

ICR USER REPORT (Tuesday, November 01, 2005)

GENERAL: Now that ICR is part of the NHMFL Core Grant, this is a great opportunity to re-assess the ICR program and allocation of NHMFL resources.

In general, the User community is highly satisfied with the level of support and especially the quality of hardware for truly world class FT ICR MS. Sharing a desire to see the “footprint” of NHMFL to reach yet further *significance and impact*, an expansion of the type and scope of applications is recommended (*vide infra*). The goal is to translate the raw power of magnetic field into scientific pay off, ultimately validating and funding a 21 Tesla FT ICR MS system.

ICR User Support: There were 130 external users in 2004 calendar year. Carol Nilson is doing a fine job in her role of facilitating User activities and research. There is a strong recommendation to continue the ICR apartment. This is a critical component of facilitating visitor traffic to NHMFL.

21 Tesla ICR System: Alan Marshall is doing a great job in planning for this system in finding academic and corporate partners. PNNL (a DOE lab) and KBSI (in Korea) are validated as key partners to incentivize vendors to work with MS & T to get the job done in about 4-5 years. Specific requests:

- That this project be established as a main line item in the MS&T Budget.
- That funds not spent by the efficient ICR NSF facility be rolled into this MAIN line item in the MS&T Budget.

Below are four main concerns of the FT ICR MS User Community:

- 1. That** the new MIDAS data station for ICR systems is slow to be released to the community.
- 2. That** the impact of NHMFL in ICR could be even greater, particularly in natural products research and in proteomics, microbiology, and human cancer biology. The highest performance mass spectrometer in the world should be driving the next phase of maturation in the field (*i.e.*, large molecule mass spectrometry) and one or two large scale proteomics projects.
- 3. That** ICR is not requesting enough or getting enough resources from the Core Grant. New hardware (totaling about 200-300K) could and should be requested to expand the scientific scope and impact of the ICR program.

The User committee has a general concern that –relative to other programs not in condensed matter physics - the ICR program is not requesting or getting a requisite share of resources from the Core Grant. An interesting study would be to evaluate impact of such programs. No matter the result of such a study (often contentious), when impact would be normalized to resources infused, the ICR User committee is confident that the

results would show a startlingly high amount of value added to NHMFL by the ICR program. Further, with strategic planning supplied by key ICR, NMR, and EPR users, the “center of mass” of the entire renewal proposal can be elevated (Powerpoint slides for ICR to be provided to AGM and GB).

4. That expanded capacities for computational support in chemometrics and bioinformatics should be added to accelerate the realization of project endpoints and ultimately to amplify impact in these areas of application: petroleum research, small molecules (natural products), and high throughput proteomics.

Personnel: Two salary lines. An increased budget should be allocated for personnel in these categories:

1. senior analyst (a most important hire, since such a person can herd many young and inexpensive cats)
2. masters level computer scientist or statistician
3. Computational Support (2-3 undergraduates)

Proposal: “Strategic Users Program”: For EPR, ICR, and NMR, a Strategic Partners Program is proposed for the Director to muse about. This would consist of 2-4 external PIs that would have 1-2 grad student or postdoctoral lines of support (shared and run by committee and in association with Cross or Marshall). Strategic Users would compete for this status. This would draw top people in different fields into using EPR, ICR, and NMR technologies. Of course, supporting a broad User base without access to hardware will be maintained. The two most excited PIs were Kelleher (ICR) and Smith (NMR) by the prospect of such a program. At the time of renewal, such PIs –properly incentivized - could also add significant vision and energy to the renewal proposal.