

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

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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

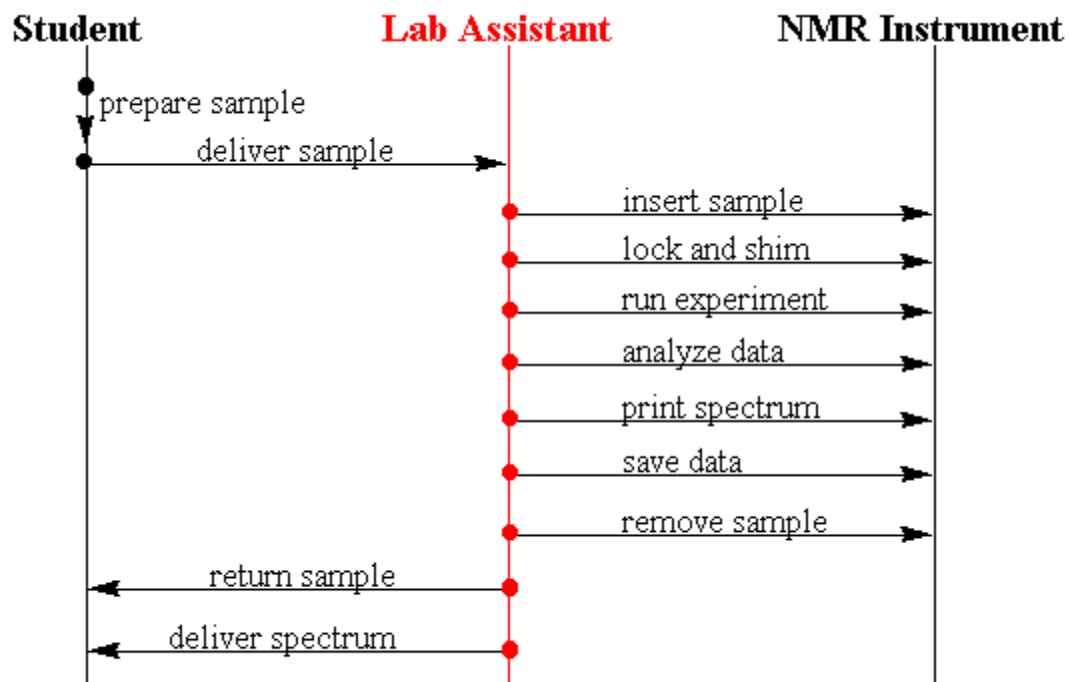
St. Olaf College **NMR** Laboratory

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



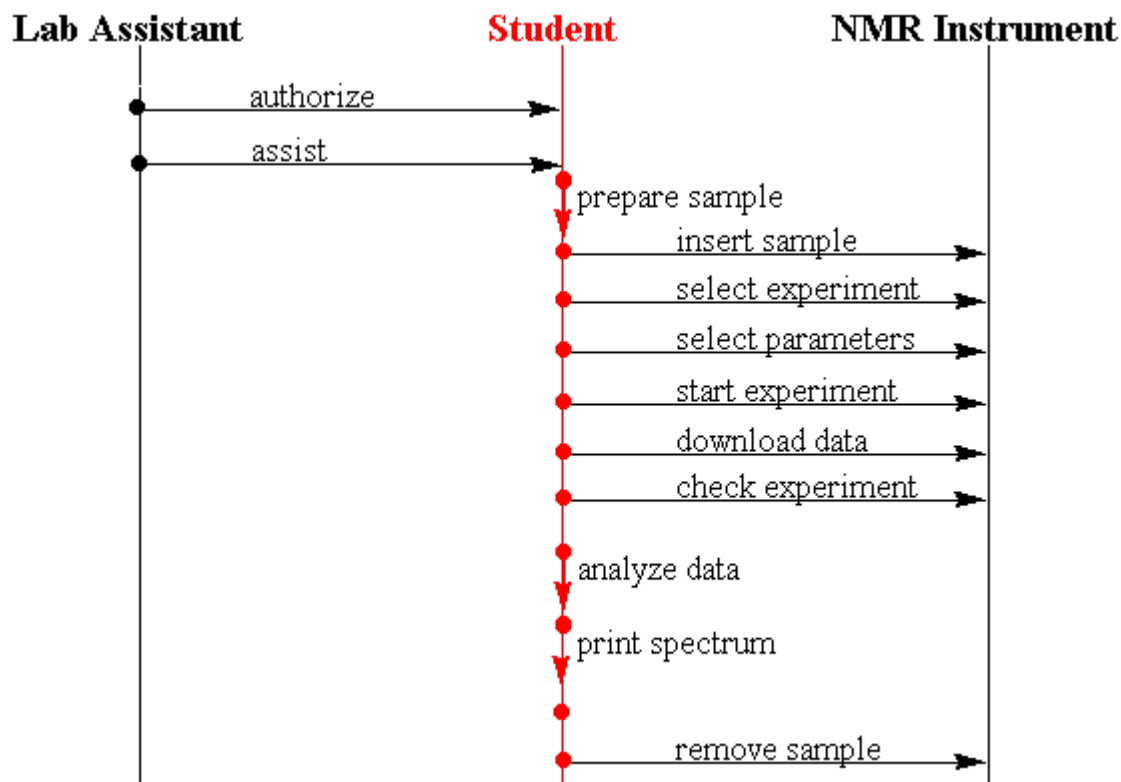
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The OLD way...



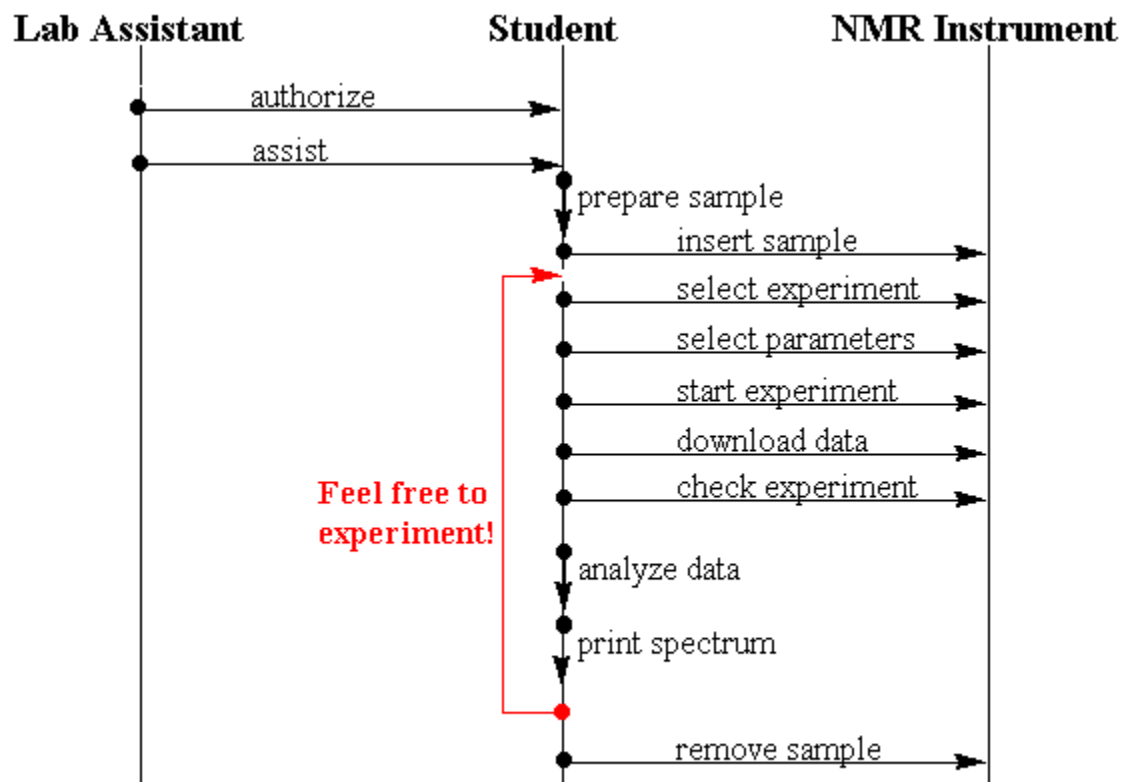
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...and the new way...



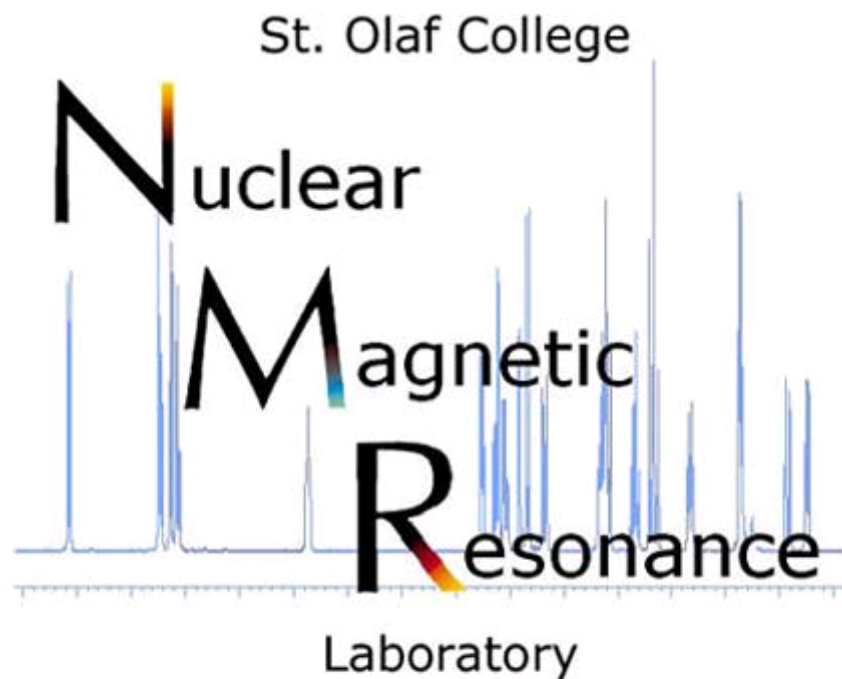
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...with a twist!



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<https://chemapps.stolaf.edu/nmr>



[Bruker Avance 400 MHz NMR Spectrometer \(on-campus users only\)](#)

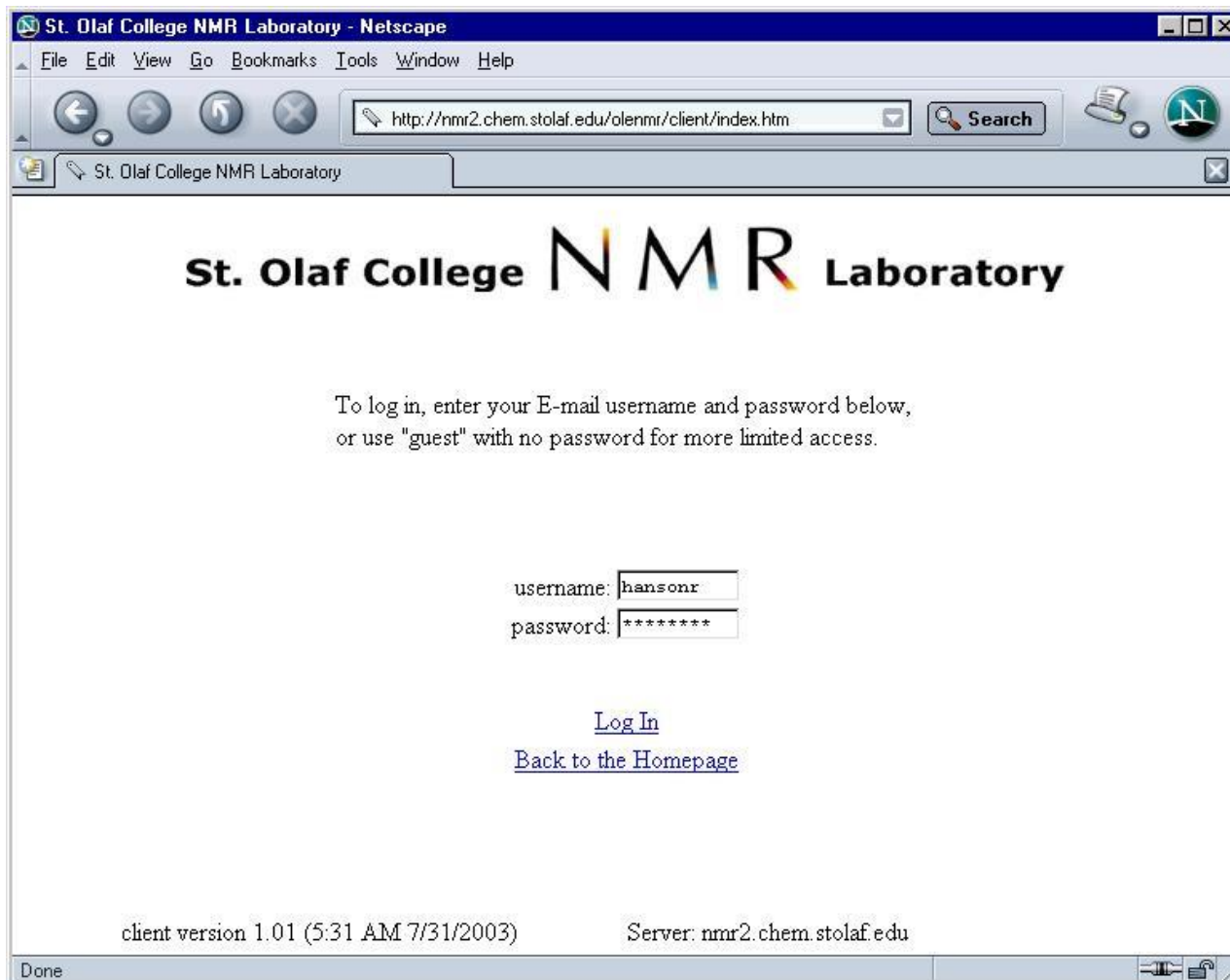
[Liquid Helium Level Log](#) [Experiment Status](#) [Holder Status](#)

[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...



