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# ARP User Guide for Neutron and Deuteration Proposal Submissions

# Purpose

This guide provides information to Australian Centre for Neutron Scattering (ACNS) and National Deuteration Facility (NDF) users regarding submission of all proposal types (Neutron, Deuteration / Neutron, Deuteration) for merit access to ACNS and NDF capabilities through the ANSTO Research Portal (ARP).

For further information, contact <a href="mailto:user.office.nsw@ansto.gov.au">user.office.nsw@ansto.gov.au</a>

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# 1. ANSTO Research Portal

Access to the <u>Australian Centre for Neutron Scattering (ACNS)</u> and the <u>National Deuteration Facility</u> (<u>NDF</u>) will be through the ANSTO Research Portal (ARP). Using the tabs/links provided in the ARP, access to specific proposal types will be available – Neutron (Normal), Neutron Program, Deuteration / Neutron (combined for experiments requiring access to both NDF and the Australian Centre for Neutron Scattering – ACNS), Deuteration, Deuteration / Neutron Program (for NDF and ACNS) and Deuteration Program.

The ACNS Customer Portal will eventually be phased from use and all data will be transferred to the ARP during a later phase of the transition. Until this occurs, approved proposals will have attending users and scheduling done through the ACNS Customer Portal.

ANSTO accepts merit access applications/proposals from researchers in universities, research organisations and industry. Merit access applications/proposals are subject to technical feasibility, safety and competitive scientific review processes.

Before starting your application, we strongly recommend you contact the relevant ACNS and NDF scientists who are expert in the capabilities or instruments you seek to access. They can:

- Work with you to develop your proposal application;
- Advise on the most appropriate capability or instrument selections; and
- Help you optimise the use of ACNS and NDF capabilities

Merit access proposals must provide enough information to address the questions and information requests during the proposal preparation and submission process to enable sufficient review.

# 2. User Accounts

### 2.1. Account registration

You must be registered in the ANSTO Research Portal to be able to submit proposals. Follow the below steps to register a new account:

- 1. Go to <u>https://portal.ansto.gov.au/</u>
- 2. Click register

	Wed, 04 Aug 2021 22:41 AEST
Research Portal	
Welcome	Sign in
to The ANSTO Research Portal. This is your gateway to all of ANSTO's research facilities and experience.	Email Password: Password Login   Register Forgot your password?
3 Enter vour email address	

- 3. Enter your email address
- 4. Create a password
- 5. Verify this password

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#### 6. Click register

Note: You can reuse your existing username and password for the ACNS Customer Portal when you register. You will need to set them up in ANSTO Research Portal).

Research Portal	Fri, 25 Jun 2021 9:55 AEST
<b>Registration</b> Please enter your details below to commence the registration process <b>Email: *</b>	
Password: * Verify Password: *	
Register	

You will receive an email containing an activation link to complete your account registration. An email confirmation message will appear on your screen, confirming that an email has been sent to your listed email address.

- 7. Click the activation link provided to verify your account
- 8. After successfully activating your account, you will see a registration confirmation message. Click on the blue 'here' to complete your registration.

### 2.2. User profile

After your account has been verified, you will be required to complete your user profile. Profile fields that are marked with a red asterisk \* are mandatory and must be filled in.

To complete your user profile you must enter your:

- 1. **Personal information:** Full name, country of citizenship and gender
- 2. **Organisation information:** Mobile number and affiliated organisation. If your organisation is not displayed in the drop-down list, please enter your organisation name in the 'Add Organisation' field
- Additional information: Email updates tick the box if you do not want to receive emails unrelated to my proposals
- 4. Click Submit at bottom of page when ready.

Please ensure that you provide valid and correct details as this can affect your ability to access the portal and submit future proposals. To change any information in this section, you must specify your current password. Only include a new password if you want to change it.

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Registration Details		
* Mandatory Information		
ACCOUNT INFORMATION		
ACCOUNTINFORMATION		
Email *		When you first set up your account, you
		cannot edit your email address.
PERSONAL INFORMATION		
Title First Name *	Other Names	
~		
Last Name * Country of Citizenship		
	~	
ORGANISATION INFORMATION		
Organisation Add	Organisation	If your organisation is not displayed in the
v □	organisation	drop-down list, please enter your organisation name in the 'Add
		Organisation field.
Position Title Depa	artment	
Telephone (Mobile) * Telephone (Other)	Website	Please include your country and area code in your telephone number
ADDITIONAL		
Email Updates		
I do NOT want to receive emails unrelated to my proposals.		
Submit		

# 2.3. Account login

- 1. Go to <u>https://portal.ansto.gov.au/</u>
- 2. Enter your email address
- 3. Enter your password

If someone has created an account on behalf of you, then there will be no account information associated with your details. You will need to create an account as per the previous steps.

### 2.3.1. Password reset

- 1. Click forgot your password
- 2. Enter your email address
- 3. Click reset password

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If you do not receive the reset link email please contact the <u>user.office.nsw@ansto.gov.au</u>.

## 2.4. User Dashboard

When you login to the ANSTO Research Portal your user dashboard will appear. Depending on your permissions, you may see the following tabs:

- **Dashboard** This will show your five most recent proposals submitted in the ANSTO Research Portal.
- **Proposals** All proposals on which you are Principal Scientist, Co-proposer or Co-proposer (editor) are listed on this page. Available options (Edit, PDF, View, Copy) for each proposal are at the right-hand side of the page for each proposal.
- **Profile** On this page you can update your password, personal information and organisation information.

Dasl	hboard	Proposals	Profile			
My Proposals						
Crea	te new proposal					
Create new proposal						
This only sh	iows you your fiv	e most recent proposa	ls. For the complete li	st, see the P	Proposals tab.	
					·	
This only sh	iows you your fiv Round	e most recent proposa Title	ls. For the complete lis	st, see the F Owner	Proposals tab. Status	Actions

Proposal

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# 3. Proposal type selection

# 3.1. Australian Centre for Neutron Scattering

You must select one of the below proposal types for merit access proposals to access the Australian Centre for Neutron Scattering instruments.

Proposal Type	Description
Normal	Merit access proposal for ACNS experiments within a 6- month round.
Deuteration/ Neutron	Merit access proposal for ACNS instruments and NDF capabilities where deuterated molecule/s are required for the proposed neutron experiments at ACNS.
Program Proposal- Neutron	Merit access proposal for access to one or more ACNS instruments and capabilities for a program of research of up to 3 years.
Program Proposal- Deuteration/Neutron	Merit access proposal for a program of research of up to 3 years for access to both ACNS instruments and NDF capabilities, where deuterated molecule/s are required for the proposed program of research utilising ACNS neutron instruments.

For all other proposals, please use the Legacy ACNS Customer Portal.

# 3.2. National Deuteration Facility

You must select one of the below proposal types for merit access proposal submissions to access the National Deuteration Facility. Selection is determined by what type of isotopic labelling you intend to request provision of (deuteration only or multiple-labelled), where you intend to utilise these molecules (Australia or overseas) and how (neutron scattering, NMR or other applications).

Proposal Type	Description
Deuteration	Merit access proposal for NDF capabilities within a 6- month round. This proposal type is for overseas neutron experiments or for non-neutron applications (e.g. NMR, MS). More information on NDF user access can be found <u>here</u> .
Deuteration/ Neutron	Merit access proposal for ACNS instruments and NDF capabilities where deuterated molecule/s are required for the proposed neutron experiments at ACNS.
Program Proposal – Deuteration	Merit access proposal for a program of research of up to 3 years for access to NDF capabilities of biological and/or chemical deuteration or multiple isotopic labelling. This program proposal type is for overseas neutron experiments or non-neutron applications (e.g. NMR, MS).
Program Proposal- Deuteration/Neutron	Merit access proposal for a program of research of up to 3 years for access to both ACNS instruments and NDF

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	capabilities, where deuterated molecule/s are required for the proposed program of research utilising ACNS neutron instruments.
--	---

For proposal types other than merit access such as user pays/collaborative or commercial and for any enquiries, please contact the NDF via <u>ndf-enquiries@ansto.gov.au</u>.

# 4. Neutron Instrument and Deuteration Technique Selection

# 4.1. Australian Centre for Neutron Scattering

There are 15 neutron beam instruments, which are classified into four main groups: diffractometers, small-angle spectrometers imaging and reflectometry instruments and inelastic spectrometers. The suite of instruments and operating cabins are housed in the Neutron Guide Hall, which also accommodates sample preparation areas, laboratories and other technical support facilities.

The Australian Centre for Neutron Scattering also operates three X-ray instruments and a physical properties measurement system. Full information on the ACNS instruments and capabilities available can be found on the <u>Call for Proposals webpage</u>.

# 4.2. National Deuteration Facility

The National Deuteration Facility offers the facilities, staff and expertise to produce molecules where all or part of the molecular hydrogen is in the form of the isotope deuterium (<sup>2</sup>H) The NDF utilises chemical or biological (*in vivo*) processes/techniques for the deuteration and multiple-labelling of a broad range of molecules.

Deuteration of molecules is useful in studies investigating the relationship between molecular structure and function and where it leads to improved material properties in their end-use application. Deuteration can enhance contrast, and reduce background (from incoherent absorption) in studies using neutron scattering instruments (at ACNS for example), or using spectroscopic techniques such as Nuclear Magnetic Resonance (NMR), Infra-Red (IR) or Mass Spectrometry (MS).

Further information about NDF capabilities and examples of the types of molecules and labelling accessible can be found at the following links:

Deuteration Techniques	
National Deuteration Facility   Biodeuteration	
National Deuteration Facility   Chemical Deuteration	
NDF product catalogue	

Further information about NDF user access can be found here.

Enquiries can be directed to: <u>ndf-enquiries@ansto.gov.au</u>

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# 5. Proposal creation: Neutron - Normal

A normal access proposal is for all merit access proposals submitted within a 6-month round. When you click the Australian Centre for Neutron Scattering (ACNS) menu, you will find a list of proposal types available. One proposal type must be selected to request access to ACNS capabilities.

- 1. Click the proposals tab
- 2. Click create new proposal
- 3. Click Australian Centre for Neutron Scattering
- 4. Select the Normal proposal access type

Australian Centre for Neutron Scattering	
Normal	
5. Input text into questions shown below:	

- **Proposal Title\***: Please provide a short, descriptive title for your proposal. This field will not accept superscripts, subscripts, other alphabet letters etc.
- Proposal Type\*: The proposal type defaults to the type of proposal you selected on the previous page.
- Proposal Round \*: Only rounds that are currently open will be available and one must be selected.
- **Principal Scientist**: select by typing surname or first name and selecting from names available.
- 6. Click create

Proposal Creation
Normal
Merit access proposal for ACNS experiments within a 6-month round.
Proposal Title *
Provide a short descriptive title
Proposal Type *
ACNS Normal: Peer-reviewed experiments on our neutron beam lines.
Proposal Round *
○ ACNS & NDF: 2023-1: (Submissions due on September 15)
Principal Scientist
Create

Once you click create, this saves your work and takes you to the main proposal creation page.

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### 5.1. Tab 1: Main

A table with the proposal details is visible on the first tab. This table includes details such as:

- Proposal number/ ID
- Proposal round
- Proposal type
- Proposal status

This data has been populated from the previous step and cannot be modified.

Proposal Details	
ID	N:P14952
Title	test proposa
Round	ACNS & NDF: 2023-1
Туре	ACNS Normal
Status	In Preparation

# 5.1.1. Keywords

List up to four keywords or phrases which relate to this proposal, separated by commas. Keywords are index or subject words which help identify the proposals topic and objectives.

Keywords
List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help
identify the proposal's topic and objectives.

### 5.1.2. Collaborators

Enter the details of all researchers involved with this proposal including students. Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs and outcomes of this project.

Adding an existing collaborator	1.	Enter the first name and last name of your collaborator
	2.	Click on your collaborator's name
	3.	Click add user
	4.	Tick first time user if your collaborator is accessing ANSTO facilities for the first time
	5.	Select student type to indicate what level your collaborator is studying at.

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Adding a new collaborator	2. 3.	Enter the first name and last name of your collaborator – if their name does not appear you will need to follow the below steps: Click create user Complete the details in the pop-up window Click create
Selecting an organisation		Enter the beginning of the name of the organisation. The closest match will appear Click on the organisation name to select

#### Collaborators

Please enter the details of the researchers (including students) involved with this proposal. Enter the given or family name of your collaborator. Click on your collaborator's name if it appears. Click Add User. If your collaborator is not registered, click *Create User*. Complete the details in the pop-up *Add a new user* form and click *Submit* and then *Close*. Select the appropriate Role and Student Type (if applicable) and enter the student's Supervisor Name.

Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs &/or outcomes of this project.

Name	:	Add User Clear	ır	
Name	Role	First Time User <b>0</b> Student T	Type <b>0</b> Funding Approved	
	Principal Scientist 🛛 👻	First Time User     Not App	plicable 💙 🗌 Funding Approved	×
	Co-proposer (editor 🗸	First Time User Honour	rs	×
	Co-proposer (editor 💙	First Time User Masters	s	×

#### Considerations

- There can be only one Principal Scientist for each proposal and only the Principal Scientist can submit a proposal.
- If you would like any of your co-proposers to be able to edit the proposal (have read and write access) please select `*Co-proposer editor*' in the role field.
- If a person has not used the ACNS neutron instruments before, check the *First Time User* box field.
- If the person is a student, use the dropdown list to select the *Student Type* (Honours, Masters, PhD)in the field provided. If you select a Student Type, enter the student's Supervisor Name.
- It is expected that the Principal Scientist submitting the proposal has spoken with relevant ANSTO Staff about the proposal prior to submission.

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### 5.1.3. Categorisation

Under categorisation there are a series of fields and questions that are to be completed if applicable to your proposal.

1. Enter the details for the fields below where applicable:

#### • Scientific area

Indicate in which of the given scientific areas your proposal should be reviewed.

