OFFICIAL





NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP

Purpose

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

For further information, contact user.office.nsw@ansto.gov.au

Table of Contents

1.	ANS	TO Re	esearch Portal (Access)	3
2.	How	to R	egister and/or Login	3
	2.1.	Regis	tration	4
	2.2.	Email	l confirmation	5
	2.3.	Regis	tration confirmation	5
	2.4.	Regis	tration details	5
	2.5.	ANST	O Research Portal landing page	6
3.	Prop	osal	type selection and creation	7
4.	. Prop	osal	creation: Deuteration1	1
	4.1.	Main	page	2
	4.1.1		Keywords 1	2
	4.1.2		Collaborators	2
	4.1.3		Categorisation1	3
	4.2.	Scien	ce page1	4
	4.2.1		Proposed Research (PDF) *	4
	4.2.2		Molecule/s to be deuterated	4
	4.2.3		Type of NDF capability technique/s required	5
	4.2.4		Other fields1	6
	4.3.	Techr	niques page1	6
	4.3.1		NDF capability technique selection	6
	4.3.2		Other fields	7
	4.4.	Figure	es page1	7
	4.5.	Propo	psal Navigation and Submission1	8
	4.5.1		Navigation of the proposal application1	8
	4.5.2		Proposal Submission1	8
5.	Prog	ram	Proposal creation and submission1	9
	5.1.	Neutr	ron	9
	5.1.1		Proposal creation1	9
	5.1.2		Proposal information	0
	5.2.	Deute	eration / Neutron 2	2
	5.2.1		Proposal creation	2
	5.2.2		Proposal information	2
	5.3.	Deute	eration	5
	5.3.1		Proposal creation	5
	5.3.2		Proposal information	5
6.	Reco	ords		9
7.	Revi	sion I	record2	9

Revision: 0 Approved by: Approved Review Due: 17/08/2026

Page 1 of 29 Effective Date: 17/08/2021 Custodian: User Office Manager



OFFICIAL

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 2 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

1. ANSTO Research Portal (Access)

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) from round 2022-1. 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 Legacy ACNS Customer Portal (the online portal where NDF and ACNS proposals were previously submitted) will eventually be phased from use and data will be transferred to the ANSTO Research Portal during a later phase of the transition.

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

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

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

Enquiries can also be directed to the following email addresses:

- NDF <u>ndf-enquiries@ansto.gov.au</u>
- ACNS <u>ACNSenquiries@ansto.gov.au</u>

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. How to Register and/or Login

You must be registered in the ANSTO Research Portal to be able to submit proposals.

To register, please go to <u>https://portal.ansto.gov.au/</u> and select the 'Register' option in the Sign In box (refer to image below).

If you already have an account in the ANSTO Research Portal, you can use your current username and password and do not need to register again. Please check that your contact information is correct and up to date.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 3 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	



2.1. Registration

	Wed, 04 Aug 2021 22:43 AF	
Research Portal		
Registration		
Please enter your details below to commence the registration process		
Email: *		
Password: *		
Verify Password: *		
Register		
Register		

- <u>Please note</u>: any field marked with a red asterisk '*' is compulsory and must be completed. This applies throughout all sections within the ARP (e.g. for some information requests within each available proposal type).
- Please provide your email address and set up a password.

Note: you can reuse your existing username and password for the Legacy ACNS Customer Portal when you register (you will just need to set them up in ARP).

- Once you have completed the required fields, click on 'Register'. You will receive an email containing an activation link.
- You will see the Email Confirmation message as shown below which confirms that an email has been sent to your listed email address.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 4 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	



An email has been sent to the address specified. It contains an activation link you must click in order to confirm your email address and activate your account at the ANSTO Research Portal

Thank you for your registration.

2.2. Email confirmation

After clicking on register, you will receive an email containing an activation link. This will be sent from the ANSTO Research Portal to the email address you provided in the previous steps.

Click on the link to activate your account.



2.3. Registration confirmation

After successfully activating your account you will be see a registration confirmation message as shown below. Click on the blue <u>here'</u> to continue as described in 2.4 to complete registration.



Please click here to continue.

2.4. Registration details

You will now need to add further information including your name, country of citizenship, gender and your affiliated organisation to complete the registration.

