St. Olaf College NMR Laboratory

# Putting it all together: Fully automated NMR spectrometer, web-based analysis, and spectral simulation with 2D/3D structure correlation for first-year organic chemistry

Robert M. Hanson

St. Olaf College, Northfield, MN

http://www.stolaf.edu/people/hansonr

SMASH 2019/NMReData symposium, Sept. 26, 2019

St. Olaf College NMR Laboratory

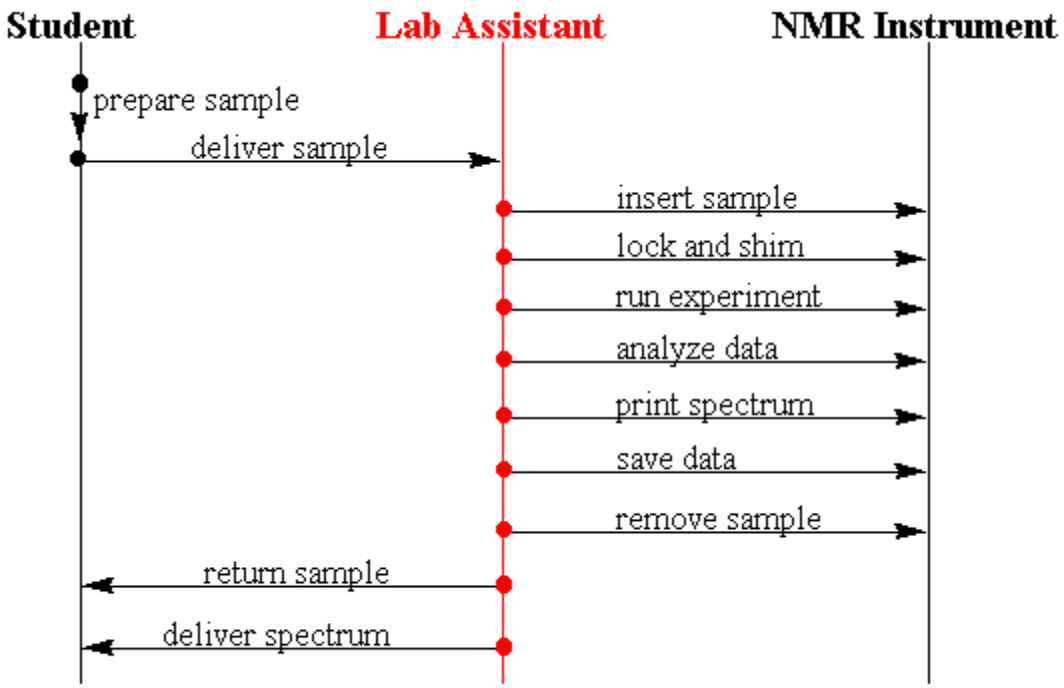
Part I: The instrument and interface

Part II: Analysis involving JSME, JSpecView, NIH/chemical resolver, and nmrDB

# St. Olaf College NMR Laboratory

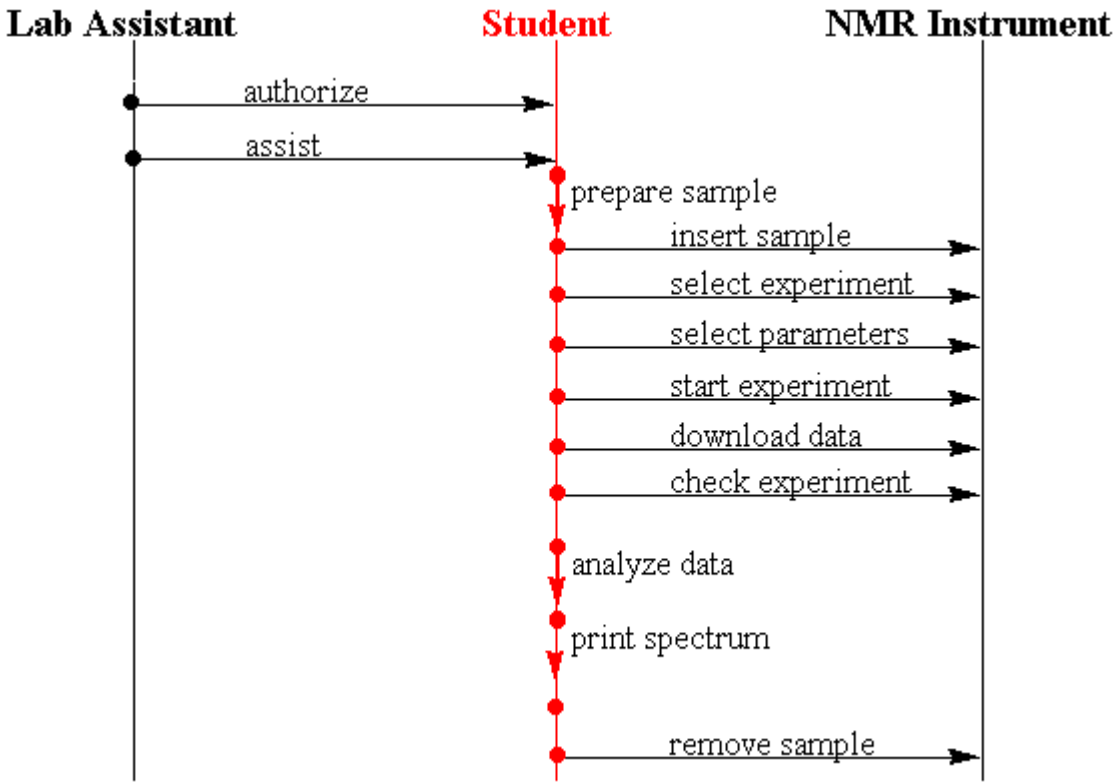
Instrumentation: Bruker 400 MHz Avance III spectrometer
with 120-position BACS autosampler, BSMS-2, GRASP II SmartProbe

# The OLD way…


Student
Lab Assistant
NMR Instrument
prepare sample
deliver sample
insert sample
lock and shim
run experiment
analyze data
print spectrum
save data
remove sample
return sample
deliver spectrum

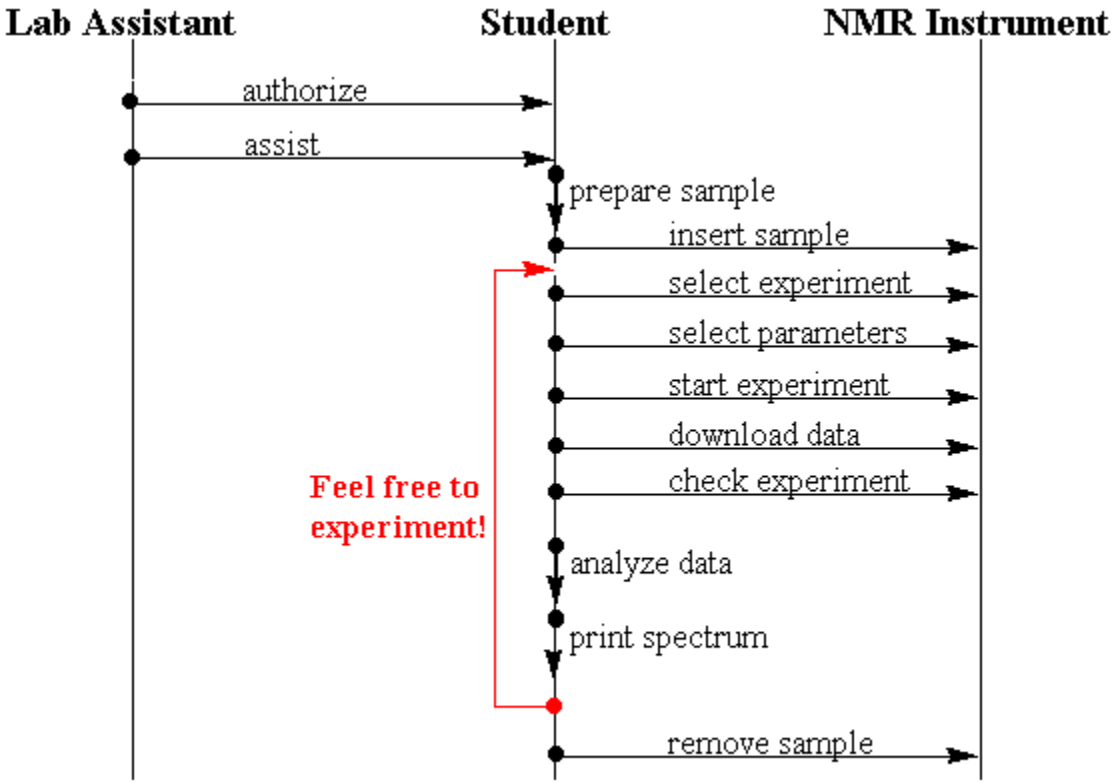
# St. Olaf College NMR Laboratory

…and the new way…



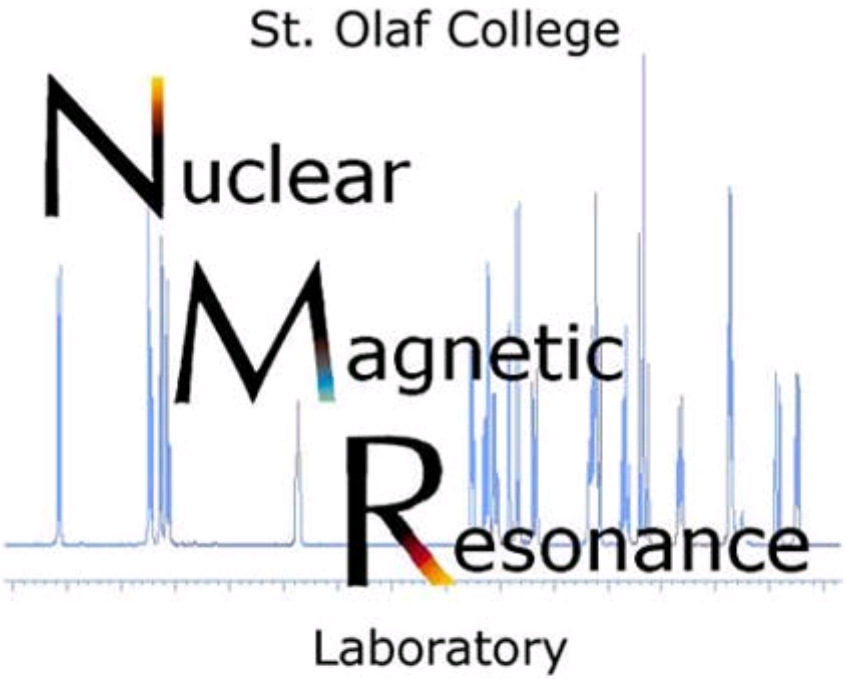
# St. Olaf College NMR Laboratory

…with a twist!



# St. Olaf College NMR Laboratory

https://chemapps.stolaf.edu/nmr




Bruker Avance 400 MHz NMR Spectrometer (on-campus users only)

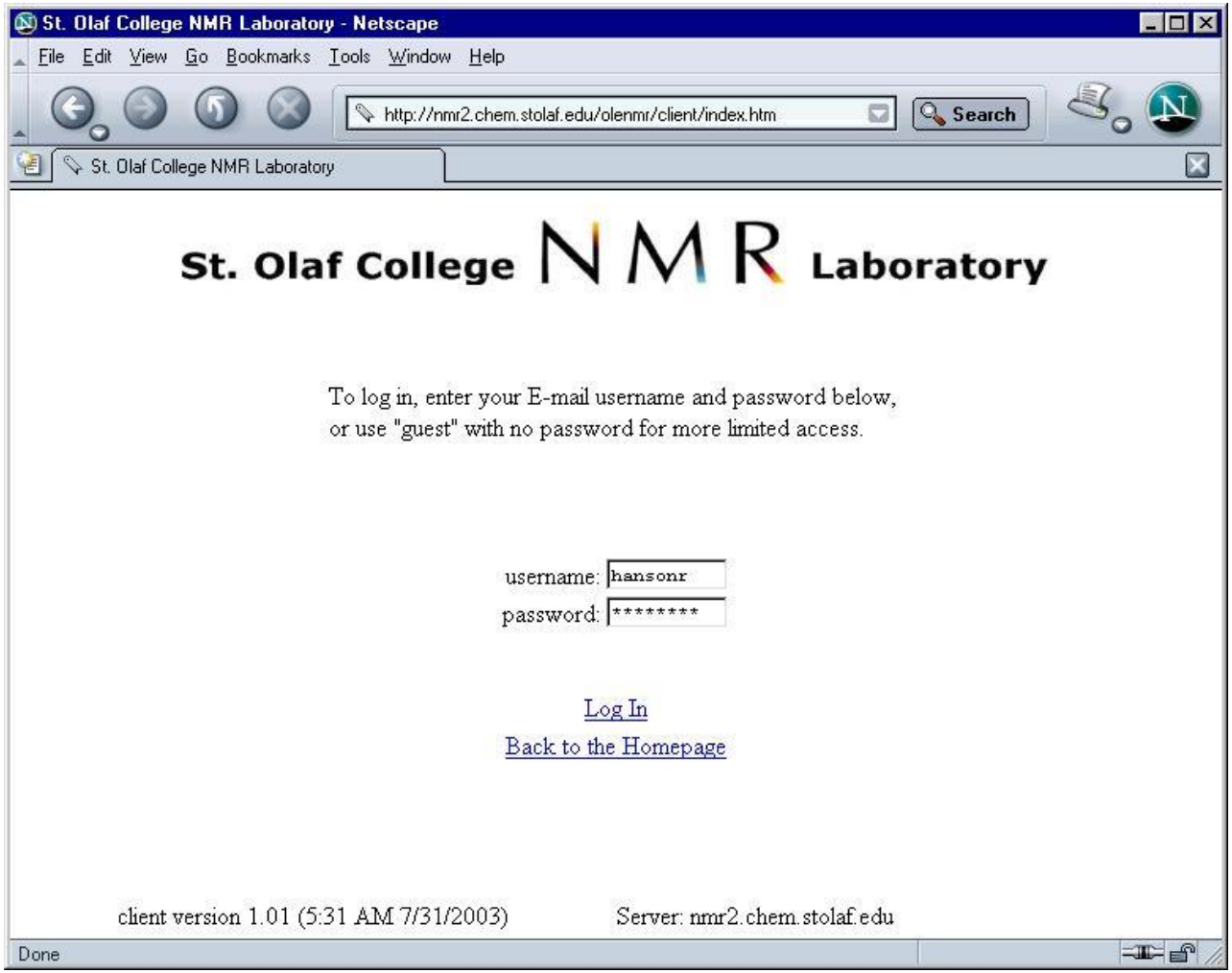
Liquid Helium Level Log  Experiment Status  Holder Status

on/off-campus demo version  Overnight Status (available on/off campus)

