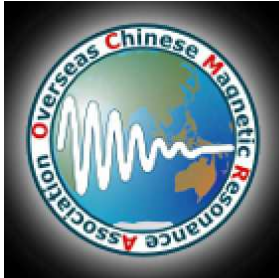


January, 2010

Issue 3

Overseas Chinese Magnetic Resonance Association

NEWSLETTER



Chair: Yi-Qiao Song

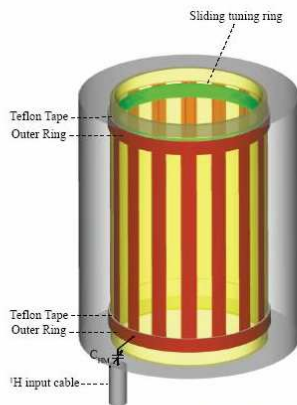
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In this issue:

Holidays are over... Getting Back to Work! by Yan-Yan Hu

High Field Imaging by Dr. Chunqi Qian

Automation of NMR in Drug Discovery by Dr. Jun Hu

From A Single Spark to A Prairie Fire by Dr. Peng Chen

Dr. Wang's Greetings and Trip to China by Dr. Jin-Shan Wang

Holidays are Over...Getting Back to Work!

- *Message from the editor*

Hope everyone enjoyed a wonderful holiday season! It is always so short that you do not even realize you had a break! Now it is time back to work. You may feel overwhelmed when staring at a stack of books, folders, papers, or cryptic computer files that seem to have been created by someone else. The clear and steady path that you had been following before the holidays appears to be a distant memory. With these mixed emotions, you can easily take the joy out of the first OCMRA newsletter for the year of 2010 which marks the start of an exciting brand-new decade! Work can wait till tomorrow...

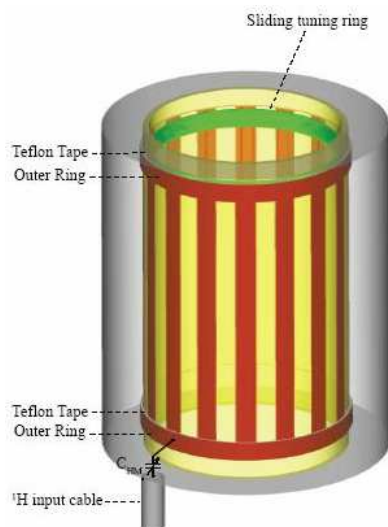
Through the holiday season, I have been thoroughly enjoying the process of corresponding to our newsletter contributors. We chatted about our busy lives (as everybody else's), career, and future unknowns; we share the news, the holiday cheers as well as all the best wishes. Special congratulations to Dr. Chunqi Qian for his research achievement on high field MRI coil design, which recently won him the **ICMRM Young Investigator Award** at the 10th International Conference on Magnetic Resonance Microscopy. In this issue, Chunqi shares his perspectives on the past ICMRM conference and delivers his art of constructing a coil with big enough tuning range without disturbing the B₁ homogeneity. Thanks to Dr. Jun Hu's generous contribution and hard work during his vacation time, we have the eye-opening opportunity of being inspired and amazed by a fantastic automated NMR system employed in drug discovery. This makes me wonder what Jun Hu does at work if everything is automated. Actually, he has already revealed this in his write-up: *watching the needles traveling up and down and the robotic arm moving back and forth is super fun!*

Our very own webmaster and coordinator, Chen Peng, conveys the legends of Mestrelab Research at its 5th anniversary - From A Single Spark to A Prairie Fire (星星之火, 可以燎原). To those of you, who dare to be inspired to build a business kingdom from a smart idea, this is an incredible story that you do not want to miss.

Dr. Jin-Shan Wang has been a true celebrity among us and a huge supporter for our Oversea Chinese Nuclear Magnetic Resonance Association. In April 2009 he and his wife were invited back to China to involve in the project of installing a 500 MHz 5 mm High Resolution NMR system in Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences. Here, he embraces and spreads the delight of his trip to Beijing, Wuhan and Guilin.

