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## CA 15209 European Network on NMR Relaxometry (EURELAX)

# Workshop: NMR Relaxometry for Interdisciplinary and Industrial Applications

**Location: CEA, Grenoble, France**

**Dates: 19.03.2019 - 22.03.2019**

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**Aim of workshop:** This workshop is aimed at participants from industry and academics who wish to form collaborations with industry on industrial applications of NMR relaxometry. The goal is to educate non-specialists from industry on the basic principles of NMR relaxometry and how this technique can be applied for potential industrial applications (in research, development and quality control environments), such as medical and pharmaceutical, oil and gas exploration, battery materials, polymers and food and agriculture.

### List of speakers and affiliations

Danuta Kruk, University Warmia & Mazury in Olzstyn, Poland (COST action Chair)  
Prof. Belorizky, CEA, Grenoble, France  
Lucia Calucci, ICCOM-CNR, Pisa, Italy  
Jean-Pierre Korb, Sorbonne Université – CNRS, Paris, France  
Pascal Fries, CEA, France  
Ioan Ardelean, Cluj-Napoca University, Romania  
Jordan Ward-Williams, Cambridge University, UK  
Oscar Tutusaus, Toyota USA  
Mauro Botta, Università Piemonte Orientale, Alessandria, Italy  
Fabio Tedoldi, Bracco, Colletterto Giacosa, Italy  
Simonetta Geninatti-Crich, Università degli studi di Torino, Italy  
Hana Lahrech, INSERM, France  
Lionel Broche, University of Aberdeen, UK  
Dominique Petit, Université de Montpellier, France  
Roberto Anedda, Porto Conte Ricerche Srl, Alghero, Italy  
Donatella Capitani, CNR, Monterotondo, Rome, Italy (to confirm)  
Rahima Sidi-Boulenouar, Université de Montpellier, France  
Guillaume Meriguet, Sorbonne Université – CNRS, Paris, France  
Sabine Bouguet-Bonnet, Université de Lorraine, France  
Carmine D'Agostino, University of Manchester, UK  
Giacomo Parigi, CERM, Università degli studi Firenze, Italy  
Marco Geppi, Università degli studi di Pisa, Italy  
Pedro Sebastião, Universidade de Lisboa, Portugal

### Organizing committee

Danuta Kruk, University Warmia & Mazury in Olzstyn, Poland (COST action Chair)  
Pascal Fries, CEA, France  
Hana Lahrech, INSERM, France  
Gianni Ferrante, Stelar Srl, Italy  
Rebecca Steele, Stelar Srl, Italy

## Local Organizers

Pascal Fries, CEA, France  
Hana Lahrech, INSERM, France

## General information for participants

General information on travel and accommodation:

Please note that coffee break refreshments will be provided by the local organizers of the training school.  
Lunch?

# WORKSHOP PROGRAM

## DAY 1 – TUESDAY 19<sup>th</sup> MARCH

08.00-09.00	REGISTRATION
09.00-09.30	Welcome introduction and practical instructions to participants - <i>COST action Chair, Danuta Kruk &amp; local organizers</i>
09.30-10.30	Measurement of relaxation data - <i>Lucia Calucci</i>
10.30-10.50	COFFEE BREAK
10.50–11.35	<i>The analysis of longitudinal relaxation times T1 of water protons over a large range of external applied magnetic field is shown to provide important information about the dynamics of liquids, solutions and living tissues– Elie Belorizky</i>
11.35-12.30	How to extract useful parameters from relaxation data (general molecular dynamics information – rotation, diffusion) – <i>Danuta Kruk (to confirm)</i>
12.30-13.00	
13.00–14.00	LUNCH
14.00–15.00	Basic theories and experiments of nuclear magnetic relaxation dispersion of liquids in confinement – <i>JP Korb</i>
-16.00	Dynamics of water in biological cells by NMR relaxometry - <i>Pascal Fries</i>
16.00-16.30	COFFEE BREAK
16.30–17.30	Analysis of relaxometry data – an overview of available software for data transformations -
17.30-19.00	Poster session and networking