Overview  227th ACS National Meeting Presentation

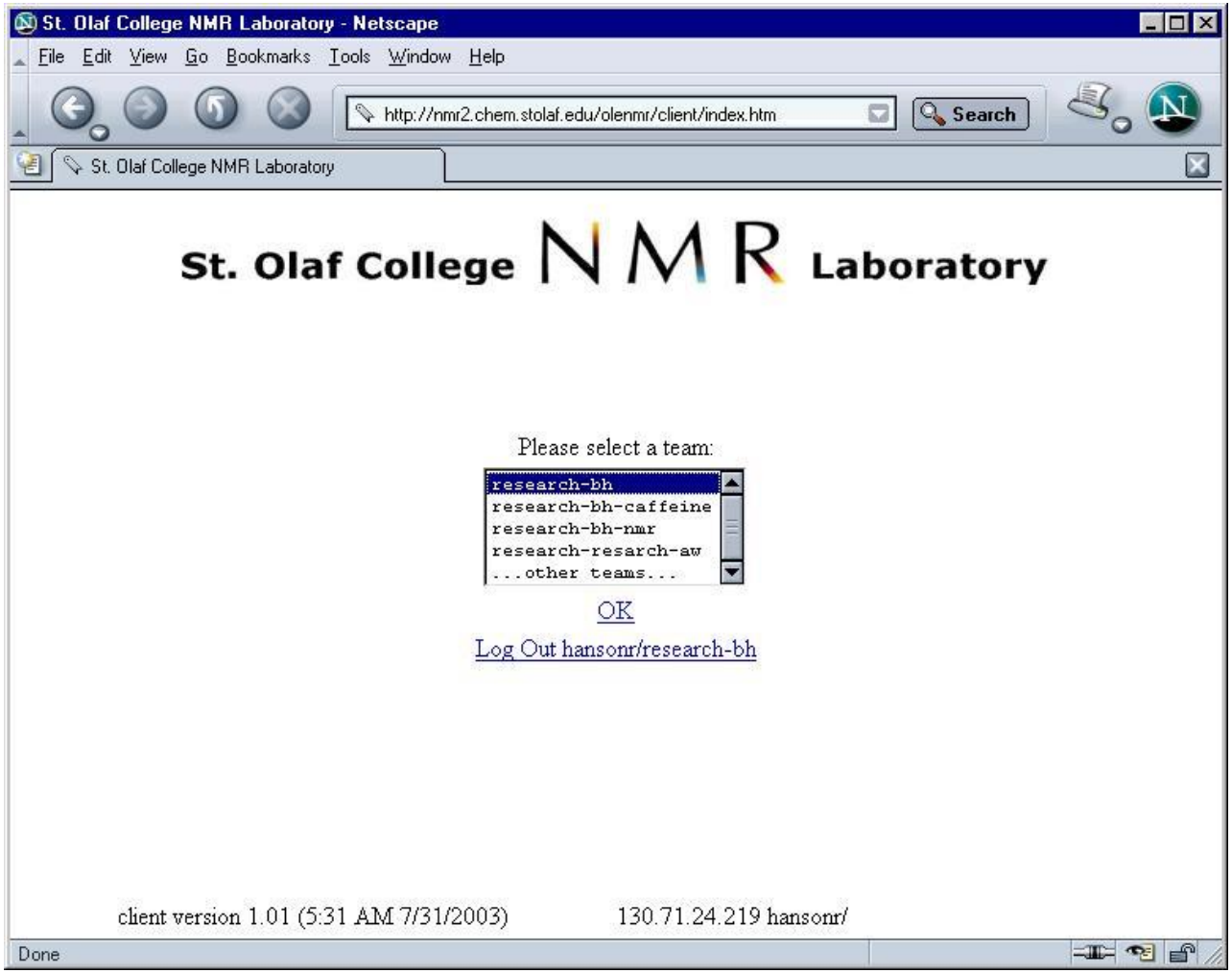
# St. Olaf College NMR Laboratory

Implementation involves “standard” St. Olaf login…



# St. Olaf College NMR Laboratory

Each user is a member of one or more IconNMR “teams”…



# St. Olaf College NMR Laboratory

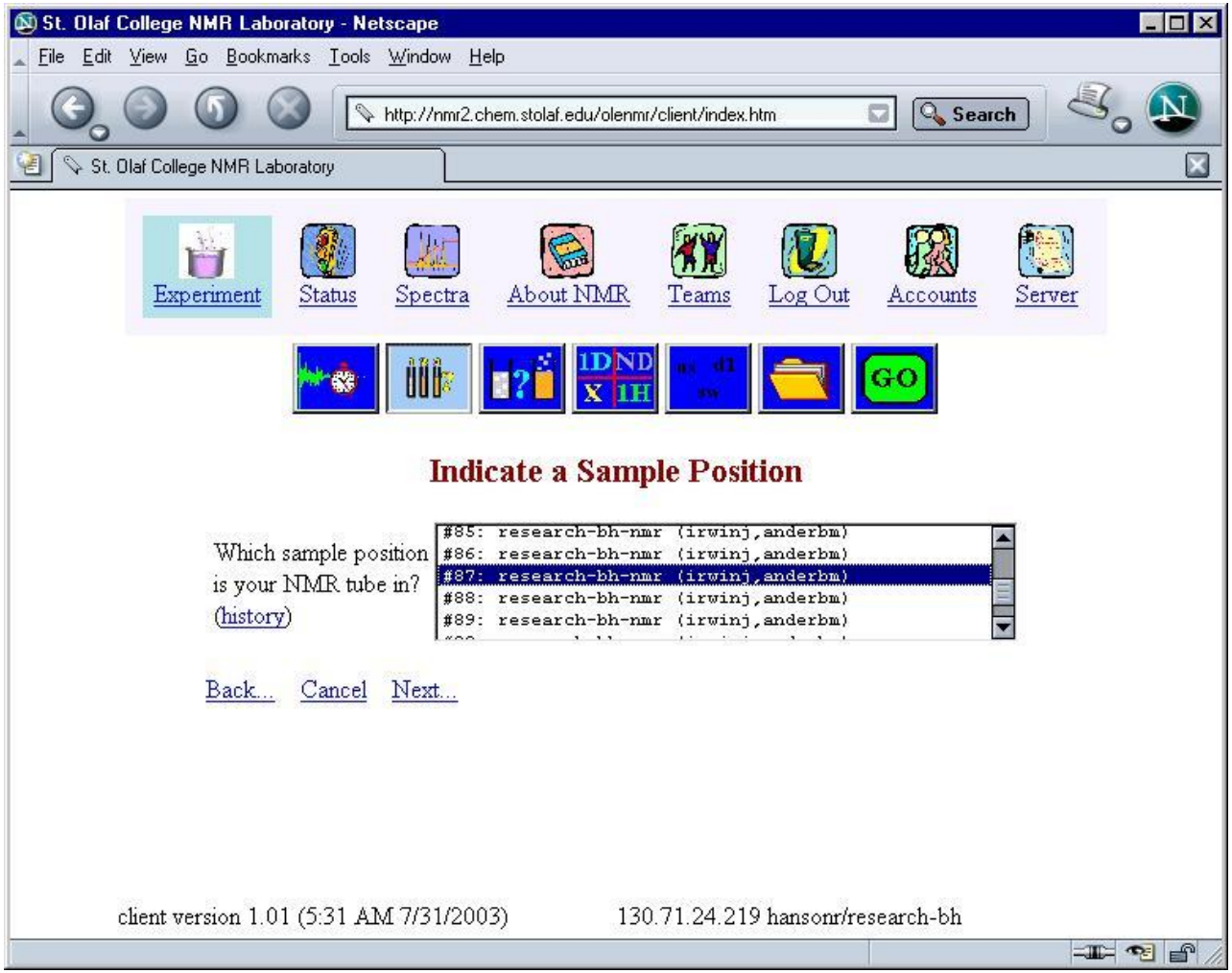
For this simulation we will run an experiment…

# St. Olaf College NMR Laboratory

Initially we see a “current status” screen…

# St. Olaf College NMR Laboratory

One or more sample positions will have been assigned to the team…



# St. Olaf College NMR Laboratory

Solvent options are automatically loaded from the Bruker database…

# St. Olaf College NMR Laboratory

Experiments are drawn from an OleNMR database…

# St. Olaf College NMR Laboratory

Permissions are experiment-based, not *user*-based…

# St. Olaf College NMR Laboratory

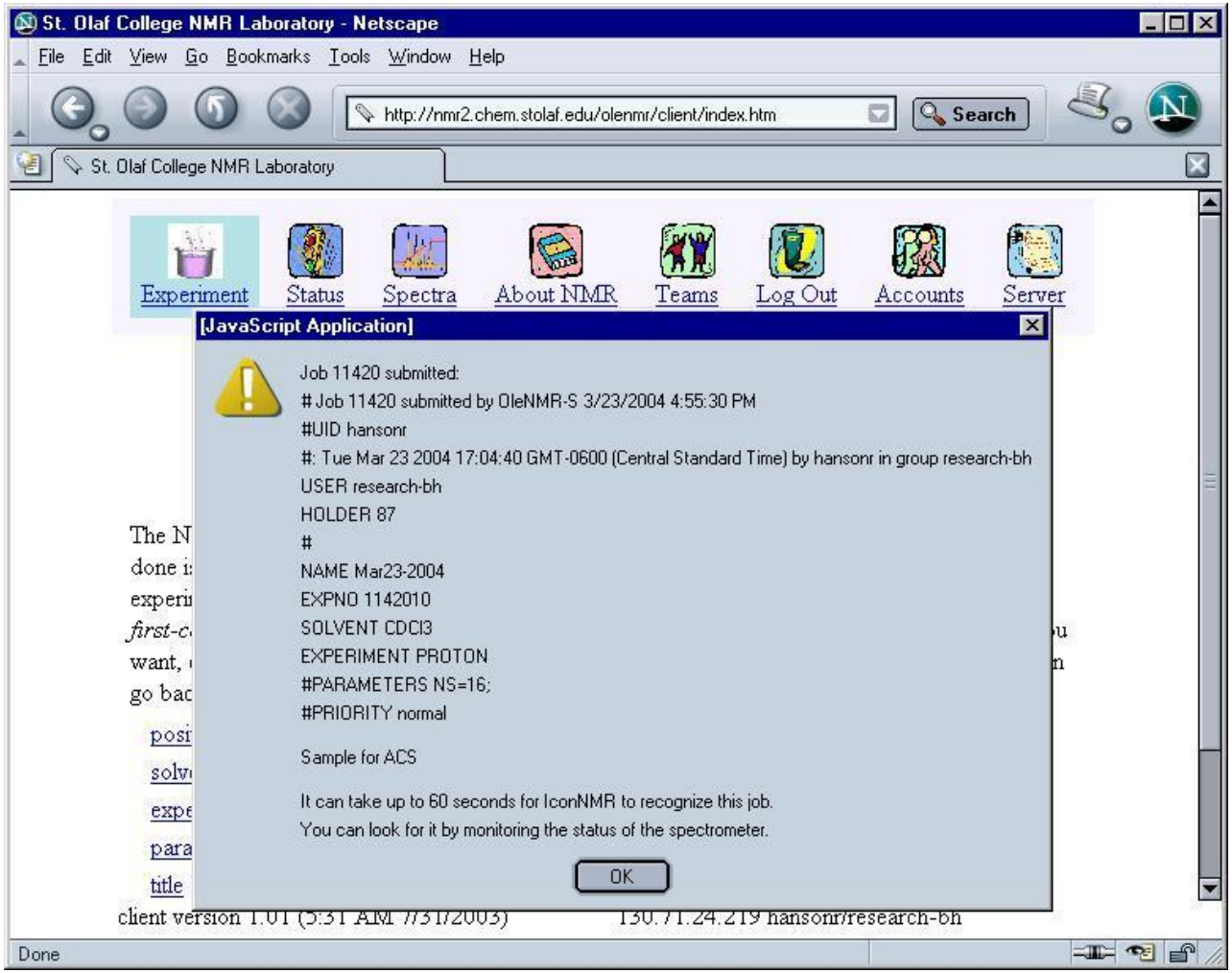
A little instruction to guide novices is on each panel…