Fields with a red asterisk $'^*$ must be filled in.

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.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 5 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

OFFICIAL

Registration Details					
ACCOUNT INFORMATION					
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 *	Gender Y	~		
ORGANISATION INFORMATION	Add Orgai	nisation	If your organisation is not displayed in th		
Position Title	~ Departme	nt	drop-down list, please enter your organisation name in the 'Add Organisation' field.		
Telephone (Mobile) *	Telephone (Other)	Website	Please include your country and area coo		
			п учи стерлоте поптоет		
ADDITIONAL					
Email Updates					
L 1 do Not want to receive em	ans un elated to my proposals.				

2.5. ANSTO Research Portal landing page

There will be three or four selections across the top menu. Click on any of these selections to access:

		Wed, 04 Aug 2021 22:50 AEST
Research Portal		[Logout]
Dashboard	Proposals	Profile

• **Dashboard** - This will show your five most recent proposals once the data from the Legacy ACNS Customer Portal is transferred in Phase 2 of the portal transition.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 6 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

- **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. Proposals entered in earlier rounds through the Legacy ACNS Customer Portal will be transferred in Phase 2 of the portal transition.
- **Reviews** If you are not a reviewer (currently in ARP), you will not see this tab. This page lists all proposals which have been assigned to you for technical feasibility, safety or scientific review. At the right-hand side are links for a PDF of the assigned proposal and a review popup.
- **Profile** On this page you can update your password, personal information and your affiliated organisation details etc.

3. Proposal type selection and creation

To create a new proposal you can do this from both the Dashboard or Proposals pages. At the top of

these pages you will see the link to "Create new proposal" next to this symbol 👽. Please click here to start a new proposal.

Example shown below of what you will find on the Dashboard page.



Once you click on the "Create new proposal" link, you will be taken to the Proposal Creation page as shown below.

On this Proposal Creation page you will find the list of ANSTO facilities for the proposal types which can be submitted through the ARP.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 7 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

OFFICIAL



On this page you will find both "National Deuteration Facility" and "Australian Centre for Neutron Scattering" tabs available to select (click on):



NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 8 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

National Deuteration Facility: Select for merit access proposal submissions to the National Deuteration Facility capabilities for provision of deuterated and multiple isotopically labelled molecules for neutron scattering and other applications. 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>. Further information about NDF user access and capabilities can be found <u>here</u>.

Australian Centre for Neutron Scattering: Select for merit access proposals to the Australian Centre for Neutron Scattering instruments and capabilities. For all other proposals, please use the Legacy ACNS Customer Portal tab. Click for more information about the <u>ACNS and the Neutron Beam facility</u>.

When you make a selection you will find the list of proposal types available (with descriptions) to submit through the ARP for NDF and ACNS.

National Deuteration Facility	=	Select for merit access proposal submissions to the National Deuteration Facility capabilities for provision of deuterated and multiple isotopically
Deuteration	Merit access proposal for NDF capabilities within a 6-month round. This proposal type is	labelled molecules for neutron scattering and other applications. For proposal types other than merit access such as user pays/collaborative or commercial and for
	experiments or for non- neutron applications (e.g. NMR, MS). Applications for rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review. More information on NDF user access can be found here.	any enquiries, please contact the NDF via ndf-enquiries@ansto.gov.au. Further information about NDF user access and capabilities can be found here.
Deuteration / Neutron	Merit access proposal for ACNS instruments and NDF capabilities where deuterated molecule/s are required for the proposed neutron experiments at ACNS. Applications for rounds 2022-1 and 2022-2 will be subjected to Anonymised Review. More information can be found here.	
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) and will NOT be subject to Anonymised Review in rounds 2022-1 and 2022-2.	
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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.	

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 9 of 29
Revision: 0	Effective Date: 17/08/2021

OFFICIAL

OFFICIAL



In this user guide, you will find a description of how to create the following proposal types:

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). Applications for rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review. More information on NDF user access can be found <u>here</u>.

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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.

Program Proposal – Deuteration / Neutron (*this proposal type can be selected under both NDF and ACNS tabs*): 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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.

