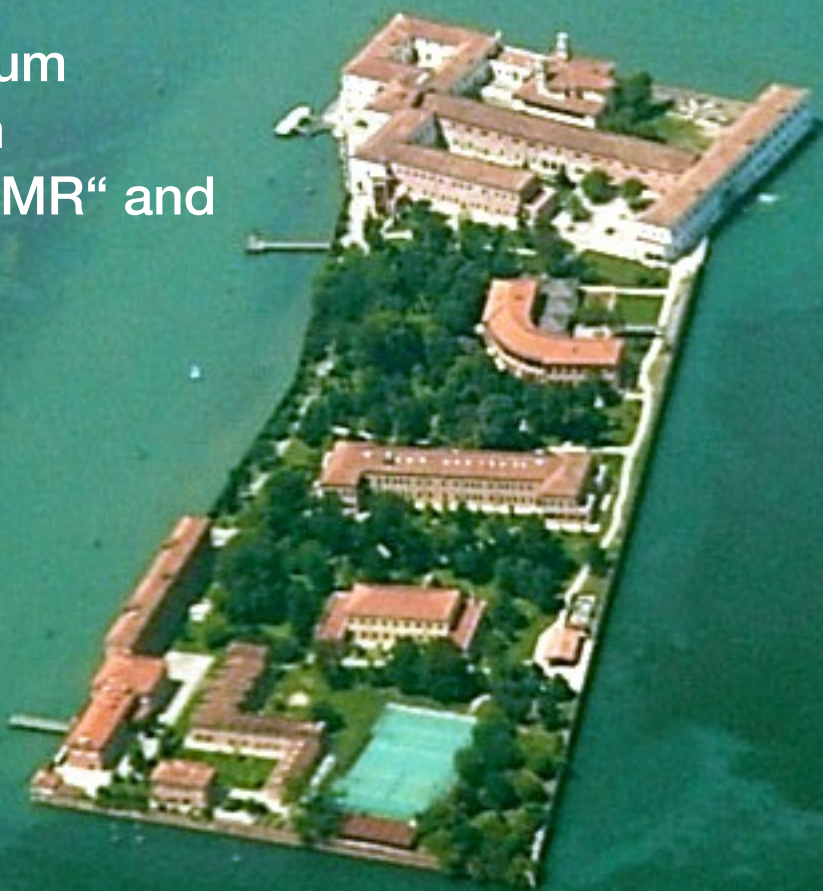


# Europe meets Italy with paramagnetic NMR

A joint symposium  
of the European  
consortium “pNMR” and  
the GIDRM



Venice,  
Isola di San Servolo  
28 September 2016  
[venice.pnmr.eu](http://venice.pnmr.eu)

A journey into paramagnetic NMR, between theory and experiments, solution and the solid-state, with applications ranging from chemistry to biology, including catalysts, battery materials, metalloproteins and large protein-protein assemblies

## Speakers include:

Michael Assfalg (Verona)  
Ladislav Benda (Lyon)  
Steven Brown (Warwick)  
Christophe Copéret (Zurich)  
Lyndon Emsley (Lausanne)

Clare Grey (Cambridge)  
Nicolas Giraud (Paris Orsay)  
Jozef Kowalewski (Stockholm)  
Claudio Luchinat (Florence)  
Federico Rastrelli (Padova)  
Tomas Åkerud (AstraZeneca)





