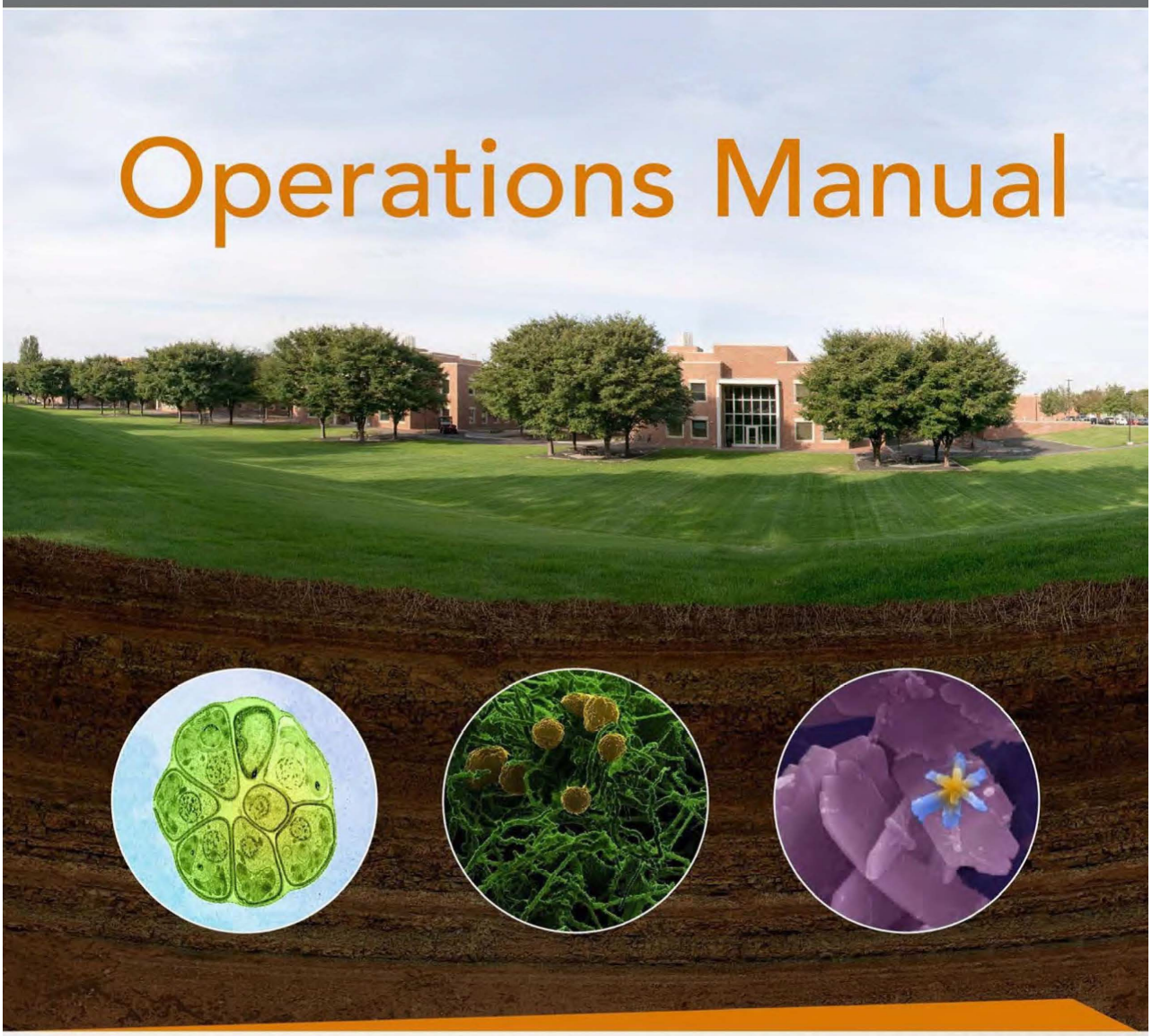
EMSL

Operations Manual



Prepared for the U.S. Department of Energy, Office of Biological and Environmental Research, Climate and Environmental Sciences Division

U.S. DEPARTMENT OF ENERGY

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EMSL Operations Manual

Contact: Rick Washburn, Lead Project Manager

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under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99354

Acronyms and Abbreviations

AI	Artificial intelligence
AP	Additional Protocol
BAM	Budget Allocation Meeting
BER	DOE Office of Science, Office of Biological and Environmental Research
CAM	Computing, Analytics, and Modeling
CDO	Chief data officer
CLA	Contributor License Agreement
CM	Commercialization manager
COI	Conflict of interest
COO	Chief operations officer
CRADA	Cooperative Research and Development Agreements
CSO	Chief science officer
DOE	U.S. Department of Energy
DOI	Digital Object Identifier
EBSD	Earth and Biological Sciences Directorate
EMSD	Environmental Molecular Sciences Division
EMSL	Environmental Molecular Sciences Laboratory
ERecords	Electronic Records *(formerly HPRM and TRIM)*
ESS&H	Environment, Safety, Security and Health
ETI	Environmental Transformations and Interactions
FICUS	Facilities Integrating Collaborations for User Science
FSB	Functional and Systems Biology
FY	Fiscal year
HBCU	Historically black college and university
HDI	PNNL's How Do I instruction system
HUPO	Human Proteome Organization
ISNI	International Standard Name Identifier
IRB	Institution Review Board
IRP	Integrated research platform
IRPL	Integrated research platform leader
JGI	Joint Genome Institute
LOI	Letter of intent
LPM	Lead project manager
ML	Machine learning
MOA	Memorandum of Agreement
MONet	Molecular Observation Network