# St. Olaf College NMR Laboratory

We designed a “fair queue” that prevents monopolization…

# St. Olaf College NMR Laboratory

A message from the server indicates successful job submission…

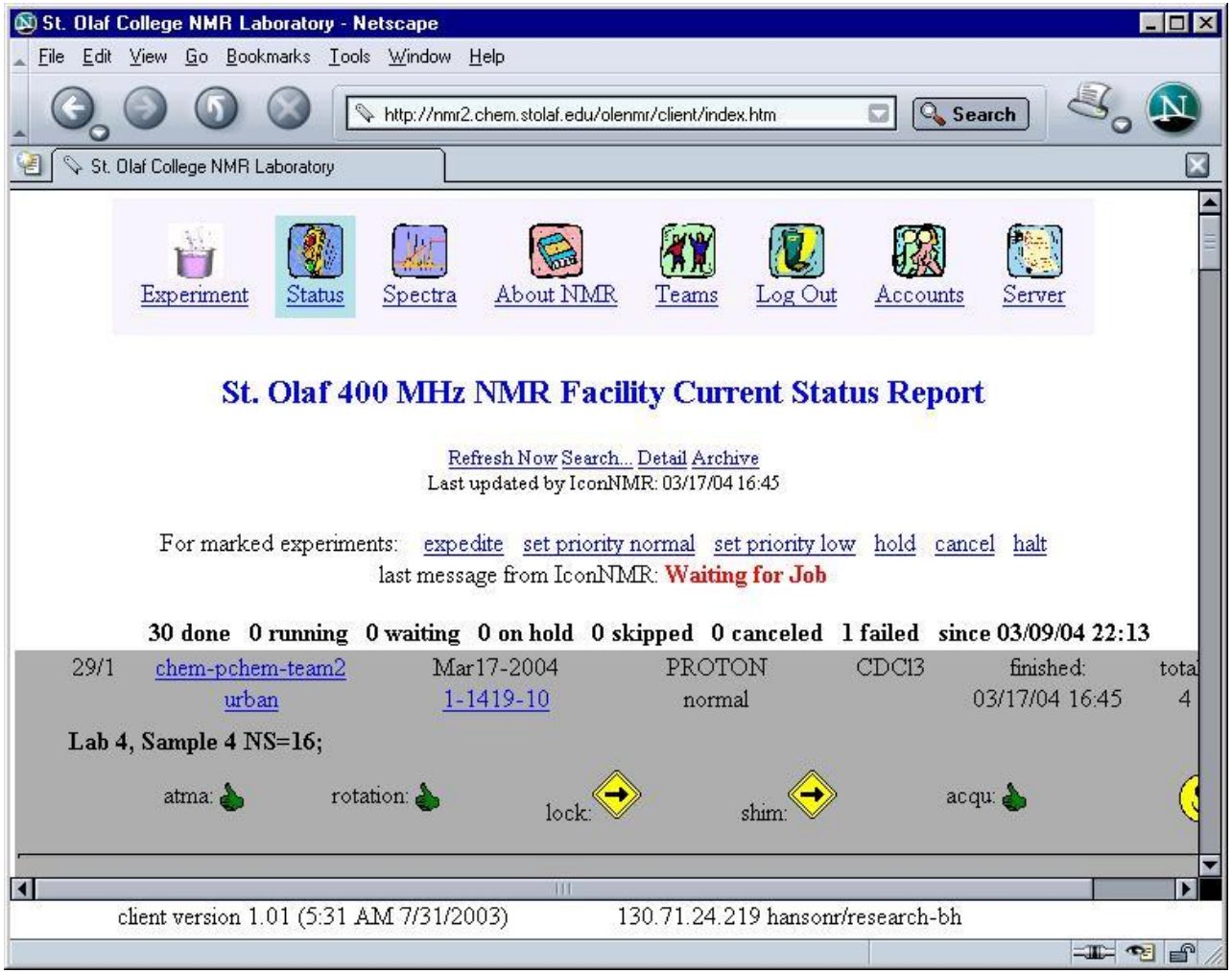


# St. Olaf College NMR Laboratory

OK, the experiment is submitted; now we will view status…

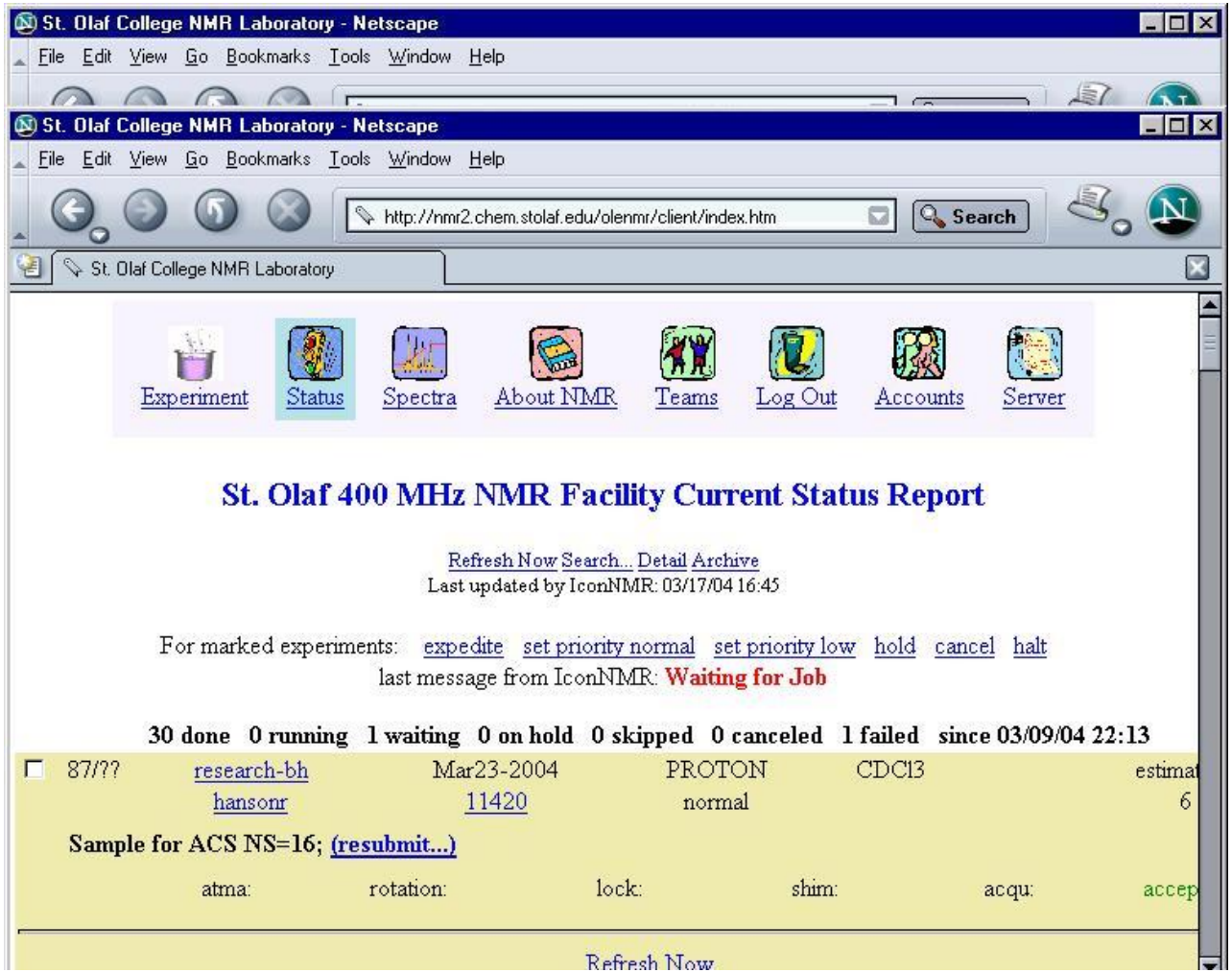
# St. Olaf College NMR Laboratory

This is a running list of active and pending jobs…



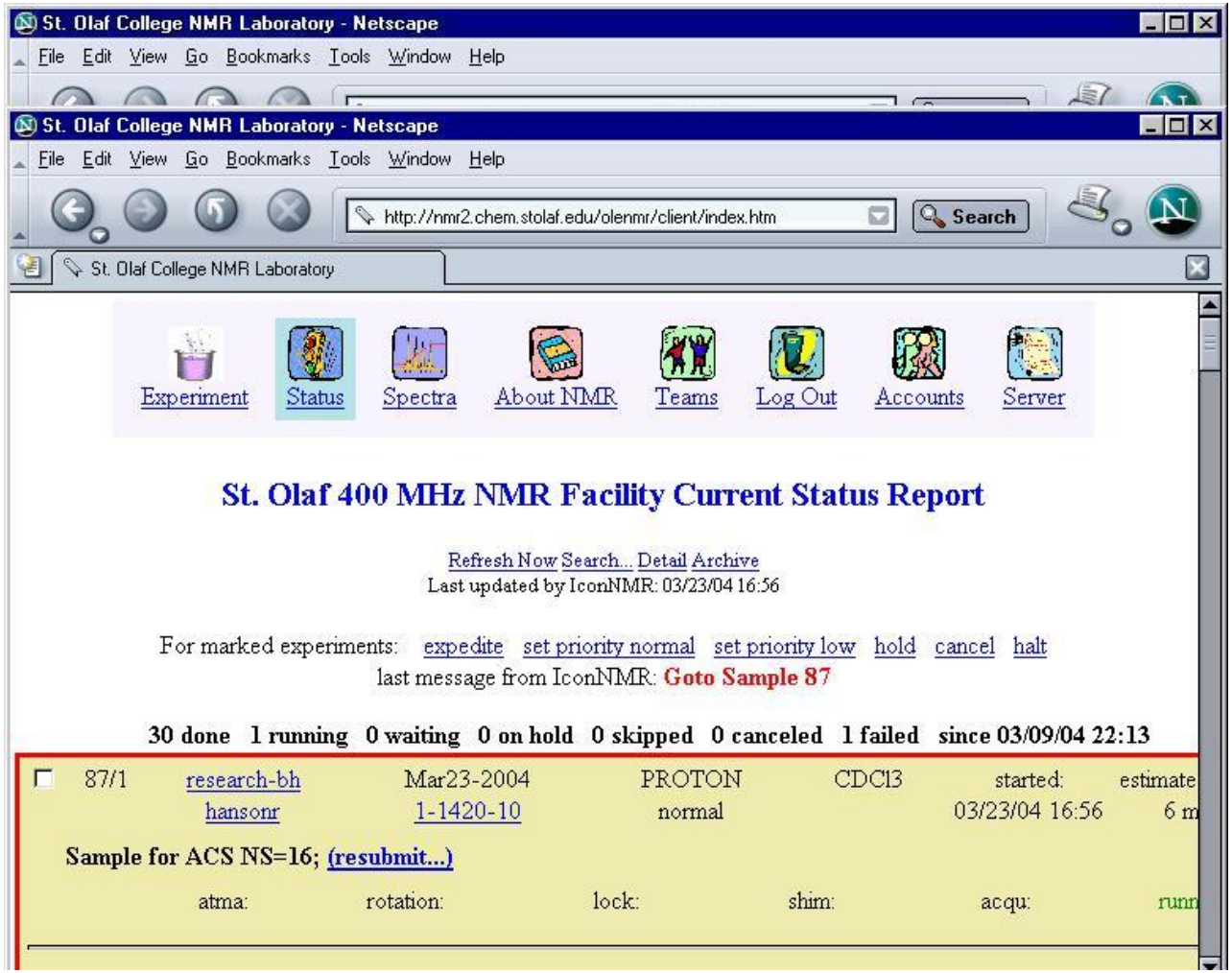
# St. Olaf College NMR Laboratory

Within one minute our job shows up…



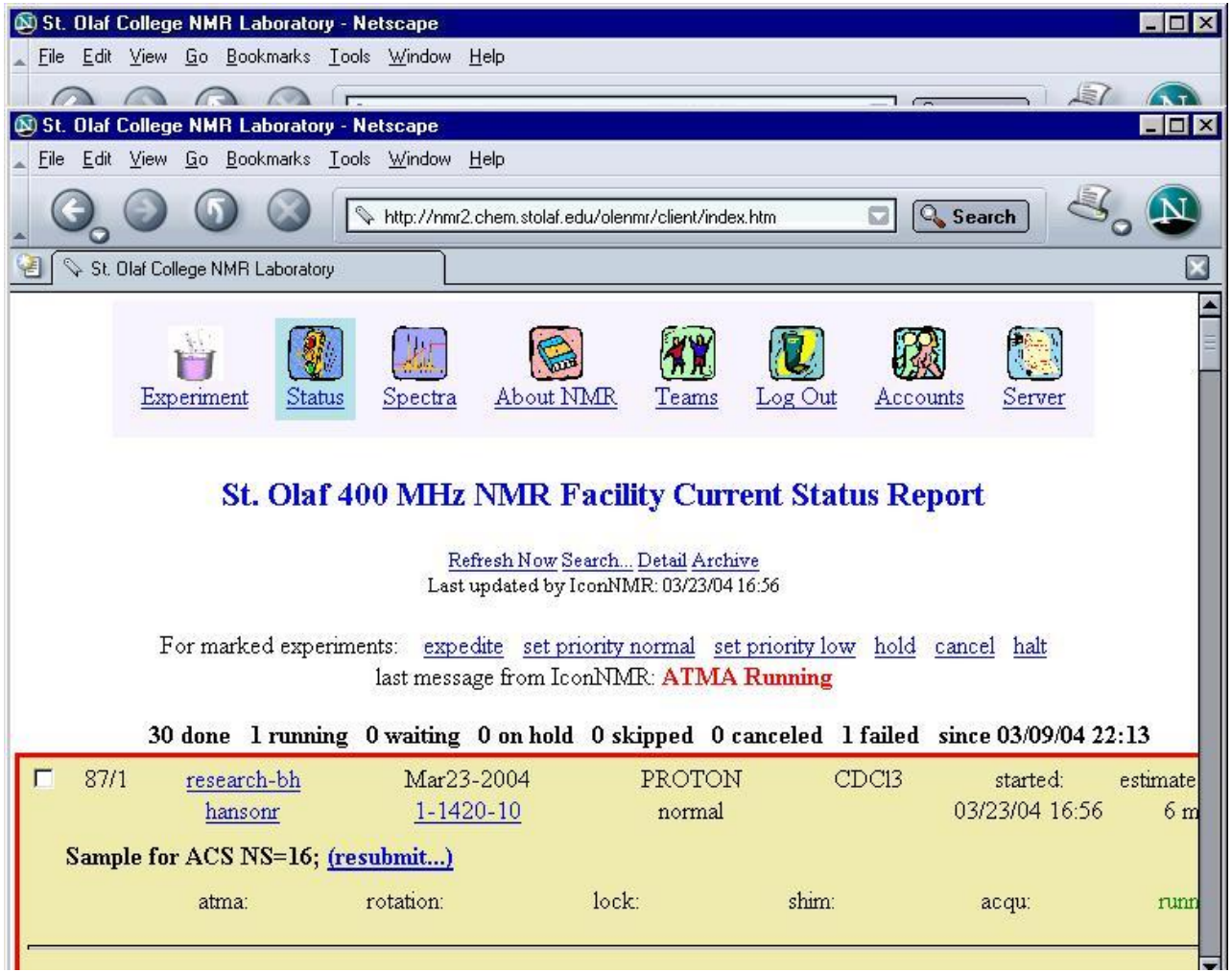
# St. Olaf College NMR Laboratory

The “last message” indicates that our job is active. The robot is working…



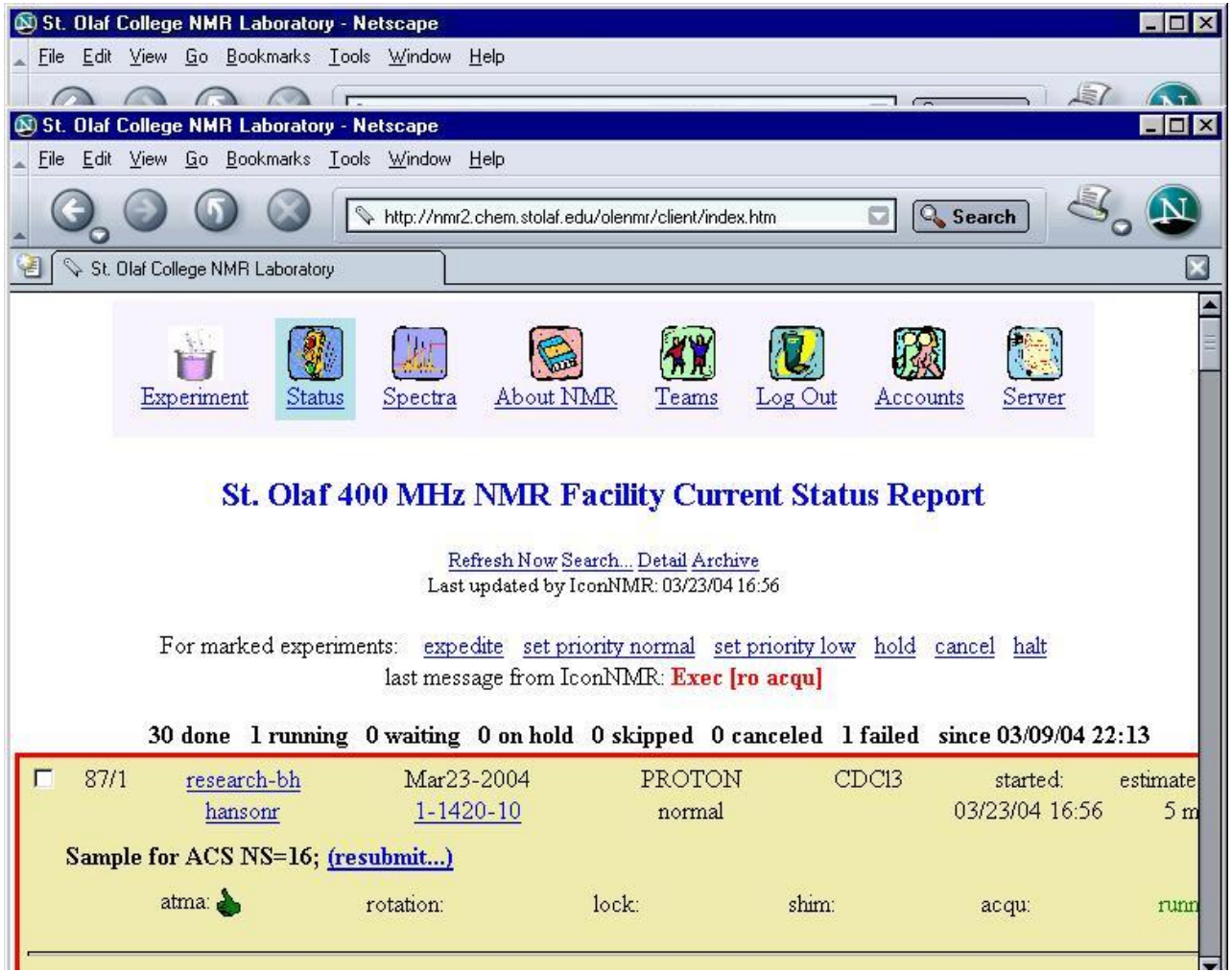
# St. Olaf College NMR Laboratory

Automatic Tuning and Matching is taking care of solvent changes…



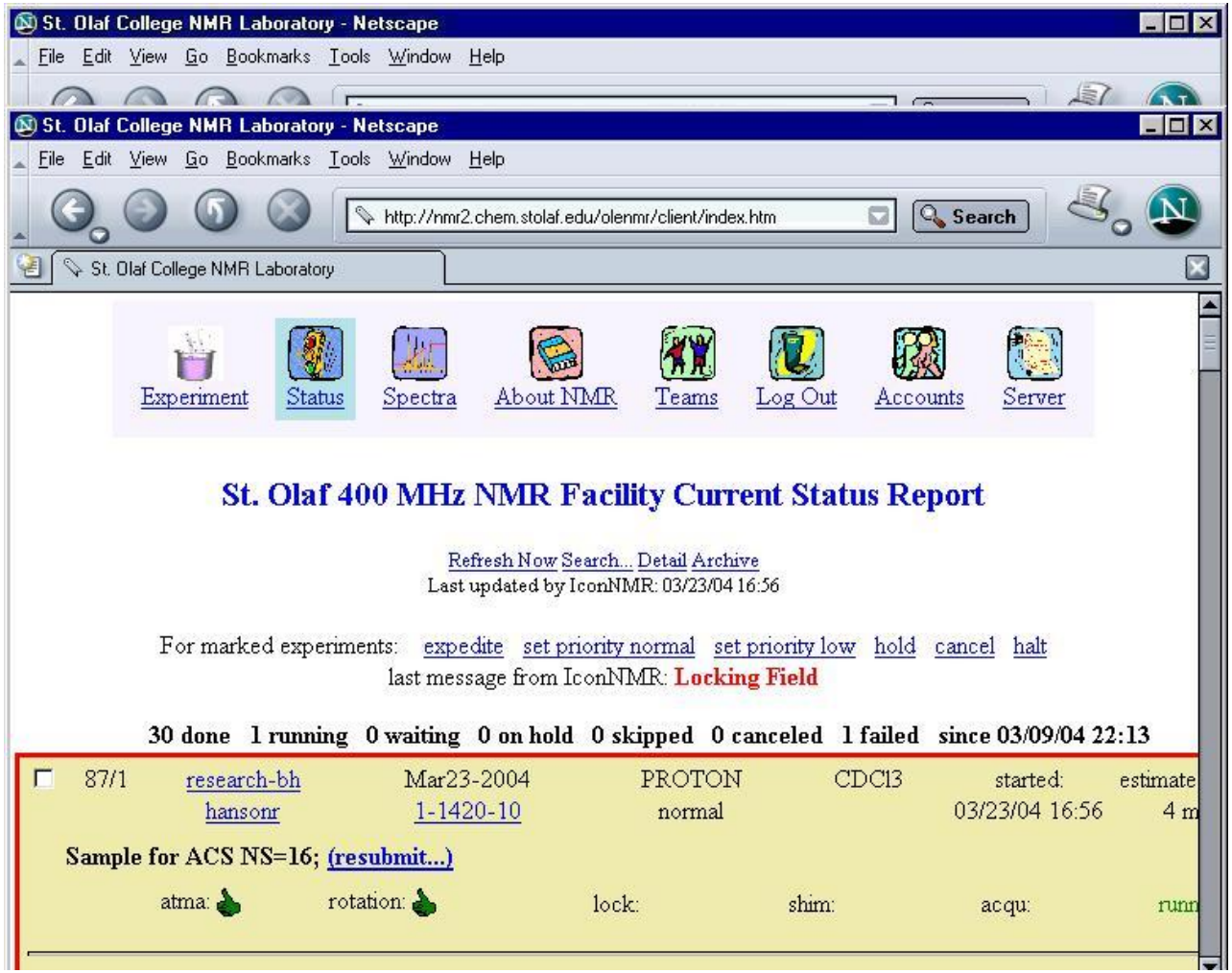
# St. Olaf College NMR Laboratory

The sample is starting to rotate…



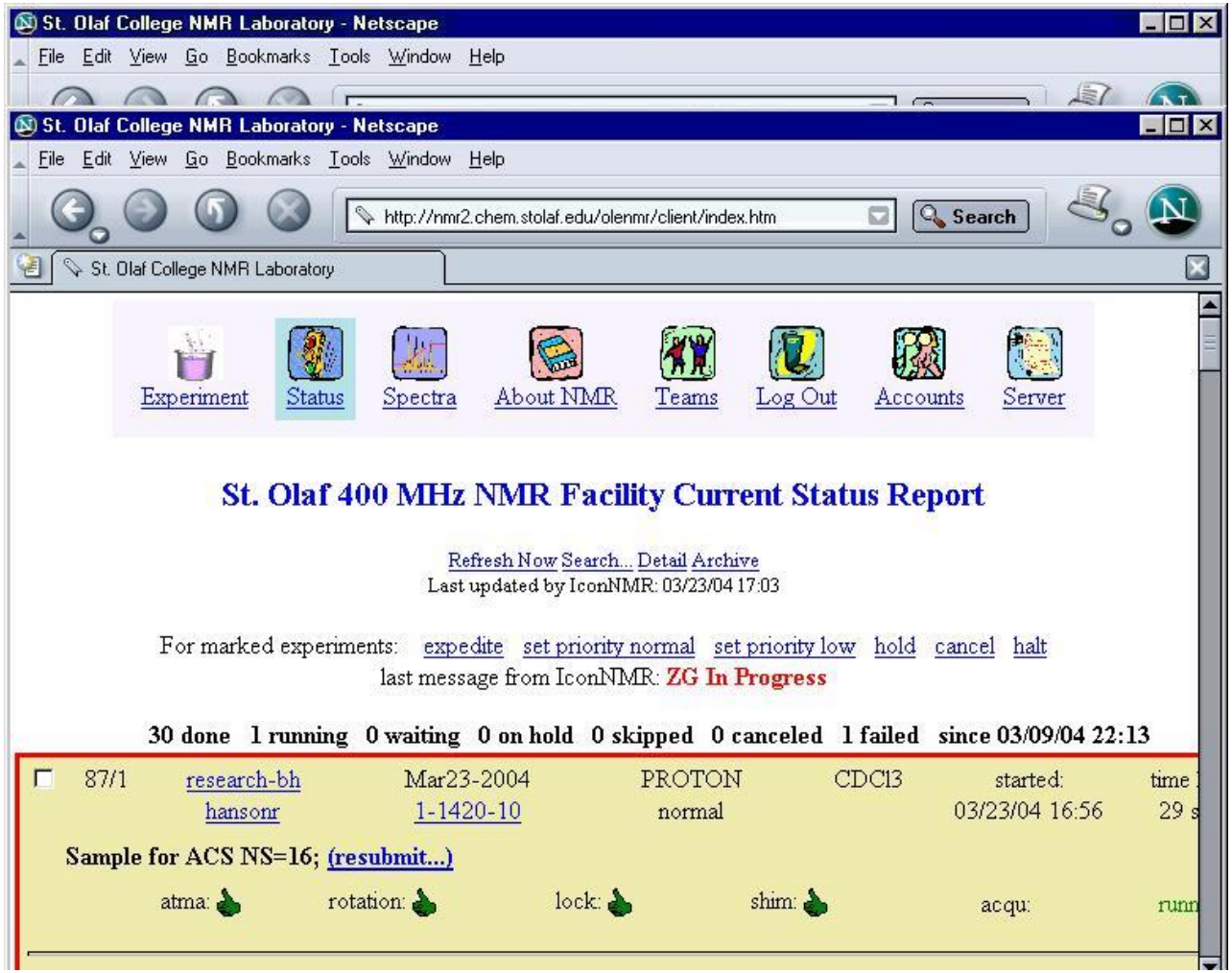
# St. Olaf College NMR Laboratory

the field is locked and shimmed using deuterium gradient shimming…



# St. Olaf College NMR Laboratory

ZG stands for “zero go”; the NMR experiment is now running…



# St. Olaf College NMR Laboratory

Thumbs-up and a happy-face indicates all is well…

# St. Olaf College NMR Laboratory

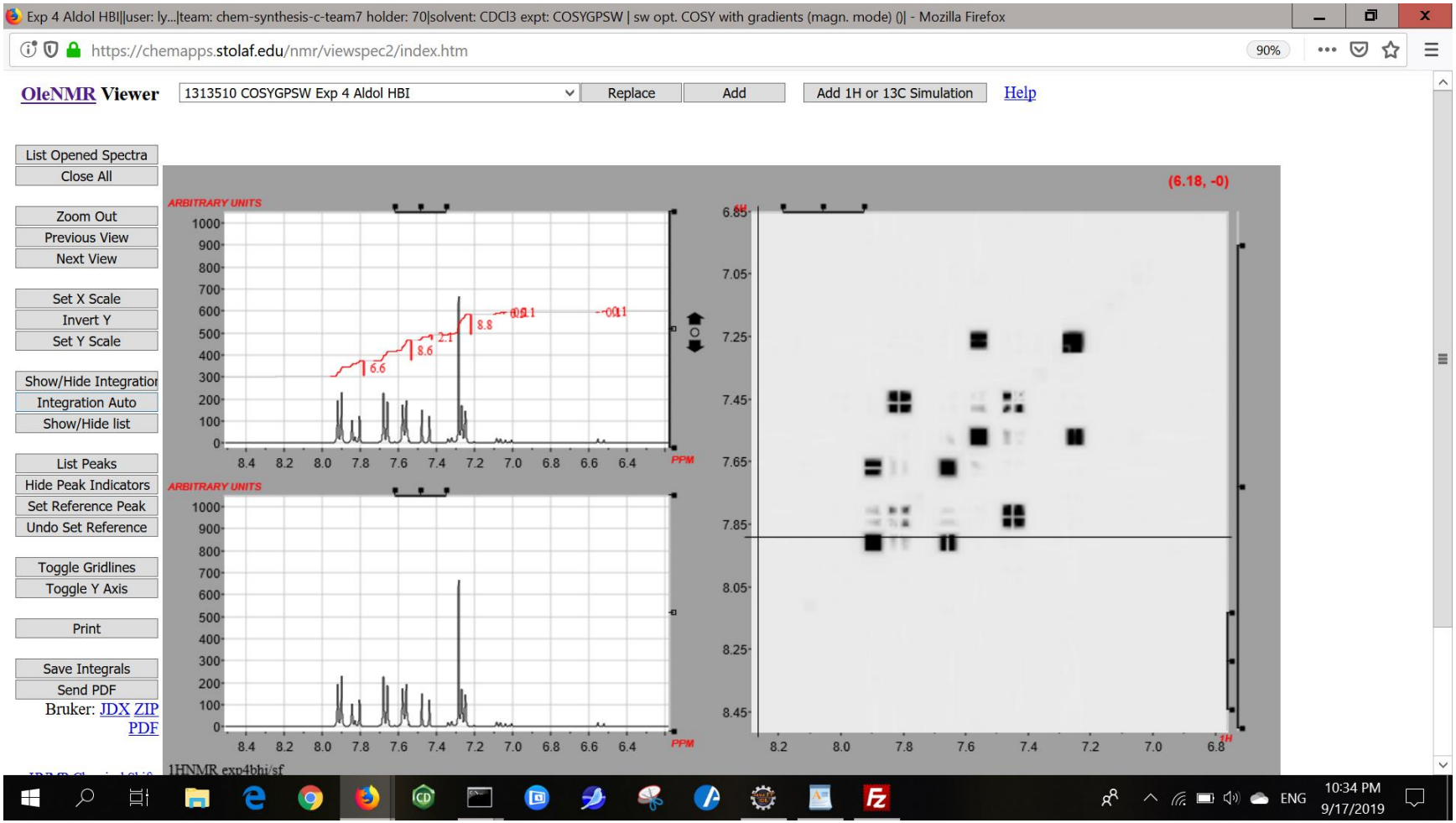
Back to the main interface, we select “view spectra”…

