

Report on NMRS-2012

A Symposium on New Developments in NMR and the Conference of the National Magnetic Resonance Society

(Submitted by K.V. Ramanathan, Convener, Organising Committee)

National Magnetic Resonance Society (India) has been holding its annual meetings at different centres in India. The 18th meeting of the society was held in Bangalore during February 5-8, 2012 and was organized by the NMR Research Centre, Indian Institute of Science, Bangalore. The focal theme of this latest meeting was new developments in NMR. A new feature of the meeting was the initiation of the ISMAR-NMRS Lecture. The opening lecture of the Conference was the ISMAR-NMRS Lecture, which was given by Lyndon Emsley on the use of Dynamic Nuclear Polarization surface enhanced NMR spectroscopy. This was followed by several talks on modern developments such as nano-scale NMR and MRI, novel isotope labeling techniques, new orienting media, novel pulse methodologies, NMR applications in metabonomics, new MRI and fMRI studies, recent applications of NMR for protein structure determination and in material science, current developments in NMR methodologies and instrumentation and so on. There were more than 250 participants and 65 oral and 132 poster presentations. While the majority of the participants were from India, there was a sizable international participation with speakers from other Asian countries, Europe, USA and Canada. There were special sessions for oral presentation by students which were judged for student oral presentation awards. There were also student poster presentation awards. Lectures in the morning were held in parallel sessions in order to accommodate as many oral presentations as possible. The presentations were of very high quality and the discussions that followed were very useful. There were also presentations by vendors of NMR spectrometers where the current status of developments in some specific areas was presented. The meeting provided an opportunity for the participants to exchange ideas. It also helped students to connect with senior scientists working in related areas for help in their research as well as explore Ph.D., post-doctoral and career opportunities.

The meeting was supported by several government funding agencies and by industry sponsors. The involvement of ISMAR gave the meeting higher visibility and also helped in attracting financial support. The Organizing Committee thanks the ISMAR Council for the support for the Conference.

The next meeting of NMRS (India) will be held in Mumbai in the year 2013. The dates and the venue of the Conference will be available shortly in the website: www.nmrsin.org

(The scientific programme and the abstract booklets are available in the web-site

<http://nrc.iisc.ernet.in/nmrs2012/nmrs2012.pdf>)

**Symposium on
New Developments in NMR
and Conference of the
National Magnetic Resonance Society**

February 5-8, 2012

**NMR Research Centre
Indian Institute of Science, Bangalore**



**Symposium on
New Developments in NMR
and Conference of the
National Magnetic Resonance Society
18th Annual Meeting**

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Indian Institute of Science, Bangalore**

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NMRS 2012
SCIENTIFIC PROGRAMME
VENUE : FACULTY HALL/ CHOKSI HALL
INDIAN INSTITUTE OF SCIENCE, BANGALORE

5th FEBRUARY 2012 (FACULTY HALL)

14.00 – 15.00 Hrs REGISTRATION
15.00 - 15.15 Hrs INAUGURATION
Session I ISMAR – NMRS Lecture 15.15 - 16.00 Hrs Lyndon Emsley Visualising Modern Materials by DNP Surface Enhanced NMR Spectroscopy
16.00 – 16.30 Hrs High Tea
Session II Methods-I
16.30 – 17.00 Hrs Masatsune Kainosho Retrieving missing NMR information by selective SAIL methods
17.00 – 17.30 Hrs Gopalakrishnan Balasubramanian Towards nanoscale NMR and MRI using diamond spins.
Session III Prof. S. Subramanian's 60th Birthday Award Lecture 17.30 – 18.15 Hrs H. S. Atreya NMR methods for structural studies of challenging systems
DINNER

6th FEBRUARY 2012

Session IV Plenary Lecture 09.00 – 9. 45 Hrs (Faculty Hall) Stanley J. Opella Structure Determination of a GPCR in Phospholipid Bilayers by Solid-State NMR	
Session Va Small Molecules (Faculty Hall)	Session Vb Biomolecular NMR-I (Choksi Hall)
9.50 – 10.20 Hrs N. Suryaprakash Evidence for Intra-Molecular Hydrogen Bonding with Organic Fluorine: Two Dimensional ¹⁵ N- ¹ H DQ-SQ and ZQ-SQ Correlation Techniques	10.00 -10.30 Hrs Gianluigi Veglia Ground and Excited States of Membrane Protein-Protein Complexes by Solid-State NMR Spectroscopy
10.20 – 10. 50 Hrs Philippe Lesot Evaluating the spectral enantiodiscrimination potential of DNA-based orienting medium using deuterium 1D and 2D NMR spectroscopy	10.30 -11.00 Hrs Siddhartha P. Sarma Solution structural studies of the regulatory subunit (IlvN) of Acetohydroxy acid synthase isoenzyme I (AHAS I)
10.50 – 11.05 Hrs Tea	11.00 – 11. 15 Hrs Tea
Session VIa Solid State NMR-I (Faculty Hall)	Session VIb NMR in Medicine-I (Choksi Hall)
11.05 -11.35 Hrs Steven P. Brown Characterising Solid-State Structures Formed by Organic Molecules: What Can NMR Contribute?	11.15 – 11. 45 Hrs G. A. Nagana Gowda Advanced Analytical Methods in the Discovery of Disease Biomarkers
11.35 – 12.05 Hrs P. K. Madhu Elucidating metal ion-A β interaction at a molecular level	11.45 - 12.15 Hrs J. W. VanMeter Cholinergic Changes Related to Deactivation of the Default Mode Network
12.05 – 12.35 Hrs Pierre Thureau Residual Dipolar Couplings in Solid-state NMR	12.15-12.45 Hrs Amarnath Jena Optimizing MRI scan time in the computation of pharmacokinetic parameters in breast cancer Diagnosis