#### Scientific Area

Please indicate in which of the given scientific areas your proposal should be reviewed. You can provide more details in the keyword section.

#### • Intellectual Property

Select 'yes or no' if there is intellectual property associated with this proposal. If yes, add the intellectual property details in the text box provided.

#### I.P. Issues

⊖ Yes

⊖ No

Intellectual Property Details Maximum 1000 characters

#### • Student thesis

Select 'yes or no' if this work forms a critical part of a student thesis. If yes, add the thesis details in the text box provided.

Does this form a critical part of a student thesis?

#### O Yes

O No

#### Thesis Details

If so, please provide the name of the student, organisation, thesis title and expected submission date.

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#### • Research Funding

Check relevant option(s) for any funding bodies who have awarded funds to this project. More than one option can be selected.

Research Funding
Name any funding bodies who have awarded funds to this project.
Internal Funding
C ARC Funding
NH&MRC Funding
Industry Funding

#### • **Industrial Relevance and Industrial Involvement** Select the industrial relevance category appropriate for this project.

Industrial Relevance	
	~
Industrial Involvement	
Name of Company involved	

- 2. Click **save**
- 3. Click **next**.

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### 5.2. Tab 2: Science

## 5.2.1. Proposed Research (PDF) \*

- 1. Upload a two-page PDF (maximum) describing your proposed research. The file must include the following information:
  - Scientific background and significance
  - Aim of the proposed experiment
  - Scientific importance of the proposed measurements
  - Detailed description of experiment (remember that referees might not be experts in the field). If requesting more than one instrument, indicate any experimental dependencies
  - Results of preliminary work carried out (e.g. using X-rays, NMR, etc.)
  - Results of previous work using neutrons (as per anonymised review guidelines)
  - Reason for choice of requested instrument/s
  - Calculation of beamtime indicate how you calculate the requested beam time (depending on number of samples, and sample-environment conditions such as temperature, etc. for each sample),
  - Data analysis provide an overview of how the data will be analysed.
  - References Clearly identify documents referenced with doi if available
  - Relevant figures
- 2. Click upload
- 3. Click choose file
- 4. Click upload

× File upload
Use the form below to upload a file. Unlike other fields, changes to files do not need to be saved.
File to upload * Choose File No file chosen
Max file size: 3mb Allowed formats: PDF, PNG, and JPG
Cancel Upload

- 5. Click save
- 6. Click next.

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#### Proposed Research (PDF) \*

Please upload a 2 page PDF (PORTRAIT ONLY, NOT LANDSCAPE USING A 12-POINT FONT) of your proposed research, which must include the information listed below. The maximum file size is 3MB.

- scientific background and significance
- aim of the proposed experiment
- scientific importance of the proposed measurements
- detailed description of experiment (remember that referees might not be experts in the field). If requesting more than one instrument, indicate any experimental dependencies
- results of preliminary work carried out (e.g. using x-rays, NMR, etc.)
- results of previous work using neutrons
- reason for choice of requested instrument/s
- calculation of beamtime indicate how you calculate the requested beam time (depending on number of samples, and sampleenvironment conditions such as temperature, etc. for each sample),
- data analysis provide an overview of how the data will be analysed.
- references Clearly identify documents referenced with doi if available

No file loaded

Upload

#### **PDF Upload Considerations**

- The maximum file size is 3MB.
- Two-page maximum can be uploaded only.
- The PDF layout must be portrait only. Landscape layout is not accepted.
- 12-point font can be used only.



## 5.3. Tab 3: Instruments

You must select the instruments required as part of your project. Additional resources may be requested on this page for laboratories and sample environment equipment.

#### 5.3.1. Neutron Instrument selection

- 1. Select neutron instrument
- 2. Select a specific instrument from the adjacent drop-down menu
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add the number of requested days
  - Describe the experimental setup\*
  - Request a scientist
  - Add sample environment equipment
  - Add laboratory ancillaries
- 5. Repeat the steps above for any additional instruments
- 6. Click save

	Instruments
Main	N:P1: Neutron Test
Science	Previous Save Next Cancel
Instruments	
Samples	Instruments: Manage the ACNS instruments required by your proposal. You may request additional resources here also, such as
Figures	Sample Environment. For more information about the choices, consult the ACNS Sample Environment Handbook.
Admin	Neutron Instrument   Add Instrument  Add Instrument
Submit	
	Analysis Type Instrument Requested
	Neutron Instrument DINGO 2 Days 🗸
	Experimental Setup * Please provide the instrumental settings you require on the instrument in order to carry out your experiment, such as resolution, wavelength, Q-range, and so on.
	Scientists     Choose     Choose       Sample Env     Choose     Choose

# 5.3.2. Non- Neutron Instrument selection

- 1. Select ACNS non- neutron instrument
- 2. Select a specific instrument from the adjacent drop-down menu
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add the number of requested days
  - Describe the experimental setup\*
  - Request a scientist
- 5. Repeat the steps above for any additional non-neutron instruments
- 6. Click save

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ACNS: Non-Neutron Instrument	Imaging Ellipsometer	5 Days	~ ×
Experimental Setup * Please provide the instrumental set as resolution, wavelength, Q-range,		ment in order to carry	out your experiment, such
Scientists Choose	~	Requested	

### 5.3.3. Impossible dates

Enter any impossible dates that you will not be able to perform the experiment. This applies to all instrument requests.

Impossible Dates	
Applies to all Instrument requests. Maximum 250 characters.	

# 5.3.4. Laboratory Requirements

Add details about any standard laboratory chemicals and equipment you would like us to supply, including equipment needed for sample storage and preparation (inert atmosphere, refrigeration).

Laboratory Requirements Please detail any standard laboratory chemicals and equipment you would like us to supply, including equipment needed for sample storage and preparation (inert atmosphere, refrigeration).

# 5.3.5. Sample Environment Requirement(s)

Describe your sample environment set up needs.

Sample Environment Requirements

Please describe your sample environment set up needs, e.g. temperature range, magnetic field range, need for electric field, in-situ requirements, need for additional equipment such as temperature baths, power supplies, etc).

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# 5.3.6. User Supplied Equipment

Describe any equipment you will bring onsite and how any hazards will be managed.

User Supplied Equipment Please describe any equipment you will bring onsite with you, and how any hazards will be managed.

Click save.

Click **next**.



### 5.4. Tab 4: Samples

This section provides a space for you to add samples and chemicals (such as solvents) related to your proposal. Each sample will need to be added separately and detailed sample information will need to be provided, including an SDS (where possible).

All items that are going to be irradiated in the neutron beam (for example your sample container/holder, or equipment/vessel you provide) must also be listed as a sample in this section.

By providing detail information regarding your samples will enable ANSTO to fulfil regulatory requirements and to assist the completion of a risk-based safety review of your proposal.

#### 5.4.1. Sample Creation

- 1. Click create new sample
- 2. Enter the following information for each sample:
  - Description\*
  - Sample Form\* (select from drop down list)
  - Chemical Formula or Chemical Composition\*
  - o CAS Number
  - Hazards\* (click in box, select 1 or more from drop down list)
  - Amount (mass g or volume ml)\*
  - Safety Comment
  - Crystalline sample\*; if yes then add lattice parameters
  - Sample prepared\* (select from drop down list)
  - o Date ready
  - Disposal method (select from drop down list)
  - Australian Safety Data Sheet\* file upload available
- 3. Click save

	Samples		
Main	N:P1: Neutron Test		
Science	Previous Next Exit		
Instruments			
Samples	Please add each sample separately. When you add a sample you will also be asked for detailed sample in possible). This information allows us to fulfil our regulatory requirements and to assist the completion o		
Figures	your proposal. Make sure you also add any extra samples and any other chemicals (for example: solvent	s) that you may	y be bringing
Admin	with you. This ensures that we have an SDS for every chemical brought to ANSTO. All items that are goin neutron beam (e.g. your sample container/holder, or equipment/vessel you provide) must be listed as a	0	
Submit	mandatory activation calculations can be performed for all materials in the beam. If you need to add a s proposal has been approved, contact the ACNS User Office.		
	Create new sample		
	Sample	Details	Сору
	Test sample	Edit	名

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Description *	
Sample Form *	
Solid	~
Chemical Formula or Chemical Composition *	
CAS Number	
Hazards *	
Amount (mass g or volume ml) *	

**Note:** If there is no Australian Safety Data Sheet available at the time of submission, you must declare the following information. If you have a sample for which these questions do not apply, leave them blank:

- Contact Details/Ownership
- Date Completed
- Precautions for Handling
- Dangerous Goods Class Primary and Secondary
- Packing Group
- UN Number
- Appearance
- Odour
- Solubility (water/solvents)
- pKa
- Flash point
- Specific Gravity
- Bulk density
- Particle Size
- Viscosity
- Boiling Point
- Melting Point



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<b>afety Data Sheet Questions</b> you have a sample for which these questions do not apply, leave them blank	
ontact Details/Ownership	
Pate Completed	
his is the date that safety information was last reviewed. It should be no more than 5 years old.	
recautions for Handling *	
	/
Dangerous Goods Class (Primary)	
	~
Dangerous Goods Class (Secondary #1)	
Dangerous Goods Class (Secondary #2)	
Packing Group	
UN Number	
Appearance	
Odour	
Solubility (water/solvents)	
pKa	
Flash point	
Specific Gravity	
Bulk density	
Particle Size	
Viscosity	
Boiling Point	
Melting Point	

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## 5.4.2. Creating additional samples

If additional samples are required, add each sample separately. To add a new sample you must:

- 1. Click create new sample
- 2. Enter the following information for each sample:
  - Description\*
  - Sample Form\* (select from drop down list)
  - Chemical Formula or Chemical Composition\*
  - CAS Number
  - Hazards\* (click in box, select 1 or more from drop down list)
  - Amount (mass g or volume ml)\*
  - Safety Comment
  - Crystalline sample\*; if yes then add lattice parameters
  - Sample prepared\* (select from drop down list)
  - Date ready
  - Disposal method (select from drop down list)
  - Australian Safety Data Sheet\* file upload available
- 3. Click save
- 4. Click **next**

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### 5.5. Tab 5: Submit

When you have finished compiling your proposal you are required to select the submit tab. On the submit tab you will need to correct any highlighted errors in the application and accept the terms and conditions displayed.

### 5.5.1. Error correction

If there are missing compulsory fields (indicated throughout by a red asterisk \*), error messages will be highlighted in red on your screen. Fix any omissions if you see any error messages, as you will not be able to submit the proposal until this is done.

This is where you submit your proposal for review. Error: You cannot submit due to the following errors:		
Instruments Tab		
Go to question		
Samples Tab		
Sample: test sample		
Upload the SDS *		
This value should not be blank.		
Go to question		

### 5.5.2. Terms and conditions

Before submitting a proposal, you must review the terms and conditions for the use of neutrons at ANSTO. A proposer will be unable to submit a proposal until the terms and conditions have been accepted.



### 5.5.3. Submission

Once the terms and conditions have been accepted, click submit. Once a proposal has been submitted no further edits can be made to the proposal.

If an error or addition needs to be made after submission, please contact <u>user.office.nsw@ansto.gov.au</u>.

You have successfully submitted proposal N:PP15020

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# 6. Program Proposal creation: Neutron

The Neutron Program Proposal is for access to one or more ACNS instruments for a program of research of up to 3 years.

- 1. Click the proposals tab
- 2. Click create new proposal
- 3. Click Australian Centre for Neutron Scattering
- 4. Select Program Proposal- Neutron

# Australian Centre for Neutron Scattering

Ŧ

#### Program Proposal - Neutron

- 5. Input text into questions shown below:
  - **Proposal Title\***: Please provide a short, descriptive title for your proposal. This field will not accept superscripts, subscripts, other alphabet letters etc.
  - Proposal Type\*: The proposal type defaults to the type of proposal you selected on the previous page.
  - Proposal Round \*: Only rounds that are currently open will be available and one must be selected.
  - **Principal Scientist**: select by typing surname or first name and selecting from names available.
- 6. Click create

# **Program Proposal - Neutron**

Merit access proposal for access to one or more ACNS instruments and capabilities for a program of research of up to 3 years.

```
Proposal Title *
```

Provide a short descriptive title

Proposal Type *
ACNS: Neutron Program Proposal: Peer-reviewed experiments on our neutron beam lines.
Proposal Round *
○ ACNS & NDF: 2023-1: (Submissions due on September 15)
Principal Scientist
Create

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### 6.1. Tab 1: Main

A table with the proposal details is visible on the first tab. This table includes details such as:

- Proposal number/ ID
- Proposal round
- Proposal type
- Proposal status

This data has been populated from the previous step and cannot be modified.

Proposal Details	
ID	N:PP14958
Title	Test proposal
Round	ACNS & NDF: 2023-1
Туре	ACNS: Neutron Program Proposal
Status	In Preparation

### 6.1.1. Keywords

List up to four keywords or phrases which relate to this proposal, separated by commas. Keywords are index or subject words which help identify the proposals topic and objectives.

#### Keywords

List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

### 6.1.2. Collaborators

Enter the details of all researchers involved with this proposal including students. Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs and outcomes of this project.

Adding an existing collaborator	1. Enter the first name and last name of your collaborator
	2. Click on your collaborator's name
	3. Click add user
	4. Tick first time user if your collaborator is accessing ANSTO facilities for the first time
	<ol> <li>Select student type to indicate what level your collaborator is studying at</li> </ol>

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Adding a new collaborator	<ol> <li>Enter the first name and last name of your collaborator – if their name does not appear you will need to follow the below steps:</li> <li>Click create user</li> <li>Complete the details in the pop-up window</li> <li>Click create</li> </ol>
Selecting an organisation	<ol> <li>Enter the beginning of the name of the organisation. The closest match will appear</li> <li>Click on the organisation name to select</li> </ol>
Adding a new organisation This step is only required if your organisation is not listed in the drop-down menu when creating a new collaborator.	<ol> <li>Click create</li> <li>Click close</li> </ol>

#### Collaborators

Please enter the details of the researchers (including students) involved with this proposal. Enter the given or family name of your collaborator. Click on your collaborator's name if it appears. Click Add User. If your collaborator is not registered, click *Create User*. Complete the details in the pop-up *Add a new user* form and click *Submit* and then *Close*. Select the appropriate Role and Student Type (if applicable) and enter the student's Supervisor Name.

Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs &/or outcomes of this project.

	Name:	Add User Clear			
Name		Role	First Time User 🚯	Student Type	Funding Approved
		Principal Scientist 🛛 🗸	🗍 First Time User	Not Applicable 🗸	Funding Approved
		Co-proposer (editor 💙	First Time User	Honours 🗸	Funding Approved
		Co-proposer (editor 🗸	First Time User	Masters 🗸	Funding Approved

#### Considerations



- There can be only one Principal Scientist for each proposal and only the Principal Scientist can submit a proposal.
- If you would like any of your co-proposers to be able to edit the proposal (have read and write access) please select `*Co-proposer – editor*' in the Role field.
- If a person has not used the ACNS neutron instruments before, check the *First Time User* field.
- If the person is a student, use the dropdown list to select the *Student Type* (Honours, Masters, PhD). If you select a Student Type, enter the student's Supervisor Name.
- It is expected that the Principal Scientist submitting the proposal has spoken with relevant ANSTO Staff about the proposal prior to submission.

#### 6.1.3. Categorisation

Under categorisation there are a series of fields and questions that are to be completed if applicable to your proposal. These fields include:

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#### 1. Enter the details for the fields below where applicable:

#### • Scientific area

Indicate in which of the given scientific areas your proposal should be reviewed.

#### **Scientific Area**

Please indicate in which of the given scientific areas your proposal should be reviewed. You can provide more details in the keyword section.

#### • Intellectual Property

Select 'yes or no' if there is intellectual property associated with this proposal. If yes, add details in the text box provided.

I.P. Issues
O Yes
O No
Intellectual Property Details
Maximum 1000 characters

#### • Student thesis

Select 'yes or no' if this work forms a critical part of a student thesis. If yes, add details in the text box provided.

Does this form a critical part of a student thesis?

⊖ Yes

⊖ No

#### Thesis Details

If so, please provide the name of the student, organisation, thesis title and expected submission date.

#### Research Funding

Check relevant option(s) for any funding bodies who have awarded funds to this project.

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Research Funding		
Name any funding bodies who have awarded funds t	o this project.	
Internal Funding		
ARC Funding		
NH&MRC Funding		
Industry Funding		

~

• **Industrial Relevance and Industrial Involvement** Select the industrial relevance category appropriate for this project.

Industrial Relevance

Industrial Involvement Name of Company involved

- 2. Click **save** to save all entries
- 3. Click **next** to navigate to the next part of the proposal



### 6.2. Tab 2: Science

### 6.2.1. Proposed Program of Research (PDF)\*

- 1. You must upload a PDF that describes your neutron experiment/s for the proposed program of research and you must include the following information:
  - Aim/s of the proposed research and scientific background/significance
  - Scientific importance of the proposed experiments
  - The vision that demonstrates that this research merits the status of an integrated program, rather than a series of normal (6-month round) proposals
  - Indicative description of the experiments to be carried out over the course of the program, including a generic list of samples and a provisional schedule of expected beamtime requirements
  - A plan for implementation of the program including timeline
  - Reason for choice of requested instrument/s
  - Description of the results of preliminary work and/or characterisation (e.g. using x-rays, NMR, etc.)
  - Brief description of your experience and track record with neutron scattering techniques
  - Please reference publications relevant to your proposed research (add DOI links if available)

#### **PDF Upload Considerations**



- The maximum file size is 3MB.
- The maximum word limit (including characters) is 5000 words.
- A maximum of 6 pages only.
- The PDF layout must be portrait only. Landscape layout is not accepted.
- 12-point font to be used only.

#### Proposed Program of Research (PDF)

Please upload a PDF (MAX 6 PAGES, PORTRAIT ONLY, NOT LANDSCAPE USING A 12-POINT FONT) of your proposed research. The maximum file size is 3MB with maximum 5000 words.

- Describe your neutron experiment/s for the proposed program of research and you must include the following information:
  - · Alm/s of the proposed research and scientific background/significance
  - Scientific importance of the proposed experiments
  - The vision that demonstrates that this research merits the status of an integrated program, rather than a series of normal (6month round) proposals
  - Indicative description of the experiments to be carried out over the course of the program, including a generic list of samples and
    a provisional schedule of expected beamtime requirements
  - A plan for implementation of the program including timeline
  - Reason for choice of requested instrument/s
  - Description of the results of preliminary work and/or characterisation (e.g. using x-rays, NMR, etc.)
  - Brief description of your experience and track record with neutron scattering techniques
     Please reference publications relevant to your proposed research (add DOI links if available)

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Upload

- 2. Click upload
- 3. Click choose file
- 4. Click upload

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File upload	×
Use the form below to upload a file. Unlike other fields, changes to files do not ne to be saved.	ed
File to upload *	
Choose File No file chosen	
Max file size: 3mb Allowed formats: PDF, PNG, and JPG	
	_
Cancel Uplo	bad

- 5. Click **save**
- 6. Click **next**.

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## 6.3. Tab 3: Instruments

On the instruments tab, you must select the instruments required as part of your project. Additional resources may be requested on this page for laboratories and sample environment equipment.

# Information entered and selections made here should reflect the first six months of your proposed program of work.

#### 6.3.1. Neutron Instrument selection

- 1. Select neutron instrument
- 2. Select a specific instrument from the adjacent drop-down menu
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add the number of requested days
  - Describe the experimental setup\*
  - Request a scientist
  - Add sample environment equipment
  - Add laboratory ancillaries
- 5. Repeat the steps above for any additional instruments
- 6. Click save

Neutron Instrument	BILBY	6	Days	~	×	
Experimental Setup * Please provide the instrumental settings you requir and so on.	e on the instrument in order to carry out y	our exper	iment, such	n as resolu	ution, wavelength, Q-rang	je,
Scientists     Choose       Sample Env     Choose       Lab Ancillaries     Choose		Request	ted			

#### 6.3.2. Non- Neutron Instrument selection

- 1. Select ACNS non- neutron instrument
- 2. Select a specific instrument from the adjacent drop-down menu
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add the number of requested days
  - Describe the experimental setup\*
  - Request a scientist
- 5. Repeat the steps above for any additional non-neutron instruments
- 6. Click save

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Analysis Type	Instrument	Requested
ACNS: Non-Neutron Instrument	Imaging Ellipsometer	9 Days 🗸
Experimental Setup * Please provide the instrumental settings you require and so on. No	on the instrument in order to carry out	your experiment, such as resolution, wavelength, Q-range,
Scientists Choose		Requested

### 6.4. Tab 4: Submit

When you have finished compiling your proposal you are required to select the submit tab. On the submit tab you will need to correct any highlighted errors in the application and accept the terms and conditions displayed.

#### 6.4.1. Error correction

If there are missing compulsory fields (indicated throughout by a red asterisk \*), error messages will be highlighted in red on your screen. Fix any omissions if you see any error messages, as you will not be able to submit the proposal until this is done.

N:PP15020: est
Previous Exit
This is where you submit your proposal for review.
Error: You cannot submit due to the following errors:
Instruments Tab
Go to question

### 6.4.2. Terms and conditions

Before submitting a proposal, you must review the terms and conditions for the use of neutrons at ANSTO. A proposer will be unable to submit a proposal until the terms and conditions have been accepted.



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## 6.4.3. Submission

Once the terms and conditions have been accepted, click submit. Once a proposal has been submitted no further edits can be made to the proposal. If an error or addition needs to be made after submission, please contact <u>user.office.nsw@ansto.gov.au</u>.

You have successfully submitted proposal N:PP15020

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# 7. Proposal creation: Deuteration proposal

A normal deuteration proposal is for all merit access proposals submitted within a 6-month period for use at overseas neutron facilities or for non-neutron applications (e.g. NMR, MS). For provision of deuterated molecules for use with ACNS neutron instruments, a Deuteration/Neutron proposal must be submitted. When you click the National Deuteration Facility (NDF) menu, you will find a list of proposal types available. One proposal type must be selected to request access to NDF techniques.

- 1. Click the proposals tab
- 2. Click create new proposal
- 3. Click National Deuteration Facility
- 4. Select the Deuteration proposal type

National Deuteration Facility	=
Deuteration	

5. Input text into questions shown below:

**Proposal Title\***: Please provide a short, descriptive title for your proposal. This field will not accept superscripts, subscripts, other alphabet letters etc.

**Proposal Type\***: The proposal type defaults to the type of proposal you selected on the previous page.

**Proposal Round \***: Only rounds that are currently open will be available and one must be selected.

**Principal Scientist**: select by typing surname or first name and selecting from names available. If the required name is not available, please select the '*Create User'* option. If you choose this option a pop-up '*Add a new user'* box will appear.

6. Click create

Deuteration
Merit access proposal for NDF capabilities within a 6-month round. This proposal type is for overseas neutron experiments or for non-neutron applications (e.g. NMR, MS). More information on NDF user access can be found here.
Proposal Title *
Provide a short descriptive title
Proposal Type *
National Deuteration Facility: Deuteration
Proposal Round *
O ACNS & NDF: 2023-1: (Submissions due on September 15)
Principal Scientist
Create

Once you click create, this saves your work and takes you to the main proposal creation page.

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### 7.1. Tab 1: Main

A table with the proposal detail is visible on the first tab. This table includes details such as:

- Proposal number/ ID
- Proposal round
- Proposal type
- Proposal status

This data has been populated from the previous step and cannot be modified.

NDF14956: test deut       Save     Next       Cancel	teration proposal
Proposal Details	
ID	NDF14956
Title	test deuteration proposal
Round	ACNS & NDF: 2023-1
Туре	National Deuteration Facility: Deuteration
Status	In Preparation

### 7.1.1. Keywords

List up to four keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

#### Keywords

List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

### 7.1.2. Collaborators

Enter the details of all researchers involved with this proposal including students. Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs and outcomes of this project.

Adding an existing collaborator	1. Enter the first name and last name of your collaborator
	2. Click on your collaborator's name
	3. Click add user
	4. Tick first time user if your collaborator is accessing NDF facilities for the first time
	<ol> <li>Select student type to indicate what level your collaborator is studying at.</li> </ol>

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Adding a new collaborator	<ol> <li>Enter the first name and last name of your collaborator – if their name does not appear you will need to follow the below steps:</li> <li>Click create user</li> <li>Complete the details in the pop-up window</li> <li>Click create</li> </ol>
--	--
Selecting an organisation	<ol> <li>Enter the beginning of the name of the organisation. The closest match will appear</li> <li>Click on the organisation name to select</li> </ol>
Adding a new organisation This step is only required if your organisation is not listed in the drop-down menu when creating a new collaborator.	<ol> <li>Click create</li> <li>Click close</li> </ol>

### Considerations

- There can be only one Principal Scientist for each proposal and only the Principal Scientist can submit a proposal.
- If you would like any of your co-proposers to be able to edit the proposal (have read and write access) please select `*Co-proposer editor*' in the Role field.
- If a person has not used NDF facilities before, check the *First Time User* field.
- If the person is a student, use the dropdown list to select the *Student Type* (Honours, Masters, PhD). If you select a Student Type, please enter the student's Supervisor Name.
- It is expected that the Principal Scientist submitting the proposal has spoken with relevant ANSTO Staff about the proposal prior to submission.

## 7.1.3. Categorisation

Under categorisation there are a series of fields and questions that are to be completed if applicable to your proposal. These fields include:

1. Enter the details for the fields below where applicable:

## Scientific area Indicate in which of the given scientific areas your proposal should be reviewed.

Scientific Area	
Please indicate in which of the given scientific areas your proposal should be reviewed. You can provide more details in the keyword	ł
section.	
	~

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### • Intellectual Property

Select 'yes or no' if there is intellectual property associated with this proposal. If yes, add details in the text box provided.

I.P. Issues		
⊖ Yes		
⊖ No		
Intellectual Property Details		
Maximum 1000 characters		

### • Student thesis

Select 'yes or no' if this work forms a critical part of a student thesis. If yes, add details in the text box provided.

Does this	form a	critical	part of a	student	thesis?
○ Yes					

O No

Thesis Details

If so, please provide the name of the student, organisation, thesis title and expected submission date.

### Participation\*

You must indicate if you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF. If yes, please indicate who and their career details.

### Participation \*

Do you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF?

- Yes
- O No

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If yes, please indicate who, their career stage (e.g. PhD student) and what type of involvement is being requested. It is recommended to discuss this with the NDF pre-submission.

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### • Research Funding

Check relevant option(s) for any funding bodies who have awarded funds to this project.

Research Funding	
Name any funding bodies who have awarded funds to this p	project.
Internal Funding	
ARC Funding	
NH&MRC Funding	
Industry Funding	

### Financial Information\*

You must indicate if you have budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials? If yes, provide details, including details of any discussions you have had with NDF staff.

Financial Information \*
Have you budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials?
If yes, please provide details, including details of any discussions you have had with NDF staff.

### • Experience

Indicate if you or any of your listed collaborators, are an early career researcher or a novice user of neutrons.

Are you an early career researcher (ECR, less than 5 years post doctoral experience)? Are you a novice user of neutrons (less than 3 years experience)?

Please indicate answers to these questions here and add any further information you deem relevant.

Industrial Relevance and Industrial Involvement

Select the industrial relevance category appropriate for this project.

