Neutron Scattering and Muon Spectroscopy Integrated Infrastructure Initiative (II): February 2012 – 2016

Created in 2003 – FP6 funding

NMI3-I funded by FP7 (9.9 M€ for February 2009 – 2013)

NMI3-II funded by FP7 (13.35 M€)

Trans National Access (6.7 M€)

Networking Activities (1.8 M€)

Joint Research Activities (4.2 M€)

18 partners from 11 countries

10 produce neutrons and muons at 8 facilities (from France, UK, Germany, Switzerland, Hungary, Czech Rep, Netherlands)

8 'non-producing' partners (from Spain, Italy, Denmark, Sweden)

Objectives of project

Networking/Coordination Activities (Juergen Neuhaus)

- "To further develop the culture of co-operation between NMI3 partners, in particular in the areas of training and outreach"

- Management – ***inc. industry events*** (WP1)
- Dissemination (WP2)
- E-learning (WP3)
- Education – Umbrella of 14 supported schools (WP4)
- ***Integrated user access*** (WP5)
- ***Data analysis software*** (WP6)

Objectives of project

Joint Research Activities (JRAs)

- "To respond to new challenges in instrumentation and methods via focussed joint research collaborations"

- New topics:
  - ***Imaging*** (RTD, WP18: Nikolay Kardjilov, HZB)
  - ***Advanced Methods and Techniques*** (RTD, WP19: Phil Bentley, ESS → Javier Campo, ICMA)
  - ***Advanced tools for Soft and Biomaterials*** (RTD, WP20: Annie Brulet, LLB)
- Continuing topics:
  - ***Muons*** (RTD, WP17: Steve Cottrell, ISIS)
  - ***Detectors*** (RTD, WP21: Nigel Rhodes, ISIS)

NMI3-II

The Transnational Access Programme:

a success story for more than 20 years

Stefan Janssen
Paul Scherrer Institute
Villigen, Switzerland

What is the Transnational Access Programme?

User facilities (e.g. neutron, muon, synchrotron, ... facilities) **provide beamtime** (access) to users from foreign countries (**transnational**)

Those users are **supported by Travel and Subsistence (T&S)** by the access programme

Beam time allocation is based on hard (**scientific excellence**) and soft (new user groups, Ph.D. students, users from countries without national source, ...) criteria

Facilities get **reimbursed by beam fees** (user fees) through the access programme and are free how to use that money (e.g. for hiring instrument scientists to **support the user programme**, buying sample environment equipment etc)