<p>12.35-12.55 Hrs</p> <p>Bibhuti B. Das Experiments optimized for Rotationally Aligned solid-state NMR of Membrane Proteins</p>	<p>12.45-13.05 Hrs</p> <p>Omkar B. Ijare Recent Developments in MRS Applications for the Diagnosis of Hepatopancreaticobiliary Diseases</p>
<p>LUNCH</p>	
<p>14.00 – 16.00 Hrs</p> <p>Session VII POSTER SESSION-I (Faculty Hall Reception Area) ODD NUMBERED POSTERS</p>	
<p>Session VIII Methods-II (Faculty Hall)</p>	
<p>16.00 – 16.30 Hrs</p> <p>Dimitris Argyropoulos Software Tools for Extracting Quantitative Data from NMR Spectra</p>	
<p>16.30 – 17.00 Hrs</p> <p>Detlef Moskau PGI's Discovered and Characterized by NMR</p>	
<p>17.00 – 17.30 Hrs</p> <p>Katsuo Asakura The Leading-edge Solid-State NMR Technologies</p>	
<p>BANQUET</p>	

7th FEBRUARY 2012

Session IX Plenary Lecture 09.00 – 9. 45 Hrs (Faculty Hall) Thomas Szyperski NMR for Structural Genomics: Methodology Development and Application	
Session Xa Solid State NMR-II (Faculty Hall)	Session Xb Biomolecular NMR-II (Choksi Hall)
9.50 -10.20 Hrs R.W. Schurko New Methods for ¹⁴ N Solid-State NMR	10.00 – 10. 30 Hrs Peter Güntert Reliable and flexible automated assignment with CYANA
10.20 -10.50 Hrs Neeraj Sinha Hydrogen bonding network in bone by solid state NMR spectroscopy	10.30 – 11. 00 Hrs Ashish Arora NMR Solution Structures of Eukaryotic ADF/Cofilins
10.50 – 11.05 Hrs Tea	11.00 – 11. 15 Hrs Tea
Session XIa Solid State NMR-III (Faculty Hall)	Session XIb NMR of Materials/Peptides (Choksi Hall)
11.05 -11.35 Hrs B. Jagadeesh Scaling of Scalar Couplings and Residual Dipolar Couplings in Solution and Solid State	11.15 – 11. 45 Hrs S. Raghobhama Conformational analysis of Proline containing Model Tri-peptides by Solution and Solid State NMR
11.35 – 12.05 Hrs Amir Goldbourt Magic angle spinning NMR studies of filamentous bacteriophage viruses	11.45 -12.15 Hrs P. R. Rajamohan NMR of Hybrid Materials
12.05 – 12.35 Hrs T. Narasimhaswamy ¹³ C- ¹ H Dipolar couplings of mesogens: A source of information for Molecular Topology	12.15 – 12. 45 Hrs T. G. AjithKumar Understanding the mechanical properties of amorphous and semi-crystalline polymers by probing their functional group, and segmental motions