The screenshot shows a Netscape browser window with the title "St. Olaf College NMR Laboratory - Netscape". The address bar contains the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". The page content includes the St. Olaf College NMR Laboratory logo, a login instruction, and two input fields for "username" and "password". The "username" field contains "hansonr" and the "password" field contains "*****". Below the fields are links for "Log In" and "Back to the Homepage". The footer of the page displays "client version 1.01 (5:31 AM 7/31/2003)" and "Server: nmr2.chem.stolaf.edu".

St. Olaf College NMR Laboratory

To log in, enter your E-mail username and password below,
or use "guest" with no password for more limited access.

username:

password:

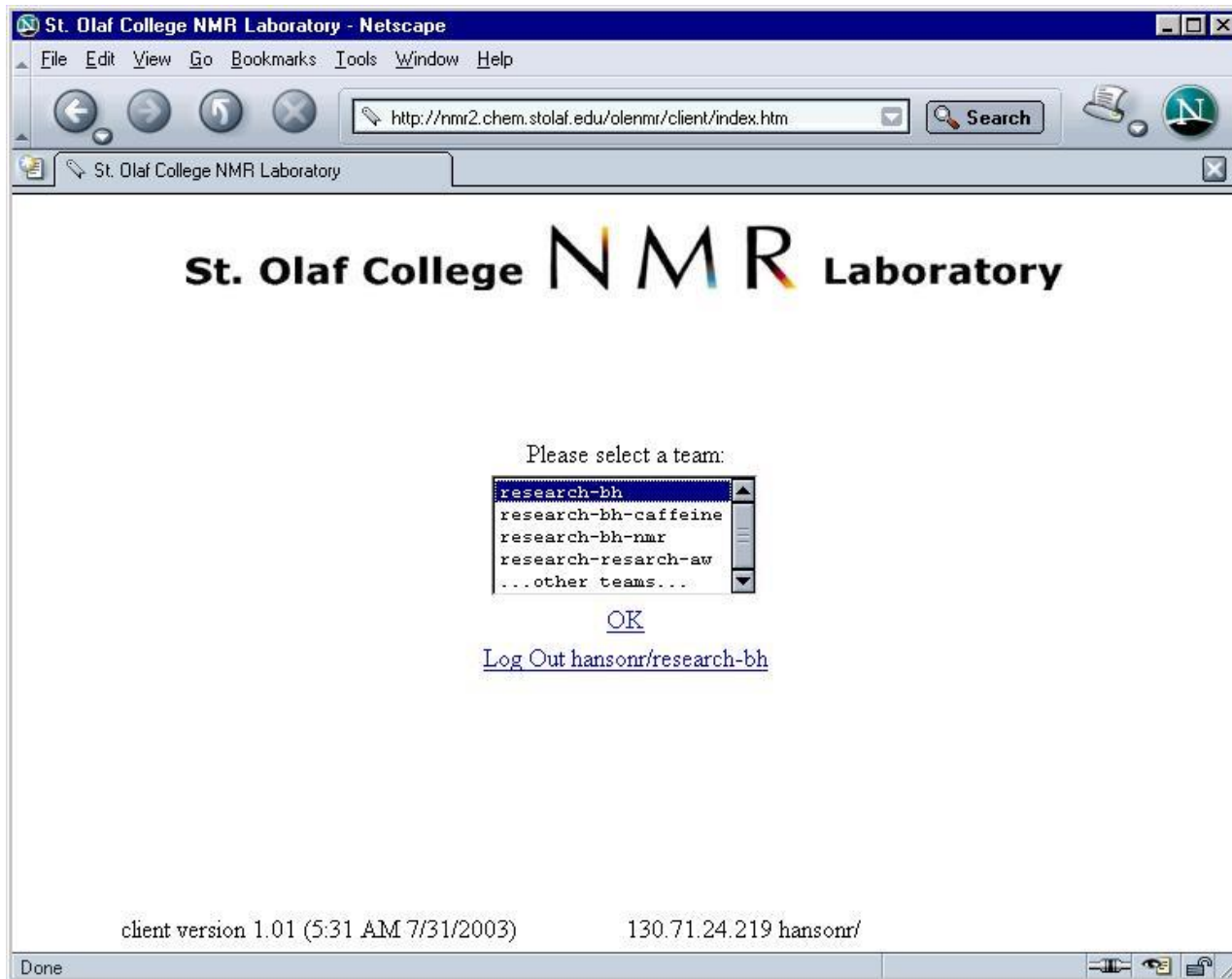
[Log In](#)

[Back to the Homepage](#)

client version 1.01 (5:31 AM 7/31/2003) Server: nmr2.chem.stolaf.edu

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 - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

St. Olaf College NMR Laboratory

St. Olaf College NMR Laboratory

What would you like to do as research-bh?

 Run Experiment	 View Status	 View Spectra	 Learn About NMR
 Switch Teams	 Log Out	 Edit Accounts	 Show Server Log

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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Initially we see a “current status” screen...

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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[Experiment](#) [Status](#) [Spectra](#) [About NMR](#) [Teams](#) [Log Out](#) [Accounts](#) [Server](#)

[GO](#)

Run an NMR Experiment

In order to carry out a nuclear magnetic resonance experiment, you will need to answer a few questions.

Current Instrument Status (as of 03/18/04 16:43)

Holder/Experiment	29/PROTON
Group/Data Set	chem-pchem-team2/Mar17-2004
Experiment/Processing Numbers	1-1419-10/1
Time Left/Status	4 Sec/Waiting for job

[update now...](#)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

Done

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

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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Experiment Status Spectra About NMR Teams Log Out Accounts Server

Indicate a Sample Position

Which sample position is your NMR tube in?
([history](#))

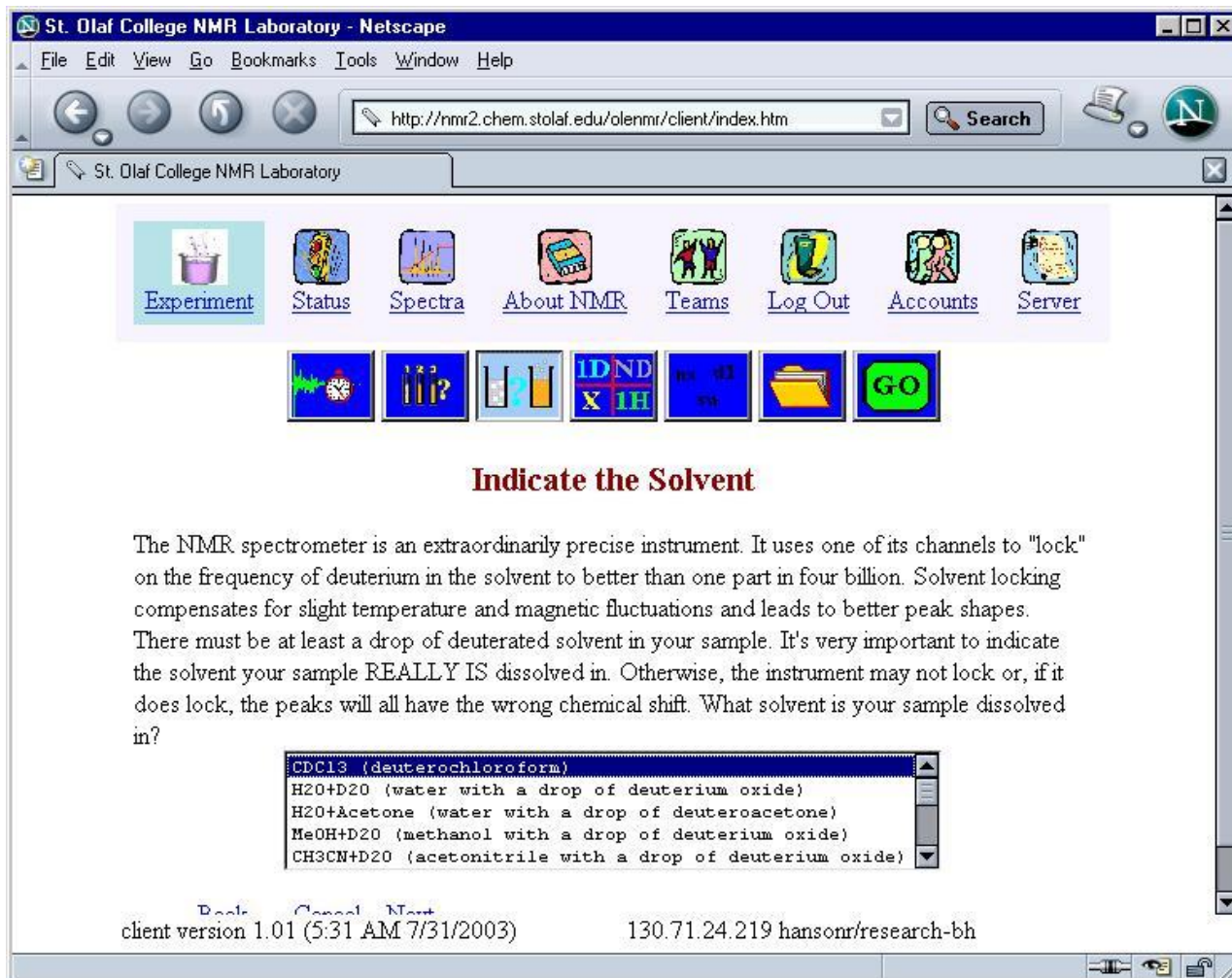
#85:	research-bh-nmr	(irwinj, anderbm)
#86:	research-bh-nmr	(irwinj, anderbm)
#87:	research-bh-nmr	(irwinj, anderbm)
#88:	research-bh-nmr	(irwinj, anderbm)
#89:	research-bh-nmr	(irwinj, anderbm)

[Back...](#) [Cancel](#) [Next...](#)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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Solvent options are automatically loaded from the Bruker database...



St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm

St. Olaf College NMR Laboratory

Experiment Status Spectra About NMR Teams Log Out Accounts Server

Indicate the Solvent

The NMR spectrometer is an extraordinarily precise instrument. It uses one of its channels to "lock" on the frequency of deuterium in the solvent to better than one part in four billion. Solvent locking compensates for slight temperature and magnetic fluctuations and leads to better peak shapes. There must be at least a drop of deuterated solvent in your sample. It's very important to indicate the solvent your sample REALLY IS dissolved in. Otherwise, the instrument may not lock or, if it does lock, the peaks will all have the wrong chemical shift. What solvent is your sample dissolved in?

CDCl₃ (deuteriochloroform)
H₂O+D₂O (water with a drop of deuterium oxide)
H₂O+Acetone (water with a drop of deuterioacetone)
MeOH+D₂O (methanol with a drop of deuterium oxide)
CH₃CN+D₂O (acetonitrile with a drop of deuterium oxide)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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Experiments are drawn from an OleNMR database...

The screenshot shows a Netscape browser window titled "St. Olaf College NMR Laboratory - Netscape". The address bar contains the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". The page features a navigation menu with icons and labels for "Experiment", "Status", "Spectra", "About NMR", "Teams", "Log Out", "Accounts", and "Server". Below this is a second row of icons, including a "GO" button. The main content area is titled "Select an Experiment" and contains a paragraph of text explaining the database and a list of available experiments. The first experiment listed is "1H experiment 16 scans", which is described as a "PROTON" experiment. The browser status bar at the bottom shows "client version 1.01 (5:31 AM 7/31/2003)" and "130.71.24.219 hansonr/research-bh".

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

St. Olaf College NMR Laboratory

Experiment Status Spectra About NMR Teams Log Out Accounts Server

Select an Experiment

There are hundreds of possible NMR experiments that can be carried out. The experiments your team is authorized to carry out are listed below. Select one of these experiments.

Note that you may carry out more than one NMR experiment on the same sample. For example, it's common to run a proton experiment, a carbon experiment, and a DEPT experiment (which identifies carbons as being C, CH, CH₂, or CH₃) all on the same sample (i.e., in the same data set).

Composite experiments such as this take somewhat longer for data collection.

1H experiment 16 scans C13 exp. comp. pulse dec. 32 scans sw opt. COSY with gradients (magn. mode) sw opt. HMQC with gradients (magn. mode) sw opt. HMBC with low pass J-filter (magn. mode)	PROTON The standard NMR experiment. Provides a proton spectrum.
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[more info...](#)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

St. Olaf College NMR Laboratory

[Experiment](#) [Status](#) [Spectra](#) [About NMR](#) [Teams](#) [Log Out](#) [Accounts](#) [Server](#)

[?](#) [?](#) [?](#) [IDND X 1H](#) [ns d1 sw](#) [GO](#)

Set the Parameters

Each NMR experiment involves a number of variable parameters. You may decide to adjust parameters at this time. Listed below are several parameters, along with their default values. You can leave these values as they are, or you can change them to see what happens.

Parameters For the PROTON Experiment

Number of scans Number of scans (NS)

NS determines the number of times data are collected. Each scan takes time, but increasing the number of scans results in less baseline noise in the spectrum

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

javascript:parent.fraClient.setup_invokeGifButton(6)

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A little instruction to guide novices is on each panel...

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File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

St. Olaf College NMR Laboratory

Experiment Status Spectra About NMR Teams Log Out Accounts Server

Indicate a Title

The title might be a unique reference from your research or laboratory notebook (such as *BH-II-24b*), the name of a compound (such as *cholesterol* or *unknown acid*), or the name of an experiment (such as *lab 3*). You can combine this sort of information any way you like. So, for example, the title might be *BH-II-24b, chromatography fractions 2-20 or lab 3, white crystals, page 23*.

Sample for ACS

[Back...](#) [Cancel](#) [Next...](#)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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We designed a “fair queue” that prevents monopolization...



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File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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Experiment Status Spectra About NMR Teams Log Out Accounts Server

Submit the Experiment

The NMR spectrometer can only run one experiment at a time. Each experiment that needs to be done is added to a list of experiments waiting to be done called the *spectrometer queue*. Your experiments will be carried out based on a *fair queue* schedule (which is not quite *first-come-first-served*). Shown below is a summary of the job you have set up. If this is what you want, click on **Submit Experiment** to add this job to the spectrometer queue. Otherwise, you can go back and change aspects of the job that don't appear to be correct.

