How to get Neutron Beamtime:

*Writing a Successful Neutron Proposal*

Victoria Garcia Sakai
Idea & Research problem

+ sample

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?
Before writing a proposal

• Literature review on similar experiments
Before writing a proposal

• Literature review on similar experiments
• Talk to colleagues
Before writing a proposal

• 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  [http://neutronsources.org/](http://neutronsources.org/)

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)
Before writing a proposal

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


Before writing a proposal

• 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
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)
Before writing a proposal

- 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?
Before writing a proposal

- 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?
Before writing a proposal

• 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 PI’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.
Proposal Ingredients (Part I)

• 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...
NIST Center for Neutron Research
Proposal for Neutron Beam Experiment

Submission ID: 13104  Proposal Number: E23-19

**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

**Estimated Duration:** 6 days

**Participants**

<table>
<thead>
<tr>
<th>Name</th>
<th>Affiliation</th>
<th>Country</th>
<th>Telephone</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td>Principal Investigator</td>
<td>National Institute of Standards and Technology</td>
<td>United States</td>
<td>0000000000</td>
<td><a href="mailto:vicente.garcia-villegas@nist.gov">vicente.garcia-villegas@nist.gov</a></td>
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<tr>
<td>User 1</td>
<td>National Institute of Standards and Technology</td>
<td>United States</td>
<td>0000000000</td>
<td><a href="mailto:user1@nationalinst.gov">user1@nationalinst.gov</a></td>
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**Instrument**

<table>
<thead>
<tr>
<th>Instrument Requested</th>
<th>NIST - Neutron Beam Instrument Center (NBIC)</th>
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<tbody>
<tr>
<td>Suggested Contact</td>
<td>Antonio Ponce</td>
</tr>
<tr>
<td>Instrument Resolution</td>
<td>Default instrument configuration</td>
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**Sample Description**

<table>
<thead>
<tr>
<th>Sample</th>
<th>Name</th>
<th>Chemical Formula</th>
<th>Mass (grams)</th>
<th>Form</th>
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</thead>
<tbody>
<tr>
<td>Sample 1</td>
<td>DPPC/D2O/maltose</td>
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<td>Liquid</td>
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**Sample Environment**

<table>
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<tr>
<th>Temperature Measurement Range (K)</th>
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<tr>
<td>Number of Runs</td>
<td></td>
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<tr>
<td>Total Collection Time (hrs)</td>
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</tr>
<tr>
<td>Sample Availability</td>
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**Sample info**

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<tr>
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<th>Name</th>
<th>Chemical Formula</th>
<th>Mass (grams)</th>
<th>Form</th>
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<tbody>
<tr>
<td></td>
<td>DPPC/D2O/sucrose</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

**Sample Environment Equipment:**

**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:

<table>
<thead>
<tr>
<th>Research Area</th>
<th>Biomolecular Science</th>
</tr>
</thead>
<tbody>
<tr>
<td>Funding Agency</td>
<td>NRC and STFC UK</td>
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</table>

**Publications**
Proposal Ingredients (Part II)

Two-page description of proposed research (incl. references)
Proposal Ingredients (Part II)

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?
Proposal Ingredients (Part II)

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?*
- Clear justification of need for neutrons and particular instrument- *why do you need beamtime on X?*
Proposal Ingredients (Part II)

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?**
- Clear justification of need for neutrons and particular instrument- **why do you need beamtime on X?**
- Description of preliminary characterisation or work on the sample/system- **do you understand your sample?**
Proposal Ingredients (Part II)

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?
- Clear justification of need for neutrons and particular instrument- why do you need beamtime on X?
- Description of preliminary characterisation or work on the sample/system- do you understand your sample?
- Aims of the experiment- What and how are you going to measure, and is the time requested justified?
Proposal Ingredients (Part II)

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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• Description of preliminary characterisation or work on the sample/system- do you understand your sample?
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• Description of data analysis/modelling – What will you do with the data?
Proposal Ingredients (Part II)

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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• Evidence team’s productivity and experience – **Will they publish in a timely manner?**
Proposal Ingredients (Part II)

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?**
- Clear justification of need for neutrons and particular instrument- **why do you need beamtime on X?**
- Description of preliminary characterisation or work on the sample/system- **do you understand your sample?**
- Aims of the experiment- **What and how are you going to measure, and is the time requested justified?**
- 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

SUBMISSION OF A PROPOSAL

Experiment Title

Proposer
Name
Email
Affiliation
Co-Proposers

Scientific background and detailed description of the proposed experiment

Abstract (~100 words)

Introduction

Reference

Previous results

(a) before shaking
(b) after shaking

50 µm

Q (Å⁻¹)

