

CONFERENCE PROGRAM

THURSDAY 13TH

9.00 – 11.30	Registration (+ coffee)
11.30 – 11.45	Opening Session
Chairperson: Carlos González Ibáñez - Institute of Physical Chemistry Rocasolano, Madrid, Spain	
11.45 – 12.25	Invited lecture 1: NMR structural insights into DNA G-rich repeats Janez Plavec - University of Ljubljana; National Institute of Chemistry, Slovenia
12.25 – 12.45	Oral Communication 1: Non canonical DNA structures and their conformational transitions studied by ¹ H and ¹⁹ F NMR spectroscopy Cristina Cabrero - Institute of Physical Chemistry Rocasolano, IQFR- CSIC, Madrid, Spain
12.45 – 13.00	Flash 1: Analysis of the interactions between midkine and pleiotrophin with chondroitin sulfate and mimetics by NMR and modelling Pedro Nieto – Institute for Chemical Research, Seville, Spain Flash 2: Molecular recognition of DNA helicase FBH1 by PCNA Francisco J. Blanco – Biological Research Centre, CIB-CSIC, Madrid, Spain
13.00 – 14.00	Lunch time (UNIVERSITY CANTEEN)
14.00 – 15.15	Poster Session 1 (HALL AULARIO IV)
Chairperson: Miquel Pons Vallés – University of Barcelona, Barcelona, Spain	
15.15 – 15.55	Invited lecture 2: NMR spectroscopic structural and stability studies pave the way for polyproline II helices as the next LEGO® for protein design Douglas V. Laurents – Institute of Physical Chemistry Rocasolano, IQFR- CSIC, Madrid, Spain
15.55 – 16.15	Oral Communication 2: The hidden order of intrinsically disordered proteins and its role in molecular recognition Borja Mateos López – Institute for Research in Biomedicine, IRB, Barcelona, Spain
16.15 – 16.35	Flash 3: Functional amyloid assembly in immunity response Paula Polonio – Institute of Physical Chemistry Rocasolano, Madrid, Spain Flash 4: Identification of a new DC-SIGN binding pentamannoside epitope within complex structure of <i>Candida albicans</i> mannan Marcos Gómez – CICbioGUNE, Bizkaia, Spain Flash 5: Structural insights of the interaction of Siglec-9 with natural and synthetic glycan analogues Unai Atxabal – CICbioGUNE, Bizkaia, Spain

16.35 – 17.05	Coffee break
Chairperson: Juan Miguel López del Amo – CICenergiGUNE, Vitoria-Gasteiz, Spain	
17.05 – 17.45	Invited lecture 3: Solid-state NMR: from small molecules to complex materials Juan Manuel Lázaro Martínez – University of Buenos Aires – CONICET, Argentina
17.45 – 18.05	Oral Communication 3: NMR of gases and polymers in dense membranes Leoncio Garrido – Institute of Polymers Science and Technology, ICTP-CSIC, Madrid, Spain
18.05 – 18.25	Oral Communication 4: Metal ion dopants in inorganic materials: From paramagnetic relaxation to DNP Daniel Jardón Álvarez – Weizmann Institute of Science, Israel
18.25 – 19.05	Invited lecture 4: Established and advanced solid-state NMR techniques for a better understanding of the nature of biochar Heike E. Knicker – Institute for Natural Resources and Agrobiolgy, IRNAS-CSIC, Seville, Spain
19.15	GERMN annual meeting
21.00	Welcome reception

FRIDAY 14TH	
Chairperson: Ignacio Alfonso Rodríguez – Institute for Advanced Chemistry of Catalonia, Barcelona, Spain	
9.00 – 9.40	Invited lecture 5: Non-stationary NMR spectroscopy Krzysztof Kazimierczuk – University of Warsaw, Poland
9.40 – 10.20	Invited lecture 6: Seeking simplicity in spectral complexity? Cutting-edge NMR methods at your disposal Laura Castañar – University of Manchester, Manchester, Great Britain
10.20 – 10.40	Oral Communication 5: Reduced relaxation matrix analysis of STD NMR initial slopes build-up curves of protein-ligand complexes Juan C. Muñoz-García – Institute for Chemical Research, Seville, Spain
10.40 – 11.00	Oral Communication 6: Monitoring anomerization reactions by ¹¹⁹ Sn NMR spectroscopy Antonio Franconetti – CICbioGUNE, Bizkaia, Spain
11.00 – 11.30	Coffee break
Chairperson: María Luisa García Martín – Andalusian Centre for Nanomedicine and Biotechnology, Málaga, Spain	
11.30 – 12.10	Invited lecture 7: The role of NMR metabolomics in current molecular epidemiology Daniel Monleón Salvadó – University of Valencia, Valencia, Spain
12.10 – 12.30	Oral Communication 7: Towards quantitative metabolic profiling of biological samples using Pure Shift NMR Covadonga Lucas-Torres – Université Paris-Saclay, France
12.30 – 13.00	Flash 6: NMR metabolomics as a powerful technique in the discovery of potential biomarkers for COVID-19 disease in serum and urine samples Ana Isabel Tristán – University of Almería, Almería, Spain Flash 7: Liquid crystalline phase behavior and hydration of hydroxypropyl cellulose in water: A liquid and solid NMR investigation Manuel Martin Pastor – University of Santiago Compostela, S. Compostela, Spain Flash 8: Study of the interaction of TEPO with silica surface by ³¹ P solid state NMR José M. Fraile – CSIC-University of Zaragoza, Zaragoza, Spain Flash 9: Multidimensional solid state NMR characterization of polymer-ceramic composite electrolytes Pedram Ghorbanzade – CICenergiGUNE, Vitoria-Gasteiz, Spain
13.00 – 14.00	Lunch time (UNIVERSITY CANTEEN)
14.00 – 15.15	Poster Session 2 (HALL AULARIO IV)