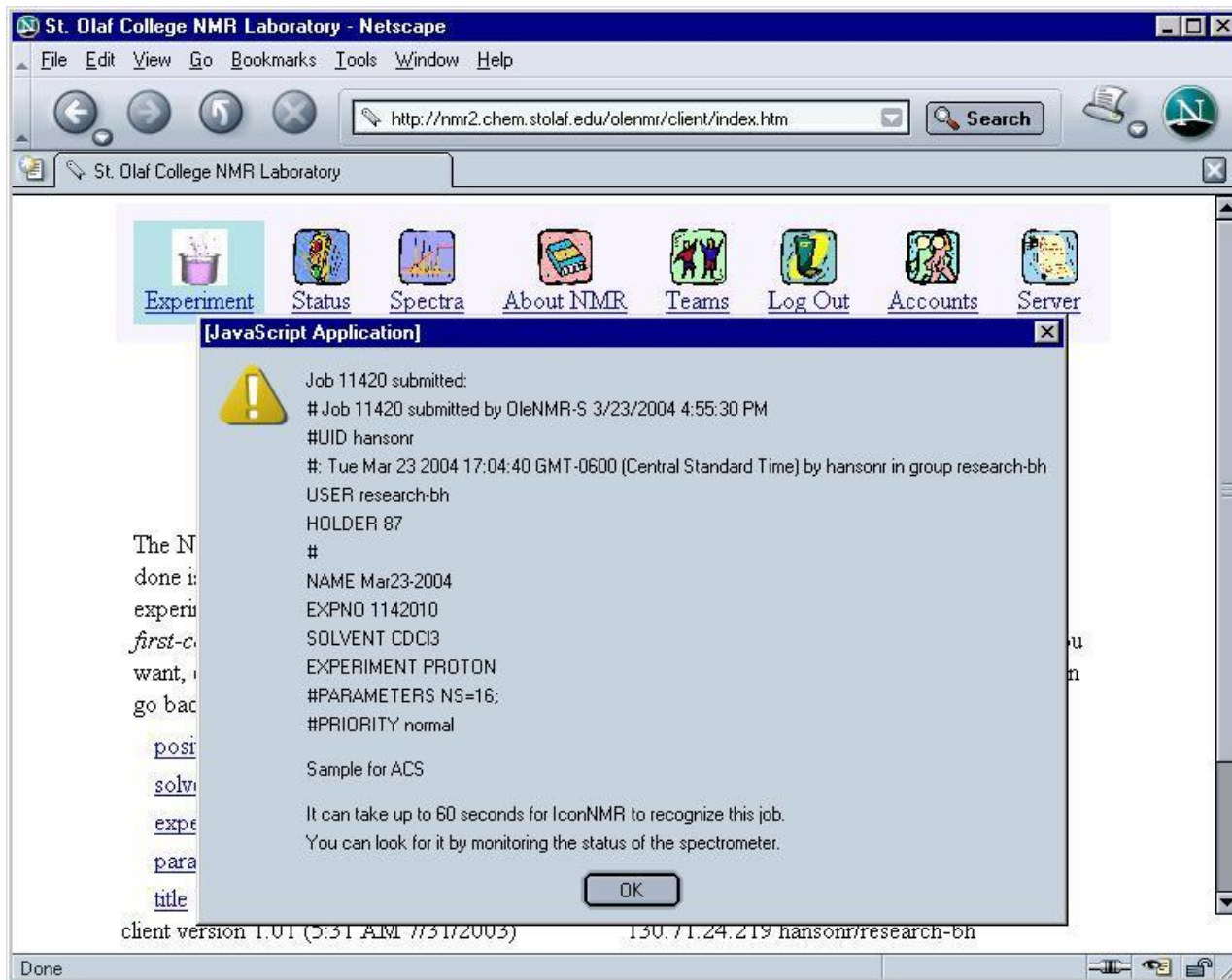
position 87
solvent CDCl₃ (deuteriochloroform) **priority: normal**
experiment PROTON This experiment will be queued for carrying out based on a "fair queue."
parameters NS=16;
title Sample for ACS

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

Done

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A message from the server indicates successful job submission...



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

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File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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What would you like to do as research-bh?

 [Run Experiment](#)  [View Status](#)  [View Spectra](#)  [Learn About NMR](#)

 [Switch Teams](#)  [Log Out](#)  [Edit Accounts](#)  [Show Server Log](#)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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This is a running list of active and pending jobs...

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File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail Archive](#)
Last updated by IconNMR: 03/17/04 16:45

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **Waiting for Job**

30 done 0 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

29/1	chem-pchem-team2	Mar17-2004	PROTON	CDC13	finished:	total
	urban	1-1419-10	normal		03/17/04 16:45	4

Lab 4, Sample 4 NS=16;

atma: 🍀 rotation: 🍀 lock: ⚠️ shim: ⚠️ acqu: 🍀

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

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Within one minute our job shows up...

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File Edit View Go Bookmarks Tools Window Help

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm

St. Olaf College NMR Laboratory

[Experiment](#) [Status](#) [Spectra](#) [About NMR](#) [Teams](#) [Log Out](#) [Accounts](#) [Server](#)

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail](#) [Archive](#)
Last updated by IconNMR: 03/17/04 16:45

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **Waiting for Job**

30 done 0 running 1 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

<input type="checkbox"/>	87/??	research-bh	Mar23-2004	PROTON	CDCI3	estim
		hansomr	11420	normal		6

Sample for ACS NS=16; [\(resubmit...\)](#)

atma: rotation: lock: shim: acqu: accep

[Refresh Now](#)

St. Olaf College NMR Laboratory

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

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm

St. Olaf College NMR Laboratory

Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail](#) [Archive](#)
Last updated by IconNMR: 03/23/04 16:56

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **Goto Sample 87**

30 done 1 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

<input type="checkbox"/>	87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDC13	started: 03/23/04 16:56	estimate 6 m
Sample for ACS NS=16; (resubmit...)							
	atma:	rotation:	lock:	shim:	acqu:	runn	

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Automatic Tuning and Matching is taking care of solvent changes...

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File Edit View Go Bookmarks Tools Window Help

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File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail Archive](#)
Last updated by IconNMR: 03/23/04 16:56

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **ATMA Running**

30 done 1 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

<input type="checkbox"/>	87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDC13	started: 03/23/04 16:56	estimate 6 m
Sample for ACS NS=16; (resubmit...)							
		atma:	rotation:	lock:	shim:	acqu:	runn

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The sample is starting to rotate...

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File Edit View Go Bookmarks Tools Window Help

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm

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Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail](#) [Archive](#)
Last updated by IconNMR: 03/23/04 16:56

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **Exec [ro acqu]**

30 done 1 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

<input type="checkbox"/>	87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDC13	started: 03/23/04 16:56	estimate 5 m
Sample for ACS NS=16; (resubmit...)							
	atma:		rotation:	lock:	shim:	acqu:	runn

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the field is locked and shimmed using deuterium gradient shimming...

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File Edit View Go Bookmarks Tools Window Help

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm

St. Olaf College NMR Laboratory

Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail Archive](#)
Last updated by IconNMR: 03/23/04 16:56

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **Locking Field**

30 done 1 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

<input type="checkbox"/>	87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDC13	started: 03/23/04 16:56	estimate 4 m
Sample for ACS NS=16; (resubmit...)							
	atma:	👍	rotation:	👍	lock:	shim:	acqu: runn

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

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

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Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now](#) [Search...](#) [Detail](#) [Archive](#)
Last updated by IconNMR: 03/23/04 17:03

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **ZG In Progress**

30 done 1 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

<input type="checkbox"/>	87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDC13	started: 03/23/04 16:56	time 29 s
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Sample for ACS NS=16; [\(resubmit...\)](#)

atna: 🍀 rotation: 🍀 lock: 🍀 shim: 🍀 acqu: runn

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

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

St. Olaf College NMR Laboratory - Netscape

File Edit View Go Bookmarks Tools Window Help

http://nmr2.chem.stolaf.edu/olenmr/client/index.htm Search

St. Olaf College NMR Laboratory

Experiment Status Spectra About NMR Teams Log Out Accounts Server

St. Olaf 400 MHz NMR Facility Current Status Report

[Refresh Now Search...](#) [Detail Archive](#)
Last updated by IconNMR: 03/23/04 17:03

For marked experiments: [expedite](#) [set priority normal](#) [set priority low](#) [hold](#) [cancel](#) [halt](#)
last message from IconNMR: **Waiting for Job**

31 done 0 running 0 waiting 0 on hold 0 skipped 0 canceled 1 failed since 03/09/04 22:13

87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDCl3	finished: 03/23/04 17:03	total 7
------	--	---	------------------	-------	-----------------------------	------------

Sample for ACS NS=16; [\(resubmit...\)](#)

atna: 🍀 rotation: 🍀 lock: 🍀 shim: 🍀 acqu: 🍀

St. Olaf College NMR Laboratory

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

The screenshot shows a Netscape browser window titled "St. Olaf College NMR Laboratory - Netscape". The address bar contains the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". The main content area displays the "St. Olaf College NMR Laboratory" logo and the question "What would you like to do as research-bh?". Below this, there are eight icons with corresponding text links: "Run Experiment" (a beaker with bubbles), "View Status" (a traffic light), "View Spectra" (an NMR spectrum), "Learn About NMR" (a book), "Switch Teams" (two people), "Log Out" (an "EXIT" sign), "Edit Accounts" (two people), and "Show Server Log" (a scroll of paper). At the bottom of the page, the text "client version 1.01 (5:31 AM 7/31/2003)" and "130.71.24.219 hansonr/research-bh" is visible.

St. Olaf College NMR Laboratory

What would you like to do as research-bh?

[Run Experiment](#) [View Status](#) [View Spectra](#) [Learn About NMR](#)

[Switch Teams](#) [Log Out](#) [Edit Accounts](#) [Show Server Log](#)

client version 1.01 (5:31 AM 7/31/2003) 130.71.24.219 hansonr/research-bh

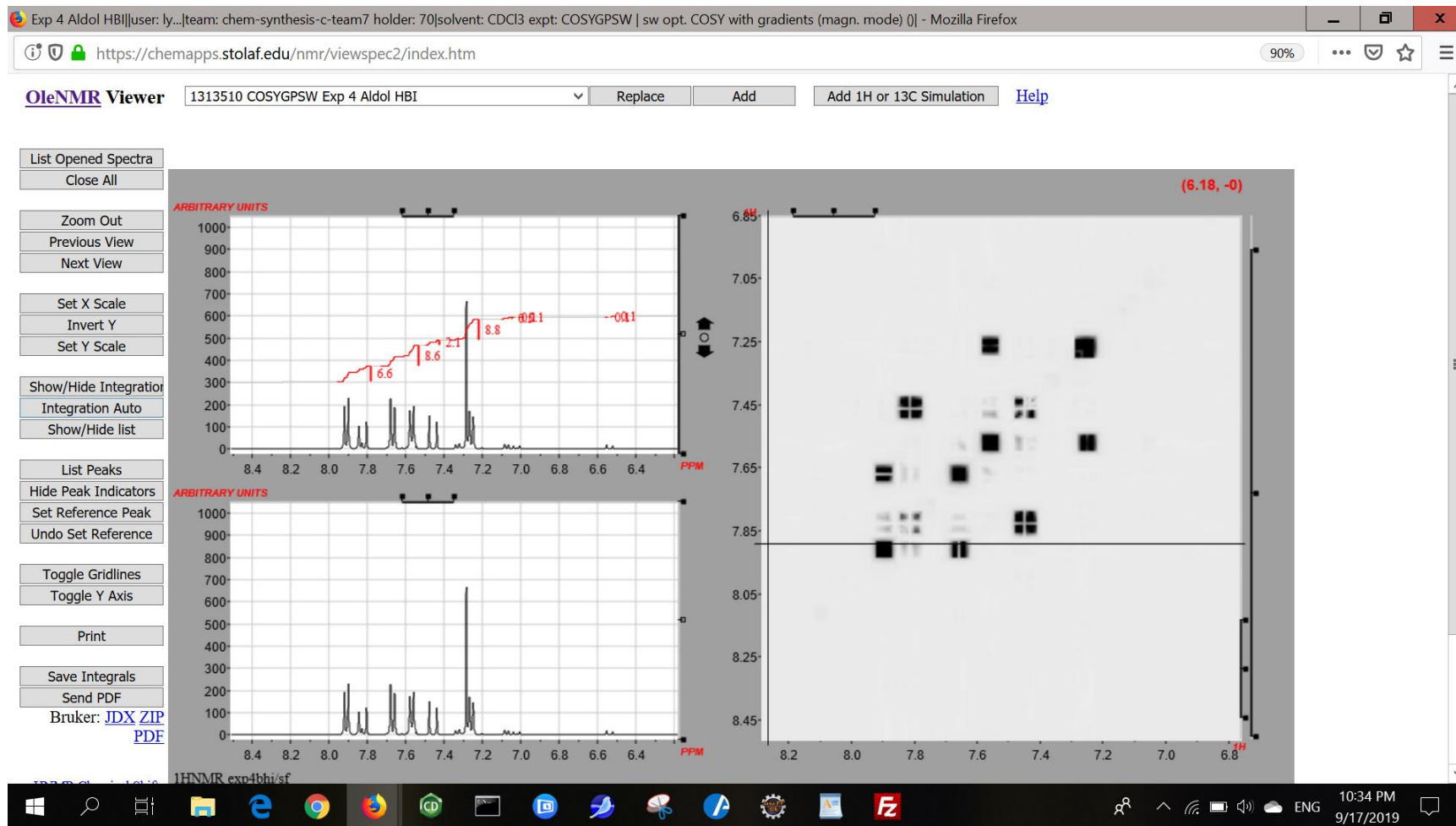
St. Olaf College NMR Laboratory

There are many options for selecting specific experiments...