12.35 – 13.05 Hrs Stefano de Gironcoli Complete NMR Chemical Shifts Assignment for Cholesterol Crystals by Combined CP-MAS Spectral Editing and ab-initio GIPAW Calculations	12.45 – 13.05 Hrs A. K. Mahapatra Intraoperative NMR
LUNCH	
14.00 – 16.00 Hrs Session XII POSTER SESSION-II (Faculty Hall Reception Area) EVEN NUMBERED POSTERS	
Session XIII Student Talks –I (Faculty Hall)	
16.00-16.15 Hrs Deepak Chatterjee NMR Studies of the Folding Patterns in Homo-Oligomers of (<i>R</i>)- $\beta^{2,2}$ -Amino Acids with Carbohydrate Side Chain	
16.15-16.30 Hrs Durgesh Kumar Dwivedi Clinical utility of diffusion MRI: ADC values in various Gleason scores	
16.30-16.45 Hrs Hemanth Kumar B.S. FA and MD changes in CMS rat model of depression – A DTI approach.	
16.45-17.00 Hrs V. S. Manu Use of Genetic Algorithm for Quantum Information Processing by NMR	
17.00-17.15 Hrs Y. Jayasubba Reddy Heteronuclear Double Quantum Correlation Experiments Involving Protons for the Study of Partially Ordered and Rigid Systems	
17.15-17.30 Hrs Jithender G Reddy (4,3)D-HN(C)NH experiment for direct sequential connection of $^1\text{H}^{\text{N}}$ - ^{15}N HSQC peaks in labeled proteins	
17.30-17.45 Hrs Arjun Sengupta Temporal changes in urine profile of <i>Plasmodium vivax</i> infected patients: Metabonomic studies using ^1H NMR spectroscopy	
17.45-18.00 Hrs Geetanjali Singh EPR Study of Electron-Hole Asymmetry in Bulk and Nanoparticles of $\text{Bi}_{1-x}\text{Ca}_x\text{MnO}_3$ ($x = 0.4, 0.6$): A Comparison	
18.00-18.15 Hrs K. Jugeshwar Singh Ultra high magnetic field and temperature dependence of NMR T1 and charge transport studies in organic conductor (PF_6^- doped poly-3-methylthiophene)	
18.30 – 20.00 Hrs CULTURAL PROGRAM	
DINNER	

8th FEBRUARY 2012

Session XIV Plenary Lecture 09.00 – 9. 45 Hrs (Faculty Hall)	
Hartmut Oschkinat Structural investigations on the ABC transporter ArtMP-J and on the interaction of α B-Crystallin with substrates by Solid-State NMR	
Session XVa NMR in Medicine-II (Faculty Hall)	Session XVb Methods-III (Choksi Hall)
9.50 – 10. 20 Hrs S. Senthil Kumaran Functional imaging during motor task	10.00 -10.30 Hrs Vikram Bajaj Applications of Remotely Detected NMR and MRI at the Microscale
10.20 – 10. 40 Hrs Anant B. Patel NMR Studies of Brain Metabolism in Animal models of Alzheimer's and Parkinson's Disease	10.30 -11.00 Hrs Victor Jaravine Fast Hyper-Dimensional NMR spectroscopy of short-lived biological samples
10.40 – 11. 00 Hrs Uttam Kumar Role of Amygdala and Pre-frontal cortex in meditation and spirituality: fMRI and Voxel Based Morphometry (VBM) investigation	
11.00 – 11.15 Hrs Tea	11.00 – 11. 15 Hrs Tea
Session XVIa Biomolecular NMR-III (Faculty Hall)	Session XVIb Methods-IV (Choksi Hall)
11.15– 11.35 Hrs Mandar V. Deshmukh Solution NMR studies of proteins involved in RNA recognition and regulation	11.15 – 11. 45 Hrs Olivier Lafon Why wait hours to acquire NMR spectra? High-field DNP and non-uniform sampling
11.35- 11.55 Hrs Neel S. Bhavesh Structural insight into the RNA recognition by ETR-3	11.45 – 12.15 Hrs Kavita Dorai Diffusion studies and quantum computing using NMR

11.55 – 12.15 Hrs Radhakrishnan Mahalakshmi Membrane Proteins and Peptides: Addressing Biophysical Questions using Spectroscopic Tools	12.15 – 12.45 Hrs T. S. Mahesh NMR implementation of Quantum Delayed-Choice Experiment
12.15 – 12.35 Hrs Sujoy Mukherjee Probing pre-amyloidogenic states of human immunoglobulin (light chain) variable domains by relaxation dispersion NMR spectroscopy	12.45 – 13.05 Hrs Arindam Ghosh Clean Absorption Mode (CAM) NMR Data Acquisition General Theory and Applications
12.35 – 12.55 Hrs Sunita Patel Structural characterization of a calcium binding protein from <i>Entamoeba histolytica</i> (EhCaBP1) at physiological pH by NMR spectroscopy	
LUNCH	
14.00 – 16.30 Hrs Session XVII Student Talks –II (Faculty Hall)	
14.00-14.15 Hrs Prashant K. Rai Spectroscopic analysis and antioxidant potential of polyherbal formulation	
14.15-14.30 Hrs Puneet Bagga In vivo NMR studies on evaluation of neuroprotective effects of dietary restriction in Pitx3 knockout mouse model of Parkinson's Disease	
14.30-14.45 Hrs Rajesh Sonti NMR study of Contryphans from cone snails: Cis/trans isomerisation in disulfide bonded cyclic peptides	
14.45-15.00 Hrs Rustam Ali Structural and Interaction Studies of GMP Synthetase from <i>Methanocaldococcus jannaschii</i> by Solution NMR	
15.00-15.15 Hrs C. Sai Chaitanya Structural and mechanistic details of RDE-4, an RNAi initiator in <i>C. elegans</i>	

