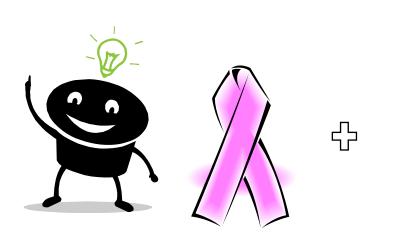
How to get Neutron Beamtime: Writing a Successful Neutron Proposal

Victoria Garcia Sakai





ß

sample



Idea & Research problem

Pre- characterisation



the unique information obtained from neutron experiments Can neutrons help me?





Are you sure?

Can you obtain the information with a different technique?

Are you completely sure?



• Literature review on similar experiments

- Literature review on similar experiments
- Talk to colleagues

- Literature review on similar experiments
- Talk to colleagues
- Research available instruments worldwide

Where should I go to get my neutrons?

- Where can I do the best science?
 - Instrument specs
 - Flux
 - Sample environment
 - Technical/user support
 - Laboratory space/facilities
 - PhD programmes
 - Software
- Proximity/ease of access
- Funding
- Personal connections/collaborations
- Food/Scenery

Where should I go to get my neutrons?

Sources <u>http://neutronsources.org/</u>



Europe (25) Americas (9) Asia-Oceania (12) Africa (1)

Sources with Significant User Programmes

Europe

- Institut Laue Langevin ILL (France)
- Heinz Maier-Leibnitz Zentrum MLZ (Germany)
- Laboratoire Leon Brillouin LLB (France)
- Helmholtz-Zentrum Berlin HZB (Germany)
- Budapest Neutron Centre BNC (Hungary)
- ISIS (UK)
- Swiss Spallation Neutron Source SINQ (Switzerland)
- European Spallation Source ESS (Sweden under construction)

Americas

- NIST Centre for Neutron Research NCNR (USA)
- High Flux Isotope Reactor HFIR (USA)
- Canadian Neutron Beam Centre CNBC (Canada)
- Spallation Neutron Source SNS (USA)
- Los Alamos Neutron Science Centre LANSCE (USA reduced user programme)

Sources with Significant User Programmes

Asia - Oceania

- Japan Research Reactor 3 JRR3 (Japan awaiting permission to restart)
- Australia Nuclear Science and Technology Organisation ANSTO, OPAL
- reactor (Australia)
- High flux Advanced Neutron Application Reactor HANARO (South Korea)
- Bombay Atomic Research Centre BARC (India)
- South Africa Nuclear Energy Corporation NECSA, Safari reactor (South Africa)
- China Advanced Research Reactor (CARR not yet operational)
- China Mianyang Research Reactor(CMRR)
- J-PARC Materials and Life Science Facility MLF (Japan)
- China Spallation Neutron Source (CSNS under construction)

- Literature review on similar experiments
- Talk to colleagues
- Research available instruments worldwide
- Contact instrument scientist and ask questions!
 - instrument configuration
 - sample environment
 - time required
 - ...

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- Decide on proposal type

Access Types

- Normal proposal rounds twice per year
- Rapid access for urgent studies or 'hot topics', submit at any time
- **Xpress access**, including postal service
- Industrial access (collaborative or for cash)
- **Back door** collaboration/tests with institute scientists
- **Programme access** long time proposals
- Joint access with other facilities ask (eg. Diamond)

- Literature review on similar experiments
- Talk to colleagues
- Research available instruments worldwide
- Contact instrument scientist and ask questions!
 - instrument configuration
 - sample environment
 - time required
 - ..
- Decide on proposal type
- Preliminary sample characterisation?

- Literature review on similar experiments
- Talk to colleagues
- Research available instruments worldwide
- Contact instrument scientist and ask questions!
 - instrument configuration
 - sample environment
 - time required
 - ..
- Decide on proposal type
- Preliminary sample characterisation?
- How will neutrons answer my questions?

- Contact instrument scientist and ask questions!
- Have I done preliminary characterisation?
- Will neutrons answer my questions?

the Proposal Process (in general)

- Two proposal calls per year
- Deadline is real!
- Technical reviews (by facility scientists) feasibility, safety...
- Scientific Review
 - Classification is done by subject or technique
 - At least 2 reviewers per proposal by external experts
 - Panel meetings at facilities
 - Time recommended
- Final balance (eg. national funding)
- Letters sent out to Pl's

Things to keep in mind...

