

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 N M R Laboratory

Part I: The instrument and interface

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

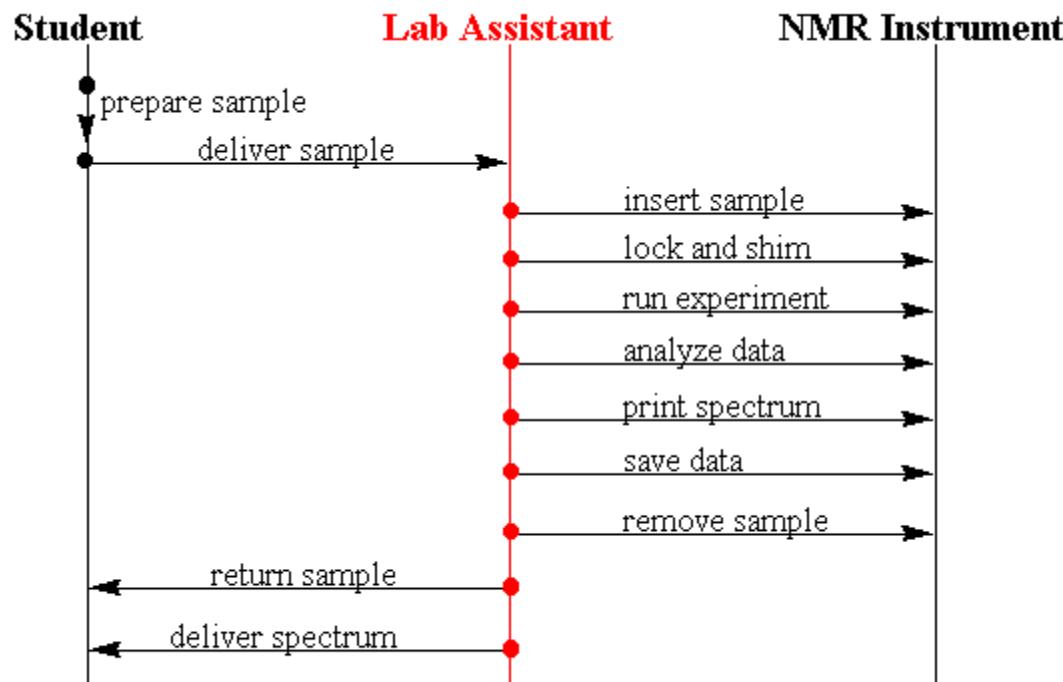
St. Olaf College N M R Laboratory

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



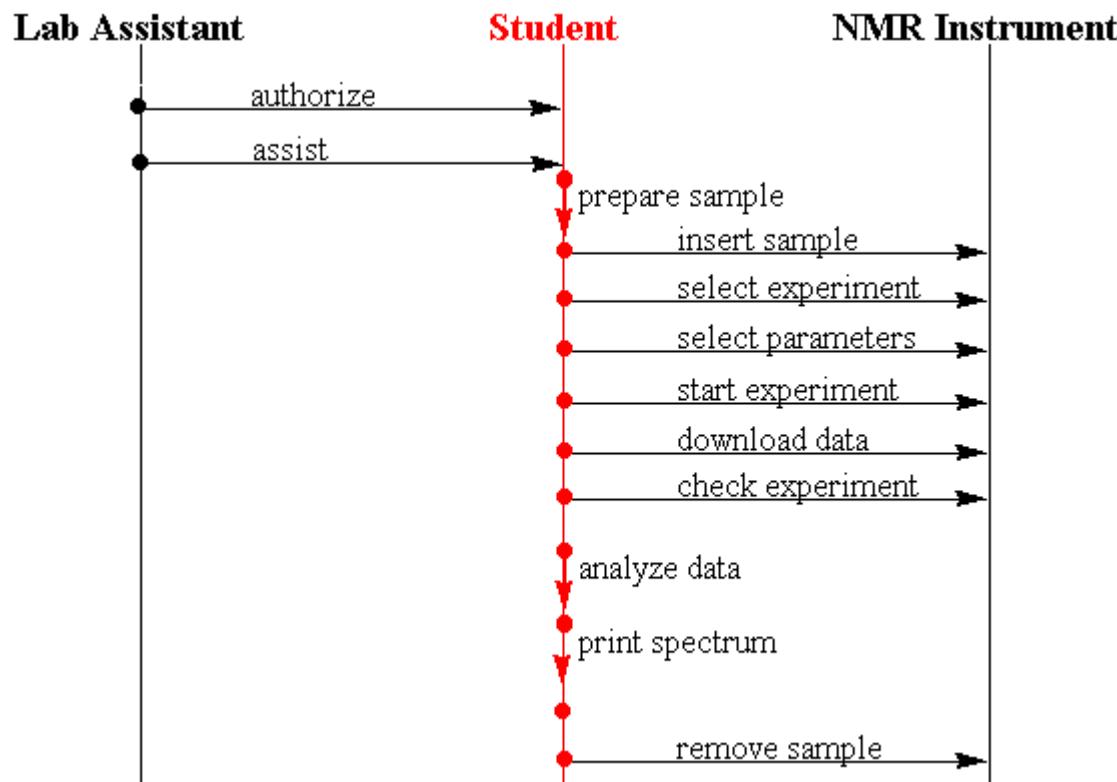
St. Olaf College N M R Laboratory

The OLD way...



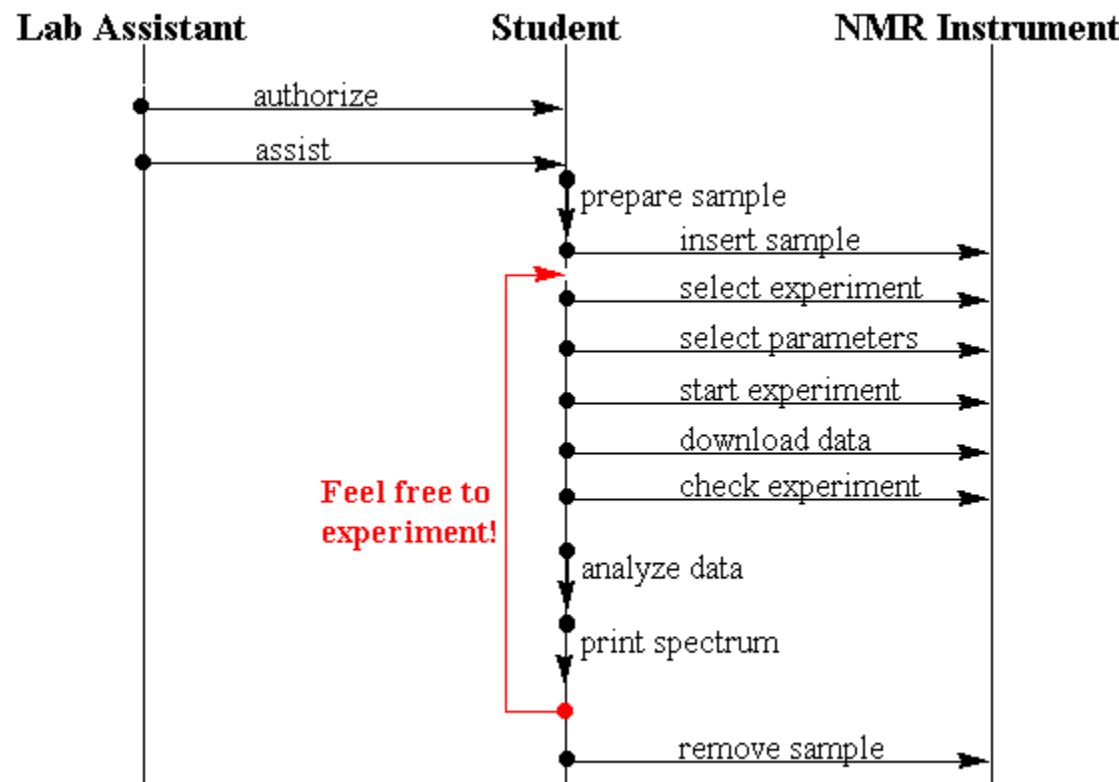
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...and the new way...



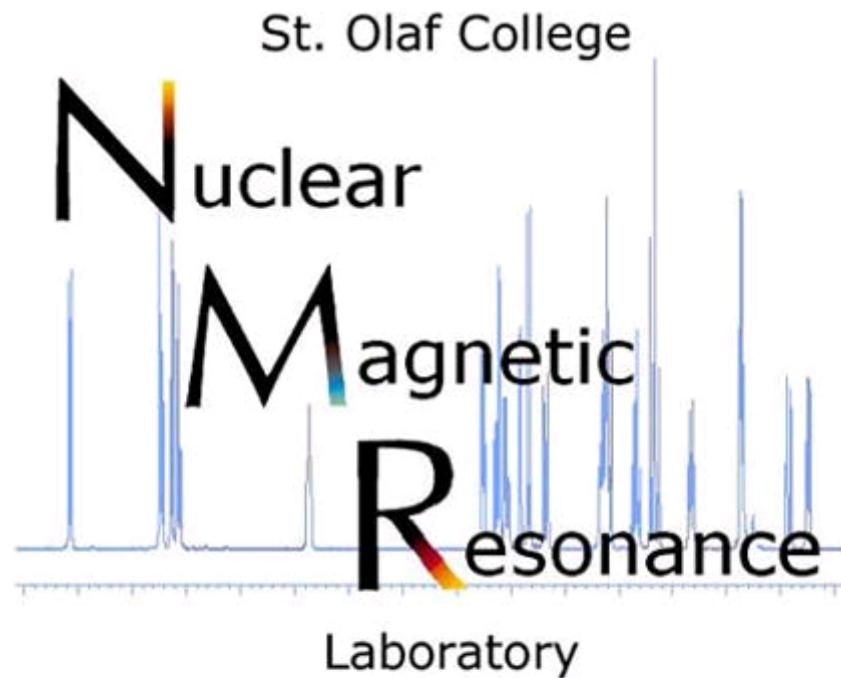
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...with a twist!



St. Olaf College NMR Laboratory

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



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

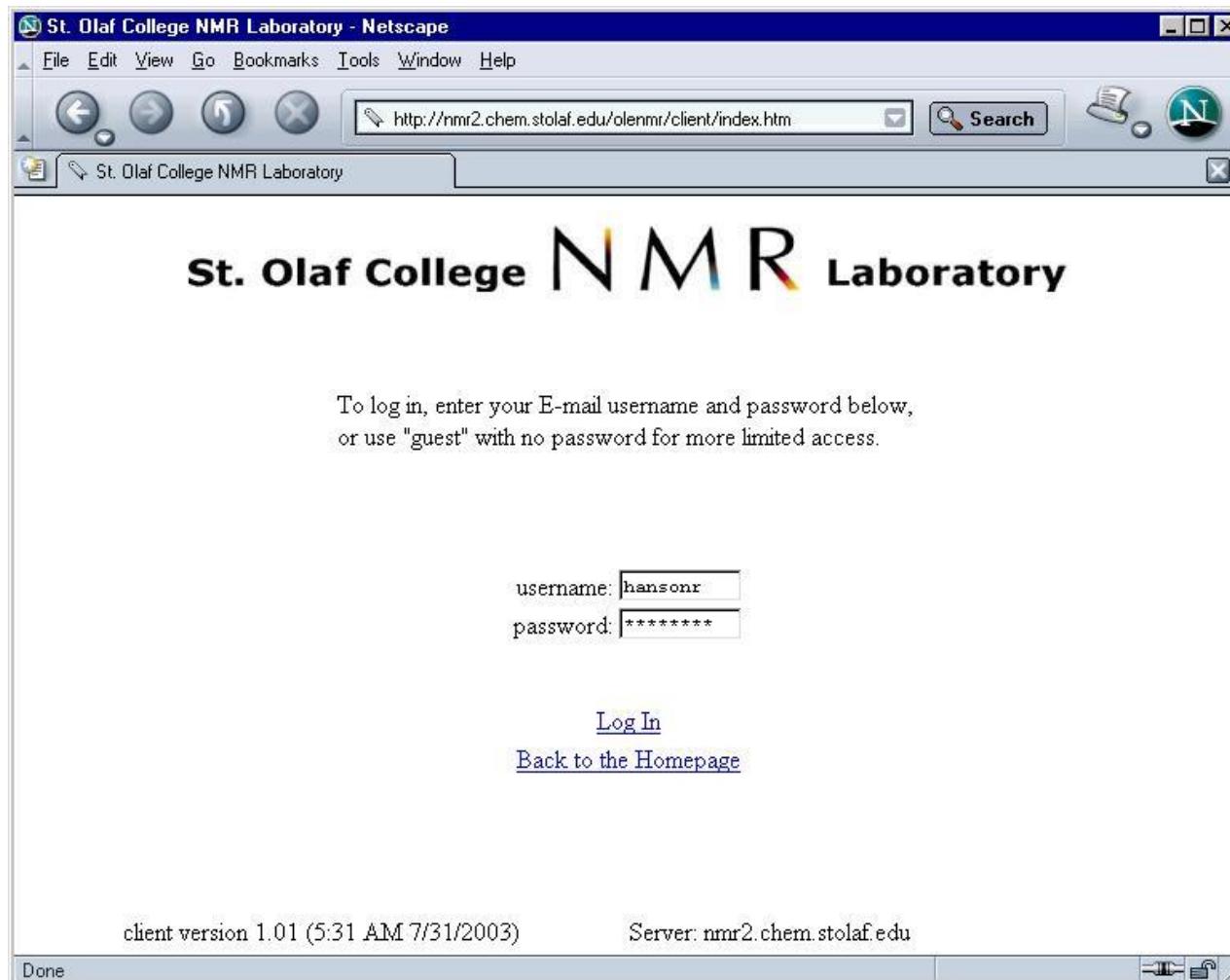
[Liquid Helium Level Log](#) [Experiment Status](#) [Holder Status](#)

[on/off-campus demo version](#) [Overnight Status \(available on/off campus\)](#)

[Overview](#) [227th ACS National Meeting Presentation](#)

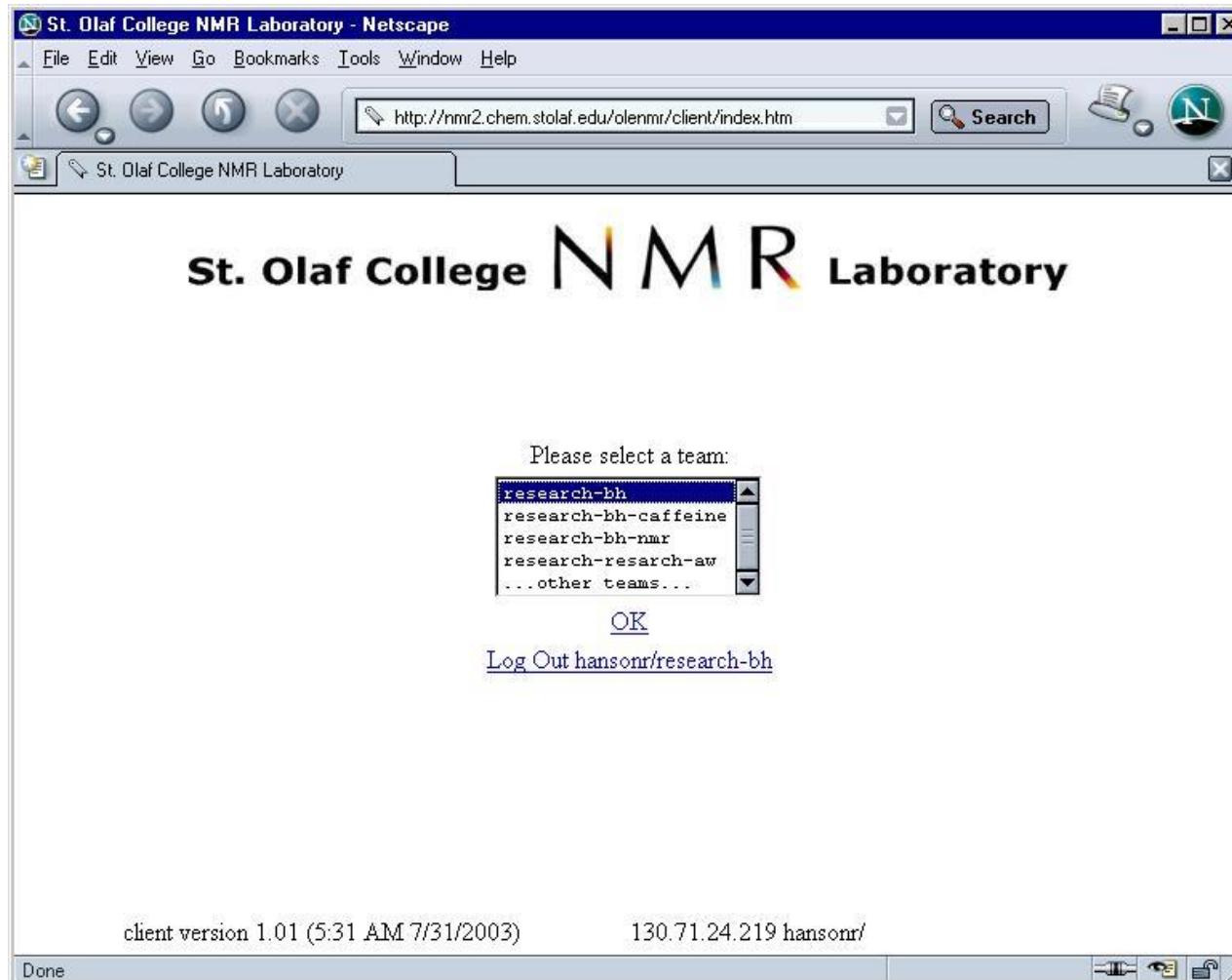
St. Olaf College N M R Laboratory

Implementation involves “standard” St. Olaf login...