15.15-15.30 Hrs Santosh Kumar Bharti Metabolomic Profiling of Amoebic and Pyogenic Liver Abscesses: An in-vitro NMR Study
15.30-15.45 Hrs Soumya Singha Roy Investigation of the Leggett-Garg Inequality for Precessing Nuclear Spins
15.45-16.00 Hrs M. Saxena Dysarthria in Parkinsonism: Neural or articulatory?
16.00-16.15 Hrs K. Veera Mohana Rao Simultaneous Measurement of Selective Multiple J-Couplings by Solid State NMR
16.15 – 16.35 Hrs Session XVIII (Faculty Hall) CBMR-NMRS Gold Medal Award Lecture U. Venkateswara Reddy Liquid Crystalline Phase of the Polysaccharide Xanthan as an aligning medium for enantiodiscrimination and measurement of Residual Dipolar Couplings
16.35 Hrs Tea
NMRS General Body Meeting
DINNER

NMRS2012 - Poster Presentations

Poster No.	Presenting Author	Abstract Title
P1	Anil Kumar Yadav	Structural and dynamics studies on a salt tolerance protein from a basidiomycete fungus
P2	Anjali Ganjiwale	E2 glycoprotein of Chickungunya virus: a molecular drug target, stereodynamic investigation
P3	Anushikha Thakur	Solution Structure and Function Analysis of Human J-protein by NMR Spectroscopy
P4	Arvind Kumar	Two Dimensional NMR studies of fast -pyrolytic Bio-oil: NMR finger printing of Bio-oil
P5	Asampille Gitanjali	Probing the mechanism and developing the applications of self assembled nanotubular structures by hIGFBP-2
P6	Ashok Kulkarni V S	¹ H-NMR and Molecular Dynamics Studies of Active Site of Vasopressin: Towards Modifications for Pharmacological Effects of Vasopressin
P7	Chandrappa S	Helix and Hairpin Nucleation in Short Peptides Using Centrally Positioned Conformationally Constrained Dipeptide Segments
P8	Deepti Chaturvedi	Refolding and Stability Studies of beta-Barrel Membrane Proteins
P9	Dharma Rao N	Drug Design through Multinuclear NMR Studies - Identification of site of donation and reactivity of selected drugs through ¹⁵ N – NMR Spectra
P10	Dinesh B	Designed β-Hairpin Peptides Containing ω-Amino acids
P11	Garima Jaipuria	Structure and Dynamics of intrinsically disordered middle domain of IGFBP2
P12	Gaurav Sharma	NMR metabolomics and anticancer potential evaluation of an ayurvedic formulation
P13	Harshesh Bhatt (Dipesh Trivedi)	Structure and RNA binding studies on a stress tolerance protein from a basidiomycete fungus
P14	Himanshu Singh	Live cell metabolomics by NMR: Acetate assimilation in <i>C. reinhardtii</i>

P15	Kamlesh Madhusudan Makwana	Structural and Biophysical Studies of ^D Pro - ^L Pro Nucleated Water-Soluble Peptide beta-Hairpins
P16	Kanchan Sonkar	¹ H Nuclear Magnetic Resonance (NMR) metabonomic study of breast cancer in Indian population
P17	Kanchan Sonkar	Metabonomic study of human serum in gallbladder cancer by ¹ H NMR spectroscopy
P18	Krishnarjuna B	NMR investigation of Amyloid peptide fragments Aβ1-12, Aβ1-16 and their interactions with Aluminium.
P19	Lakshmi Bala	Irritable bowel syndrome: Metabolomic study of upper gut aspirate
P20	Mahammad Yasin U	A Coarse View of the Energy landscape of Lysozyme by Cross-relaxation NMR
P21	Mamta Sharma	¹ H NMR analysis for metabolites in plasma from rats administrated acute dose of sarin - A Nerve agent
P22	Muruga Poopathi Raja	NMR Analysis of SL3 Analogue of HIV-1 Packaging Signal Ψ-RNA
P23	Neeraj Rastogi	Metal Ions as Catalyst for Aggregation of Therapeutic Peptide Salmon Calcitonin
P24	Piyush Gupta	NMR studies of fast pyrolytic jatropha Bio-oil and its upgrading through hydro treatment
P25	Pradeep T.P	Interaction of flavonoid, rutin with telomeric G-quadruplex sequence d-(TTGGGGT) ₄
P26	Priyanka Sharma (Pamita Awasthi)	Synthesis and spectroscopic study of Juvenile Hormone Analogues containing sulphonamide feature as a potential pesticides
P27	Pushpa Mishra	NMR Structural Insights into the Plasmodium Falciparum P2 Protein
P28	Rakhi Sharma	Solution structure of Crc and RNA Interaction Studies
P29	Rama Jayasundar	NMR spectroscopic analysis and anti-oxidant evaluation of dietary and non-dietary parts of medicinal plants
P30	Ravi S	Robust turn structures in α ₃ β cyclic tetrapeptides induced and