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) and will NOT be subject to Anonymised Review in rounds 2022-1 and 2022-2.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 10 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

4. Proposal creation: Deuteration

Select 'Deuteration' proposal type under the NDF selection tab, you will be taken to the following screen:

Proposal Creation

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). Applications for rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review. 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: 2022-1: (Open for submission)

Principal Scientist

Create

All questions which have a red asterisk * must be completed.

- 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 as shown below to be filled in:

dd a new user			
Add User			
First Name *			
Last Name *			
Email *			
Organisation			
Department			
Position Title			
	Create	2	
	Cancel		
			Clo

• Click on 'Create'. This saves your work and takes you to the Main page.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 11 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

Please note: Admin page option in top left hand side navigation menu which is visible in screen shots throughout this guide are only available to ANSTO Research Portal Administrators. This does not form part of the proposal creation process.

4.1. Main page

The Main page shows the information you have previously entered and allocates a unique proposal number/ID. Please save your work frequently – 'Save' buttons are at the top and bottom of the screen.

	Main			
Main	NDF2: Deuteration	Test		
Science	Save Next Cancel			
Techniques				
Figures	Proposal Details			
Admin	ID	NDF2		
Submit	Title	Deuteration Test		
	Round	ACNS & NDF: 2022-1		
	Туре	National Deuteration Facility: De	euteration	
	Status	In Preparation		
	identify the proposal's to	pic and objectives.	sposal, separated by commost key f	norda are moex of addject worda miner riep
	Collaborators Please enter the detail collaborator. Click on y Complete the details in Type (if applicable) and Please ensure you incl outputs &/or outcome	s of the researchers (including your collaborator's name if it ap n the pop-up Add a new user for d enter the student's Superviso ude all ANSTO staff who will co s of this project.	students) involved with this propos opears. Click Add User. If your collab m and click <i>Submit</i> and then <i>Close</i> . S r Name. ntribute to this proposal and any pe	al. Enter the given or family name of your porator is not registered, click <i>Create User</i> . Select the appropriate Role and Student eople who will be associated with the
	Name:		Add User Clear	
	Name	Role	First Time User 🛛	Student Type 🗿

4.1.1. 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.

4.1.2. Collaborators

Please enter the details of all the researchers (including students) involved with this proposal.

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

• Enter the first name and last name of your collaborator. The field will search on either name. Click on your collaborator's name if it appears. Click *Add User*.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 12 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

If your collaborator's name does not appear in the dropdown list, click *Create User* at the bottom of the dropdown list. Complete the details in the pop-up '*Add a new user'* box as shown in Section 4. You need to add the following information, click *Submit* and then *Close*:

- First name
- o Last name
- o Email
- o Organisation
- Options for affiliated Organisation are available to select from a dropdown list. Please enter the beginning of the name of the Organisation and the closest match will appear. Click on the organisation name to select.

If the organisation is not listed please enter the name of the organisation. Click *Create* and then *Close*. For each name added, select the appropriate User role.



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/capabilities before, check the *First Time User* box.
- 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.

4.1.3. Categorisation

Add information where relevant to the following fields:

- Scientific area (select from drop down list)
- Intellectual Property (I.P.) Issues (select Yes or No)
 - If Yes, add Details
- Select Yes or No if this work forms a critical part of a student thesis
 - If Yes, add Thesis Details
- Participation (select *Yes* or *No*)
- Research Funding (check relevant option/s)
- Financial Information*
- Are you an ECR?
- Industrial Relevance (select from drop down list)
- Industrial Involvement (add name/s)

Click on 'Save' to save all entries.

Click on 'Next' or 'Science' on top left hand side of screen to navigate to the next part of the proposal.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 13 of
	29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

4.2. Science page

	Science
Main	NDF2: Deuteration Test
Science	Previous Save Next Cancel
Techniques	
Figures	Do you know if synthesis of your molecule/s requires Biodeuteration (for deuteration or multiple isotopic labelling) or Chemical deuteration techniques?
Admin	If you are not sure, please contact the NDF via ndf-enquiries@ansto.gov.au to discuss your proposal.
Submit	Proposed Research (PDF) *

4.2.1. Proposed Research (PDF) *

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 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)

4.2.2. Molecule/s to be deuterated

Use the following as headings to describe each molecule you are requesting in the free text field:

- Type of experimental application (where labelled molecule/s will be used e.g. neutron, NMR)
- *Molecule name* full and any abbreviation (Note: maximum of 2 molecules per proposal. Please contact NDF if you require more).
- *Molecule structure* (as applicable, add to Figures section)
- *Isotopic labelling required* (²H only or multiple-labelling with ¹³C and/or ¹⁵N. *Note*: labelling capability dependent on molecule request)
- *Deuteration level* (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 (e.g. 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.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 14 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

4.2.3. Type of NDF capability technique/s required

Do you require Biodeuteration - protein or other biosynthetically produced molecules? *

If you answer Yes, you will be prompted for more information.