MSI	Minority serving institution
NMR	Nuclear magnetic resonance
NPUA	Non-Proprietary User Agreement
OSTI	DOE Office of Scientific and Technical Information
PB	petabyte(s)
PC	Project coordinator
PI	Principal investigator
PM	Project manager
PNNL	Pacific Northwest National Laboratory
PNSO	Pacific Northwest Site Office
PPE	Personal protective equipment
PRP	Proposal review panel
PUA	Proprietary User Agreement
R&D	Research and development
ROO	Research operations officer
ROR	Research Organization Registry
S&T	Science and technology
SAL	Science Area leader
SC	DOE Office of Science
SPP	Strategic Partnership Project
STAC	Science and Technology Advisory Committee
SC	DOE Office of Science
STI	scientific and technical information
TDO	PNNL's Office of Technology Deployment and Outreach
TTO	Technology Transfer Ombudsman
UEC	User Executive Committee
UPS	User Program Services
WBS	Work breakdown structure

Contents

1.0 Introduction

EMSL - Environmental Molecular Sciences Laboratory is a Department of Energy (DOE) Office of Science national scientific user facility that is funded and sponsored by DOE's Office of Biological and Environmental Research (BER). As a user facility, our scientific capabilities—people, instruments, and facilities—are available for use by the global research community. We support BER's mission to achieve a predictive understanding of complex biological, Earth, and environmental systems for energy and infrastructure security, independence, and prosperity. BER seeks to understand the biological, biogeochemical, and physical processes that span from molecular and genomics-controlled scales to the regional and global scales that govern changes in watershed dynamics, climate, and the Earth system. We believe that a deeper understanding of critical molecular-level processes is necessary in each of these areas to understand, predict, and ultimately manipulate and control complex environmental and energy systems.

EMSL approaches science differently than many institutions. We believe in—and have proven—the value of drawing together members of the scientific community and assembling the people, resources, and facilities to solve problems. We integrate experts across disciplines and experiment with computing and simulation, and our user program proposal calls with other user facilities demonstrate this integration.

Operationally, our approaches and systems are designed to be transparent in support of a diverse, productive, collaborative, and highly impactful user community. In support of this, EMSL is officially registered with the International Standard Name Identifier (ISNI) organization (ISNI ID: 0000 0004 0373 6523). ISNI acts as a bridge identifier across multiple domains, including Ringgold Inc. (124574), Research Organization Registry (https://ror.org/04rc0xn13), Global Research Identifier Database (grid.436923.9), OrgRef (19642725), and Wikidata (Q5381141). In addition, EMSL data products can be found using the DOI prefix 10.25582, and EMSL awards can be found using the DOI prefix 10.46936.

EMSL's Operations Manual is a general resource tool to assist EMSL users and laboratory staff within EMSL to locate official policy, practice, guidance, and associated subject matter experts. It is updated at least annually at the beginning of each fiscal year and as needed based on budgetary changes, BER priorities, management decisions, advisory committee recommendations, etc. All changes are recorded in the change control record, which can be found at the end of this manual in Section 21.0. It is not intended to replace or amend any formal Battelle policy or practice. Users of this manual should rely only on Battelle's How Do I (HDI) for official policy. No contractual commitment or right of any kind is created by this manual. Battelle management reserves the right to alter, change, or delete any information contained within this manual without prior notice.

2.0 Mission and Vision

EMSL's mission as a national scientific user facility is to provide access to premier multimodal molecular science instruments, data analytics, production computing, and multiscale modeling to enable researchers to study biotic and abiotic processes and understand their function in a systems context for energy and environmental security and infrastructure resilience.

EMSL's vision is for a research community empowered to study the role of molecular processes in controlling the functioning of biological and ecological systems across spatial and temporal scales and to enable a predictive understanding of the living Earth system.

3.0 EMSL Science Areas

3.1 EMSL Science Areas

During its third decade of operation, EMSL plans to optimize scientific productivity by focusing scientific leadership and capability development on grand science challenges within three EMSL Science Areas: Functional and Systems Biology, Environmental Transformations and Interactions, and Computing, Analytics, and Modeling. These Science Areas were developed in collaboration with the scientific community and leadership from the DOE-BER leadership. More information on each Science Area is provided in the next three sections. Each Science Area is led by a Science Area leader (SAL), and each Science Area is organized into integrated research platforms (IRPs). Each IRP also has a leader (IRPL). Although each Science Area focuses on drivers important to that field of science, there are significant mutual and complementary scientific interests, including the common need to understand the impacts of complexity and the importance of many types of interfaces. Thus, the scope of a user/research project in EMSL may impact all three Science Areas and may extend to other valid scientific questions that can make use of EMSL's capabilities. Science Area research is enhanced when combined with advanced data analytics and visualization, computational modeling and simulation, and efficient parallel software. Thus, users are encouraged to combine computation with EMSL's state-of-the-art experimental tools to create an integrated platform for scientific discovery.