	Ampapathi	controlled by Carbo- β^3 Amino acid
P31	Reddy P.P.	Search for New Helical Folds in Peptides from α -Amino Acids with Alternating Chirality
P32	Rudra N. Purusottam	Probing water-protein interactions in bacteriophage pfl by solid state NMR spectroscopy
P33	Rustam Ali	Solution NMR studies of GMP Synthetase from <i>M. Jannaschii</i>
P34	Santosh Kumar Bharti	Magic Angle Spinning NMR Spectroscopic Metabolic Profiling of Gall Bladder Tissues for Differentiating Malignant from Benign Disease
P35	Anupam Jain, Ashok Kumar, Vaibhav Shukla, Sarita Tripathi	Dynamics study of LdCof and TgADF and its comparison
P36	Sashikanth Reddy	Effect of bulk solvent friction on aromatic ring-flip rates in cytochrome <i>c</i> studied by pure exchange spectroscopy
P37	Shilpa Dogra	Study on complex of mitoxantrone with d-(ATCGAT) ₂ DNA hexamer sequence using Phosphorous-31 and Proton Nuclear Magnetic Resonance Spectroscopy
P38	Shivanand Pudakalakattai	Pyruvate uptake as a biomarker for assessing the implantation potential of embryos in human <i>In-vitro</i> fertilization.
P39	Sneha Bagle	In search of novel antifertility agent, exploring in-vitro metabolic inhibition and antifertility effect of nifedipine analogues
P40	Somnath Mondal	Methodological development and application of NMR spectroscopy to the Ubiquitin and full length IGFBP-2
P41	Soumita Ghosh	Multivariate modelling with ¹ H NMR of pleural effusion in cerebral malaria in mice.
P42	Soumita Ghosh	Predictive biomarkers for cerebral malaria in mice.
P43	Supriya Pratihari	Insight into Mechanism of Action of Cathelicidin-Derived Antimicrobial Peptide (AMP) and their Structure-Function Relationship
P44	Susmitha A.L	Structure based rational redesign of eye lens proteins
P45	Svetlana Rajkumar Maurya	Biophysical Characterization of gp33 – A Transcriptional Co-Activator

P46	Sweta Tripathi	Interaction of flavone, luteolin with Parallel β -stranded G-quadruplex sequence d-(TTGGGGT) ₄
P47	Umashankara M	Evaluation of Diverse α/γ -Backbone Patterns in β -Turn mimicry
P48	Uttam Pal	Hydroxyl-Hydrogen Bond and Deuterium Isotope Effect on ¹³ C Chemical Shift
P49	Vaibhav K. Shukla	NMR Assignment of UNC-60A: Divergence with conventional ADF/Cofilin family
P50	Vasantha Gowda	Effect on helical transformations by insertion of an extra C-C bond in the main chain of designed heptapeptides
P51	Veena Hegde	NMR metabonomics of differentiation study of human saliva samples collected at different trimesters of pregnant women
P52	Venkatraman R	Structural Characterization of the Natively Unfolded $\beta\gamma$ -Crystallin from <i>Hahella chejuensis</i>
P53	Vidya Raghunathan	Theoretical and in vitro studies of a C-terminal peptide from PGKC of <i>Leishmania mexicana mexicana</i> .
P54	Ajay Rakkesh	High Resolution Solid State ⁶⁷ Zn and ^{47, 49} Ti NMR Investigation of ZnO/TiO ₂ Core-Shell nanostructures
P55	Bindhu Baby	27 Al Solid State NMR evidence for two hexa coordinated Al sites in LaAlO ₃
P56	Chandan Singh	Experimental aspects of solid state NMR study of bone
P57	Cyril Augustine	Heteronuclear Dipolar Decoupling in the NMR Spectroscopy of Liquid Crystals and Solids using a Phase-wiggled SW _f -TPPM Sequence
P58	KowsalyaDevi P	Extracting Narrow Lines in the Presence of Inhomogeneous Magnetic Fields - Use of Nutation Echoes
P59	Mohana Krishna	Solid State ¹³ C NMR Spectral study of coal samples for advance detection of fires in coal mines.
P60	Navdeep Gogna	HRMAS NMR investigation of fungicide on the metabolic profile of seed germination
P61	Nitin P. Lobo	Molecular Order of Mesogens by Chemical Shift Anisotropy and ¹³ C- ¹ H Dipolar Couplings
P62	Pattabi Rama Krishna	Solid State ¹³ C NMR Spectral study for analyzing the aliphatic and aromatic moieties of plant materials used in Homam.