# St. Olaf College NMR Laboratory

There are many options for selecting specific experiments…

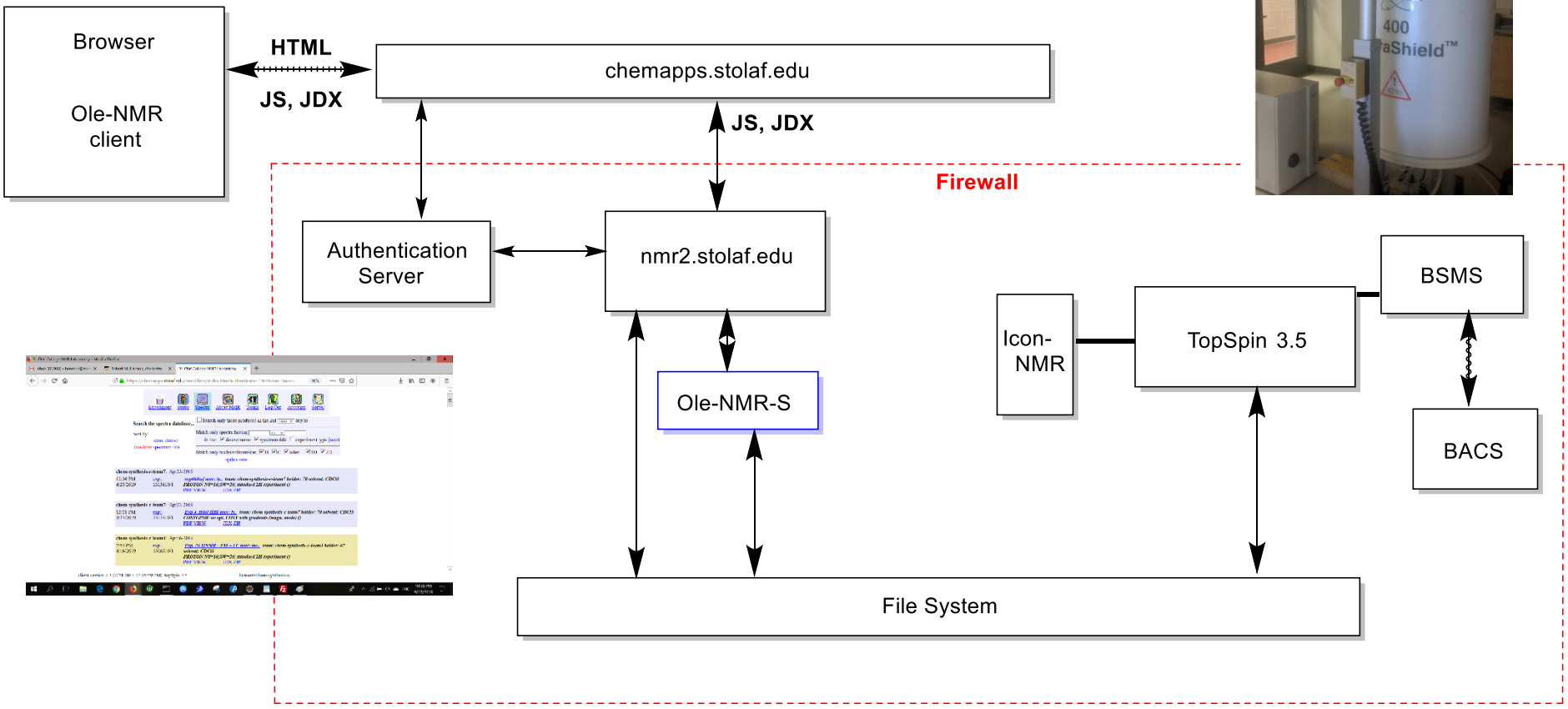
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



St. Olaf College NMR Laboratory

# Ole-NMR/TopSpin Overall Schematic

St. Olaf College NMR Laboratory

Part I: The instrument and interface

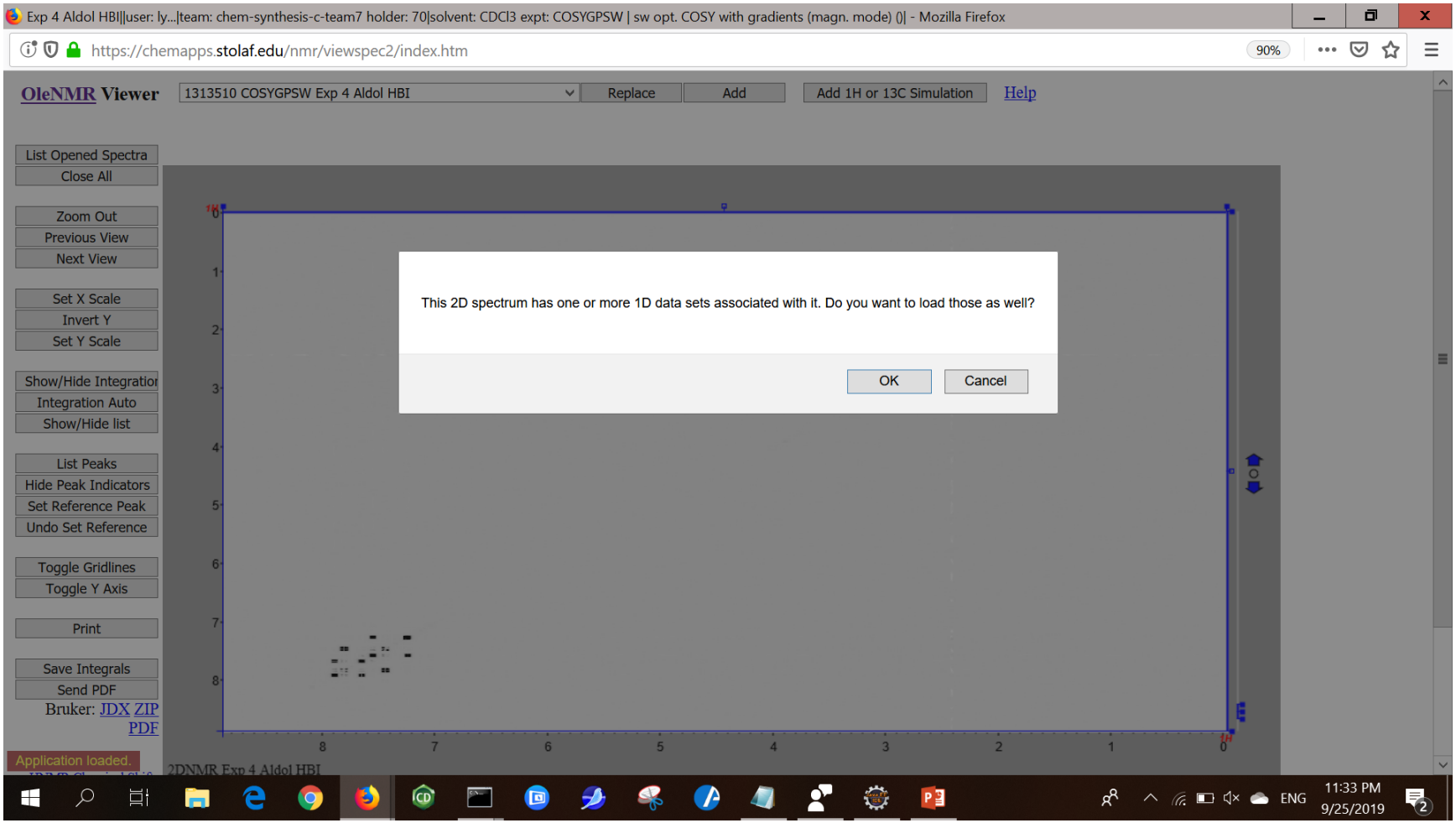
Part II: Analysis Involving JSME, JSpecView, NIH/Chemical Resolver, and nmrDB

# St. Olaf College NMR Laboratory

There are many options for selecting specific experiments…

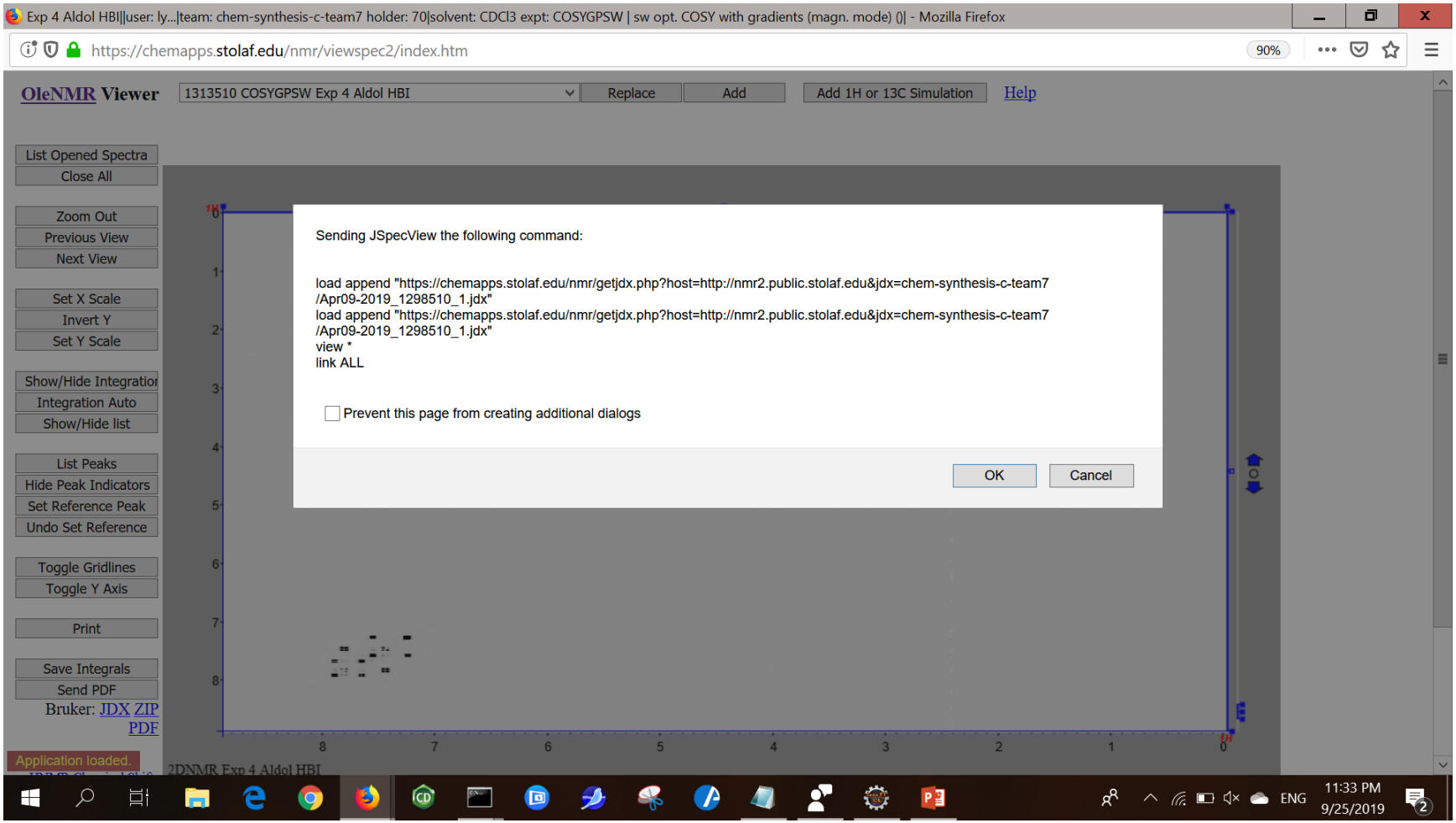
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



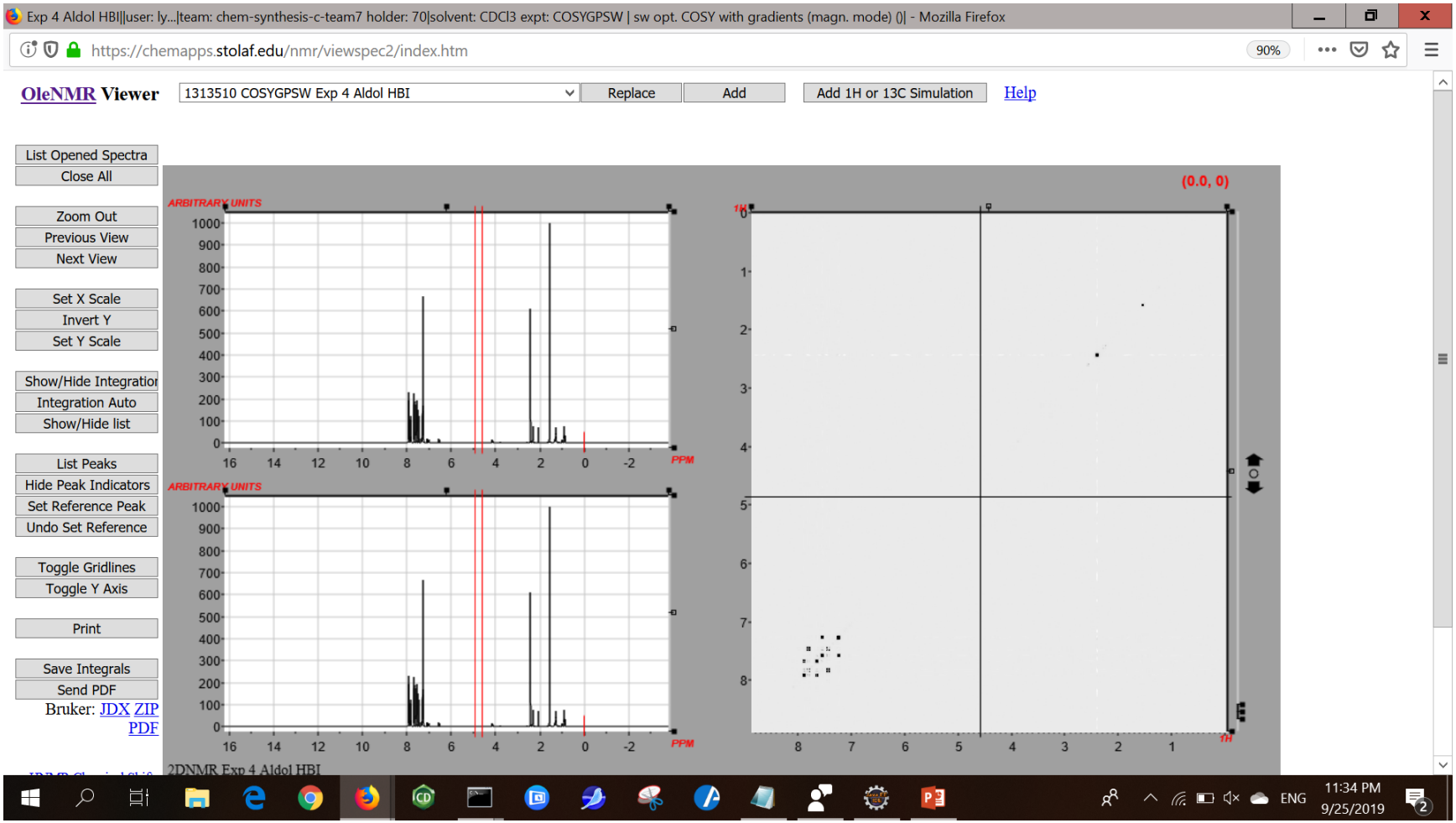
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



