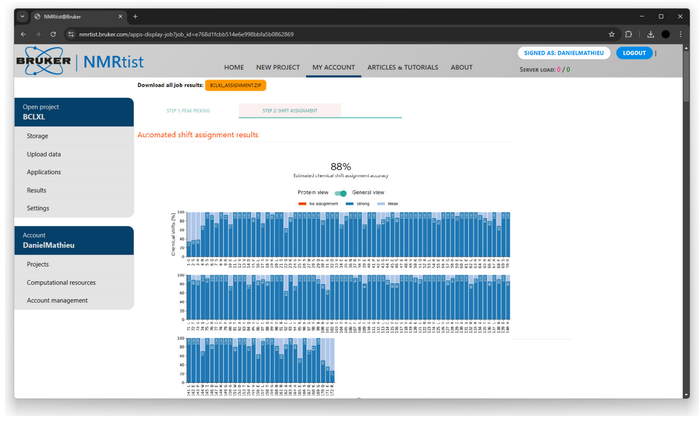
NMRtist
Protein NMR Data Anlaysis with Ease

NMRtist[1] is a cloud based, AI supported software platform, which has been developed by the group of Roland Riek at the ETH Zurich. It utilizes the underlying ARTINA[2,3] algorithm to perform protein spectra analysis including peak picking and assignment in full automation.

Bruker and the group at the ETH in Zurich have entered a collaboration to provide an even easier to use platform to perform these traditionally very time-consuming tasks, executed by a trained expert.



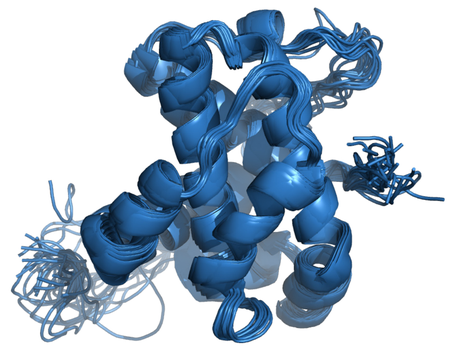


Fig. 1: Example of an assignment task in the NMRtist Web Interface on the left and the structure of a 20 kDa cancer related protein, determined using NMRtist on the right

Peak Picking

The ARTINA algorithm consists of the three individual steps which can be executed separately or in consecutive order.

The ARTINA peak picking application uses a deep convolutional neural network to detect positions of signals in the selected NMR spectra. For each spectrum, the method returns peak lists in various formats. Additionally, the application performs a spectrum referencing check, verifying relative shifts between pairs of spectra that record frequencies of the same atoms.

ARTINA
peak picking

Resonance Assignment

The second step is resonance assignment. What usually is a days or weeks long undertaking can be automated and executed in a matter of minutes or hours.

The ARTINA shift assignment application first uses a deep convolutional neural network to detect positions of signals in the selected NMR spectra (see ARTINA peak picking application above). Afterwards, the detected signals undergo FLYA[4] automated chemical shift assignment. The method returns protein chemical, together with assigned peak lists for the individual NMR spectra.