Access programme – member facilities

6.7 M€

10 facilities

- 8 neutron sources
- 2 muon sources

10 institutions

Overview – NMI3-II access data

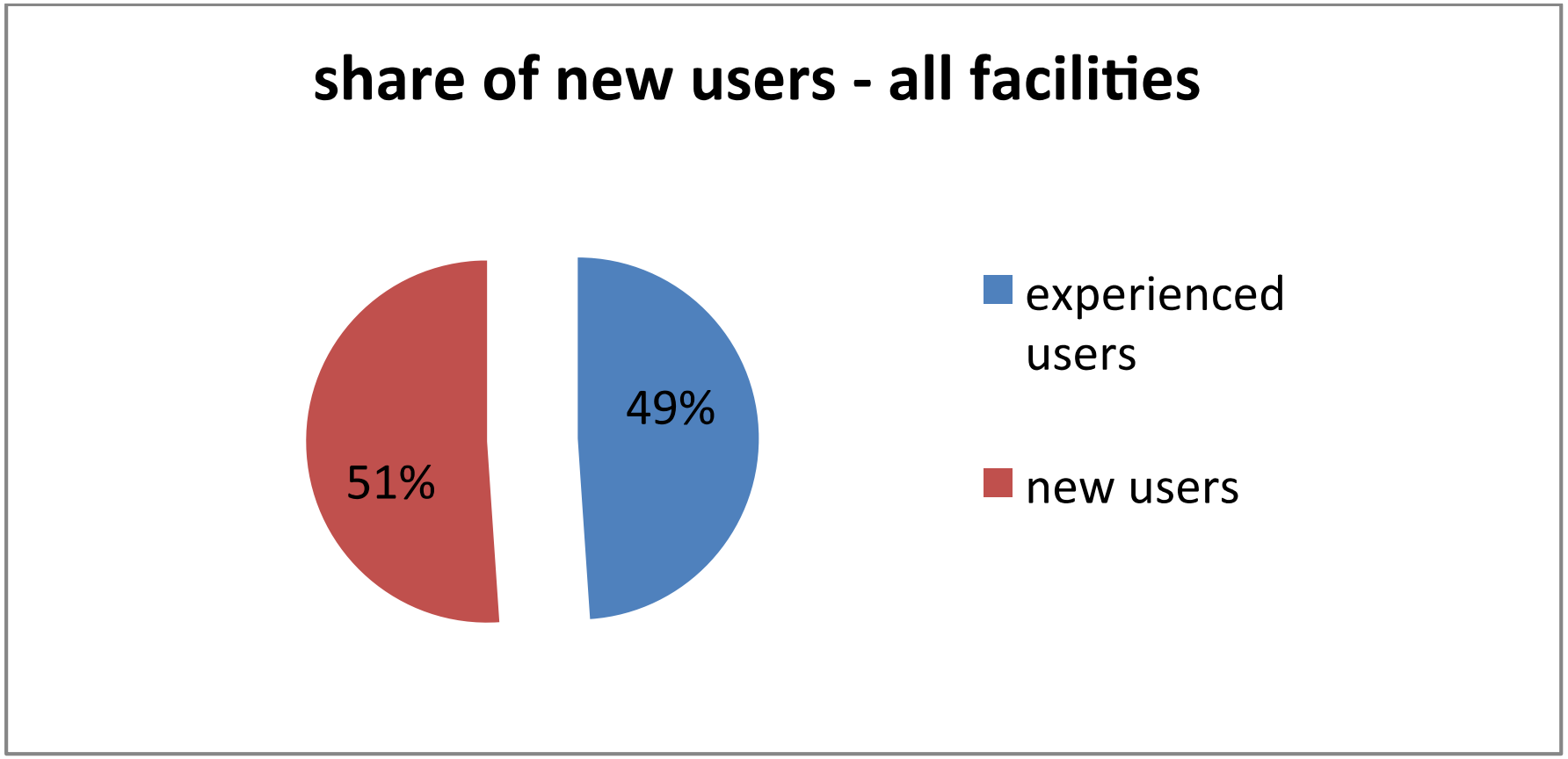
Parti-cipant number	Organisation short name	Short name of infrastructure	Operator country code	Min quantity of access to be provided	Estimated unit cost (€)	Fraction of unit cost charged to EC project	Estimated total quantity of access to be provided over project period	Estimated Access cost	Estimated number of experiment	Estimated number of users
2	**STFC**	ISIS Neutrons	UK	68	15865.75	100%	11004	1 078 871	64	125
2	**STFC**	ISIS Muons	UK	14	15865.75	100%	11004	222 121	13	26
3	**TUM**	FRM II	DE	462	3300	48.1%	21120	1 524 600	120	215
5	**PSI**	SINQ	CH	262	2897	52.5%	6750	759 014	80	110
5	**PSI**	SμS	CH	123	2898.72	63.2%	2700	356 543	50	65
6	**HZB**	BER II	DE	300	2493.54	56.7%	19800	748 062	75	150
7	**CEA**	LLB	FR	271	3352.94	70%	16560	908 647	54	92
9	**MTA EK**	BRR	HU	150	1599.29	55%	1800	239 894	32	45
12	**TUD**	RID	NL	90	2013	89%	6400	181 176	10	20
13	**NPI**	NPI	CZ	92	1203.66	100%	2688	110 737	10	17

Minimum: 1800 days **500 expts 850 users**

Overview – delivered days – PR1 (37% of duration):

	eligible user projects	funded projects	beam days	% delivered
STFC Neutrons	167	32	32	**47.1**
STFC Muons	27	6	6	**42.9**
TUM	107	107	515	**111.5**
PSI Neutrons	331	59	276	**105.3**
PSI Muons	160	26	89	**72.4**
HZB	175	71	517	**172.3**
CEA	19	19	105	**38.7**
MTA EK	38	21	112	**74.7**
TUD	14	10	75	**82.9**
NPI	10	6	61	**66.3**
Total	**1048**	**357**	**1788**	

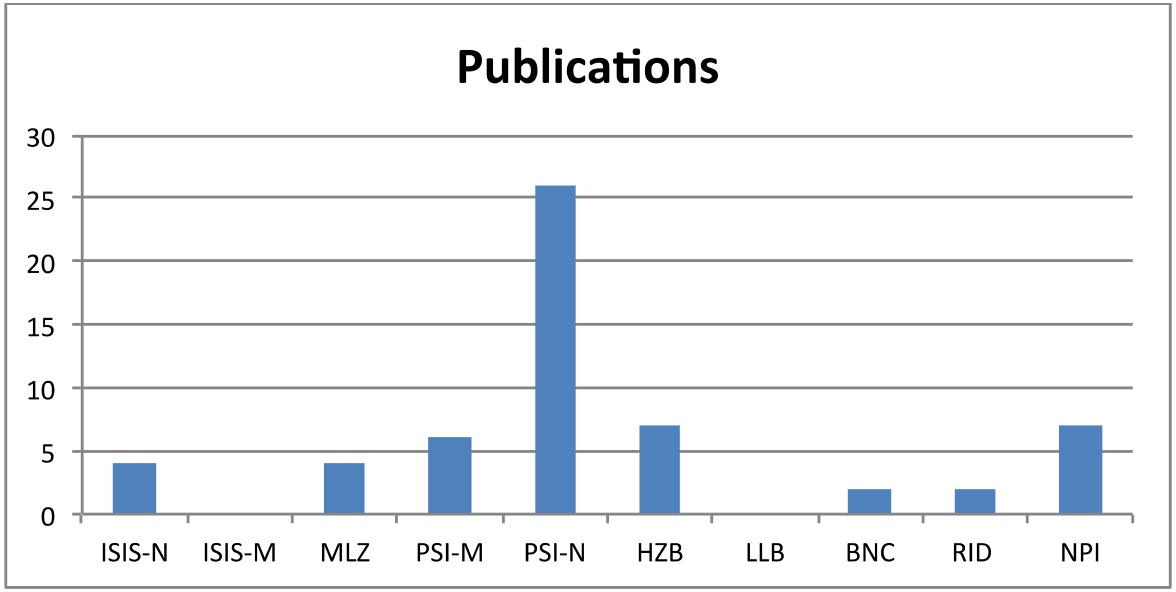
The access programme attracts many new neutron/muon users



