20th Symposium of National Magnetic Resonance Society, India; NMRS-2014

February 2 – 5, 2014
Tezpur University

Organizer: Department of Chemical Sciences, Tezpur University

Contact: Convenors, Dr. Ashim J. Thakur & D. Bipul Sarma; Department of Chemical Sciences, Tezpur University, Tezpur-784028, Email: nmrs2014attu@gmail.com

SCIENTIFIC PROGRAM

Sunday, February 2, 2014
Venue: KBR auditorium, TU

09.00 – 14.00	Registration
14.00 – 14.30	Inauguration Hon'ble Vice Chancellor Prof. M. K. Chaudhuri, Tezpur University, India Hon'ble Vice Chancellor Prof. A. S. Brar, Guru Nanak Dev University, India
	Session 1: Chair: Prof. C. L. Khetrapal, CBMR, Lucknow
14.30 – 15.15	**IT-1:** Claire Grey, University of Cambridge, UK [**ISMAR-NMRS Lecture**] -
	Session 2: Chair: Prof. A. S. Brar, GND University, Amritsar
15.20 – 15.50	**IT-2:** T. S. Mahesh, IISER Pune [Prof. S. Subramanian's 60th Birth Day Lecture Award 2013] Multi-spin Quantum Control: Applications in NMR and Quantum Information
15.50 – 16.05	**OP-1:** Sachin R Chaudhari, IISc, Bangalore [Jharana Rani Best Student Award for 2013] Extraction of Magnitudes and Relative Signs of $^{n}J_{HF}$ couplings: A Pure Shift and RES-TOCSY Methodologies
16.05 – 16.35	Tea
	Session 3: Chair: Prof. Anil Kumar, IISc, Bangalore
16.35 – 17.05	**IT-3:** Daniel Huster, University of Leipzig, Germany Molecular Dynamics of G Protein-Coupled Receptors in Membranes
17.05 – 17.35	**IT-4:** Bernhard Blumich, RWTH Aachen University, Germany Compact NMR
17.35 – 18.05	**IT-5:** Nico Tjandra, National Heart Lung and Blood Institute, USA Principles of Efficient IgE Antibody response revealed by the structure of Grass Pollen Allergen Phl p 5a
20.00 – 10.00	Dinner **Venue: Cafeteria, TU**

Monday, February 3, 2014
Venue: Council Hall, TU

9.00-9.40 **PLENARY TALK:** **IT-6:** Robert G. Griffin, MIT, USA
High Frequency Dynamic Nuclear Polarization
Chair Prof. K. V. Ramanathan

	Session 4: Chair: Prof. N. Suryaprakash, IISc Bangalore **Venue: Council Hall, TU**	**Session 5:** Prof. Gabriele Varani, University of Washington, USA **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
09.40 – 10.10	**IT-7:** Asher Schmidt, Israel Institute of Technology, Israel The interplay of phosphate and water in tuning ACC metastability - from stabilization to crystallization via a nano-scale solid-solid phase separation: A molecular NMR view.	**IT-8:** Koichi Kato, Nagoya City University, Japan NMR approaches for elucidating the functional roles of carbohydrate chains
10.10 – 10.40	**IT-9:** Matthias Ernst, ETH Zurich Optimized Proton-Driven Spin Diffusion by Tailored RF-Irradiation Schemes	**IT-10:** Rolf Boelens, Utrecht University, The Netherlands Structure and dynamics in gene regulation and DNA repair
10.40 – 11.10	**IT-11:** Philippe Lesot, University de Paris-	**IT-12:** K. V. Ramanathan, IISc, Bangalore