- *by Yan-Yan Hu*





High Field Imaging

The 10th International Conference on Magnetic Resonance Microscopy was held during Aug 30 - Sep 4, 2009 in the beautiful town of West Yellowstone. This is a biannual conference focusing on the non-medical aspects of MRI with topics ranging from development in hardware and methodology to application in materials especially in porous media. As a first-time attendant to the conference, I was really impressed by the high quality of science as well as the open communication among people of diverse backgrounds. More remarkably, I was honored to be selected as a finalist to participate in the Young Investigator Competition session at the conference. Also, among the six finalists who made oral presentations, I stood out by winning the Young Investigator Award.

Low field and portable MRI is one of the major themes of this conference. However, I took my presentation as an opportunity to demonstrate the progress in ultrahigh field imaging. Although the high field MRI is more costly compared to its low field counterpart, it plays an indispensable role in achieving higher resolution and better sensitivity especially for the direct detection of low- γ nuclei, such as ^{23}Na and ^{13}C . Most importantly, the National High Magnet Field Lab in Florida, where my work was conducted, provides the scientific community with free access to its facility. It allows users from all over the world to utilize its high field capability to enhance their experiments or observe new phenomena not seen at lower field.

In my presentation, I addressed a specific requirement in high field MRI coil design, i.e. the construction of a coil with big enough tuning range without disturbing the B_1 homogeneity. Operated in the field as high as 21.1 Tesla, the coil needs a big enough tuning range to compensate for the sample induced frequency shift. But the tuning capacitor used in most low frequency coils is unsuitable for our purpose because the variable capacitor is the asymmetric element that often perturbs the B_1 homogeneity. To overcome this limitation, we incorporated a sliding tuning ring into a volume coil and varied the overlapping capacitance between the ring and the coil, thus symmetrically adjust the resonance frequency over a broad tuning range. This design principle has been tested in several different versions of volume coils, and it is anticipated to work equally efficiently even for coils operating for a 1.5 T clinical magnet as well.

The entire conference was filled with exciting oral presentations and versatile poster sessions. Several well-known Chinese scholars, including Dr. Yiqiao Song, Dr. Yang Xia and Dr. Lizhi Xiao, gave enlightening speeches on their latest research topics. The conference also features the picturesque landscape in the Yellow Stone National Park. As to the 11th ICMRM, I believe that there will be a larger group of Chinese attendants since will be hosted in Beijing with Dr. Lizhi Xiao as the conference chair. I look forward to the conference taking place later next year.



- by Chunqi Qian, NIH



Introduction to a Bruker NMR Automation system applied in Drug Discovery

NMR spectroscopy has proven to be a very powerful tool and well incorporated into the drug discovery process. NMR techniques in both small molecules and proteins have been extensively applied at a variety of stages of drug discovery. It is not the purpose of this essay to review NMR methods used in drug discovery, as they have been well documented in the literature. Instead, an automated NMR setup aiming at NMR compound library screening and compound titration will be briefly introduced. Also, only a Bruker-based NMR automation system is discussed here.



As shown in the left figure below, the whole system consists of three major components, a SampleRail that transfers NMR tubes, a Tecan robot that prepares

samples and certainly ICONNMR platform in TopSpin manages the NMR experiments during automation. Each component is controlled by specific softwares. Therefore, communication among these softwares is very critical of fulfilling an automated experiment. In addition, the NMR probe should be equipped with automated tuning and matching probehead, so called ATMA in Bruker.

A typical NMR screening experiment starts with setting up optimal NMR parameters which are saved for all automation experiments. Multiple NMR experiments for one sample are certainly feasible in ICONNMR. The Tecan robotic system (right in the figure) is the core for sample preparation. Due to some technical and communication reasons, unfortunately the Tecan is controlled by three softwares. The Tecan platform can hold protein stocks in cold box which can be set to 4 °C, compound plates (384 or 96 wells), ligand or substrate eppendorfs, buffer solution and empty NMR tubes. Normally, the needles pipette certain amount buffer to a NMR tube, then certain amount of protein, compound in DMSO stock or substrates in eppendorfs can be added and mixed thoroughly according to the protocol designed by the operator. Once the sample preparation is finished, the robotic arm grabs the NMR tube and transfers it to the shuttle on the SampleRail. The shuttle carries the NMR tube to the magnet and NMR experiments start as planned. NMR tube washing is implemented in Tecan systems so the tubes in the trail can be reused many times. Last but certainly not least, watching the needles traveling up and down and the robotic arm moving back and forth is super fun!