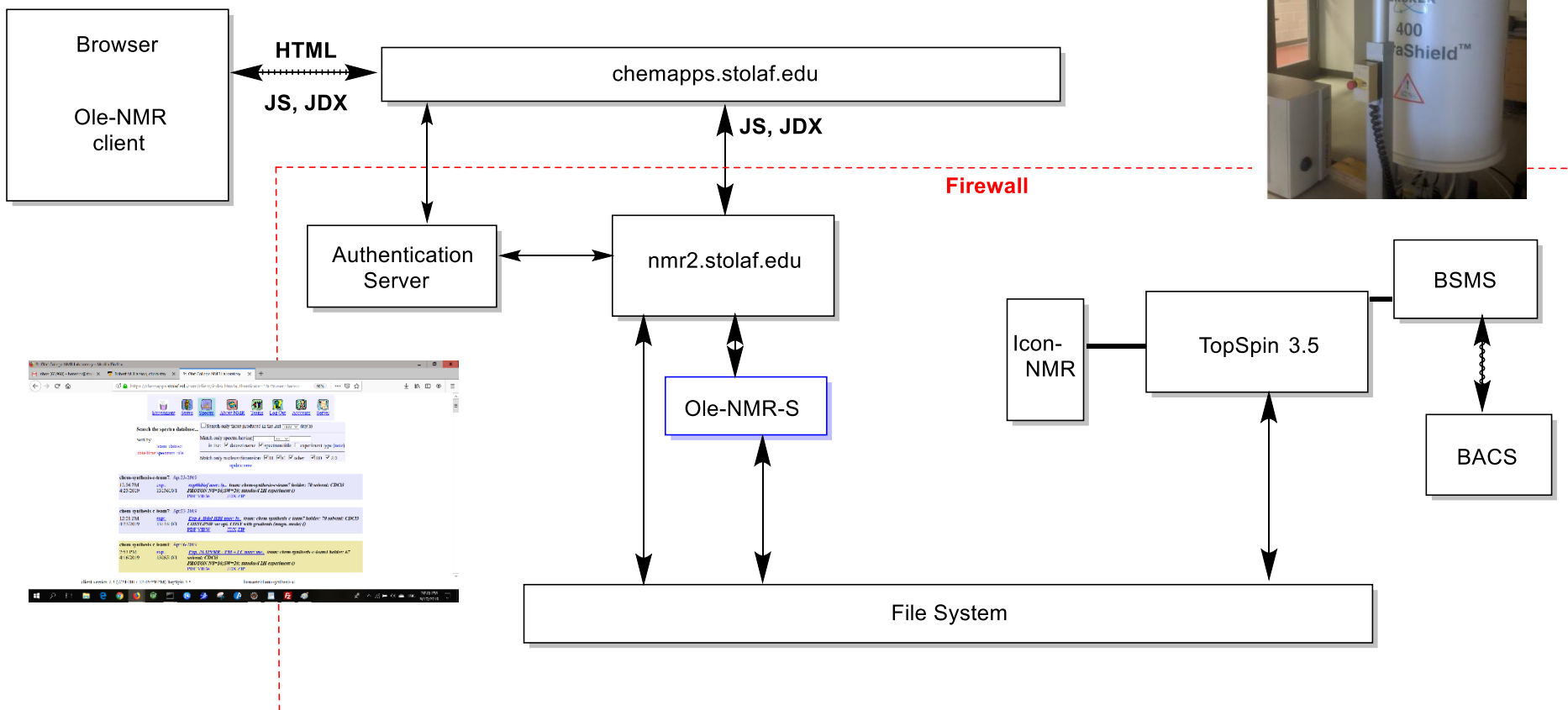
The screenshot shows a Netscape browser window displaying the St. Olaf College NMR Laboratory website. The browser's address bar shows the URL `http://nmr2.chem.stolaf.edu/olenmr/client/index.htm`. The website features a navigation menu with icons and labels for [Experiment](#), [Status](#), [Spectra](#), [About NMR](#), [Teams](#), [Log Out](#), [Accounts](#), and [Server](#). Below the navigation menu is a search section titled "Search the spectra database...". This section includes a search input field, a dropdown menu for "Search only those produced in the last" with a value of "7" and "day(s)", and a "Match only spectra having" section with a dropdown menu set to "or". The "Match only spectra having" section includes checkboxes for "dataset name", "spectrum title", and "experiment type (note)". Below this is a "Match only nucleus/dimension:" section with checkboxes for "H", "C", "other", "1D", and "2D". A link "update now" is also present. The main content area displays a search result for "research-bh: Mar23-2004" with a timestamp of "5:03 PM 3/23/2004" and an experiment ID of "expt. 1142010/1". The result description is "*Sample for ACS team: research-bh holder: 87 solvent: CDCl3 PROTON NS=16; standard 1H experiment (1 Min 34 Sec)*". Below the description are links for "PDF (dir)", "EXPT", and "JDX (dir)".

St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



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...

The screenshot shows a Netscape browser window displaying the St. Olaf College NMR Laboratory website. The browser's address bar shows the URL `http://nmr2.chem.stolaf.edu/olenmr/client/index.htm`. The website features a navigation menu with icons and labels for [Experiment](#), [Status](#), [Spectra](#), [About NMR](#), [Teams](#), [Log Out](#), [Accounts](#), and [Server](#). Below the navigation menu is a search section titled "Search the spectra database...". This section includes a search input field, a dropdown menu for "Search only those produced in the last" with a value of "7" and "day(s)", and a "Match only spectra having" section with a dropdown menu set to "or". The "Match only spectra having" section includes checkboxes for "dataset name", "spectrum title", and "experiment type (note)". Below this is a "Match only nucleus/dimension:" section with checkboxes for "H", "C", "other", "1D", and "2D". A link "update now" is also present. The main content area displays a search result for "research-bh: Mar23-2004" with a timestamp of "5:03 PM 3/23/2004" and an experiment ID of "expt. 1142010/1". The result description is "*Sample for ACS team: research-bh holder: 87 solvent: CDCl3 PROTON NS=16; standard 1H experiment (1 Min 34 Sec)*". Below the description are links for "PDF (dir)", "EXPT", and "JDX (dir)".

St. Olaf College NMR Laboratory

Analysis using JSpecView-JS

The screenshot displays the OleNMR Viewer application window. The title bar indicates the experiment name: "Exp 4 Aldol HBI". The address bar shows the URL: "https://chemapps.stolaf.edu/nmr/viewspec2/index.htm". The main window contains a 2D NMR spectrum plot with a vertical axis from 0 to 8 and a horizontal axis from 0 to 8. A dialog box is overlaid on the plot, asking: "This 2D spectrum has one or more 1D data sets associated with it. Do you want to load those as well?". The dialog has "OK" and "Cancel" buttons. The left sidebar contains various controls such as "List Opened Spectra", "Zoom Out", "Set X Scale", and "List Peaks". The Windows taskbar at the bottom shows the system tray with the date and time: "11:33 PM 9/25/2019".

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Analysis using JSpecView-JS

The screenshot displays the OleNMR Viewer software interface. The main window shows a 2D NMR spectrum with a grid. The x-axis is labeled from 8 to 0, and the y-axis is labeled from 1 to 8. A dialog box is overlaid on the spectrum, containing the following text:

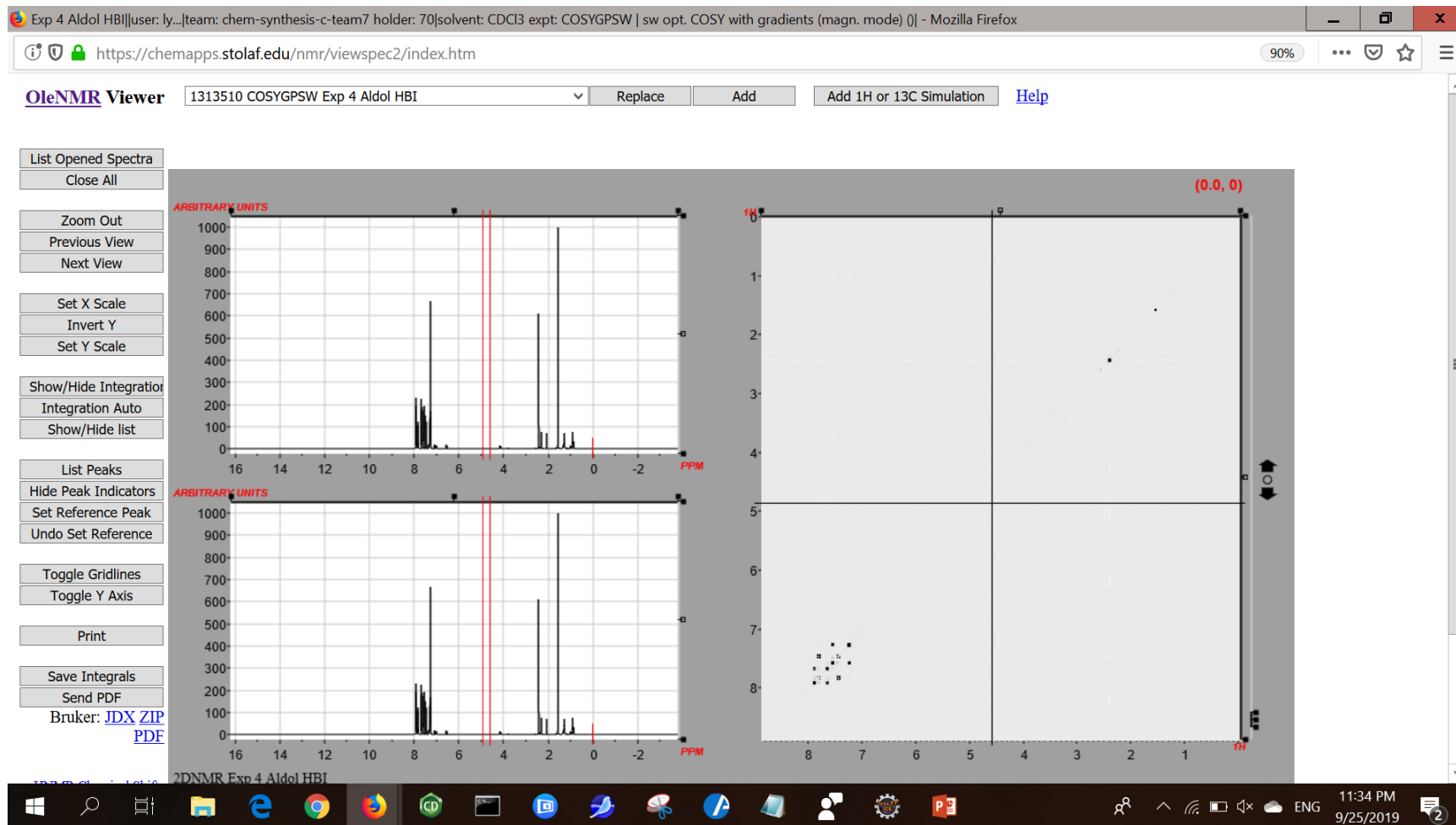
```
Sending JSpecView the following command:  
  
load append "https://chemapps.stolaf.edu/nmr/getjdx.php?host=http://nmr2.public.stolaf.edu&jdx=chem-synthesis-c-team7/Apr09-2019_1298510_1.jdx"  
load append "https://chemapps.stolaf.edu/nmr/getjdx.php?host=http://nmr2.public.stolaf.edu&jdx=chem-synthesis-c-team7/Apr09-2019_1298510_1.jdx"  
view *  
link ALL
```

Below the command text is a checkbox labeled "Prevent this page from creating additional dialogs" which is currently unchecked. At the bottom right of the dialog box are "OK" and "Cancel" buttons.

The software interface includes a top menu bar with "Replace", "Add", "Add 1H or 13C Simulation", and "Help". On the left side, there is a vertical toolbar with various functions such as "List Opened Spectra", "Zoom Out", "Previous View", "Next View", "Set X Scale", "Invert Y", "Set Y Scale", "Show/Hide Integration", "List Peaks", "Hide Peak Indicators", "Set Reference Peak", "Undo Set Reference", "Toggle Gridlines", "Toggle Y Axis", "Print", "Save Integrals", and "Send PDF". The bottom status bar shows "Application loaded.", "2DNMR Exp 4 Aldol HBI", and the system clock "11:33 PM 9/25/2019".

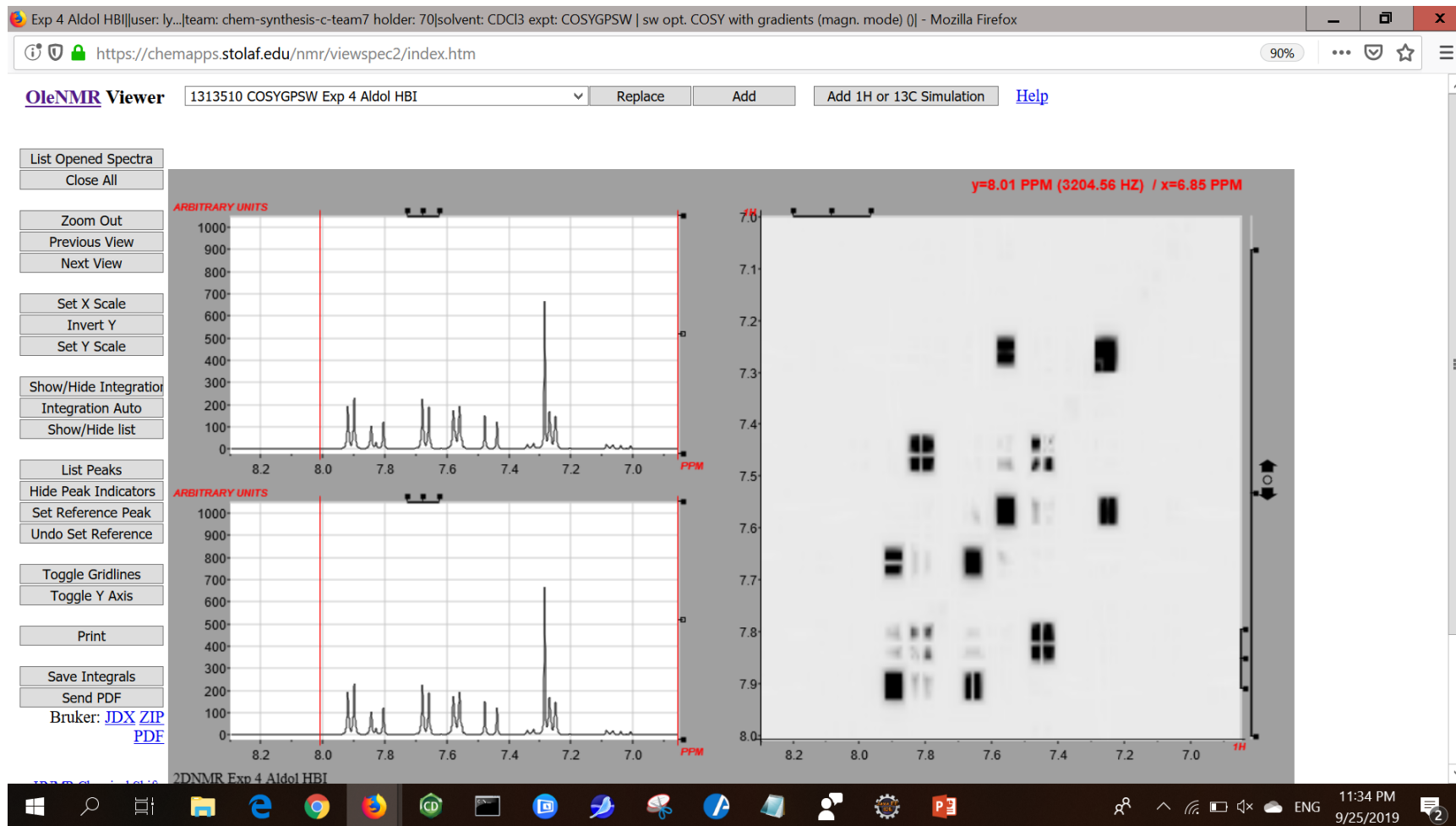
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Analysis using JSpecView-JS