3.2 Functional and Systems Biology

The **Functional and Systems Biology (FSB)** Science Area focuses on characterizing enzymes and biochemical pathways to connect protein structures and metabolic functions to complex phenotypic responses. EMSL's rich approach to phenotyping incorporates interactions within cells, among cells in communities, and between cellular membrane surfaces and their environment for microbes (archaea, bacteria, protists, viruses, algae, and fungi) and plants. A fundamental understanding of biological processes is enabled by multiscale experimental observations, metabolic reconstruction, and modeling, leading to rich datasets. These datasets can be used to improve strategies for designing plants and microbes for biofuels and biobased products, as well as unraveling the complexities of carbon, nutrient, and elemental cycles within cells and their immediate environment.

Three IRPs support FSB scientific research:

- The Structural Biology IRP enables users to obtain structural, biochemical, and dynamic information about proteins, protein complexes, and other biomolecules at nanoscale spatial and temporal resolutions to infer function.
- The Biomolecular Pathways IRP enables users to investigate the translation of genomic information into functional relationships among biomolecules within cells in response to changes in their internal or external environment.
- The Cell Signaling and Communications IRP enables users to reveal dynamic interactions and trafficking of molecular signals between cells, populations, and communities to understand complex inter-relationships between organisms in response to their environment.

Point of Contact: Scott Baker, John Bargar, and Jay Bardhan, Science Area Leaders
Note: Level 1 Document; requires DOE approval
Current Version: July 15, 2024
Previous Version: June 15, 2023
Last Reviewed: July 15, 2024

3.3 Environmental Transformations and Interactions

The **Environmental Transformations and Interactions (ETI)** Science Area seeks to understand molecular and microscale processes controlling the transformation and transport of critical constituents across scales to predict ecosystem response to change. These include carbon, critical nutrients, minerals, volatile emissions, and aerosols. ETI user science focuses on developing mechanistic and predictive understanding of environmental (physiochemical, hydrological, biogeochemical), microbial, plant, and ecological system function in soil and subsurface ecosystems, in the atmosphere, and across their interfaces. EMSL provides experimental, computational, and simulation expertise along with a wide variety of advanced capabilities to enable users to understand the functioning of environmental and ecological systems from the subsurface to the atmosphere, from the terrestrial to aquatic, and from land surface to atmospheric interfaces. Experiment and modeling approaches and their associated data and simulation outputs, in collaboration with the Computing, Analytics, and Modeling group, accelerate mechanistic understanding of coupled soil–microbe–plant–atmosphere molecular processes and their interdependencies, ultimately informing models of ecosystem processes and land–atmosphere interactions at larger scales. Three IRPs support ETI scientific research:

- The Biogeochemical Transformations IRP enables users to investigate the biochemical, physical, and microbial processes that affect chemical speciation, transformation, and transport of carbon, critical nutrients, and minerals within the environment.
- The Terrestrial-Atmospheric Processes IRP enables users to discern the emission mechanisms of aerosols and gases from plants and soil into the atmosphere and developing an understanding of the multiphase interfacial chemistry and aging processes occurring near Earth's surface and extending up to the atmospheric boundary layer.
- The Rhizosphere Function IRP enables users to investigate the impact of the root system architecture and rhizodeposition on the molecular and structural mechanisms of root–soil–microbe interactions. A primary goal is to improve the prediction of root-controlled processes and their impacts on plant resilience, nutrient cycling, and volatile emissions under environmental change.

3.4 Computing, Analytics, and Modeling

The **Computing, Analytics, and Modeling (CAM)** Science Area brings advanced data analytics, visualization, and computational modeling and simulation to bear on increasingly complex multimodal experimental data to develop a predictive understanding of biological and environmental systems. A major focus is on improving the integration of experimental and computational methods that both advances predictive approaches to biodesign for biofuel and bioproduct production and accelerates research to understand the molecular mechanisms underlying biological and hydro-biogeochemical processes controlling the flux of materials (e.g., carbon and nutrients) in the environment.

Currently, two IRPs support CAM scientific research:

- The Systems Modeling IRP enables users to focus on delivering state-of-the-art modeling approaches to accelerate the prediction and control of complex systems in BER priority areas. The System Modeling IRP's priorities are to enable scientific discovery in biological and environmental sciences using scientific computing approaches and to accelerate the integration of modeling and EMSL's experiments through advances in artificial intelligence/machine learning (AI/ML).
- The Data Transformations IRP enables users to deliver state-of-the-art data science capabilities for exploratory data analysis and data integration and for curating and preparing datasets for release to the data science community to catalyze data science research in directions relevant to BER. The Data Transformations IRP is also

leading efforts to realize the potential of generative AI (e.g., large language models) to accelerate discovery by facilitating access to diverse, distributed datasets that span multiple disciplines.

4.0 Definition of an EMSL User

To uphold the value of user statistics, the Office of Science has established a set of shared core principles for defining and counting users. These principles, along with definitions for each user facility, can be found at http://science.energy.gov/user-facilities/. For the purposes of reporting EMSL user data to DOE, the following definitions will apply.

