

## **2005-2007 LITRE Grant Proposal**

---

### **1. Project Title:**

Nuclear Magnetic Resonance integrated solution for Chemist , Biochemist and Polymer Scientist - FT-NMR- under Unity

---

### **2. Project Coordinator:**

**First Name:** Hanna

**Last Name:** Gracz

**Campus Address:** 128 Polk Hall, Molecular and Structural Biochemistry

**Email Address:** hanna\_gracz@ncsu.edu

**Campus Phone:** 919-515-8907

**Unity ID:** gracz

---

### **3. Other Participants:**

1. Dr. Ken Hanck

\*\*\*\*\*

September 12, 2005

MEMORANDUM

TO: Hanna Gracz

FROM: Kenneth Hanck, Associate Chair  
Interim Director NMR Facility

SUBJECT: LITRE Proposal

I am delighted that you have decided to re-submit your LITRE proposal for a second time. I am familiar with your project and I strongly support your idea of providing NCSU students and Faculty with NMR-(Nuclear Magnetic Resonance ) processing (FT-fourier transform) software, NMR prediction software (H1 proton and C13 carbon spectra) and data managing software which would be widely available under the NC State Eos/Unity network and environment. This software will be compatible with the existing software on a nine(9) high resolution and solid state NMR spectrometers available throughout the NCSU Campus. Students can easily generate high quality reports from acquired raw NMR data. The software enables the user to automate work and data flow.

As Director of the NMR Facility I would be more than happy to help implement an effective plan to acquire the new software. I oversee the use of the NCSU NMR Facility and I have been instrumental in keeping the facility at a level which addresses campus needs.

Based on my own experience, I am confident that the acquisition of new software can be a critically important addition to the instrumentation resources

available to the scientists in our University. We operate a variety of NMR instruments at NCSU NMR Facility. These instruments are fully subscribed on a 24 hr/day, 7 day/week schedule for state-of-the-art studies as well as a service samples.

It is critical that we do all the processing off line and distribute the data electronically. Doing so offers several advantages including:

\$ making the NMR method more visible in the University strong science and technology environment

\$ providing common platform –NMR processing software for users in different departments: Chemistry, Biochemistry, Plant Pathology, Botany, Wood & Paper Science, Chemical Engineering, Food Science, Toxicology, Soil Science, Textile and Polymer Science. etc.

\$ facilitating communication by improving the access and use of available NMR resources both within the NMR Facility and within NC State University

\$ providing the Faculty with the NMR expertise they need, to facilitate interdepartmental collaboration and project sharing

\$ helping Faculty to accommodate students individual learning style by enhancing available teaching and learning NMR tools

\$ providing students with modern electronic tools for NMR data analysis, spectra prediction and report writing with new technology.

I wish you the best of luck with your proposal, and if I can be of any additional help, please do not hesitate to call.

---

#### **4. College or Unit:**

: College of Agriculture and Life Sciences and College of Physical and Mathematical Sciences

---

#### **5. Department:**

Chemistry and Molecular and Structural Biochemistry

---

#### **6. Project Description:**

I would like to provide the NCSU students and Faculty with the NMR-(Nuclear Magnetic Resonance ) processing (FT –Fourier transformation) software , NMR prediction software (H-1 proton and C13-carbon spectra) and data managing software. The newly installed software would be widely available under the NC State Eos/Unity network and environment at every workstation through the Campus. This software will be compatible with the existing software on eight high resolution and solid state NMR spectrometers available at four locations- three building at NCSU Campus. Students will easily generate the report based on acquire raw NMR data. The software enables the user to automate work and data flow.

## 7. Project Objectives:

- 1.To improve general student learning skills in a field of physical chemistry and analytical chemistry
- 2.To make the FT-NMR method more visible in the University strong science and technology environment
- 3.To provide common platform –NMR Fourier transformation processing software for users in different Departments : Chemistry, Molecular and Structural Biochemistry, Plant Pathology, Botany, Wood & Paper Science, Chemical Engineering, Food Science, Toxicology, Soil Science, Textile and Polymer Science, Mechanical & Aerospace Engineering etc.
- 4.To facilitate the communication, improve the access and increase the use of available NMR resources within the NMR Facility and within the NC State University
5. To bring closer the Faculty with the NMR expertise and needs, to facilitate interdepartmental collaboration and project sharing
6. To help Faculty to accommodate students individual learning style by enhancing available teaching and learning NMR tools
- 7.To provide students with modern electronic tools for the NMR data analysis , spectra prediction and report writing. Learning with the new technology-electronic tools for the NMR research.