# Europe meets Italy with Paramagnetic NMR

Last annual workshop of the pNMR consortium

*Isola di San Servolo, Venice, Italy*

## Schedule

### Wednesday, September 27<sup>th</sup>

- 10.00 Registration
- 10.30 **Guido Pintacuda** (CNRS Lyon, FR)  
Introductory remarks
- 10.40 **Claudio Luchinat** (GIOTTO BioTech, University of Florence, IT)  
*"Past present and future of paramagnetic NMR"*
- 11.30 **Ladislav Benda** (TU Berlin, DE /CNRS Lyon, FR)  
*"What we understand and what we don't in paramagnetic NMR"*
- 12.00 **Jozef Kowalewski** (Stockholm University, SE)  
*"Paramagnetic relaxation in solution: an overview"*
- 12.30 Lunch, *Sala Basaglia/Church Cloister*
- 14.00 **Tomas Åkerud** (AstraZeneca, Molndal, SE)  
*"Paramagnetic NMR in the pharmaceutical industry"*
- 14.30 **Federico Rastrelli** (University of Padova, IT)  
*"A study on the topology of mixed monolayer nanoparticles by paramagnetic tagging"*
- 15.00 **Nicolas Giraud** (Université Paris-Sud, Orsay, FR)  
*"Paramagnetic NMR : a toolbox for probing supramolecular interactions involving lanthanide complexes"*
- 15.30 **Michael Assfalg** (University of Verona, IT)  
*"Transient protein-nanoparticle interactions investigated by solution NMR"*
- 16.00 Coffee Break, *Atrio Colone*
- 16.30 **Lyndon Emsley** (EPFL Lausanne, CH)  
*"Paramagnetic Polarization sources for DNP"*
- 17.00 **Christophe Copéret** (ETH Zürich, CH)  
*"Title TBC"*
- 17.30 **Steven P. Brown** (University of Warwick, UK)  
*"Ab-Initio Random Structure Searching, Powder X-Ray Diffraction and NMR crystallography for Molecular Organic Solids"*
- 18.00 **Clare P. Grey** (University of Cambridge, UK)  
*"New advances in the development and applications of p-NMR to transition metal oxides: applications to battery and fuel cell electrode materials"*
- 19.45 **Dinner**, *Sala Basaglia/Church Cloister*

# Schedule

## Thursday, September 29<sup>th</sup>

- 9.00 **Andrea Bertarello** (ENS/CNRS Lyon)  
*"Paramagnetic metalloproteins and fast magic-angle spinning: experiments and theory meet at the metal center"*
- Jury:** Claudio Luchinat (Giotto Biotech SRL, Florence)/ Moreno Lelli (University of Florence) / Juha Vaara (University of Oulu)
- 10.00 Coffee Break, *room 3*
- 10.15 **Mathilde Lescanne** (University of Leiden)  
*"Paramagnetic NMR with lanthanoid tags for methyl group assignment and protein studies"*
- Jury:** Giacomo Parigi (CIRMMP)/ Michael Odelius (University of Stockholm)/Guido Pintacuda (CNRS Lyon)
- 11.15 Coffee Break, *room 3*
- 11.30 **Witold Andralojc** (CIRMMP, Florence)  
*"Conformational heterogeneity in multidomain biological systems studied through paramagnetic NMR"*
- Jury:** Jozef Kowalewski (University of Stockholm) / Claudio Luchinat (Giotto Biotech SRL, Florence)/ Tomas Åkerud (Astra Zeneca)
- 12.30 Lunch, *room 3*
- 14.00 **Roberta Pigliapochi** (University of Cambridge)  
*"Combined first principles and experimental investigation of paramagnetic solid-state NMR: application to Li-ion battery cathode materials"*
- Jury:** Lyndon Emsley (EPFL) / Frank Engelke (Bruker BioSpin GmbH) / Ladislav Benda (CNRS Lyon)
- 15.00 Coffee Break, *room 3*
- 15.15 **Arobendo Mondal** (TU Berlin)  
*"Bridging the gap between paramagnetic molecular and solid-state calculations using CP2K"*
- Jury:** Christophe Copéret (ETH Zürich) / Clare Grey (University of Cambridge) / Vladimir Malkin (Slovak Academy of Sciences)
- 16.15 Coffee Break, *room 3*
- 16.30 **Kevin Sanders** (ENS/CNRS Lyon)  
*"Development and application of new NMR methods for paramagnetic inorganic materials"*
- Jury:** Lyndon Emsley (EPFL) / Clare Grey (University of Cambridge) / Frank Engelke (Bruker BioSpin GmbH)
- 17.30 End of the meeting.

