

User Survey Summary

EMSL is committed to continually improving the users' experience. Although change cannot always be implemented overnight, we rely strongly on the input received from our user community and encourage you to continue providing feedback to our technical staff, our [User Support Office](#), and through the bi-annual survey. Users can also provide comments and feedback to the [User Executive Committee](#) and should feel free to contact anyone on the committee at any time.

Currently, user surveys are administered biannually for experimental users and are sent only to those individuals who have accessed our resources during the prior six months or annually for computational-only users and are sent only to those individuals who have accessed computing resources during the prior year. The results of the most recent survey are posted here with management responses to concerns or issues identified by our user community.

October 2014 Survey

Surveys Submitted Between October 11, 2014, and November 1, 2014.

Survey Satisfaction: 92.9 %

Survey Responses: 129

Surveys Sent: 532

Survey Response Rate: 24.2%

1. How satisfied were you with the availability of facilities and equipment?

- 80 Very Satisfied
- 47 Satisfied
- 5 Neither Satisfied nor Dissatisfied
- 0 Dissatisfied
- 1 Very Dissatisfied
- 1 Not Applicable

2. How satisfied were you with performance of facilities and equipment (e.g., were they maintained to specifications for your intended use, ready when scheduled, etc.)?

- 78 Very Satisfied
- 43 Satisfied
- 6 Neither Satisfied nor Dissatisfied
- 1 Dissatisfied
- 1 Very Dissatisfied

- 3 Not Applicable

3. List additional capabilities that you think EMSL should have.

User comments to this and other survey questions are below.

4. With the new knowledge gained at EMSL, I expect to (check all that apply):

- 125 Disseminate new knowledge via publication in peer-reviewed open literature
- 101 Disseminate new knowledge via presentations at professional society meetings
- 10 Acquire a patent
- 57 Further Department of Energy mission(s)
- 83 Facilitate collaborative interactions (e.g., stimulated new ideas for future experiment; increased work; etc.)
- 53 Train students (undergraduate, graduate or postdoctoral associate)
- 70 Use data for a future proposal
- 56 Establish or grow network and/or further collaboration
- 0 Other

5. How satisfied were you with the assistance provided by the EMSL technical staff?

- 88 Very Satisfied
- 36 Satisfied
- 5 Neither Satisfied nor Dissatisfied
- 2 Dissatisfied
- 0 Very Dissatisfied
- 2 Not Applicable

6. How satisfied were you with the assistance provided by the EMSL administrative staff?

- 87 Very Satisfied
- 34 Satisfied
- 7 Neither Satisfied nor Dissatisfied
- 0 Dissatisfied
- 0 Very Dissatisfied
- 6 Not Applicable

7. How appropriate and user friendly were the training and safety procedures?

- 55 Very Satisfied
- 48 Satisfied
- 6 Neither Satisfied nor Dissatisfied
- 3 Dissatisfied
- 0 Very Dissatisfied

- 22 Not Applicable

8. How satisfied were you with the proposal process (e.g. submission & review)?

- 47 Very Satisfied
- 46 Satisfied
- 11 Neither Satisfied nor Dissatisfied
- 4 Dissatisfied
- 1 Very Dissatisfied
- 24 Not Applicable

9. How did you learn about EMSL?

- 24 Scientific meeting/conference
- 8 Internet search
- 12 Journal publication
- 41 Previous EMSL use
- 49 Colleague
- 70 PNNL staff member
- 4 Other

USER ENDORSEMENTS AND COMMENTS

Although not all comments are shown, below is a representative sampling of the positive user comments received.

- Absolutely outstanding.
- Everything was perfectly organized and instruments were available as soon as I arrived.
- EMSL is a world-class facility, and it shows.
- The assistance of EMSL technical staff was invaluable to me and my research group.
- The point of contact was exceptionally well organized. I like the idea of working with a single point of contact, rather than each of the individual instrumentalists.
- The administrative staff was very helpful and they had everything sorted out ahead of time, so that we could work efficiently while we were at PNNL.
- The data has been fantastic and the results novel. We will have no problem publishing the data, primarily because of the well targeted use of these state-of-the-art instruments.
- The [scientific consultant] not only provided exceptional support, but has become an essential scientific collaborator on this project.

EMSL's Response

We appreciate your recognition of the efforts we make to provide outstanding facility operations, a stellar suite of instruments and dedicated scientific, technical and administrative staff. We especially want to call out Bruce Arey, Doug Baxter, Mark Engelhard, Andy Lipton, Danny Perea, Toni Quackenbush, Shuttha Shutthanandan, and Andreas Vasdekis who received special recognition for their outstanding expertise and assistance.

User Concerns and Suggestions

While user satisfaction rates very highly, we carefully review any comments in which users expressed concerns or suggestions for improvement. These have been compiled into several topical areas and representative comments are provided below, along with EMSL's response.