Industrial Relevance
Industrial Involvement
Name of Company involved

- 2. Click save
- 3. Click next

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## 7.2. Tab 2: Science

## 7.2.1. Proposed Research (PDF) \*

Do you know if synthesis of your molecule/s requires Biodeuteration (for deuteration or multiple isotopic labelling) or Chemical deuteration techniques? If you are not sure, please contact the NDF via <u>ndf-enquiries@ansto.gov.au</u>to discuss your proposal.

- 1. Upload a two-page PDF (maximum) describing your proposed research which includes the information listed below. Please note, other specific details will be requested further within the proposal (e.g. protein sequence information). This must include:
  - Scientific background and significance
  - Aim and scientific importance of the proposed experiment/s using the requested molecule/s (neutron, NMR or other)
  - Describe how the requested molecule/s will be utilised in the proposed experiments and how deuteration or multiple isotope labelling will assist the investigation/s
  - Describe what preliminary or previous work and/or characterisation you have done on the target molecule/s
  - Add detail on which instrument/s, where and when you intend to use the requested molecule/s. If you have neutron beamtime granted, please indicate where and when. If not, where and when will a proposal be submitted?
  - Please reference publications relevant to your proposed research (add DOI links if available)
  - Relevant figures

#### Proposed Research (PDF) \*

Please upload a 2 page PDF (PORTRAIT ONLY, NOT LANDSCAPE USING A 12-POINT FONT) of your proposed research which must include the information listed below. The maximum file size is 3MB.

- NOTE: other specific details will be requested further within the proposal (e.g. protein sequence information).
  - Scientific background and significance,
  - · Aim and scientific importance of the proposed experiment/s using the requested molecule/s (neutron, NMR or other),
  - Describe how the requested molecule/s will be utilised in the proposed experiments and how deuteration or multiple isotope labelling will assist the investigation/s,
  - Describe what preliminary or previous work and/or characterisation you have done on the target molecule/s,
  - Add detail on which instrument/s, where and when you intend to use the requested molecule/s. If you have neutron beamtime
    granted, please indicate where and when. If not, where and when will a proposal be submitted?
  - · Please reference publications relevant to your proposed research (add DOI links if available)

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### PDF Upload Considerations

- The maximum file size is 3MB.
- The maximum word limit (including characters) is 5000 words.
- A maximum of 2 pages only.
- The PDF layout must be portrait only. Landscape layout is not accepted.
- 12-point font only.
  - o Click upload
  - Click choose file

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• Click upload

File upload	×
Use the form below to upload a file. Unlike other fields, changes to files do not need to be saved.	d
File to upload * Choose File No file chosen	
Max file size: 3mb Allowed formats: PDF, PNG, and JPG	
Cancel Uploa	d

- Click save
- Click **next**.

## 7.2.2. Molecule/s to be deuterated or multiple labelled

Molecule/s to be deuterated or multiple labelled (Note: maximum of 2 per proposal unless otherwise agreed to by NDF management)		
Molecule name	Full and any abbreviation	
Molecule structure	As applicable	
Deuteration level	Add as percentage required. Include justification for the desired level	
Isotopic labelling details	Describe if uniform, selective or segmental labelling required. If selective or segmental labelling, please describe in detail and/or attach a drawing to the Figures section showing sites required and optional sites	
Form of molecule requested	For example biomass/cell paste, partially purified, fully purified	
Quantity required	Specify minimum workable quantity and ideal quantity for your experimental application/s. Please indicate if the quantity requested will be utilised in multiple experiments.	

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## 7.2.3. Additional Questions: Biodeuteration

**Do you require Biodeuteration - protein or other biosynthetically produced molecules?** If you select '*yes'* to this question you will be required to provide additional information in the field provided in regards to the following:

Method for production For 1H (protonated) form of molecule (if known), use the following as headings to provide information and describe as applicable for each molecule (add references as needed):	<ul> <li>Host microorganism (e.g. <i>E.coli</i> BL21, <i>S. cerevisiae</i>). Indicate if you can provide the microbe if you have a bio-engineered or specific microbe for production of your requested molecule.</li> <li>Scale of production</li> <li>Culture inoculation preparation</li> <li>Growth conditions (medium – rich or minimal, temperature, timeframes etc)</li> <li>Expression conditions (induction OD/temperature for proteins, expression time etc)</li> <li>Solubility and stability characteristics</li> <li>Storage conditions</li> <li>Add any relevant data to indicate method outcomes (e.g. yield)</li> <li>Add expression SDS-PAGE images in the Proposed Research PDF for protein/s</li> <li>If purification method is known, please describe in the Purification section or add relevant reference/s.</li> </ul>	
Recombinant protein expression Use the following as headings to provide information and describe for each protein and corresponding plasmid (add references as needed):	<ul> <li>Protein and Expression Plasmid</li> <li>Do you have a plasmid readily for provision to the NDF?</li> <li>If you don't currently have a plasmid, please</li> <li>contact NDF to discuss further.</li> </ul>	
	<b>Note:</b> NDF preferred plasmids for reliable protein deuteration encode for kanamycin resistance and the <i>lacI</i> repressor (e.g. pET28a or similar).	
	<ul> <li>Protein UniProt/SwissProt ID</li> </ul>	
	<ul> <li>Species of origin (e.g. human, mouse, bacterial)</li> </ul>	
	<ul> <li>Plasmid (name and describe, indicate commercial/non-commercial and history)</li> </ul>	
	<ul> <li>Antibiotic selection</li> </ul>	
	<ul> <li>Induction (e.g. IPTG)</li> </ul>	
	$_{\odot}$ Expression tags (describe any N- or C- terminal)	
	<ul> <li>Molecular weight, kDa (of expressed protein with and without tags as applicable)</li> </ul>	
	<ul> <li>Mutations or modifications (if applicable)</li> </ul>	
	<ul> <li>Protein toxicity to host organism (if applicable)</li> </ul>	
	1	

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## 7.2.4. Additional Questions: Chemical Deuteration

<b>Do you require Chemical Deuteration via exchange and synthesis?</b> If you select ' <i>yes'</i> to this question you will be required to provide additional information in the field provided in regards to the following:				
Method for production	Have you produced the molecule in <sup>1</sup> H (protonated) form? If yes, please add the following:			
	<ul> <li>Reaction scheme – add drawing as Figure or reference/s</li> </ul>			
	$_{\odot}$ Method (as much detail as possible) or reference/s			
	<ul> <li>If purification method known, please describe in the Purification section or add relevant reference/s.</li> </ul>			

## 7.2.5. Purification Method

This field has been provided for the proposer to describe proven purification method (in 1H or 2H, or multiple labelled form) for each molecule requested. You must include materials and equipment required and quantification method along with references if known.

<b>Purification Method (if</b> Describe proven purificat Include materials and equinot available).	tion method (					ner of method if reference/s
$ \begin{array}{c c} \hline \begin{tabular}{c} \hline \end{tabular} \\ \hline \hline \end{tabular} \end{array} \end{array} \end{array} \begin{array}{c} \hline \begin{tabular}{c} \hline \end{tabular} \\ \hline \begin{tabular}{c} \hline \end{tabular} \\ \hline \end{tabular} \end{array} \end{array} \begin{array}{c} \hline \begin{tabular}{c} \hline \end{tabular} \\ \hline \end{tabular} \end{array} \end{array} \begin{array}{c} \hline \begin{tabular}{c} \hline \end{tabular} \\ \hline \end{tabular} \end{array} \end{array} \begin{array}{c} \hline \begin{tabular}{c} \hline \end{tabular} \\ \hline \end{tabular} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array} \end{array} \end{array} \end{array} \begin{array}{c} \hline \end{tabular} \end{array} \end{array}$	<ul><li>☐ ☐ ☐</li><li>Gize →</li></ul>	← → X □ ▲- ▲-	B I <u>U</u>	<u>J</u> <del>S</del> × <sub>e</sub> x <sup>e</sup> <u>I</u> x	]= :=  = = =	≣ © © ⊨
						4

## 7.2.6. Safety hazards for deuterated molecule synthesis\*

If the requested molecule/s represent any actual or potential hazard to human health, other organisms or the environment, this must be explained further in the field provided. You must describe each molecule, indicating handling and hazard minimisation conditions required; and also information on what approval/s and/or conditions have been required to fulfil for each molecule at your institution/s?

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Safety Hazards for Deuterated Molecule Synthesis \*
Does the requested molecule/s represent any actual or potential hazard to human health, other organisms or the environment?
Please describe for each molecule, indicating handling and hazard minimisation conditions required.
What approval/s and/or conditions have you been required to fulfil for each molecule at your institution/s?

# 7.2.7. Regulatory requirements for deuterated molecule synthesis\*

If there are any regulatory requirements associated with the requested molecule/s, provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

Regulatory Requirements for Deuterated Molecule Synthesis \*

Are there any regulatory requirements associated with your requested molecule/s?

Please provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

Click **save** Click **next** 

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## 7.3. Tab 3: Techniques

Select the NDF technique(s) required for your proposal (NDF - Biodeuteration or NDF - Chemical Deuteration). If your research requires both NDF capability techniques, please submit separate proposals. You must select the NDF Scientist(s) with whom you have discussed this proposal (if any).

## 7.3.1. Technique Selection

For each NDF technique selected, you must select the technique required for your proposal including Biodeuteration or Chemical Deuteration. You will need to enter the requested number of molecules and choose a local contact for the proposal.

- 1. Select Deuteration
- 2. Select a technique from the adjacent drop-down menu
- 3. Click add technique
- 4. Enter the following information for the requested instrument:
  - Add number of requested molecules
  - Scientists (this should indicate any NDF team members you have discussed the proposal with)
- 5. Click save

Deuteration		NDF - Biodeuteration	~	Add Technique
Capability Type	Technique	Requested		
Deuteration	NDF - Biodeuteration	9 Molecul 🗸		×
Scientists Choose	~	Requested		

## 7.3.2. Requested Supply Date/s

Please indicate date/s required for provision of requested molecule/s and where they are to be delivered.

### Requested Supply Date/s \*

Please indicate date/s required for provision of requested molecule/s and where they are to be delivered.

### Click save

Click **next** 

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## 7.4. Tab 4: Submit

When you have finished compiling your proposal you are required to select the 'submit' tab. The research portal will check there are no errors and the terms and conditions have been accepted prior to submission.

## 7.4.1. Error correction

If there are missing compulsory fields (indicated throughout by a red asterisk \*), error messages will be highlighted in red on your screen. Fix any omissions if you see any error messages, as you will not be able to submit the proposal until this is done.

Please review and accept the sections below to submit your proposal for review. If you have any queries regarding these items, please contact the NDF via ndf-enquiries@ansto.gov.au.

Error: You cannot submit due to the following errors:

### Main Tab

Financial Information *
Have you budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials? If yes, please provide details, including details of any discussions you have had with NDF staff.
It is value should not be blank.
Co to question

## 7.4.2. Potential Cost Recovery Fees

Requests for multiple-labelled proteins (e.g. with 2H plus 13C and/or 15N) will involve some recovery of the cost of isotopically labelled materials used in production. Proposals for experimental applications in countries other than Australia will be subject to partial cost recovery/collaboration.

Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments). Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery.

l accept the Potential Cost Recovery Fees
Requests for multiple-labelled proteins (e.g. with <sup>2</sup> H plus <sup>13</sup> C and/or <sup>15</sup> N) will involve some recovery of the cost of isotopically labelled materials used in production.
Proposals for experimental applications in countries other than Australia will be subject to partial cost recovery/collaboration. Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments). Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery.
O Yes

## 7.4.3. Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) – an Australian Government initiative."

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### I accept the Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) – an Australian Government initiative."

⊖ Yes

⊖ No

### 7.4.4. Submission

Once the terms and conditions have been accepted, click submit.

Further information on NDF user access can be found <u>here</u>. If you have any queries about these items please contact the NDF Leader and NDF User Program Manager via <u>ndf-enquiries@ansto.gov.au</u>

No further edits can be made to the proposal once it is submitted. If an error or addition needs to be made after submission, please contact <u>user.office.nsw@ansto.gov.au</u> and provide the Proposal ID along with your request for help.

You have successfully submitted proposal N:PP15020

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## 8. Proposal creation: Program Proposal Deuteration

A deuteration program proposal is for a merit access proposal for a program of research of up to 3 years for access to NDF capabilities of biological and/or chemical deuteration or multiple isotopic labelling. This program proposal type is for overseas neutron experiments or non-neutron applications (e.g. NMR, MS). When you click the National Deuteration Facility (NDF) menu, you will find a list of proposal types available. One proposal type must be selected to request access to NDF techniques.

- 1. Click the proposals tab
- 2. Click create new proposal
- 3. Click National Deuteration Facility
- 4. Select the Program Proposal Deuteration proposal type

## National Deuteration Facility

## Program Proposal – Deuteration

5. Input text into questions shown below:

**Proposal Title\***: Please provide a short, descriptive title for your proposal. This field will not accept superscripts, subscripts, other alphabet letters etc.

**Proposal Type\***: The proposal type defaults to the type of proposal you selected on the previous page.

**Proposal Round** \*: Only rounds that are currently open will be available and one must be selected. This defaults to NDF: Deuteration Program Proposal.

**Principal Scientist**: select by typing surname or first name and selecting from names available. If the required name is not available, please select the '*Create User'* option. If you choose this option a pop-up '*Add a new user'* box will appear.

6. Click create

Program Proposal – Deuteration
Merit access proposal for a program of research of up to 3 years for access to NDF capabilities of biological and/or chemical deuteration or multiple isotopic labelling. This program proposal type is for overseas neutron experiments or non-neutron applications (e.g. NMR, MS).
Proposal Title *
Provide a short descriptive title
test
Proposal Type *
NDF: Deuteration Program Proposal
Proposal Round *
ACNS & NDF: 2023-1: (Submissions due on September 15)
Principal Scientist
Create

Once you click create, this saves your work and takes you to the main proposal creation page.