Scientific output: publications

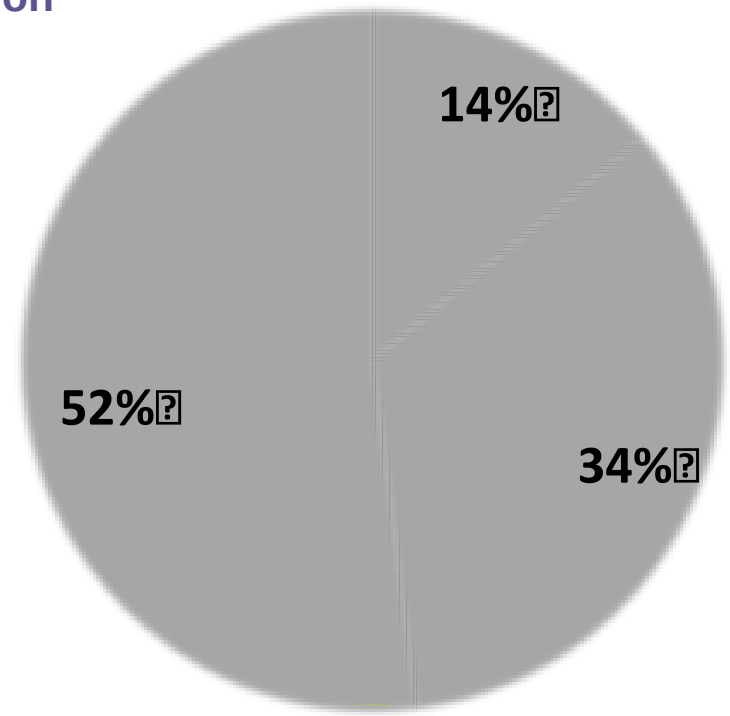
PR1:

- 854 eligible proposals,
  380 selected for funding (44%)
- 50 publications based on NMI3 funded experiments have already appeared



Impact of publications:

- Angew. Chemie – Int. Edition
- Physical Review Letters
- New Phytologist
- Soft Matter
- Langmuir
- Inorganic Chemistry
- J. Applied Cryst.
- Appl. Physics Letters
- Physical Review B
- .....



win – win situation for:

the users:

they can perform their experiments at world class facilities and get the best possible results

the facilities:

they get partly re-imbursed for their immense operation costs (20 – 50 M€/year)

the EC:

the access programme helps the EC to meet the **Grand Challenges** by hundreds of publications

NMI3-II

Integrated User Access – WP5

Stefan Janssen
Paul Scherrer Institute
Villigen, Switzerland

Integrated User Access – what is it about?

Work package number	5		Start date or starting event:							M0
Work package title	Integrated User Access									
Activity Type	COORD									
Participant number	6	3	9	8	4	1	2	7	13	5	12
Participant short name	HZB	TUM	BNC-AEKI	HZG	Jülich	ILL	STFC	CEA	NPI	PSI	TUD
Person-months per participant (total incl. own contribution):	8	48	4	8	4	4	4	8	2	4	2

11 partner facilities

- mainly user offices -

In order to structure and harmonize an integrated access format to European national neutron and muon facilities for the scientific users an 'Integrated User Access (IUA)' Networking Activity should consider and develop

- **strategies and forms for a common integrated user registration (prototype)**
- **harmonized proposal forms and templates**
- **optimized peer review processes and**
- **possible platforms for cross source beam time access**