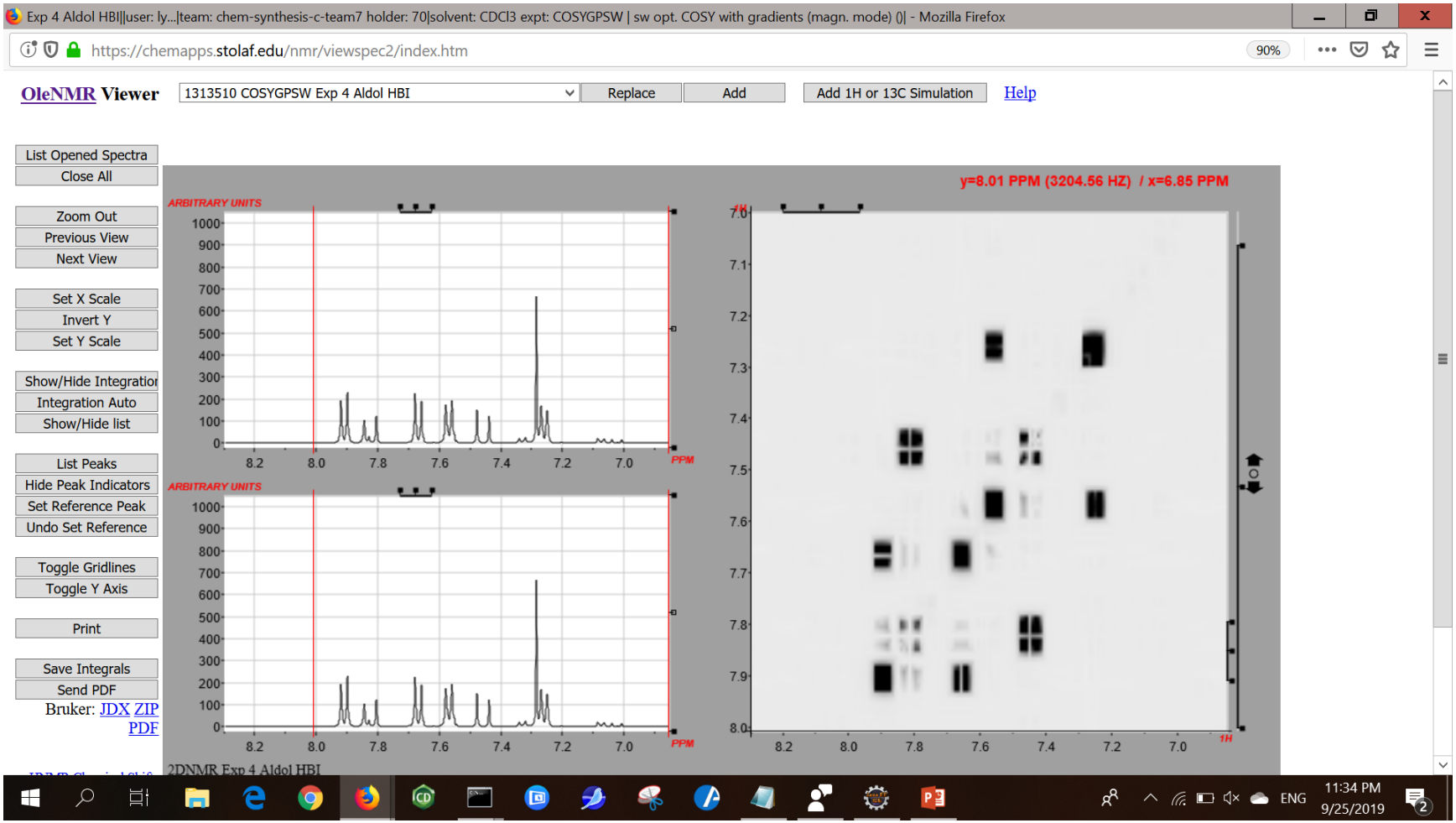
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



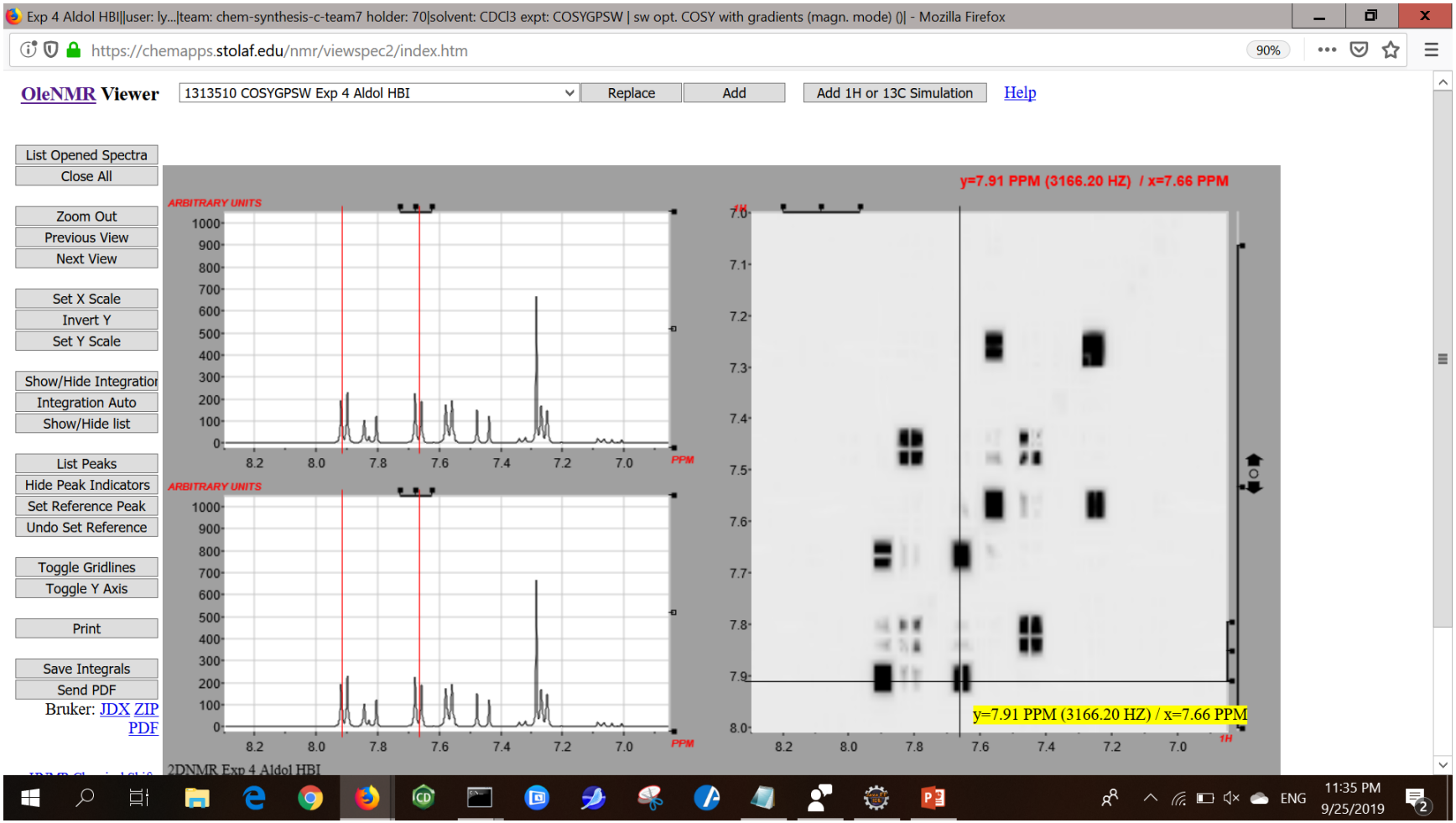
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



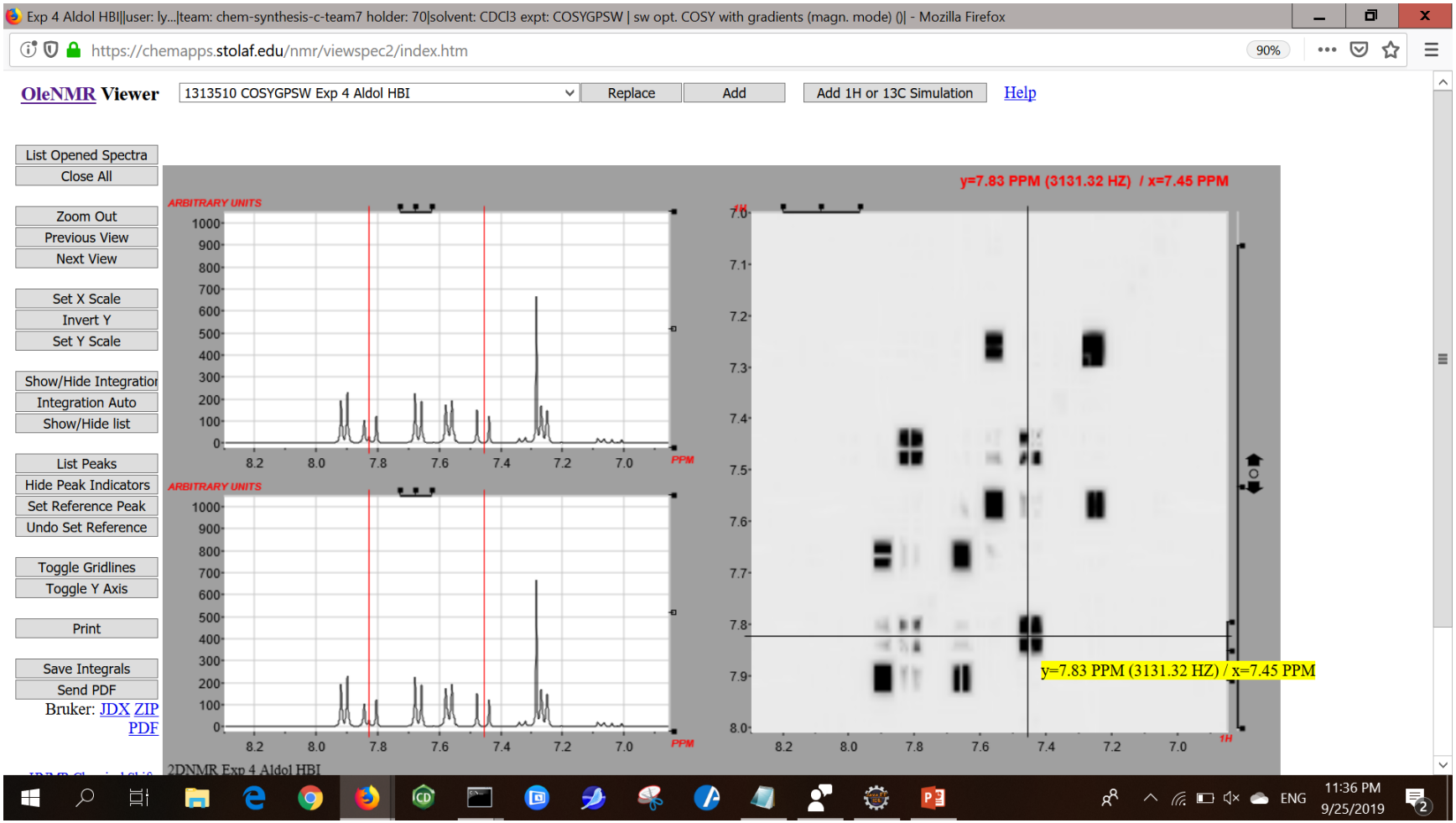
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



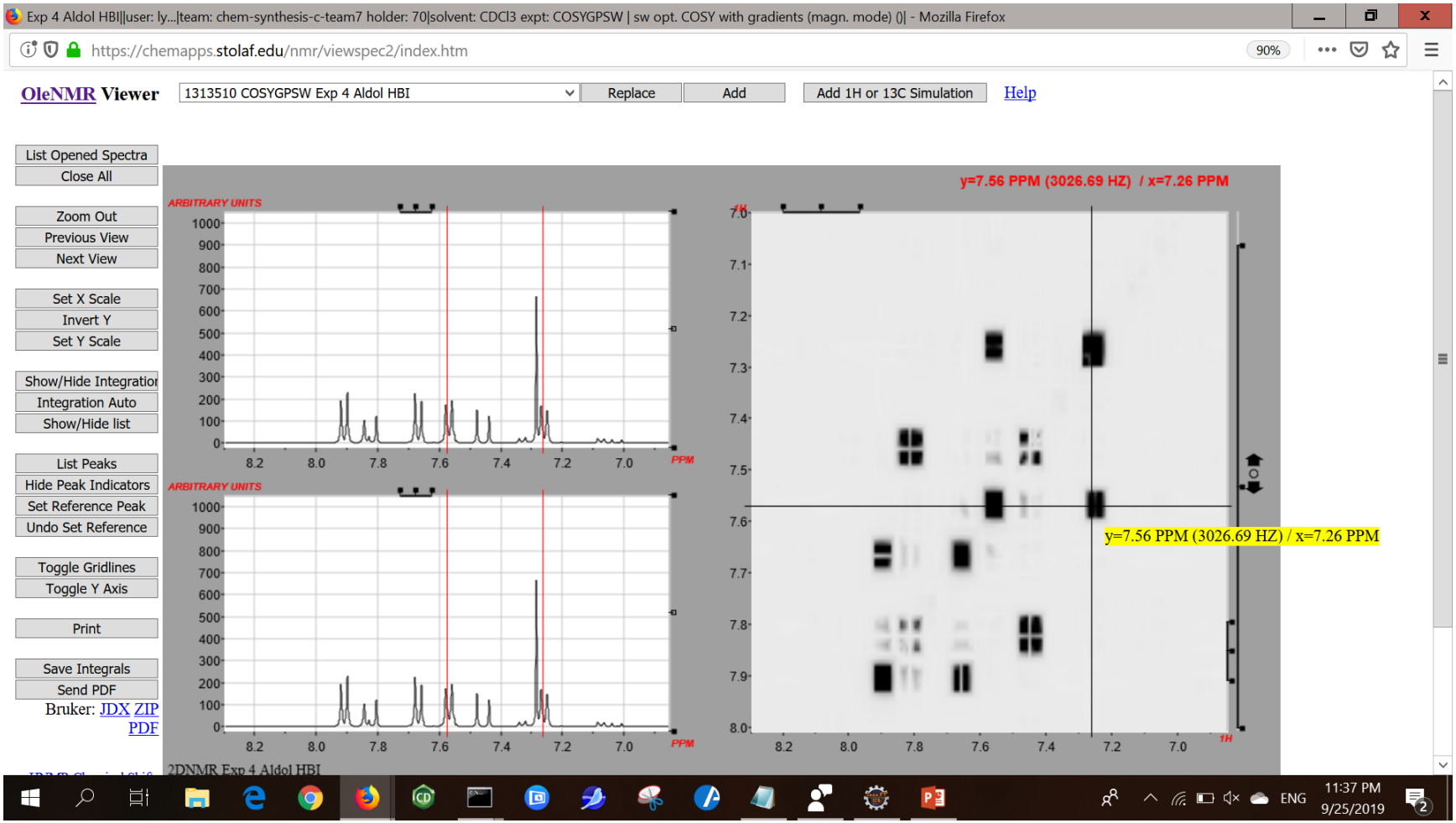
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



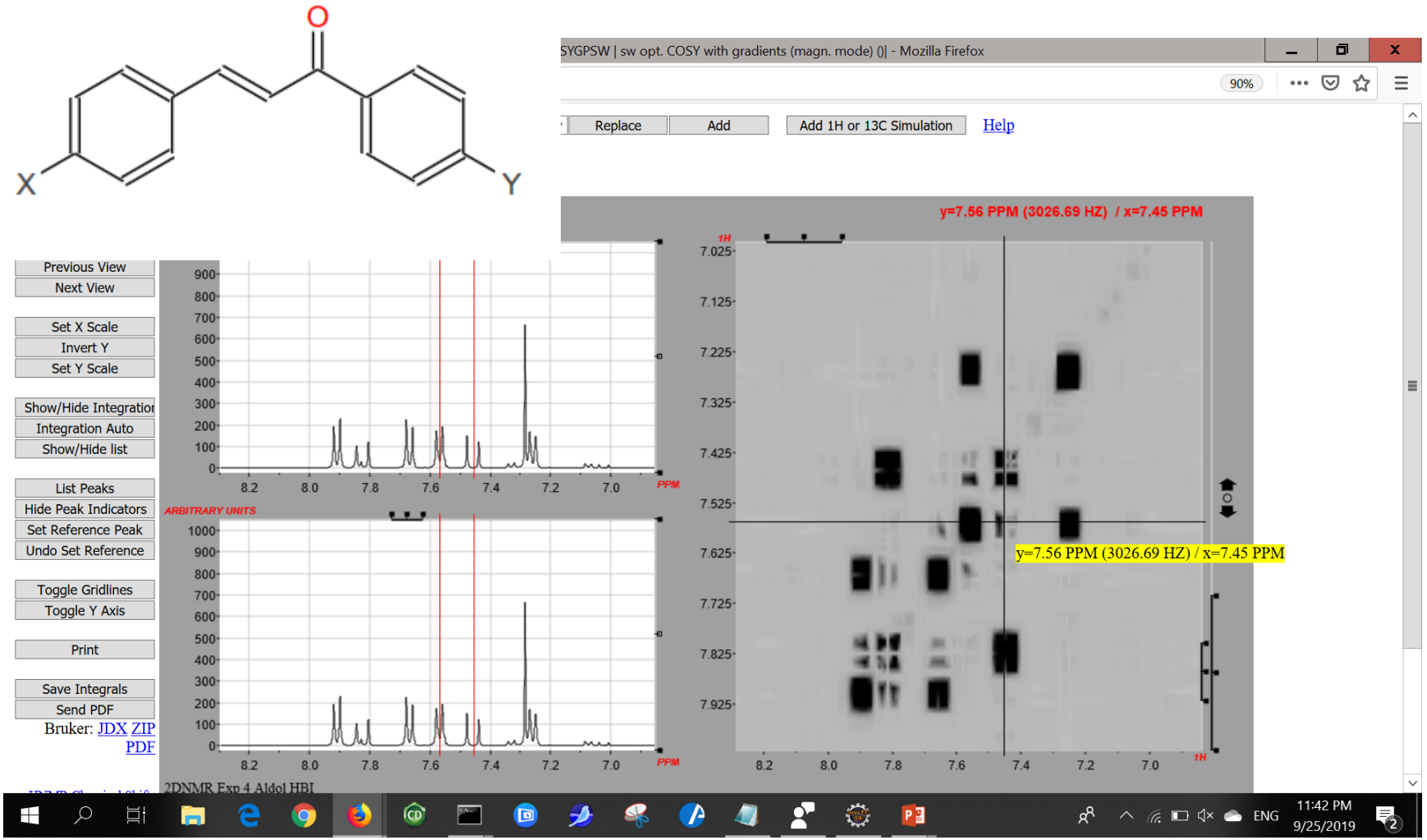
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