- O Yes
- No

Do you require Chemical Deuteration via exchange and synthesis? *

If you answer Yes, you will be prompted for more information.

- Yes
- No

If you select *Yes*' to either of these questions, additional free text fields with requested information lists become available to fill in.

Note: if your research requires both NDF capability techniques, please submit separate proposals.

For Biodeuteration requests, the following information is requested in the free text field:

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):

- Host microorganism (e.g. *E.coli* BL21, *S. cerevisiae*). Indicate if you can provide the microbe if you have a bio-engineered or specific microbe for production of your requested molecule.
- Scale of production
- Culture inoculation preparation
- Growth conditions (medium rich or minimal, temperature, timeframes etc)
- Expression conditions (induction OD/temperature for proteins, expression time etc)
- Solubility and stability characteristics
- Storage conditions
- Add any relevant data to indicate method outcomes (e.g. yield)
- Add expression SDS-PAGE images to Figures for protein/s

If purification method is known, please describe in the Purification section or add relevant reference/s.

Recombinant protein expression

Use the following as headings to provide information and describe for each protein and corresponding genetic construct (add references as needed):

- Protein and Expression/genetic construct If you don't currently have an expression construct, please contact NDF to discuss further.
 - UniProt/SwissProt ID
 - Species of origin (e.g. human, mouse, bacterial)
 - o DNA and amino acid sequences
 - Vector (name and describe, indicate commercial/non-commercial)
 - Antibiotic selection

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 15 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

- Induction (e.g. IPTG)
- Tags (describe any N- or C- terminal)
- Molecular weight, kDa (of expressed protein with and without tags as applicable)
- Mutations or modifications (if applicable)
- Toxicity to host organism (if applicable)

For Chemical Deuteration requests, the following information is requested in the free text field: Method for production

If known, please provide the following information and describe as applicable for each molecule:

- Have you produced the molecule in ¹H (protonated) form? If yes, please add the following:
 - Reaction scheme add drawing as Figure or reference/s
 - Method (as much detail as possible) or reference/s
 - $\circ~$ If purification method known, please describe in the Purification section or add relevant reference/s.

4.2.4. Other fields

Fill out the following information request fields as applicable:

- Purification Method (if known)
- Safety hazards for deuterated molecule synthesis*
- Regulatory requirements for deuterated molecule synthesis*

Click on 'Next' or 'Techniques' on top left hand side of screen to navigate to the next part of the proposal.

4.3. Techniques page

4.3.1. NDF capability technique selection

	NDE2: Deuteration Tes	t		
Main	NDF2. Dedteration res			
Science	Previous Save Next	Cancel		
Techniques				
Figures	Techniques: Select NDF tec	hnique required by your proposa	l (NDF - Biodeuteration and/or NDF -	Chemical Deuteration).
Admin				
Submit	Deuteration	✓ N	DF - Biodeuteration	
	Capability Type	Technique	Requested	
	Deuteration	NDF - Biodeuteration	1 Molecul 🗸	
	Scientists Choose	~	Requested	
	Requested Supply Date/s *			
	Please indicate date/s required for provision of requested molecule/s and where they are to be delivered.			

NDF - ACNS User Guide for Deuteration and Program Proposal Type	s in ARP Page 16 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

On the Techniques page, you can select the NDF capability technique required for your molecule/s request (NDF – Biodeuteration or NDF – Chemical Deuteration), request number of molecules, and NDF scientists.

- Select NDF Deuteration technique from drop down list and click on *Add Instrument*. In the box that opens up:
 - Add number of requested molecules
 - Scientists (drop down selection list of NDF scientists)



Note: if your research requires both NDF capability techniques, please submit separate proposals.