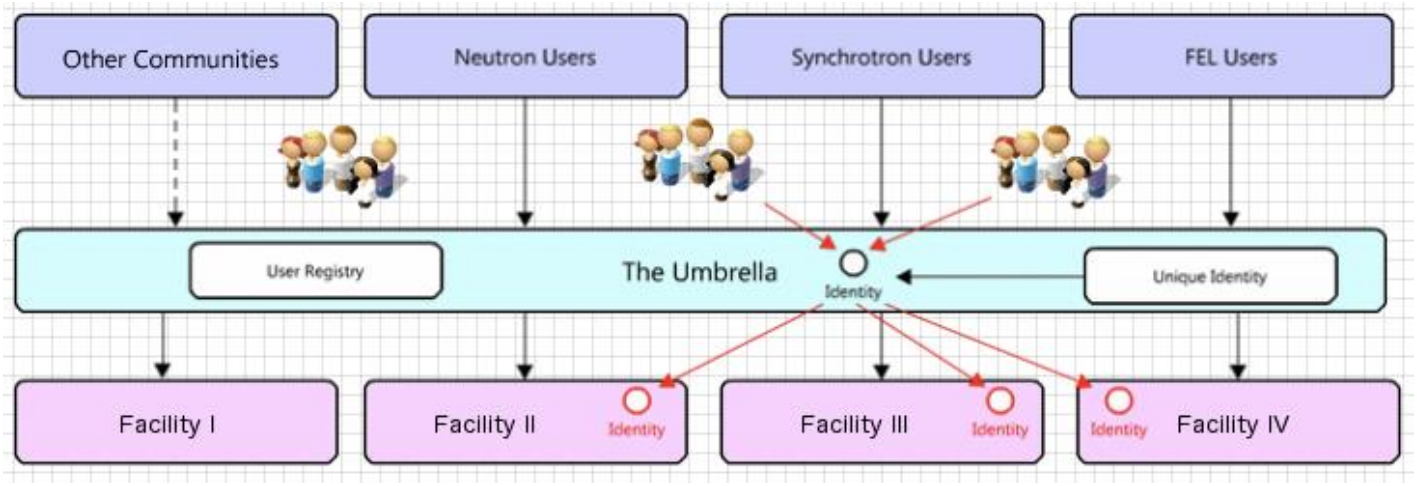
In addition, better statistical survey on European user access could be possible.

strategies and forms for a common integrated user registration (prototype)

Umbrella is the pan-European federated identity system for the users of the European large photon / neutron / muon facilities. Such a kind of an IT platform is offered to this community for the first time:

- EU wide unique, persistent ID
- community overlapping
- commonly developed within several EU Projects (PanData, CRISP, EuroFEL, NMI3, BioStruct-X,...