- By Jun Hu, AstraZeneca R&D Boston



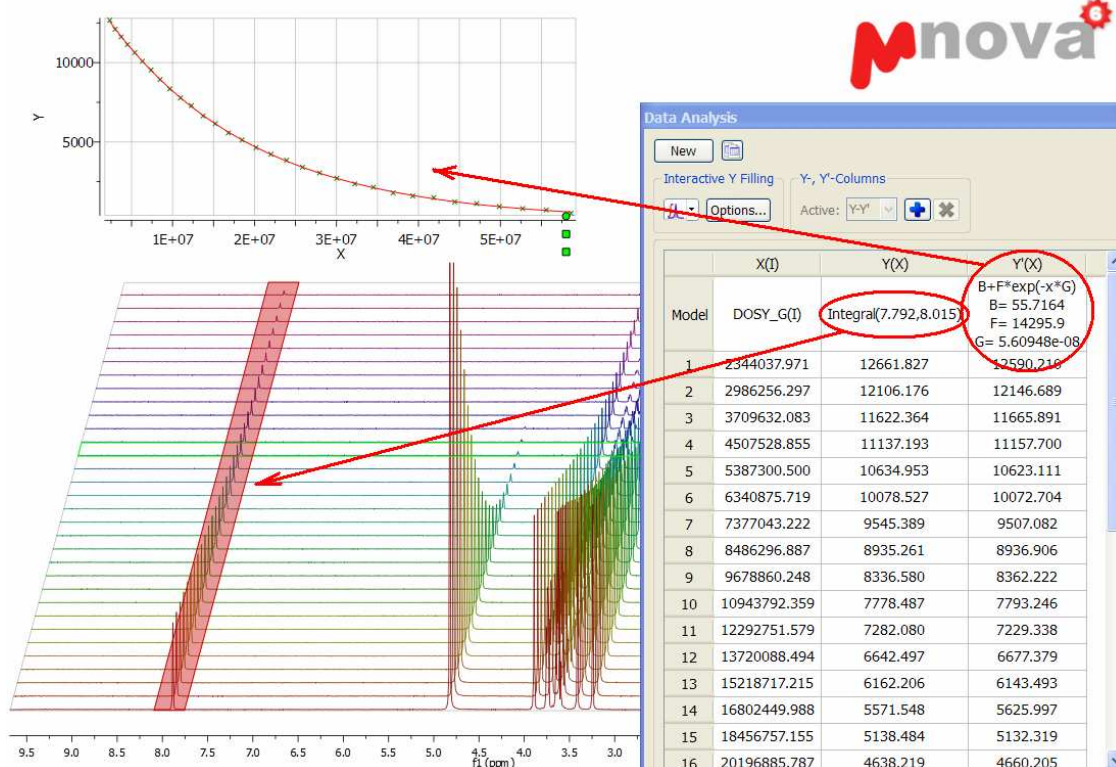
星星之火, 可以燎原- From A Single Spark to A Prairie Fire: Mestrelab Research Celebrates Its 5th Anniversary



MESTRELAB IS 5 YEARS OLD!

The past December of 2009 marked the 5th anniversary of Mestrelab Research SL, a small yet fast growing software company well known for its sophisticated yet inexpensive NMR and MS software. This company is located at Santiago de Compostela in the northwest of Spain. It started with a free 3rd party NMR processing software, MestreC, developed by Carlos Cobas then an organic chemistry PhD working in Professor Javier Sardina's group in the University of Santiago de Compostela (USC). The free MestreC software became surprisingly popular with about 30,000 users registered by 2004. After several years of support, however, USC ceased funding it, and Carlos decided to spin off from USC and seek partnership with his childhood friend Santiago Dominguez, who is a business graduate with extensive international experience in multinationals and start ups. In December 2004, Carlos and Santiago co-founded a commercial company, Mestrelab Research. In the following 5 years, they have continued to develop MestreC by adding numerous new features and a completely renovated user interface to the program, and eventually renamed it MestreNova (Mnova). Not only for multi-vendor data (Bruker, Varian, JEOL and others), Mnova also benefits multi-platform users (Windows, Macintosh and Linux). Not only for NMR processing, Mnova provides also a set of easy-to-use tools for routine and advanced data analysis, prediction and reporting. Not only for NMR, Mnova has evolved into a multi-technique chemistry software since the successful development of an MS plugin that processes and analyzes LC/GC-MS data. This trend will continue at an even faster pace as we are going to introduce more exciting new plugins in the near future.