St. Olaf College N M R Laboratory

Each user is a member of one or more IconNMR "teams"...



St. Olaf College N M R Laboratory

For this simulation we will run an experiment...

The screenshot shows a vintage-style web browser window titled "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains standard icons for Back, Forward, Stop, and Refresh. The address bar shows the URL <http://nmr2.chem.stolaf.edu/olenmr/client/index.htm>. A search bar with a magnifying glass icon is also present. The main content area features the college's logo and the text "What would you like to do as research-bh?". Below this are eight buttons arranged in two rows of four:

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

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" are displayed, along with a set of small navigation icons.

St. Olaf College NMR Laboratory

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

The screenshot shows a vintage-style web browser window for the St. Olaf College NMR Laboratory. The title bar reads "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains standard icons for back, forward, search, and refresh. The address bar shows the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". Below the toolbar is a navigation bar with links: Experiment (highlighted), Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. Underneath the navigation bar are several small icons: a red and white striped ball, a blue and yellow striped ball, a blue and yellow striped ball with question marks, a blue and yellow striped ball with an 'ID ND X 1H' label, a blue and yellow striped ball with a question mark, a blue and yellow striped ball with a folder icon, and a green 'GO' button. The main content area features a red header "Run an NMR Experiment" followed by a paragraph: "In order to carry out a nuclear magnetic resonance experiment, you will need to answer a few questions." Below this is a section titled "Current Instrument Status (as of 03/18/04 16:43)". It lists the following information:

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...](#)

At the bottom, it says "client version 1.01 (5:31 AM 7/31/2003)" and "130.71.24.219 hansonr/research-bh". The status bar at the bottom right shows icons for volume, screen orientation, and other system controls.

St. Olaf College NMR Laboratory

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

The screenshot shows a vintage-style web browser window for the St. Olaf College NMR Laboratory. The title bar reads "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains icons for Back, Forward, Stop, Home, Search, and a magnifying glass. The address bar shows the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". Below the toolbar is a navigation bar with links: Experiment (highlighted in blue), Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. Underneath the navigation bar are several small icons representing different NMR functions. The main content area features a red header "Indicate a Sample Position". A question "Which sample position is your NMR tube in?" is followed by a scrollable list of sample positions. The list contains the following entries:

- #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)
- ...

At the bottom of the page are links for Back..., Cancel, and Next... . The footer displays "client version 1.01 (5:31 AM 7/31/2003)" and "130.71.24.219 hansonr/research-bh".

St. Olaf College NMR Laboratory

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

The screenshot shows a vintage-style web browser window for the St. Olaf College NMR Laboratory. The title bar reads "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains icons for Back, Forward, Stop, Home, and Search. The address bar shows the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". Below the toolbar is a navigation bar with links: Experiment (selected), Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. A row of small icons follows: a green circle with a question mark, a blue square with a flame, a red square with a grid, a blue square with a 1H, a yellow folder, and a green "GO" button. The main content area features a red header "Indicate the Solvent". Below it is a paragraph explaining the importance of solvent indication for NMR locking. At the bottom is a scrollable list of solvent options:

- CDC13 (deuterochloroform)
- 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)

At the very bottom, the status bar displays "Date: Client: Next:" and "client version 1.01 (5:31 AM 7/31/2003)". To the right of the status bar are several small icons.

St. Olaf College NMR Laboratory

Experiments are drawn from an OleNMR database...

The screenshot shows a vintage-style web browser window titled "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains icons for Back, Forward, Stop, Home, and Search. The address bar shows the URL <http://nmr2.chem.stolaf.edu/olenmr/client/index.htm>. Below the toolbar is a title bar with the text "St. Olaf College NMR Laboratory". The main content area features a navigation menu with links: Experiment (highlighted), Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. Below the menu are several experiment selection icons: 1H, 13C, DEPT, HMQC, HMBC, a folder icon, and a GO button. A red header "Select an Experiment" is centered above a text block. The text explains that there are hundreds of possible NMR experiments and provides examples of common experiments like proton, carbon, and DEPT experiments. It also notes that composite experiments take longer. On the left, a scrollable list of experiment options includes: 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), and sw opt. HMBC with low pass J-filter (magn. mode). To the right of this list is a section titled "PROTON" with the text: "The standard NMR experiment. Provides a proton spectrum." and a "more info..." link. At the bottom of the page, the client version is listed as "client version 1.01 (5:31 AM 7/31/2003)" and the IP address is "130.71.24.219 hansonr/research-bh". The bottom right corner contains standard browser control icons.

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

1H 13C DEPT HMQC HMBC

GO

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.

[more info...](#)

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

St. Olaf College NMR Laboratory

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

The screenshot shows a vintage-style web browser window for the St. Olaf College NMR Laboratory. The title bar reads "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar has standard icons for Back, Forward, Stop, and Search. The address bar shows the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". Below the address bar is a toolbar with icons for Experiment, Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. A second row of icons includes a multi-channel NMR spectrum, a question mark, a 1D ND X 1H sequence, a folder labeled "ns d1 sw", and a green "GO" button. The main content area features a red header "Set the Parameters". Below it, text explains that each NMR experiment involves variable parameters and lists several parameters with their default values. A section titled "Parameters For the PROTON Experiment" shows a dropdown menu set to "16" for "Number of scans". To the right, a detailed description of the "Number of scans (NS)" parameter is provided, stating that it determines the number of times data are collected, noting that more scans result in less baseline noise. At the bottom, the client version is listed as "client version 1.01 (5:31 AM 7/31/2003)", and the IP address is "130.71.24.219 hansonr/research-bh". The status bar at the bottom contains the JavaScript command "javascript:parent.fraClient.setup_invokeGifButton(6)".

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

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)

St. Olaf College N M R Laboratory

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

The screenshot shows a vintage-style web browser window titled "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains standard icons for back, forward, search, and refresh. The address bar shows the URL <http://nmr2.chem.stolaf.edu/olenmr/client/index.htm>. The title bar of the main content area also reads "St. Olaf College NMR Laboratory". Below the title bar is a horizontal menu with icons and labels: Experiment (selected), Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. Underneath this menu is a row of small, colorful icons representing various NMR functions. The central content area features a red header "Indicate a Title" above a text input field containing the placeholder "Sample for ACS". At the bottom of the page are navigation links: Back..., Cancel, Next..., and client version 1.01 (5:31 AM 7/31/2003). The footer also displays the IP address 130.71.24.219 and the path 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

Sample for ACS

Back... Cancel Next...

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

St. Olaf College NMR Laboratory

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

The screenshot shows a vintage-style web browser window for the St. Olaf College NMR Laboratory. The title bar reads "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar has icons for Back, Forward, Stop, Home, and Search. The address bar shows the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". Below the address bar is a toolbar with icons for Experiment, Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. A row of smaller icons below the main toolbar includes a green starburst, three blue squares with white question marks, a red square with a blue question mark, a blue square with a yellow question mark, a blue square with a green question mark, a blue folder icon, and a green "GO" button. The main content area features a red header "Submit the Experiment". Below it is a paragraph explaining the experiment queue system. At the bottom, there is a table of experimental parameters and a note about the queue.

Submit the Experiment

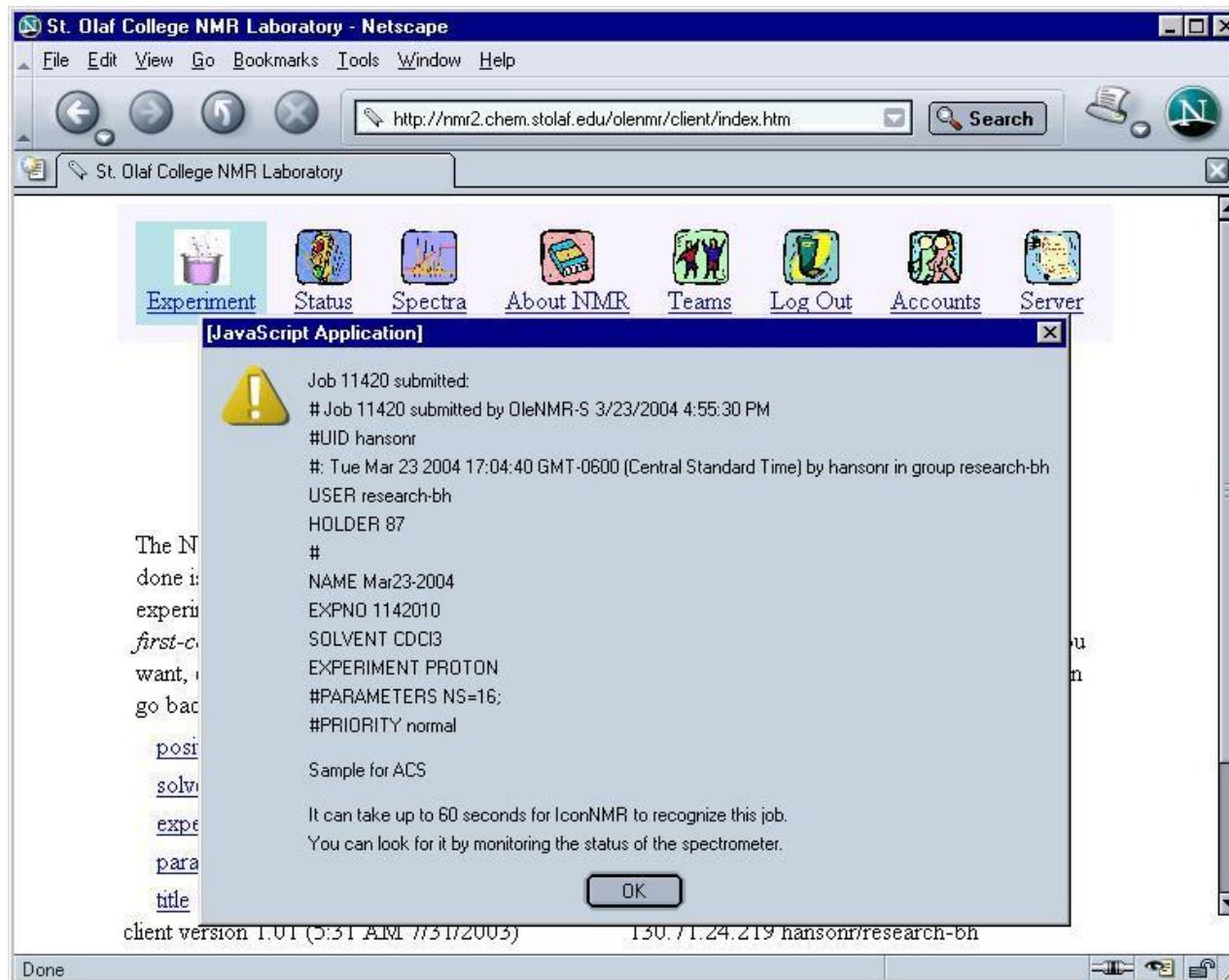
The NMR spectrometer can only run one experiment at a time. Each experiment that needs to be done is added to a list of experiments waiting to be done called the *spectrometer queue*. Your experiments will be carried out based on a fair queue schedule (which is not quite *first-come-first-served*). Shown 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.

<u>position</u>	87	priority: normal
<u>solvent</u>	CDCl ₃ (deuterochloroform)	This experiment will be queued for carrying out
<u>experiment</u>	PROTON	based on a "fair queue."
<u>parameters</u>	NS=16;	
<u>title</u>	Sample for ACS	

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

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...

The screenshot shows a vintage-style Netscape browser window with a blue title bar and menu bar. The title bar reads "St. Olaf College NMR Laboratory - Netscape". The menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. Below the menu is a toolbar with icons for Back, Forward, Stop, Home, and Search. The address bar shows the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". The main content area displays the "St. Olaf College NMR Laboratory" logo at the top. Below it, a blue header asks "What would you like to do as research-bh?". Eight buttons are arranged in two rows of four:

- Run Experiment (Icon: flask with liquid)
- View Status (Icon: traffic light)
- View Spectra (Icon: NMR spectrum)
- Learn About NMR (Icon: book)

- Switch Teams (Icon: two people high-fiving)
- Log Out (Icon: exit sign)
- Edit Accounts (Icon: two people)
- Show Server Log (Icon: server tower)

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" are visible, along with standard browser navigation buttons.

St. Olaf College NMR Laboratory

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

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 03/17/04 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	CDCI3	finished:	03/17/04 16:45	total 4
	urban	1-1419-10	normal				

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

St. Olaf College NMR Laboratory

Within one minute our job shows up...

The screenshot displays two instances of the St. Olaf College NMR Laboratory website within Netscape browsers. Both windows have identical titles: "St. Olaf College NMR Laboratory - Netscape". The top menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. Below the menu is a toolbar with standard navigation icons (Back, Forward, Stop, Home) and a search bar containing the URL "http://nmr2.chem.stolaf.edu/olenmr/client/index.htm". The search button is labeled "Search". A logo featuring a stylized letter 'N' is visible on the right side of the toolbar.

The main content area features a navigation bar with eight icons: Experiment, Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. The "Status" icon is highlighted with a blue glow, indicating it is the active page. Below this is a section titled "St. Olaf 400 MHz NMR Facility Current Status Report". It includes links for Refresh Now, Search..., Detail, and Archive. A note states "Last updated by IconNMR: 03/17/04 16:45".

Instructions for marked experiments are provided: expedite, set priority normal, set priority low, hold, cancel, and halt. A message from IconNMR indicates "Waiting for Job".

Summary statistics: 30 done, 0 running, 1 waiting, 0 on hold, 0 skipped, 0 canceled, 1 failed, since 03/09/04 22:13. A table lists experimental details:

87/??	research-bh hansonr	Mar23-2004 11420	PROTON normal	CDC13	estimat 6
Sample for ACS NS=16; (resubmit...)					
atma:	rotation:	lock:	shim:	acqu:	accep

A "Refresh Now" button is located at the bottom of the page.

