



Round Table Discussion Session 10:

Development of a Roadmap for Ultrahigh Field NMR/MRI/MRS Science in the US

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Discussion panel:
Jean Baum, Joanna Long, Chad Rienstra

Session Agenda

- ✓ Sustainable Mechanisms To Enable Transformational Science Requiring UHF MRI/NMR Technologies In The US
- ✓ Development Of A Roadmap For UHF NMR/MRI/MRS Science In The US
- ✓ UHF NMR/MRI/MRS Science In The US Workshop: Feedback From Program Officers
- ✓ Closing Remarks


Sustainable Mechanisms To Enable Transformational Science Requiring UHF MRI/NMR Technologies In The US

Models for sustained instrument deployment, infrastructure, funding, support

Infrastructure- models for national facilities (Joanna Long, Chad Rienstra)

Mechanisms for sustained support (Jean Baum)

Discussion (Everyone)



***Models for Sustained Instrument Deployment,
Infrastructure, Funding, Support***

Current Challenges for UHF Science In The US

- ✓ Establishing a good mechanism for extensive cooperation between facilities as if the facilities were one large consortium. (Think Advanced Photon Source and Beam lines as a set of facilities)
 - Each facility does not have to be optimized for all user activities. While many activities will likely be in common others such as ultra high temperature for materials would be only established at one or two facilities until the demand merits expansion into other facilities. Different focus in each center, complementary expertise, with some overlaps in capabilities and scientific themes.
 - Shared protocols equipment and reagents may lead to improved efficient usage of the instruments. The community has demonstrated their interest and willingness to cooperate in this way.
 - Involve broader community of non-NMR researchers as users of UHF facilities.
- ✓ Bleeding edge technologies
- ✓ Establish a coherent roadmap for development of multiple shared facilities with clear prioritization

Infrastructure- Models for Shared UHF Facilities in the US

The establishment of a sufficient number of National High Field NMR & MRI Facilities that develop enabling technologies in a broad range of science to take optimal advantage of ultrahigh magnetic fields and make them available to broad scientific communities throughout the US.

- ✓ These facilities will have state of the art commercial instrumentation as well as the ability to develop instrumentation for specific needs at the cutting edge of the spectroscopy and science. There is a great deal of room for these developments especially in an environment in which there is only one major NMR spectrometer manufacturer.
- ✓ These facilities will serve the entire high field NMR spectroscopy community in the US, much of it through remote access. While remote access works quite well today (as exemplified by the NHMFL facilities) there is much room for enhancing this capability. In order to serve the broad community an excellent web site must be developed that provides critical information and facilitates access.
- ✓ These facilities will establish working relationships with other facilities (such as APS) to leverage complementary technologies, e.g., SAXS, crystallography, cryo-EM, computation.

Instrument Deployment: Timelines, Instrumentation Types

- ✓ While the establishment of National High Field Facilities is the vision for housing the next generations of high field magnets, there is an urgent need for current and immediate next generation instruments for the biological, chemical and biomedical communities in the United States.
- ✓ An interim solution must be found so that American scientists can continue to pursue cutting edge materials, chemical, and biological science. This includes the need for 1 and 1.2 GHz as well as DNP instruments housed in local or regional facilities.

Toward Integrative Science Infrastructures

- ✓ Identify infrastructure opportunities for integrating NMR/MRI/MRS science with other complementary methodologies.

Infrastructure- Mechanisms for Sustained Support

Establish models for continued and sustainable funding mechanisms to support:

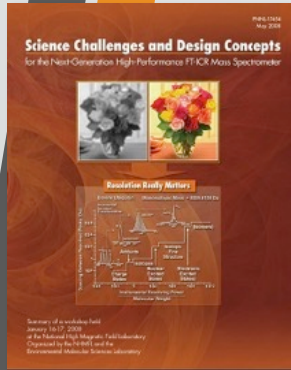
- ✓ Innovative infrastructure, equipment and highly qualified in-house personnel
- ✓ Equipment acquisition, operation, and maintenance in these facilities.
- ✓ Research and training of in-house and off-campus investigators.
- ✓ Off-campus investigator access (travel and accommodations) and usage of the facilities.

Likely sustainable support models will include partnerships between Federal, State, industry, philanthropy.