## DAY 2 – WEDNESDAY 20<sup>th</sup> MARCH

08.30-09.30	Applications of nuclear magnetic relaxation dispersion in petroleum industry – <i>Jean-Pierre Korb</i>
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09.30-10.30	Fast Field Relaxometry, the Mesoscopic Part of Multi-scale NMR Approach for Proton Dynamics in Porous Media: Industrial Applications – <i>Dominique Petit</i>
10.30-10.50	COFFEE BREAK
10.50-11.20	Applications of Field Cycling relaxometry to cement materials - <i>Ioan Ardelean</i>
11.20-12.20	<i>Relaxing liquids in porous catalysts: Applications and potential - Carmine D'Agostino</i>
12.20-12.50	Fast Field Cycling Relaxometry and its Application to Porous Catalytic Systems – <i>Jordan Ward-Williams</i>
12.50–14.00	LUNCH
14.00 – 15.00	Battery electrolytes – <i>Danuta Kruk</i>
15.00-15.30	Oscar Tutusaus, Toyota USA
15.30-16.00	
16.00–16.20	COFFEE BREAK
16.20-17.20	<i>Combining NMR relaxometry with other techniques - Guillaume Meriguet [1 hour?]</i>
17.20-17.50	<i>1H relaxometry for studying the solvent behavior in an organo-gelation process – Sabine Bouquet-Bonnet [30 min]</i>
17.50-18.20	Industrial application presentation

### DAY 3 – THURSDAY 21<sup>st</sup> MARCH

08.30-09.30	Food applications of relaxometry? – <i>Donatella Capitani</i>
09.30-10.00	MR relaxometry for quality assessment and authentication of dairy products - <i>Roberto Anedda</i>
10.00-10.30	Plants and relaxometry - <i>Rahima Sidi-Boulenouar</i>
10.30-10.50	COFFEE BREAK
10.50-11.50	Role of intracellular water lifetime as a tumour biomarker by <i>in vivo</i> FFC - <i>Simonetta Geninatti [1 hour]</i>
11.50-12.20	Potential of FFC NMR in cancer diagnostics - <i>Hana Lahrech [30 min?]</i>
12.20-12.50	FFC-MRI – <i>Lionel Broche [30 min?]</i>
12.50–14.00	LUNCH
14.00–15.15	Relaxation enhancement of Gd-based MRI probes: from small chelates to nanosized systems - <i>Mauro Botta (75 min)</i>
15.15-16.00	Macrocyclic paramagnetic agents for MRI: Determinants of relaxivity and strategies for their improvement - <i>Fabio Tedoldi (30 min then 15 min q's for both presentations combined)</i>
16.00–16.20	COFFEE BREAK
16.20-17.20	NMR relaxometry of proteins - <i>Giacomo Parigi [1 hr]</i>
17.20-	
	SOCIAL DINNER???

### DAY 4 – FRIDAY 22<sup>nd</sup> MARCH

08.30-	Pharmaceuticals (high field relaxometry) – <i>Marco Geppi</i>
	Pharmaceutical applications (formulations – liquids – viscous liquids – authentication (viagra)) - <i>Danuta Kruk</i>

10.30-10.50	COFFEE BREAK
10.50-11.50	<i>Polymers – Lucia Calucci [1 hour?]</i>
11.50-12.20	<i>NMR Relaxometry in Complex Soft-Matter Systems: Experimental Results and Model Fitting – Pedro Sebastiao [30 min]</i>
12.20-12.50	
12.50–14.00	LUNCH
14.00–16.00	<i>Round table discussion – useful industrial applications of NMR relaxometry – All (session chair &amp; panel – mix of academia &amp; industry)</i>
16.00–16.20	COFFEE BREAK
16.20-17.50	
17.50-18.20	Closing remarks - COST action Chair, Danuta Kruk & local organizers