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

The screenshot displays two instances of the St. Olaf College NMR Laboratory website within Netscape browsers. Both windows have identical titles, 'St. Olaf College NMR Laboratory - Netscape'. The top menu bar includes 'File', 'Edit', 'View', 'Go', 'Bookmarks', 'Tools', 'Window', and 'Help'. The toolbar below the menu contains standard icons for back, forward, search, and refresh. The address bar shows the URL 'http://nmr2.chem.stolaf.edu/olenmr/client/index.htm'. The main content area features a navigation bar with icons for 'Experiment' (selected), 'Status', 'Spectra', 'About NMR', 'Teams', 'Log Out', 'Accounts', and 'Server'. Below this is a section titled 'St. Olaf 400 MHz NMR Facility Current Status Report'. It includes links for 'Refresh Now', 'Search...', 'Detail Archive', and a note that it was last updated by IconNMR on 03/23/04 at 16:56. A message for marked experiments provides options like 'expedite', 'set priority normal', 'set priority low', 'hold', 'cancel', and 'halt', followed by a red link 'Goto Sample 87'. A summary table shows the status of 30 experiments: 1 done, 1 running, 0 waiting, 0 on hold, 0 skipped, 0 canceled, 1 failed, and the last update was on 03/09/04 at 22:13. A specific experiment entry for sample 87 is highlighted with a red border. The entry details are: ID 87/1, Name research-bh_hanson, Date Mar 23-2004, Time 1-1420-10, Type PROTON, Shimming normal, Solvent CDCl3, Started 03/23/04 at 16:56, and Estimated time 6 m. A note below says 'Sample for ACS NS=16; (resubmit...)'.

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 hanson	Mar 23-2004 1-1420-10	PROTON normal	CDCl3 normal	started: 03/23/04 16:56	estimate: 6 m
Sample for ACS NS=16; (resubmit...)							
atma:		rotation:	lock:	shim:	acqu:	runn:	

St. Olaf College NMR Laboratory

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

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 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	CDCI3	started: 03/23/04 16:56	estimate 6 m
Sample for ACS NS=16; (resubmit...)							
atma:		rotation:	lock:	shim:	acqu:	runn	

St. Olaf College NMR Laboratory

The sample is starting to rotate...

The screenshot shows two instances of the St. Olaf College NMR Laboratory website in Netscape browsers. The top window displays the main navigation menu with links for Experiment, Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. The bottom window displays a status report titled "St. Olaf 400 MHz NMR Facility Current Status Report". It includes links for Refresh Now, Search..., Detail, and Archive, and a note that it was last updated by IconNMR on 03/23/04 at 16:56. Below this, it shows statistics for marked experiments: 30 done, 1 running, 0 waiting, 0 on hold, 0 skipped, 0 canceled, 1 failed, and the last update time of 03/09/04 22:13. A table lists experiment details: ID 87/1, title research-bh_hanson, date Mar 23-2004, 1-1420-10, type PROTON, status normal, solvent CDCl3, started 03/23/04 16:56, and estimate 5 m. A note below the table says "Sample for ACS NS=16; ([resubmit...](#))". At the bottom, it shows rotation status: atma: rotation: lock: shim: acqu: run:

St. Olaf College NMR Laboratory

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

The screenshot displays two instances of the St. Olaf College NMR Laboratory website within Netscape browsers. Both windows have a dark blue header bar with the title "St. Olaf College NMR Laboratory - Netscape". Below the header is a menu bar with options: File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The main content area shows a navigation bar with icons and labels: Experiment, Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. The "Status" icon is highlighted with a light blue background. Below this is a section titled "St. Olaf 400 MHz NMR Facility Current Status Report". It includes links for Refresh Now, Search..., Detail, and Archive. A timestamp indicates the data was last updated by IconNMR on 03/23/04 at 16:56. A message for marked experiments provides links to expedite, set priority normal, set priority low, hold, cancel, and halt. It also mentions the last message from IconNMR: "Locking Field". Below this, a summary of experiment statistics is shown: 30 done, 1 running, 0 waiting, 0 on hold, 0 skipped, 0 canceled, 1 failed, and the last run since 03/09/04 at 22:13. A detailed table lists individual experiments, including sample names like "research-bh_hanson", dates (e.g., Mar23-2004), and parameters (e.g., PROTON, CDCI3, normal). The table also includes columns for start time (03/23/04 16:56), estimate time (4 m), and other status indicators. A note at the bottom states "Sample for ACS NS=16; ([resubmit...](#))".

	87/1	research-bh hanson	Mar23-2004 1-1420-10	PROTON normal	CDCI3 normal	started: 03/23/04 16:56	estimate 4 m
Sample for ACS NS=16; (resubmit...)							
		atma:	rotation:	lock:	shim:	acqu:	runn:

St. Olaf College NMR Laboratory

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

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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		Mar23-2004		PROTON		CDCI3		started:		03/23/04 16:56	time	
		hansonr			1-1420-10			normal						

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

atma: rotation: lock: shim: acqu: runn:

St. Olaf College NMR Laboratory

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

The screenshot displays two instances of the St. Olaf College NMR Laboratory website within Netscape browsers. Both windows have identical titles: "St. Olaf College NMR Laboratory - Netscape". The top menu bar includes File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The toolbar contains standard icons for Back, Forward, Stop, Home, and Search. The address bar shows the URL <http://nmr2.chem.stolaf.edu/olenmr/client/index.htm>. The main content area features a navigation bar with icons and labels: Experiment, Status, Spectra, About NMR, Teams, Log Out, Accounts, and Server. Below this is a section titled "St. Olaf 400 MHz NMR Facility Current Status Report". It includes links for Refresh Now, Search..., Detail, and Archive. A note states "Last updated by IconNMR: 03/23/04 17:03". A message for marked experiments lists options: expedite, set priority normal, set priority low, hold, cancel, and halt. A red message indicates the last update was "Waiting for Job". Below this, a summary of experiment statistics is provided: 31 done, 0 running, 0 waiting, 0 on hold, 0 skipped, 0 canceled, 1 failed, and the last successful run was on 03/09/04 at 22:13. A detailed table follows:

87/1	research-bh hansonr	Mar23-2004 1-1420-10	PROTON normal	CDC13	finished: 03/23/04 17:03	total 7
------	------------------------	-------------------------	------------------	-------	-----------------------------	------------

A note below the table says "Sample for ACS NS=16; ([resubmit...](#))". At the bottom, status indicators show thumbs-up for atma, rotation, lock, shim, and acqu, while a yellow smiley face icon is present.

St. Olaf College N M R Laboratory

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

The screenshot shows a vintage-style web browser window titled "St. Olaf College NMR Laboratory - Netscape". The address bar displays the URL <http://nmr2.chem.stolaf.edu/olenmr/client/index.htm>. The main content area features the college's logo and the text "What would you like to do as research-bh?". Below this, there are eight icons arranged in two rows of four, each with a corresponding link:

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

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" are visible, along with standard browser control buttons.

St. Olaf College NMR Laboratory

There are many options for selecting specific experiments...

The screenshot displays two instances of the St. Olaf College NMR Laboratory website, likely from different versions of Netscape. Both windows have a dark blue header bar with the title "St. Olaf College NMR Laboratory - Netscape". Below the header is a menu bar with File, Edit, View, Go, Bookmarks, Tools, Window, and Help. The main content area contains several icons: Experiment, Status, Spectra (which is highlighted in light blue), About NMR, Teams, Log Out, Accounts, and Server. Below these icons is a search section titled "Search the spectra database...". It includes a checkbox for "Search only those produced in the last [7] day(s)" and dropdown menus for "Sort by" (team: dataset or date/time spectrum title) and "Match only spectra having" (dataset name, spectrum title, experiment type). There are also checkboxes for "dataset name", "spectrum title", and "experiment type (note)". Another section allows filtering by nucleus/dimension: H, C, other, 1D, and 2D, with an "update now" button. At the bottom, there is a footer with the text "research-bh: Mar23-2004", the date and time "5:03 PM 3/23/2004", the experiment number "expt. 1142010/1", and a link to a sample entry: "Sample for ACS team: research-bh holder: 87 solvent: CDCl₃ PROTON NS=16; standard 1H experiment (1 Min 34 Sec)". It also provides links to PDF and EXPT files.

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

Search the spectra database...

Sort by:

team: dataset
date/time spectrum title

Match only spectra having [] or []
in the: dataset name spectrum title experiment type (note)

Match only nucleus/dimension: H C other 1D 2D

update now

research-bh: Mar23-2004

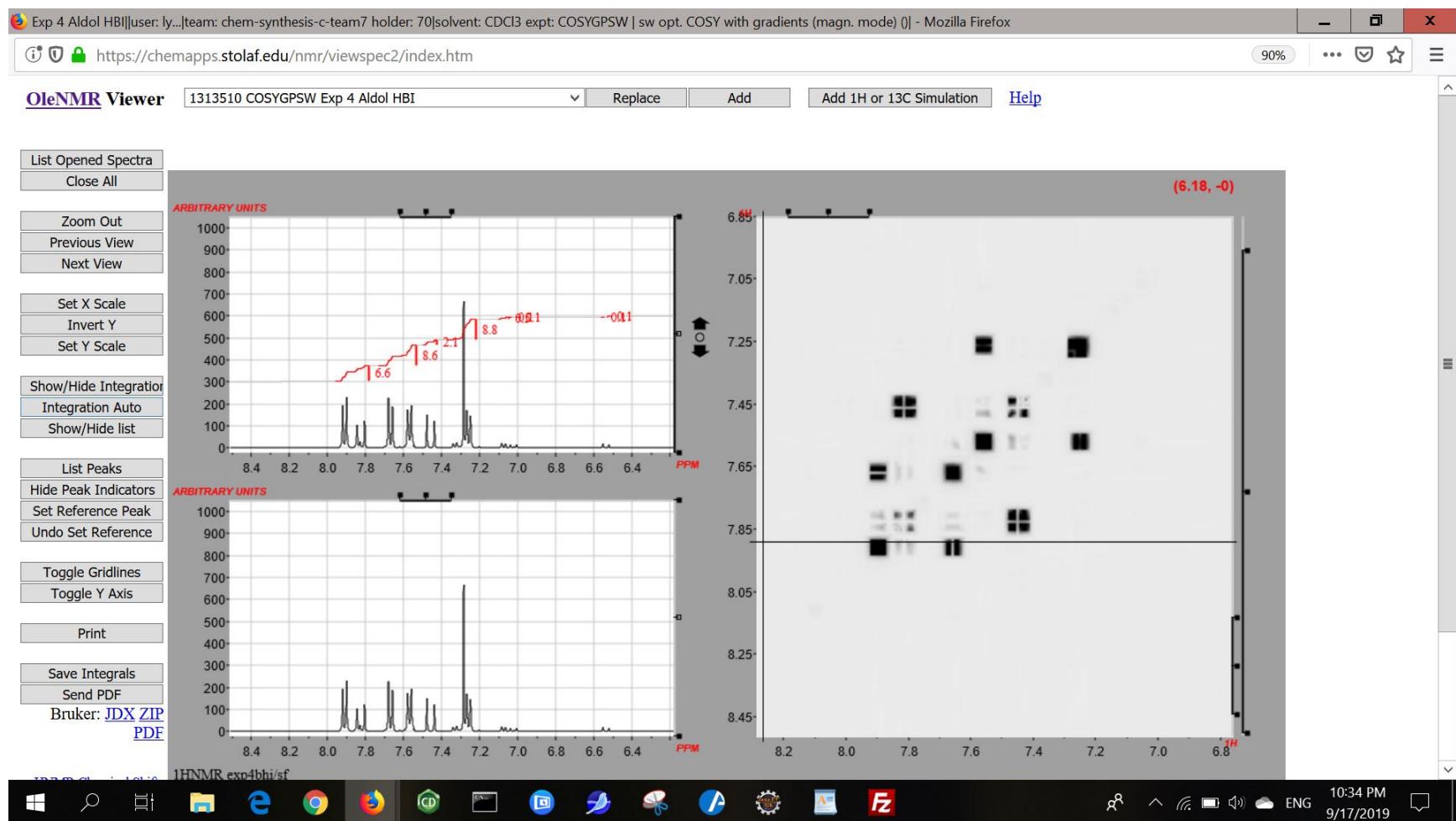
5:03 PM 3/23/2004 expt. 1142010/1

[Sample for ACS](#) team: research-bh holder: 87 solvent: CDCl₃
PROTON NS=16; standard 1H experiment (1 Min 34 Sec)

[PDF \(dir\)](#) [EXPT](#) [IDX \(dir\)](#)

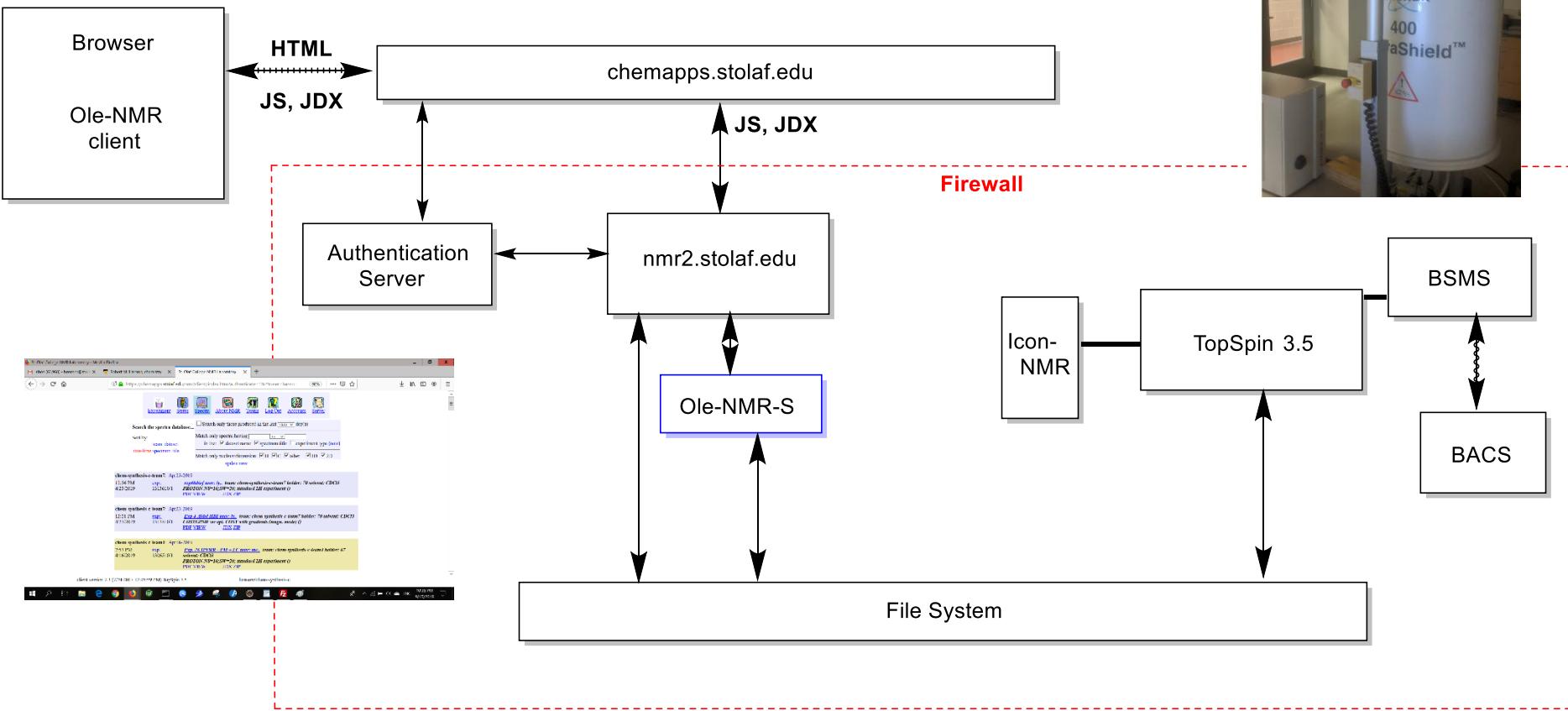
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



St. Olaf College NMR Laboratory

Ole-NMR/TopSpin Overall Schematic



St. Olaf College N M R 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...

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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

Search the spectra database...