User Definition: An individual who makes use of EMSL resources. Each user will be categorized as one of the following:

- **On-site User** – An individual who is a member of an approved research team, has signed all required user agreements, and is physically present using an EMSL capability, at least once during the reporting period, to conduct research on an active peer-reviewed project.
- **Remote User** – An individual who is a member of an approved research team, has signed all required user agreements, and has been granted authority by the principal investigator (PI) to participate remotely in experimental planning, execution (including remote operation of instrumentation/computing hardware or engaging with EMSL staff on sample submission/delivery), and data analysis on an active peer-reviewed project.
- **Data User** – An individual who registers for an EMSL user account and downloads data from EMSL's public data portal during the current reporting year, but did not participate in the collection, calibration, or reconstruction of those data.

User Counts: An individual is counted as a user only once per fiscal year (FY) despite their number of active projects or data downloads. When a user qualifies in more than one category, EMSL follows a hierarchical scheme, in which On-site takes precedence over Remote and Data, and Remote takes precedence over Data. EMSL staff and Resource Owners are not included in user counts.

Reporting: Reports sent to the DOE program manager for EMSL and DOE leadership will contain year-to-date counts, unless otherwise specified by DOE, and the user data will be posted on EMSL's website.

Note: For reporting the numbers of users or institution types by proposal type, users with multiple user proposal types will be counted once per proposal type. However, only distinct users are included when reporting the total number of users per FY. EMSL Staff and Resource Owner proposals are not included when reporting User proposal data.

"EMSL resources" are defined as all resources purchased or co-purchased by the User Program and all resources located in space that EMSL maintains or manages.

Example of EMSL's reporting mechanism for user and proposal statistics:

User and Proposal Statistics

Fiscal Year 2023 (October 1, 2022 to September 30, 2023)

	Breakdown by Proposal Type				Total Distinct	
	Call Responders	Capacity	Limited Scope	Scientific Partner	FY2023	Year End FY2022
Active Proposals					**Distinct Active Proposals**	
Total Active Proposals	150	64	23	2	239	244
Users					**Distinct Users**	
Total Users	492	204	33	2	683	744
Users by Type					**Distinct Users by Type**	
Onsite Users	97	78	6	1	175	174
Remote Users	395	126	27	1	508	570
Data Users	0	0	0	0	0	0
Users by Institution					**Distinct Users by Institution**	
Academic	253	18	25	0	289	330
DOE Laboratory (Other)	63	2	2	0	66	60
Foreign	42	0	1	0	43	47
PNNL	115	184	1	1	263	290
Industry	4	0	2	1	7	6
Other	15	0	2	0	15	11

Call Responders: User proposals that are part of EMSL's advertised call for proposals include Exploratory Research, Facilities Integrating Collaborations for User Science (FICUS) Research, Large-Scale EMSL Research, and Molecular Observation Network (MONet).

5.0 EMSL Proposal Types, Review Process, and Peer Review Criteria

Access to EMSL is governed by a merit-reviewed proposal process with different proposal opportunities available to facilitate access based on user needs while assuring EMSL capabilities are used to address cutting-edge science questions. The processes described below for proposal solicitation, review, and allocation continually evolve and leverage user feedback to provide a clear and reasonable process that remains consistent with the expectations of our users and BER.

5.1 Proposal Types

To maximize the impact of EMSL research, there are a variety of proposal opportunities available for both users and staff members. All proposals, whether user or staff, are submitted via EMSL's User Portal and undergo management and merit reviews. Although access may be available for research whose information or intellectual property is restricted, most research conducted at EMSL is nonproprietary with results shared with the scientific community through publications in open literature or conference presentations and papers.

5.1.1 Proposal Review

EMSL follows a graded management and merit review process based on the proposal type and scope of the project as identified by the author on the application. Proposals may be denied at any point during the review process, at which point the author receives electronic notification of the reasons for denial along with requirements for resubmittal if the author is eligible.

5.1.1.1 Internal Management and ESS&H Review

Once the proposal has passed the screening and technical review, concurrent internal management reviews occur. Proposals likely to be funded or approved are reviewed by qualified individuals in the following EMSL support offices:

- **Business:** To ensure all research is conducted under a fully executed DOE user agreement or other contracting mechanism, such as a Cooperative Research and Development Agreements **(**CRADA) or subcontract. For details regarding the DOE user agreements, see Section 14.0. Proprietary work is assessed for appropriate cost reimbursement, etc.
- **Environment, Safety, Security, and Health (ESS&H):** To assess hazards and work scope to ensure work is appropriate for both EMSL's operating envelope and the specific workspace involved and compliant with current export control regulations.

Depending on the research scope as identified by the author in the request, the proposal may also be reviewed by the following subject matter experts below. Proposals involving these above-standard hazards require a special appendix to provide detailed information on the study.

- **Animal and/or Human Subjects:** To ensure review and approval by the Animal Care and Use Committee and/or the Institution Review Board (IRB) for Human Subjects.

