

SBR-SERCAT Sample Submission Tutorial

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SBR-SERCAT customers Sample Submission

- Customers must fill out the web form in order to have samples shipped to SERCAT for analysis.
- All of the information is either required for management of the service, preparing shipment of samples to SERCAT, and preparing a Experiment Safety Assessment Form (ESAF) for APS.

To get started...

- Using your favorite web browser, go to the following web page:
<http://harvest.cals.ncsu.edu/structural-biochemistry-resource/>

This is the Structural Biochemistry Resource home page

Select the **X-Ray Crystallography** pull down tab.

Select **Scheduling** from that tab.

The screenshot shows the homepage of the Structural Biochemistry Resource. At the top, there is a navigation bar with a red logo containing the letters 'TY', a 'RESOURCES' menu, and a search bar. Below the logo, the text 'College of Agriculture and Life Sciences' is visible. The main title 'Structural Biochemistry Resource' is centered above a horizontal menu bar with four tabs: 'Home' (which is highlighted in red), 'NMR Spectroscopy', 'X-Ray Crystallography', and 'Bio-molecular Interaction'. The central image is a 3D molecular model of a protein structure, colored in red, blue, and green, set against a background of a circular grid with various data points and numbers.

Fostering the development of an integrated research network

Structural biology brings together the interrelated disciplines of molecular biology, biochemistry, and biophysics. The molecular structure of biological macromolecules, proteins, and nucleic acids at atomic resolution have helped to revolutionize modern biology. Characterizing biological structures at the atomic level is crucial for understanding the functions of biological macromolecules, including interactions with small ligands (such as substrates and inhibitors) and other macromolecules (nucleic acids and/or proteins). Therefore, structural biology is a pillar of basic biomedical research, indispensable for understanding the details of biological processes and for characterizing the differences between natural and diseased states.

The Scheduling page has a calendar that indicates the SERCAT access dates.

SERCAT access schedules will never show more than two access times ahead

In most cases, both ID and BM beamlines are available on the same days. If access dates for beamlines are not on the same day, the calendar will specifically indicate which beam line is accessed on which day.

Beamline time is for a 24 hour period starting at 10:00 AM Eastern for the ID and 12:00 PM Eastern for the BM.

NC STATE UNIVERSITY

RESOURCES Search College of Agriculture and Life Sciences →

Structural Biochemistry Resource

Home NMR Spectroscopy X-Ray Crystallography Bio-molecular Interaction

The X-ray crystallography facility offers many services. Below are a list of services (SER-CAT and in-house x-ray data collection) that can be scheduled through the use of Google Forms. For all other services please contact [Dr. Paul Swartz](#).

Calendar



Scheduling Form

SBR - X-ray Time Request

Customers must fill out the web form in order to have samples shipped to SERCAT for analysis.
All of the information is either required for management of the service, preparing shipment of samples to SERCAT, and preparing a Experiment Safety Assessment Form (ESAF) for APS.

* Required

User Name: Last, First *
ex// Washington, George who will actually be collecting the data and the primary contact person for the samples

SERCAT Sample registration

Samples must be registered 24 hours prior to shipping and must be in the hands of SBR-SERCAT at that time as well.

The USER and USER email refer to the person who will actually be collecting the data and the primary contact person for the samples.

The PI and PI email refers to the person whose account number is being supplied for fee charges.

SBR - X-ray Time Request

- Customers must fill out the web form in order to have samples shipped to SERCAT for analysis.
- All of the information is either required for management of the service, preparing shipment of samples to SERCAT, and preparing a Experiment Safety Assessment Form (ESAF) for APS.

* Required

User Name: Last, First *

ex// Washington, George who will actually be collecting the data and the primary contact person for the samples

Swartz, Paul

User's email address *

ex// ncsu-bionmr-facility AT ncsu DOT edu

paul_swartz@ncsu.edu

PI Name: Last, First *

ex// Adams, Samuel whose account number is being supplied for fee charges

Swartz, Paul

SERCAT Sample registration

The account number provided will be billed for the time usage during data collection at SERCAT. Time is calculated from the time and date stamps of the files that appear on the data files. Time will be rounded up to the nearest full hour.

Click on the **NEXT** button to continue the submission.

PI's email address *

ex// ncsu-bionmr-facility AT ncsu DOT edu

paul_swartz@ncsu.edu

Account number to charge
(#Required for NCSU requestors) ex// 123456-78901

000000-00000

Billing Details *

Academic (NCSU user)

Academic (non-NCSU user)

Industrial/Commerical

NEXT

Never submit passwords through Google Forms.