Sort by:

team: dataset
date/time spectrum title

Match only spectra having [] or []
in the: dataset name spectrum title experiment type (note)

Match only nucleus/dimension: H C other 1D 2D

update now

research-bh: Mar23-2004

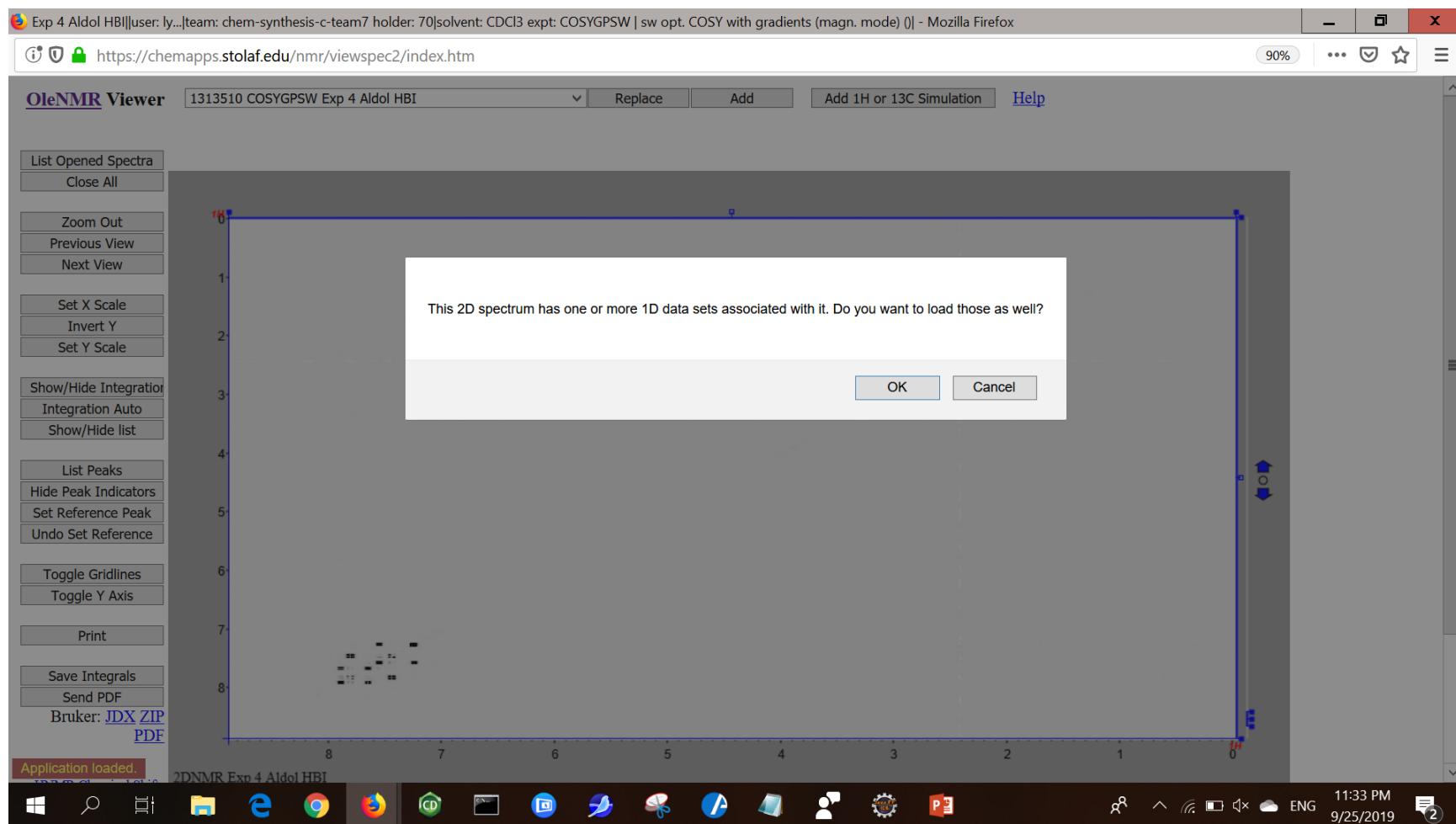
5:03 PM 3/23/2004 expt. 1142010/1

[Sample for ACS](#) team: research-bh holder: 87 solvent: CDCl₃
PROTON NS=16; standard 1H experiment (1 Min 34 Sec)

[PDF \(dir\)](#) [EXPT](#) [IDX \(dir\)](#)

St. Olaf College NMR Laboratory

Analysis using JSpecView-JS

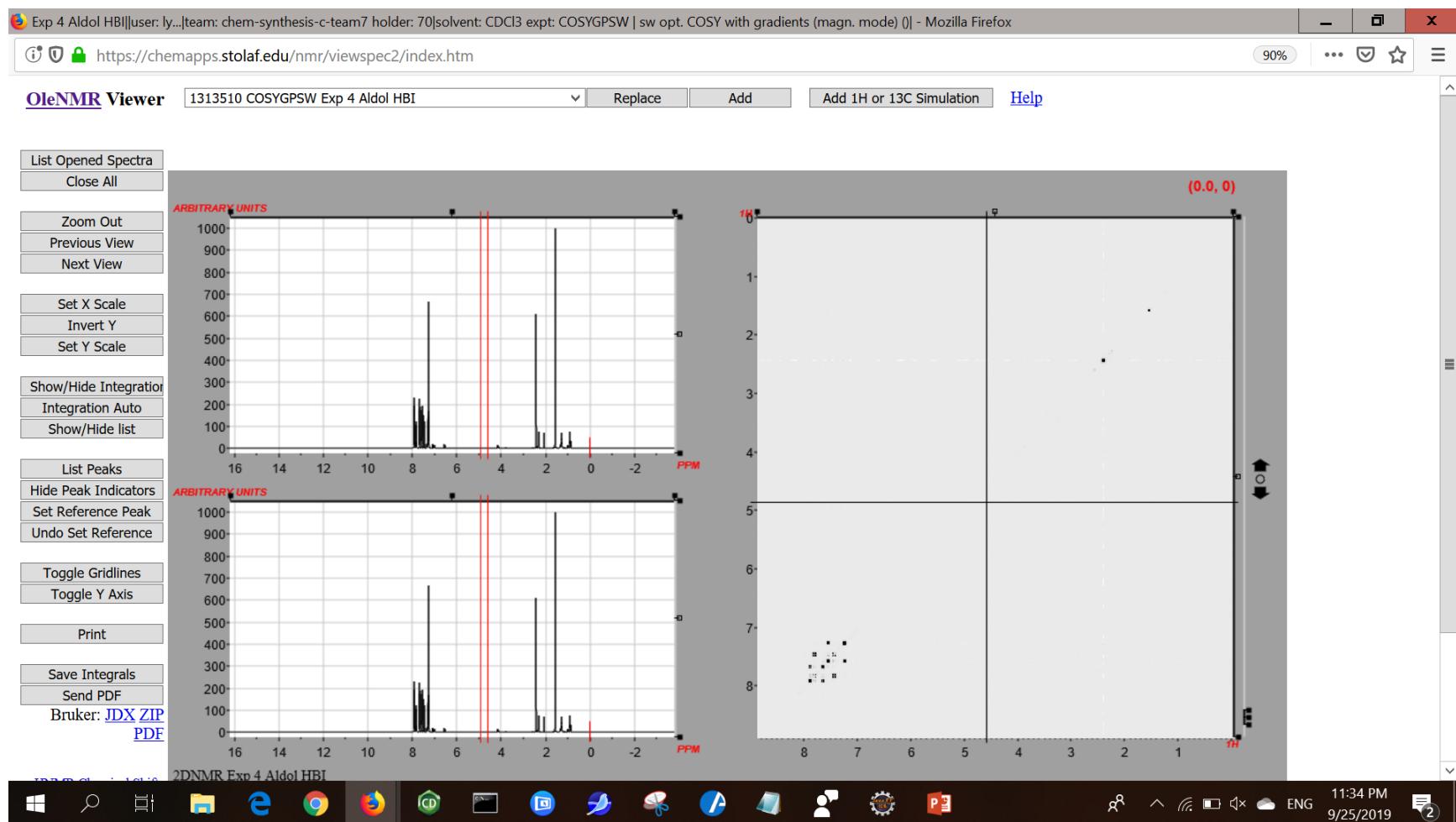


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Analysis using JSpecView-JS

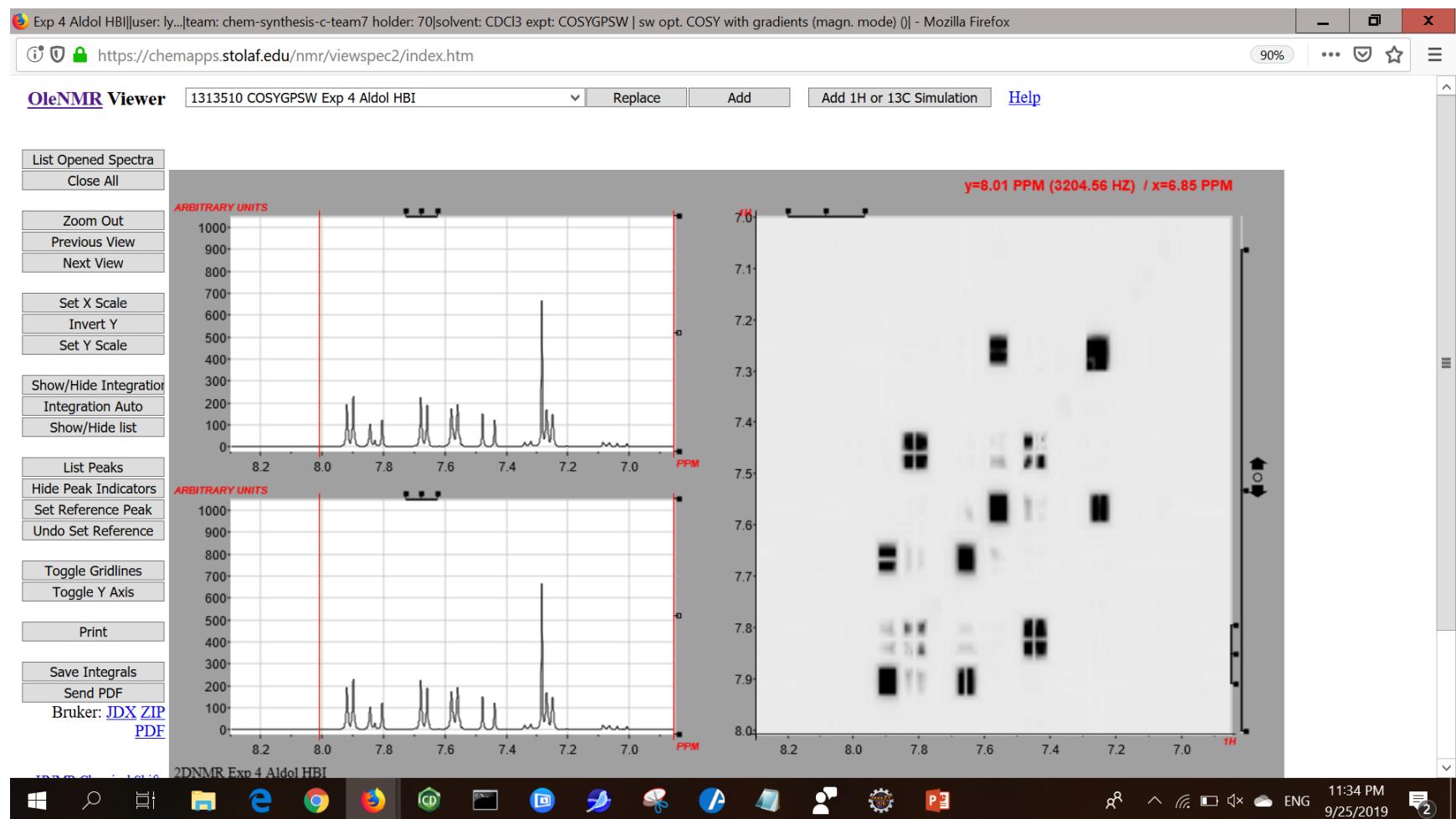
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



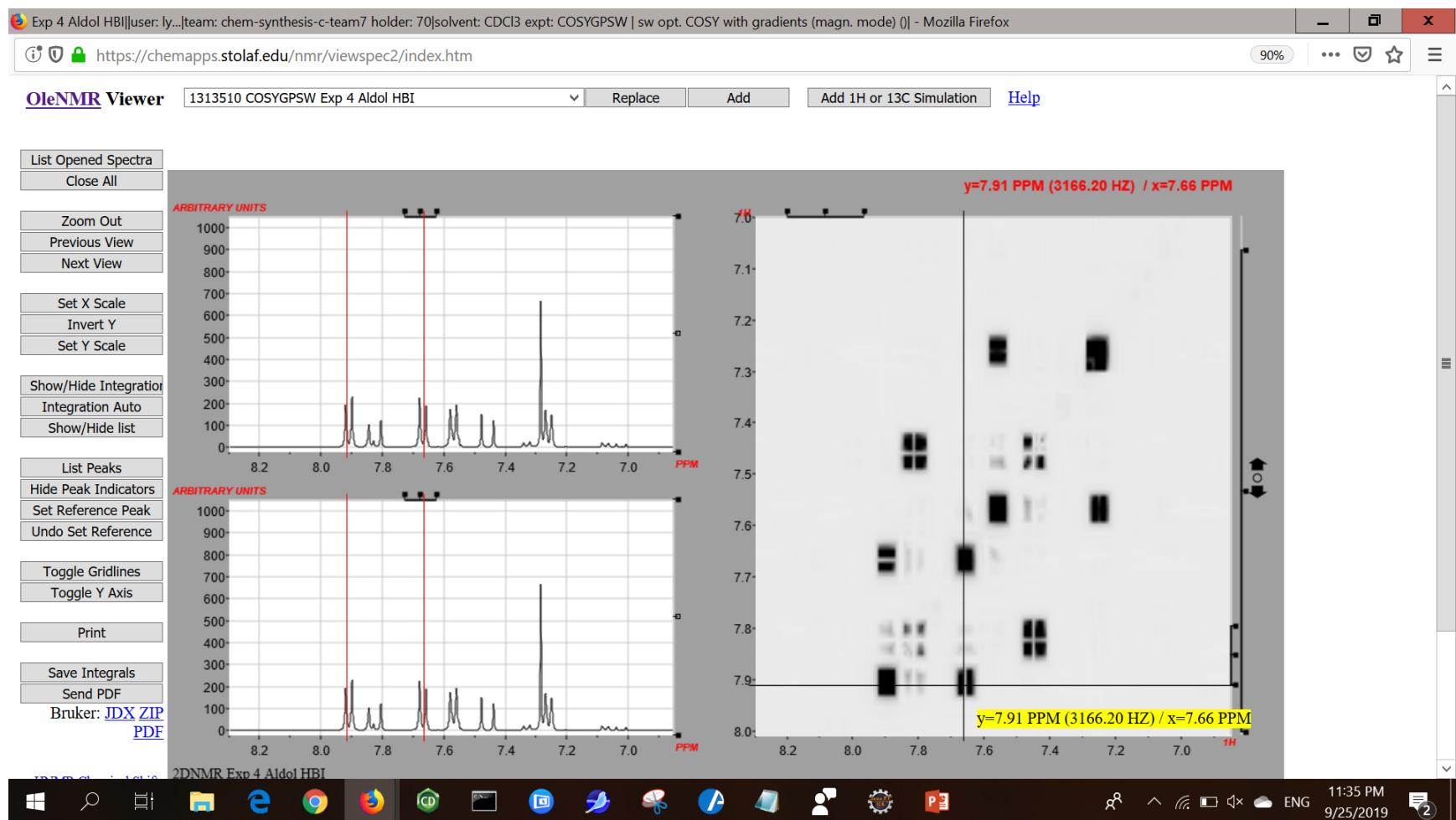
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