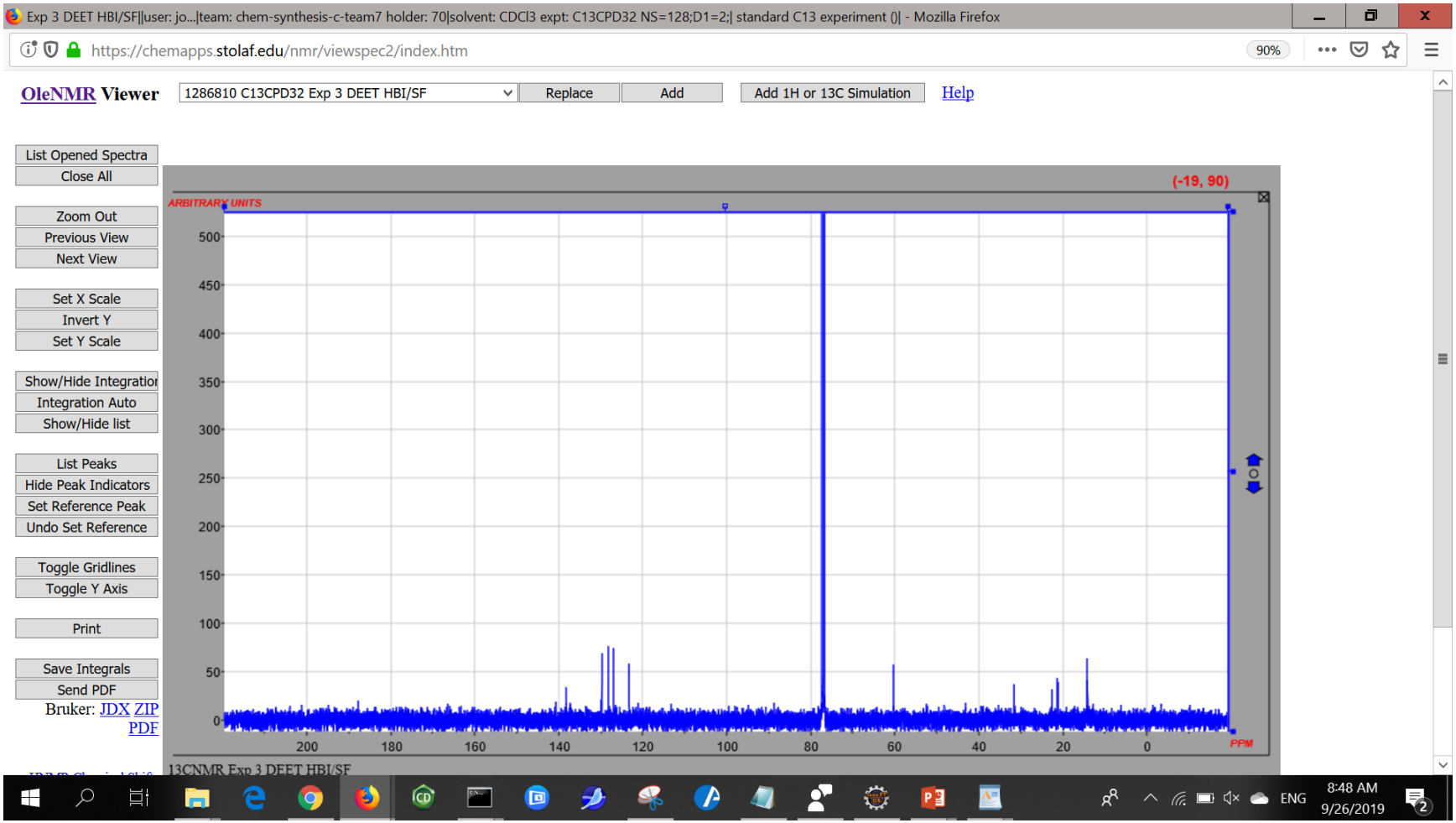
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



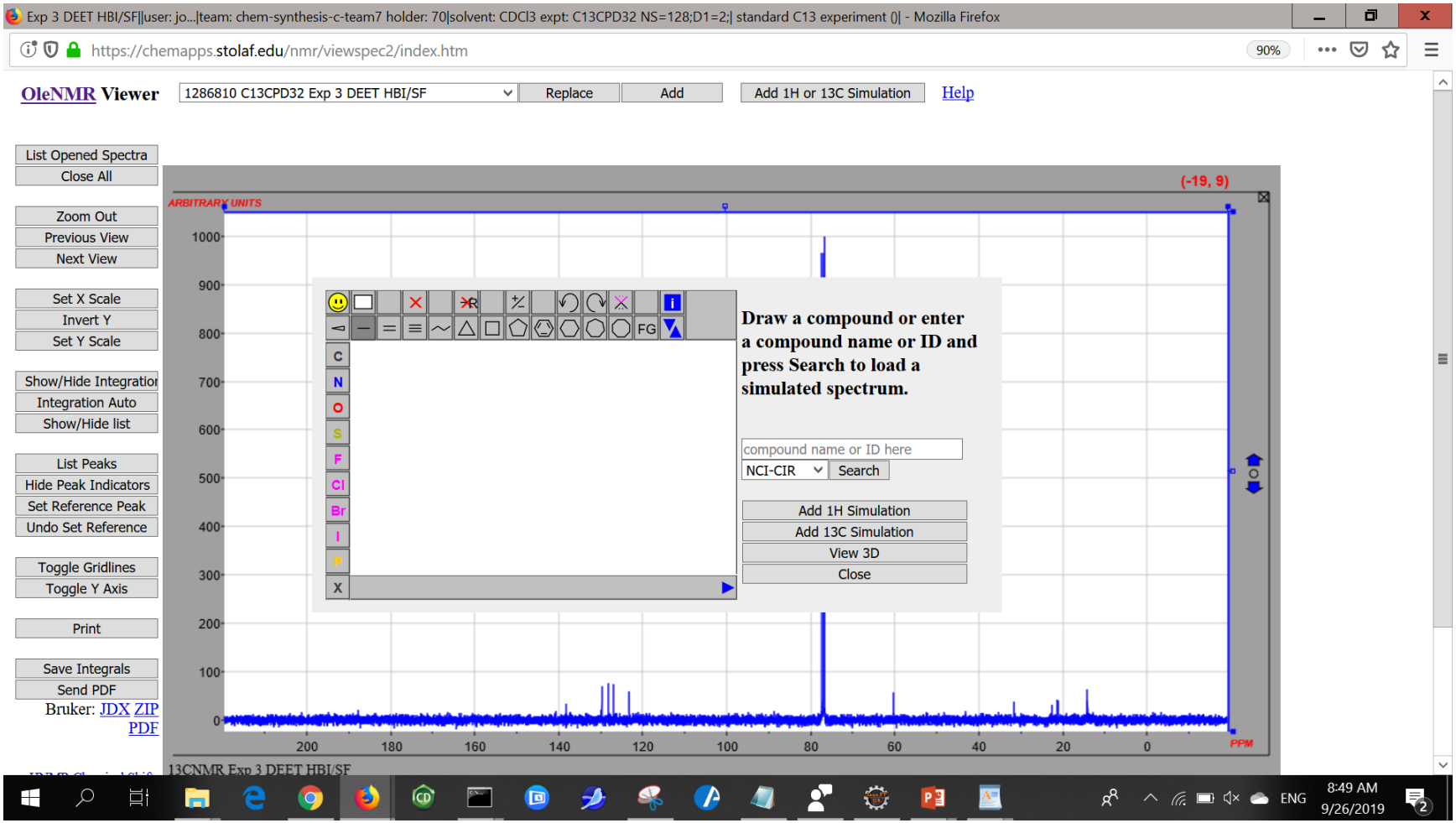
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



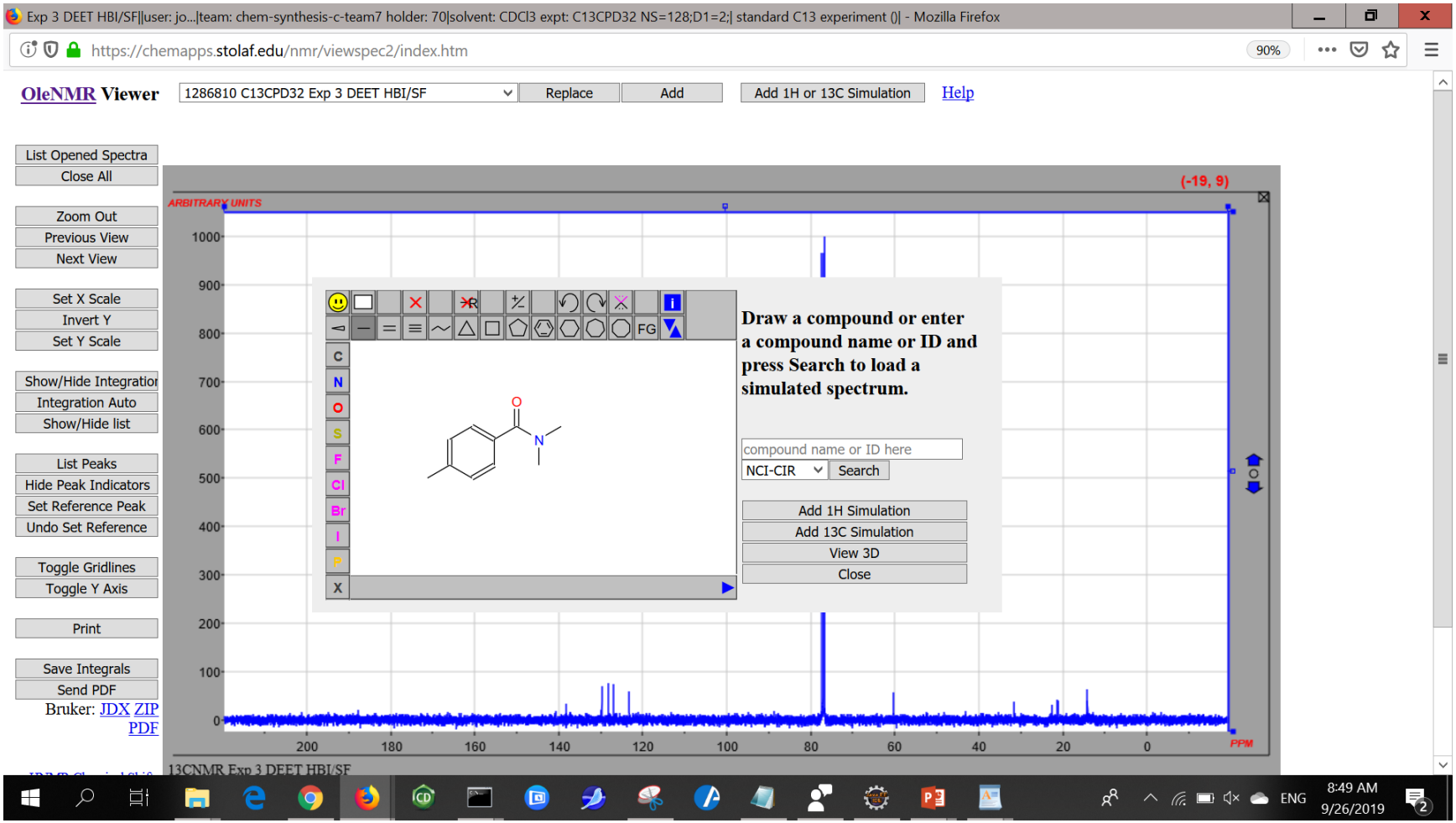
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



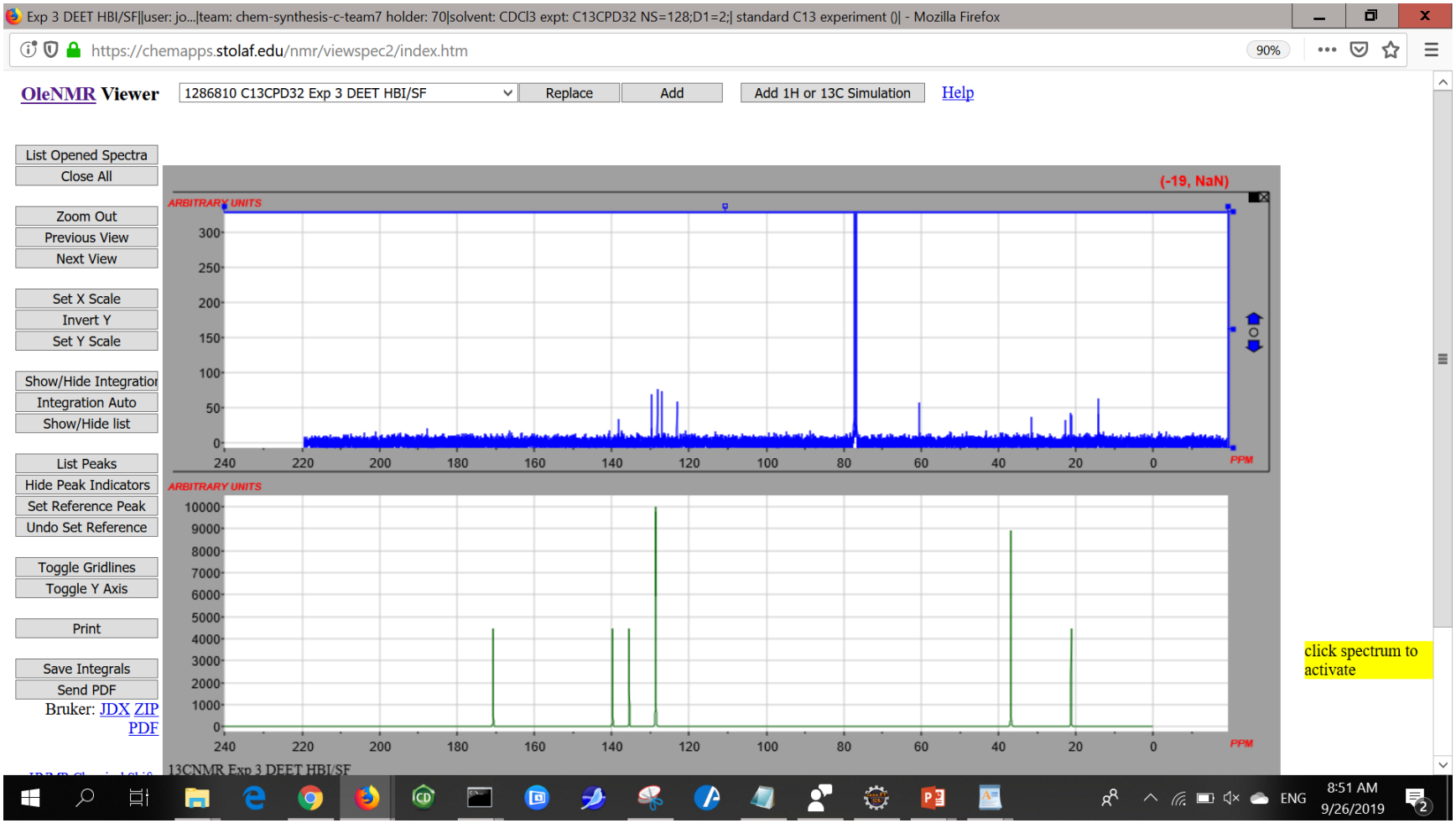
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



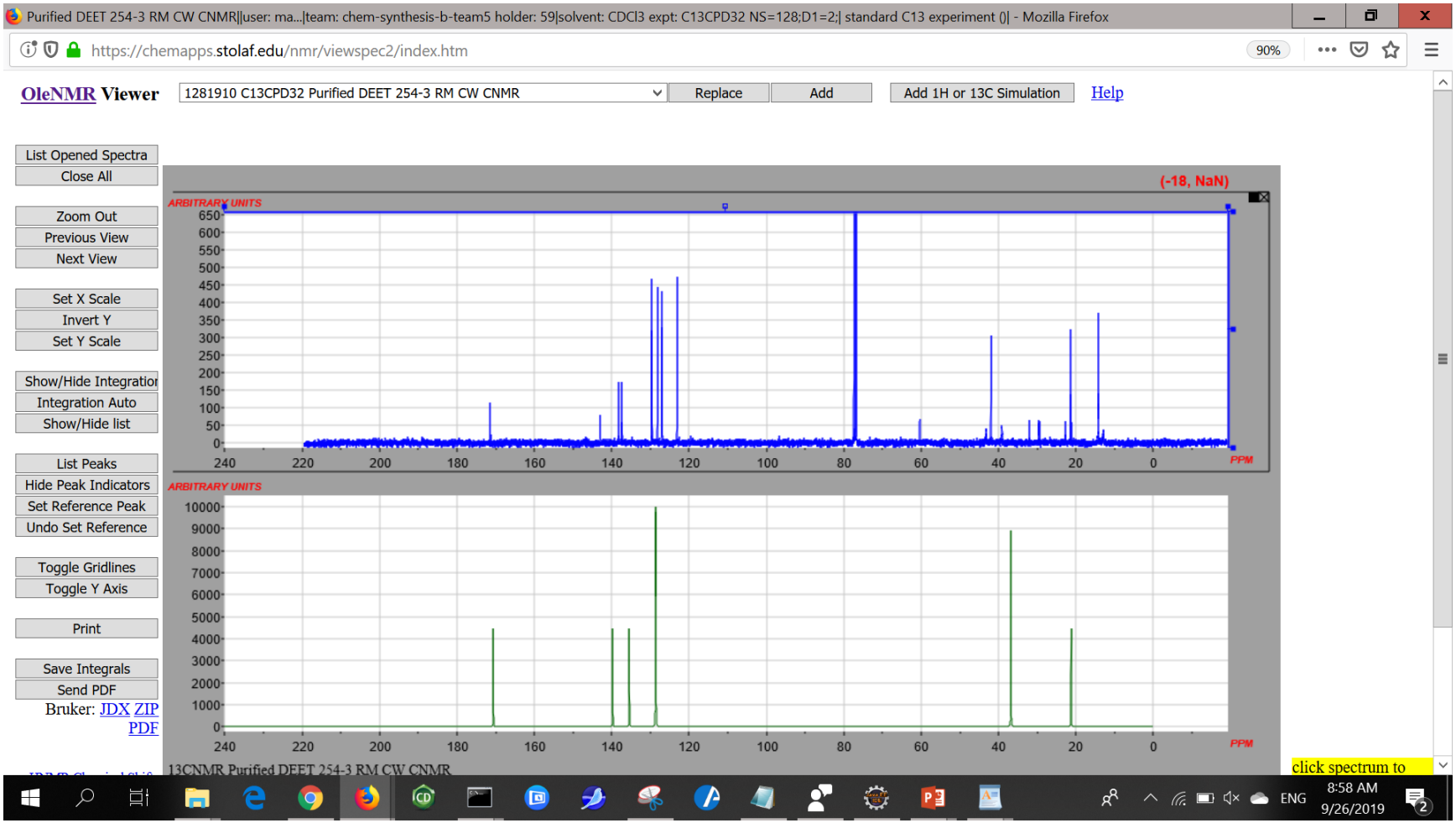
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