Infrastructure- Mechanisms for Sustained Support

- ✓ Establish mechanisms for attracting and sustaining young investigators for high field technology and applications.
- ✓ Establish mechanisms to recruit and retain trained technical and scientific personnel of the highest caliber in shared resources; this will ensure that users and on-site scientists will mutually push technological advances forward.
- ✓ Need to have agility in scheduling instrument time.

A Recent Timeline for a Large Instrument Acquisition



Science needs workshop held, recommendations



CD2/3a approved. (8/11)
EMSL begins spectrometer development (9/11)

Agilent begins magnet mfg (9/11); but late wire delivery

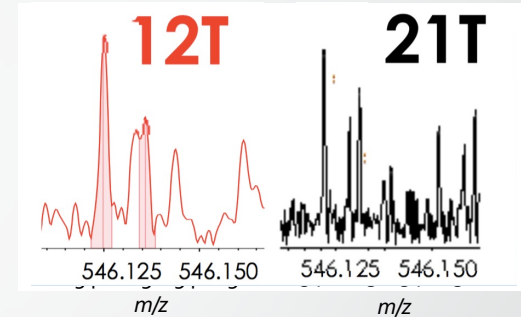
Magnet reaches field at Agilent factory (7/14)



Magnet delivered (11/14)

Magnet comes to field at EMSL (2/15)

First spectra obtained (3/15); first papers (4-6/15)



2008

2009

2010

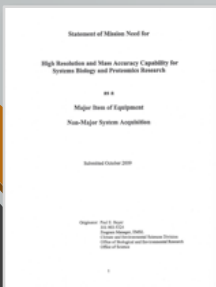
2012

2013

2014

2015

DOE approves Mission Need Statement (CDo) for HRMAC (10/09)



CD1 approved (9/10)

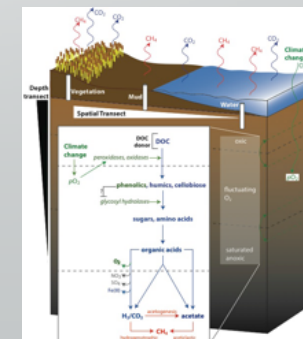
Magnet fails to reach field. Rework plans begin (12/13)

CD 2/3b approved (10/14)



Magnet accepted, HRMAC system completed (3/15)

Performance criteria met (6/30)



First science projects underway (7/15)

Project completion! (9/15)



***Roadmap for Ultrahigh Field
NMR/MRI/MRS Science In The US***

Post-Workshop

- ✓ **(1 week)** Disseminate the report of the meeting to the broader scientific community, through the workshop website
- ✓ **(4-6 weeks)** **Develop a roadmap for UHF NMR/MRI/MRS science in the US**
 - *Feedback from the broader scientific community including non-MR and MR researchers*
- ✓ **(sustained effort)** Work, as a community, to implement the roadmap

Roadmap for Ultrahigh Field NMR/MRI/MRS Science In The US

I. SCIENCE NEEDS AND BENEFITS

1. *Task force on science drivers for health sciences*
2. *Task force on science drivers for materials, catalysis, energy sciences*

II. TECHNOLOGY DEVELOPMENT

1. *Task force on superconductor development*
2. *Task force on cryostat and magnet design*

III. INSTRUMENT DEPLOYMENT AND FUNDING MECHANISMS, SHARED FACILITIES INFRASTRUCTURE

1. *Task force to establish sustainable models for shared UHF NMR/MRI centers in the US*
2. *Task force on the campaign for advancing UHF NMR and MRI in the US*

IV. SUMMARY RECOMMENDATIONS

Thank you!

- **Program committee**

William Brey, Brad Chmelka, Jeff Duyn, Angela Gronenborn, Jeff Hoch, Alexej Jerschow, Karl Mueller, Kamil Ugurbil

- **Task force leaders**

Brad Chmelka, Tim Cross, Lucio Frydman, Bob Griffin, Angela Gronenborn, Jeff Hoch, Alexej Jerschow, Kamil Ugurbil, Larry Wald

- **Leaders of EU UHF NMR Centers**

Lucia Banci, Lyndon Emsley

- **Speakers**

- **Session chairs**

- **Scribes**

- **All participants**

Thank you!

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