---

## 8. Estimated number of students affected:

Short term impact: 100 students/semester- All graduate students and postdoctoral fellows from NCSU working with Nuclear Magnetic Resonance Spectroscopy (NMR) as an analytical tool.

Long term impact: 200/semester- All undergraduate students taking the courses which includes NMR in their curriculum for example course #725 Chemistry - Analytical methods in Organic Chemistry.

\*\*\*\*\*

9 September, 2005

Dear Hanna,

I am excited that you are applying for the LITRE funding. I wholeheartedly support your idea to provide the NCSU students and Faculty with the NMR (Nuclear Magnetic Resonance) processing (FT - Fourier Transformation) software, NMR prediction software (1H proton and 13C carbon spectra), and data management software, which would be widely available under the NC State Eos/Unity network and environment. A great advantage to us is that this software is compatible with the existing software on a nine high resolution and solid state NMR spectrometers available on NCSU campus. Students will easily generate their reports based on acquired raw NMR data. The software enables the user to automate work and data flow.

As graduate student in Mechanical Engineering at NCSU I am more than happy to help implement an effective plan to acquire the new software. This software is especially useful to students such as myself, who are studying cross-disciplinary fields and may not have as much experience as a chemist. Based on my own experience, I am confident that the acquisition of new software can be a critically important addition to the instrumentation resources available to the scientists in our University. As the technology age drives us to more complex research, this software will undoubtedly help solidify our

university and as a leader in research.

This software package will allow us to do all data processing offline and distribute the data electronically. Thus we can provide a common platform for the entire university, i.e. NMR processing software for user in different Departments such as Chemistry, Biochemistry, Plant Pathology, Botany, Wood and Paper Science, Chemical Engineering, Food Science, Toxicology, Soil Science, Textile and Polymer Science. etc.

This will also help to facilitate communication between our scientists and increase the use of available NMR resources within the NMR Facility and within the entire NC State University.

Providing students with modern electronic tools for the NMR data analysis, spectra prediction and report writing is truly invaluable. I wish you the best of luck with your proposal, and if I can be of any additional help, please do not hesitate to call.

Sincerely

Brian P. Mosher

Graduate Student, Dept. of Mechanical and Aerospace Engineering  
North Carolina State University

\*\*\*\*\*

---

## 9. Outcomes of the Project:

If this project is successful:

- 1.It will improve general student learning skills in a field of analytical chemistry. It will break prejudice to the nuclear magnetic resonance methodology
2. Students will get more familiar with NMR.It will make the FT-NMR method more visible in the University strong science and technology environment.
- 3.It will provide common platform –NMR Fourier transformation processing software for user in different Departments : Chemistry, Molecular and Structural Biochemistry, Plant Pathology, Botany, Wood &Paper Science, Chemical Engineering, Food Science, Toxicology, Soil Science, Textile and Polymer Science, Mechanical &Aerospace Engineering etc.
- 4.It will facilitate the communication, improve the access and increase the use of available NMR resources within the NMR Facility and within the NC State University
5. It will bring closer the Faculty with the NMR expertise and needs, to facilitate interdepartmental collaboration and project sharing
6. It will help Faculty to accommodate students individual learning style by enhancing available teaching and learning NMR tools
- 7.It will provide students with modern electronic tools for the NMR data analysis , spectra prediction and report writing. Learning with the new technology-electronic tools for the NMR research.

---

## 10. Project impact on NCSU:

1. It will increase the awareness among the NCSU students and Faculty of importance of the NMR analytical methodology (See example Liposcience

–NMR based method patented and developed at  
NCSU-<http://www.liposcience.com/>)

2. It will enhance learning environment by providing the state of –the - art NMR software for every day use under Eos/ Unity academic computing environment
  3. It will increase speed and productivity in student learning
  4. It will close the existing gap of lack of standard electronic mechanism for NMR data distribution and processing at NCSU
  5. Long term impact will include cost savings. There will be substantial time savings for the staff of the NMR Facility.. Data will be distributed electronically and process by the person submitting a sample. It will shorten the turn around time and save the money to operate the NMR spectrometers.
  6. It will be in line with long term plans from Academic Affairs in CALS and PAMS: "Provide students with access to state-of-the-art equipment and technology"
- 