umbrella

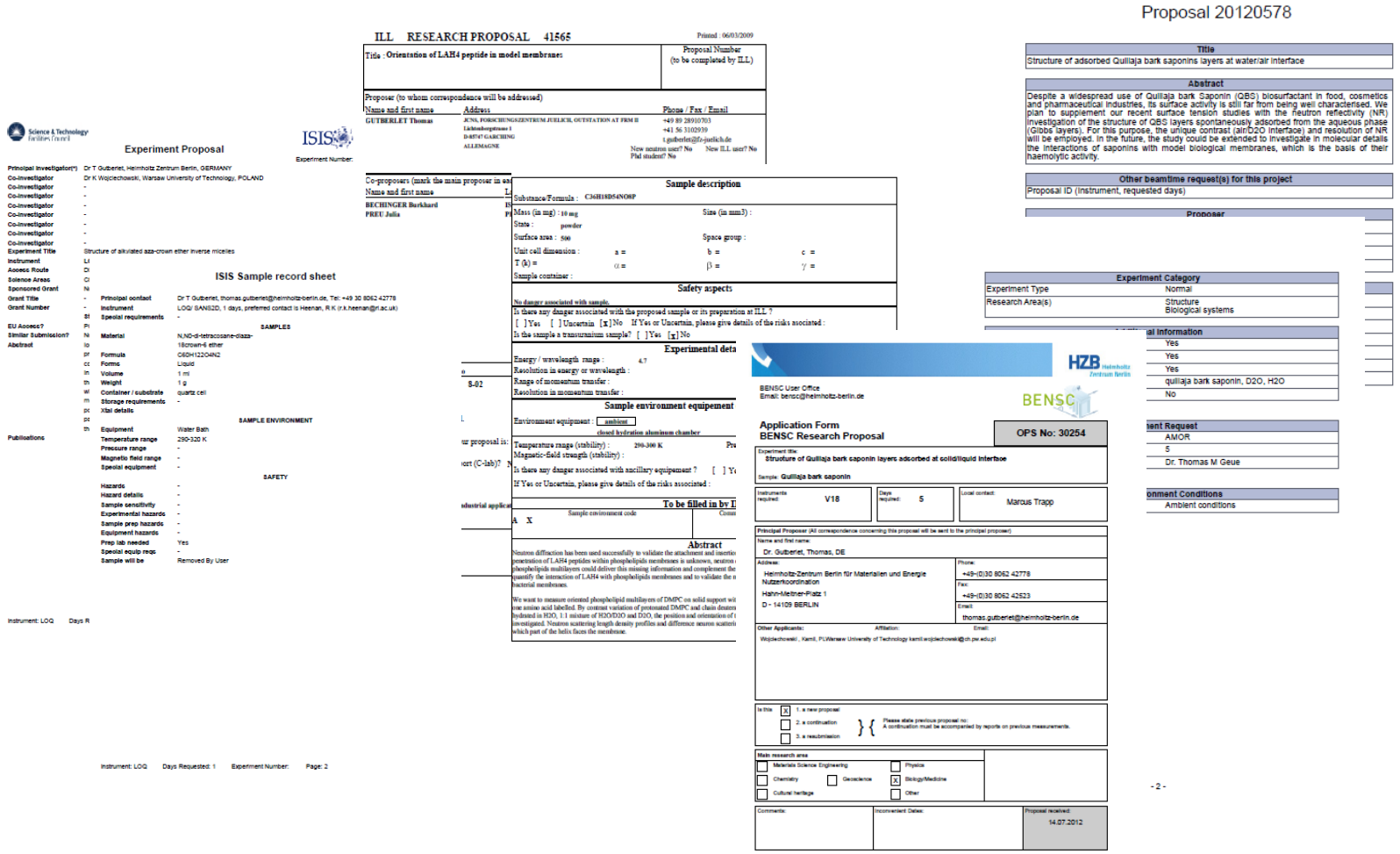


Harmonized proposal forms

- **Forms and templates** of proposal submissions at existing DUO applications **will be compared.**

- **Harmonized proposal template** adopted for the individual requirements **will be proposed** and prepared for implementation.

Harmonized proposal forms



Science & Technology Facilities Council

Experiment Proposal

ISIS

Experiment Number:

Principal Investigator(*) Dr T Gutberlet, Helmholtz Zentrum Berlin, GERMANY

Co-Investigator Dr K Wojciechowski, Warsaw University of Technology, POLAND

Co-Investigator -

Co-Investigator -

Co-Investigator -

Co-Investigator -

Co-Investigator -

Co-Investigator -

Experiment Title Structure of alkylated aza-crown ether inverse micelles

Instrument LI

Access Route DI

Science Areas CI

Sponsored Grant Nu

Grant Title -

Grant Number -

EU Access?

Similar Submission?

Abstract

Publications

ISIS Sample record sheet

Principal contact Dr T Gutberlet, thomas.gutberlet@helmholtz-berlin.de, Tel: +49 30 8062 42778

Instrument LOQ/ SANS2D, 1 days, preferred contact is Heenan, R K (r.k.heenan@rl.ac.uk)

Special requirements -

SAMPLES

Material N,N-di-tetracosane-diaza-18crown-6 ether

Formula C60H122O4N2

Forms Liquid

Volume 1 ml

Weight 1 g

Container / substrate quartz cell

Storage requirements -

Xtal details

SAMPLE ENVIRONMENT

Equipment Water Bath

Temperature range 290-320 K

Pressure range -

Magnetic field range -

Special equipment -

SAFETY

Hazards -

Hazard details -

Sample sensitivity -

Experimental hazards -

Sample prep hazards -

Equipment hazards -

Prep lab needed Yes

Special equip req -

Sample will be Removed By User

Instrument: LOQ Days R

Instrument: LOQ Days Requested: 1 Experiment Number: Page: 2

ILL RESEARCH PROPOSAL 41565

Printed : 06/03/2009

Title : Orientation of LAH4 peptide in model membranes

Proposal Number (to be completed by ILL)

Proposer (to whom correspondence will be addressed)

Name and first name | Address | Phone / Fax / Email

GUTBERLET Thomas | JCNS, FORSCHUNGSZENTRUM JUELICH, OUTSTATION AT FRM II, Lichtenbergstrasse 1, D-85747 GARCHING, ALLEMAGNE | +49 89 28910703, +41 56 3102939, t.gutberlet@fz-juelich.de

New neutron user? No New ILL user? No Phd student? No

Co-proposers (mark the main proposer in ea

Name and first name

BECHINGER Burkhard

PREU Julia

Sample description

Substance/Formula : C36H18D54NO8P

Mass (in mg) : 10 mg Size (in mm3) :

State : powder

Surface area : 500 Space group :

Unit cell dimension : a = b = c =

T (k) = α = β = γ =

Sample container :

Safety aspects

No danger associated with sample.

Is there any danger associated with the proposed sample or its preparation at ILL ?

[ ]Yes [ ]Uncertain [x]No If Yes or Uncertain, please give details of the risks asociated :

Is the sample a transuranium sample? [ ]Yes [x]No

Experimental deta

Energy / wavelength range : 4.7

Resolution in energy or wavelength :

Range of momentum transfer :

Resolution in momentum transfer :

Sample environment equipement

Environment equipement : ambient

closed hydration aluminum chamber

Temperature range (stability) : 290-300 K

Magnetic-field strength (stability) :

Is there any danger associated with ancillary equipement ? [ ] Y

If Yes or Uncertain, please give details of the risks associated :

To be filled in by I

Sample environment code

A X

Abstract

Neutron diffraction has been used successfully to validate the attachment and insertio penetration of LAH4 peptides within phospholipids membranes is unknown, neutron phospholipids multilayers could deliver this missing information and complement the quantify the interaction of LAH4 with phospholipids membranes and to validate the bacterial membranes.