SERCAT Sample registration

Select the **SERCAT data collection** button.
Also fill in the access date that you wish the samples to be available at SERCAT for analysis.

SBR - X-ray Time Request

Which service? *

Beamline time is for a 24 hour period starting at 10:00 AM Eastern for the ID and 12:00 PM Eastern for the BM.

- SER-CAT data collection
- In house x-ray data collection

SER-CAT or In house x-ray source use date

Please see calendar above for SER-CAT dates

MM DD YYYY

04 / 21 / 2016

Protein Name(s) *

Provide the non-abbreviated name of the biological contents of the crystal (protein, DNA, RNA, complex, etc.). Include any mutations that have been introduced. Make a unique submission for each different protein (including different mutations). If the USER has proprietary information concerns about using the name of the target, contact SBR-SERCAT Administration (sbr@scranton.edu, 010-512-0170) to arrange alternate names.

SERCAT Sample registration

Provide the non-abbreviated name of the biological contents of the crystal (protein, DNA, RNA, complex, etc.) along with its species origin and whether the protein is purified from human tissues. Include any mutations that have been introduced.

If the USER has proprietary information concerns about using the name of the target, contact SBR-SERCAT Administration (paul_swartz@ncsu.edu, 919-513-0173) to arrange alternate means.

Make a unique submission for each different protein or experiment (including different mutations).

Indicate the number of crystals to be shipped. It is recommended that, if possible, at least 6 crystals from each experiment be shipped. In the past, 6 crystals have almost always yielded results.

Indicate the source of the protein or its expression system if locally produced.

Protein Name(s) *

Provide the non-abbreviated name of the biological contents of the crystal (protein, DNA, RNA, complex, etc.). Include any mutations that have been introduced. Make a unique submission for each different protein (including different mutations). If the USER has proprietary information concerns about using the name of the target, contact SBR-SERCAT Administration (paul_swartz@ncsu.edu, 919-513-0173) to arrange alternate means.

Hen Egg White Lysozyme

Number of Crystals *

It is recommended that, if possible, at least 6 crystals from each experiment be shipped. In the past, 6 crystals have almost always yielded results.

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Expression System *

Indicate the source of the protein –either its native source if it was purified from that source or the bacterium that was used to expressed a cloned product.

urchased from Sigma Chemical Company

Heavy Atoms (Element/N) *

SERCAT Sample registration

List any heavy atoms that have been introduced into the protein for phasing or naturally are present.

Indicate if the sample can be considered a biohazard either from its function, its source, or the heavy atoms that are resident in the crystals.

Select the type of experiment that you intend to perform.

Heavy Atoms (Element/N) *

ex // Gold Chloride

Gold Chloride

Biohazard *

Indicate if the sample can be considered a biohazard either from its function or its source.

- Yes
 No

Experiment *

Select the type of experiment that you intend to perform.

- Gen. Diff
 Phasing
 Other : _____

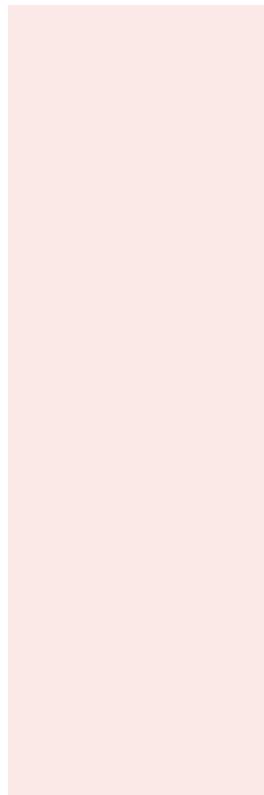
Wavelengths *

ex// 1 \AA , Indicate the wavelength(s) of light that you expect to be using.

SERCAT Sample registration

Indicate the wavelength(s) of light that you expect to be using.

Finally, click on either **BACK** if you want to abandon your submission or **SUBMIT** to register the sample.



The form contains the following fields:

- A question "Is this a sample for an experiment?" with options "No" (radio button) and "Yes" (checkbox). "No" is selected.
- A section "Experiment *":
 - "Gen. Diff" (radio button)
 - "Phasing" (radio button, selected)
 - "Other : _____" (text input field)
- A section "Wavelengths *":
 - "1.0" (text input field with a red underline)
- Buttons at the bottom: "BACK" (grey) and "SUBMIT" (blue).