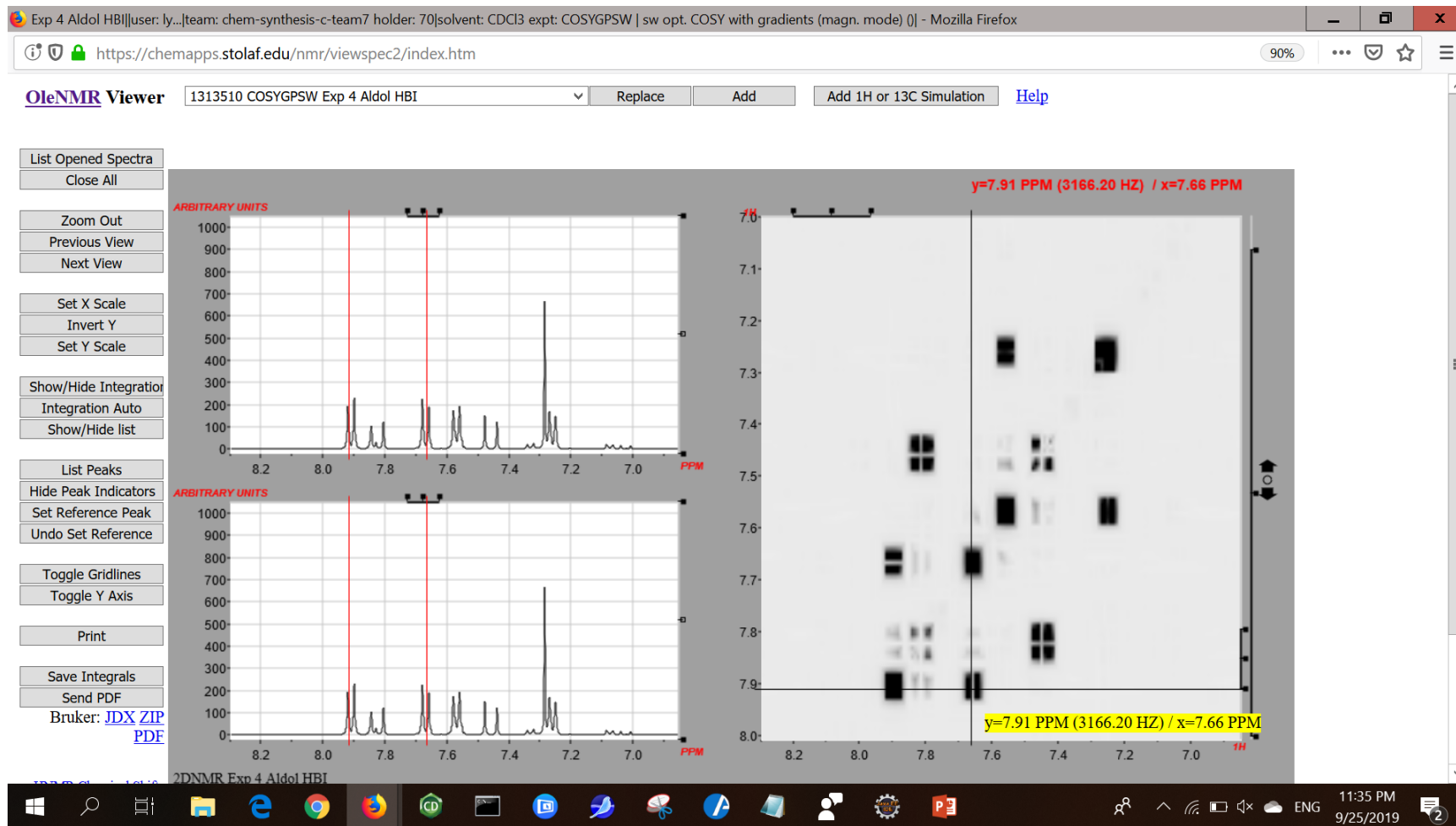
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Analysis using JSpecView-JS



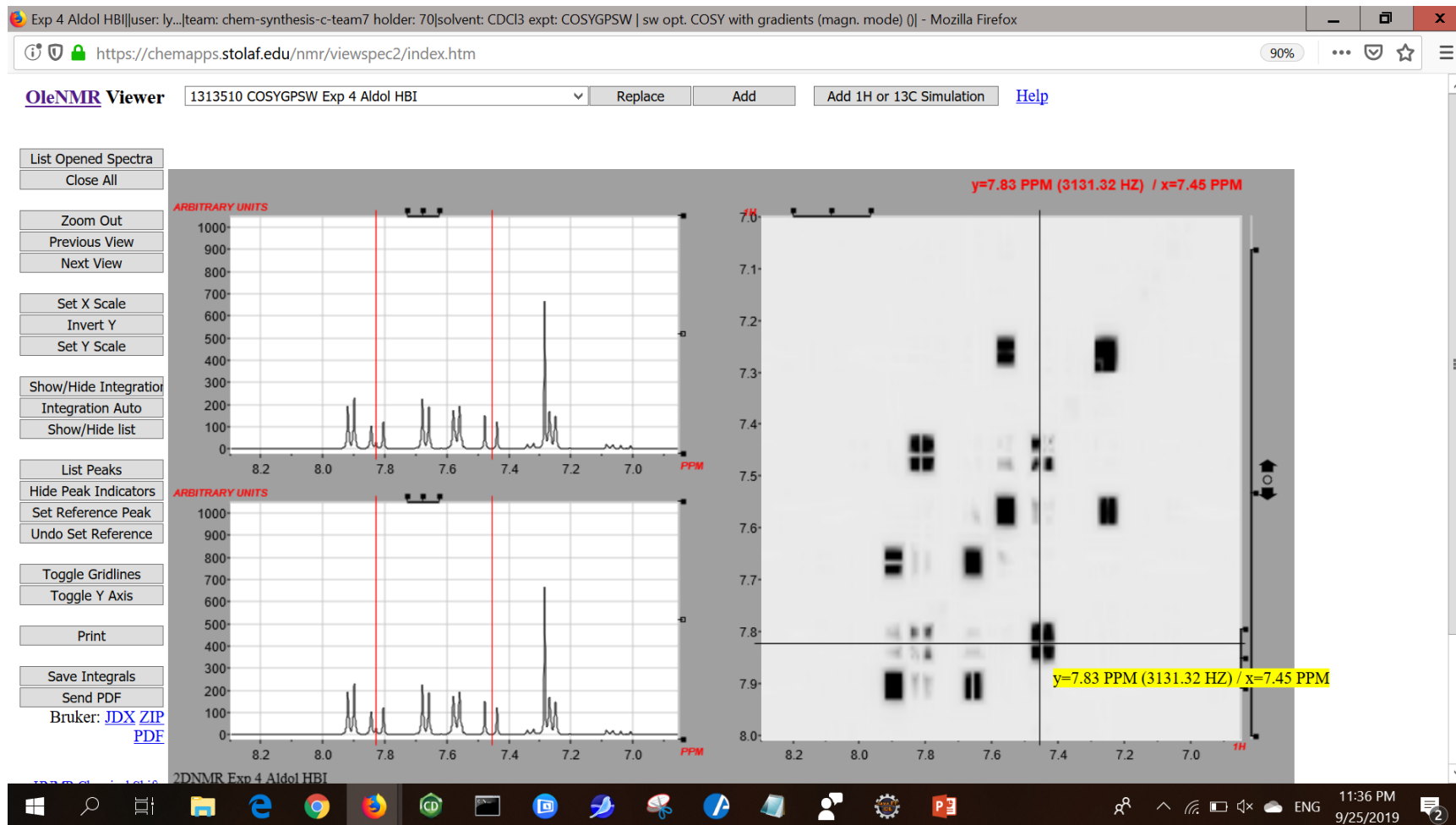
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Analysis using JSpecView-JS



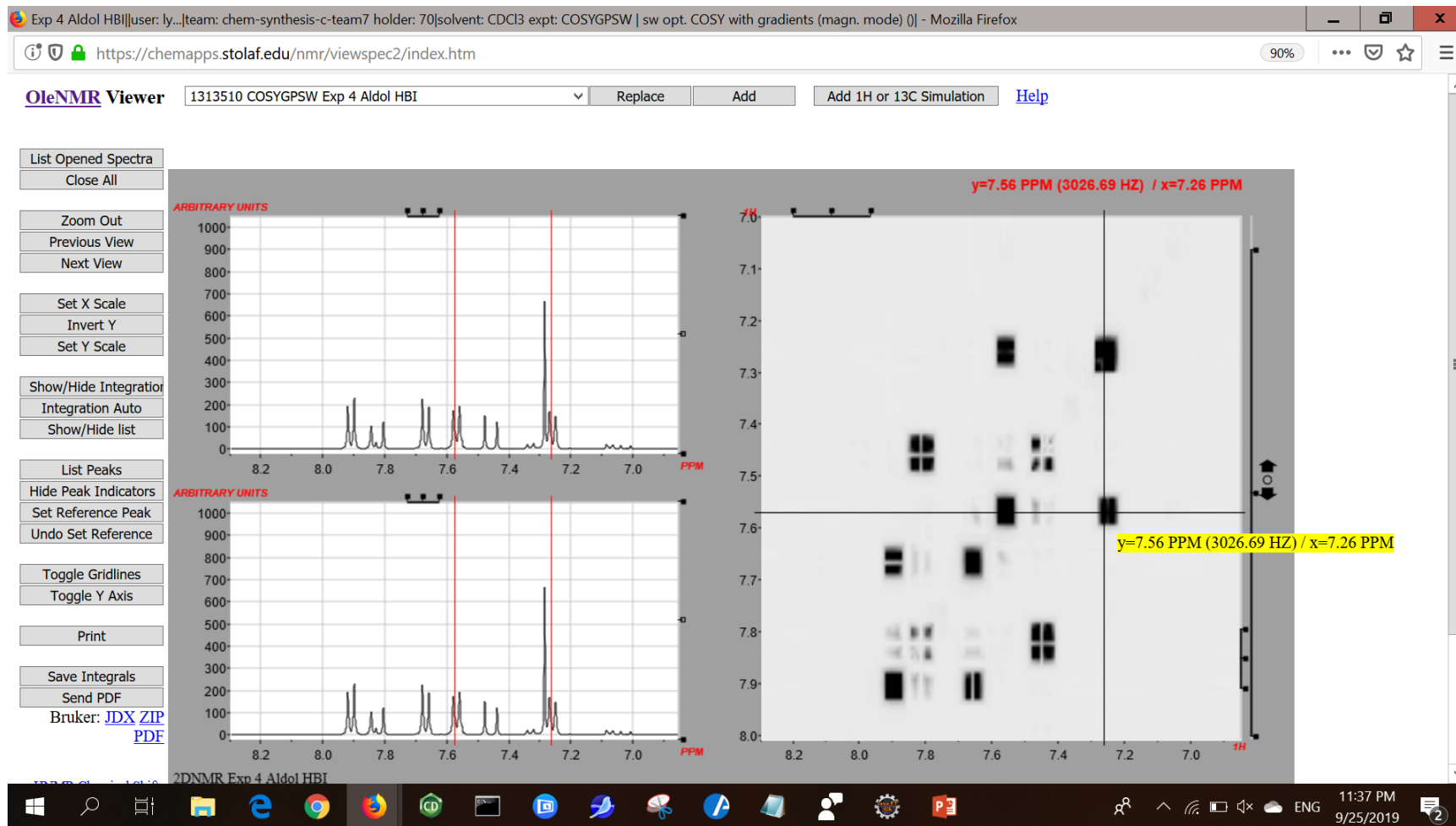
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Analysis using JSpecView-JS



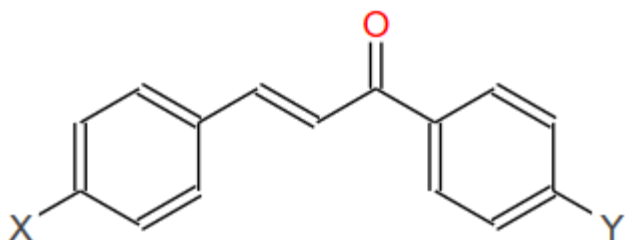
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Analysis using JSpecView-JS



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Analysis using JSpecView-JS



- Previous View
- Next View
- Set X Scale
- Invert Y
- Set Y Scale
- Show/Hide Integration
- Integration Auto
- Show/Hide list