ARTINA
shift
assignment

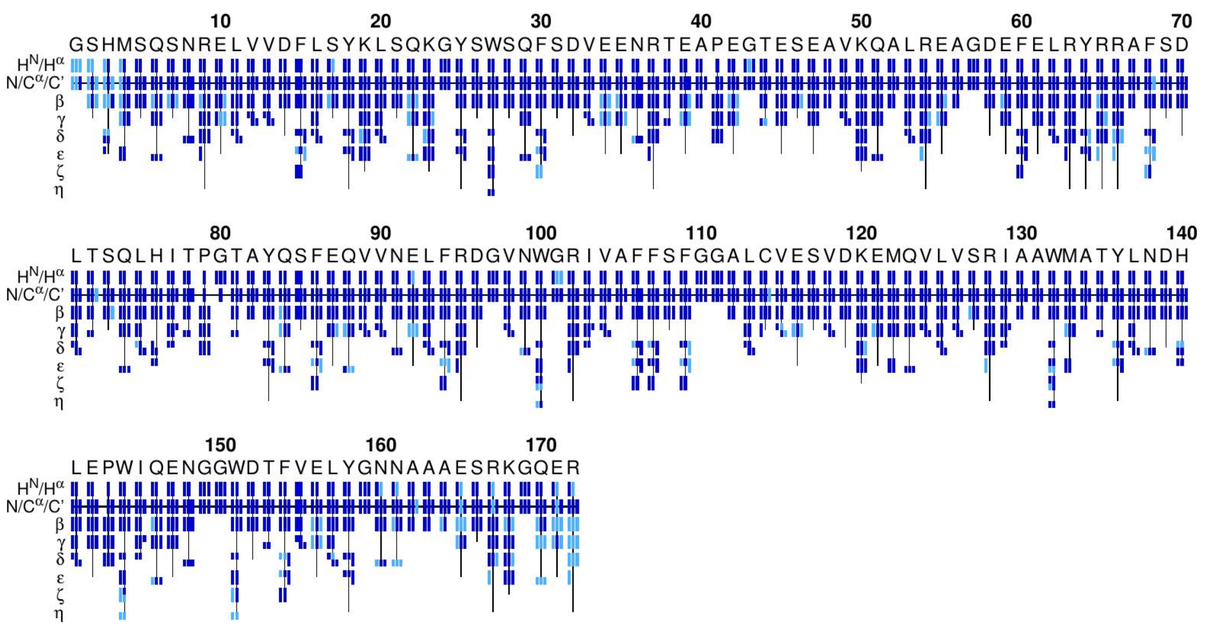


Fig. 2: Example of an automated assignment result succeeding fully automated peak picking

3D Structure Calculation

3D Structure determination using NMR is very often turned towards when proteins or other biomolecules cannot be crystallized or, more likely nowadays, AI based predictions are questioned and have to be verified or refined. The task however is time-consuming and often requires an expert with experience in the required software packages.

The ARTINA structure determination application implements end-to-end protein structure solving. Given a set of spectra and a protein sequence as input, the application generates the abovementioned peak lists and assignments, followed by a fully automated structure calculation using CYANA[5].

ARTINA
structure
determination

New Features

NMRtists now allows for additional input data, most importantly existing structures, such as crystal structures or AlphaFold predictions. Using such a model helps in the assignment process, reducing the number of datasets required.

With a combination of code improvements and infrastructure upgrades, performance could be improved, especially working with large numbers of data sets or when performing structure calculations.

References

1. Klukowski, P., Riek, R. & Güntert, P. NMRtist: an online platform for automated biomolecular NMR spectra analysis, Bioinformatics, 2023.

2. Klukowski, P., Riek, R. & Güntert, P. Rapid protein assignments and structures from raw NMR spectra with the deep learning technique ARTINA (2022). Nature Communications 13, 6151.

3. Klukowski, P., Riek, R. & Güntert, P. Time-optimized protein NMR assignment with an integrative deep learning approach using AlphaFold and chemical shift prediction, Science Advances, 2023.

4. Schmidt, E., & Güntert, P. (2012). A new algorithm for reliable and general NMR resonance assignment. Journal of the American Chemical Society, 134, 12817-12829.

5. Güntert, P. & Buchner, L. (2015). Combined automated NOE assignment and structure calculation with CYANA. J. Biomol. NMR 62, 453-471.

From spectra to assignment and structures

- Cloud based, AI supported software platform
- Fully automated peak picking of multidimensional NMR spectra
- Performs resonance assignment, thereby simplifying the most time-consuming task in biomolecular NMR
- Fully automated structure determination
- High performance, secure cloud architecture
- **Try it now:** Sign up on *nmrtist.bruker.com* and enjoy free testing for a limited time