P63	Rajendra Singh Thakur	Solid-State NMR investigation of spherical NaCl agglomerates
P64	Sudheer Kumar	Deuterium NMR Methods for Studies in the Solid state
P65	Veera Prakash B	Role of spacer on Orientational order parameter of mesogens: Investigation of ^{13}C - ^1H dipolar couplings by Solid State ^{13}C NMR spectroscopy
P66	Venus Singh Mithu	Investigation of efficiency of heteronuclear dipolar decoupling schemes in solid state NMR
P67	Akshay Bhatt	Quantitative application of NMR in ropivacaine hydrochloride and its related impurity-A with correlation by alternate techniques
P68	Ankeeta	Visual cortex reorganization for language task in late blind subjects and controls
P69	Bhasin A	BOLD activation in chronic stroke patients after administration of autologous mononuclear and mesenchymal stem cells
P70	Chandan Sinha	Metabolic profiling by NMR spectroscopy of serum from patients of Acute Lung Injury (ALI) and Acute Respiratory Distress Syndrome (ARDS)
P71	Chaudhary K	Semantic & Comprehension Lexical processing in left temporal lobe epilepsy patients using fMRI
P72	Deepika Bagga	Assessment of Semantic Judgment abilities in Alcohol Dependents: An fMRI Study
P73	Hemanth Kumar B.S	Neurometabolite fluctuations during onset of depression in CMS rats as detected by in vivo proton MRS at 7T.
P74	Kavita Singh	Radiation induced early changes in brain: DTI perspective
P75	Mamta Gupta	Diffusion tensor imaging screening of radiation induced changes in mice brain after single and fractionated cranial irradiation
P76	Mamta Gupta	In vivo assessment of Brain metabolites following Whole Body and Cranial Irradiation: A 7T ^1H MRS study
P77	Nisha Sainia	Design and Synthesis of Novel DO3A-BTA MR Contrast Agent
P78	Pandichelvam Veeraiah	Does the routes of administration of Alcohol has variable effect on Brain Function?
P79	Pandichelvam Veeraiah	Evaluation of Cerebral Metabolism in Mice Brain with Different Amount of Alcohol Exposure

P80	Priya Saxena	Lewis base coordinated cadmium(II) acetate aggregates: Efforts to unravel the role of steric/basic properties of Lewis base upon the degree of aggregation
P81	Puja Panwar Hazari	Design and Synthesis of Gd(III)-DTPA Bis-(Methionine) as Contrast Agent for MRI
P82	Rajeswari Moganty	MRI To Evaluate The Therapeutic Effect Of Bleomycin And Doxorubicin On Skin Tumors
P83	Rajiv Ramaswamy	Topological Connectivity and Elastic Responsivity of Brain as a window to the Alzheimer-type Neurodegenerative process
P84	Rani Gupta Sah	Longitudinal assessment of tumor response to neo-adjuvant chemotherapy in locally advanced breast cancer (LABC) patients using in-vivo MRS and MRI
P85	Richa Trivedi	Quantification of Cortico-Callosal Wallerian Degeneration using Diffusion Tensor Tractography
P86	Sadhana Singh	Z-Assessment of motor function deficit in thyroid dysfunction: An fMRI study
P87	Sarkar B.K	Micro Magnetic Resonance Imaging Technique for the investigation of water diffusion in the plant vascular bundles
P88	Sidhu O. P.	Changes in the metabolome and histopathology of Amaranthus mosaic begomovirus-infected Amaranthus hypochondriacus L. using NMR spectroscopy and magnetic resonance imaging
P89	Sidhu O. P., Anil Bhatiya	Metabolite profiling of medicinal plant chemo types using HR-MAS NMR spectroscopy
P90	Sunil Koundal	T2 -Weighted MR Imaging on Heat Stress induced changes in Rat Brain at 7 Tesla.
P91	Surbhi Prakash	A Novel Gd(III) Based Target Specific MRI Contrast Agent with DOTA-Bis(Triazole-Biotin) System Constructed Via VersatileCu(I) Catalyzed Click Chemistry
P92	Uttam Kumar	Semantic Processing and impact of language proficiency in bilingual: An fMRI investigation.
P93	Virendra K Meena	Deferoxamine-Cysteine: MRI based contrast agents of paramagnetic complex with Mn ²⁺ and Gd ³⁺
P94	Vivek Tiwari	Reduced Cerebral Metabolism upon Alcohol Exposure During Developmental Period
P95	Vivek Tiwari	NMR Investigations of Glutamatergic and GABAergic Energetic

