

Editorial

NMR Spectroscopy and Imaging in Biological Chemistry and Medicine

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In recent years, research in the areas of Biological Chemistry and Medicine has been advancing along many directions including those centered around NMR spectroscopy and imaging. Some of these directions are already established and some have just emerged. This multitude of ways the NMR phenomenon and related methods can be applied to Biochemistry and Medicine is astonishing. This Special Issue of Magnetochemistry on “NMR Spectroscopy and Imaging in Biological Chemistry and Medicine” presents a total of six representative interdisciplinary contributions. Below is an overview of these exciting reports.

The first work “Artifacts’ Detection for MRI Non-Metallic Needles: Comparative Analysis for Artifact Evaluation Using K-Means and Manual Quantification” by Marwah AL-Maatoq*, Melanie Fachet, Rajatha Rao and Christoph Hoeschen from Otto von Guericke University (Magdeburg, Germany) [1] explores the potential of utilizing non-metallic materials for interventional biopsy needles utilized during MRI recordings. For example, the traditional MRI needles for spinal cord interventions are constructed from metallic alloys (e.g., nickel–titanium) and are known to introduce into the recorded data highly disruptive artifacts. The work presented here explores the possibility of utilizing non-metallic materials for the construction of such needles. The team reports encouraging results with seven non-metallic needle prototypes designed as enforced fiber bundles for an inner core with different outer hollow sheets. Also, approaches for the quantitative assessment and comparison of the newly designed needles are proposed.

The second paper “NMR of Paramagnetic Proteins: ^{13}C Derived Paramagnetic Relaxation Enhancements Are an Additional Source of Structural Information in Solution” by Leonardo Querci, Inês B. Trindade, Michele Invernici, José Malanho Silva, Francesca Cantini, Mario Piccioli* from University of Florence (Sesto Fiorentino, Italy) and Ricardo O. Louro* from Universidade Nova de Lisboa (Oeiras, Portugal) [2] reports the team’s success in utilizing ^{13}C detected experiments tuned to measure longitudinal relaxation rates of $^{13}\text{C}'$ and $^{13}\text{C}\alpha$ nuclei. These relaxation rates can be utilized to generate highly powerful electron-nuclear spin distance restraints affording a powerful type of structural restraints in paramagnetic metalloproteins. In this proof-of-concept work, the authors demonstrate that the effects of ^{13}C and ^1H PREs restraints can be synergistic especially in cases when the paramagnetic effects are stronger. The two types of PREs if used together can minimize the blind spheres centered around the metal. This in turn can greatly improve the quality of the solution NMR structure determination of paramagnetic metalloproteins and ultimately benefit biomedical research and applications.

The third report “Slow Methyl Axes Motions in Perdeuterated Villin Headpiece Subdomain Probed by Cross-Correlated NMR Relaxation Measurements” by Liliya Vugmeyster* (University of Colorado, Denver, CO, USA), Parker J. Nichols (University of Colorado, Anschutz Medical Campus, Aurora, CO, USA), Dmitry Ostrovsky (University of Colorado,



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Denver, CO, USA), C. James McKnight (Boston University Chobanian and Avedisian School of Medicine, Boston, MA, USA) and Beat Vögeli (University of Colorado, Anschutz Medical Campus, Aurora, CO, USA) [3] highlights the intricate probing of unusually slow motions (sub-nanosecond to nanosecond time scale) of the methyl axes in valine and leucine residues in the 35-residue folded villin headpiece C-terminal subdomain, a highly impactful model protein fragment. In this sample, all the non-exchangeable protons except for the methyls in Val and Leu residues were deuterated. This afforded an unobstructed probing of the NMR relaxation interference between the methyl H-H and H-C dipoles, which are sensitive to the methyl axes' motions. Using the data acquired at different temperatures, the authors were able to delineate the contributions from the comparably paced slow internal motions in the methyls and the overall molecular tumbling of the sample. The methods developed and applied here by the author team will have applications in probing the structure and dynamics of key methyl groups in protein samples in liquid and solid states as well as in medically relevant wet powders.

The fourth article "Structural Parameters of the Interaction between Ciprofloxacin and Human Topoisomerase-II β Enzyme: Toward New ^{19}F NMR Chemical Shift Probe" by Thais Aparecida Sales, Mateus Aquino Gonçalves and Teodorico Castro Ramalho* from Federal University of Lavras (Lavras, Brazil) [4] introduces an elegant application of a fluorine (^{19}F) containing drug ciprofloxacin as an ^{19}F -NMR traceable ligand for human topoisomerase-II β whose elevated expression is linked with aggressive forms of breast cancer. Binding of ciprofloxacin to topoisomerase-II β is tight, which allows for straightforward quantification of the levels of the enzyme–ciprofloxacin complex by ^{19}F NMR. This method affords a rapid and robust way of assessing the level of expression of the target enzyme, thus facilitating and expediting the breast cancer diagnosis.

The fifth manuscript "Solution NMR Backbone Assignment of the C-Terminal Region of Human Dynein Light Intermediate Chain 2 (LIC2-C) Unveils Structural Resemblance with Its Homologue LIC1-C" by Morkos A. Henen, Natasia Paukovich, Rytis Prekeris and Beat Vögeli* from the School of Medicine, University of Colorado Anschutz Medical Campus (Aurora, CO, USA) [5], is a brief report which describes the NMR backbone resonance assignment of the C-terminal region of the light intermediate chain 2 of human dynein 1 (LIC2-C) and related structural conclusions. The mutations in dynein motor proteins are linked with dynein diseases, or dyneinopathies, which are a group of genetic disorders impacting nerves and muscles. The structural characterization of the LIC2-C fragment will assist in deciphering the structural biology of dyneins and molecular mechanisms of the related medical conditions.

The sixth publication "Old Discovery Leading to New Era: Metabolic Imaging of Cancer with Deuterium MRI" by Hao Ding* (Imperial College London, UK), Athar Haroon (Barts Health NHS Trust, London, UK), Simon Wan (University College London, UK), Thoralf Niendorf (Freie Universität Berlin, Humboldt Universität zu Berlin, Max-Delbrueck Center for Molecular Medicine in the Helmholtz Association, Berlin, Germany) and Sola Adeleke (Guy's and St Thomas' NHS Foundation Trust, London, UK and King's College London, UK) [6] is an opinion piece which outlines the potential of deuterium metabolic spectroscopy (DMS) and metabolic imaging (DMI) as tools for in vivo tumor metabolism visualization. The opinion describes the potential of the DMS/DMD approach as a robust diagnostic method as well as the obstacles remaining before the applications become straightforward and widely adopted.

Conflicts of Interest: The author declares no conflict of interest.

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