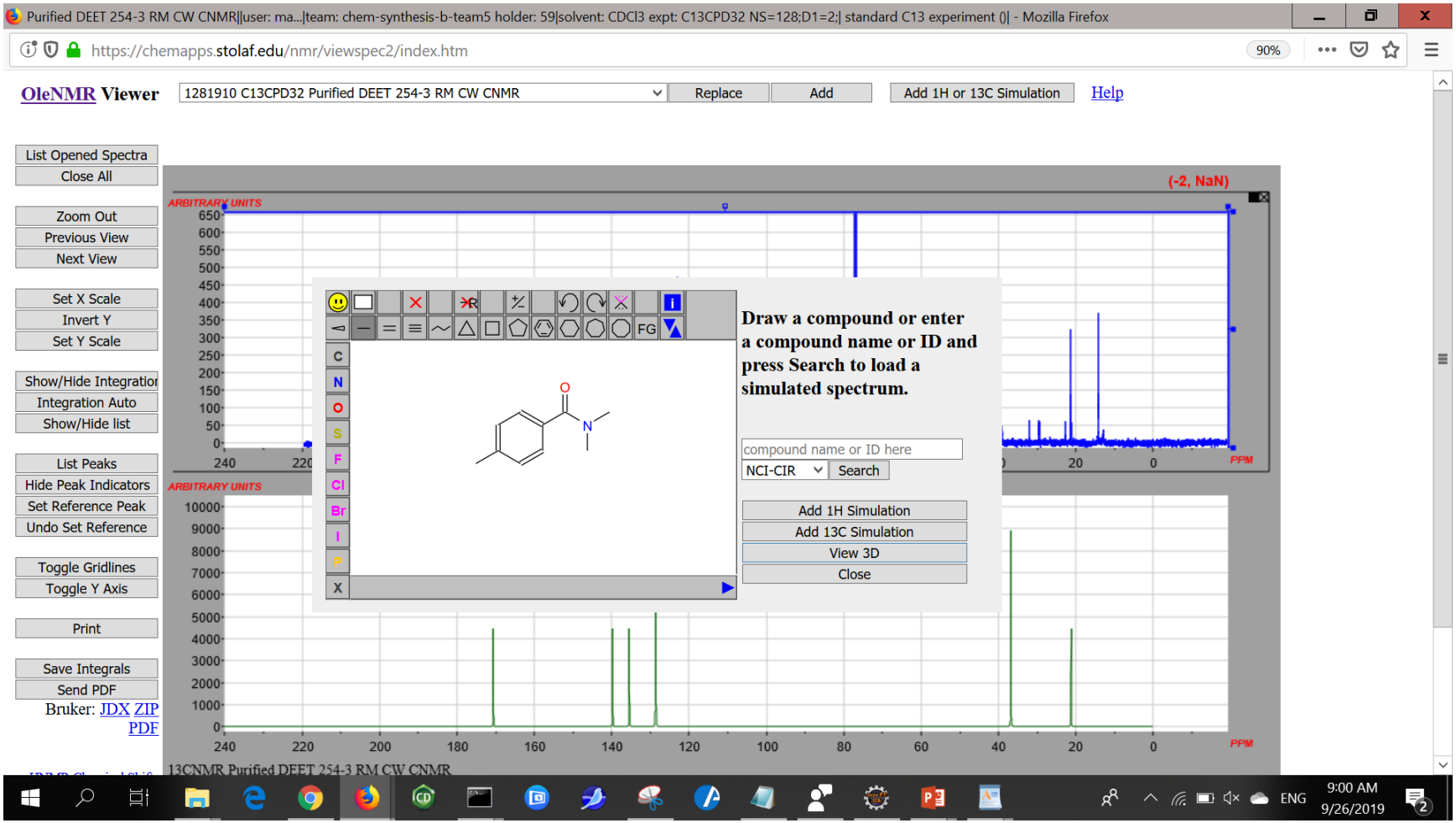
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



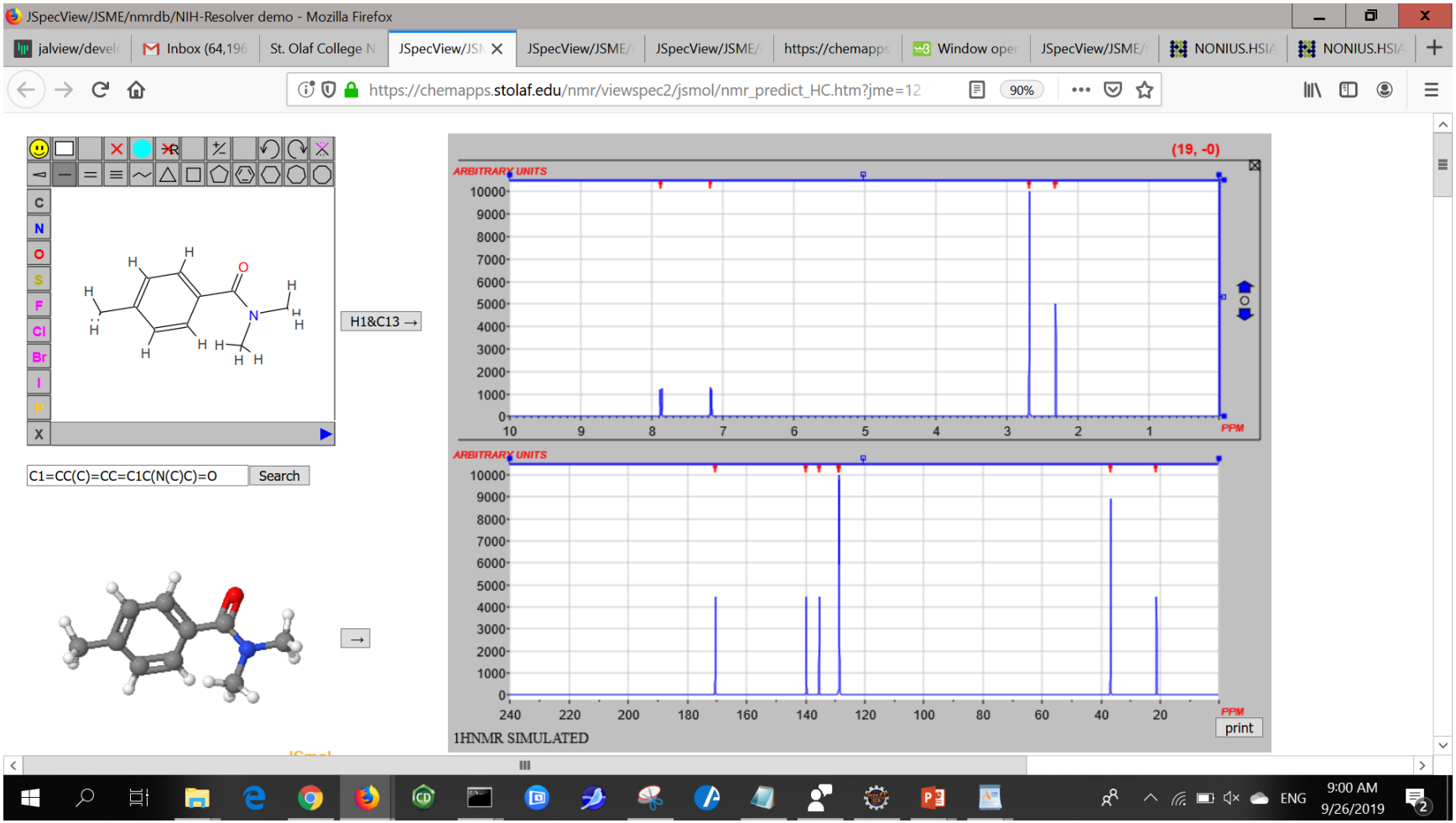
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



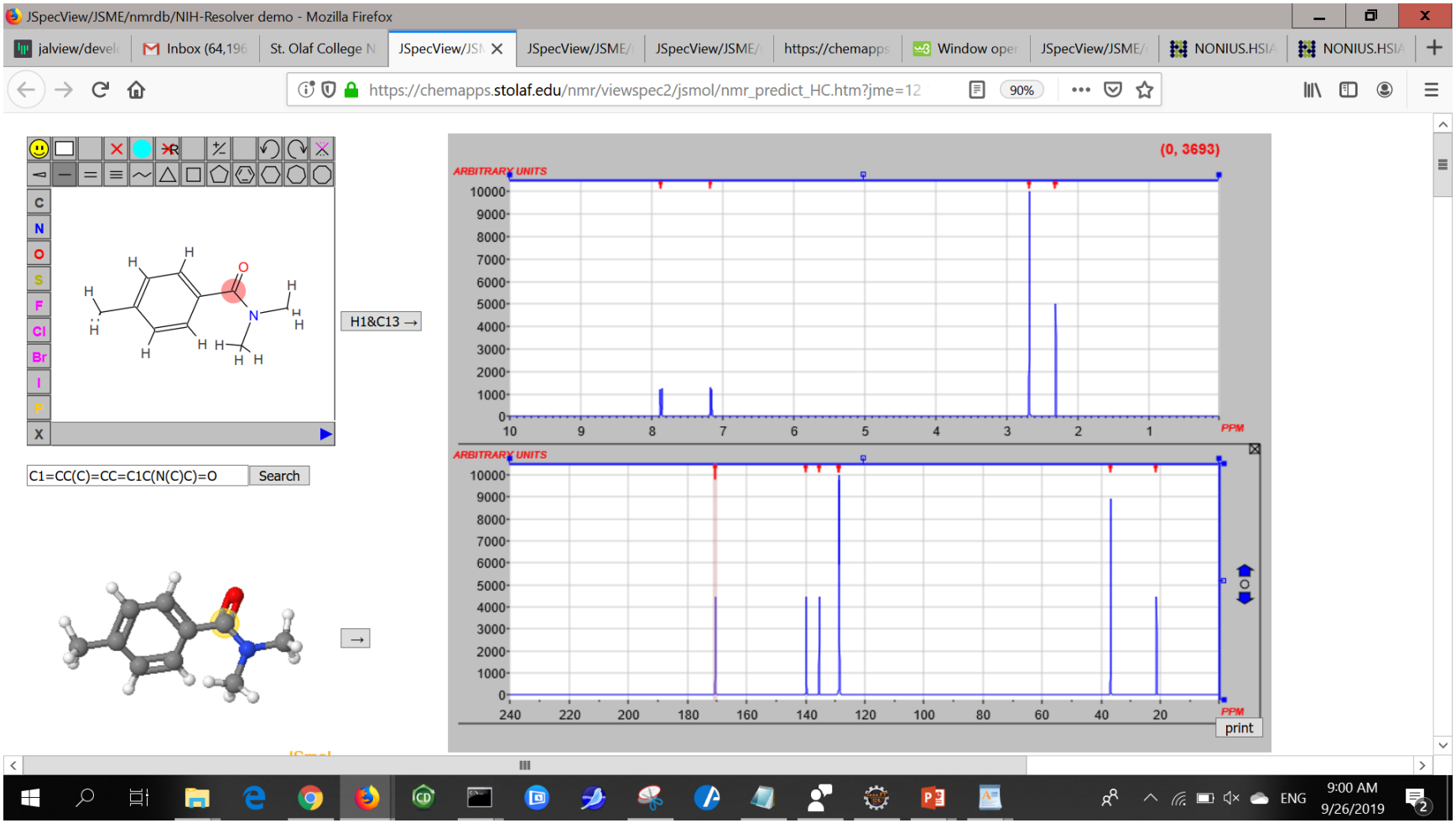
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS



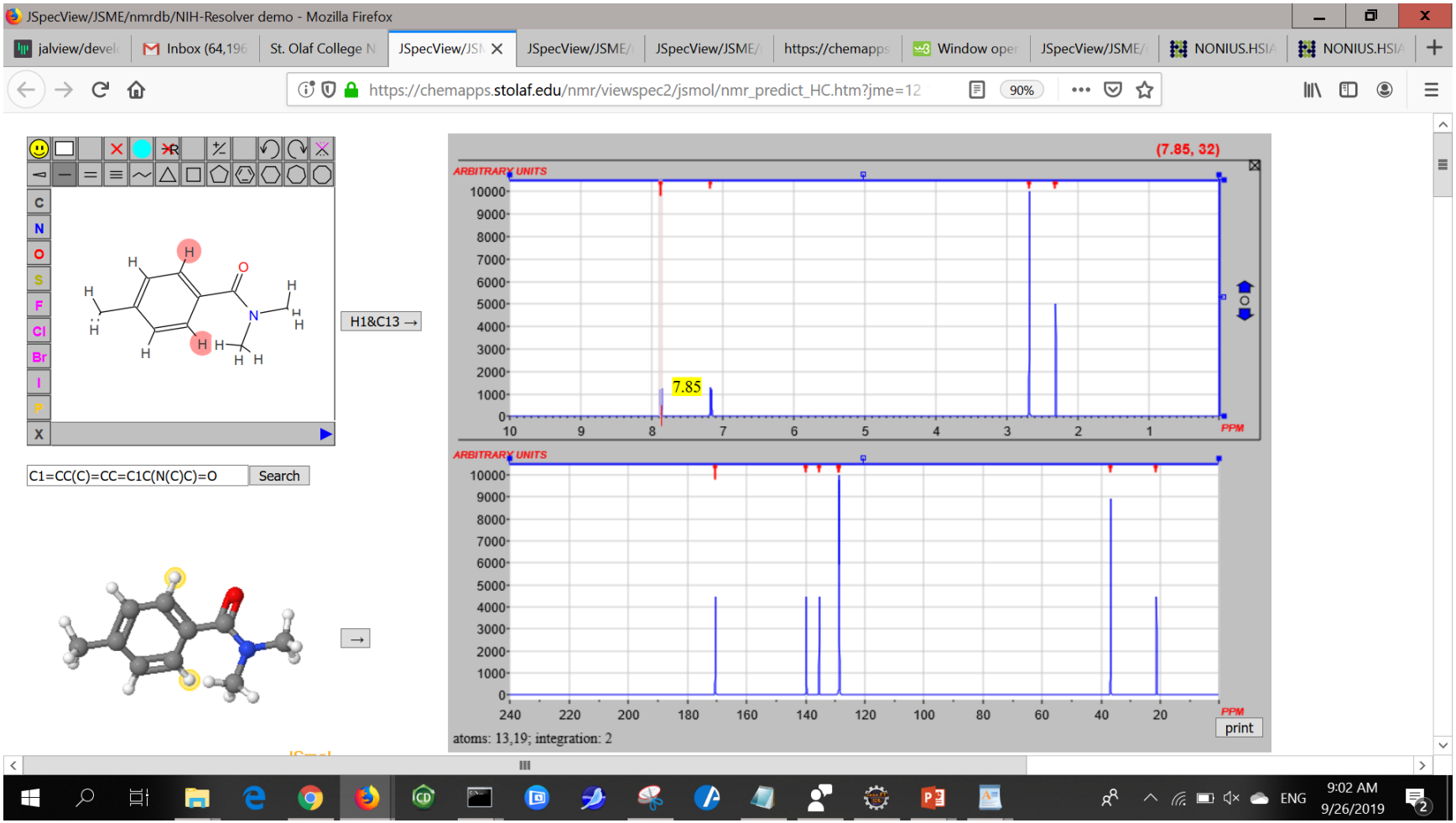
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS

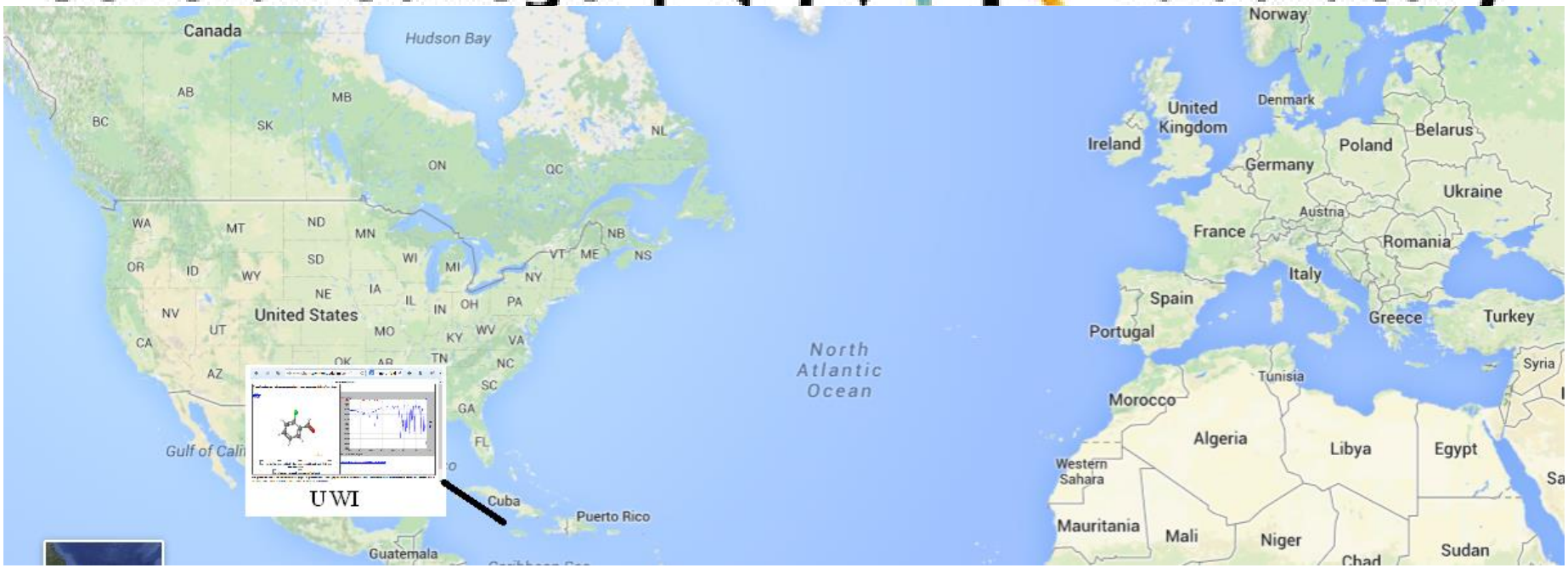


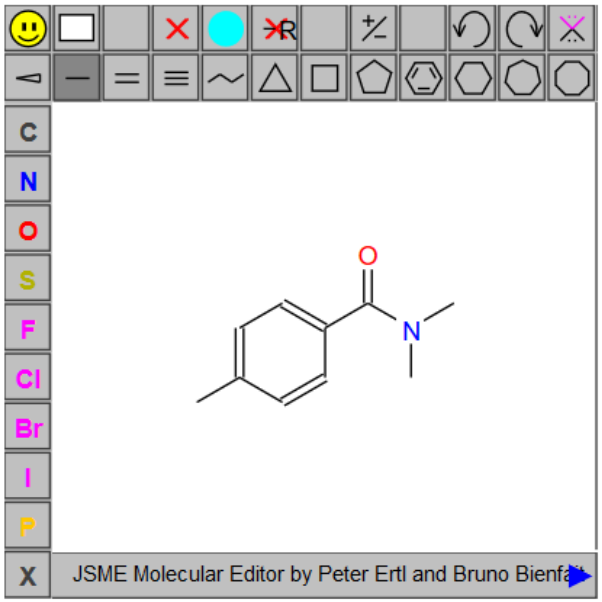
# St. Olaf College NMR Laboratory

## Analysis using JSpecView-JS

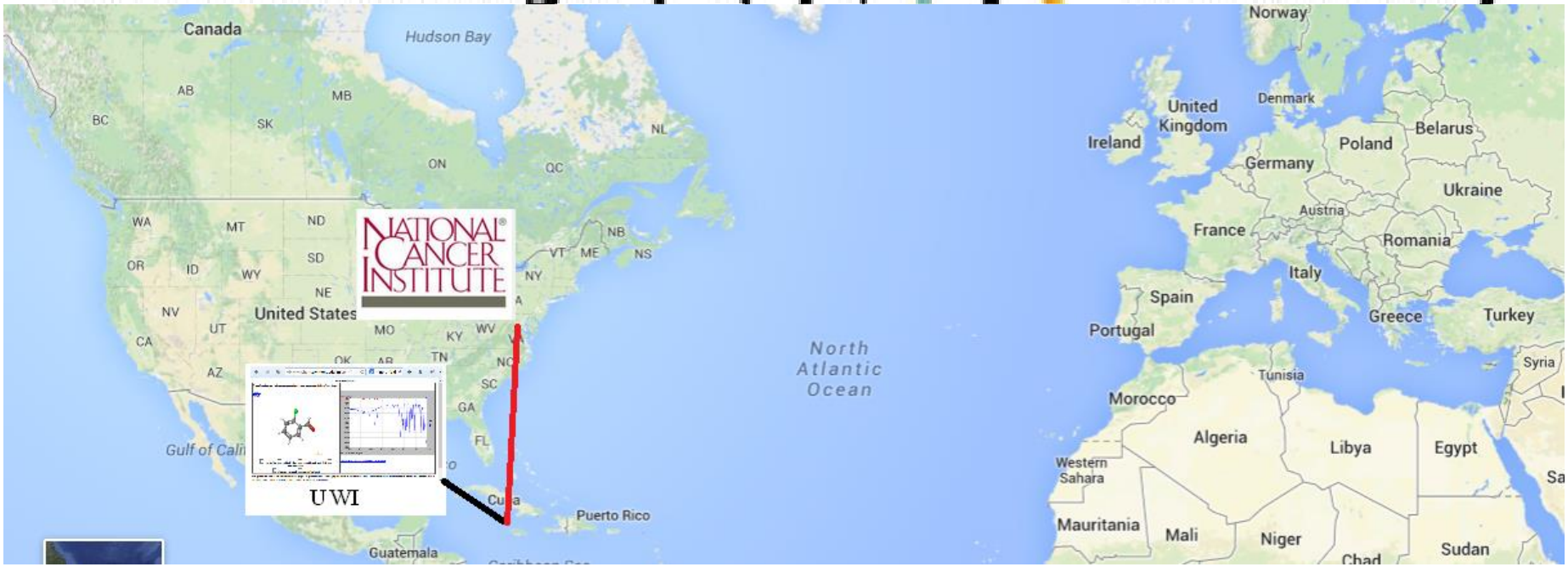


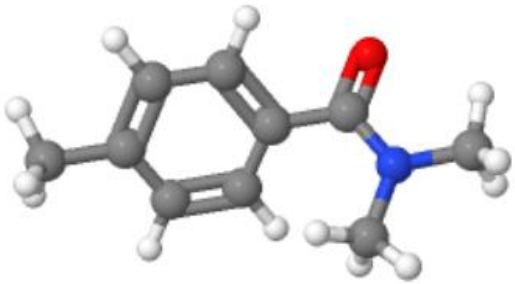
# St. Olaf College NMR Laboratory



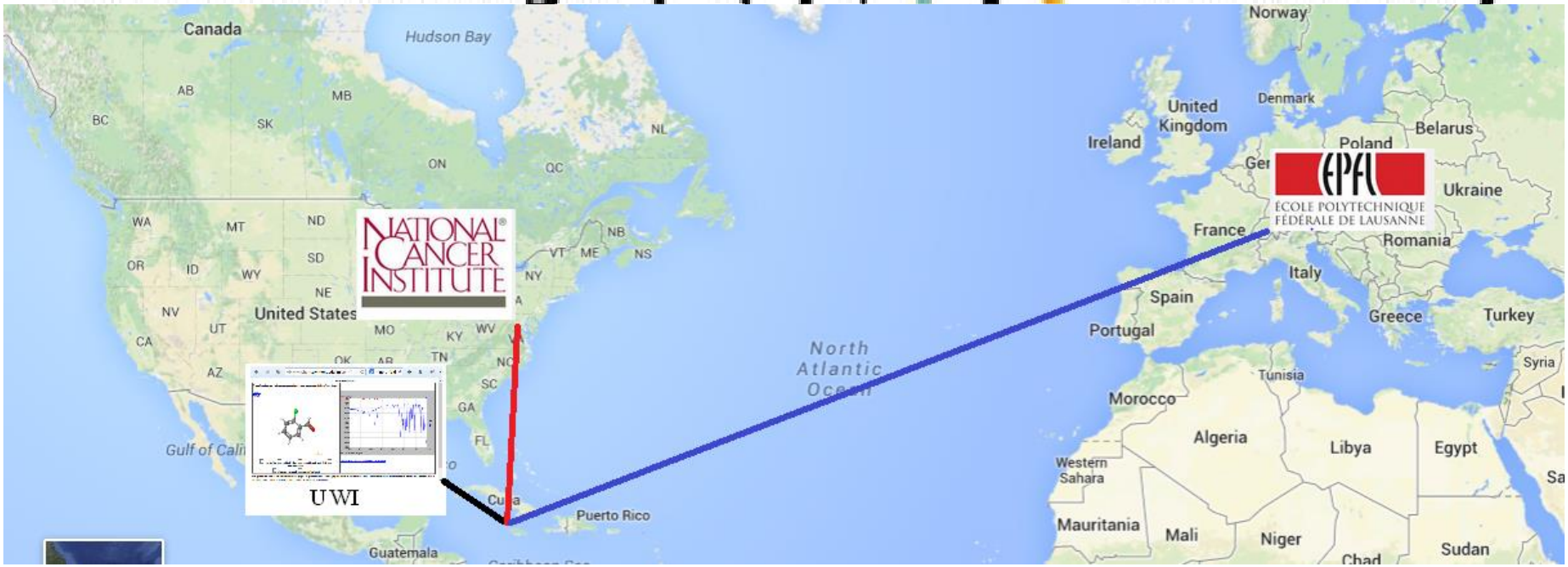
# St. Olaf College NMR Laboratory

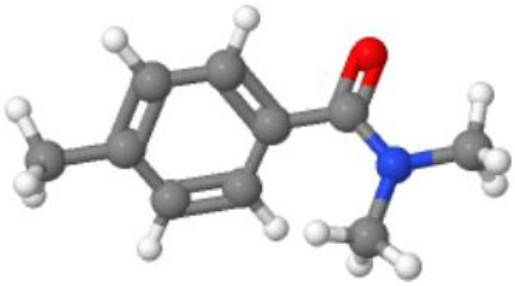


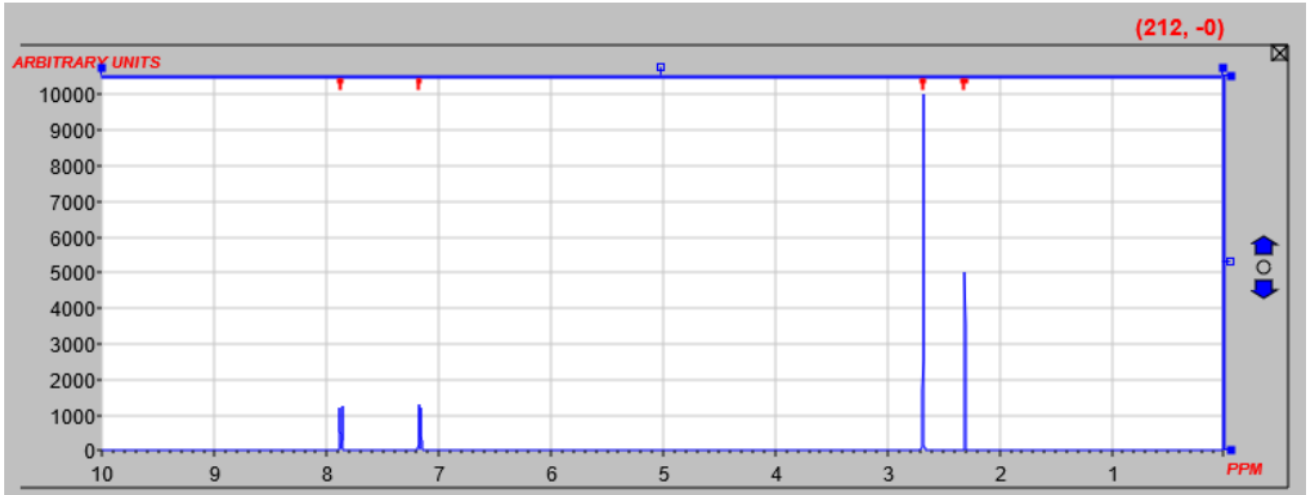



JSmol

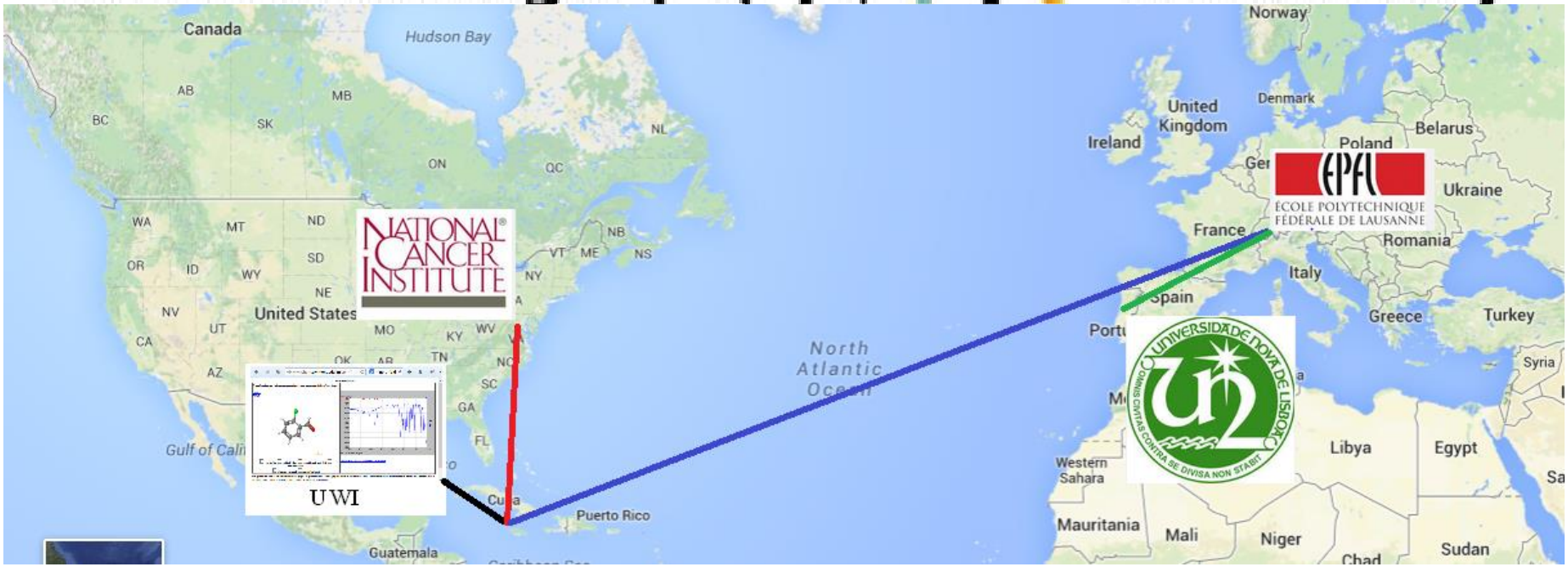
# St. Olaf College NMR Laboratory

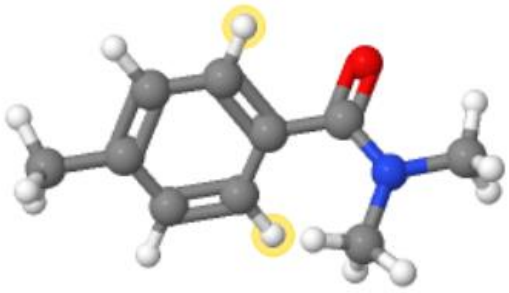


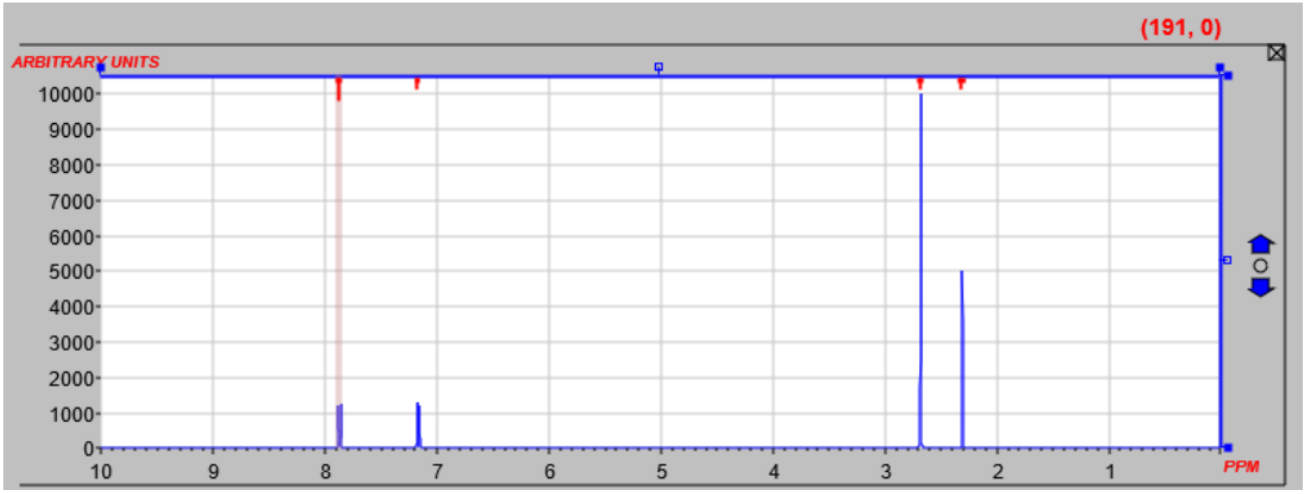



# St. Olaf College NMR Laboratory



JSmol



Acknowledgments…

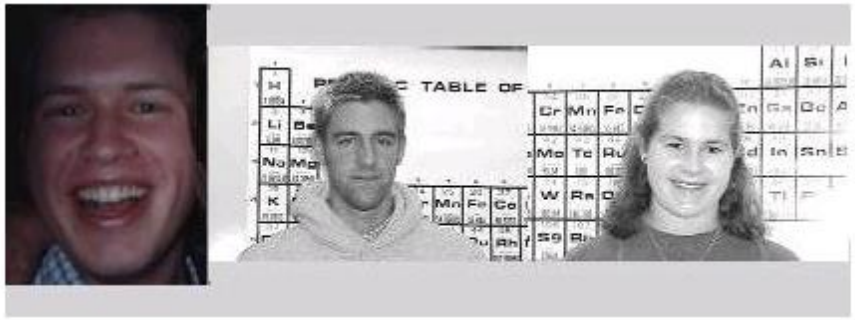
- St. Olaf College

- Peter Ertl, Novartis
- Robert Lancashire, UWI-Mona
- Clemens Anklin, Bruker

# St. Olaf College NMR Laboratory

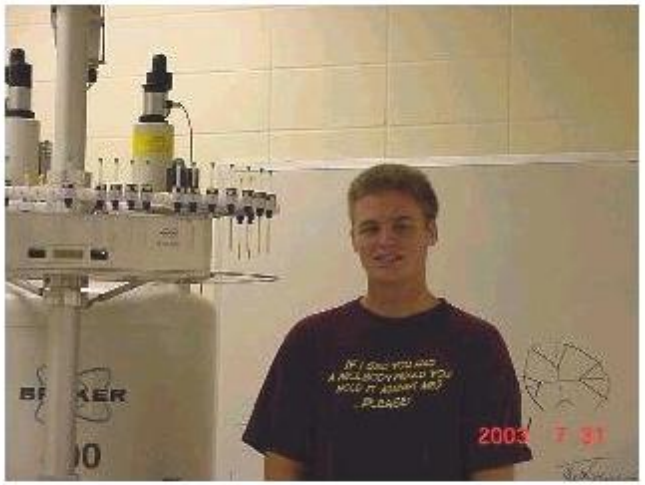
Thanks to the students who really made this possible.

(Can you tell they had fun?)



Mike Purnell, Gregg Sydow, and Stephanie Skladzien

Jared Irwin



Bryan Anderson