USER COMMENTS

OVERSUBSCRIBED INSTRUMENTATION OR STAFFING

- Scheduling has been a problem and we had periods where we had sent samples as requested, but nothing happened. I marked "satisfied" because when we do get results, they've been very good.
- Here is something that could be improved. It was not clear when [mass spectrometry] resources would be available and when samples would be processed once shipped to EMSL. It seemed like there was no specific order of when projects/samples are being processed. An online system that would allow the user to monitor sample processing would be great. Specifically, a system that tells the user how many other samples are in the queue in front of a particular sample of interest would be great.
- The performance is great, but I can't run a [computing] job long enough to get any results.
- ...When you get assistance, it's great. It just seems like the technical staff is over committed.
- The new policy on Cascade of a maximum job duration of 48 hours means that I cannot use the machine. My productivity has suffered. Unfortunately my code and the application - quantum mechanics on uranium oxides - with diagonalizing very dense matrices - does not parallelize well. Running them on 32 processors instead of 8 results in factor of 10 SLOWDOWN. LINPACK is what it is. Running on tacoma or olympus, my jobs will take more than a month. It's possible for me to run more than one job on a 32-processor core without much of an increase in latency, so I would put that processor to good use.

EMSL'S RESPONSE

The comments related to our mass spectrometry capability are certainly valid, and queue times have been increasing for several reasons. Older instruments are no longer being able to generate adequate data for our 'omics samples, requested analysis has proven more challenging than initially anticipated on some metabolomics samples, and we have not had enough staff to assist with the increased number of projects using mass spectrometry for their analyses. As a result, we

continue to invest in EMSL mass spectrometry capabilities and have planned for several instrument acquisitions in the coming year. In addition, plans are in place for adding new staff to support our users. Both the new state-of-the-art instruments and additional staffing should help address the difficulties with metabolomic samples and improve overall queue times.

EMSL's computing policies are in line for best practices at other supercomputing centers. We restrict jobs on Cascade from exceeding 48 hours because they tend to use just a few processors, which creates significant problems for scheduling large jobs. Cascade was designed to enable large jobs utilizing tens to hundreds, and occasionally thousands, of nodes. For smaller, but long-running jobs, users are encouraged to break them into consecutive shorter runs that generate a restart point partway through for improved scheduling. [MSC Consulting](#) and software staff are available to provide advice on the best approach for setting up your codes on Cascade, and users are encouraged to contact [Dr. Karol Kowalski](#) to discuss software applications before starting their Cascade use.

USER COMMENTS

TRAINING

- Several videos did not work on MAC computers.
- I approve of the approach, but more info should be given as to what training is needed when and when it needs to be repeated.
- I think the "test out" option on a few of the modules was very useful. This saved me a lot of time since I've completed this training many times.
- Computer documents inadequate

EMSL'S RESPONSE

PNNL's training department continues their multi-year plan to revamp both course content and delivery methodologies for their training courses. We want to especially thank the user who noted the new ability to "test out" of some of the training modules. This was implemented on more courses as just one step among many being considered.

PNNL training staff informed us that video performance issues in most cases are related to the web-browser or computer settings. For Mac users, they recommend launching training in Firefox (vs. Safari) and making sure pop-up blockers are off and computers are running the most recent version of Flash Play Plug-in. They also informed us that they are still in the initial conversion effort for course improvement, which focused on PC implementation. Once this effort is complete, they will expand the development standards to include Mac systems. To better assist you in the future with these types of problems, please be sure to contact the User Support Office directly and provide details regarding the training, specific video problems and error messages.

USER COMMENTS

TRANSPARENT PROCESSES AND COMMUNICATION

- My proposals were rejected in 3 years. The reviewer recommends to award my proposal but the committee rejected it without reasons.
- At the supposed user meetings the attendance was very low - i.e. 2 or 3 people (there should be at least 15 users) - and the CSMs did sometimes not attend and I did not have the feeling that I was at all informed about microscope issues in these meetings.
- Listing all of the collaborators and former students for all of the proposal participants was an unnecessary burden. Obviously, the panel can just see if there is a conflict by the names of the people on the proposal.
- I think the new review system is very worthwhile. However, it seems that the score cutoff is not calibrated properly and leads to a great deal of stress and confusion. My proposal ranked third in the specific science theme and had nothing but positive comments in the referee reviews. However, my proposal missed the cutoff and required an appeal by the science theme lead to be approved for the coming year. This just does not make sense to me, particularly since the referees noted nothing that needed work or could be improved in their written reviews. I recommend devoting effort to re-calibrating the proposal scoring cutoff.

EMSL'S RESPONSE

The proposal review process involves several steps. Proposals are reviewed by two to three members of the panel most closely aligned with your research. These individuals are responsible for providing the review comments and leading the discussion with the entire panel. They may recommend acceptance of a proposal during their initial evaluation, but may adjust their scores as proposals are calibrated during panel discussions. The entire review panel, however, is responsible for assigning the final score and ranking the proposals in priority order. This calibration of proposals is essential to ensure EMSL is selecting the best science within limited resource levels.

The panel is also responsible for setting a cut-off score for consideration. This score is set based on levels of resources available and quality of competing proposals. This cut-off score is then used throughout the following fiscal year to maintain equitable selection decisions between proposal calls and cycles. General cycles, for example, may receive fewer proposals and a proposal could rank 4 out of 6 but have an overall score that falls below proposals that could not be accepted in the annual Call due to resource limitations.