We want to measure oriented phospholipid multilayers of DMPC on solid support wit row amino acid labelled. By contrast variation of protonated DMPC and chain deuter hydrated in H2O, 1:1 mixture of H2O/D2O and D2O, the position and orientation of investigated. Neutron scattering length density profiles and difference neuron scatteri which part of the helix faces the membrane.

Proposal 20120578

Title

Structure of adsorbed Quillaja bark saponins layers at water/air interface

Abstract

Despite a widespread use of Quillaja bark Saponin (QBS) biosurfactant in food, cosmetics and pharmaceutical industries, its surface activity is still far from being well characterised. We plan to supplement our recent surface tension studies with the neutron reflectivity (NR) investigation of the structure of QBS layers spontaneously adsorbed from the aqueous phase (Gibbs layers). For this purpose, the unique contrast (air/D2O interface) and resolution of NR will be employed. In the future, the study could be extended to investigate in molecular details the interactions of saponins with model biological membranes, which is the basis of their haemolytic activity.

Other beamtime request(s) for this project

Proposal ID (Instrument, requested days)

Proposer

Experiment Category

Experiment Type Normal

Research Area(s) Structure, Biological systems

al information

Yes

Yes

Yes

quillaja bark saponin, D2O, H2O

No

ent Request

AMOR

5

Dr. Thomas M Geue

onment Conditions

Ambient conditions

HZB Helmholtz Zentrum Berlin

BENSC User Office

Email: bensc@helmholtz-berlin.de

BENSC

Application Form

BENSC Research Proposal

OPS No: 30254

Experiment title: Structure of Quillaja bark saponin layers adsorbed at solid/liquid interface

Sample: Quillaja bark saponin

Instruments required: V18

Days required: 5

Local contact: Marcus Trapp

Principal Proposer (All correspondence concerning this proposal will be sent to the principal proposer)

Name and first name: Dr. Gutberlet, Thomas, DE

Address: Helmholtz-Zentrum Berlin für Materialien und Energie, Nutzerkoordination, Hahn-Meitner-Platz 1, D - 14109 BERLIN

Phone: +49-(0)30 8062 42778

Fax: +49-(0)30 8062 42523

Email: thomas.gutberlet@helmholtz-berlin.de

Other Applicants: Affiliation: Email:

Wojciechowski , Kamil, PLWarsaw University of Technology kamil.wojciechowski@ch.pw.edu.pl

Is this [X] 1. a new proposal, [ ] 2. a continuation, [ ] 3. a resubmission

Please state previous proposal no:

A continuation must be accompanied by reports on previous measurements.

Main research area

[ ] Materials Science Engineering [ ] Physics

[ ] Chemistry [ ] Geoscience [X] Biology/Medicine

[ ] Cultural heritage [ ] Other

Comments: Inconvenient Dates: Proposal received: 14.07.2012

- 2 -

Harmonized proposal forms – 3 parts

General Part

Proposer
Prename
Surname
Nationality
Gender
Institution
Department
Street
ZIP
Town
Phone
Fax
e-mail
Organisation
Status

Technical Part

Instrument
Wavelength
Polarization
excitation energy
energy resolution
momentum transfer ra
momentum transfer re
temperature range
temperature stability
pressure range
field range
field homogeneity
sample environment
on-site lab use

Scientific Part

Scientific description
abstract/summary
scientific context/background
necessity of neutron use
choice of instrument
preliminary work
detailed experimental plan
publication record

requirements
can/mounting device
le
associated
after experiment

Possible platforms for cross source beam time access

- **Idea:** one proposal asks for **beamtime at several facilities**, e.g. neutrons and photons
- Various models have been **evaluated and discussed**
- Works where single centres have N and X, also ILL & ESRF for SAS

