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Rowan-BMS Collaboration

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Rowan – BMS Research Collaboration

Rowan Team:

- Randolph Bushman and Mark Vadeika (NMR Data Analysis)
- Christopher Lange and Brett Amberge (Laboratory Information Management System)
- Thomas Keane and Mathew Fiduk (NLP Models and Named Entity Recognition for the Autonomous Processing of Text Corpora)
- Dominick Profico, Izhar Ali, Ben Chau, and Ethan Colby-Witanek (Text Summarization and Processing as Knowledge Graph)
- Dr. Vasil Hnatyshin (Department Head – Computer Science, Student Advisor)

BMS Team:

- Dr. Serhiy Hnatyshyn (Scientific Advisor)
- Jan-Lucas Ott (Technical Advisor)



NMR Data Analysis Laboratory Information Management System

- **Nuclear Magnetic Resonance (NMR)**
 - Analysis raw spectrometer data using machine learning techniques
 - LeNet-5 Deep Neural Network that classification of peak shapes (tested using amino acids data)
 - Multithreaded environment with GUI written using WXPYthon
- **Laboratory Information Management System**
 - Web-based software to support the drug discovery
 - Developed parser to display raw data in meaningful format
 - Front end web components with CRUD (Create, Read, Update, Delete) capabilities
 - Database design for data storage
 - Scripts to facilitate automatic testing when new changes are pushed on Git

The screenshot displays the DeconvTotal software interface. The top window shows an NMR spectrum plot with 'new experiment' data and several deconvoluted peaks. The plot includes a legend for 'Experiment Spectrum' and 'Deconvoluted Peak 0' through 'Deconvoluted Peak 15'. Below the plot is a console window with statistical data: 'reduced chi-square = 2.7912e+10', 'Akaike info crit = 7531.36402', and 'Bayesian info crit = 7542.60263'. It also lists peak parameters such as 'peak15Amplitude: 30621.3431 +/- 541.596241 (1.77%)' and 'peak15Height: 2588128.33 +/- 29779.8651 (1.15%)'. A message at the bottom states 'Peak deconvolution was successful!'.

The bottom window is a web-based 'Assay List' interface. It features a search bar, a 'Show 10 entries' dropdown, and a table with columns for 'Status', 'Assay Name', and 'Functions'. The table lists three entries: 'PK', 'PD', and 'Massspec', each with a checkmark in the status column and three function icons (green, blue, orange). Below the table, there are input fields for 'Program' (containing 'Program1'), 'BMS Program ID' (containing '123456'), and a 'CREATE PROGRAM' button.