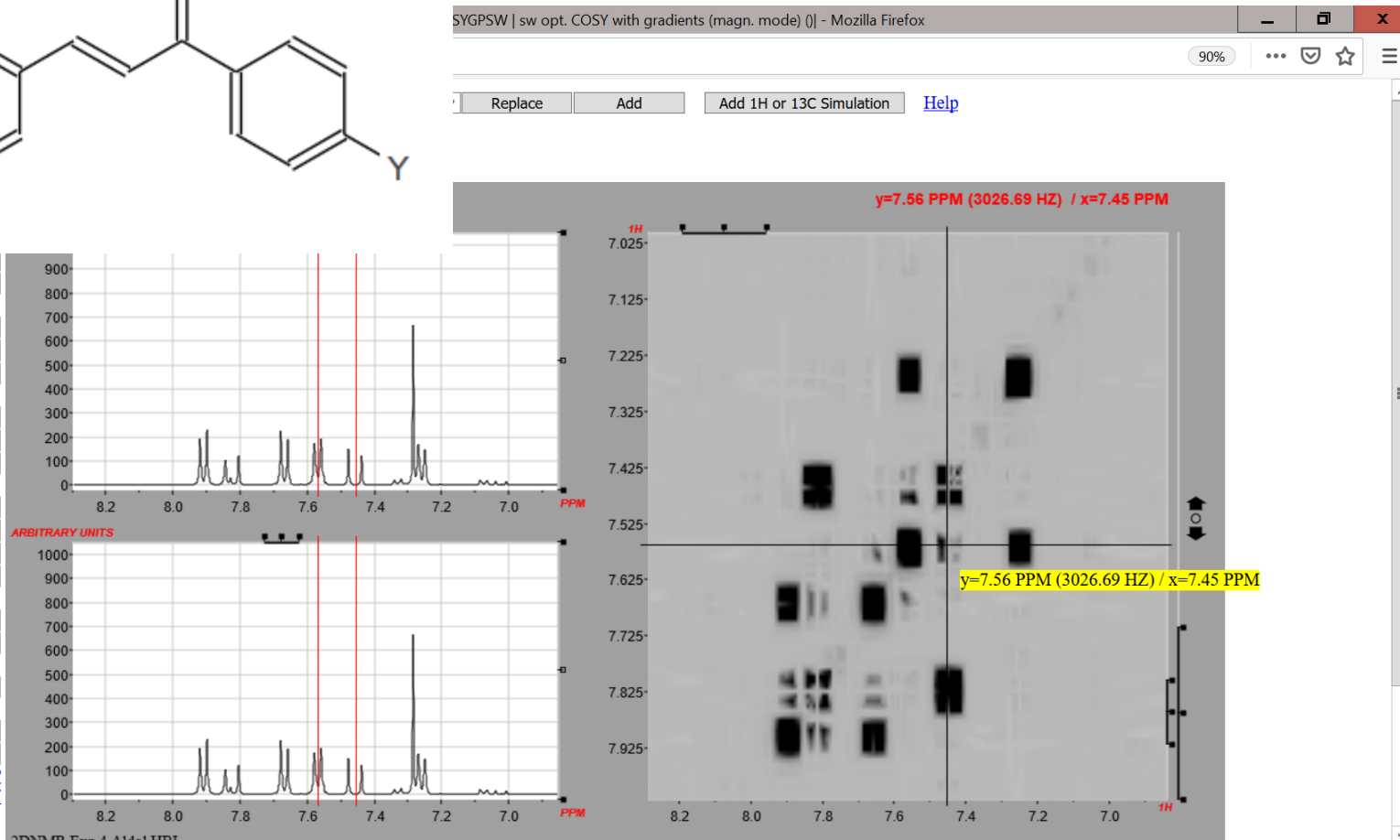
- List Peaks
- Hide Peak Indicators
- Set Reference Peak
- Undo Set Reference

- Toggle Gridlines
- Toggle Y Axis

Print

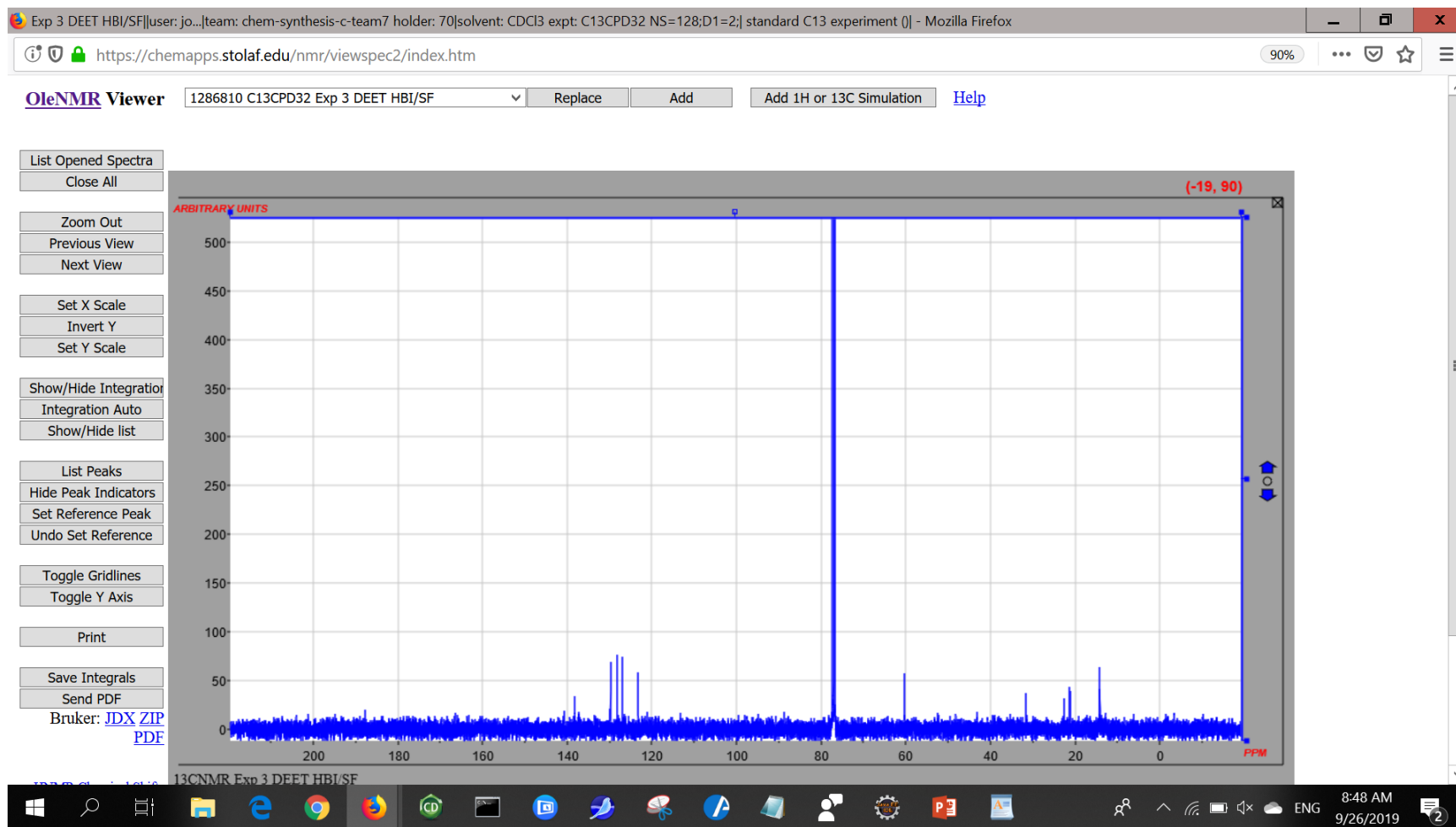
- Save Integrals
- Send PDF

Bruker: [JDX ZIP](#)
[PDF](#)



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Analysis using JSpecView-JS



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Analysis using JSpecView-JS

Exp 3 DEET HBI/SF|user: jo...|team: chem-synthesis-c-team7 holder: 70|solvent: CDCl3 expt: C13CPD32 NS=128;D1=2;| standard C13 experiment (0) - Mozilla Firefox

https://chemapps.stolaf.edu/nmr/viewspec2/index.htm 90%

OleNMR Viewer 1286810 C13CPD32 Exp 3 DEET HBI/SF Replace Add Add 1H or 13C Simulation Help

List Opened Spectra
Close All

Zoom Out
Previous View
Next View

Set X Scale
Invert Y
Set Y Scale

Show/Hide Integration
Integration Auto
Show/Hide list

List Peaks
Hide Peak Indicators
Set Reference Peak
Undo Set Reference

Toggle Gridlines
Toggle Y Axis

Print

Save Integrals
Send PDF
Bruker: [JDX ZIP](#)
[PDF](#)

ARBITRARY UNITS (-19, 9)

1000
900
800
700
600
500
400
300
200
100
0

200 180 160 140 120 100 80 60 40 20 0 PPM

Draw a compound or enter a compound name or ID and press Search to load a simulated spectrum.

compound name or ID here
NCI-CIR Search

Add 1H Simulation
Add 13C Simulation
View 3D
Close

13CNMR Exp 3 DEET HBI/SF

8:49 AM
9/26/2019

The screenshot displays the OleNMR Viewer web application. The main window shows a 13C NMR spectrum with a y-axis labeled 'ARBITRARY UNITS' ranging from 0 to 1000 and an x-axis labeled 'PPM' ranging from 200 to 0. A prominent peak is visible at approximately 77 ppm. A simulation overlay is active, featuring a toolbar with various icons and a search box. The search box contains the text 'compound name or ID here' and 'NCI-CIR'. Below the search box are buttons for 'Add 1H Simulation', 'Add 13C Simulation', 'View 3D', and 'Close'. The browser's address bar shows the URL 'https://chemapps.stolaf.edu/nmr/viewspec2/index.htm' and the page title 'OleNMR Viewer'. The Windows taskbar at the bottom shows the system time as 8:49 AM on 9/26/2019.

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Analysis using JSpecView-JS

Exp 3 DEET HBI/SF|user: jo...|team: chem-synthesis-c-team7 holder: 70|solvent: CDCl3 expt: C13CPD32 NS=128;D1=2;| standard C13 experiment (0) - Mozilla Firefox

https://chemapps.stolaf.edu/nmr/viewspec2/index.htm 90%

OleNMR Viewer 1286810 C13CPD32 Exp 3 DEET HBI/SF Replace Add Add 1H or 13C Simulation Help

List Opened Spectra
Close All

Zoom Out
Previous View
Next View

Set X Scale
Invert Y
Set Y Scale

Show/Hide Integration
Integration Auto
Show/Hide list

List Peaks
Hide Peak Indicators
Set Reference Peak
Undo Set Reference

Toggle Gridlines
Toggle Y Axis

Print

Save Integrals
Send PDF
Bruker: [JDX ZIP](#)
[PDF](#)

Draw a compound or enter a compound name or ID and press Search to load a simulated spectrum.

compound name or ID here
NCI-CIR Search

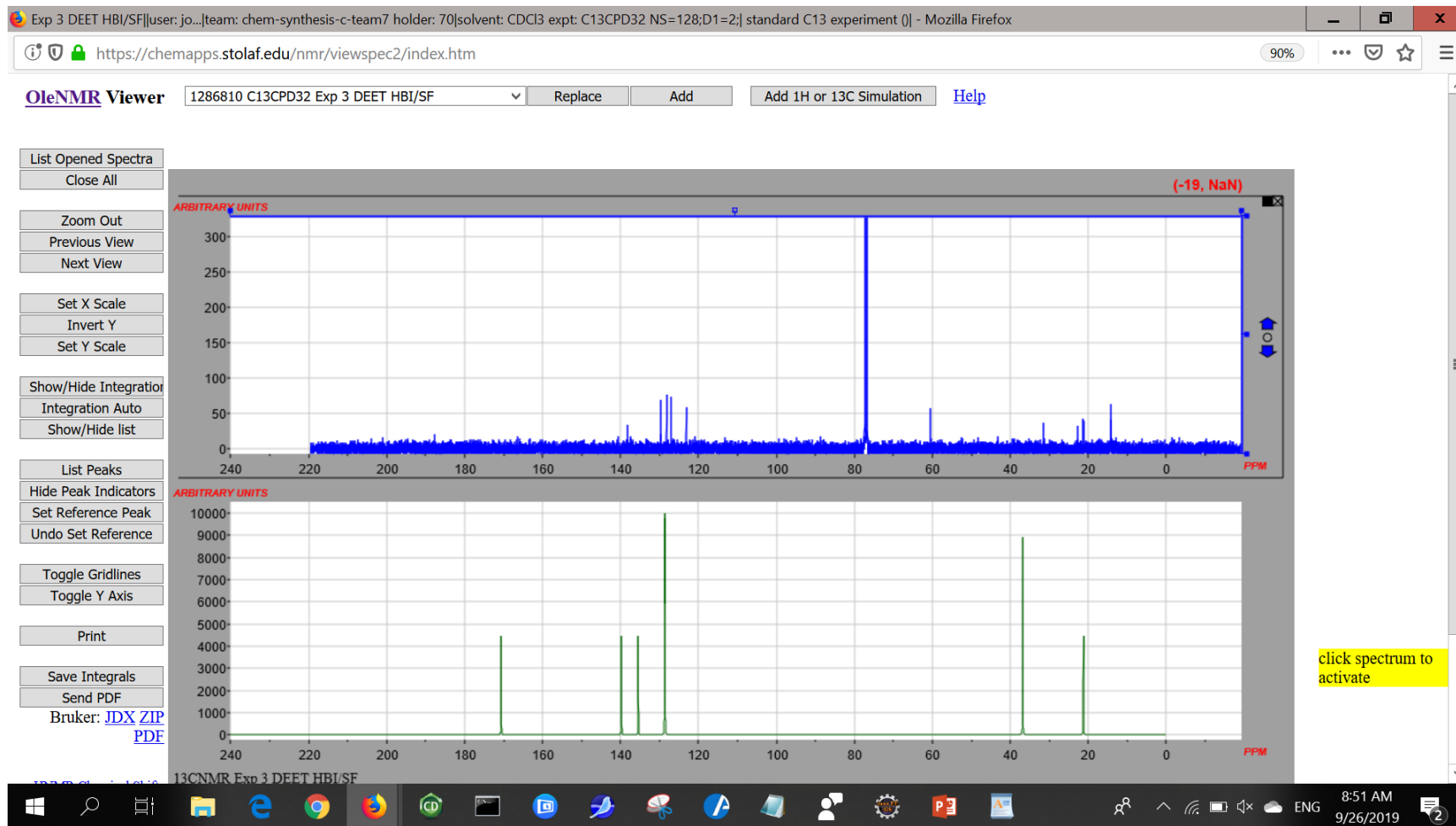
Add 1H Simulation
Add 13C Simulation
View 3D
Close