NMI3-II

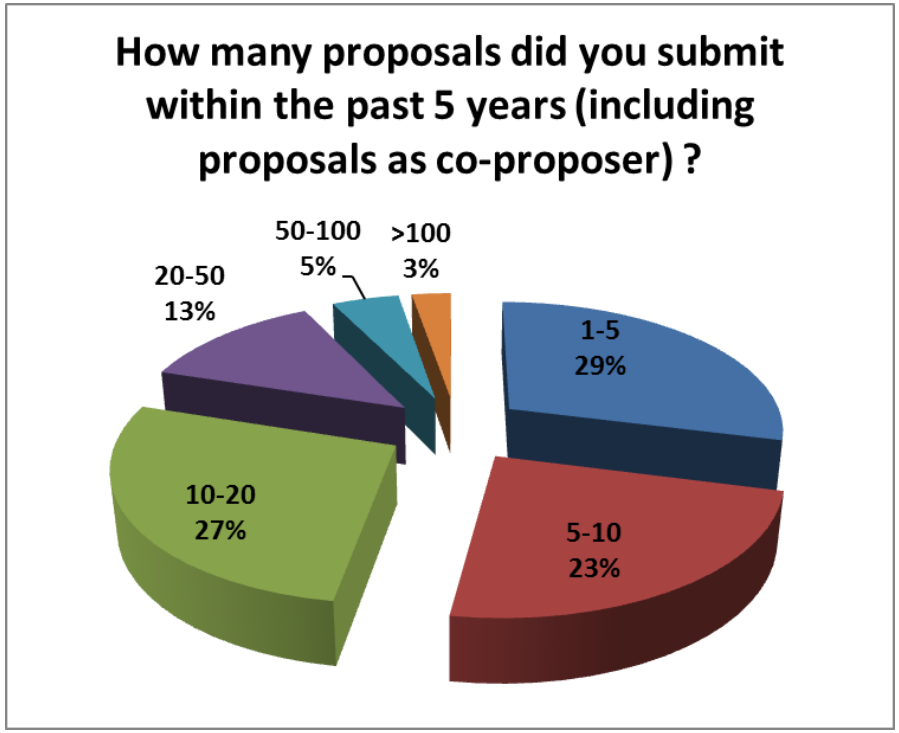
User survey -

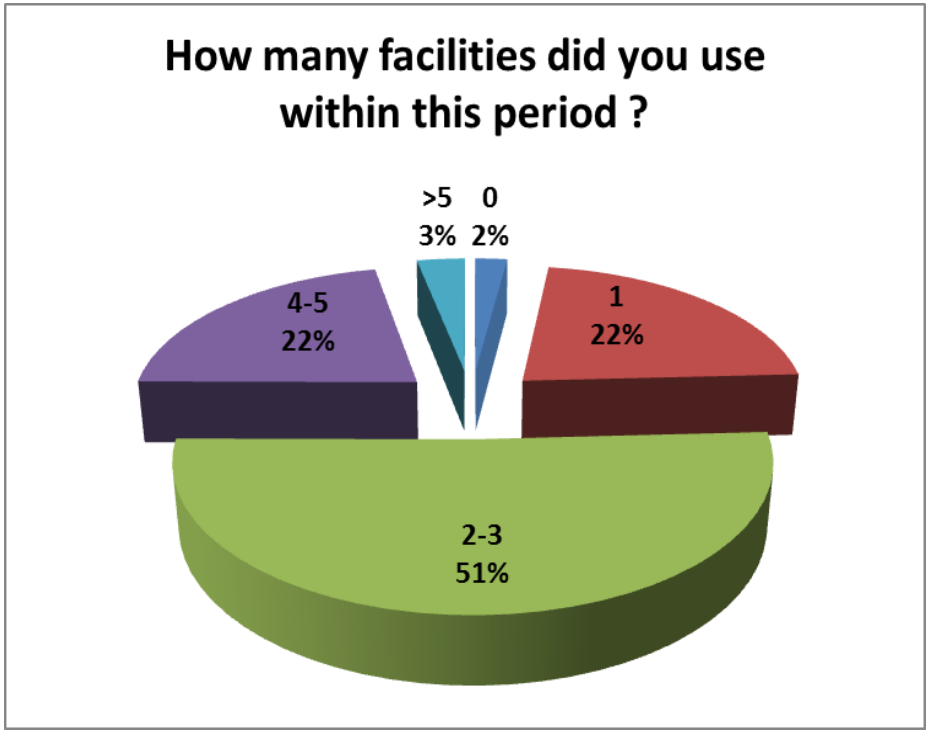
Where the users are and what the users do:
A survey on users of European neutron/muon facilities