		at Late Stage of Alzheimer's Disease
P96	Arun Kumar Bar	NMR & X-Ray diffraction techniques to determine geometry of ligand-co-ordination driven supramolecular architectures
P97	Avik Mazumder	Proton-decoupled phosphorus-31 diffusion ordered spectroscopy of a model mixture of phosphitylated markers of chemical warfare agents
P98	Chandrakala.M	Activation of – N=CH – bond in a Schiff base by divalent nickel monitored by NMR Evidence
P99	Dey K. K.	Enhancing sensitivity of the central transition by multiple inversion of satellite transitions
P100	Dey K. K.	New Methods for Separating Quadrupolar Interaction and Chemical Shift Anisotropy under static and MAS conditions for Integer Quadrupolar Nuclei
P101	Divya Kumari	Study of Hydrogen Bond Directed Conformations in Organofluorine Molecules by NMR Spectroscopy and DFT
P102	Hadi Ghaffari	Structural characterization and antioxidant activity of a novel antioxidant compound from Hyptis suaveolens (L.) Poit.
P103	Lokesh	Folic acid salts as Weak Orienting Media for NMR Spectroscopic Enantiomeric Visualization of Water Soluble Chiral Molecules
P104	Manasi Ghosh	³¹ P NMR study of trimer spin chain compound Ca ₃ Cu ₂ Ni(PO ₄) ₄
P105	Manjunatha M.N.	Spectral studies of Zn(II), Cd(II) and Hg(II) complexes with 1-(p-methoxybenzyl)-2-(p-methoxyphenyl)benzimidazole
P106	Matsyendra Nath Shukla	3D COMPACT-IDOSY : A new tool for the analysis of complex mixtures.
P107	Nitesh Kumar	Synthesis and Characterisation of titanium complexes as anti-cancer agents
P108	Phani Kumar B.V.N	Influence of Water-insoluble Nonionic PEO-PPO-PEO Copolymer on the Microstructure and Self-aggregation Dynamics of SDS Aqueous Solution - A NMR Investigation
P109	Radhakrishnan S	¹ H and ¹³ C NMR spin-lattice relaxation studies on 2,6-dibenzylidenecyclohexanones
P110	Ramu L.	Temperature and Pressure dependences of ³⁵ Cl NQR frequency and spin lattice relaxation time in 3, 4 – Dichloronitrobenzene

P111	Ranjeet Tiwari	The utility of NMR spectroscopy for grade analysis of polymeric excipients where separate end groups are not discriminated in the spectrum
P112	Sachin Rama Chaudhari	Simple Three Components Chiral Derivatizing Protocols for NMR Spectroscopic Enantiodiscrimination of Hydroxy Acids, Primary Amines and Diacids
P113	Sankeerth Hebbar	Correlation of combination transitions with single quantum coherences of Dipolar Coupled Spins
P114	Somenath Ghatak	NMR spectroscopy of medicinally important plants
P115	Somenath Ghatak	Spectroscopic analysis and in-vitro anti-oxidant efficacy of tribulus terrestris
P116	Srinivasa	Pilot study of soil organic components in farming by NMR Spectroscopy
P117	Srinivasa	Resolution of isomers by Matrix assisted DOSY using α -cyclodextrin as a co-solute
P118	Sudeshna Sen	Characterization of Hydroxyl Hydrogen Bond Properties During Phosphodiester Bond Hydrolysis by Ribonucleases
P119	Thirupathaiah A	Isolation and structure determination of a chalcone "spinosine" from the roots of <i>Tephrosia spinosa</i> .
P120	Venkatesh G.B.	Synthesis and Characterisation of Some Novel Trimethylsilyl-Substituted 4-Aza-tricyclo[5.2.2.0 _{2,6}]undec-8-ene-3,5-dione Derivatives
P121	Vijaya Bhaskar K	Synthesis and antimicrobial activity of Tetrahydrobenzo [b] pyran and its derivatives.
P122	Abhishek Shukla	Measurement of Translational Diffusion Constant using Noon State
P123	Bhagyashree K.S.	Temperature Dependent Sign Reversal of Magnetocrystalline Anisotropy in Nanoparticles of La _{0.875} Sr _{0.125} MnO ₃
P124	Honnavar G.V	EPR investigation of Mixed Alkali Effect in Oxy - fluoro Vanadate glasses
P125	Karthik Gopalakrishnan	Filter Diagonalisation method as an alternative to spectral deconvolution for accurate estimation of NMR signals

P126	Rama Koteswara Rao K	Quantum simulation of frustrated Ising spins by NMR
P127	Santosh Kumar Upadhyay	Application of NMR methodology to the Cultural Heritage
P128	Shruti Dogra	Numerically Optimized band-selective and refocusing pulses in SOFAST-HMQC and BEST-HMQC experiments
P129	Siddesh B.M	Towards building a broad band pulsed heterodyne NMR spectrometer.
P130	Soumya S. Roy	Nuclear Spins as Quantum Test-beds
P131	Srinivas Chinthalapalli	High-resolution NMR in inhomogeneous magnetic fields
P132	Swagata Chakraborty	Simultaneous acquisition of $^{13}\text{C}^{\alpha}$ - ^{15}N and ^1H - ^{15}N - ^{15}N sequential correlations in proteins: Application of dual receivers in 3D HNN

Plenary Lectures

Visualizing Modern Materials by DNP Surface Enhanced NMR Spectroscopy

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We have shown over the last few years that multi-dimensional magic-angle-spinning solid-state NMR spectroscopy can play a major role in characterizing a range of difficult materials, from macromolecules to polymorphs to catalysts. An overview of this progress will be given.

In particular, sensitivity is a key problem in NMR, and we will demonstrate different approaches to increasing sensitivity. For example, we will show how surface NMR spectra can be greatly enhanced using DNP. Polarization is transferred from the protons of the solvent to the rare nuclei (at natural isotopic abundance) at the surface, yielding at up to a hundred-fold signal enhancement for surface species in silica frameworks.