13CNMR Exp 3 DEET HBI/SF

8:49 AM
9/26/2019

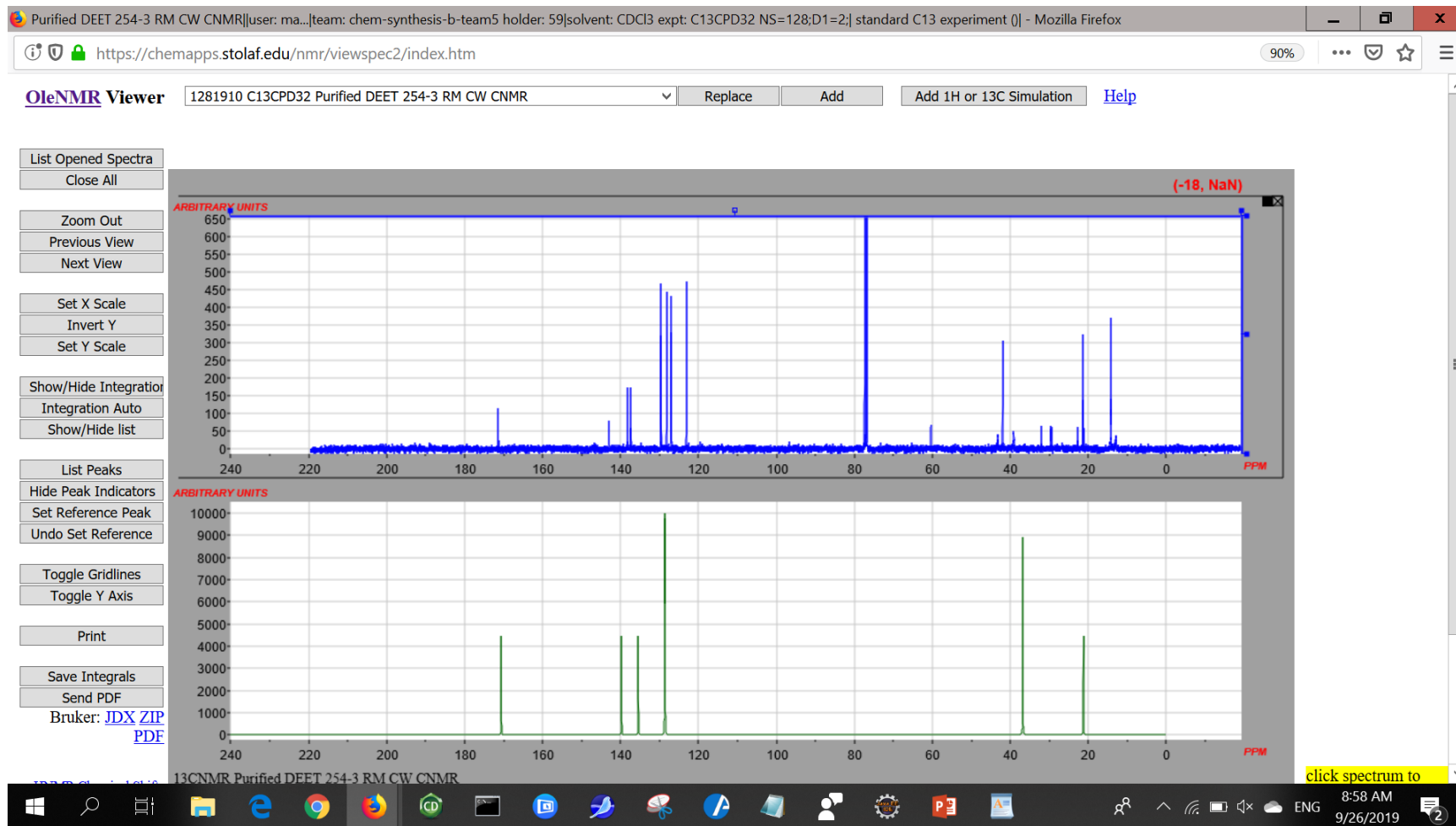
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Analysis using JSpecView-JS



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Analysis using JSpecView-JS



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Analysis using JSpecView-JS

Purified DEET 254-3 RM CW CNMR[user: ma...|team: chem-synthesis-b-team5 holder: 59|solvent: CDCl3 exp: C13CPD32 NS=128;D1=2;] standard C13 experiment (0) - Mozilla Firefox

https://chemapps.stolaf.edu/nmr/viewspec2/index.htm 90%

OleNMR Viewer 1281910 C13CPD32 Purified DEET 254-3 RM CW CNMR Replace Add Add 1H or 13C Simulation Help

List Opened Spectra
Close All

Zoom Out
Previous View
Next View

Set X Scale
Invert Y
Set Y Scale

Show/Hide Integration
Integration Auto
Show/Hide list

List Peaks
Hide Peak Indicators
Set Reference Peak
Undo Set Reference

Toggle Gridlines
Toggle Y Axis

Print

Save Integrals
Send PDF
Bruker: [JDX](#) [ZIP](#) [PDF](#)

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Analysis using JSpecView-JS

JSpeView/JSME/nmrdb/NIH-Resolver demo - Mozilla Firefox

jalview/develop | Inbox (64,196) | St. Olaf College N | JSpeView/JSME | JSpeView/JSME/ | JSpeView/JSME/ | https://chemapps | Window oper | JSpeView/JSME/ | NONIUS.HSI/A | NONIUS.HSI/A

https://chemapps.stolaf.edu/nmr/viewspec2/jsmol/nmr_predict_HC.htm?jme=12

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ARBITRARY UNITS

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10 9 8 7 6 5 4 3 2 1 PPM

H1&C13 →

C
N
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S
F
Cl
Br
I
P
X

C1=CC(C)=CC=C1C(N(C)C)=O Search

ARBITRARY UNITS

10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
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240 220 200 180 160 140 120 100 80 60 40 20 PPM

1HNMR SIMULATED

print

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Analysis using JSpecView-JS

JSpecView/JSME/nmrdb/NIH-Resolver demo - Mozilla Firefox

jalview/develop | Inbox (64,196) | St. Olaf College N | JSpecView/JSME | JSpecView/JSME/ | JSpecView/JSME/ | https://chemapps | Window oper | JSpecView/JSME/ | NONIUS.HSI/A | NONIUS.HSI/A

https://chemapps.stolaf.edu/nmr/viewspec2/jsmol/nmr_predict_HC.htm?jme=12

90%

0, 3693

ARBITRARY UNITS

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4000
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2000
1000
0

10 9 8 7 6 5 4 3 2 1 PPM

ARBITRARY UNITS

10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0

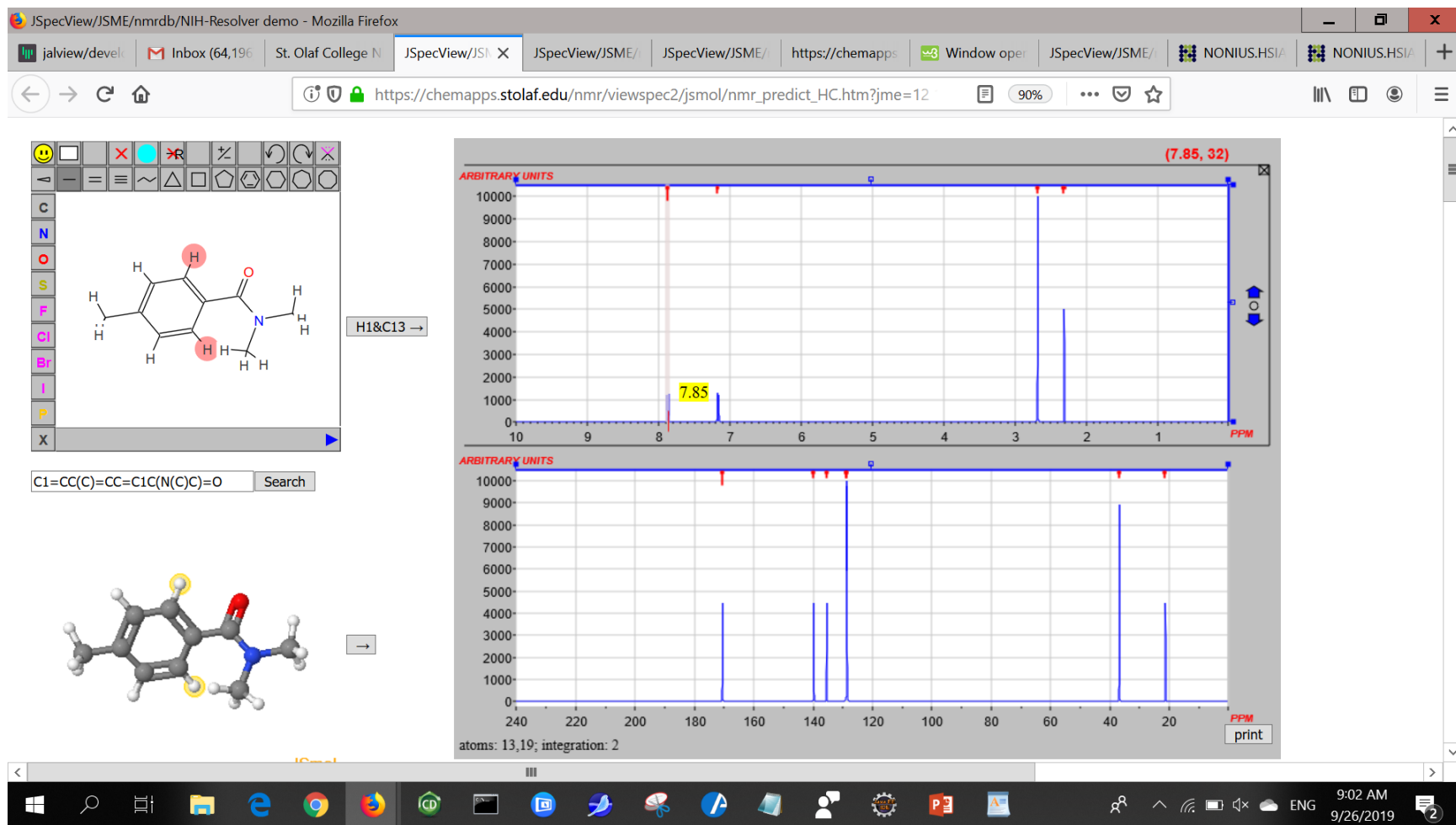
240 220 200 180 160 140 120 100 80 60 40 20 PPM

print

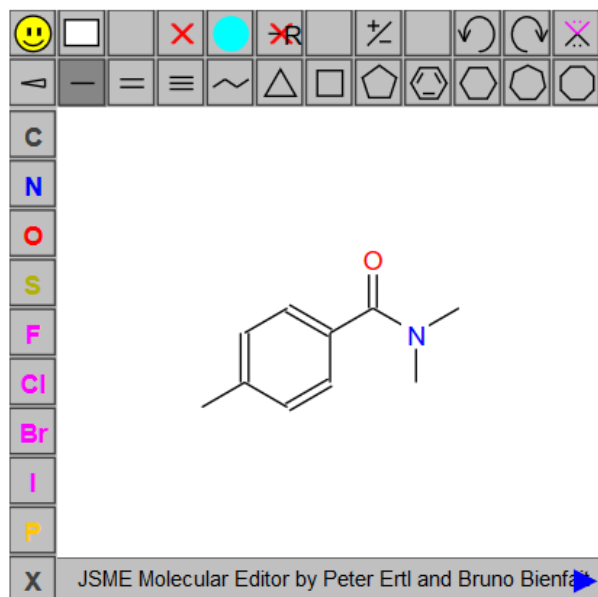
C1=CC(C)=CC=C1C(N(C)C)=O Search

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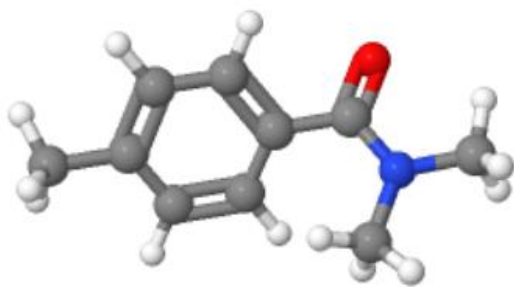
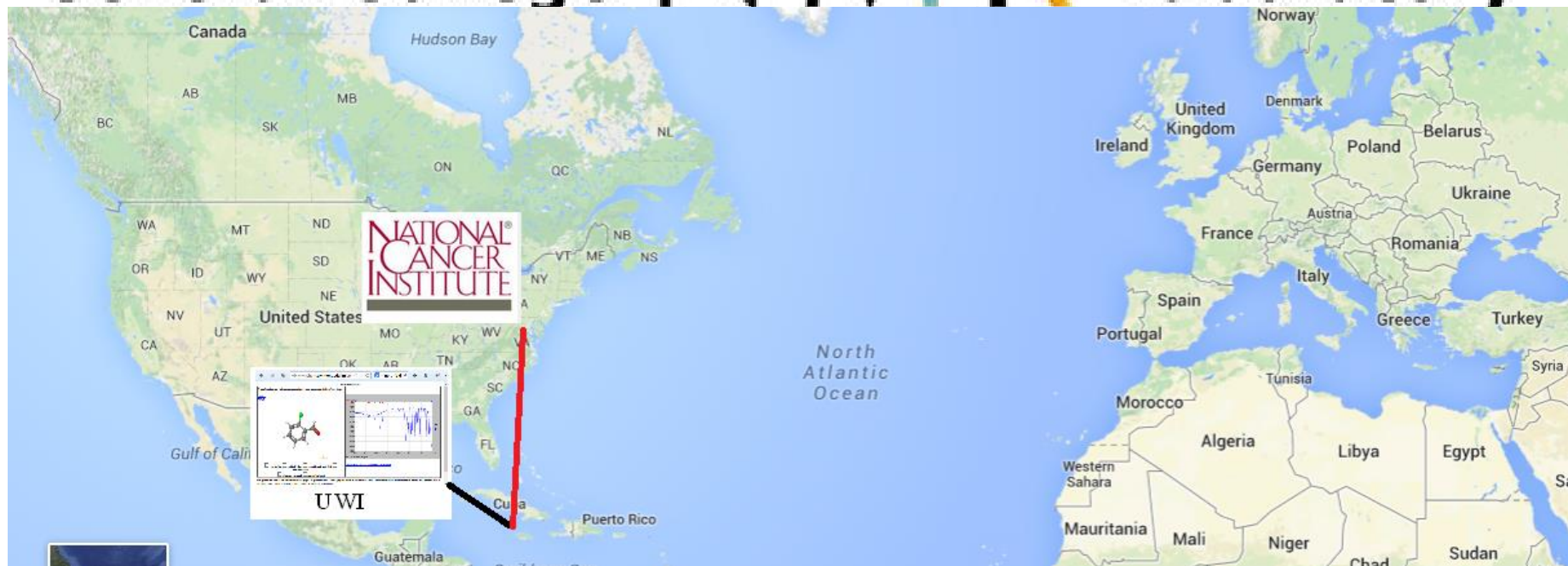
Analysis using JSpecView-JS