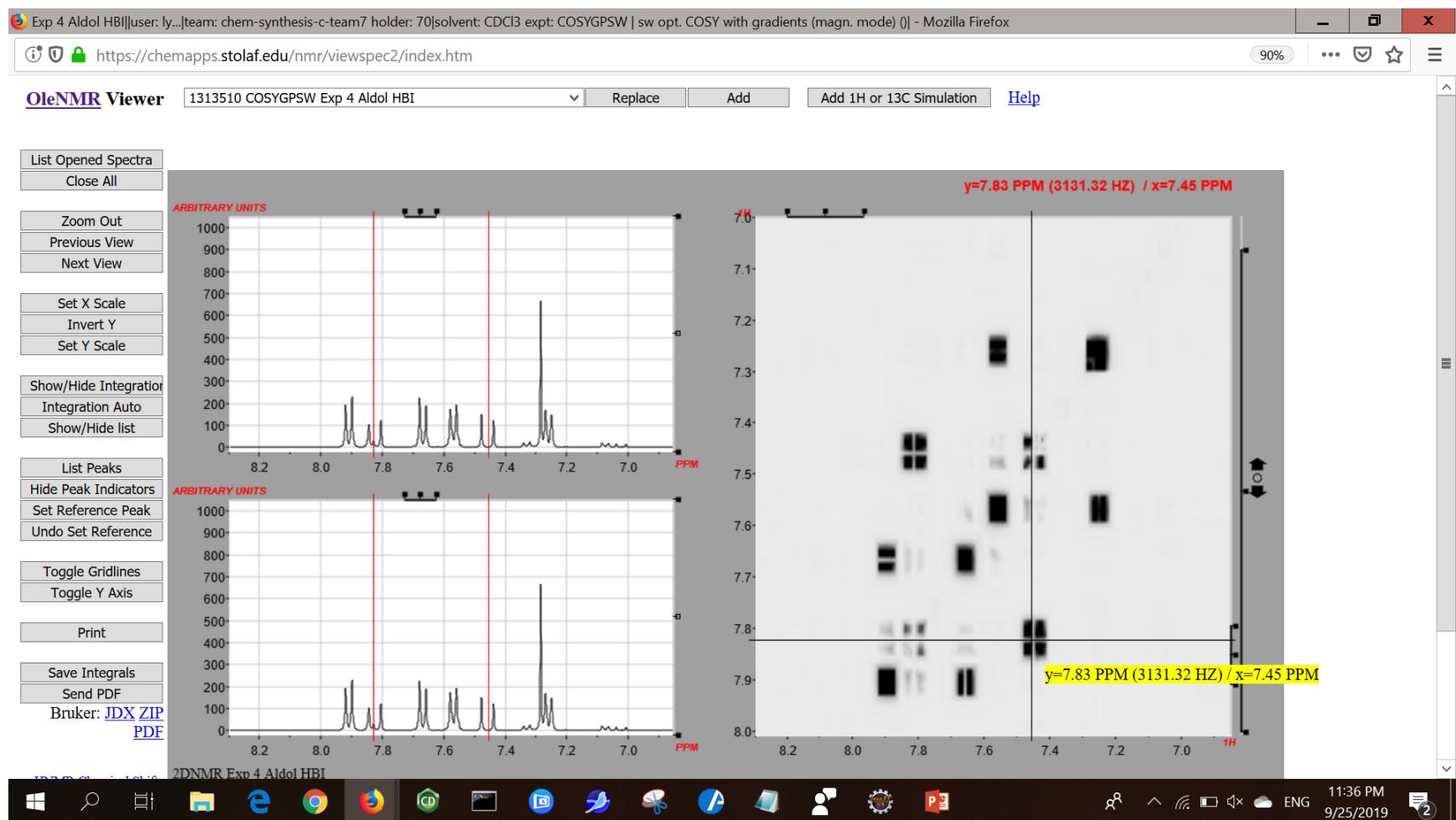
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



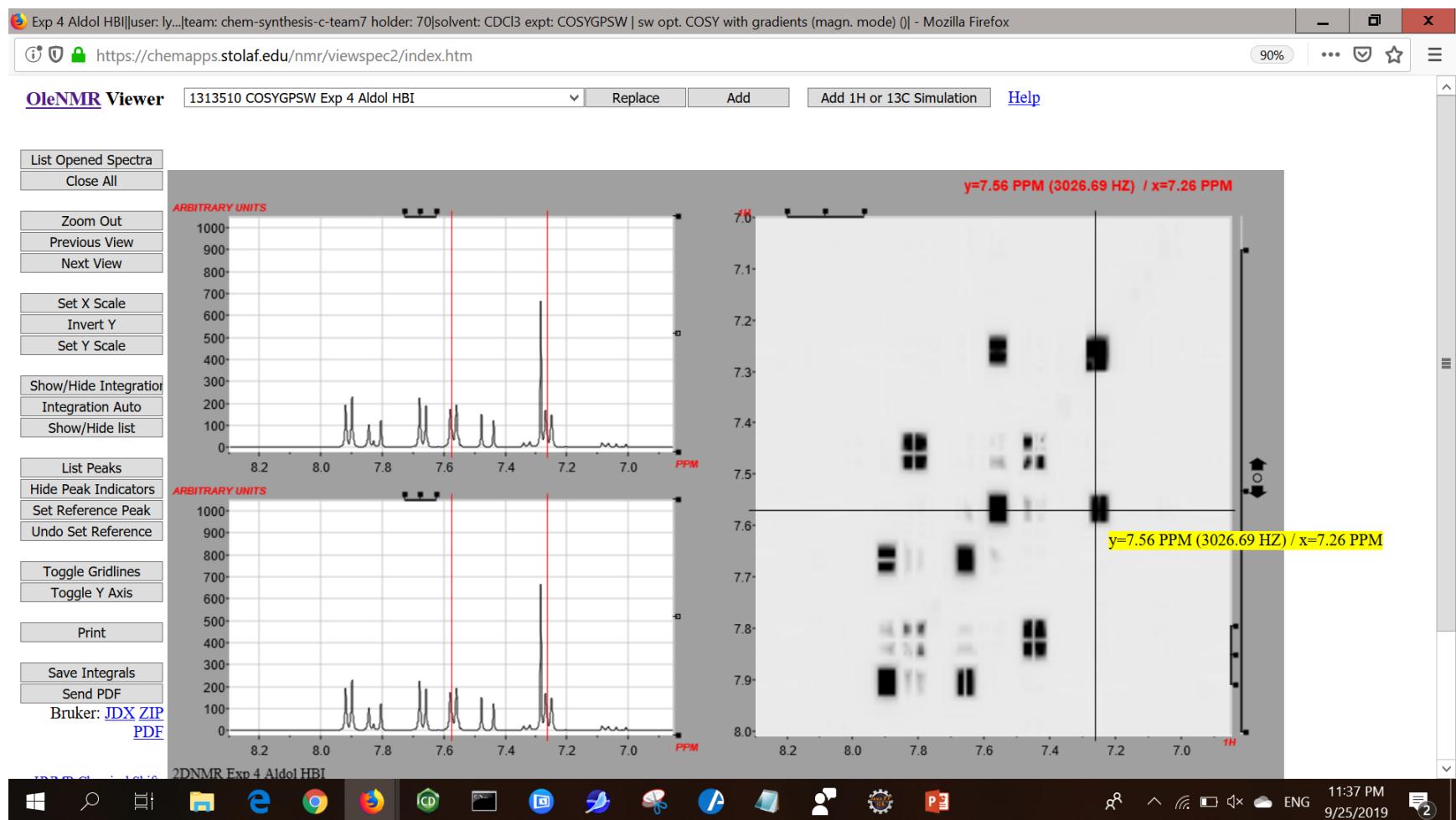
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



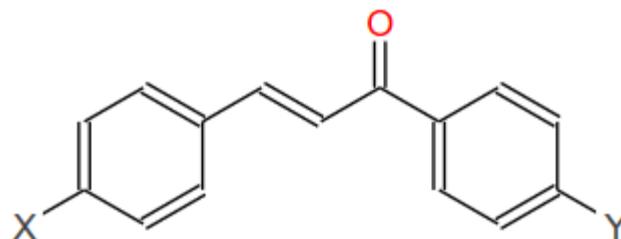
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Analysis using JSpecView-JS



St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



Previous View
Next View

Set X Scale
Invert Y
Set Y Scale

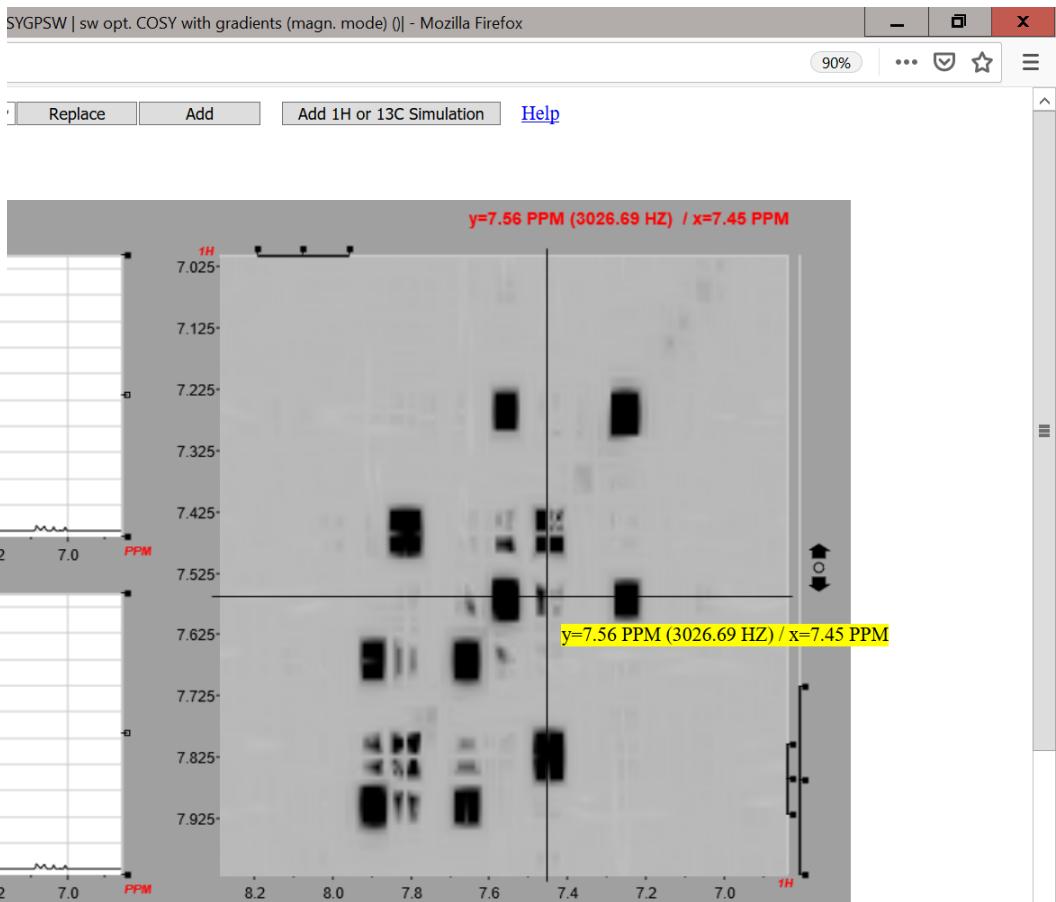
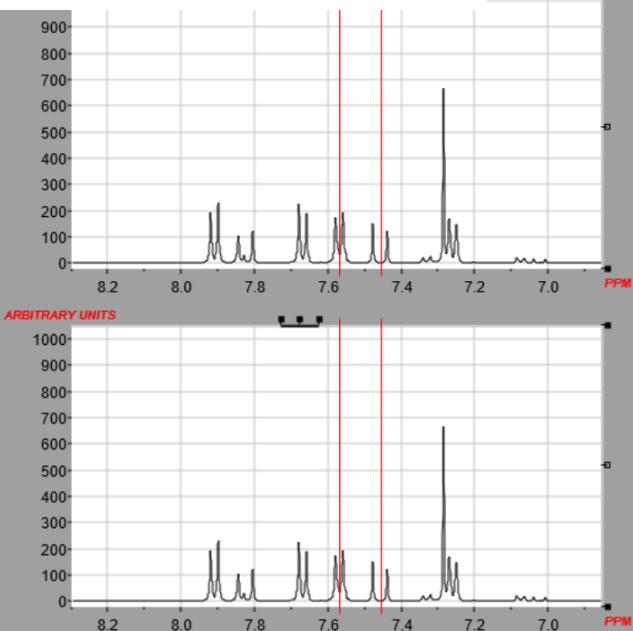
Show/Hide Integration
Integration Auto
Show/Hide list

List Peaks
Hide Peak Indicators
Set Reference Peak
Undo Set Reference

Toggle Gridlines
Toggle Y Axis

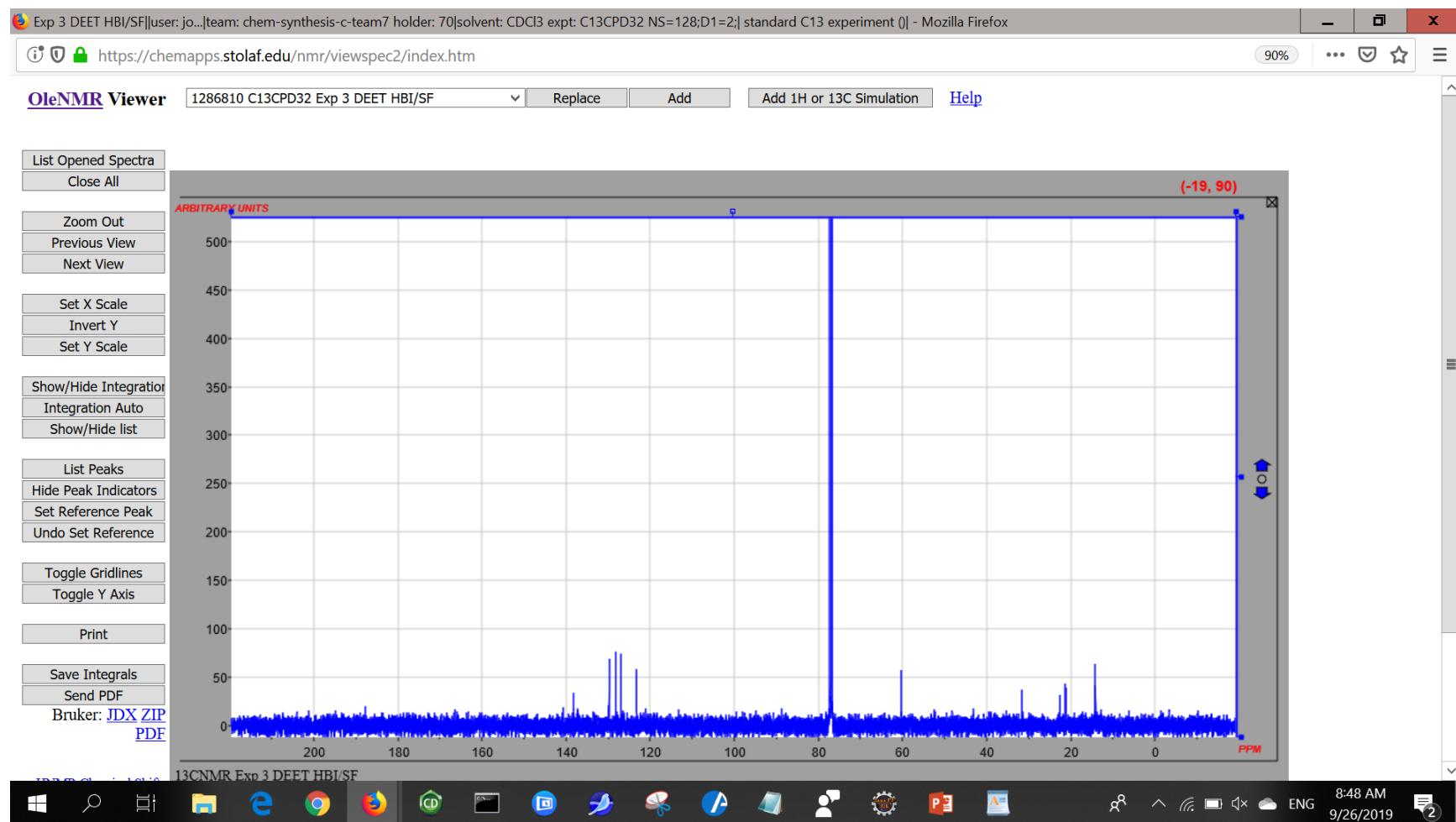
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Save Integrals
Send PDF
Bruker: [DX ZIP](#)
[PDF](#)