4.3.2. Other fields

Requested Supply Date/s*

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

Click on 'Save' to save all entries.

Click on 'Next' or 'Figures' or 'Submit' on top left hand side of screen menu to navigate to the next part of the proposal you are ready for.

4.4. Figures page

Research I	NSTO Portal	Add figures
Dashboar	d	
	Figure	Drop files here
Main	NDF2: D	Click here to select a figure to upload, or drop your figures here
Science	Previous	Browse
Techniques	Add Figur	
Admin		Max file size: 3mb
Submit	No figure	Allowed formats: PDF, PNG, and JPG
		Close Upload
	Add Figure	
	Previous	Save Next Cancel

Figures relevant to your application can be dropped into the proposal. Please ensure reference is made to these Figures as appropriate within the proposal text. Multiple Figures can be added (or be left blank). To add:

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 17 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

- Click on 'Add Figure'
- Drop file into area highlighted on screen or click on "Browse" to select a file from your computer. Maximum file size 3MB. PDF, PNG and JPG formats permitted.
- Click on 'Upload'
- Click on 'Save'

Click on 'Next' or 'Submit' on top left hand side of screen to navigate to the next part of the proposal

4.5. Proposal Navigation and Submission

4.5.1. Navigation of the proposal application

Navigate between proposal pages by:

- The menu on the left hand side of the portal screen
- 'Previous' and 'Next' buttons at the bottom of each page

Remember to click on 'Save' button to save your proposal often and especially after data is entered on each proposal page.

4.5.2. Proposal Submission

When you have completed all data entry required:

- Select "Submit" tab in menu on top left hand side of portal screen
- If there are missing compulsory fields (indicated throughout by a red asterisk *), error messages will be highlighted in red (example shown below)
- Fix any omissions if you see any error messages

	Submit
Main	NDF2: Deuteration Test
Science	Previous Exit
Techniques	
Figures	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.
Admin	Error: You cannot submit due to the following errors:
Submit	Techniques Tab
	Requested Supply Date/s * Please indicate date/s required for provision of requested molecule/s and where they are to be delivered. This value should not be blank. Go to question

If you don't see any error messages, the following will be visible:

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 18 of
	29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

	Submit
Main	NDF2: Deuteration Test
Science	Previous Exit
Techniques	
Figures	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.
Admin	I accept the Potential Cost Recovery Fees
Submit	Requests for multiple-labelled proteins (e.g. with ² H plus ¹³ C and/or ¹⁵ 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
	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."
	O Yes
	O No
	Submit

Please read and review the information sections on NDF potential cost recovery and authorship agreement. You must select '*Yes*' to accept both sections to be able to submit your proposal for review.

When you are ready click on 'Submit' button.

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.

5. Program Proposal creation and submission

There are 3 Program Proposal types which can be selected for access to ACNS, NDF and both facilities in ARP.

All Program Proposal submissions require upload of a PDF in the 'Science' page outlining in detail the 'Proposed Program of Research' addressing the information requested for each proposal type and covering a timeframe of up to 3 years.

Refer to details in 5.1.2.2, 5.2.2.2 and 5.3.2.2 for each proposal type.

5.1. Neutron

5.1.1. Proposal creation

Select 'Program Proposal – Neutron' proposal type under the ACNS tab:

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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.
Vou will be taken to the following careers	

You will be taken to the following screen:

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 19 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

Proposal Creation

P

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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.

roposal Title *
rovide a short descriptive title
roposal Type *
ACNS: Neutron Program Proposal: Peer-reviewed experiments on our neutron beam lines.
roposal Round *
ACNS & NDF: 2022-1: (Submissions due on September 15)
rincipal Scientist
Create

Fill out all fields and click on 'Create' (refer to Section 4.)

5.1.2. Proposal information

Please fill out each proposal page section with the requested information outlined in the fields:

- 5.1.2.1. Main page
 - Keywords
 - Collaborators
 - Scientific area (select from drop down list)
 - Intellectual Property (I.P.) Issues (select Yes or No)
 - o If Yes, add Details
 - Select Yes or No if this work forms a critical part of a student thesis
 - If Yes, add Thesis Details
 - Research Funding (check relevant option/s)
 - Industrial Relevance (select from drop down list)
 - Industrial Involvement (add name/s)

5.1.2.2. Science page

Proposed Program of Research

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 including 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

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 20 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

- 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)

5.1.2.3. Instruments page

On the Instruments page, you can select one or more ACNS neutron instruments and non-neutron instruments, describe experimental setup for each instrument selection, request number of days, ACNS instrument scientists and laboratory ancillaries.