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## 8.1. Tab 1: Main

A table with the proposal detail is visible on the first tab. This table includes details such as:

- Proposal number/ ID
- Proposal round
- Proposal type
- Proposal status

This data has been populated from the previous step and cannot be modified.

Proposal Details	
ID	NDF:P15024
Title	test
Round	ACNS & NDF: 2023-1
Туре	NDF: Deuteration Program Proposal
Status	In Preparation

## 8.1.1. Keywords

List up to four keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

#### Keywords

List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

## 8.1.2. Collaborators

Enter the details of all researchers involved with this proposal including students. Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs and outcomes of this project.

Adding an existing collaborator	1. Enter the first name and last name of your collaborator
	2. Click on your collaborator's name
	3. Click add user
	<ol> <li>Tick first time user if your collaborator is accessing NDF facilities for the first time</li> </ol>
	<ol><li>Select student type to indicate what level your collaborator is studying at.</li></ol>
Adding a new collaborator	<ol> <li>Enter the first name and last name of your collaborator – if their name does not appear you will need to follow the below steps:</li> </ol>

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	<ol> <li>Click create user</li> <li>Complete the details in the pop-up window</li> <li>Click create</li> </ol>
Selecting an organisation	<ol> <li>Enter the beginning of the name of the organisation. The closest match will appear</li> <li>Click on the organisation name to select</li> </ol>
Adding an existing collaborator	1. Enter the first name and last name of your collaborator
	2. Click on your collaborator's name
	3. Click add user
	4. Tick first time user if your collaborator is accessing ANSTO facilities for the first time
	5. Select student type to indicate what level your collaborator is studying at.

### Considerations



There can be only one Principal Scientist for each proposal and only the Principal Scientist can submit a proposal.

- If you would like any of your co-proposers to be able to edit the proposal (have read and write access) please select `*Co-proposer editor*' in the Role field.
- If a person has not used NDF facilities before, check the *First Time User* field.
- If the person is a student, use the dropdown list to select the *Student Type* (Honours, Masters, PhD). If you select a Student Type, please enter the student's Supervisor Name.
- It is expected that the Principal Scientist submitting the proposal has spoken with relevant ANSTO Staff about the proposal prior to submission.

## 8.1.3. Categorisation

Under categorisation there are a series of fields and questions that are to be completed if applicable to your proposal. These fields include:

- 1. Enter the details for the fields below where applicable:
  - Scientific area Indicate in which of the given scientific areas your proposal should be reviewed.

Scientific Area	
Please indicate in which of the given scientific areas your proposal should be reviewed. You can provide more details in the keyword	d
section.	
	~

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### • Intellectual Property

Select 'yes or no' if there is intellectual property associated with this proposal. If yes, add details in the text box provided.

I.P. Issues	
⊖ Yes	
O No	
Intellectual Property Details	
Maximum 1000 characters	

### • Student thesis

Select 'yes or no' if this work forms a critical part of a student thesis. If yes, add details in the text box provided.

○ Yes	
O No	
Thesis Details	
If so, please provide the name of the student, organisation, thesis title and expected	submission date.

### Participation\*

You must indicate if you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF. If yes, please indicate who and their career details.

Participation	*
_	~

Do you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF?

- Yes
- ⊖ No

If yes, please indicate who, their career stage (e.g. PhD student) and what type of involvement is being requested. It is recommended to discuss this with the NDF pre-submission.

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### • Research Funding

Check relevant option(s) for any funding bodies who have awarded funds to this project.

Research Funding	
Name any funding bodies who have awarded funds to this project.	
Internal Funding	
C ARC Funding	
NH&MRC Funding	
Industry Funding	

### • Financial Information\*

You must indicate if you have budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials? If yes, provide details, including details of any discussions you have had with NDF staff.

Financial Information \*
Have you budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials?
If yes, please provide details, including details of any discussions you have had with NDF staff.

### Experience

Indicate if you or any of your listed collaborators, are an early career researcher or a novice user of neutrons.

Are you an early career researcher (ECR, less than 5 years post doctoral experience)? Are you a novice user of neutrons (less than 3 years experience)?

Please indicate answers to these questions here and add any further information you deem relevant.

• Industrial Relevance and Industrial Involvement

Select the industrial relevance category appropriate for this project.

Industrial Relevance	
	~
Industrial Involvement	
Name of Company involved	

- 2. Click save
- 3. Click next

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## 8.2. Tab 2: Science

## 8.2.1. Proposed Program of Research (PDF) \*

Do you know if synthesis of your molecule/s requires Biodeuteration (for deuteration or multiple isotopic labelling) or Chemical deuteration techniques? If you are not sure, please contact the NDF via <u>ndf-enquiries@ansto.gov.au</u>to discuss your proposal.

- 1. Upload a PDF describing your proposed program of research and justification of requests for deuterated and/or multiple isotopically labelled molecule/s. You must include the following information:
  - Aim/s of the proposed research and scientific background/significance
  - Scientific importance of the proposed experiments utilising the deuterated and/or multiple isotopically labelled molecule/s
  - The vision that demonstrates that this research merits the status of an integrated program, rather than a series of normal (6-month round) proposals
  - Indicative description of the experiments to be carried out over the course of the program including a description of how the deuterated and/or multiple isotopically labelled molecule/s will be utilised and how they will assist the investigation
  - A provisional schedule of expected isotopically labelled molecule/s requirements
  - A plan for implementation of the program including timeline
  - · Reason for choice of requested isotopically labelled molecule/s
  - Description of results of preliminary work and/or characterisation
  - Brief description of your experience and track record with use of deuterated and/or multiple isotopically labelled molecules and your proposed experimental application/s (e.g. neutron scattering, NMR etc)
  - Please reference publications relevant to your proposed research (add DOI links if available)
- 2. Click upload
- 3. Click choose file
- 4. Click upload

File upload	×
Use the form below to upload a file. Unlike other fields, changes to files do not nee to be saved.	ed
File to upload * Choose File No file chosen	
Max file size: 3mb Allowed formats: PDF, PNG, and JPG	
Cancel	ad

- Click save
- 5. Click next.

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### Considerations

- The maximum file size is 3MB.
- The maximum word limit (including characters) is 5000 words.
- A maximum of 6 pages only.
- The PDF layout must be portrait only using a 12-point font. Landscape layout is not accepted.

#### Proposed Program of Research (PDF) \*

Please upload a PDF (MAX 6 PAGES, PORTRAIT ONLY, NOT LANDSCAPE USING A 12-POINT FONT) of your proposed research. The maximum file size is 3MB with maximum 5000 words.

NOTE: specific Deuteration details will be requested in other fields within this Science section.

Describe your proposed program of research and justification of requests for deuterated and/or multiple isotopically labelled molecule/s. You must include the following information:

- · Aim/s of the proposed research and scientific background/significance
- Scientific importance of the proposed experiments utilising the deuterated and/or multiple isotopically labelled molecule/s
- The vision that demonstrates that this research merits the status of an integrated program, rather than a series of normal (6-month round) proposals
- Indicative description of the experiments to be carried out over the course of the program including a description of how the deuterated and/or multiple isotopically labelled molecule/s will be utilised and how they will assist the investigation
- A provisional schedule of expected isotopically labelled molecule/s requirements
- A plan for implementation of the program including timeline
- Reason for choice of requested isotopically labelled molecule/s
- Description of results of preliminary work and/or characterisation
  Brief description of your experience and track record with use of deuterated and/or multiple isotopically labelled molecules and your proposed experimental application/s (e.g. neutron scattering, NMR etc)
- Please reference publications relevant to your proposed research (add DOI links if available)

La Test document.pdf

## 8.2.2. Molecule/s to be deuterated or multiple labelled

Molecule/s to be deuterated or multiple labelled (Note: maximum of 2 per proposal unless otherwise agreed to by NDF management)

Molecule name	Full and any abbreviation		
Molecule structure	As applicable		
Deuteration level	Add as percentage required. Include justification for the desired level		
Isotopic labelling details	Describe if uniform, selective or segmental labelling required. If selective or segmental labelling, please describe in detail and/or attach a drawing to the Figures section showing sites required and optional sites		
Form of molecule requested	<b>d</b> For example biomass/cell paste, partially purified, fully purified		
Quantity required	Specify minimum workable quantity and ideal quantity for your experimental application/s. Please indicate if the quantity requested will be utilised in multiple experiments.		

## 8.2.3. Additional Questions: Biodeuteration

**Do you require Biodeuteration - protein or other biosynthetically produced molecules?** If you select '*yes'* to this question you will be required to provide additional information in the field provided in regards to the following:

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Method for production For 1H (protonated) form of molecule (if known), use the following as headings to provide information and describe as applicable for each molecule (add references as needed):	<ul> <li>Host microorganism (e.g. <i>E.coli</i> BL21, <i>S. cerevisiae</i>). Indicate if you can provide the microbe if you have a bio-engineered or specific microbe for production of your requested molecule.</li> <li>Scale of production</li> <li>Culture inoculation preparation</li> <li>Growth conditions (medium – rich or minimal, temperature, timeframes etc)</li> <li>Expression conditions (induction OD/temperature for proteins, expression time etc)</li> <li>Solubility and stability characteristics</li> <li>Storage conditions</li> <li>Add any relevant data to indicate method outcomes (e.g. yield)</li> <li>Add expression SDS-PAGE images in the Proposed Research PDF for protein/s</li> <li>If purification method is known, please describe in the Purification section or add relevant reference/s.</li> </ul>		
<b>Recombinant protein</b> <b>expression</b> Use the following as headings to provide information and	<ul> <li>Protein and Expression Plasmid</li> <li>Do you have a plasmid readily for provision to the NDF?</li> <li>If you don't currently have a plasmid, please</li> <li>contact NDF to discuss further.</li> </ul>		
describe for each protein and corresponding plasmid (add references as needed):	<b>Note:</b> NDF preferred plasmids for reliable protein deuteration encode for kanamycin resistance and the <i>lacI</i> repressor (e.g. pET28a or similar).		
	<ul> <li>Protein UniProt/SwissProt ID</li> </ul>		
	<ul> <li>Species of origin (e.g. human, mouse, bacterial)</li> </ul>		
	<ul> <li>Plasmid (name and describe, indicate commercial/non-commercial and history)</li> </ul>		
	<ul> <li>Antibiotic selection</li> </ul>		
	<ul> <li>Induction (e.g. IPTG)</li> </ul>		
	$\circ$ Expression tags (describe any N- or C- terminal)		
	<ul> <li>Molecular weight, kDa (of expressed protein with and without tags as applicable)</li> </ul>		
	<ul> <li>Mutations or modifications (if applicable)</li> </ul>		
	<ul> <li>Protein toxicity to host organism (if applicable)</li> </ul>		

## 8.2.4. Additional Questions: Chemical Deuteration

<b>Do you require Chemical Deuteration via exchange and synthesis?</b> If you select ' <i>yes</i> ' to this question you will be required to provide additional information in the field provided in regards to the following:			
Method for production	<ul> <li>Have you produced the molecule in <sup>1</sup>H (protonated) form? If yes, please add the following:         <ul> <li>Reaction scheme – add drawing as Figure or reference/s</li> </ul> </li> </ul>		

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0	Method (as much detail as possible) or reference/s
0	If purification method known, please describe in the Purification section or add relevant reference/s.

## 8.2.5. Purification Method

This field has been provided for the proposer to describe proven purification method (in 1H or 2H, or multiple labelled form) for each molecule requested. You must include materials and equipment required and quantification method along with references if known.

Purification Method (if known)				
Describe proven purification method (in <sup>1</sup> H or <sup>2</sup> H, or multiple labelled form) for each molecule requested. Include materials and equipment required and quantification method along with references (indicate designer of method if reference/s not available).				
O Source   Q × □ ii ii ii i → → X II B I U + × × × I <sub>x</sub> Ii Ii = = = = ■				
$\blacksquare \equiv \Omega$ Format - Size - $\underline{A}$ - $\underline{A}$ -				
A				

## 8.2.6. Safety hazards for deuterated molecule synthesis\*

If the requested molecule/s represent any actual or potential hazard to human health, other organisms or the environment, this must be explained further in the field provided. You must describe each molecule, indicating handling and hazard minimisation conditions required; and also information on what approval/s and/or conditions have been required to fulfil for each molecule at your institution/s?



# 8.2.7. Regulatory requirements for deuterated molecule synthesis\*

If there are any regulatory requirements associated with the requested molecule/s, provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

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### Regulatory Requirements for Deuterated Molecule Synthesis \*

Are there any regulatory requirements associated with your requested molecule/s? Please provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

Click save Click next

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## 8.3. Tab 3: Techniques

Select the NDF technique(s) required for your proposal (NDF - Biodeuteration or NDF - Chemical Deuteration). If your research requires both NDF capability techniques, please submit separate proposals. You must select the NDF Scientist(s) with whom you have discussed this proposal (if any).

## 8.3.1. Technique Selection

For each NDF technique selected, you must select the technique required for your proposal including Biodeuteration or Chemical Deuteration. You will need to enter the requested number of molecules and choose a local contact for the proposal.

- 1. Select Deuteration
- 2. Select a technique from the adjacent drop-down menu
- 3. Click add technique
- 4. Enter the following information for the requested instrument:
  - Add number of requested molecules
  - Scientists (this should indicate any NDF team members you have discussed the proposal with)
- 5. Click save
- 6. Click next

Deuteration	~	NDF - Biodeuteration	~	Add Technique
Capability Type	Technique	Requested		
Deuteration	NDF - Biodeuteration	9 Molecul 🗸		×
Scientists Choose	~	Requested		

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## 8.4. Tab 4: Submit

When you have finished compiling your proposal you are required to select the 'submit' tab. The research portal will check there are no errors and the terms and conditions have been accepted prior to submission.

## 8.4.1. Error correction

If there are missing compulsory fields (indicated throughout by a red asterisk \*), error messages will be highlighted in red on your screen. Fix any omissions if you see any error messages, as you will not be able to submit the proposal until this is done.