	Sud, France NMR using Chiral Anisotropic Solvents: Recent Methodological Advances and new Analytical Applications	NMR Experiments for the Ordered Phases - Assignment, Structure and Dynamics
11.10 – 11.30	Tea Break	
	Session 6: Prof. S. K. Dolui, Tezpur University **Venue: Council Hall, TU**	**Session 7:** Chair: Prof. B. K. Patel, IIT-Ghy **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
11.30 – 12.00	**IT-13:** Thomas Szyperski, University at Buffalo, NY, USA	**IT-14:** Donghan Lee, Max Planck Institute, Germany Molecular Recognition through Concerted Backbone and Side Chain Motion
12.00 – 12.30	**IT-15:** Hanudutta Atreya, IISc Bangalore New NMR methods for rapid data acquisition and analysis: Application to Metabolomics	**IT-16:** Ashutosh Kumar, IIT Bombay, India Native structure governs the amyloid formation and fibril reversibility of a short cyclic peptide hormone
12.30 – 13.00	**IT-17:** Arindam Ghosh, NISER Bhubneswar Are the wavelet based de-noising techniques necessary or optimum for NMR spectroscopy?	**IT-18:** Nilamoni Nath, MPI, Germany Probing supra-τ_c Dynamics on GB3 through $^{13}C_\alpha$–H_α Order Parameters
13.00 – 14.00	Lunch Break **Venue: Cafeteria, TU**	
14.00-16.00	Group Photo + Poster Session I + Tea Break **Venue: Council Hall, TU**	
	Session 8: Chair: Dr. B. Jagadeesh, IICT Hyderabad **Venue: Council Hall, TU**	**Session 9:** Chair: Dr. Romesh C. Boruah, CSIR-NEIST-Jorhat **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
16.00 – 16.30	**IT-19:** N. Suryaprakash, IISc Bangalore Testing Enantiopurity by NMR Spectroscopy: Our Recent Strategies	**IT-20:** Norbert Muller, Johannes Kepler University, Austria
16.30 – 17.00	**IT-21:** Bikash Baishya, CBMR Lucknow ‘‘Perfect Echo’’ INEPT	**IT-22:** Rama Jayasunder, AIIMS, New Delhi NMR in validating Ayurveda
17.00 – 17.15	**OP-2:** Shivanand M. P., IISc Bangalore Accelerating 3D HSQC-DOSY with projection NMR spectroscopy and non-uniform sampling	**OP-3:** Lokesh, IISc Bangalore RES-TOCSY: A Simple Approach to Resolve Overlapped 1H NMR Spectra of Enantiomers
17.15 – 17.45	**IT-23:** Hironao Sajiki, Gifu Pharmaceutical University, Japan. Heterogeneous Platinum Metal-Catalyzed Deuterium Labeling Methods Characterized by the Simplification of NMR Charts	**OP-4:** Veena Bansal, IOCL Faridabad Solid State NMR Studies for Structural insights of Lignocellulosic biomass **OP-5:** Nigel Crossley, Oxford Instruments India Pvt Ltd
17.45 – 18.00		**OP-6:** Rajagopal Bhaskaran, Claflin University NMR Structural Studies on a Human Lymphatic Filarial Aspartic Protease Inhibitor
18.30 – 19.45	Cultural Program Venue: KBR auditorium, TU	
20.00 – 22.00	Dinner **Venue: Cafeteria, TU**	

Tuesday, February 4, 2014
Venue: Council Hall, TU

09.00-9.40	**PLENARY TALK:** **IT-24:** Prof. Stephan Grzesiek, University of Basel, Switzerland Atomic details of protein folding, interactions and function revealed by NMR Chair: Dr. A. C. Kunwar, IICT, Hyderabad
	Session 10: Chair: Prof. Robert G. Griffin, MIT, USA
09.40 – 10.10	**IT-25:** Lyndon Emsley, Universite de Lyon, France Powder NMR Crystallography from Proton Chemical Shifts
10.10 – 10.40	**IT-26:** Gabriele Varani, University of Washington, USA NMR structures allow the design of pharmaceutically active and potent inhibitors of RNA
10.40 – 11.10	**IT-27:** Lucia Banci, University of Florence, Italy