Scientific reviewers are not always experts in your specialty since science at the facilities is so diverse. So, don't assume they know everything.

Most reviewers spend 5-8 minutes per proposal! Many will not have time to read through the references!

So, you must get all relevant information in the proposal. Make your point, clearly and succinctly.

- User/participant information
- Title and abstract
- Sample description
- Sample environment requirements
- Instrument specs requested and time
- Publications, student thesis, scientific area, grants, submission status, safety...

JCNS, Munich

CONS.	utron Science
Julich Centre for Ne	utron Science

Proposal No. : 8744 Proposer : Affiliation : Short Name :

Subject		
Title		Title
Scientifique area	Soft Condensed Matter	
Grand Challenges	Soft Matter, Macromolecules, Complex fluids	Instrument
Instrument	KWS-1	Tusciallicite
Continuation of experiment No.	7211	
Resubmission of proposal nr.		

Rapid Access only available for instruments KWS-2, PGAA and SPODI. Each accepted Rapid Access proposal will receive up to a maximum of 12 hours of beamtime.

Rapid Access Proposal?	No
Internal beam time	No
Did you submit this proposal also to another facility?	No
Measuring time [days]	
Abstract (max 200 words)	AbstraCt
Experimental team	
Co-authors name, affiliation	User info

name, affiliation Local contact

Sample		
Substance	deuterium oxide	
Elemental formula	D2O	-
Sample type	liquid	
sample size [mm] weight [mg]	1 (mm) thickness, 20 (g)	Sample info
Number of samples	2	
Availability of samples	2013-07-19	
Space group		
unit cell parameters		

Sample environment			
No sample environment	Yes		
needed			
Cryostat		— Sample -	
High temperature furnace			
Pressure cell		environment	
Magnetic field		environment	
other sample environment	shear cell (Anton Paar)		
Temperature range		— info -	
Temperature stability			
Pressure range			
Magnetic field			
Security aspects			
Toxic	No		
explosive	No		
radioactive	No		
Sample gets activated	No		
activity after experiment [Bq / isotope]			
Other risks			
Miscellaneous	-		
Sample preparation laboratory (neutron guide hall)	No		
Typ of work, materials, equipment in use			
Special technical support	No		
Details(e.g. own equipment, special configurations, mechanics, control, software)			

ISIS, UK

Science & Technolo Facilities Council			ISIS .
Experiment Proposal			viment Number: 020169
Principal investigator(*) Co-investigator Co-investigator Co-investigator Co-investigator Co-investigator Co-investigator Co-investigator Co-investigator Experiment Title	Dr V Garcia Sakai, STFC, United Ki		Title
Instrument	IRIS/ OSIRIS	Days Requested: 7	
Access Route Science Areas	Direct Access - Resubmission Biology and Bio-materials	Previous RB Number: -	Time 4
Sponsored Grant	No	Sponsor: -	•
Grant Title	-	· 1	nstrument
Grant Number	-	_	
	Start Date: -	Finish Date: -	
EU Access?			
Similar Submission?	No		
Abstract		Abstract	
Publications			

ISIS Sample record sheet

Principal contact Instrument Special requirements	Dr V Garcia Sakai, Victoria.garcia-sakai@stfc.ac.uk, Tel: 00-44-1235-446703 IRIS/ OSIRIS, 7 days, preferred contact is Garcia Sakai, V (Victoria.garcia-sakai@stfc.ac.uk)		
opecial requirements	-	SAMPLES	
Material	protein		
Formula	-		
Forms	Solid		Sample info
Volume	1 cc		panipic into
Weight	-		
Container / substrate	-		
Storage requirements	-		
Xtal details			
		SAMPLE ENVIRONMENT	
Equipment	CCR		Cample
Temperature range	10-330 K		Sample
Pressure range	-		environment
Magnetic field range	-		environment
Special equipment			info
		SAFETY	MF0
Hazards	-		
Hazard details	-		
Sample sensitivity	-		
Experimental hazards	-		
Sample prep hazards	-		
Equipment hazards	-		
Prep lab needed	Yes		
Special equip reqs	-		
Sample will be	Removed By User		



NCNR, USA

Title

Time

NIST Center for Neutron Research

Proposal for Neutron Beam Experiment

Experiment Title Title: Dynamics of phospholipid vesicles in the presence of bioprotectants Proposal Type: New Proposal Time Received: 21-MAR-08 17:52