- **Radiological:** To ensure research involving radiological samples is reviewed and approved by EMSL's radiological engineer and chief operating officer as appropriate for the operating envelope for EMSL space. In addition, although not a formal reviewer, EMSL's research operations manager is notified of these proposal requests.
- **Project Management:** If any of the additional hazards above are identified, the proposal will be reviewed by EMSL's Project Management Office Director to ensure project risks are appropriately managed within EMSL's operating envelope.

5.1.1.2 Merit Review

Concurrent with the management and ESS&H reviews, merit review is conducted on a graded approach, balancing the effort of assessment against the impact on EMSL resources. Depending on the type of use requested, some proposals require both external and internal review; others require internal merit review only. In general, review is based on five review criteria that were developed in concert with BER.

Internal Merit Review

General proposals undergo internal review only to meet the special needs of the project. The IRP obtains an internal scientific review to assess the merit of the research objectives. For EMSL Staff Time proposals, the team leader or group leader provides the merit review. For EMSL's intramural research and development (R&D) program, the CSO or their delegate convenes a review panel consisting of internal and external reviewers to assess the merit of the research against EMSL's strategic science objectives. For further details about the EMSL staff proposal review processes, see Sections 8.0 and 9.0.

External Peer Review

All user proposals competing for budgetary support from the User Program are reviewed by scientific experts from the external research community.

- ***Proposal Review Panels.*** A proposal review panel, or PRP, is established for each Science Area and at a minimum comprises the SAL, the lead project manager (LPM), and external experts from the Science Areas represented in the annual call. Each proposal is assigned to at least two members of the PRP, who each comment and score the proposal on the criteria in Section 5.3. The PRPs then review the recommended score and adjust it based on their discussion.

  The combined criteria scores establish a preliminary ranking of the proposals. PRP members assigned to the proposal serve as the spokespersons to initiate panel discussion. The PRP members are not required to come to a consensus of the criteria scores, but they are responsible for confirming the final score for each criterion and ranking the proposals according to the composite scores. Although preference may be given to proposals related to the specific topics within the annual call, PRPs may also identify high-quality proposals that do not fit within the call and recommend these in a prioritized list for consideration at the EMSL director's discretion.

  Projects that will begin their second year will be evaluated by the project manager (PM) and IRP leader. Projects lacking progress and/or communication with EMSL without sufficient justification will not continue into the second year. Projects denied a second year will have the concurrence of the PM, IRP leader, SAL, and LPM.

- ***Special Independent Reviews.*** Because of the strategic scope and unique purposes of the scientific partner projects, a special merit review process is followed. Proposals are first reviewed for strategic alignment with the EMSL User Program, user/scientific impact and need, resource and time requirements, and impact to staff development. If the proposal passes this evaluation, external review is conducted by select members of EMSL's advisory committees and/or identified experts in the scientific field. See Section 7.0 for further details.

5.1.2 User Proposals

EMSL offers three types of user proposals that are grouped into (1) annual calls, (2) general proposals, and (3) scientific partner proposals. In addition, EMSL may from time to time announce **special calls** outside the annual call schedule. Preference is given to user proposals submitted in response to announced calls for proposals.

Annual Call Proposals: EMSL has two primary award cycles each year: one beginning December (winter cycle) and one beginning June (summer cycle).

- The winter cycle typically involves several options, including calls to focus on topics of interest in EMSL's Science Areas (Large-Scale EMSL Research), use multiple facilities (as part of FICUS), or team with EMSL scientists on larger projects (Research Campaigns). Projects typically have an award duration of up to 24 months. Projects are reviewed after 1 year and can be closed because of inadequate progress and/or communication from the PI team.
- The summer cycle is targeted toward exploratory research in topics of interest in EMSL's research program that can be accomplished in 9 months. This cycle may also be used to target the call to certain audiences or groups of researchers.

Both cycles encourage proposals that couple experiments with modeling or simulation, and proposals are awarded time on a full or partial FY basis. These proposals receive priority access to instrument time and receive the bulk of EMSL-funded staff support to work with the research team.

For applications to the annual calls, an initial letter of intent (LOI) must be submitted before a full proposal, and full proposals may only be submitted by invitation.

Calls for proposals are advertised through a variety of formal and informal methods. These include notices on our website, alerts in the User Portal (EMSL's web-based user tool), email, social media announcements, targeted emails to BER program managers for distribution to their PIs, internal Laboratory notifications, and informal correspondence by our scientists to colleagues. Details of the annual calls and any special requirements are provided in the call announcements.

Winter Cycle (for access beginning October 1 following award decisions):

- **Large-scale EMSL research topics.** Each year, the call for Large-Scale EMSL Research proposals identifies selected topics of interest within each of EMSL's Science Areas. The topics announced in each call are developed by the Science Area leads, in concert with EMSL and DOE leadership, to focus user activities to accelerate results in emerging science areas of interest to EMSL, BER, and DOE. Accepted projects are valid for 24 months.
- **Requests to use multiple facilities.** The call for FICUS Research proposals includes opportunities to request the use of multiple user facilities with one proposal. Joint facility applications are part of the FICUS program,

which was initially developed by user facilities stewarded by DOE-BER. Applications typically follow special proposal requirements and review processes, and details are provided with the call. For example, the call between EMSL and DOE's Joint Genome Institute (JGI) provides a unique opportunity for researchers to combine the power of JGI's genomics and EMSL's unique imaging, -omics, and computational resources in one research project. Accepted projects are valid for 24 months.