I first heard about MestreC in early 2000s, but did not think that it would survive in this small and crowded NMR software market. Yet I continued to be surprised by how fast the program evolved and how popular it became. One thing that caught my eye a few years ago was how Mnova allows the user to select multiple 1D and 2D raw files and drag-and-drop them to Mnova. One by one, all of selected spectra are automatically processed and displayed in separate pages like in Power Point. The program itself figures out the file format and the processing parameters instead of expecting the users to input them. On the other hand, the applied processing parameters can be verified by the user, who can change any of them and then see the results immediately. Even better, once you are satisfied with the parameter setting, you can save it as a template and apply it to multiple spectra using a simple script. Another example is the Data Analysis function for extracting and analyzing data from multiple spectra. As shown in the picture and caption below, with only a few clicks you will get the integrals, curve fitting and calculation done, and have the table and picture ready for publication:



Easy calculation of diffusion constant from multiple spectra in Mnova: Click and drag to define the integration area (pink area) and the integrals are listed in the Y(X) column and displayed as crosses in the diagram. Next select a model function and the fitted values and parameters are listed in the Y'(X) column and the curve displayed in the diagram. All pictures and data can be copied to Word document for publication.

The company itself evolves quickly too. Starting from Carlos as the only full-time employee working in his bedroom in 2004, the company has expanded to about 15 people plus many collaborators, a global sales network and over 60,000 registered users. In last year, over 30 universities in China have purchased Mnova. Since I joined this company in May 2008, I got to know Mnova people in person. I have been constantly impressed by their friendliness, openness, generosity, passion, diligence, and efficiency. It is a company full of energy and creativity. If you have a few minutes, take a look at Santi's blog <http://mestrelab.com/5-years.html>, you will see what I mean. Certainly, at conferences such as ENC, SMASH, ACS, and ASMS, you are welcome to stop by our exhibition booth and have a fun chat with us.



-By Chen Peng, Mestrelab Research



A Message from Dr. Jin-Shan Wang

Dear OCMRA friends:

Best wishes to all of you for Health and Happy New Year in 2010.

I hope you will be successful in your career and your dream will come true in this year.



J.S. Research 15th Anniversary

Thank you very much for your support and help to our company in past years. I hope to see you again in the upcoming 51st ENC at Daytona Beach FL in April 2010. We will celebrate the 15th anniversary of our company together!

On this wonderful occasion, I would like to tell you good news in China as following:

A 500 MHz 5 mm High Resolution NMR system has just completed in Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences. It passed the examination and got accepted by the consultant committee of specialists on December 29, 2009.

This research project is funded by Chinese National Plan of Development of Sciences and Technologies. The leaders of this project are Professor Chaohui Ye and Professor Jianqing Qiu. Our company was extensively involved this project.

My wife and I were invited to visit China to discuss about this project in April 2009.

During that time I introduced the history of ENC and OCMRA to the old friends. Also, I forward OCMRA web address and its newsletter to them. Finally, I would like to share some pictures from China in Beijing, Wuhan and Giulun with you.



Sincerely yours,

Jin-Shan

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Wuhan 武汉

Guilin 桂林



*****The End*****

Dear Friends,
 Our OCMRA committee wishes you and your family all the best for the year of 2010! Please join us at www.ocnmra.org. Let us stay connected as a strong community, help and support one another for many years to come! Please send your comments regarding our newsletter to Shan Liu (lius5@mail.nih.gov) or Yan-Yan Hu (huyy02@gmail.com). Hope to see you soon at our annual OCMRA meeting at 51st ENC!