Scheduling Desired Dates: 07-01-2008 to 12-31-2008 Impossible Dates: Estimated Duration: 6 days

Participants				User info
	Name	Address	Country	Telephone/e-mail
Principal	Garcia-Sakai,	Rutherford Appleton Laboratory	United Kingdom	000-000-0000
Investigator	Victoria	ISIS Facility		victoria.garcia-sakai@stfc.ac.uk
		Chilton, Didcot		
		Oxon, OX11 0QX		
User 2	Nanda, Hirsh	National Institute of Standards and	United States	hirsh.nanda@nist.gov
		Technology		
		NIST Center for Neutron Research		
		100 Bureau Drive, MS6102		
		Gaithersburg, MD		
		20899-6102		

Instrument

Instrument Requested:	NG-5 NSE, Neutron spin echo spectrometer (CH	RNS)
Suggested Local Contact:	Antonio Faraone	1
Instrument Resolution:		Instrument
Instrument Configuration:	Default instrument configuration	Tuscianciic

Sample Description		
	Sample 1	
Name	DPPC/D2O/maltose	
Chemical Formula		
Mass (grams)		
Form	Liquid	

		💳 Sample info
Temperature Measurement Range (K)	300-330	
Number of Runs		
Total Collection Time (hrs)		
Sample Availability	2008-03-01 00:00:00.0	
	Sample 2	
Name	DPPC/D2O/sucrose	
Chemical Formula		
Mass (grams)		
Form	Liquid	
Temperature Measurement Range (K)	300-330	
Number of Runs		
Total Collection Time (hrs)		
Sample Availability	2008-03-01 00:00:00.0	

Sample Environment

Sample Environment Equipment:

Sample environment info

Special Requirements

Please describe any non-routine needs for sample temperature, magnetic field, etc., or other ancillary equipment. Specify any equipment needed at NIST for sample loading, treatment, storage, etc. (inert atmosphere, refrigeration, dry box, etc.). Also describe any equipment you plan to bring to NIST.

Safety

Check *at least* one box that describes your sample [X] No Hazards [] Toxic [] Corrosive [] Radioactive [] Explosive [] Flammable If there are any hazards associated with your proposed experiment, please indicate how any risks are to be handled.

Categorization

For reporting purposes, please categorize your proposal:

L	Research Area:	Biomolecular Science
L	Funding Agency:	NRC and STFC UK

Publications

Two-page description of proposed research (incl. references)

• Brief background, state the problem clearly and why the experiment is important, why it will make a difference – Why should one care?

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- Clear justification of need for neutrons and particular instrument- why do you need beamtime on X?

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- Description of preliminary characterisation or work on the sample/system- do you understand your sample?

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- Evidence team's productivity and experience Will they publish in a timely manner?

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- Description of data analysis/modelling What will you do with the data?
- Evidence team's productivity and experience Will they publish in a timely manner?
- Be clear and specific not vague and general!
- Think of yourself as a reviewer! What would annoy you?

2-page Case including references and figures/tables



User Office Lichtenbergstr. 1, 85748 Garching/ Germany Tel: +49.(0)89.10703/10794 Fax: +49.(0)89.10799 Email: userintric@jtrm2.tum.de Web: user.frm2.tum.de

SUBMISSION OF A PROPOSAL

Experiment Title

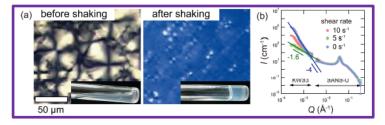
Proposer Name Email Affiliation Co-Proposers

Scientific background and detailed description of the proposed experiment

Abstract (~100 words)



User Office Lichtenbergetr. 1, 85748 Garching/ Germany Tel: +49.(0)89.10703/ 10794 Fax: +49.(0)89.10799 Email: userinfo@ffm2.tum.de Web: user.frm2.tum.de



Aim	of	proposed	work

Introduction

Reference

[1] K. Sadakane, A. Onuki, K. Nishida, S. Koizumi, and H. Seto, Phys. Rev. Lett., 103, 167803 (2009). [2] A. Onuki, J. Chem. Phys., 128, 224704 (2008).