	NMR in Molecular Systems Biology: from structures to function	
11.10 – 11.25	Tea Break	
	Session 11: Chair: Prof. Nasreen Islam, Tezpur University **Venue: Council Hall, TU**	**Session 12:** Chair: Prof. Pradeep Phukan Gauhati University **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
11.25 – 11.40	**OP-7:** Detlef Moskau, Bruker Biospin, Switzerland	**OP-8:** G. S. Kapur, IOCL Haryana
11.40 – 11.55	**OP-9:** Kavita Dorai, IISER Mohali Explorations of multiqubit entanglement and decoherence mitigation on an NMR quantum computer	**OP-10:** M. Srinu, IISc Bangalore Characterization and Solution NMR Studies of Natural Compounds
11.55 – 12.10	**OP-11:** Suresh Kumar Vasa, Max Planck Institute, Germany Bactofilins β-sheet enriched bacterial cytoskeleton proteins	**OP-12:** Pritam Deb, Tezpur University
12.10 – 12.25	**OP-13:** Virendra Kumar, AIIMS, New Delhi In Vivo Quantitation of Metabolites using Proton Magnetic Resonance Spectroscopy of Brain at 3T in Obstructive Sleep Apnea	**OP-14:** Harindranath Kadavath, MPI Gottingen NMR Spectroscopy of Human Neuronal Tau Protein: Interaction of Different Isoforms with Microtubules
12.25 – 12.40	**OP-15:** Amol S. Kotmale, NCL Pune NMR Studies on a Synthetic Zipper Peptide Motif Orchestrated via Co-operative Interplay of Hydrogen Bonding, Aromatic Stacking and Backbone Chirality	**OP-16:** Rajkumar Sharma, CBMR, Lucknow Structural studies on major coat protein of bacteriophage M13 by solid state NMR spectroscopy
12.40 – 12.55	**OP-17:** Shivam Dixit, Integral Bioscience, Delhi qNMR - A quantitative tool for purity determination	**OP-18:** Deepti Upadhyay, AIIMS, New Delhi Abnormal metabolism in Celiac Disease: ^{1}H NMR study of blood plasma
12.55 – 14.00	Lunch Break **Venue: Cafeteria, TU**	
14.00-16.00	Poster Session II + Tea Break **Venue: Council Hall, TU**	
	Session 13: Chair: Prof. Manoj Mishra, IIT Bombay **Venue: Council Hall, TU**	**Session 14:** Chair: Prof. Christian Griesinger, Max Planck Institute, Germany **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
16.00 – 16.30	**IT-28:** Walter Kockenberger, University of Nottinghum, UK Spin Diffusion and Solid Effect Dynamic Nuclear Polarization	**IT-29:** Isabella C. Felli, University of Florence, Italy Novel methods based on ^{13}C detection to study intrinsically disordered proteins
16.30 – 17.00	**IT-30:** Ajith Kumar, NCL Pune Structural Insights into Magnetic Materials from Solid State NMR Studies on Isostructural Nonmagnetic Materials	**IT-31:** B. Jagadeesh, IICT-Hyderabad Real-time homodecoupled pure-shift NMR methodologies for unambiguous analysis of organic molecules
17.00 – 17.15	**OP-19:** Christy George, IIT-Madras Chemical shift resolved 'low' field ^{19}F NMR: DNP (OE) enhanced, diagonal suppressed correlation spectroscopy at X-band	**OP-20:** Pravin Kumar Mishra, CCMB, Hyderabad ^{1}H-[^{13}C]-NMR study for understanding antidepressant effect of ketamine in social defeat model of depression
17.15 – 17.30	**OP-21:** Harpreet Singh, IISER Mohali Preserving quantum states in subspace and entangle state using super zeno effect on an NMR quantum computer	**OP-22:** Jithender G. Reddy, TIFR Mumbai Complete Backbone and DENQ Side chain NMR Assignments in Proteins from a Single Experiment: Implications to Structure – Function studies
17.30 – 17.45	**OP-23:** Sai Chaitanya Chiliveri, CCMB-Hyderabad On structural aspects of dsRBD containing proteins in the RNAi pathway across organisms	**OP-24:** A. L. Susmitha, TIFR Mumbai Deciphering the functional role of Ca^{2+} in the beta/gamma crystallins by NMR spectroscopy
17.45-18.00	**OP-25:** Bappaditya Chandra, TIFR Mumbai Combining fast fluorescence and slow NMR techniques to determine the atomic level structure of transient toxic Amyloid beta oligomers	**OP-26:** K K Bhagchandini, ACD Labs Five different approaches for Verification & Elucidation of unknowns; using NMR!
20.00 – 22.30	Dinner (Banquet) **Venue: Cafeteria, TU**	