Chairperson: Jesús Angulo Álvarez – Institute for Chemical Research, Seville, Spain	
15.15 – 15.55	Invited lecture 8: An NMR-based metabolomic view of the natural history of COVID-19 disease Oscar Millet – CICbioGUNE, Bizkaia, Spain
15.55 – 16.15	Oral Communication 8: NMR-based design of a short Gαi3 protein for crystallography Mariola Ferreras-Gutiérrez – Biological Research Centre, CIB-CSIC, Madrid, Spain
16.15 – 16.35	Oral Communication 9: Immobilization of biantennary N-glycans leads to branch specific epitope recognition by LSEctin Sara Bertuzzi – CICbioGUNE, Bizkaia, Spain
16.35 – 17.05	Coffee break
Chairperson: Jesús Jiménez Barbero – CICbioGUNE, Bizkaia, Spain	
17.05 – 17.45	Invited lecture 9: NMR-based strategies to unravel the role of glycans in infectious diseases Luca Unione - CICbioGUNE, Bizkaia, Spain
17.45 – 18.00	Flash 10: Structural insights into the molecular recognition of pseudomannobioside ligands of C-type lectins by NMR and computational techniques Irene Herrera-González – University of Seville, Seville, Spain Flash 11: Brain biomarkers of autism in rats exposed to chlorpyrifos: An NMR-based metabolomics approach Ana del Mar Salmerón López – University of Almería, Almería, Spain
18.00 – 18.40	Invited lecture 10: Towards the use of NMR in clinical diagnostics Manfred Spraul – Bruker Biospin, Mannheim, Germany
21.00	Conference dinner

SATURDAY 15TH	
Chairperson: Pilar Romero Soria – Universidad de Zaragoza, Zaragoza, Spain	
9.00 – 9.40	Invited lecture 11: NMR studies on the elucidation of the (unusual) structure of selector-selectand aggregates between daclatasvir and some cyclodextrins Antonio Salgado – University of Alcalá, Madrid, Spain
9.40 – 10.20	Invited lecture 12: New multiple nuclei and ultra-high resolution/solvent suppression Spinsolve benchtop NMRs Sanel Suljić – Magritek Ltd., Düsseldorf, Germany
10.20 – 10.40	Oral Communication 10: Application of advanced NMR methods to the structure elucidation of complex small molecules Josep Saurí – Autonomous University of Barcelona, Barcelona, Spain
10.40 – 11.00	Flash 12: Structure and Conformational Mobility of 1,3,5-Triazine Derivatives for OLED Applications Nikolay G. Vassilev – Bulgarian Academy of Sciences, Sofia, Bulgaria Flash 13: ¹⁹⁵ Pt NMR in high-valent pyrazolate-bridged Pt ₂ complexes: a picture of the chemical structure Lorenzo Arnal – University of Zaragoza, Zaragoza, Spain Flash 14: Multinuclear Multidimensional NMR spectroscopy on a single microcoil for unprecedented NMR detection limits María Victoria Gómez Almagro – University of Castilla la Mancha, Ciudad Real, Spain
11.00 – 11.30	Coffee break
Chairperson: María Ángeles Jiménez López - Institute of Physical Chemistry Rocasolano, Madrid, Spain	
11.30 – 12.10	Invited lecture 13: Using NMR methods to investigate supramolecular systems Nuno Basilio – Universidade NOVA de Lisboa, Lisboa, Portugal
12.10 – 12.30	Oral Communication 11: Phosphorylation and allosteric interactions of c-Src investigated by multinuclear NMR methods Alejandro Fernández – University of Barcelona, Barcelona, Spain
12.30 – 12.50	Oral Communication 12: Understanding and development of advanced electrode materials by <i>in-situ/ex-situ</i> solid state NMR Nahom Enkhubari Asres – CICenergiGUNE, Vitoria-Gasteiz, Spain
12.50 – 13.20	Awards and closing ceremony
13.00 – 14.00	Lunch time (UNIVERSITY CANTEEN)

WORKSHOP. NMR SERVICES: COLLABORATION, AUTOMATION, MANAGEMENT AND TRAINING PROGRAM

Chairperson: José Ignacio Delso Hernández – University of East Anglia, Norwich, United Kingdom

15.00 – 15.05	Welcome
15.05 – 15.30	Topic: Sharing of information among NMR Services Ignacio Alfonso Rodríguez – IQAC-CSIC, Barcelona, Spain Isabel Merino Natal – University of Oviedo, Spain David Pantoja Uceda – IQFR-CSIC, Madrid, Spain
15.30 – 16.00	Topic: The implementation of NUS and NOAH experiments Juan Miguel Expósito López – University of Almería, Spain
16.00 – 16.30	Topic: Collaboration among NMR Services and research groups. Where does the technical work ends and where the research begins? José Ignacio Santos González – University of the Basque Country, Bilbao, Spain Elena Sáez Barajas – Complutense University of Madrid, Madrid, Spain
16.30 – 17.00	Coffee break
17.00 – 17.30	Topic: Management of NMR Services Isabel Merino Natal – University of Oviedo, Spain Ángel Jimeno Marco – University of Zaragoza, Zaragoza, Spain
17.30 – 18.00	Topic: Training of NMR users and technicians Roundtable