Previous results

Proposed experiments

Here is our experimental plan:

- 1) Instrument: KWS1 with rheo-meter (Anton Paar)
- 2) Shear-rate: 0 s⁻¹, 0.1 s⁻¹, 1 s⁻¹, 3 s⁻¹, 5 s⁻¹, 7 s⁻¹, 10 s⁻¹, 50 s⁻¹, 100 s⁻¹, 1000 s⁻¹
- The measured spatial domain: Q = 0.003 Å⁻¹ to 0.3 Å⁻¹
- 4) Sample: (i) D₂O / 3-methylpydine / NaBPh₄
- (ii) D₂O / C₁₄E₅
- 5) Temperature: 298 K

We assume that one measurement takes 45 minutes (15 minutes at high-Q and 45 minutes at low-Q region). Then, the total measurement time is estimated as

0.75 (hours) \times 10 (shear rate) \times 2 (samples) \times 1 (temperature) = 15 (hours). Additionally, we need 8 hours for setting rheo-meter and changing the detector length. Threfore, we request 1 days beam-time.

Your publication record (give references to papers published in the last two years arising from experiments at FRM II instruments) There is no paper arising from experiments at FRM II instruments.

2 of 2

Changes in lipid dynamics induced by melittin absorption on membrane surfaces

The rise of infectious bacterial strains resistant to current antibiotic treatments is a growing concern universally. This has spurred an intensified interest both in the discovery and understanding of naturally occurring anti-microbial agents and the molecular mechanism by which they function. Most anti-microbial compounds associate with the cellular membrane and disrupt the delicate electro-chemical balance required for bacterial cellular life. One such naturally occurring molecule is melitin (MLT), found in the venom of honeybees. MLT posses many characteristics shared among known anti-microbial peptides. It is a single domain a-helix with a strong amphipathic quality (Fig. 1a). Structural studies from X-ray diffraction experiments [1] show partitioning into the lipid membrane of cells - intercalating with the headgroup region (Fig. 1b). Significant perturbations to the lipid chains are also observed: a thinning of the hydrocarbon region as well as a broadening of the terminal methyl distribution suggest an increase in chain disorder due to MLTs presence. At higher concentrations, MLT fully penetrates the membrane as self-assembled helical bundles that form large pores in the membrane, leading to cell death.

Detailed structural data from diffraction experiments has helped elucidate the function of MLT. However the mechanism for biological activity stems from the dynamics. We propose to use quasielastic neutron scattering (QENS) to characterize the changes in mobility of a model dioleov/phosphatidylcholine (DOPC) phospholipid membrane, in the presence of MLT. The protein:lipid system will be divided into three major components, the phospholipid headgroups, the lipid hydrocarbon tails and the MLT itself. Selective deuteration will allow us to follow the mobility of each of the three components separately. Regions of lipid that interact with MLT the most will be identified by comparison of dynamical changes with the pure DOPC bilayer measurements. Furthermore a study combining molecular dynamic (MD) simulations with neutron results on a similar system [2] suggests that regulating the mobility of phospholipid headgroups controls melting transitions. Measuring the effect on the membrane Tm provides another method for probing the balance between headgroup and chain interactions with MLT.

Previous QENS measurements of ordered lipid systems have used a combination of several dynamic models to describe motions in the ps to ns range of accessible time scales [1,3-4]. Given the sub ns dynamic range of the IRIS backscattering instrument our experiments will primarily be sensitive to methyl rotations, dihedral isomerization and localized diffusion (Fig. 2a). Despite the use of selective deuteration, the dynamical processes are still complex and may prove difficult to dissect into their individual contributions. Therefore, we will use an experimentally validated MD simulation [5] to provide a powerful method for aiding in the interpretation of QENS data, since there is total overlap in time and length scales accessed by both methods. Preliminary analysis of a DOPC/MLT simulation already provides some insights into potential perturbation in lipid dynamics caused by the peptide. Fig. 2b shows a snapshot of the simulation in which lipids within the vicinity of the protein are either highly kinked or extended. Furthermore the less mobile headgroups adjust their packing behavior around MLT. The results already suggest a possible framework for interpreting QENS data for this system.