As examples of this approach, we demonstrate the fast characterization of the distribution of surface bonding modes and interactions in a series of functionalized materials using this technique. Surface enhanced carbon-13, silicon-29, nitrogen-15 and aluminum-27 DNP NMR spectra were obtained by using incipient wetness impregnation of samples with a solution containing a polarizing radical. Furthermore, the remarkable gain in time provided by surface enhanced DNP NMR spectroscopy (up to a factor 10 000) allows the facile acquisition of two-dimensional correlation spectra, allowing access to conformational features of the surface groups.

Structure Determination of a GPCR in Phospholipid Bilayers by Solid-State NMR

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G-protein coupled receptors (GPCRs) are the largest class of membrane proteins with essential roles transducing signals into the cell and functioning as drug receptors. As a result, they present important targets for structure determination. They are technically challenging because of their size and their requirement for a membrane environment. We have developed an NMR approach specifically tailored for structure determination of membrane proteins, including GPCRs, in phospholipid bilayers under physiological conditions. Notably, no modifications to the protein sequence are required, and no detergents or non-natural lipids are present in the samples. The method merges magic angle spinning (MAS) solid-state NMR and oriented sample (OS) solid-state NMR for application to samples of uniformly $^{13}\text{C}/^{15}\text{N}$ labeled membranes prepared by expression in bacteria and refolded into proteoliposomes. The MAS solid-state NMR spectra are resolved and assigned using two- and three- dimensional homo- and hetero-nuclear correlation experiments. Chemical shift anisotropy and heteronuclear dipolar coupling powder patterns are measured using three-dimensional triple-resonance ROCSA and SLF experiments. The method is based on the inherent rotational diffusion of membrane proteins in liquid crystalline phospholipid bilayers motionally averaging the powder patterns such that their parallel edges provide the same angle-dependent frequency that is measured from a stationary aligned sample with its normal parallel to the direction of the magnetic field. The structure is calculated with a two step procedure that first utilizes Rosetta to derive an initial structure, and then XPLOR-NIH for refinement using the experimental constraints. The method will be demonstrated with the determination of the three-dimensional structure of the 350-residue chemokine receptor CXCR1 in DMPC bilayers at 25°C and pH7.

NMR for Structural Genomics: Methodology Development and Application

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The Northeast Structural Genomics Consortium (NESG; <http://www.neg.org>) has contributed more than 450 NMR structures to the Protein Data Bank (<http://www.pdb.org>) within the framework of the 'Protein Structure Initiative' (PSI) of the U.S. National Institutes of Health. For such HTP structure determination, the development of methodology focuses on increasing (i) the data acquisition speed, (ii) the spectral resolution and precision of chemical shift measurements, (iii) the reliability of semi-automated data processing and analysis, including structure calculations, and (iv) the precision and accuracy of NMR structures. Recent developments and the impact on the structure determination of selected targets are presented, and future perspectives are discussed.

Structural investigations on the ABC transporter ArtMP-J and on the interaction of α B-Crystallin with substrates by Solid-State NMR

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Small heat shock proteins occur as polydisperse oligomers and are vital to maintain long-living cells in a functional state. A main player in higher organisms is α B-crystallin which is accompanied by α A-crystallin in the eye lens. γ -S-crystallin, another eye lens protein, is one of its 'tasks' since it needs to be kept stably folded for the life time of the organism. Previously, we determined a structure of the α -crystallin domain, and obtained first insights into the structure of the oligomer. Now we were investigating further the activation mechanism of α B-crystallin and its interaction with substrates such as γ -S-crystallin as well as the structure of its N-terminus.

Investigations of membrane proteins may be facilitated by extensive deuteration, and subsequent detection of protons under magic-angle spinning conditions. Various schemes for the usage of proton chemical shifts for achieving sequence-specific assignments will be discussed. Samples of Outer membrane protein G and an ABC transporter reconstituted into native lipid bilayers are investigated in variously labelled forms, and spectra of different functional states of the will be presented together with initial assignments and functional considerations.

The application of dynamic nuclear polarisation (DNP) to the investigation of these systems requires further optimization of samples, experimental parameters and concepts. The application of DNP to various proteins systems will be discussed, and spectra of different types of membrane protein samples presented. Spectra with reasonable line width are obtained on membrane integrated complexes. Various technical aspects of the application of DNP to protein systems will be discussed. During the DNP process, the electron polarization is transferred to the surrounding core nuclei and subsequently to the bulk nuclei. The enhanced signal reaches its maximum intensity after a certain period of time. This process depends on several factors such as; relaxation behavior, proton concentration, spin-diffusion and type of the nucleus. As a result, for each nucleus to be polarized there is a characteristic exponential polarization build-up behavior, with different time constant (τ_B) for each nucleus of interest. A systematic investigation of the polarization build-up behavior for different nuclei (^1H , ^2H , ^{13}C , ^{15}N) is presented and for protonated and deuterated SH3 proteins. This information will shed light on the choice of the nucleus to be polarized.