Aim of proposed work

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
3) The measured spatial domain: Q = 0.003 Å⁻¹ to 0.3 Å⁻¹
4) Sample: (i) D₂O / 3-methylpyridine / NaBH₄
   (ii) D₂O / CsCl
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 x 10 (shear rate) x 2 (samples) x 1 (temperature) = 15 hours. Additionally, we need 8 hours for setting rheo-meter and changing the detector length. Therefore, 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.
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 increased interest both in the discovery and understanding of naturally occurring antimicrobial agents and the molecular mechanism by which they function. Most antimicrobial compounds associate with the cellular membrane and disrupt the delicate electrochemical balance required for bacterial cellular life. One such naturally occurring molecule is melittin (MLT), found in the venom of honeybees. MLT possesses many characteristics shared among known antimicrobial peptides. It is a single domain entity with a strong amphipathic character (Fig. 1a). Structural studies from X-ray diffraction experiments [1] show partitioning into the lipid membrane of cells - interacting 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 MLT's presence. At higher concentrations, MLT fully generates the membrane as self-assembled hexagonal 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 quasistatic neutron scattering (GENS) to characterize the changes in mobility of a model dioleoylphosphatidylcholine (DOPC) phospholipid membrane, in the presence of MLT. The proteolipid 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's Tm provides another method for probing the balance between headgroup and chain interactions with MLT.

Previous GENS measurements of ordered lipid systems have used a combination of several dynamical methods to describe motions in the ps to ns range of accessible time scales [3–4]. Given the sub-nanosecond range of the IRIS backscattering experiments, our sample will primarily be sensitive to motional reorientations, chain 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 GENS 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 linked or extended. Furthermore, the less mobile headgroups adjust their packing behavior around MLT. The results already suggest a possible framework for interpreting GENS data for this system.

We propose to perform experiments on the following samples:

1. Fully hydrogenated DOPC (h-DOPC)
2. Fully hydrogenated DOPC with melittin (h-DOPC+melittin)
3. Hydrogenated headgroup DOPC (h-DOPC)
4. Hydrogenated headgroup DOPC with melittin (h-DOPC+melittin)

The experiments proposed are presented in turn below:

(a) Elastic window scans (10–98 MeV) 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) changes in Tm and in the dynamic regimes within the timescale of the IRIS spectrometer. Comparing lipid labeled with fully hydrogenated [signal dominated by tail proteins] DOPC will indicate if the gel-to-fluid transition is specific 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.

References:
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!)

INSTITUT MAX VON LAUE - PAUL LANGEVIN (ILL)

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 Proposal System. 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)

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<th>Focus Area</th>
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<td>College 1</td>
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<tr>
<td>College 2</td>
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<tr>
<td>College 3</td>
<td>Nuclear and Particle Physics</td>
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<td>College 4</td>
<td>Magnetic Excitations</td>
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<td>College 6</td>
<td>Magnetism</td>
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<tr>
<td>College 7</td>
<td>Structure and dynamics of liquids and solids</td>
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<tr>
<td>College 8</td>
<td>Structure and dynamics of biological systems</td>
</tr>
<tr>
<td>College 9</td>
<td>Structure and dynamics of soft-condensed matter</td>
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@ the SNS-HFIR (USA)

<table>
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<th>Focus Area</th>
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<tbody>
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<td>Subcommittee 9</td>
<td>Disordered Materials</td>
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<td>Subcommittee 10</td>
<td>Low Energy/Chemical Spectroscopy</td>
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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 documented. 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
<table>
<thead>
<tr>
<th>Pair No.</th>
<th>Student A</th>
<th>Student B</th>
<th>Student C</th>
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<tbody>
<tr>
<td>1</td>
<td>Alexander Hawkins</td>
<td>Chao-Lung Chiang</td>
<td>Jack Parsons</td>
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<td>2</td>
<td>Alexandra Turrini</td>
<td>Heather Mutch</td>
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<td>4</td>
<td>Guratinder Kaur</td>
<td>Richard Waite</td>
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<td>5</td>
<td>Gavin Irvine</td>
<td>Michael Barter</td>
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<td>Fenfen Chang</td>
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<td>Lauren Cane</td>
<td>Xiaoyu Xu</td>
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<td>Ana Catarina Araujo</td>
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<td>11</td>
<td>Mario Valvo</td>
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<td>12</td>
<td>Ka Hou (Jacky) Hong</td>
<td>Philip Welch</td>
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<td>13</td>
<td>Brinda Vyas</td>
<td>Andrés Martín Cid</td>
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<td>Karthika Chandran</td>
<td>Virgile Favre</td>
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<td>Cristina Castro Vargas</td>
<td>Jhuma Sannighahi</td>
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<td>16</td>
<td>Belinda Dewi</td>
<td>Bei Tian</td>
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<td>17</td>
<td>Fu Song</td>
<td>Sarah O’Sullivan</td>
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<td>18</td>
<td>Giuseppe Paladini</td>
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<td>Haiyan He</td>
<td>Kai-chi Lo</td>
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<td>Johannes Nicol</td>
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<td>Purushottam Shashikumar</td>
<td>Juan Mora Cardozo</td>
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<td>Oleksandr Zagorodko</td>
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<td>23</td>
<td>Michaela Buscemi</td>
<td>Gregory Moody</td>
<td>Maxim Podlesnyi</td>
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<td>Sophie Ayscough</td>
<td>Sebastian Köhler</td>
<td>Benjamin Thomas</td>
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<td>Yifan Quan</td>
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