Please review and accept the sections below to submit your proposal for review. If you have any queries regarding these items, please contact the NDF via ndf-enquiries@ansto.gov.au.

Error: You cannot submit due to the following errors:

### Main Tab

Financial Inform	ation *
, ,	ed for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled please provide details, including details of any discussions you have had with NDF staff.
This value shows the sh	uld not be blank.
Go to question	

## 8.4.2. Potential Cost Recovery Fees

Requests for multiple-labelled proteins (e.g. with 2H plus 13C and/or 15N) will involve some recovery of the cost of isotopically labelled materials used in production. Proposals for experimental applications in countries other than Australia will be subject to partial cost recovery/collaboration.

Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments). Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery.

l accept the Potential Cost Recovery Fees
Requests for multiple-labelled proteins (e.g. with <sup>2</sup> H plus <sup>13</sup> C and/or <sup>15</sup> N) will involve some recovery of the cost of isotopically labelled materials used in production.
Proposals for experimental applications in countries other than Australia will be subject to partial cost recovery/collaboration. Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments). Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery.
O Yes
O No

## 8.4.3. Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) – an Australian Government initiative."

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### I accept the Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) – an Australian Government initiative."

⊖ Yes

O No

### 8.4.4. Submission

Once the terms and conditions have been accepted, click submit.

Further information on NDF user access can be found <u>here</u>. If you have any queries about these items please contact the NDF Leader and NDF User Program Manager via <u>ndf-enquiries@ansto.gov.au</u>

No further edits can be made to the proposal once it is submitted. If an error or addition needs to be made after submission, please contact <u>user.office.nsw@ansto.gov.au</u> and provide the Proposal ID along with your request for help.

You have successfully submitted proposal N:PP15020

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## 9. Proposal creation: Deuteration/ Neutron proposal

This proposal type is for access proposal to ACNS instruments and NDF techniques where deuterated molecule/s are required for the proposed neutron experiments at ACNS.

- 1. Click the proposals tab
- 2. Click create new proposal
- 3. Click Australian Centre for Neutron Scattering or National Deuteration Facility
- 4. Select the Deuteration/ Neutron proposal type

National Deuteration Facility	=
Deuteration / Neutron	

### Deuteration / Neutron

5. Input text into questions shown below:

**Proposal Title\***: Please provide a short, descriptive title for your proposal. This field will not accept superscripts, subscripts, other alphabet letters etc.

Australian Centre for Neutron Scattering

**Proposal Type\***: The proposal type defaults to the type of proposal you selected on the previous page.

**Proposal Round \***: Only rounds that are currently open will be available and one must be selected.

**Principal Scientist**: select by typing surname or first name and selecting from names available. If the required name is not available, please select the '*Create User*' option. If you choose this option a pop-up '*Add a new user*' box will appear.

6. Click create

Deuteration / Neutron
Merit access proposal for ACNS instruments and NDF capabilities where deuterated molecule/s are required for the proposed neutron experiments at ACNS.
Proposal Title *
Provide a short descriptive title
Proposal Type *
Deuteration and Neutron Proposal: Deuteration/Neutron
Proposal Round *
○ ACNS & NDF: 2023-1: (Submissions due on September 15)
Principal Scientist
Create

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## 9.1. Tab 1: Main

A table with the proposal detail is visible on the first tab. This table includes details such as:

- Proposal number/ ID
- Proposal round
- Proposal type
- Proposal status

This data has been populated from the previous step and cannot be modified.

Main		
D/N14954: tset		
Save Next Cancel		
Proposal Details		
ID	D/N14954	
Title		
Round	ACNS & NDF: 2023-1	
Туре	Deuteration and Neutron Proposal	
Status	In Preparation	

#### Keywords

List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

## 9.1.1. Keywords

List up to four keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

### Keywords

List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

## 9.1.2. Collaborators

Enter the details of all researchers involved with this proposal including students. Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs and outcomes of this project.

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Adding an existing collaborator	1. Enter the first name and last name of your collaborator
	2. Click on your collaborator's name
	3. Click add user
	4. Tick first time user if your collaborator is accessing ANSTO facilities for the first time
	5. Select student type to indicate what level your collaborator is studying at.
Adding a new collaborator	<ol> <li>Enter the first name and last name of your collaborator – if their name does not appear you will need to follow the below steps:</li> <li>Click create user</li> <li>Complete the details in the pop-up window</li> <li>Click create</li> </ol>
Selecting an organisation	<ol> <li>Enter the beginning of the name of the organisation. The closest match will appear</li> <li>Click on the organisation name to select</li> </ol>
Adding a new organisation This step is only required if your organisation is not listed in the drop-down menu when creating a new collaborator.	<ol> <li>Click create</li> <li>Click close</li> </ol>

### Considerations



- There can be only one Principal Scientist for each proposal and only the Principal Scientist can submit a proposal
- If you would like any of your co-proposers to be able to edit the proposal (have read and write access) please select `*Co-proposer editor*' in the Role field.
- If a person has not used the ACNS neutron instruments/NDF capabilities before, check the *First Time User* box field.
- If the person is a student, use the dropdown list to select the *Student Type* (Honours, Masters, PhD). If you select a Student Type, enter the student's Supervisor Name.
- It is expected that the Principal Scientist submitting the proposal has spoken with relevant ANSTO Staff about the proposal prior to submission.

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## 9.1.3. Categorisation

Under categorisation there are a series of fields and questions that are to be completed if applicable to your proposal. These fields include:

1. Enter the details for the fields below where applicable:

### Scientific area

Indicate in which of the given scientific areas your proposal should be reviewed.

```
Scientific Area
Please indicate in which of the given scientific areas your proposal should be reviewed. You can provide more details in the keyword
section.
```

### • Intellectual Property

Select 'yes or no' if there is intellectual property associated with this proposal. If yes, add details in the text box provided.

I.P. Issues
○ Yes
○ No
Intellectual Property Details
Maximum 1000 characters

### • Student thesis

Select 'yes or no' if this work forms a critical part of a student thesis. If yes, add details in the text box provided.

 Does this form a critical part of a student thesis?

 Yes

 No

 Thesis Details

 If so, please provide the name of the student, organisation, thesis title and expected submission date.

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### Participation\*

You must indicate if you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF. If yes, please indicate who and their career details.

### Participation \*

Do you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF?

Yes

O No

If yes, please indicate who, their career stage (e.g. PhD student) and what type of involvement is being requested. It is recommended to discuss this with the NDF pre-submission.

### • Research Funding

Check relevant option(s) for any funding bodies who have awarded funds to this project.

Research Funding
Name any funding bodies who have awarded funds to this project.
Internal Funding
ARC Funding
NH&MRC Funding
Industry Funding

### • Financial Information\*

You must indicate if you have budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials? If yes, provide details, including details of any discussions they have had with NDF staff.

Financial Information *
Have you budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials? If yes, please provide details, including details of any discussions you have had with NDF staff.

### • Experience

Indicate if you or any of your listed collaborators, are an early career researcher or a novice user of neutrons.

Are you an early career researcher (ECR, less than 5 years post doctoral experience)? Are you a novice user of neutrons (less than 3 years experience)?

Please indicate answers to these questions here and add any further information you deem relevant.

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## • Industrial Relevance and Industrial Involvement

Select the industrial relevance category appropriate for this project.

Industrial Relevance	
	~
Industrial Involvement	
Name of Company involved	

- 2. Click save
- 3. Click next

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## 9.2. Tab 2: Science and Synthesis

## 9.2.1. Proposed Research (PDF) \*

- 1. Upload a three-page PDF (maximum) describing their neutron experiment/s including use and justification of deuterated molecule/s using the following as headings:
  - Scientific background and significance,
  - Aim of the proposed experiment/s,
  - Scientific importance of the proposed measurements,
  - Describe how the deuterated molecule/s will be utilised in the proposed experiments and how they will assist the investigation,
  - Description of experiment (detailed)
  - Describe results of preliminary work and/or characterisation (e.g. X-rays, NMR),
  - Describe previous work using either neutrons or deuterated molecules.
  - Reason for choice of requested instrument/s
  - Describe how the requested beam time was calculated (depending on number of samples, and sample-environment conditions such as temperature, etc. for each sample),
  - Overview of how the experimental data will be analysed
  - Please reference publications relevant to your proposed research (add DOI links if available)
  - Relevant figures
- 2. Click upload
- 3. Click choose file
- 4. Click upload

File upload	×
Use the form below to upload a file. Unlike other fields, changes to files do not nee to be saved.	ed
File to upload * Choose File No file chosen	
Max file size: 3mb Allowed formats: PDF, PNG, and JPG	
Cancel Uplo	ad

- 4. Click save
- 5. Click next

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Please upload a 3 page PDF (PORTRAIT ONLY, NOT LANDSCAPE USING A 12-POINT FONT) of your proposed research. The maximum file size is 3MB.

NOTE: specific Deuteration details will be requested in other fields within this Science section.

- Describe your neutron experiment/s including use and justification of deuterated molecule/s using the following as headings:
  - Scientific background and significance,
  - Aim of the proposed experiment/s,
  - Scientific importance of the proposed measurements,
  - Describe how the deuterated molecule/s will be utilised in the proposed experiments and how they will assist the investigation,
  - Description of experiment (detailed)
  - Describe results of preliminary work and/or characterisation (e.g. X-rays, NMR),
  - Describe previous work using either neutrons or deuterated molecules.
  - Reason for choice of requested instrument/s
  - Describe how the requested beam time was calculated (depending on number of samples, and sample-environment conditions such as temperature, etc. for each sample),
  - Overview of how the experimental data will be analysed
  - Please reference publications relevant to your proposed research (add DOI links if available)

La Test document.pdf

Replace Delete

### **PDF Upload Considerations**

- The maximum file size is 3MB.
- 3 page maximum.
- The PDF layout must be portrait only. Landscape layout is not accepted.
- 12-point font only.

### 9.2.2. Molecule/s to be deuterated or multiple labelled

Molecule/s to be deuterated or multiple labelled (Note: maximum of 2 per proposal unless otherwise agreed to by NDF management) Molecule name Full and any abbreviation Molecule structure As applicable **Deuteration level** Add as percentage required. Include justification for the desired level **Isotopic labelling details** Describe if uniform, selective or segmental labelling required. If selective or segmental labelling, please describe in detail and/or attach a drawing to the Figures section showing sites required and optional sites Form of molecule requested For example biomass/cell paste, partially purified, fully purified Quantity required Specify minimum workable quantity and ideal quantity for your experimental application/s. Please indicate if the quantity requested will be utilised in multiple experiments.

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## 9.2.3. Additional Questions: Biodeuteration

9.2.3. Additional Questions: Biodeuteration		
If you select 'yes' to this question provided in regards to the following		
Method for production For 1H (protonated) form of molecule (if known), use the following as headings to provide information and describe as applicable for each molecule (add references as needed):	<ul> <li>Host microorganism (e.g. <i>E.coli</i> BL21, <i>S. cerevisiae</i>). Indicate if you can provide the microbe if you have a bio-engineered or specific microbe for production of your requested molecule.</li> <li>Scale of production</li> <li>Culture inoculation preparation</li> <li>Growth conditions (medium – rich or minimal, temperature, timeframes etc)</li> <li>Expression conditions (induction OD/temperature for proteins, expression time etc)</li> <li>Solubility and stability characteristics</li> <li>Storage conditions</li> <li>Add any relevant data to indicate method outcomes (e.g. yield)</li> <li>Add expression SDS-PAGE images in the Proposed Research PDF for protein/s</li> <li>If purification method is known, please describe in the</li> </ul>	
Recombinant protein expression	<ul> <li>Purification section or add relevant reference/s.</li> <li>Protein and Expression Plasmid Do you have a plasmid readily for provision to the NDF?</li> </ul>	
Use the following as headings to provide information and		
describe for each protein and corresponding plasmid (add references as needed):		
	<ul> <li>Protein UniProt/SwissProt ID</li> </ul>	
	<ul> <li>Species of origin (e.g. human, mouse, bacterial)</li> </ul>	
	<ul> <li>Plasmid (name and describe, indicate commercial/non-commercial and history)</li> </ul>	

- $\circ \quad \text{Antibiotic selection} \quad$
- $\circ$  Induction (e.g. IPTG)
- Expression tags (describe any N- or C- terminal)
- Molecular weight, kDa (of expressed protein with and without tags as applicable)
- Mutations or modifications (if applicable)
- Protein toxicity to host organism (if applicable)

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## 9.2.4. Additional Questions: Chemical Deuteration

<b>Do you require Chemical Deuteration via exchange and synthesis?</b> If you select ' <i>yes'</i> to this question you will be required to provide additional information in the field provided in regards to the following:		
Method for production	Have you produced the molecule in <sup>1</sup> H (protonated) form? If yes, please add the following:	
	<ul> <li>Reaction scheme – add drawing as Figure or reference/s</li> </ul>	
	$\circ$ Method (as much detail as possible) or reference/s	
	<ul> <li>If purification method known, please describe in the Purification section or add relevant reference/s.</li> </ul>	

## 9.2.5. Purification Method

This field has been provided for the proposer to describe proven purification method (in 1H or 2H, or multiple labelled form) for each molecule requested. You must include materials and equipment required and quantification method along with references if known.

Purification Method (if known) Describe proven purification method (in <sup>1</sup> H or <sup>2</sup> H, or multiple labelled form) for each molecule requested. nclude materials and equipment required and quantification method along with references (indicate designer of method if reference/ not available).
B     Source     Q     Source     Q     Source     Q     Source     Q     Source     Q     Source     Source     Z     Source     So

## 9.2.6. Safety hazards for deuterated molecule synthesis\*

If the requested molecule/s represent any actual or potential hazard to human health, other organisms or the environment, this must be explained further in the field provided. You must describe each molecule, indicating handling and hazard minimisation conditions required; and also information on what approval/s and/or conditions have been required to fulfil for each molecule at your institution/s?

