

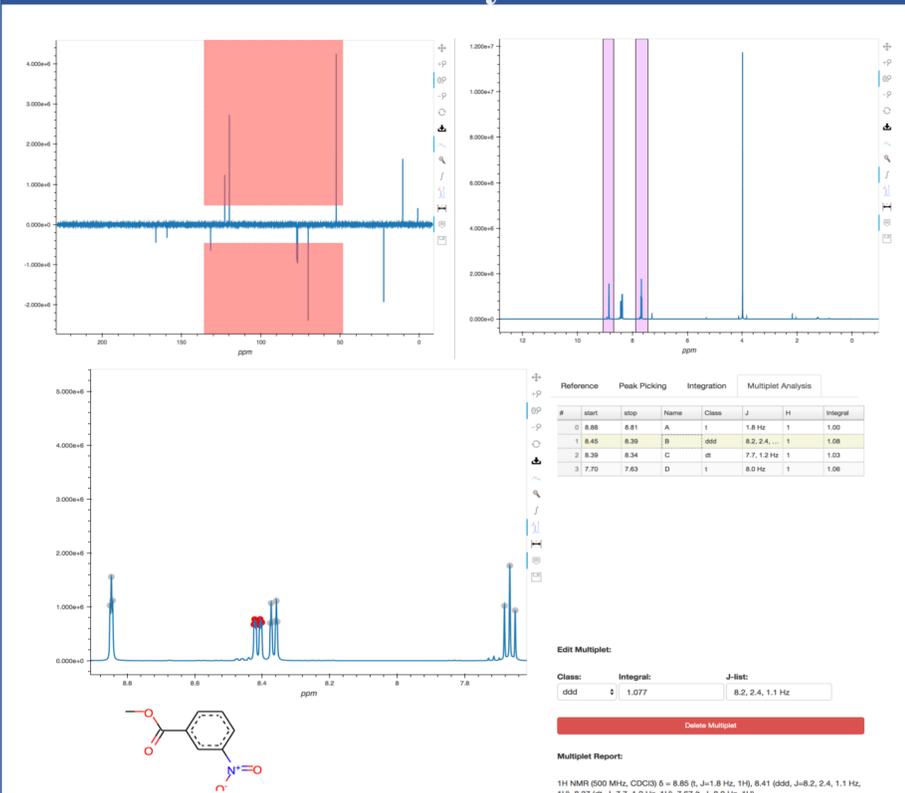
Exploration of Data Enrichment and Data Search Mechanisms for NMR Spectra via Spectrum Analysis

Michalis Psalios (mp236@) and Prof Simon Dobson (Supervisor)

Abstract

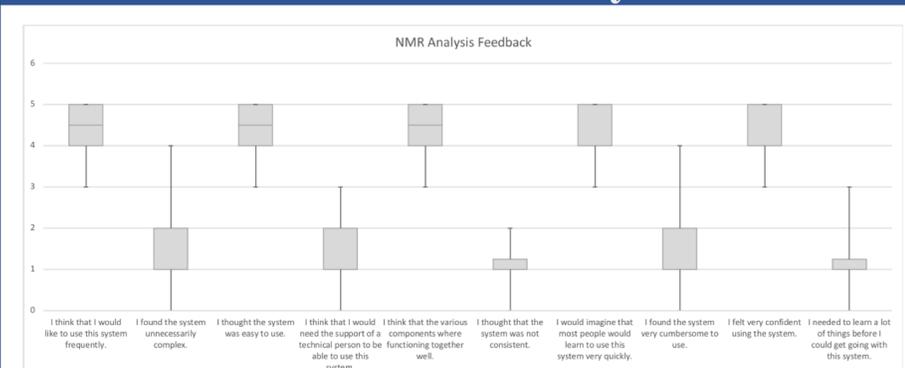
The vast amount of data in scientific research has increased the need for a reliable management system that allows people to store and search data effectively. NOMAD provides a fast and secure data store which allows users to search NMR data based on various metadata. This project extends the functionality of the NOMAD system and enhances data search based on the actual experiment data.

