TopSpin
Multiplet Analysis Tutorial
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- Report dialog and export to JMR and Japanese patent format
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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

See peaks over the spectrum as a result of the peak picking operation.
Enter Multiplet Analysis

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

Type 'mana' command in the command line and press enter.
Click this button to define multiplets in whole displayed spectrum range.

See multiplets defined.
Automatic Definition in Selected Range

Click this button to define multiplets in manually selected range

- Press left mouse button and drag to other side of the required range
- Release mouse
Automatic Definition in Selected Range

See multiplets defined
Multiplet Options Dialog

Click here to open dialog

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

- Click this button to define one single-level multiplet in manually selected range

- Press left mouse button and drag to other side of the required range

- Release mouse
Define single-level multiplet by region

See multiplet defined
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

See multiplet defined
Define single-level multiplet using Free Grid

- Step 1: Click this button to activate the ‘Free Grid’ mode

- Step 2: Right-click and choose the number of peaks should be included into a multiplet
Define single-level multiplet using Free Grid

- Step 3: Click a peak within a multiplet

- Step 4: Move the cursor to place the grid lines onto peaks should be included into a multiplet

- Step 5: Click left mouse button
Define single-level multiplet using Free Grid

See multiplet defined
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 1: Define single-level multiplets before

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

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

- Step 4: Right-click and choose ‘Define Multiplet’
Couple Existing Multiplets

See multi-level multiplet defined
Couple Existing Multiplets by ID

- Step 1: Define single-level multiplets before

- Step 2: Click this button to show the ‘Couple Existing Multiplets by ID’ dialog

- Step 3: Type multiplet IDs separated with comma and click ‘Ok’
Couple Existing Multiplets by ID

See multi-level multiplet defined
Define multi-level multiplet using Coupled Grid

1. Define a multiplet manually.
2. Click this button to activate the 'Coupled Grid' mode.
3. Right-click and choose multiplicity.
Define multi-level multiplet using Coupled Grid

- Step 4: Move the cursor to place the grid lines onto peaks should be included into a multiplet
- Step 5: Click left mouse button
Define multi-level multiplet using Coupled Grid

See multi-level multiplet defined
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 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’

Result
- 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

Result
- 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.
Decouple Multiplet

- Step 1: Select required multiplet

- Step 2: Click this button to decouple multiplet

Result
- Step 1: Select required multiplet

- Step 2: Click this button to activate mode

- 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

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’
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**

- **Step 1:** Select multiplet

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

- **Step 3:** Right click on the molecule and choose ‘Connect Selected Multiplet’
- Step 2: See atoms corresponding to the selected multiplet

- Step 1: Select multiplet
View Structure Correlations Outside Multiplet Analysis

- Step 1: Open the same dataset twice using ‘Display in new window’ and ‘Window / Arrange ...’ menus

- Step 2: Activate the Structure tab in one of the windows and press shown button

- Step 3: Move the mouse cursor over the structure: you will see cursor moving over the spectrum according with the correlations

- Step 4: Move the cursor over the spectrum: atoms will be selected automatically according with the correlations