### **11. Project Assessment Plan:**

- Ad 1. Survey among users of the NMR Facility and particularly graduate students from chemistry, biochemistry, textile and polymer science, chemical engineering., natural resources, soil science, toxicology, botany and food science
  - Ad 2. Project report including students and Faculty comments,
  - Ad 3. Survey among users of the NMR Facility. Financial implication within the NMR Facility
  - Ad 4. Survey among users of the NMR Facility, numbers of interdisciplinary research papers
  - Ad 5. Numbers of research papers citing use of the NMR Facility
  - Ad 6. Increased rate of used of the NMR Facility
  - Ad 7. Evaluation process at the college level
- 

### **12. Staffing and Support:**

1. Staff support from the Computing Consultant & Resnet Technician NC State University Computing Services/Information Technology will help to install the NMR software under Eos/Unity and make sure lockers for the first 10 graduate students who will test the software have enough available space (\$500)
  
  2. Graduate Student assistant who will help to test laptop software and Unity software as well as help to train the first group of students. This training in the long run will be supported by the Web based instruction tools. (\$1000)
- 

### **13. Financial Support Requested:**

- EPA salary total:** \$1,000
- SPA salary total:** \$500
- Other salary:** \$500
- Equipment:** \$17,550
- Cost associated with assessment:**
- Other financial support requested:**

**Total Funds requested:** \$19,600

**Additional Explanation of how funds will be used:**

Equipment (including hardware and software):Laptop from DELL after the University discount-\$1400

ACD(Advanced Chemistry Development) –software :

ACD /2D NMR Processor- \$4,190

ACD/13CNMR&1HNMR Predictor. Prediction of proton and carbon NMR spectra-two software packages \$11,960 unlimited seat-network versions.

It will allow any 9 people on a network who could see the software to simultaneously use it.

\*\*\*\*\*

Optional : NMR Manager and Processor with improved Report Editor-\$7,170.

Software manages data from all the NMR instruments and combines the techniques and data into one data base for enhanced mining. The money will be used to acquire , install and test the appropriate software.

Laptop will be used to test installed software with each NMR spectrometer located along 4 rooms in Dabney Hall, one on Centennial Campus, Partners III Bldg and one in Wood and Paper Science Bldg..

---

**14. Funding Breakdown:**

**Total funding requested for fiscal year 2005-2006:** \$9,800

**Total funding requested for fiscal year 2006-2007:** \$9,800

---

**15. Staff Support and/or Technical Support Requested:**

Staff support from the NC State University Computing Services/Information Technology

10 hours@\$50/hr=\$500

Installation of Software packages under Eos/Unity

---

**16. Timetable for Implementation:**

1.Software purchase- 5 weeks from the data funding is available

2.Laptop computer purchase –three weeks from the time funding is available

3.Installing software on a Laptop and testing it with each NMR spectrometer.

Making sure the data can be transfer and successfully processed-

8 spectrometers and two main software packages .It will take 30 working days.

4.Software installation under Eos/Unity academic computing environment

It will take approximately three working days to install all of the software packages

5.Testing software packages under Unity environment 20 working days

6.Increasing lockers space for all interested graduate students-20 working

days

7. Training first group of 30 graduate students from Chemistry, Wood@Paper Science, Chemical Engineering, Mechanical and Aerospace Engineering, Textile whose research is NMR related and who are familiar with the NMR technique. This group will include the postdocs and graduate students from Biochemistry familiar with the range of NMR tools for protein structure solution.  
-40 days

8. It will take 5 (five) months to accomplish the main phase of a project

9. Full package should be implemented in the end of spring semester 2006 and accomplished in the spring of 2007.

---

### **17. Human Subjects Protection:**

If your proposal project involves research using human subjects, you will need approval from the Institutional Review Board for the Protection of Human Subjects in Research (IRB) prior to final approval. IRB information is available at <http://www.ncsu.edu/sparcs/irb>



---

### **18. Proposal Release:**

By submitting this proposal the applicant grants the LITRE Advisory Board permission to make this proposal available as an example for future grant applicants. All personal information will be removed if this proposal is used as an example.