T. Gutberlet, S. Janssen
Neutron News **25**, 43 (2014)

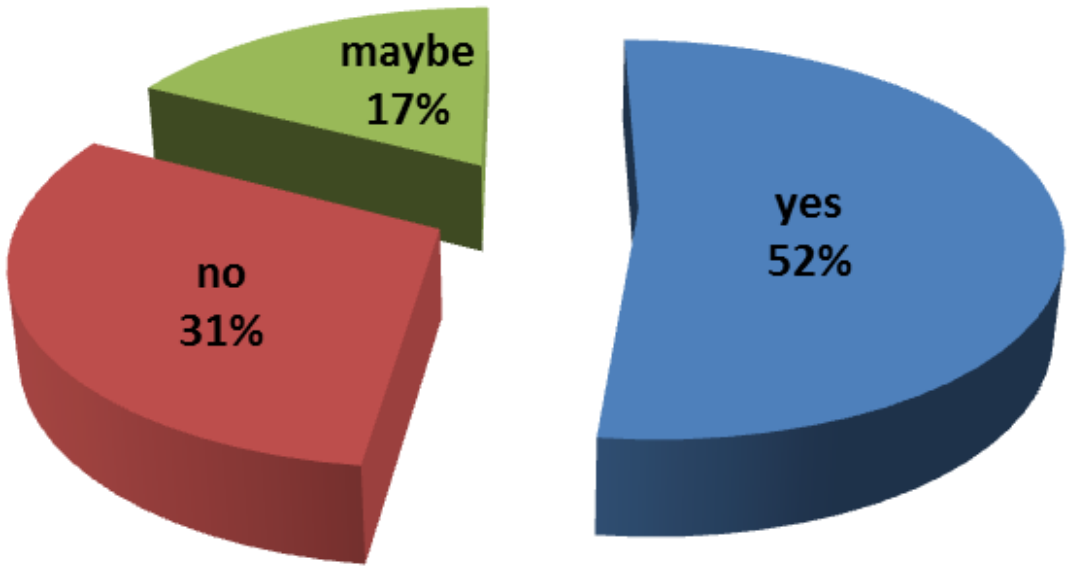
doi: 10.1080/10448632.2014.870805

Where the users are and what the users do:
A survey on users of European neutron/muon facilities

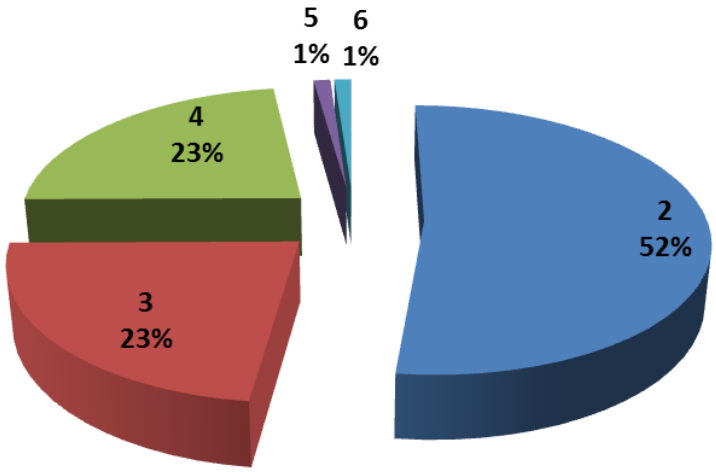




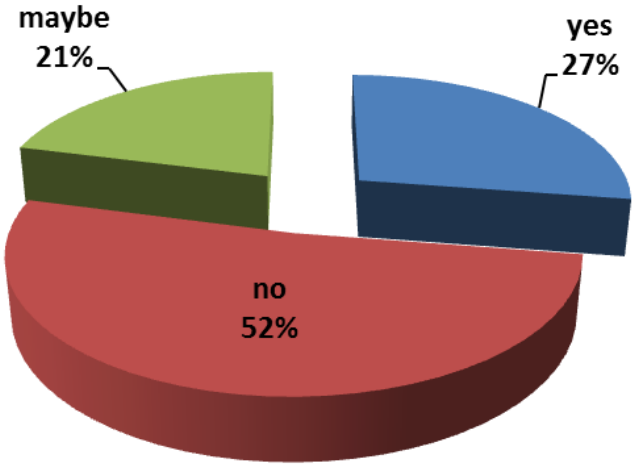
Would you like to share submitted proposals to several facilities for review ?



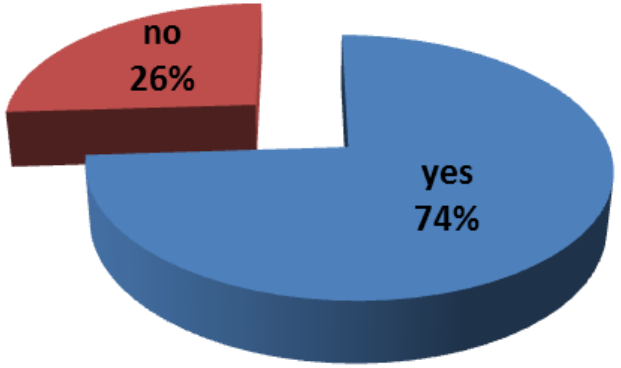
How often would you like proposal deadlines per year?



Would you prefer a continuous proposal submission process?



Are proposal deadlines as often if you want?



A few personal thoughts – *what* we do and *how* we do it:

- Consultation is a good thing
- Results can be ambiguous
- Don't wait for the majority to ask for change

  We are all conservative, anticipate change, try new things
- User profiles are changing

  Less experts, more multi-disciplinary
- More frequent proposal reviews using state-of-the-art IT
- Rapid access to beamtime
- Industry wants 1 month between idea and experiment
- Time to travel reduced

  Remote access to instruments

→ Neutron scattering in the lab (at home)!

Instrument scientists having been doing it for more than a decade