Teaming on research campaigns. The winter cycle may include opportunities to partner with EMSL staff and other research teams on topics that require multiple methods and approaches for combined experimental and computational research and advanced data integration. These campaigns are typically multi-institutional and larger in scope. Research campaigns require an LOI, and selected authors are invited to work with EMSL staff to develop more fully a project plan to be submitted as a full proposal. Research campaigns can be valid for multiple years and will be based on the selected project design.

Summer Cycle (for access beginning January following award decisions):

- **Exploratory research topics.** Each year, the call for exploratory research proposals seeks to target specific audiences or research areas and may identify topics of interest within each of EMSL's Science Areas. With PRP recommendation, this is also a chance for authors to resubmit revised proposals from the large-scale research call. There are additional requirements for the proposal package when authors are resubmitting a proposal based on the PRP recommendation.

Special Calls for Proposals. On occasion, researchers may have opportunities to request access through special science calls that are announced outside the normal call cycles. These calls will typically follow unique proposal submission, review, and access schedules.

General Proposals. General proposals are smaller-scale research projects that allow researchers to get acquainted with the staff and capabilities at EMSL outside the annual award cycles in December and June. A variety of proposal opportunities are available, and the scope can vary from a single, focused experiment to a multiresource set of studies. General proposal types can vary in duration and are based on either calendar or fiscal year.

- **Limited Scope.** Requests for short-term proposals to conduct a limited scope of work outside EMSL's advertised calls for proposals. Requests are accepted on a limited basis at the discretion of management based on current staffing, available budget, and instrument pressures. Preference is given to BER focused research. If approved, the entire scope of the project must be completed within a 90-day EMSL access window, except projects within the CAM Science Area, which must be completed within 120 days.
- **Contracted Time.** Requests to use contracted time on instruments that are owned by the EMSL User Program. Annually, a set number of hours on instruments available for contracted time will be established by the EMSL chief operations officer (COO) in consultation with the IRP leaders, instrument custodians, and the user program services office. Quarterly available hours will be advertised through the EMSL website and will be available to external and internal entities until they are expended. Available hours will be reviewed and updated as needed quarterly. External entities will need to establish a contract with Pacific Northwest National Laboratory (PNNL) to access the instruments and fund instrument custodian time. Data generated via contracted time projects not associated with a BER-funded project will be provided to the user but not archived by EMSL.
- **Proprietary.** Business sensitive or proprietary research where results are not intended to be published. Researchers who do not intend to publish results and request their information be kept as business sensitive or proprietary must provide a contract mechanism (charge code or subcontract number) to cover associated labor

and/or instrument time depending on the restriction of data. Proposals containing restricted information will be reviewed under special protocols to maintain confidentiality. For non-federally funded proprietary work, the DOE requires payment for full-cost recovery of the facilities used, which includes, but is not limited to, labor, equipment usage, consumables, materials, and EMSL staff travel. Unlike limited scope and capacity proposals, access is granted for up to one *calendar* year. Data from these projects are provided to the user but not archived by EMSL.

Scientific Partner Proposals. These proposals may be submitted at any time throughout the year by individuals or groups who wish to partner scientifically with EMSL staff to enhance an existing capability or develop and build unique new capabilities that enhance EMSL's user program. Capability development efforts that utilize collaborative multidisciplinary teams, pooled or leveraged resources, unique operating environments, or other resources that may be beyond those available to individual researchers or teams are encouraged. Scientific partner proposals are intended to leverage the combined resources, expertise, and capabilities of the partner institution to maximize impact for EMSL, the partner, and future EMSL users. In return for co-development, EMSL scientific partners may have priority access to the new capability for a negotiated and specified period. The award and timing of EMSL scientific partner projects are contingent upon EMSL strategic needs and the availability of EMSL resources.

Exploration of this type of partnership begins with an LOI that is emailed to EMSL's chief science officer (CSO). The LOI will be considered at any time throughout the year and should initiate a dialog on suitability, interest, and strategic need for the capability and include short descriptions of the significance, impact, outcome, approach, resources, EMSL and partner contributions, and the team. After approval of an LOI, the primary investigator will be asked to submit a full proposal through the EMSL User Portal, which will go through management and special independent review. Proposals are expected to address innovation, significance and impact, relevance to EMSL roadmap/users/BER science, the advantage brought by the partnership, and the resources and timing. Proposals are valid based on the agreed-upon scope and duration but are reviewed regularly for progress by the CSO and chief data officer (CDO). For full details of this program, see Section 7.0.