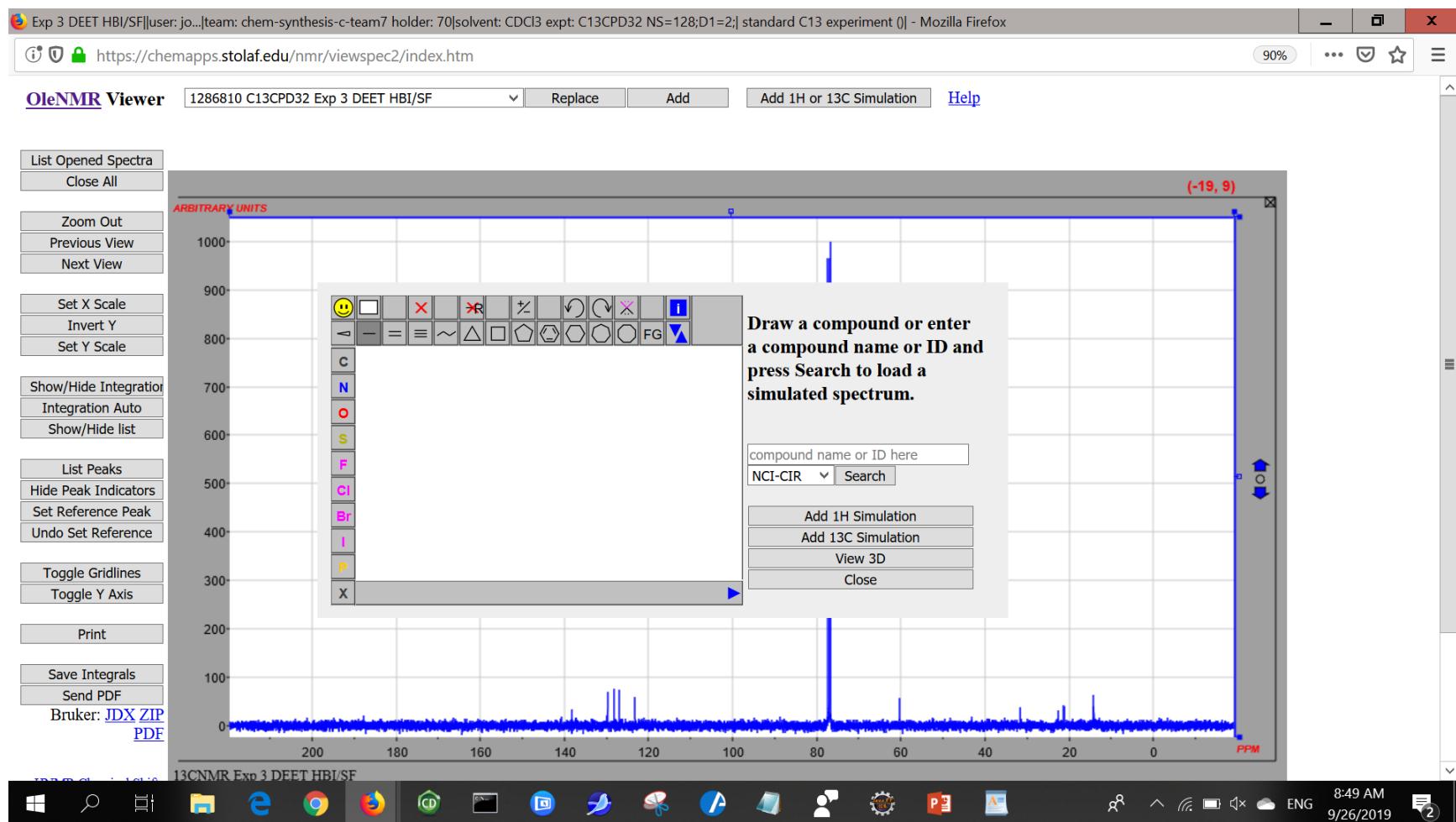
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Analysis using JSpecView-JS



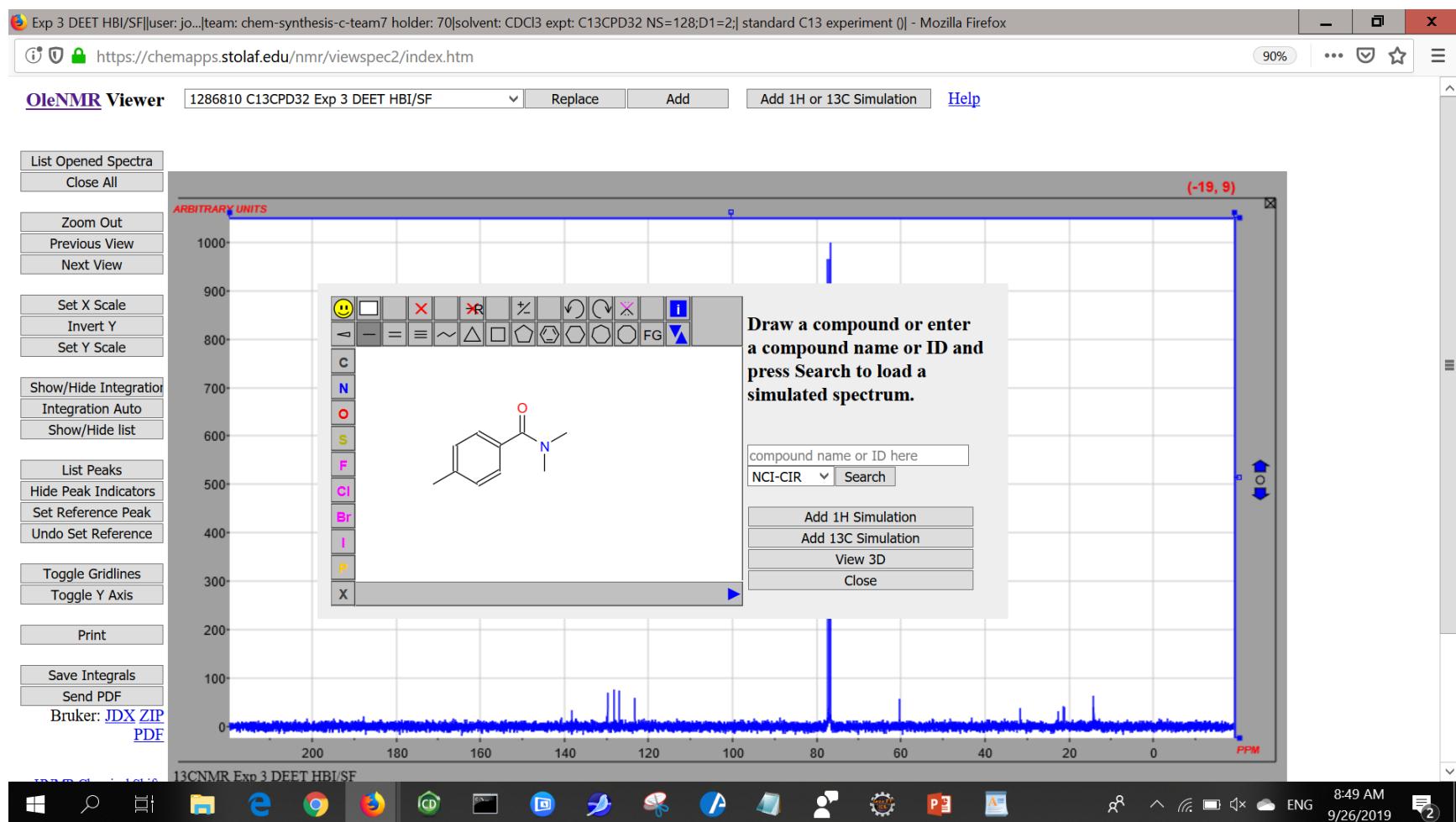
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



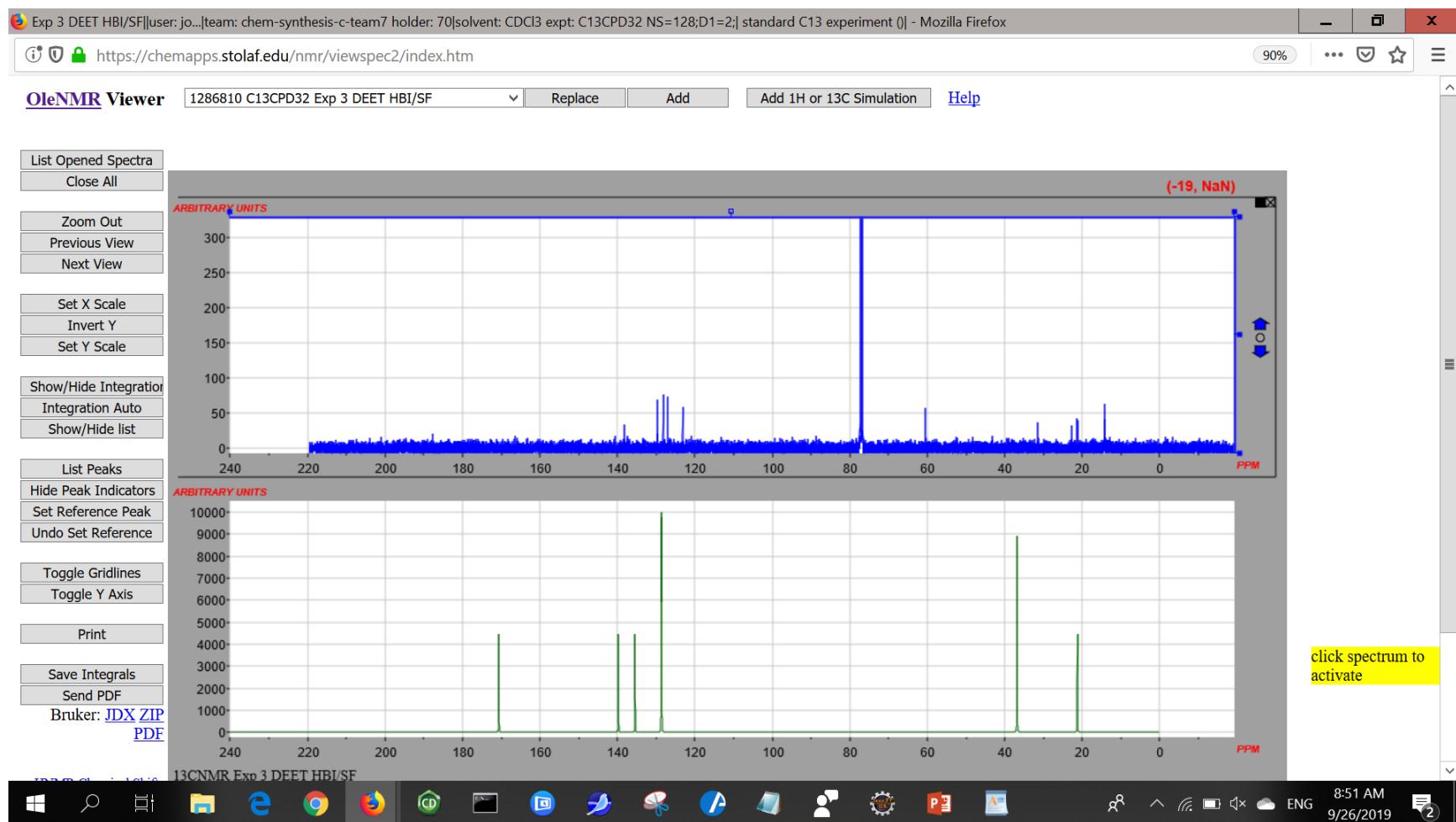
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Analysis using JSpecView-JS



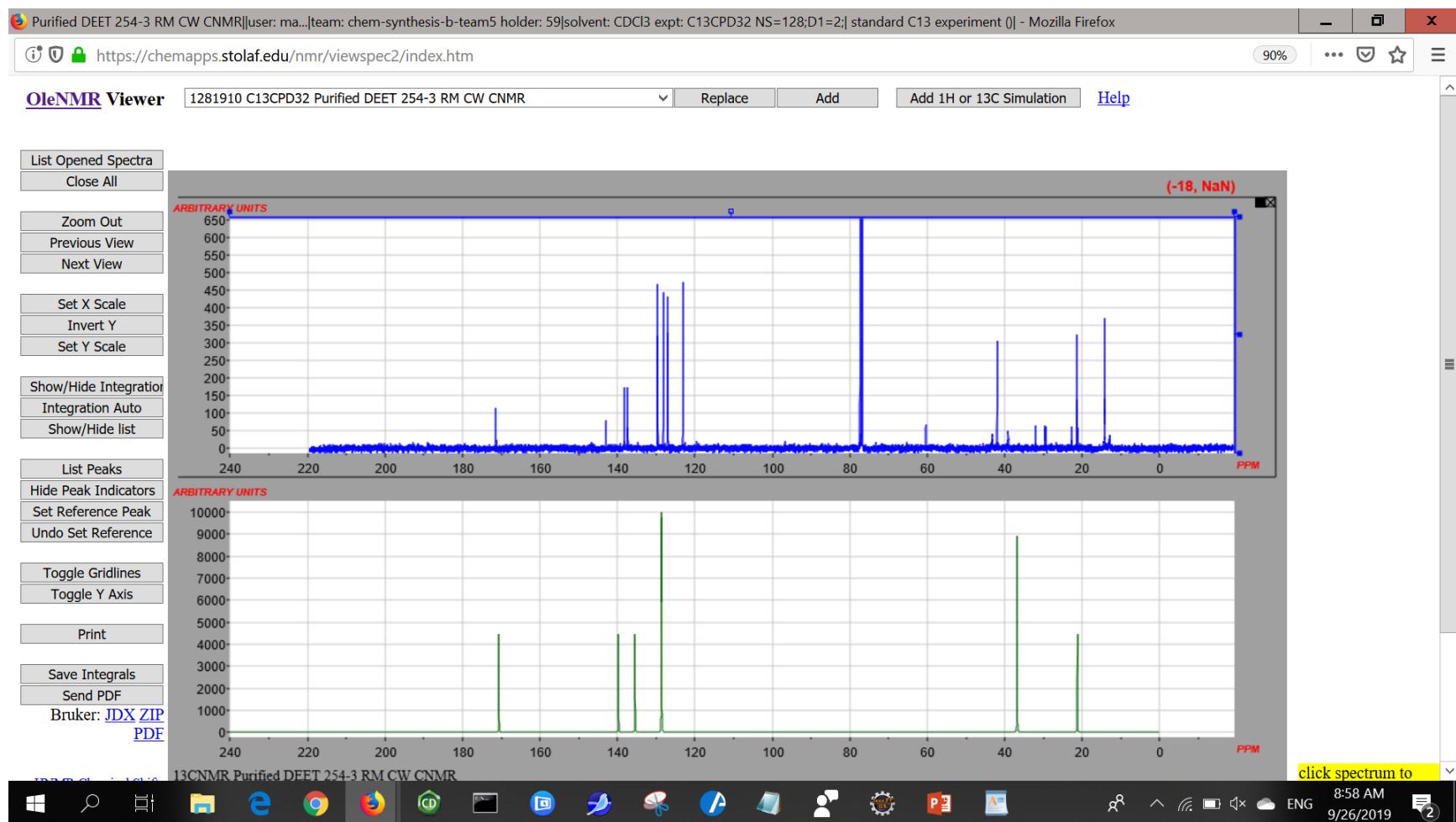
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



