



Denver

CHEMISTRY

Fall 2021

Seminar Series



11am-12pm

Aug. 27th

Via [Zoom](#)

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Buenos Aires, Argentina

“NMR Metabolomics Based on Multiplets
(Getting the most out of JRES spectra)”

Our group has come up with a simple, yet powerful solution to deal with the peak overlap issue on 1D ^1H NMR-based metabolomic studies, which causes challenges on any statistical analysis performed on the data. By executing the statistical analysis on the 2D JRES spectral set and later projecting the nontilted spectrum, which results in a trace that mimics a CPMG experiment, the output can be queried with existing 1D ^1H databases. In addition, we created the Chemical Shift Multiplet DataBase (CSMDB), which allows queries from the full JRES spectrum by searching the chemical shift on the f2 projections and matching the multiplets on the f1 traces for increased confidence. Moreover, biological correlation arising from either statistical total correlation spectroscopy (STOCSY) or multivariate data analyses (MVDA) is readily evaluated by examining the unmatched peaks on the original query. This “Consecutive Queries” feature reveals biological connections among metabolites appearing in the same spectral trace, integrating the recovery of biological information with metabolite identification. Lastly, cases of misaligned JRES spectra are processed by matching f1 traces among the spectra and building a correspondence table, which can be then subjected to statistical analyses and the results later queried with CSMDB as well.