Table 1. User Proposal Types Available

Proposal Type	Call / Submission Dates		Research Focus	Duration	Merit Review
Large-Scale EMSL Research*	Calls open late December to early January	Due dates vary by Call	PI-initiated scope based on call topics in EMSL's Science Areas	24 months	External Reviewers
FICUS Research*			PI-initiated scope based on call topics defined jointly with multiple facilities	24 months	
Research Campaign*			EMSL-initiated scope for larger campaigns to advance strategic science	Defined in Call	
Exploratory Research*	Call opens June	Due dates may vary, but usually mid-summer	PI-initiated scope on calls to targeted user communities	9 months	
Scientific Partner*	Any Time		PI-initiated scope for capability development	Negotiated	
Limited Scope			PI-initiated research scope	90 days, 120 days for CAM projects	Internal Reviewers
Contracted Time				Up to 1 fiscal year	
Proprietary*			PI-initiated research scope not intended for public dissemination	Up to 1 calendar year	

*Proposal type requires a Letter of Intent

5.1.3 EMSL Staff Proposals

Two types of proposals track utilization by EMSL staff on their own research: EMSL Staff Time and EMSL Intramural Science and Technology (S&T) Program proposals. Proposals are submitted through the User Portal and are subject to internal management, safety, and merit reviews.

EMSL Staff Time Proposals. Per the Utilization Policy, up to 10% of the available instrument time is open to Environmental Molecular Sciences Division (EMSD) staff members to help advance their scientific careers through independent or collaborative research, with an additional 10% made available at the EMSL director's discretion. This research is expected to result in EMSD staff publications or externally funded programs. To utilize this benefit and track instrument use, staff submit EMSL staff time proposals that are valid for up to three years, with annual evaluations against progress and instrument utilization. Access is subject to approval by the appropriate IRP leader, team leader, or group leader. Internal health, safety, and environmental reviews are also required. For more details, see Section 8.0.

EMSL Intramural Program Proposals. These proposals are submitted under a competitive intramural program for directed R&D efforts aligned with EMSL's strategic goals. This program offers three tiers of support for EMSL and PNNL staff to propose ideas that would add important capability or expertise to the EMSL user program and enhance the professional visibility of staff. Calls for proposals are issued internally, and proposals are routed through the User Portal for selection and merit review. Access duration varies according to the tier requested and is based on successful completion of milestones. For more details, see Section 9.0.

5.2 Submitting a Proposal

All proposals are submitted online via the EMSL User Portal (https://nexus.emsl.pnnl.gov/Portal/), following annual guidance on the website. Upon submittal, User Program Services (UPS) receives notification to initiate the screening and review process.

5.2.1 Proposal Screening and Technical Review

Proposals are screened by UPS to determine if the required information is present, and the proposal package adheres to the published guidance. If the proposal passes screening, it is assigned to a primary IRP leader, based on the scope of work, as well as a PM and project coordinator (PC). The IRP leader conducts a technical review to evaluate the impact to existing staff and resource availability, ensure the work is technically feasible and extreme hazards are identified, and assess the instrument time request against the Utilization Policy. The IRP leader includes other IRP leaders and scientific consultants as appropriate for this review.

5.2.2 Allocation of Resources

At the beginning of each FY, the User Support budget is distributed between the Science Areas to support the annual calls. The budget is allocated to support accepted projects at the Budget Allocation Meeting (BAM) based on the ranking of proposals by the PRPs. Prior to the BAM, each IRP leader evaluates the scope of the proposal against the resource request to refine the request and estimate the overall size of the project in terms of both instrument (experimental and computing) and staff time. This often involves discussions with the proposal authors to fine tune the scope of the proposal. The IRP leaders' estimates are then combined to establish the total estimated costs needed to support each proposal. The BAM is attended by the SALs, a UPS data analyst, and the LPM. At the BAM, the committee reviews the combined costs to determine if allocations are reasonable and appropriate to achieve the proposed results. The recommended allocations are then reviewed by the LPM (and/or delegate), SALs, and EMSL director to ensure resources support EMSL's strategy in each area. The review evaluates acceptance rates, as well as funding totals by proposal, Science Area portfolios, BER-relevant science, and BER PIs and by institution (PNNL vs. external). The SALs then work together and adjust the starting budget between Science Areas as needed to maintain consistency in the quality of proposals and address any concerns about the resulting mortgages in each Science Area for extending years.

The recommended list is reviewed by BER program managers for final consideration. Concurrence by the EMSL director serves as the record of decision, authorizing the creation of charge codes for each project and UPS to issue decision notifications. The final decision to conduct work on an accepted project, however, is dependent on approval by the DOE if the PI is not a U.S. citizen.

Except for limited scope requests, general proposals and EMSL staff time proposals are not normally eligible for budgetary support. Resource time is managed by the IRP leaders based on the Utilization Policy and availability.

Scientific Partner and EMSL Intramural Science and Technology Research Program (Intramural S&T Program) proposals are each supported by separate budgets that are jointly managed by the CSO and CDO.

5.2.3 Notification and Appeals

UPS issues decisions to the applicants for approved proposals and brief reasons for denied proposals. Peer reviewer comments, as well as the composite score for all user proposals, are made available to the applicants in the EMSL User Portal. Appeals may be submitted following the process outlined in Section 6.0.

5.2.4 Project Team Access and Project Closure

Team members on approved proposals work through the assigned PM or UPS to arrange visits or remote access. Prior to any direct access, users must complete required training and access requirements.