Information entered and selections made here should reflect the first 6 months of your proposed program of work.

- Select Neutron Instrument or ACNS:Non-Neutron Instrument from drop down list
- Select a specific instrument from the adjacent drop-down menu and click on *Add Instrument.* In the box that opens up:
 - Add number of requested days
 - Experimental Setup* (describe)
 - Scientists (drop down selection list corresponds to the instrument selected)
 - Sample environment (drop down selection list)
 - Laboratory Ancillaries (drop down selection list)

Repeat the steps above for any additional instruments (*Note*: each instrument is added sequentially below the first instrument selected)

5.1.2.4. Figures page

Add Figures as needed (refer to Section 4.4)

5.1.2.5. Submit page

When you have completed all data entry required:

- Select 'Submit' tab in menu on left hand side of portal screen
- If there are missing compulsory fields (indicated throughout by a red asterisk *), error messages will be highlighted in red
- Fix any omissions if you see any error messages
- Review the Terms and Conditions for use of neutrons at ANSTO. You must select '*Yes*' to be able to submit your proposal for review.
- Once ready, click on 'Submit' button.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 21 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

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.

5.2. Deuteration / Neutron

5.2.1. Proposal creation

Select 'Program Proposal – Deuteration / Neutron' proposal type under either the NDF or ACNS tab:

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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.

You will be taken to the following screen:

Proposal Creation

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. Applications for program proposals in rounds 2022-1 and 2022-2 will NOT be subject to Anonymised Review.

Proposal Title * Provide a short descriptive title Proposal Type * • ACNS & NDF: Neutron and Deuteration Program Proposal Round * • ACNS & NDF: 2022-1: (Submissions due on September 15)

Create

Fill out all fields and click on 'Create' (refer to Section 4.)

5.2.2. Proposal information

Please fill out each proposal page section with the requested information outlined in the fields:

- 5.2.2.1. Main page
 - Keywords
 - Collaborators
 - Scientific area (select from drop down list)
 - Intellectual Property (I.P.) Issues (select Yes or No)
 - o If Yes, add Details

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 22 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

- Select Yes or No if this work forms a critical part of a student thesis
 - If *Yes*, add Thesis Details
- Participation (select Yes or No, with NDF)
- Research Funding (check relevant option/s)
- Financial Information*
- Are you an ECR?
- Industrial Relevance (select from drop down list)
- Industrial Involvement (add name/s)

5.2.2.2. Science and Synthesis page

Proposed Program of Research

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.

<u>Note</u>: specific Deuteration details are also requested in other fields within this section in the portal, as per Section 4.2.3 and 4.2.4.

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)

5.2.2.3. Instruments page

On the Instruments page, you can select one or more ACNS neutron instruments and non-neutron instruments, NDF capability techniques, describe experimental setup for each ACNS instrument selection, request number of days (ACNS) or molecules (NDF), ACNS instrument scientists, NDF scientists and ACNS laboratory ancillaries.

Information entered and selections made here should reflect the first 6 months of your proposed program of work.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 23 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

- Select Deuteration, Neutron Instrument or ACNS:Non-Neutron Instrument from drop down list
- Select a specific ACNS instrument or NDF capability from the adjacent drop-down menu and click on *Add Instrument*. In the box that opens up:
 - Add number of requested days or molecules
 - Experimental Setup (describe for ACNS only)
 - \circ $\;$ Scientists (drop down selection list corresponds to the ACNS instrument selected or NDF scientists list)
 - Sample environment (drop down selection list for ACNS instrument only)
 - Laboratory Ancillaries (drop down selection list for ACNS instrument only)

Repeat the steps above for any additional instruments or NDF capabilities (*Note*: each instrument is added sequentially below the first instrument selected)

5.2.2.4. Figures page

Add Figures as needed (refer to Section 4.4)