Text at the bottom right: "Never submit passwords through Google Forms."

SERCAT Sample registration

The result of the **SUBMIT** selection allows reviewing and editing of the submission or to continue to an additional submission.

The screenshot shows a Google Form interface. At the top, there is a navigation bar with four items: 'Home', 'NMR Spectroscopy', 'X-Ray Crystallography' (which is highlighted in red), and 'Bio-molecular Interaction'. Below the navigation bar, the main content area has a title 'SBR - X-ray Time Request'. Underneath the title, a message says 'Your response has been recorded.' followed by two blue underlined links: 'Edit your response' and 'Submit another response'. At the bottom of the form, a small note states 'This form was created using Google Forms. [Create your own](#)' and the 'Google Forms' logo.

Home NMR Spectroscopy **X-Ray Crystallography** Bio-molecular Interaction

SBR - X-ray Time Request

Your response has been recorded.

[Edit your response](#)
[Submit another response](#)

This form was created using Google Forms. [Create your own](#)

Google Forms

SERCAT Sample registration

At the end of a successful submission, an Email will be sent to the USER with a summary of the submission. Further contact can be expected from the facility concerning the logistics of packing and shipping the samples.

X-Gm-Message-State:
AD7BkJLgue597AHDFJlv23OPs9S1hfzUZzQFt7C7yTEqRsNe/TWd/eJQmGCScjGtx0pkwfi3uMdr28xVQw6X
UdhVs+FXPCsNxzeTFwpQQcDZlqDQ/aC8D93l565+/X5oW/3f9bS9zJ2zQdPHdGN/0kNwxPWmExfOkQvrY
Wlt5aYH/8Y/U5I51Y4blYUaj/7+w9f8SGUKB7apZ3OZ3f
MIME-Version: 1.0
X-Received: by 10.66.216.100 with SMTP id op4mr3769504pac.9.1457633064381;
Thu, 10 Mar 2016 10:04:24 -0800 (PST)
Message-ID: <001a11c1fb0040ca5052db5a50d@google.com>
Date: Thu, 10 Mar 2016 18:04:24 +0000
Subject: SER-CAT data collection - Thu Apr 21 2016 00:00:00 GMT-0400 (EDT)
From: ncsu-bionmr-facility@ncsu.edu
To: paul_swartz@ncsu.edu
Content-Type: text/plain; charset=ISO-8859-1; format=flowed; delsp=yes

Crystal samples are shipped to SERCAT 2 days before allotted time and allotted times are usually late in the week so shipping is either on Monday or Tuesday of the week with data collection Wednesday through Friday.

Access time starts at 10:00 AM Eastern time for the ID beamline and 12:00 PM Eastern time for the BM beamline. Data collection occurs in Polk Hall 053.

There are times when equipment failures at SERCAT or APS that prevent data collection for a time. Usually, additional time will be provided at a

later date.

Shipping toxic samples requires that crystals be shipped on freight airplanes or ground and the shipping takes two days. When this is needed, shipping may have to happen more than two days before data collection time. Additional paperwork is also needed with toxic samples. When shipping virus particles, all appropriate FDA and local regulations apply so further paperwork is needed.
Specifics about your submission follows:

Timestamp :: 3/10/2016 13:04:19
User Name: Last, First :: Paul Swartz
User's email address :: paul_swartz@ncsu.edu
PI Name: Last, First :: Paul Swartz
PI's email address :: paul_swartz@ncsu.edu
Account number to charge :: 000000-00000
Billing Details :: Academic (NCSU user)
Which service? :: SER-CAT data collection
SER-CAT or In house x-ray source use date :: 4/21/2016
Protein Name(s) :: Lysozyme
Number of Crystals :: 10-15
Expression System :: E. coli
Heavy Atoms (Element/N) :: Gold Chloride
Biohazard :: No
Experiment :: Phasing
Wavelengths :: 1

SERCAT Data Return

- Data from SERCAT will be deposited on a hard drive during collection. The hard drive is transported with the samples to and from SERCAT.
- Sample and data return generally happen within 3 to 4 working days of the data collection.
- Data processing can be done while data is collected and scaled data sets and log files can be emailed to the user as soon as they are prepared. Actual diffraction frames return with the samples.
- Proprietary data issues should be brought to the attention of SBR-SERCAT administration (paul_swartz@ncsu.edu, 919-513-0173) so that an arrangement for data security that is acceptable to both SBR-SERCAT and the USER can be achieved.