NMR Analysis Tool



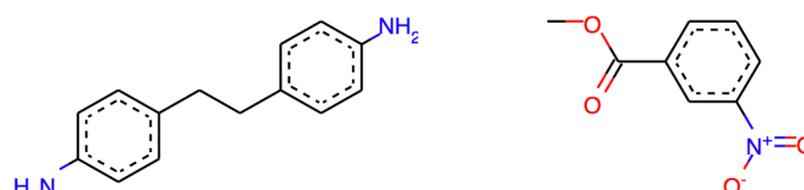
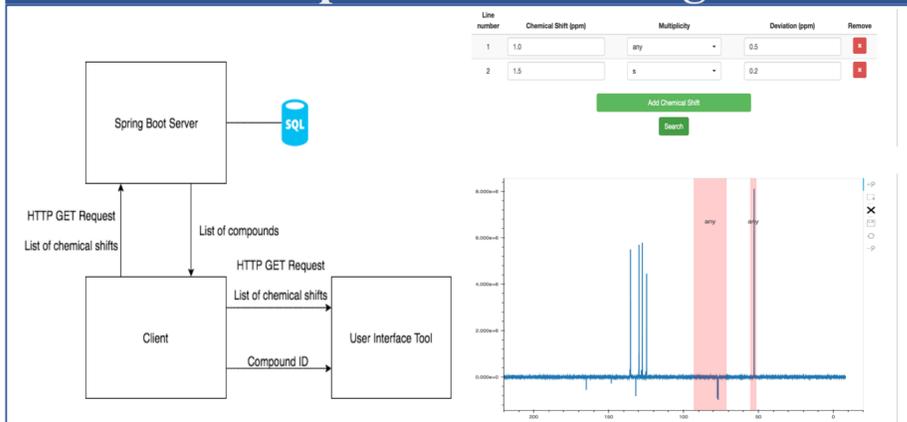
- Perform peak picking on spectrum data
- Determine integral intensity of peaks
- Classify multiplet information from NMR spectra
- Generate multiplet report required for publications

User-Case Study



- Positive feedback from users
- “Excellent” usability and user experience based on SUS [1] (System Scale Usability) questionnaire

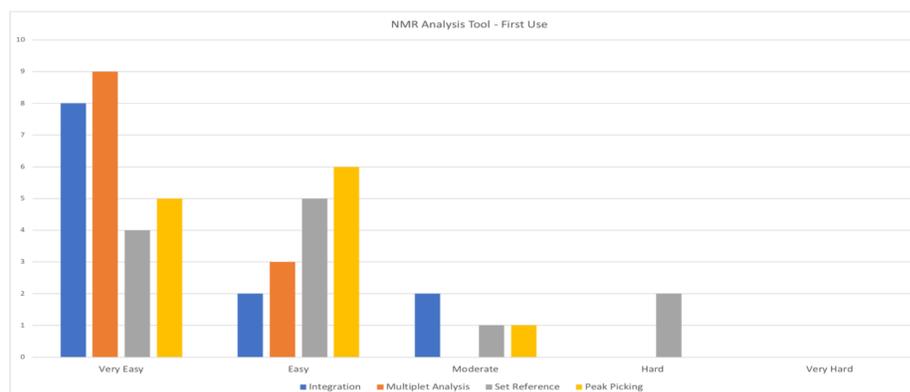
NMR Spectra Search Engine



- Search based on peaks' chemical properties using the information acquired by the NMR analysis tool
- Simple traditional user interface (UI) allows users to manually enter the input parameters.
- UI tool provides a simple, fast way to search for NMR spectra

Contributions

- An open-source tool to perform analysis of NMR data
- A search engine to search NMR data based on their multiplet information
- Novel user interface design for entering input parameters.



Conclusions and Future Work

This project implements an NMR Analysis Tool and an NMR Spectra Search Engine based on multiplet information.

The system is planned to be integrated with the NOMAD system. After integration with NOMAD, the database of NMR analysis data will increase significantly. A study on how the search engine scales with the number of classified spectra must be conducted to analyse the performance of the engine.

References:

1. Brooke, J. (1996). SUS-A quick and dirty usability scale. *Usability evaluation in industry*, 189(194), 4-7.