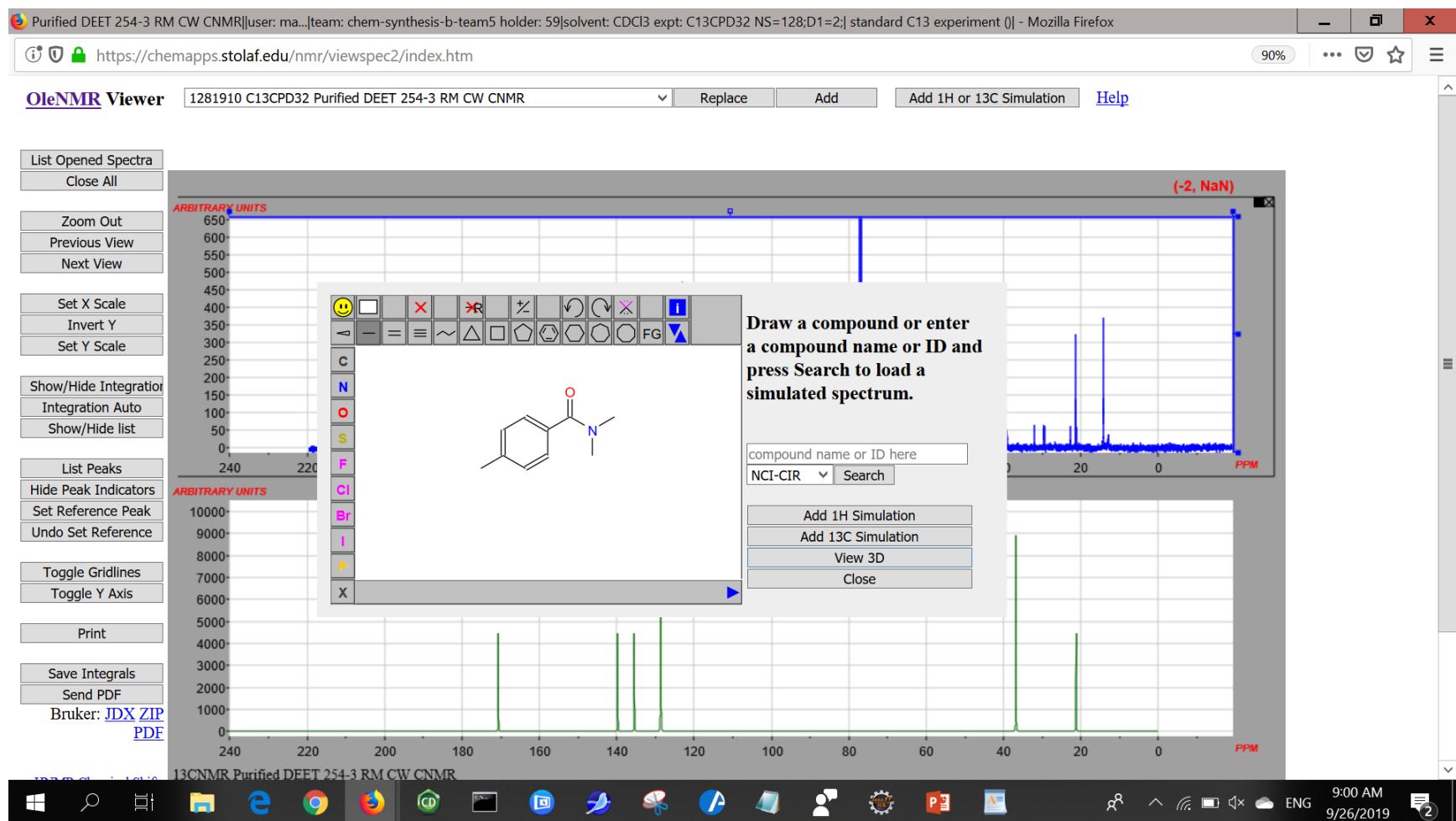
St. Olaf College NMR Laboratory

Analysis using JSPECView-JS



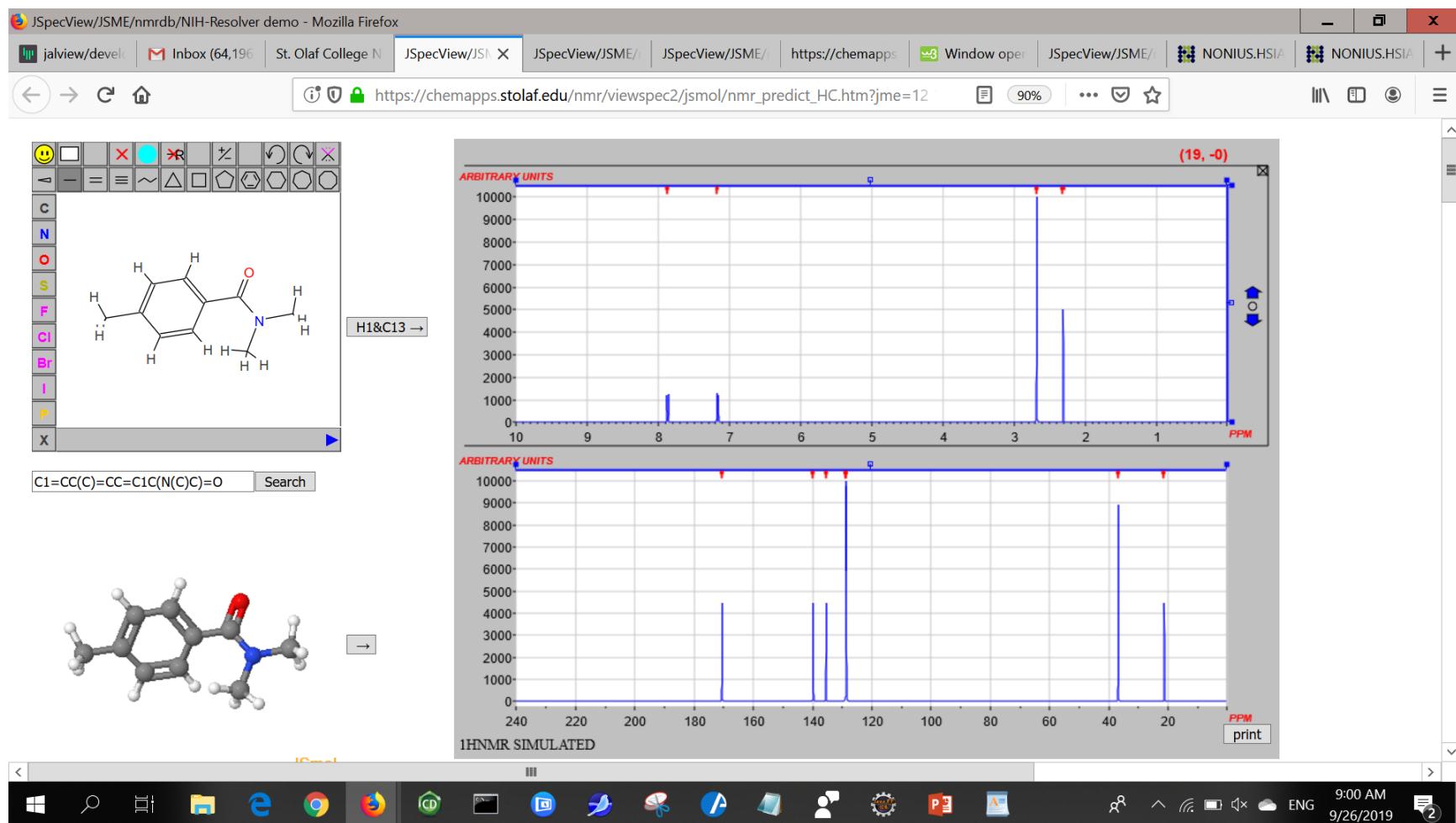
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Analysis using JSpecView-JS



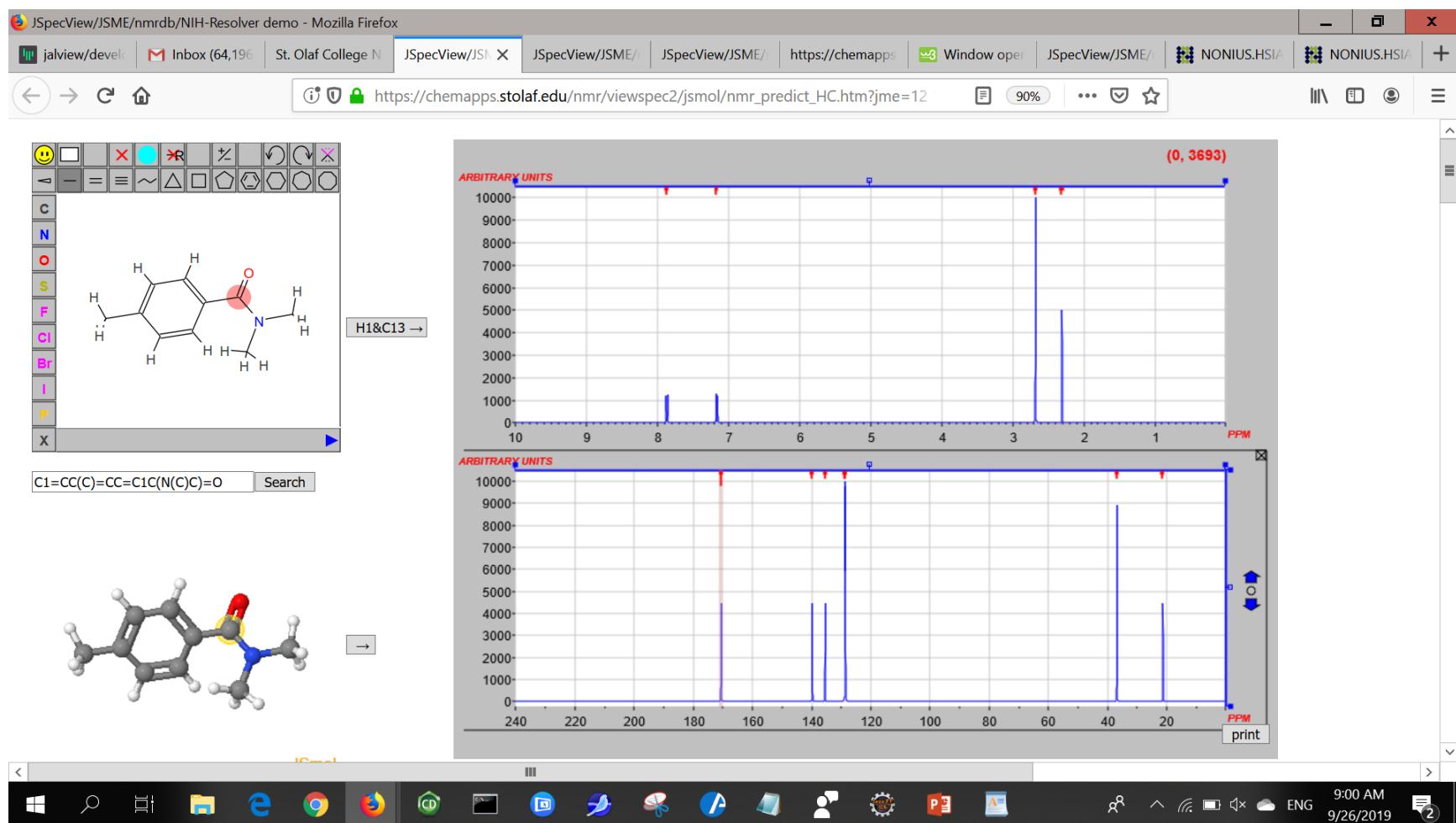
St. Olaf College NMR Laboratory

Analysis using JSpecView-JS



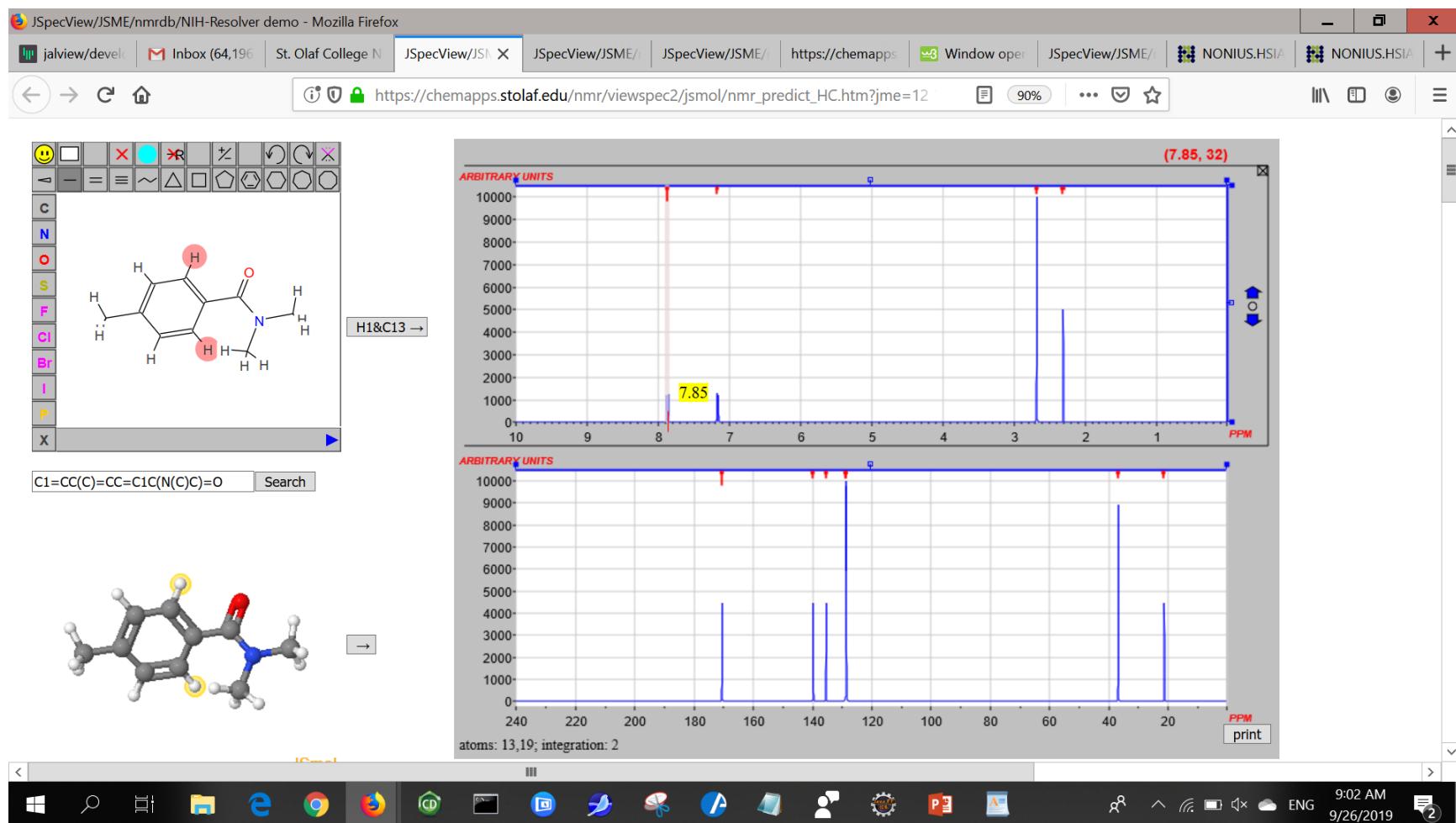
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Analysis using JSpecView-JS

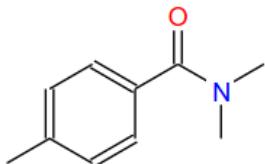
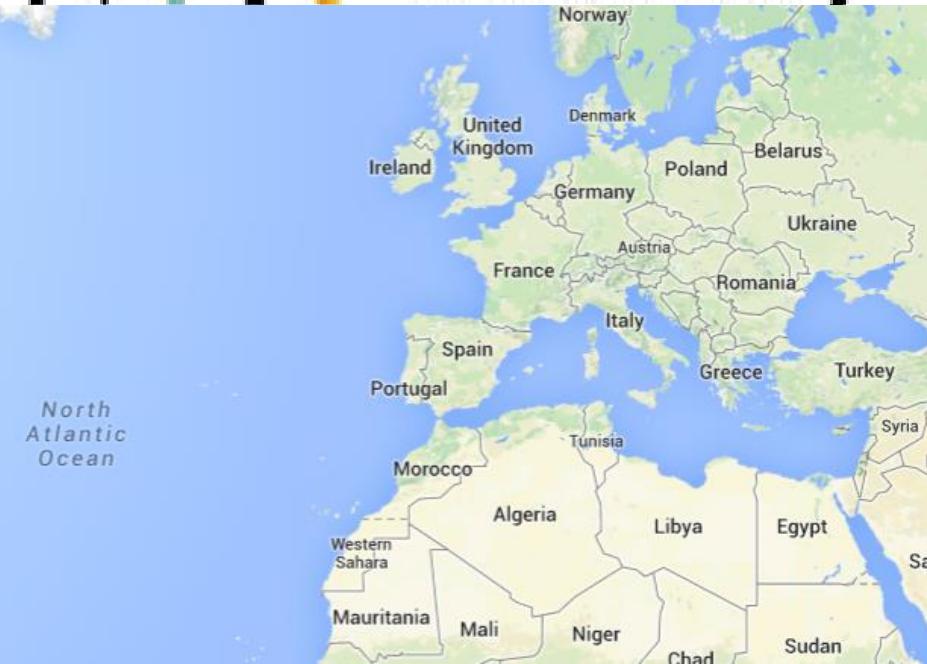