We propose to perform experiments on the following samples:

- (1) Fully hydrogenated DOPC [hh-DOPC]
- (2) Fully hydrogenated DOPC with melittin [hh-DOPC+h-melittin]
- (3) Hydrogenated head-group DOPC [hd-DOPC]
- (4) Hydrogenated head-group DOPC with melittin [hd-DOPC+h-melittin]

The experiments proposed are presented in turn below:

(a) Elastic window scans (10-350K): elastic scans will give us a number of preliminary results. A comparison of the scans of the non-labeled lipid with and without MLT (samples 1,2), will show changes in Tm and in the dynamic regimes within the timescale of the IRIS spectrometer. Comparing head labeled with fully hydrogenated (signal dominated by tail protons) DOPC will indicate if the gel-to-fluid transition is characteristic to a specific part of the lipid (samples 1,3). Addition of the MLT to the labeled DOPC will show any differences in mobility in the presence of MLT that are specific to the individual components of the lipid (samples 2,4). Finally, mean-square displacement data for all samples will reveal changes in the mobility of all three components in the system (all samples). Elastic scans will require 3 days. (b) Dynamic runs: we propose to measure the dynamics of each of samples 3-6 at two temperatures, below and above Tm. The measurements will allow analysis of the mobility of the DOPC head and tail groups quantitatively (samples 1,3), allowing for precise assessment of their response to the addition of MLT (samples 2,4). These experiments require 4 days (assumine 12hr per temperature run based on sample quantities).

The samples will consist of multilayers of DOPC and DOPC/MLT mixtures containing 1.5 mol % MLT per mol DOPC, plated onto a series of silicon wafers. Around 15 wafers are stacked in an aluminium slab-shaped cell with the face area of the same dimensions as the neutron beam. Such a cell has already been used for experiments on the backscattering spectrometer at the NIST Center for Neutron Research. The cell is contained in a humidity chamber and the samples are kept at 66 % r.h. with a NaNO2 solution in D20. Use of D20 allows minimization of incoherent scattering from the buffer and also from the exchangeable protons in the MLT. The concentration of MLT and the humidity is chosen to match the MD simulations and diffraction experiments.

We propose to use the IRIS spectrometer with the PG002 configuration at a resolution of 8.8 ueV (HWHM) and an energy range of 1.0 meV, giving us access to timescales between ca. 0.5-100 ps. The Q-range accessible is 0.3-1.8 inv. Ang. These distances and times are directly comparable to the MD simulations. For the completion of the proposed work we are requesting a total of 7 days.

We note that this is a resubmission of RB 0720585 which was awarded 7days. Since then we have been trying to synthesize MLT and encountered some difficulties, thus we have not used our beamtime and we thought it would be better to resubmit. We now have a successful route for expressing MLT and will be ready to perform the experiment.

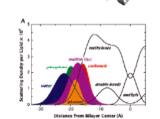


Figure 1: (a) The amphipathic MLT monomer is shown with polar residues in green, basic residues in blue and non-polar residues in grey. b) X-ray scattering length density profiles show MLT partitioning into the lipid headgroup region of a dioleov/phosphatidy/choline (DOPC) bilayer [1].

References:

K. Hristova et al, Biophysical J. 80 801 (2001).
 M. Doxastakis et al, Biophysical J. 92 147 (2007).
 S. König et al, J. Phys II France 2 1589 (1992).
 S. König et al, Biophysical J. 68 1871 (1995).
 S. R. W. Benz et al, Biophysical J. 91 3617 (2006).

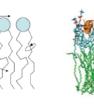


Figure 2: (a) A schematic of accessible motions on the sub ns time scale. Straight arrows represent localized mobility and circular arrows represent localized isomerization or terminal methyl rotation. (b) Snapshot of a DOPC/MLT MD simulation. Perturbation to lipid tail conformation and packing defects in lipid headgroups are evident.

Do's and Don't's'

- ✓ Use all space allocated
- ✓ Add readable
 figures/graphs
- ✓ Justify need for neutrons
- ✓ Add references
- ✓ Check before submission

- ★ Use miniture font
- Include if they do not add to proposal
- ✗ Use generic arguments
- **×** Expect reviewer to read
- **×** Make silly mistakes

Proposal Submission

- Online
- Read guidelines for given facility system
- Follow instructions carefully
- Meet the deadline (don't play tricks!)



Guidelines for the scientific background and detailed description of the proposed experiment

(For electronic proposal submission only)

Please remove this first page before creating your post-script file

The two pages of this form are to be filled in by all users or groups of users who apply for beamtime for experiments at the ILL via the Internet. Please print pages two and three of this document into a postscript file and attach it to your proposal on the Electronic **P**roposal **S**ystem. This two-page description will be reduced by the system to a one-page, A4 format in black & white, and will be attached to your web proposal.