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Safety Hazards for Deuterated Molecule Synthesis \* Does the requested molecule/s represent any actual or potential hazard to human health, other organisms or the environment? Please describe for each molecule, indicating handling and hazard minimisation conditions required. What approval/s and/or conditions have you been required to fulfil for each molecule at your institution/s?

# 9.2.7. Regulatory requirements for deuterated molecule synthesis\*

If there are any regulatory requirements associated with the requested molecule/s, provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

#### Regulatory Requirements for Deuterated Molecule Synthesis \*

Are there any regulatory requirements associated with your requested molecule/s? Please provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

Click save Click next

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## 9.3. Tab 3: Instruments

On the instruments tab you can select one or more neutron instruments, ACNS non-neutron instruments and NDF techniques.

### 9.3.1. Neutron Instrument selection

- 1. Select Neutron Instrument
- 2. Select an instrument from the adjacent drop-down menu
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add number of requested days
    - Experimental Setup\*
    - Request a scientist/s
    - Sample environment
    - Laboratory Ancillaries
- 5. Repeat the steps above for any additional neutron instruments
- 6. Click save

Analysis Type	Instrument	Requested
Neutron Instrument	BILBY	9 Days 🗸
Experimental Setup [Neutron Instrument only] Please provide the ins resolution, wavelength, Q-range, and so on.	strumental settings you require on the	instrument in order to carry out your experiment, such as
Scientists     Choose        Sample Env     Choose        Lab Ancillaries     Choose		Requested

## 9.3.2. Non-Neutron Instrument selection

- 1. Select Non-Neutron Instrument
- 2. Select an instrument from the adjacent drop-down menu.
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add number of requested days
  - Experimental Setup\*
  - Request a scientist/s
- 5. Repeat the steps above for any additional non-neutron instruments
- 6. Click save

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ACNS: Non-Neutron Instrument	Imaging Ellipsometer	8	Days	~			×
Experimental Setup [Neutron Instrument only] Please provide t resolution, wavelength, Q-range, and so on		e instrument in (	order to carr	ry out your	experiment, s	such as	
							į
Scientists Choose 🗸	]	Request	ted				

### 9.3.3. Technique Selection

For each NDF technique selected, you must select the technique required for your proposal including Biodeuteration or Chemical Deuteration. You will need to enter the requested number of molecules and choose a local contact for the proposal.

- 1. Select Deuteration
- 2. Select a technique from the adjacent drop-down menu
- 3. Click add technique
- 4. Enter the following information for the requested instrument:
  - Add number of requested molecules
    - Scientists (this should indicate any NDF team members you have discussed the proposal with)
- 5. Repeat the steps above for any additional NDF techniques.
- 6. Click save

Deuteration	NDF - Biodeuteration	8 Molecul 🗸	
Experimental Setup [Neutron Instrument only] Please p resolution, wavelength, Q-range, ai		he instrument in order to carry out your experiment, such as	
Scientists Choose	~	Requested	

# 9.3.4. Deuterated molecule/s supply\*

You must indicate how far in advance of neutron experiments you require provision of the requested deuterated molecules/s and where they are to be delivered.

Deuterated Molecule/s Supply *
Please indicate how far in advance of neutron experiments you require provision of the requested deuterated molecules/s and where
they are to be delivered.

Click save

Click next

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#### 9.4. Tab 4: Samples

#### This tab is for Neutron experiments only

This section provides a space for you to add samples and chemicals (such as solvents) related to your proposal. Each sample will need to be added separately and detailed sample information will need to be provided, including an SDS (where possible).

All items that are going to be irradiated in the neutron beam (for example your sample container/holder, or equipment/vessel you provide) must also be listed as a sample in this section.

By providing detail information regarding your samples will enable ANSTO to fulfil regulatory requirements and to assist the completion of a risk-based safety review of your proposal.

#### 9.4.1. Sample Creation

- 1. Click create new sample
- 2. Enter the following information for each sample:
  - Description\*
  - Sample Form\* (select from drop down list)
  - Chemical Formula or Chemical Composition\*
  - o CAS Number
  - Hazards\* (click in box, select 1 or more from drop down list)
  - Amount (mass g or volume ml)\*
  - Safety Comment
  - Crystalline sample\*; if yes then add lattice parameters
  - Sample prepared\* (select from drop down list)
  - Date ready
  - Disposal method (select from drop down list)
  - Australian Safety Data Sheet\* file upload available
- 3. Click save

Samples		
D/N15026: test		
Previous Next Exit		
This tab is for Neutron experiments only Please add each sample separately. When you add a sample you will also be asked for detailed sample in possible). This information allows us to fulfil our regulatory requirements and to assist the completion of your proposal. Make sure you also add any extra samples and any other chemicals (for example: solvent with you. This ensures that we have an SDS for every chemical brought to ANSTO. All items that are goin, neutron beam (e.g. your sample container/holder, or equipment/vessel you provide) must be listed as a mandatory activation calculations can be performed for all materials in the beam. If you need to add a sa proposal has been approved, contact the ACNS User Office.	f a risk-based saf s) that you may k g to be irradiated sample here so t	ety review of be bringing I in the hat
Create new sample		
Sample No samples yet	Details	Сору

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Description *	
Sample Form *	
Solid	*
Chemical Formula or Chemical Composition *	
CAS Number	
Hazards *	
Amount (mass g or volume ml) *	

If there is no Australian Safety Data Sheet available at the time of submission, you must declare the following information. If you have a sample for which these questions do not apply, leave them blank:

- Contact Details/Ownership
- Date Completed
- Precautions for Handling
- Dangerous Goods Class Primary and Secondary
- Packing Group
- UN Number
- Appearance
- Odour
- Solubility (water/solvents)
- рКа
- Flash point
- Specific Gravity
- Bulk density
- Particle Size
- Viscosity
- Boiling Point
- Melting Point

#### 9.4.2. Creating additional samples

If additional samples are required, add each sample separately. To add a new sample you must:

- 1. Click create new sample
- 2. Enter the following information for each sample:
  - Description\*

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- Sample Form\* (select from drop down list)
- Chemical Formula or Chemical Composition\*
- CAS Number
- Hazards\* (click in box, select 1 or more from drop down list)
- Amount (mass g or volume ml)\*
- Safety Comment
- Crystalline sample\*; if yes then add lattice parameters
- Sample prepared\* (select from drop down list)
- Date ready
- Disposal method (select from drop down list)
- Australian Safety Data Sheet\* file upload available
- 3. Click save
- 4. Click next

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### 9.5. Tab 5: Submit

When you have finished compiling your proposal you are required to select the 'submit' tab. The research portal will check there are no errors and the terms and conditions have been accepted prior to submission.

### 9.5.1. Error correction

If there are missing compulsory fields (indicated throughout by a red asterisk \*), error messages will be highlighted in red on your screen. Fix any omissions if you see any error messages, as you will not be able to submit the proposal until this is done.

# 9.5.2. Terms and conditions

Before submitting a proposal, you must review the terms and conditions for the use of neutrons at ANSTO. A proposer will be unable to submit a proposal until the terms and conditions have been accepted.

This is where you submit your proposal for review.

**Terms and Conditions \*** 

Click Yes to agree with the terms and conditions for the use of neutrons at ANSTO.

○ Yes

⊖ No

Submit

# 9.5.3. Potential Cost Recovery Fees

Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery. Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments).

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I accept the Potential Cost Recovery Fees

Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery. Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments).

⊖ Yes

⊖ No

# 9.5.1. Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) – an Australian Government initiative."

I accept the Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) – an Australian Government initiative."

⊖ Yes

O No

#### 9.5.2. Submission

Once the terms and conditions have been accepted, click submit.

Further information on NDF user access can be found <u>here</u>. If you have any queries about these items please contact the NDF Leader and NDF User Program Manager via <u>ndf-enquiries@ansto.gov.au</u>

No further edits can be made to the proposal once it is submitted. If an error or addition needs to be made after submission, please contact <u>user.office.nsw@ansto.gov.au</u> and provide the Proposal ID along with your request for help.

You have successfully submitted proposal N:PP15020

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# 9.6. Program Proposal Creation: Deuteration / Neutron

This proposal type is for a program of research of up to 3 years for access to both ACNS instruments and NDF techniques, where deuterated molecule/s are required for the proposed program of research utilising ACNS neutron instruments.

- 1. Click the proposals tab
- 2. Click create new proposal
- 3. Click Australian Centre for Neutron Scattering or National Deuteration Facility
- 4. Select Program Proposal Deuteration/ Neutron

Australian Centre for Neutron Scattering	=
Program Proposal – Deuteration / Neutron	
National Deuteration Facility	÷
Program Proposal – Deuteration / Neutron	

- 5. Input text into questions shown below:
  - **Proposal Title\***: Please provide a short, descriptive title for your proposal. This field will not accept superscripts, subscripts, other alphabet letters etc.
  - Proposal Type\*: The proposal type defaults to the type of proposal you selected on the previous page.
  - Proposal Round \*: Only rounds that are currently open will be available and one must be selected.
  - **Principal Scientist**: select by typing surname or first name and selecting from names available. If the required name is not available, please select the '*Create User'* option. If you choose this option a pop-up '*Add a new user'* box will appear.
- 6. Click create

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Program Proposal – Deuteration / Neutron
Merit access proposal for a program of research of up to 3 years for access to both ACNS instruments and NDF capabilities, where deuterated molecule/s are required for the proposed program of research utilising ACNS neutron instruments.
Proposal Title *
Provide a short descriptive title
test program combined
Proposal Type *
ACNS & NDF: Neutron and Deuteration Program     ACNS & NDF: NEUTRON AND
Proposal Round *
ACNS & NDF: 2023-1: (Submissions due on September 15)
Principal Scientist
Create

# 9.7. Tab 1: Main

A table with the proposal detail is visible on the first tab. This table includes details such as:

- Proposal number/ ID
- Proposal round
- Proposal type
- Proposal status

This data has been populated from the previous step and cannot be modified.

Proposal Details	
ID	DN:P15028
Title	test program combined
Round	ACNS & NDF: 2023-1
Туре	ACNS & NDF: Neutron and Deuteration Program
Status	In Preparation

# 9.7.1. Keywords

List up to four keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help identify the proposal's topic and objectives.

Keywords
List up to 4 keywords or phrases which relate to this proposal, separated by commas. Key words are index or subject words which help
identify the proposal's topic and objectives.

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#### 9.7.2. Collaborators

Enter the details of all researchers involved with this proposal including students. Please ensure you include all ANSTO staff who will contribute to this proposal and any people who will be associated with the outputs and outcomes of this project.

Adding an existing collaborator	1.	Enter the first name and last name of your
		collaborator
	2.	Click on your collaborator's name
	3.	Click add user
	4.	Tick first time user if your collaborator is accessing ANSTO instruments and/or NDF facilities for the first time
	5.	Select student type to indicate what level your collaborator is studying at.
Adding a new collaborator	2. 3.	Enter the first name and last name of your collaborator – if their name does not appear you will need to follow the below steps: Click create user Complete the details in the pop-up window Click create
Selecting an organisation	1. 2.	organisation. The closest match will appear
Adding a new organisation	1.	Click create
This step is only required if your organisation is not listed in the drop-down menu when creating a new collaborator.	2.	Click close

### 9.7.3. Categorisation

Under categorisation there are a series of fields and questions that are to be completed if applicable to your proposal. These fields include:

- 1. Enter the details for the fields below where applicable:
  - **Scientific area** Indicate in which of the given scientific areas your proposal should be reviewed.

Scientific Area	
Please indicate in which of the given scientific areas your proposal should be reviewed. You can provide more details in the keyword section.	
	~

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#### • Intellectual Property

Select 'yes or no' if there is intellectual property associated with this proposal. If yes, add details in the text box provided.

I.P. Issues	
O Yes	
○ No	
Intellectual Property Details	
Maximum 1000 characters	
	1

#### • Student thesis

Select 'yes or no' if this work forms a critical part of a student thesis. If yes, add details in the text box provided.

C	Does this form a critical part of a student thesis?
¢	O Yes
C	O No
т	Thesis Details
H	f so, please provide the name of the student, organisation, thesis title and expected submission date.

#### Participation\*

You must indicate if you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF. If yes, please indicate who and their career details.

Ρ	а	r	t	ic	ip	а	ti	0	n	*

Do you or any of your team wish to participate in the production, purification and/or characterisation of isotopically labelled molecules at the NDF?

- Yes
- No

If yes, please indicate who, their career stage (e.g. PhD student) and what type of involvement is being requested. It is recommended to discuss this with the NDF pre-submission.

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#### • Research Funding

Check relevant option(s) for any funding bodies who have awarded funds to this project.

Research Funding
Name any funding bodies who have awarded funds to this project.
Internal Funding
ARC Funding
NH&MRC Funding
Industry Funding

#### • Financial Information\*

You must indicate if you have budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials? If yes, provide details, including details of any discussions they have had with NDF staff.

Financial Information *	
Have you budgeted for the cost or contribution to the cost of the requested deuterated and/or multiple isotopically labelled materials If yes, please provide details, including details of any discussions you have had with NDF staff.	?
	/

#### • Experience

Indicate if you or any of your listed collaborators, are an early career researcher or a novice user of neutrons.

Are you an early career researcher (ECR, less than 5 years post doctoral experience)? Are you a novice user of neutrons (less than 3 years experience)?

Please indicate answers to these questions here and add any further information you deem relevant.

#### • Industrial Relevance and Industrial Involvement

Select the industrial relevance category appropriate for this project.