5.2.2.5. Submit page

When you have completed all data entry required:

- Select 'Submit' tab in menu on left hand side of portal screen
- If there are missing compulsory fields (indicated throughout by a red asterisk *), error messages will be highlighted in red
- Fix any omissions if you see any error messages

If you don't see any error messages, the following will be visible:

Submit

DN:P6: D/N Program Proposal Test

Previous Exit

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

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

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

Submit

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP

Page 24 of 29

Effective Date: 17/08/2021



Please read and review the sections on Terms and Conditions for use of neutrons at ANSTO, NDF potential cost recovery and authorship agreement. You must select '*Yes*' to accept all sections to be able to submit your proposal for review.

When you are ready click on 'Submit' button.

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.

5.3. Deuteration

5.3.1. Proposal creation

Select 'Program Proposal – Deuteration' proposal type under the NDF tab:

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) and will NOT be subject to Anonymised Review in rounds 2022-1 and 2022-2.

You will be taken to the following screen:

Proposal Creation

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) and will NOT be subject to Anonymised Review in rounds 2022-1 and 2022-2.

Proposal Title *

Provide a short descriptive title

Proposal Type * NDF: Deuteration Program Proposal Proposal Round * ACNS & NDF: 2022-1: (Submissions due on September 15) Principal Scientist Create

Fill out all fields and click on 'Create' (refer to Section 4.)

5.3.2. Proposal information

Please fill out each proposal page section with the requested information outlined in the fields:

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 25 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

5.3.2.1. Main page

- Keywords
- Collaborators
- Scientific area (select from drop down list)
- Intellectual Property (I.P.) Issues (select Yes or No)
- o If Yes, add Details
- Select Yes or No if this work forms a critical part of a student thesis
- If Yes, add Thesis Details
- Participation (select Yes or No)
- Research Funding (check relevant option/s)
- Financial Information*
- Are you an ECR?
- Industrial Relevance (select from drop down list)
- Industrial Involvement (add name/s)

5.3.2.2. Science page

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 ndf-enquiries@ansto.gov.au to discuss your proposal.

Proposed Program of Research

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.

<u>Note</u>: specific Deuteration details are also requested in other fields within this section in the portal, as per Section 4.2.3 and 4.2.4.

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)

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 26 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

• Please *reference publications relevant to your proposed research* (add DOI links if available)

5.3.2.3. Techniques page

On the Techniques page, you can select the NDF capability techniques required for your molecule/s request (NDF – Biodeuteration and/or NDF – Chemical Deuteration), request number of molecules, and NDF scientists.

Information entered and selections made here should reflect the first 6 months of your proposed program of work.

- Select NDF Deuteration technique from drop down list and click on *Add Instrument*. In the box that opens up:
 - Add number of requested molecules
 - Scientists (drop down selection list of NDF scientists)

Repeat the steps above for each NDF capability.

5.3.2.4. Figures page

Add Figures as needed (refer to Section 4.4)

5.3.2.5. Submit page

When you have completed all data entry required:

- Select 'Submit' tab in menu on left hand side of portal screen
- If there are missing compulsory fields (indicated throughout by a red asterisk *), error messages will be highlighted in red
- Fix any omissions if you see any error messages

If you don't see any error messages, the following will be visible:

Submit

NDF:P5: NDF Program Proposal Test



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.

l accept the 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.



O No

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."

0	Yes
0	No

Submit

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP

Page 27 of 29



Effective Date: 17/08/2021

Please read and review the sections on NDF potential cost recovery and authorship agreement. You must select '*Yes*' to accept both sections to be able to submit your proposal for review.

When you are ready click on 'Submit' button.

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.

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 28 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	

6. Records

The following records are to be maintained for ANSTO Research Portal.

File Number	Title	Туре	Storage Location	Retention
Rev 0	ACNS-NDF Submissions User Guide for ARP	Guide	P:\UserOffice\User Office NSW\ANSTO Research Portal\ARP Training Manual Revisions	5 years

7. Revision record

Rev	Description	Date
0	Original issue	14/07/2021

End of Guide

NDF - ACNS User Guide for Deuteration and Program Proposal Types in ARP	Page 29 of 29
Revision: 0	Effective Date: 17/08/2021
OFFICIAL	