***multiNMRFit***

Virtual decoupling of 2D HSQC NMR experiments - version 1.1

<https://github.com/NMRTeamTBI/MultiNMRFit/>

**User Manual**

Version 1.1

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# Introduction

MultiNMRFit is a scientific software designed to fit series of 1D spectra either acquired under a pseudo2D format or in a series of independent 1Ds. It is designed as semi-automated software that will manually clusterized peaks that belong to the same multiplet after an automated peak picking on defined region of a reference spectrum.

# Quick Start

## Installation

MultiNMRFit requires Python 3.5 or higher and run on all platforms. If you don’t have a Python environment configured on your computer, we recommend that you follow the instructions from [Anaconda](https://www.anaconda.com/products/individual).

Then, open a terminal (*e.g.* run *Anaconda Prompt* if you have installed Anaconda) and type:

pip install multinmrfit

## Usage – Data Loading

### Graphical User Interface

To start the Graphical User Interface, type in a terminal (or *Anaconda Prompt* for Windows)

|  |
| --- |
| multinmrfit |

The MultiNMRFit window will open. If the window fails to open, have a look at our help section to solve the problem.

Graphical user interface

Description automatically generated

Fill all the required entries from the *inputs*, *analysis* and *outputs* sections. Options might be used accordingly to your need. P

### Command Line Interface

To start the MultiNMRFit analysis from a terminal instead of using the graphical user interface, type in a terminal (or *Anaconda Prompt* for Windows) the multinmrfit command followed by the path to the inputs file. The inputs file

|  |
| --- |
| multinmrfit *path/inputsfile.json* |

## Usage – Clusterization

# Help - FAQ

## I cannot start MultiNMRFit graphical user interface, can you help me?

If you installed MultiNMRFit following our standard procedure and that you are unable to start MultiNMRFit by opening a terminal and typing multinmrfit, then there is indeed something wrong. Do not panic, we are here to help! Please follow this simple procedure:

1. The first step of the debugging process will be to get a *traceback*, i.e. a message telling us what is actually going wrong:
   * On Unix-based systems, you should already see it in the terminal you opened.
   * On Windows, you will have to open MultiNMRFit from your Anaconda prompt with python.exe -m multinmrfit to display the traceback.
2. Read the traceback and try to understand what is going wrong:
   * If it is related to your system or your Python installation, you will need to ask some help from your local system administrator or your IT department so they could guide you toward a clean installation. Tell them that you wanted “to use the graphical user interface of MultiNMRFit, a Python 3.5 software” and what you did so far (installation), give them the traceback and a link toward the documentation. They should know what to do.
   * If you believe the problem is in MultiNMRFit or that your local system administrator told you so, then you probably have found a bug! We would greatly appreciate if you could open a new issue on our [issue tracker](https://github.com/MetaSys-LISBP/IsoCor/issues). One of the developers will help you.