When preparing your description, please follow the instructions below:

- Give a brief statement of the **background** and the general importance of the research.
- Give a clear account of the **aims of the proposed experiment** and a detailed description of the experiment; keep in mind that not all of the subcommittee members are experts in the field.



Proposal Review Process

• Panel review

- By technique or by science area
- At least 2 reviewers per proposal
- Panel review meeting at the facility



@ the ILL (France)

College 1	Applied materials science, instrumentation and techniques
College 2	Theory
College 3	Nuclear and Particle Physics
College 4	Magnetic Excitations
College 5	Crystallography
College 6	Magnetism
College 7	Structure and dynamics of liquids and solids
College 8	Structure and dynamics of biological systems
College 9	Structure and dynamics of soft-condensed matter

@ the SNS-HFIR (USA)

-	
Subcommittee 1	Engineering and Materials
Subcommittee 2	Imaging
Subcommittee 3	Triple Axis
Subcommittee 4	Time of flight
Subcommittee 5	Low Q reflectometry
Subcommittee 6	Low Q SANS
Subcommittee 7	Single crystal diffraction
Subcommittee 8	Powder diffraction
Subcommittee 9	Disordered Materials
Subcommittee 10	Low Energy/Chemical Spectroscopy

Proposal Review Process

- Proposal is given a rating (eg. 1 to 5 in steps of 0.5)
- Typical marking definitions (NCNR, NIST)
 - 5 = E = Excellent proposal. Experiment must be carried out. Highest priority for beamtime.
 - 4 = VG = Very good proposal. Experiment is highly deserving of beamtime. No reason to deny beamtime except under conditions of unusually high demand.
 - 3 = G = Good proposal. May receive beamtime under normal circumstances, but may not, depending on demand.
 - 2 = F = Fair proposal. While scientific merit does not appear to be exceptionally high, the experiment may receive beamtime if its is available, but will probably not receive time
 - 1 = P = Poor proposal. Scientific merit not convincingly docmented. Beamtime should not be allocated to the proposal.

Success ...

... depends on many factors:

- Quality of proposal
- Days available
- Oversubscription
- Committee's feeling about high risk-high reward proposal versus unexciting but definite publication
- Mood, tiredness...
- Country balances
- ...



Neutron Proposal Exercise ...

- In pairs
- Use proposal template in your packs (1 per pair)
- To be filled in with pen/pencil, no printers
- One experiment would be ideal if you can somehow merge work
- Deadline is 5pm on Wednesday 13th
- Panel meeting will take place on the afternoon of Thursday 14th

Proposal Pairs

Pair No.	Student A	Student B	Student C
1	Alexander Hawkins	Chao-Lung Chiang	Jack Parsons
2	Alexandra Turrini	Heather Mutch	
3	Anabel Pérez Checa	Giordano Benacchio	
4	Guratinder Kaur	Richard Waite	
5	Gavin Irvine	Michael Barter	
6	Fenfen Chang	Oliver Paull	
7	Maria Vanina Chiarpotti	Alicia Ruiz Caridad	
8	Hyeyoung Kim	Meng-Hsuan Hsieh	
9	Lauren Cane	Xiaoyu Xu	
10	Ana Catarina Araujo	Lawrence Gammond	
11	Mario Valvo	Jack Kan	
12	Ka Hou (Jacky) Hong	Philip Welch	
13	Brinda Vyas	Andrés Martín Cid	
14	Karthika Chandran	Virgile Favre	
15	Cristina Castro Vargas	Jhuma Sannighahi	
16	Belinda Dewi	Bei Tian	
17	Fu Song	Sarah O'Sullivan	
18	Giuseppe Paladini	Minhao Yu	
19	Haiyan He	Kai-chi Lo	
20	Johannes Nicol	Jianbo Gao	
21	Purushottam Shashikumar	Juan Mora Cardozo	
22	Oleksandr Zagorodko	Oliver Hedge	
23	Michaela Buscemi	Gregory Moody	Maxim Podlesnyi
24	Sophie Ayscough	Sebastian Köhler	Benjamin Thomas
25	Yifan Quan	Gino Casella	