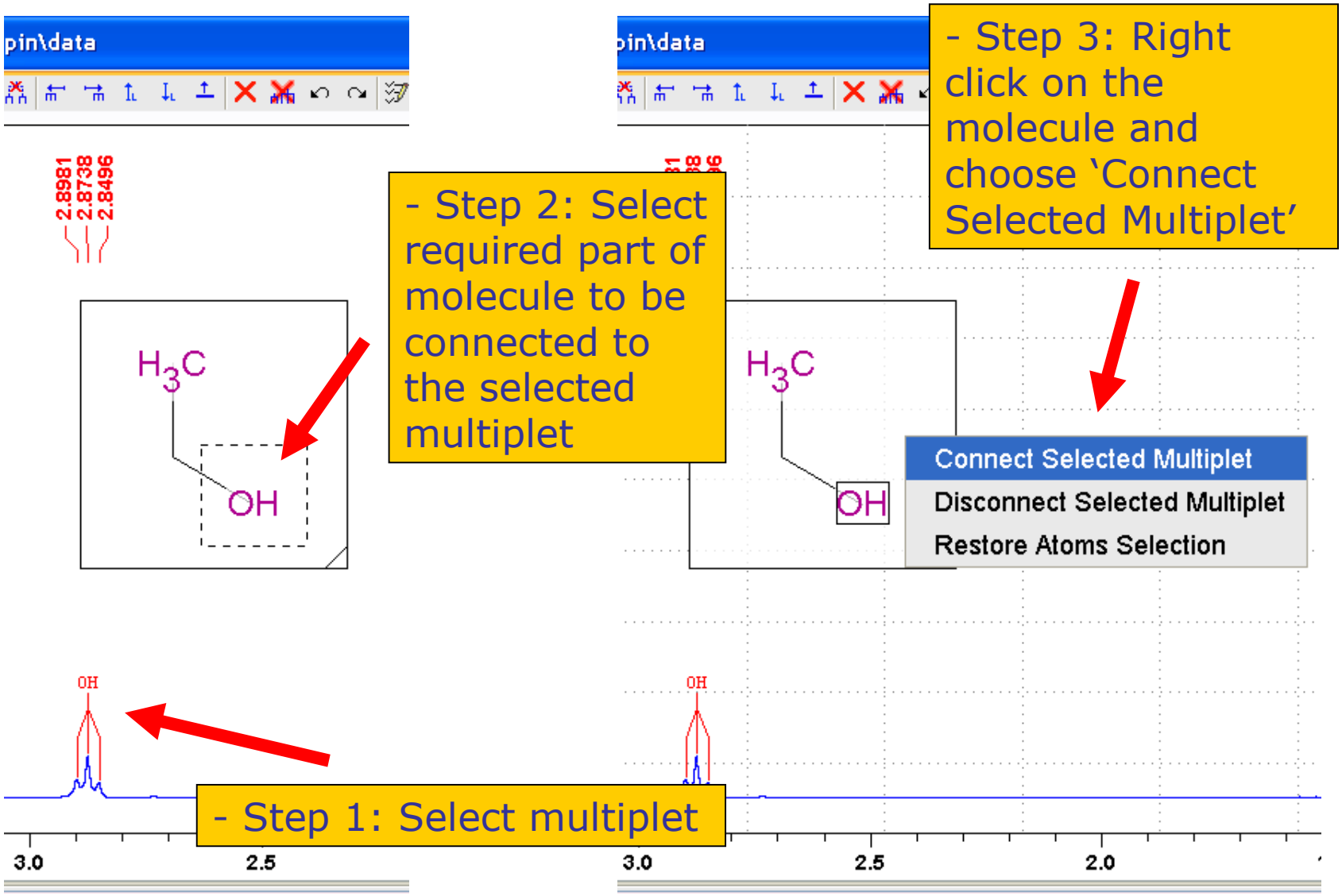
Correlations with Molecule Structure

Features:

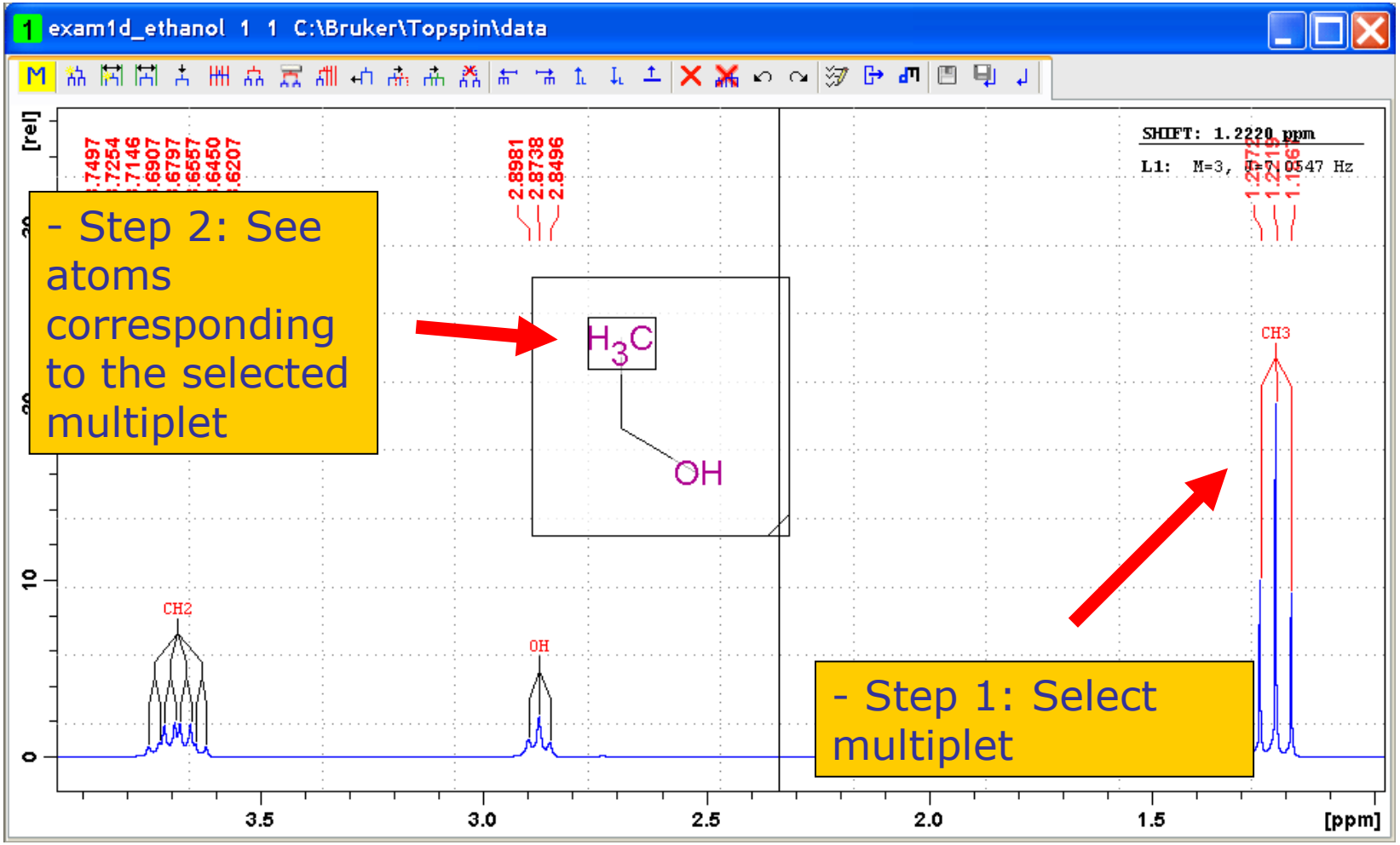
- Multiplet Analysis allows to define atoms-to-multiplet correlations if you have molecule structure defined for the dataset

- It is possible to view such correlation inside and outside of Multiplet Analysis module

Define Structure Correlations



View Structure Correlations



View Structure Correlations Outside Multiplet Analysis