Wednesday, February 5, 2014
Venue: Council Hall, TU

9.00-9.40 **PLENARY TALK:** **IT-32:** Prof. Christian Griesinger, Max Planck Institute, Germany
NMR of small and large dynamic systems
Chair: Prof. Stephan Grzesiek

	Session 15: Chair: Prof. S. K. Bhattacharjee, Prof., Gauhati University (Retired) **Venue: Council Hall, TU**	**Session 16:** Prof. Lucia Banci, University of Florence, Italy **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
09.45 – 10.15	**IT-33:** Amir Goldbourt, Tel Aviv University, Israel High resolution structure of a filamentous viral capsid, its DNA properties, and their interface, revealed by solid-state MAS NMR	**IT-34:** Anant B. Patel, CCMB Hyderabad 13C NMR Studies of Brain Energy Metabolism in Parkinson's Disease
10.15 – 10.45	**IT-35:** P. K. Madhu, TIFR Mumbai Heteronuclear spin decoupling in solid-state NMR	**IT-36:** Krishna Mohan Poluri, IIT-Roorkee Structural Analysis of Chemokine-Glycosaminoglycan Interactions
10.45 – 11.15	**IT-37:** Martin Billeter, University of Gothenburg, Sweden Intercalation of large molecules into DNA: intermediates and mechanisms	**IT-38:** Hans Vliegenthart, Utrecht University, The Netherlands NMR spectroscopy as a tool in carbohydrate and glycoprotein analysis
11.15 – 11.45	Tea Break	
	Session 17: Chair: Prof. Ganesh Pandey, CBMR Lucknow **Venue: Council Hall, TU**	**Session 18:** Prof. Amir Goldbourt, Tel Aviv University, Israel **Venue: Seminar Hall, Dept. of Chem. Sc. TU**
11.45 – 12.00	**OP-27:** Arthanari Haribabu, Harvard University, USA Solution structure of the Herpesvirus Nuclear Egress Complex Subunit Exhibits a Novel Fold	**OP-28:** Kowsalya Devi Pavuluri, IISc Bangalore Real Time Dissolution Monitoring using Spatial Encoding NMR
12.00 – 12.15	**OP-29:** Kiran Kumar Singarapu, IICT Hyderabad Solution structure determination of *Aedes Aegypti* Sterol Carrier Protein 2 Like2 (AeSCP2L2) and its complex with palmitate	**OP-30:** B. V. N. Phani Kumar, CLRI, Chennai NMR Investigations on Copolymer-Surfactant Interactions
12.15 – 12.30	**OP-31:** Sudha M. Cowsik, JNU New Delhi Molecular Recognition of Tachykinin Receptor Selective Agonists: Insights from Structural Studies	**OP-32:** Kong Ooi Tan, ETH Zürich Broadband double-quantum recoupling by combined continuous-wave and phase-alternating RF irradiation
12.30 – 13.00	**IT-39:** Sujoy Mukherjee, IICB, Kolkata Role of transthyretin's backbone conformational flexibility in amyloid fibril formation	**IT-40:** G. Balasubramanian, MPI Biophys. Chemistry, Germany -
13.10 – 14.30	Lunch Break **Venue: Cafeteria, TU**	
	Session 19: Chair: Prof. A. S. Brar, **Venue: Council Hall, TU**	
14.30 – 15.00	**IT-41:** Markus Zweckstetter, Max Planck Institute for Biophysical Chemistry, Germany NMR studies of protein folding and misfolding	
15.00 – 15.30	**IT-42:** Peter Guntert, Goethe-University Frankfurt, Germany -	
	Session 20: Concluding ceremony, **Venue: Council Hall, TU**	
16.00 – 17.30	High Tea & NMRS General Body Meeting Best Oral and Poster Awards Presentation	

Legends: IT - Invited talk; OP - Oral presentation