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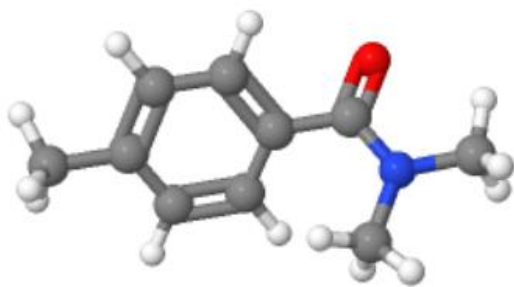
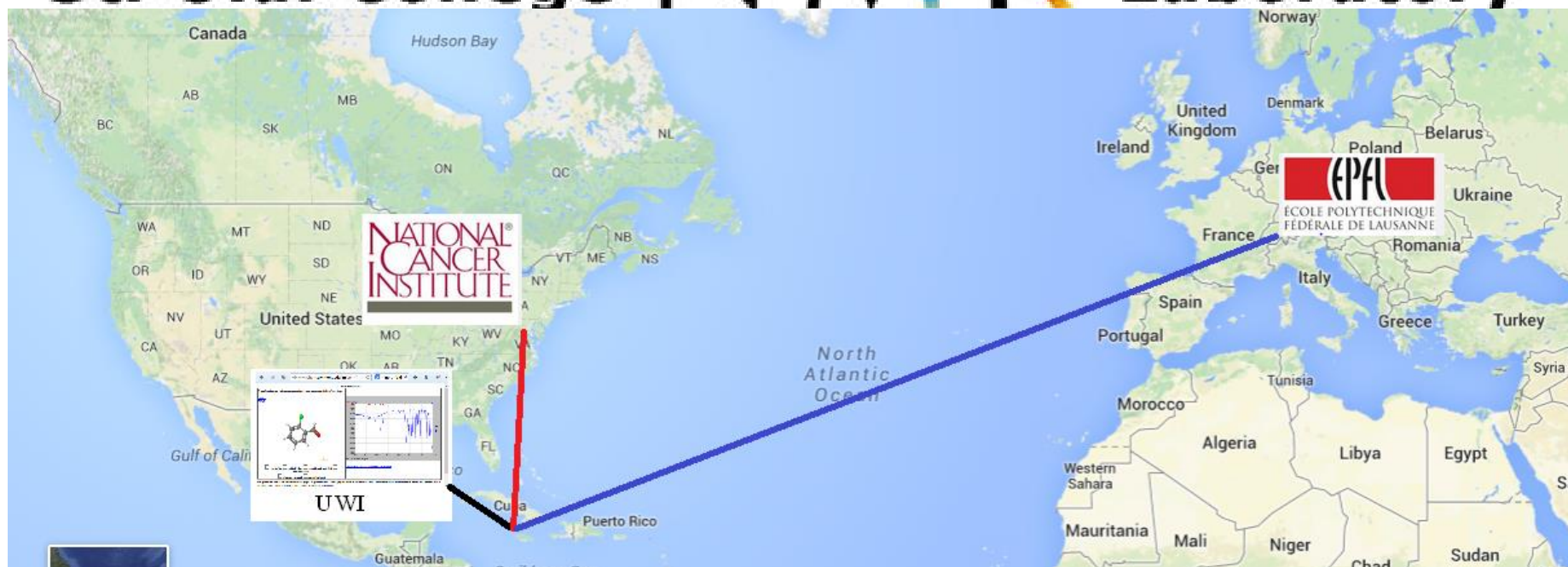


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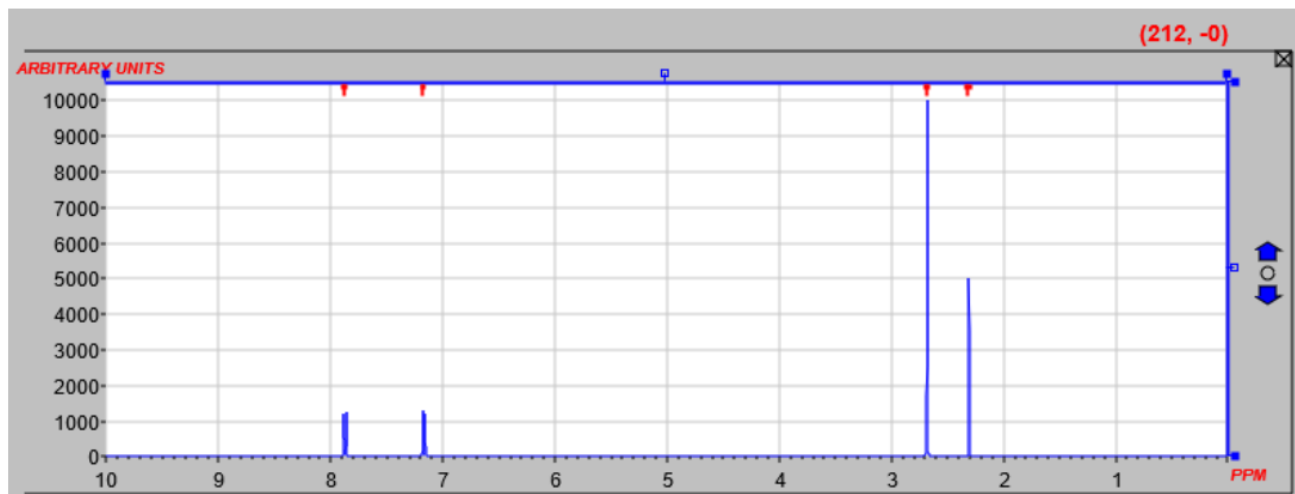


JSmol

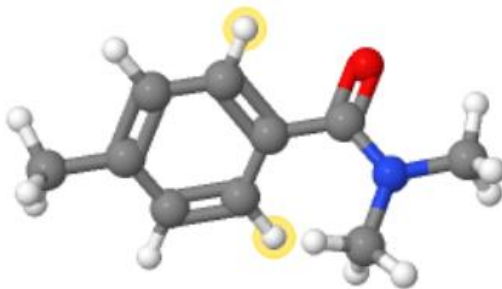
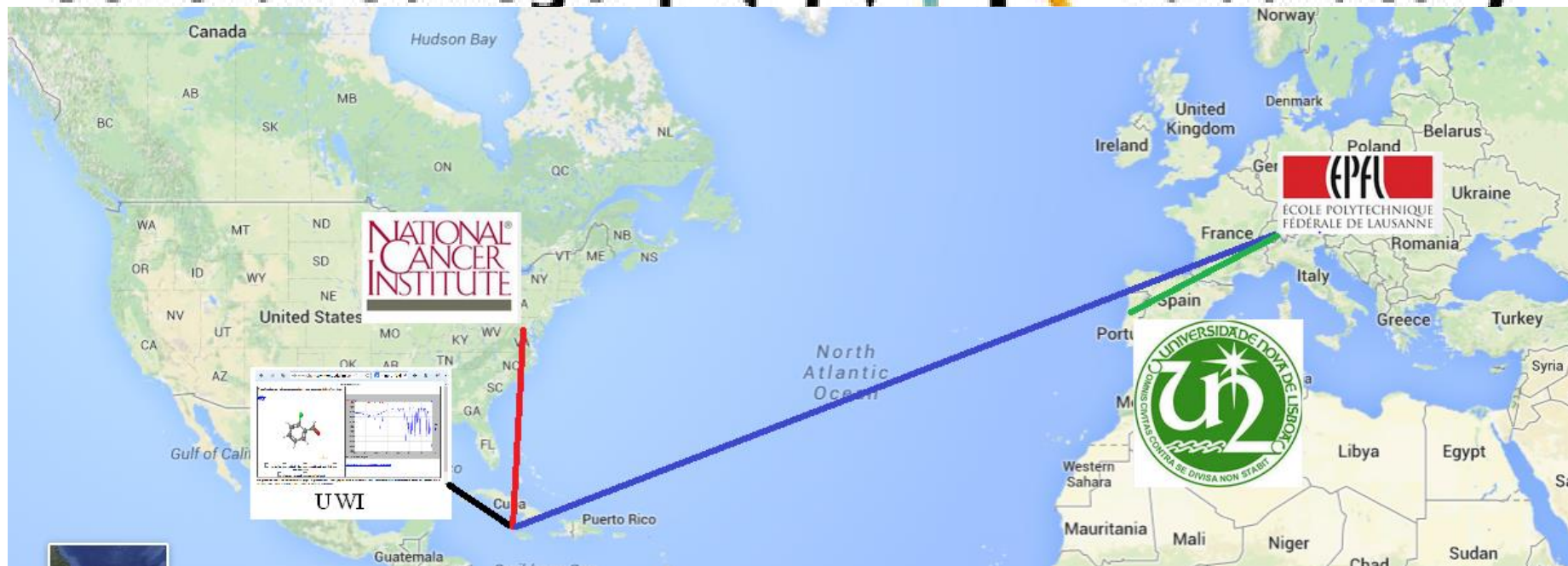
St. Olaf College **NMR** Laboratory



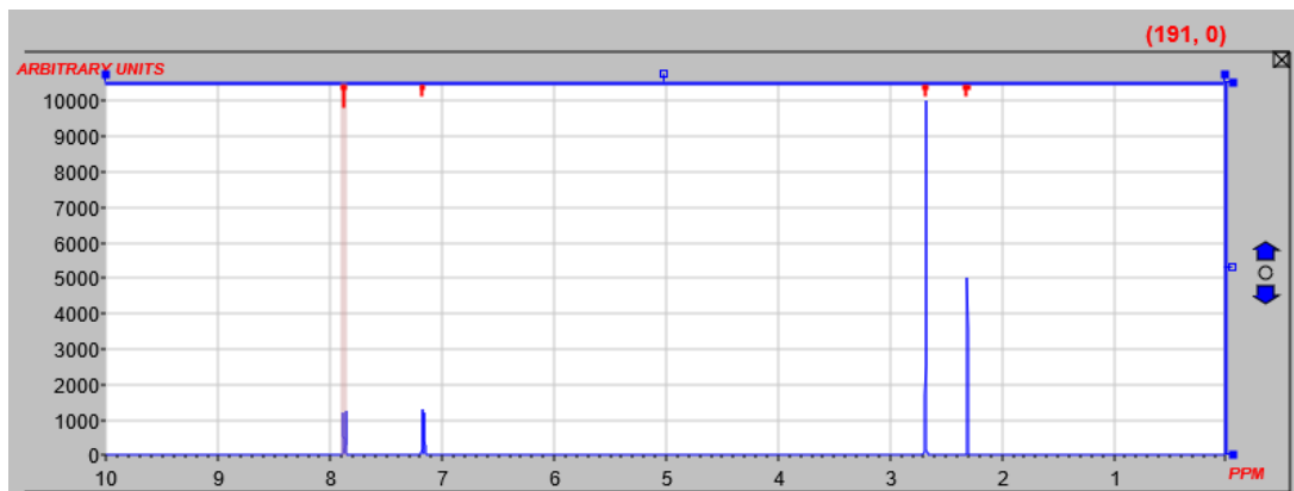
JSmol



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JSmol



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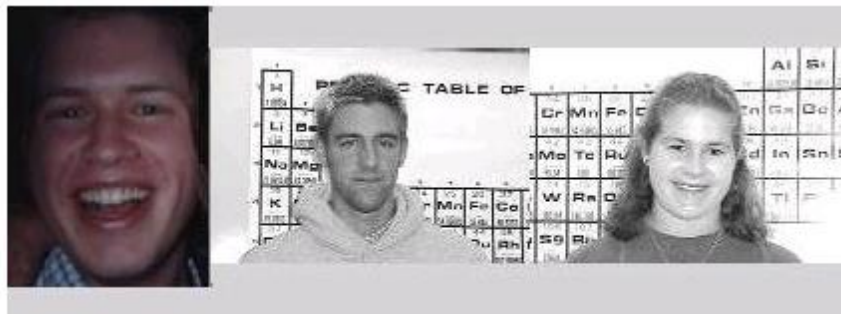
- Peter Ertl, Novartis
- Robert Lancashire, UWI-Mona
- Clemens Anklin, Bruker



St. Olaf College NMR Laboratory

Thanks to the students who really made this possible.

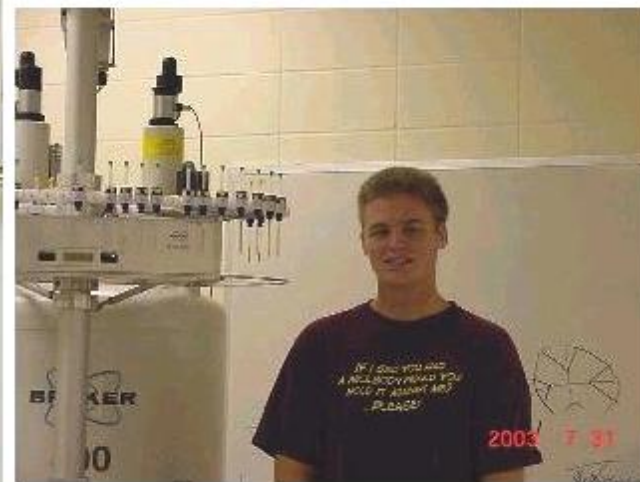
(Can you tell they had fun?)



Mike Purnell, Gregg Sydow, and Stephanie Skladzien



Jared Irwin



Bryan Anderson