Industrial Relevance	
Industrial Involvement	
Name of Company involved	

- 2. Click save
- 3. Click next

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# 9.8. Tab 2: Science and Synthesis

### 9.8.1. Proposed Program of Research (PDF) \*

- 1. You must upload a PDF of your proposed research. Please note, specific Deuteration details are also requested in other fields within this section in the portal. You must describe your neutron experiment/s including use and justification of deuterated molecule/s for the proposed program of research and you must include the following information:
- Aim/s of the proposed research and scientific background/significance
- Scientific importance of the proposed experiments
- The vision that demonstrates that this research merits the status of an integrated program, rather than a series of normal (6-month round) proposals
- Indicative description of the neutron experiments to be carried out over the course of the program including a description of how the deuterated molecule/s will be utilised and how they will assist the investigation
- A generic list of samples for the neutron experiments with a provisional schedule of expected beamtime and deuterated molecule/s requirements
- A plan for implementation of the program including timeline
- Reason for choice of requested instrument/s and deuterated molecule/s
- Description of results of preliminary work and/or characterisation (e.g. using x-rays, NMR, etc.)
- Brief description of your experience and track record with neutron scattering techniques and use of deuterated molecules
- Please reference publications relevant to your proposed research (add DOI links if available)
- 2. Click upload
- 3. Click choose file
- 4. Click upload

× File upload	
Use the form below to upload a file. Unlike other fields, changes to files do not need to be saved.	
File to upload * Choose File No file chosen	
Max file size: 3mb Allowed formats: PDF, PNG, and JPG	
Cancel Upload	

- 6. Click save
- 7. Click next

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#### Science and Synthesis

#### DN:P15028: test program combined

Previous Save Next Cancel

#### Proposed Program of Research (PDF) \*

Please upload a PDF (MAX 6 PAGES, PORTRAIT ONLY, NOT LANDSCAPE USING A 12-POINT FONT) of your proposed research. The maximum file size is 3MB with maximum 5000 words.

NOTE: specific Deuteration details will be requested in other fields within this Science section.

Describe your neutron experiment/s including use and justification of deuterated molecule/s for the proposed program of research

and you must include the following information:

- Aim/s of the proposed research and scientific background/significance
- Scientific importance of the proposed experiments
- The vision that demonstrates that this research merits the status of an integrated program, rather than a series of normal (6month round) proposals
- Indicative description of the neutron experiments to be carried out over the course of the program including a description of how the deuterated molecule/s will be utilised and how they will assist the investigation
- A generic list of samples for the neutron experiments with a provisional schedule of expected beamtime and deuterated
  molecule/s requirements
- A plan for implementation of the program including timeline
- · Reason for choice of requested instrument/s and deuterated molecule/s
- Description of results of preliminary work and/or characterisation (e.g. using x-rays, NMR, etc.)
- Brief description of your experience and track record with neutron scattering techniques and use of deuterated molecules
- Please reference publications relevant to your proposed research (add DOI links if available)

#### **PDF Upload Considerations**

- The maximum file size is 3MB.
- Maximum of 6 pages.
- The PDF layout must be portrait only using a 12-point font. Landscape layout is not accepted.

# 9.8.2. Molecule/s to be deuterated or multiple labelled

Molecule/s to be deuterated or multiple labelled (Note: maximum of 2 per proposal unless otherwise agreed to by NDF management)

Molecule name	Full and any abbreviation	
Molecule structure	As applicable	
Deuteration level	Add as percentage required. Include justification for the desired level	
Isotopic labelling details	Describe if uniform, selective or segmental labelling required. If selective or segmental labelling, please describe in detail and/or attach a drawing to the Figures section showing sites required and optional sites	
Form of molecule requested	For example biomass/cell paste, partially purified, fully purified	
Quantity required	Specify minimum workable quantity and ideal quantity for your experimental application/s. Please indicate if the quantity requested will be utilised in multiple experiments.	

#### 9.8.3. Additional Questions: Biodeuteration

**Do you require Biodeuteration - protein or other biosynthetically produced molecules?** If you select '*yes'* to this question you will be required to provide additional information in the field provided in regards to the following:

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Method for production For 1H (protonated) form of molecule (if known), use the following as headings to provide information and describe as applicable for each molecule (add references as needed):	<ul> <li>Host microorganism (e.g. <i>E.coli</i> BL21, <i>S. cerevisiae</i>). Indicate if you can provide the microbe if you have a bio-engineered or specific microbe for production of your requested molecule.</li> <li>Scale of production</li> <li>Culture inoculation preparation</li> <li>Growth conditions (medium – rich or minimal, temperature, timeframes etc)</li> <li>Expression conditions (induction OD/temperature for proteins, expression time etc)</li> <li>Solubility and stability characteristics</li> <li>Storage conditions</li> <li>Add any relevant data to indicate method outcomes (e.g. yield)</li> <li>Add expression SDS-PAGE images in the Proposed Research PDF for protein/s</li> <li>If purification method is known, please describe in the Purification section or add relevant reference/s.</li> </ul>
<b>Recombinant protein</b> <b>expression</b> Use the following as headings to provide information and describe for each protein and	<ul> <li>Protein and Expression Plasmid</li> <li>Do you have a plasmid readily for provision to the NDF?</li> <li>If you don't currently have a plasmid, please</li> <li>contact NDF to discuss further.</li> </ul>
corresponding plasmid (add references as needed):	<b>Note:</b> NDF preferred plasmids for reliable protein deuteration encode for kanamycin resistance and the <i>lacI</i> repressor (e.g. pET28a or similar).
	<ul> <li>Protein UniProt/SwissProt ID</li> </ul>
	<ul> <li>Species of origin (e.g. human, mouse, bacterial)</li> </ul>
	<ul> <li>Plasmid (name and describe, indicate commercial/non-commercial and history)</li> </ul>
	<ul> <li>Antibiotic selection</li> </ul>
	<ul> <li>Induction (e.g. IPTG)</li> </ul>
	$\circ$ Expression tags (describe any N- or C- terminal)
	<ul> <li>Molecular weight, kDa (of expressed protein with and without tags as applicable)</li> </ul>
	<ul> <li>Mutations or modifications (if applicable)</li> </ul>
	<ul> <li>Protein toxicity to host organism (if applicable)</li> </ul>

# 9.8.4. Additional Questions: Chemical Deuteration

<b>Do you require Chemical Deuteration via exchange and synthesis?</b> If you select ' <i>yes</i> ' to this question you will be required to provide additional information in the field provided in regards to the following:	
Method for production	<ul> <li>Have you produced the molecule in <sup>1</sup>H (protonated) form? If yes, please add the following:         <ul> <li>Reaction scheme – add drawing as Figure or reference/s</li> </ul> </li> </ul>

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0	Method (as much detail as possible) or reference/s
0	If purification method known, please describe in the Purification section or add relevant reference/s.

# 9.8.5. Purification Method

This field has been provided for the proposer to describe proven purification method (in 1H or 2H, or multiple labelled form) for each molecule requested. You must include materials and equipment required and quantification method along with references if known.

Purification Method (if known)				
Describe proven purification method (in <sup>1</sup> H or <sup>2</sup> H, or multiple labelled form) for each molecule requested. Include materials and equipment required and quantification method along with references (indicate designer of method if reference/s not available).				
O Source   Q X □				
$\blacksquare = \Omega  \text{Format}  \bullet  \text{Size}  \bullet  \blacktriangle \bullet$				
4				

# 9.8.6. Safety hazards for deuterated molecule synthesis\*

If the requested molecule/s represent any actual or potential hazard to human health, other organisms or the environment, this must be explained further in the field provided. You must describe each molecule, indicating handling and hazard minimisation conditions required; and also information on what approval/s and/or conditions have been required to fulfil for each molecule at your institution/s?



# 9.8.7. Regulatory requirements for deuterated molecule synthesis\*

If there are any regulatory requirements associated with the requested molecule/s, provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

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#### Regulatory Requirements for Deuterated Molecule Synthesis \*

Are there any regulatory requirements associated with your requested molecule/s? Please provide any information as necessary, including any approvals or conditions you are required to fulfil at your institution (e.g. Office of the Gene Technology Regulator - OGTR).

- 5. Click save
- 6. Click next

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### 9.9. Tab 3: Instruments

On the instruments tab you can select one or more ACNS neutron instruments, non-neutron instruments and NDF techniques. Information entered and selections made here should reflect the first 6 months of your proposed program of work.

#### 9.9.1. Neutron Instrument selection

- 1. Select Neutron Instrument
- 2. Select an instrument from the adjacent drop-down menu
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add number of requested days
  - Experimental Setup\*
  - Request a scientist/s
  - Sample environment
  - Laboratory Ancillaries
- 5. Repeat the steps above for any additional neutron instruments
- 6. Click save

Analysis Type	Instrument	Requested
Neutron Instrument	BILBY	9 Days 🗸
Experimental Setup [Neutron Instrument only] Please provide the ins resolution, wavelength, Q-range, and so on.	trumental settings you require on the	e instrument in order to carry out your experiment, such as
Scientists     Choose     V       Sample Env     Choose     V       Lab Ancillaries     Choose     V		Requested

#### 9.9.2. Non-Neutron Instrument selection

- 1. Select Non-Neutron Instrument
- 2. Select an instrument from the adjacent drop-down menu.
- 3. Click add instrument
- 4. Enter the following information for the requested instrument:
  - Add number of requested days
  - Experimental Setup\*
  - Request a scientist/s
- 5. Repeat the steps above for any additional non-neutron instruments
- 6. Click save

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ACNS: Non-Neutron Instrument	Imaging Ellipsometer	8	Days	~	×	
Experimental Setup [Neutron Instrument only] Please provide th resolution, wavelength, Q-range, and so on.	<u> </u>	e instrument in	order to carr	y out you	ir experiment, such as	
						1
Scientists Choose V		Reques	ted			

#### 9.9.3. Technique Selection

- 1. Select Deuteration
- 2. Select a technique from the adjacent drop-down menu
- 3. Click add technique
- 4. Enter the following information for the requested instrument:
  - Add number of requested molecules
  - Scientists (this should indicate any NDF team members you have discussed the proposal with)
- 5. Repeat the steps above for any additional NDF techniques.
- 6. Click save

Deuteration	NDF - Biodeuteration	8	Molecul 🗸		×
Experimental Setup [Neutron Instrument only] Please provid resolution, wavelength, Q-range, and so	le the instrumental settings you require on the ir on.	nstrument in	order to carry out y	your experiment, such a	as
					11
Scientists Choose	▼	Reques	ted		

Click save Click next

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#### 9.10. Tab 4: Submit

When you have finished compiling your proposal you are required to select the 'submit' tab. The research portal will check there are no errors and the terms and conditions have been accepted prior to submission.

#### 9.10.1. Error correction

If there are missing compulsory fields (indicated throughout by a red asterisk \*), error messages will be highlighted in red on your screen. Fix any omissions if you see any error messages, as you will not be able to submit the proposal until this is done.

This is where you submit your proposal for review. Error: You cannot submit due to the following errors:

# 9.10.2. Terms and conditions

Before submitting a proposal, you must review the terms and conditions for the use of neutrons at ANSTO. A proposer will be unable to submit a proposal until the terms and conditions have been accepted.

This is where you submit your proposal for review.

#### Terms and Conditions \*

Click Yes to agree with the terms and conditions for the use of neutrons at ANSTO.

O Yes

O No

Submit

# 9.10.3. Potential Cost Recovery Fees

Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery. Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments).

I accept the Potential Cost Recovery Fees

Large mass or number of molecules will be subject to negotiation and will potentially be subject to partial cost recovery. Some delivery charges incurred by NDF will be subject to cost recovery (e.g. dry ice shipments).

⊖ Yes

 $\bigcirc$  No

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#### 9.10.4. Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) - an Australian Government initiative."

#### I accept the Authorship agreement

Co-authorship of publications arising from use of NDF-produced molecules through the merit and user pays/collaboration access models is expected due to the substantial time (weeks to months) and degree of difficulty in isotopically labelling molecules that are not usually available from other sources.

The following acknowledgment is to be added to any resulting publications: "The National Deuteration Facility is partly funded by the National Collaborative Research Infrastructure Strategy (NCRIS) - an Australian Government initiative."

○ Yes

○ No

#### 9.10.5. Submission

Once the terms and conditions have been accepted, click 'submit'.

Further information on NDF user access can be found here. If you have any queries about these items please contact the NDF Leader and NDF User Program Manager via ndf-enguiries@ansto.gov.au

No further edits can be made to the proposal once it is submitted. If an error or addition needs to be made after submission, please contact user.office.nsw@ansto.gov.au and provide the Proposal ID along with your request for help.

You have successfully submitted proposal N:PP15020

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# **10. Contacts**

Contact details for ACNS and NDF scientists can be found using the following links

User Office NSW	Phone: +61 2 9717 9111
	Email address: <u>user.office.nsw@ansto.gov.au</u>
Australian Centre for Neutron Scattering	Email address: <u>ACNSenquiries@ansto.gov.au</u>
National Deuteration Facility	Email address: <u>ndf-enquiries@ansto.gov.au</u>

# 11. Useful Links

- <u>https://www.ansto.gov.au/our-facilities/australian-centre-for-neutron-scattering/neutron-scattering-instruments</u>
- <u>https://www.ansto.gov.au/ndf/staff-list</u>
- <u>https://www.ansto.gov.au/our-science/capabilities.</u>

# 12. Records

The following records are to be maintained.

File Number	Title	Туре	Storage Location	Retention
Rev 0	ACNS - NDF User Guide for Neutron and Deuteration/Neutron Proposal Type Submissions in ARP	Guide	P:\UserOffice\User Office NSW\ANSTO Research Portal\ARP Training Manual Revisions	5 years
Rev 1	ACNS - NDF User Guide for Neutron and Deuteration/Neutron Proposal Type Submissions in ARP	Guide		

# 13. Revision record

Rev	Description	Date
0	Original issue	16/08/2021
1	References to Anonymised Review and 2022-1 and 2022-2 rounds omitted	11/07/2022
2	Update of document title; Inclusion of screenshots and addition of user account and profile instructions	28/07/2022

#### End of Guide

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