# Schedule

## Friday, September 30<sup>th</sup>

- 9.00 **Syed Awais Rouf** (University of Oulu)  
*"NMR Chemical Shifts in Paramagnetic Molecules: A First-Principles Study"*
- Jury:** Vladimir Malkin (Slovak Academy of Sciences) / Andrew Pell (Stockholm University) / Michael Odelius (Stockholm University)
- 10.00 Coffee Break, *room 3*
- 10.15 **Florian Allouche** (ETH Zürich)  
*"Characterization of Paramagnetic Surface Species"*
- Jury:** Anne Lesage (CNRS Lyon) / Moreno Lelli (University of Florence) / Juha Vaara (University of Oulu)
- 11.15 Coffee Break, *room 3*
- 11.30 **Peter Cherry** (Slovak Academy of Sciences)  
*"Fully relativistic pNMR theory: development, interpretation and applications"*
- Jury:** Perttu Lantto (University of Oulu) / Jozef Kowalewski (University of Stockholm) / Ladislav Benda (CNRS Lyon)
- 12.30 Lunch, *room 3*
- 14.00 **Puneet Ahuja** (AstraZeneca)  
*"Paramagnetic NMR to determine the structures of ligands bound to the drug targets"*
- 15.15 **Tobias Schubeis** (CNRS Lyon)  
*"Structural biology by solid-state NMR : applications to amyloid fibrils and membrane proteins"*
- 16.15 End of the meeting

Lunch will be served on Wednesday, Thursday, Friday, as well as Dinner on Wednesday, and will be free of charge for participants. However, please do attend if you said you would so.

Wednesday 28<sup>th</sup> September dinner: **registration is compulsory.**

There will be no poster session.

**Wifi :** there is WIFI connection in the meeting rooms, in the sleeping rooms, and at San Servolo Café. Access is free and no password is required.



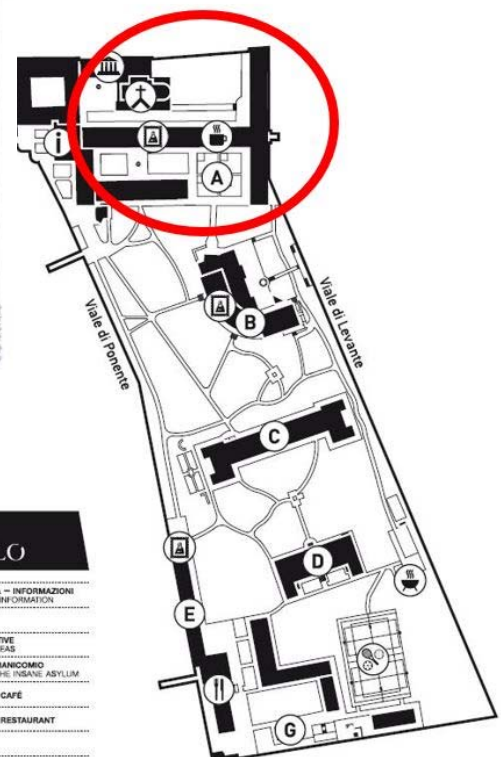
**Please beware of the waiting times between all connections.**

More information  
can be found on  
[venice.pnmr.eu](http://venice.pnmr.eu)



# On site

The meetings and catering rooms are located as shown below :



SAN SERVULO	
<b>I</b>	ACCOGLIENZA - INFORMAZIONI RECEPTION - INFORMATION
<b>C</b>	CHIESA CHURCH
<b>A</b>	AREE ESPOSITIVE EXHIBITION AREAS
<b>M</b>	MUSEO DEL MANICOMIO MUSEUM OF THE INSANE ASYLUM
<b>S</b>	SANSERVULO CAFE
<b>R</b>	SANSERVULO RESTAURANT
<b>B</b>	BARBECUE
<b>C</b>	CAMPI SPORTIVI SPORTS FACILITIES
<b>A</b>	PIAZZA BADEN-POWELL BADEN-POWELL SQUARE
<b>B</b>	PALAZZINA GRECALE BUILDING GRECALE
<b>C</b>	PALAZZINA MAESTRALE BUILDING MAESTRALE
<b>D</b>	PALAZZINA SCIROCCO BUILDING SCIROCCO
<b>E</b>	PALAZZINA LIBRECCIO BUILDING LIBRECCIO
<b>G</b>	PALAZZINA ZEPHRO BUILDING ZEPHRO