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Analysis using JSpecView-JS

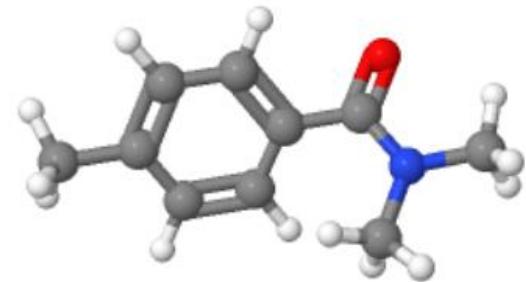
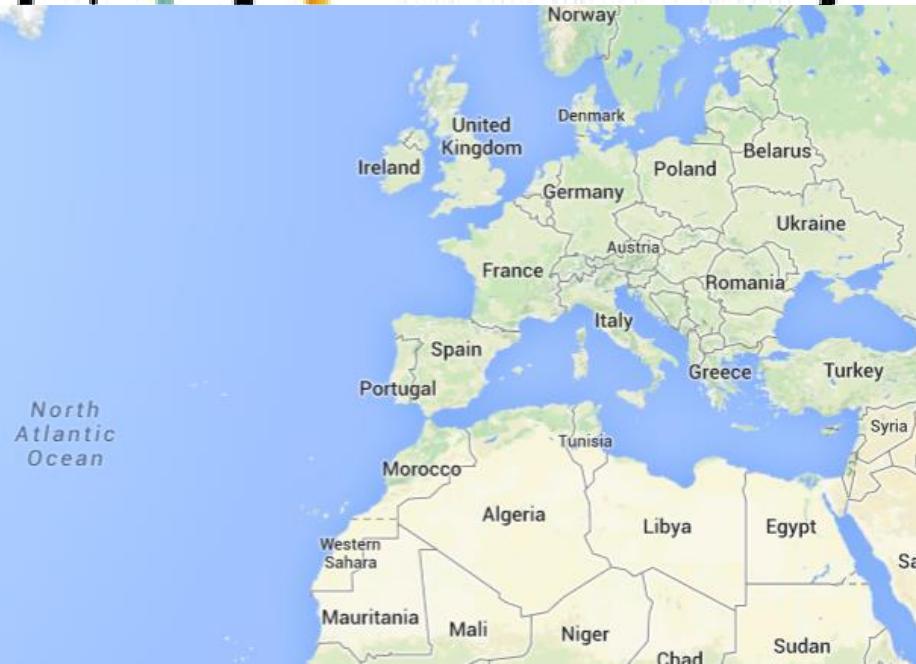


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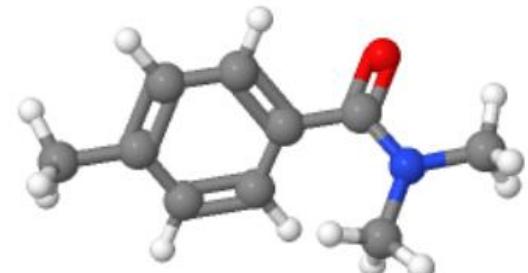
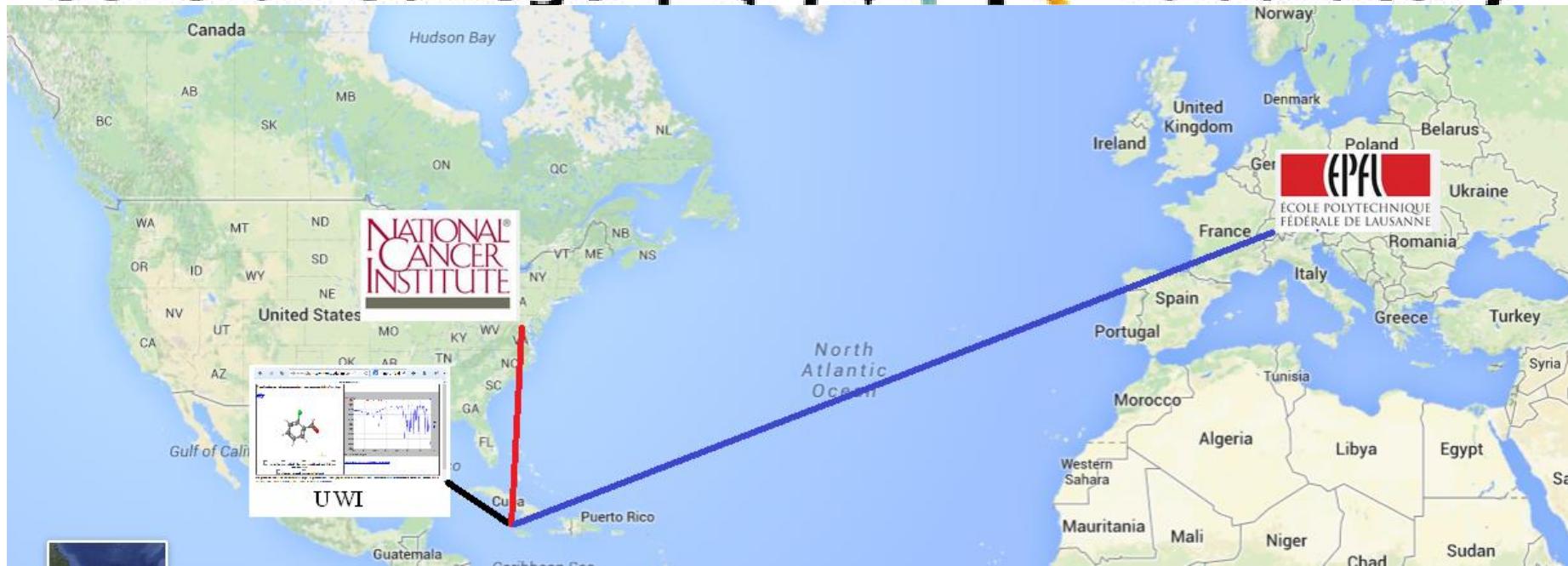
The JSME Molecular Editor interface displays a chemical structure of 4-methyl-N,N-dimethylbenzaldehyde. The structure consists of a benzene ring with a methyl group at position 1 and a formyl group (-CHO) at position 4. A dimethylamino group (-NMe₂) is attached to the carbonyl carbon. The editor's toolbar is visible on the left, featuring icons for basic operations like selection, copy/paste, and zoom, as well as buttons for common atoms (C, N, O, S, F, Cl, Br, I, P) and functional groups.

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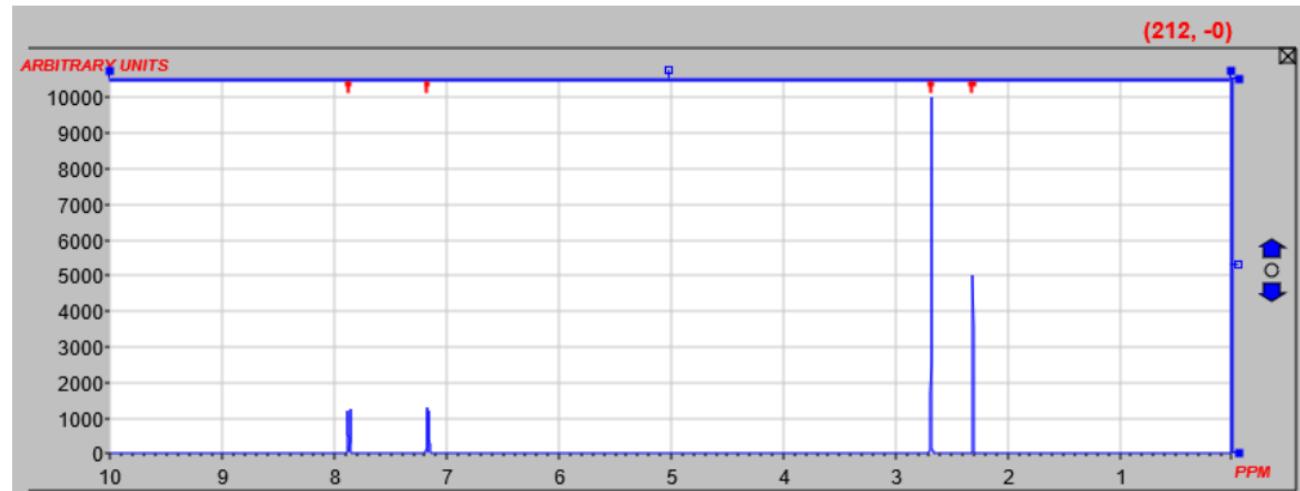


JSmol

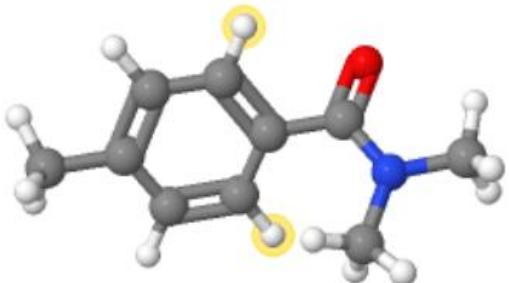
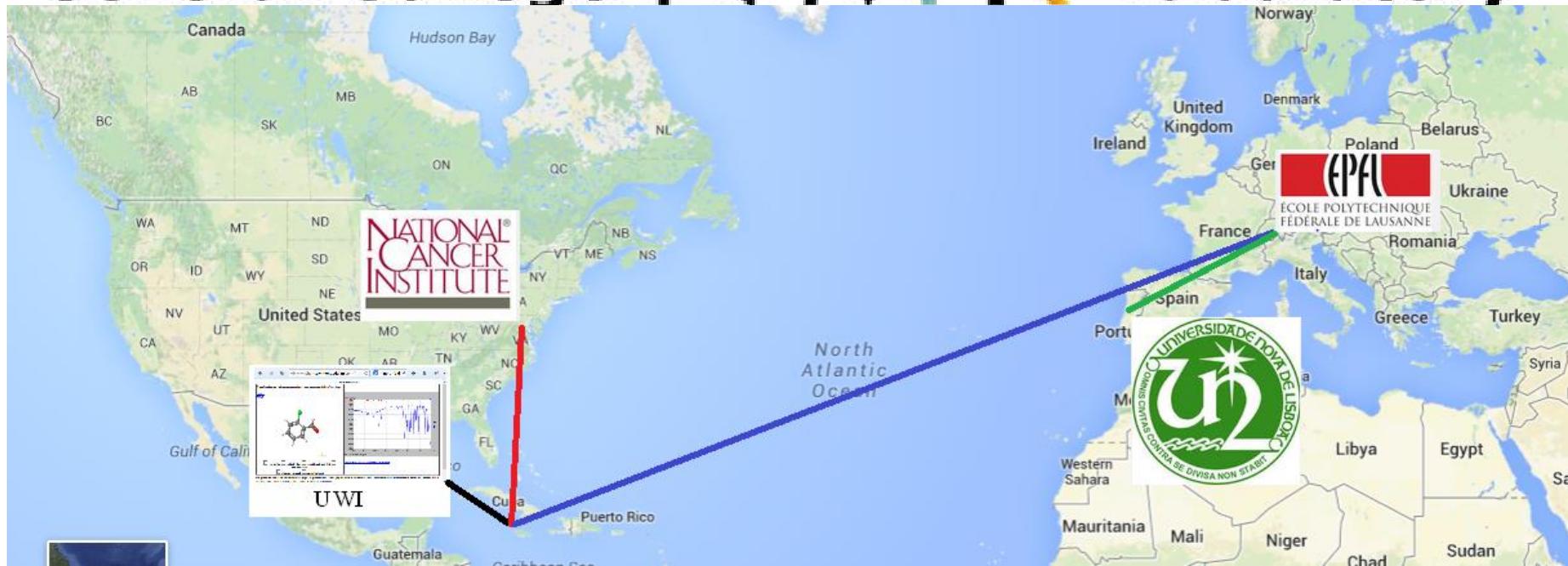
St. Olaf College NMR Laboratory



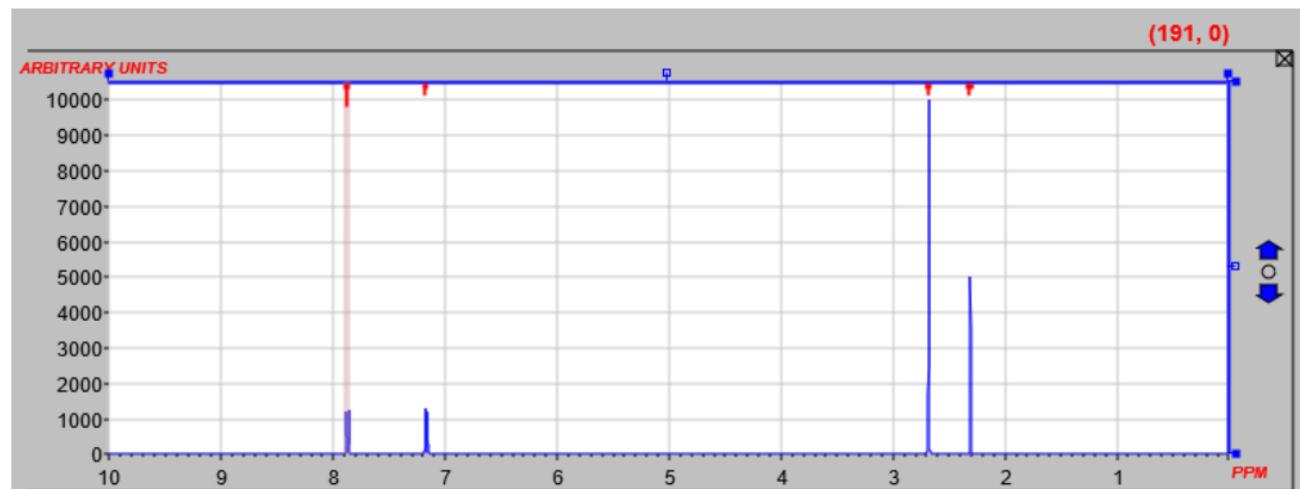
JSmol



St. Olaf College NMR Laboratory



JSmol



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Acknowledgments...

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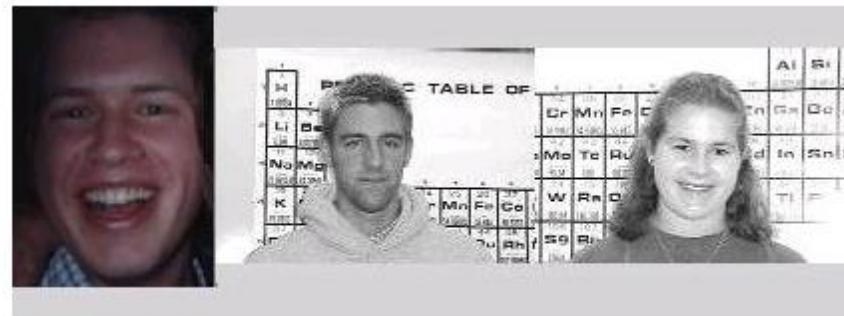
- Peter Ertl, Novartis
- Robert Lancashire, UWI-Mona
- Clemens Anklin, Bruker



St. Olaf College N M R 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