The ranked list of proposals is forwarded to the Resource Allocation Committee (RAC), which is responsible for estimating time and staff support costs needed by each proposal. Proposals are accepted by ranked order until either instrument time or staff support budgets are met. Proposals that are not accepted at this stage are rejected based solely on the lack of resources needed to support the scope. Decision notices provide the final score, the relative ranking within the proposals reviewed, and the Panel's summary comment. In addition, the letter specifies if the proposal was denied by the Panel based on overall scores or could not be accepted due to lack of

resources. If PIs receive decision letters without those details, please contact the User Support Office.

The recent requirement for a list of active collaborators was made so we could set a schedule that allows us to conduct a thorough review with the shortest turnaround possible for early notification to authors. That gives them time to find alternate resources for their research, if needed, or to begin preparing samples so they are ready as soon as the project is scheduled to start.

The list of collaborators -- a normal requirement in BER proposal calls-- allows us to identify the conflicts *prior* to assigning reviewers and avoid the delays caused when they decline assignments due to conflicts and we have to find new reviewers. Asking all panel members to look through the teams listed in all proposals submitted would similarly add significant delays.

To make this requirement more manageable, however, we revised our guidance for this year. Participation in very large collaborative efforts with an individual does not necessarily constitute a conflict of interest for purposes of our peer review process. Lists in excess of 100 collaborators per investigator can be shortened to include only the closest collaborators and we ask you to use your best judgment in these cases. In addition, PIs may substitute a list from a recent NSF, DOE, or other proposal that meets the spirit of this request.

USER COMMENTS

OPERATIONAL DELAYS OR DOWNTIME

- The project schedule got delayed for writing new safety documents for dealing with handling rad samples. The project was granted an extension to accommodate this delay. The project continues to make progress during this extension and is near completion.
- There do seem to be quite a few problems with the high pressure NMR probe for the 750 MHz NMR.
- Some problems caused by electrical outages were rather severe.

EMSL'S RESPONSE

The safety protocols for the different instruments available in our Radiochemistry Annex did take longer than expected and affected some of those proposals that were selected well in advance of our anticipated date for full operation. However, we are happy to report that all instruments are now available for radiological work.

The high pressure probe on the 750 MHz is a capability development project by our staff and is not expected to be fully accepted until mid-summer. While we allowed a few researchers to experiment with it, we thought we had adequately explained the status of the probe. Obviously there must have been some miscommunication, and we apologize for any issues our users were not expecting. Interested users can follow up with [Nancy Washton](#) to discuss the opportunities available when the capability is fully operational and online.

Unfortunately, we cannot fully prevent power outages and instrument downtime. Luckily, over our 17-year history, we have had only three power outages that lasted more than a second and we have a large standby generator for especially critical items. However, even minor interruptions, such as switching from the main power to a backup generator can cause component failures in our research instruments. We have, and will, continue working on ways to minimize the impact to our instruments, such as the use of standalone UPS connections, implementation of QC methods in our mass spectrometry capability to help identify residual problems from power outages, and the installation of a second power feed from the City of Richland with automatic switching that allows the City to provide power to EMSL if they lose one of their feeds.

USER COMMENTS

ADDITIONAL CAPABILITIES REQUESTED BY THE USERS

Molecular Science Computing:

- gp computer cluster
- "Molden" software for visualization of the geometries, vibrational frequencies, and orbitals from "Molpro" outputs

Spectroscopy and Diffraction:

- Tip-enhanced Raman imaging capability and Nsom setup (standard nsom)
- Raman spectrometer with 1800 groove/mm grating
- Small Angle X-Ray Scattering

Microscopy:

- A Vacuum transfer system from Transmission Electron Microscope to Focus Ion Beam or Atom Probe Tomography

Cell Isolation & Systems Analysis:

- Capability to culture microbes

Mass Spectrometry:

- 3D in-situ real time chemical mapping of aerosols
- Thermo FUSION
- Thermo Q Exactive HF
- Back-up generators/ (related to mass spec)
- LD FTICRMS

EMSL'S RESPONSE

Your suggestions for new capabilities have been provided to the Capability Leads and will be evaluated as part of our annual capital planning.

In response to previous concerns about the aging mass spectrometry instruments, we are in the process of acquiring a Thermo Fusion mass spectrometer that should come online by the end of FY2015. We have also partnered with PNNL to purchase a Q-Exactive system for targeted proteomics applications, and users will have access to a Q-Exactive HF system that PNNL purchased.

Recently, a 21T magnet has been installed as part of the high-resolution, mass accuracy capability (HRMAC) development project. This project is on schedule for completion in Fall 2015. A new AMS as well as GC-QTOF are also under development or have been approved for purchase. In addition, we are continually investigating advanced separation technologies including size-exclusion chromatography and will implement these into our workflows when feasible and advantageous.

For details of available instruments or to provide more information of instrument needs to support the experiments you have in mind, we encourage you to talk to the appropriate Capability Lead (<http://www.emsl.pnl.gov/contacts/>) or your host.