Projects close automatically based on their project type. Except for limited scope projects, EMSL team members, as well as the PI and PM, will be notified one month in advance of the project's planned end date. If there are special circumstances that may warrant an extension, the PMs will work with the PIs and the IRP leaders to submit a request for extension to the UPS team (IRPLs and PMs). The assigned PM will make sure existing policies are being followed for user program transparency and will acquire input from the appropriate SAL. The LPM will approve or deny based on the input. Projects may, however, be closed at any time for cause by the EMSL director.

5.3 Peer Review Criteria

EMSL's mission is to accelerate scientific discovery and pioneer new capabilities to understand biological and environmental processes across temporal and spatial scales. EMSL supports the mission of the Department of Energy, Office of Science, Biological and Environmental Research (BER) program to achieve a predictive understanding of complex biological, Earth, and environmental systems for the nation's energy and infrastructure sustainability and security. The BER program seeks to understand the biological, biogeochemical, and physical processes that span from molecular and genomics-controlled scales to the regional and global scales that govern changes in watershed dynamics, climate, and the Earth system.

Starting with the genetic information encoded in organisms' genomes, BER research seeks to discover the principles that guide the translation of the genetic code into the functional proteins and the metabolic and regulatory networks underlying the systems biology of plants and microbes as they respond to and modify their environments. This predictive understanding will enable design and reengineering of microbes and plants underpinning energy independence and a broad clean energy portfolio, including improved biofuels and bioproducts, improved carbon storage capabilities, and controlled biological transformation of materials such as nutrients and contaminants in the environment.

BER research further advances the fundamental understanding of dynamic, physical, and biogeochemical processes required to systematically develop Earth system models that integrate across the atmosphere, land masses, oceans, sea ice, and subsurface. These predictive tools and approaches are needed to inform policies and plans for ensuring the security and resilience of the Nation's critical infrastructure and natural resources.

Reviewers are asked to score each user proposal based on three criteria to ensure the proposed research is of high quality, is an appropriate use of EMSL's resources, and aligns with BER's and EMSL's missions. These criteria are

combined using a weighted average approach to generate a composite score (see Section 5.4). This composite score and the reviewers' comments are provided to the proposal author. Potential considerations are provided below to help provide consistency among reviewers. Sample scoring statements for each criterion have been developed in concert with past reviewers and are provided in Table 2 for additional calibration.

Criterion 1. Scientific merit and quality of the proposed research (50%)

Potential considerations: How important is the proposed activity to advancing knowledge and understanding within its own field or across different fields? To what extent does the proposed activity suggest and explore creative and original concepts? How well conceived and organized is the proposed activity?

Criterion 2. Relevance of the proposed research to the missions of EMSL and the BER program (25%)

Potential Considerations: What is the relationship of the proposed research to EMSL's and BER's missions? Does the research significantly advance mission goals and align with the focus topics for EMSL's Science Areas as outlined in the most recent Call for Proposals? Will the proposed research advance scientific and/or technological understanding of issues pertaining to one or more EMSL Science Areas? How well does the project plan represent a unique or innovative application or development of EMSL capabilities?

Criterion 3. Appropriateness and reasonableness of the request for EMSL resources for the proposed research (25%)

Potential Considerations: Are EMSL capabilities and resources essential to performing this research? Are the proposed methods/approaches optimal for achieving the scientific objectives of the proposal? Are the requested resources reasonable and appropriate for the proposed research? Does the complexity and/or scope of effort justify the duration of the proposed project—including any modifications to EMSL equipment to carry out research? Is the specified work plan practical and achievable for the proposed research project? Is the amount of time requested for each piece of equipment clearly justified and appropriate?

5.4 Rating Descriptions and Weighted Scores

The descriptions in the following table are sample statements intended to help distinguish between the different scores within each criterion and provide calibration among reviewers but are not intended to constrain the reviewer's evaluation or comments. For EMSL proposals, scores are weighted based on criterion (see table below) and averaged to generate an overall composite score for each proposal. For proposals submitted to a FICUS call, the review criteria are those negotiated between the partnering facilities and are included in the call announcement. For example, for the FICUS call with JGI, only science merit, team qualification, mission impact, and resource use are included in the review criteria and are weighted equally. The exploratory research call utilizes a dual anonymous review process that includes scoring for scientific merit, mission impact, Science Area impact, and resource use. The specific scoring criteria are included in the review criteria posted on the EMSL website and in the call guidance. Proposals are scored from 1 to 5, with 5 being highest.

Table 2. EMSL Project Research Review Criteria, Relative Weight, and Scoring Descriptions

Score	Science Merit	EMSL and BER Relevance	Resource Requests	Reviewer Calibration Summary
	50%	25%	25%	
5 Outstanding	Highly innovative research; will launch a new direction or have exceptional impact on existing problems in the research field. No flaws in the research plan; includes an approach or a plan for predictive understanding.	Outstanding fit to the focused topics outlined in most recent EMSL Call for the Science Area under review and the BER mission.	State-of-the-art resources are requested and are essential to perform this research, and the amount of the request highly aligns with the scope of the call.	Personally advocate for this proposal; stands above the rest and ranks within the top 5% of proposals reviewed.
4 Excellent	Well-conceived, original; strong potential for important contribution to the research field. Minor flaw(s) in the research plan; includes an approach or a plan for predictive understanding.	Strong fit to the focused topics outlined in the most recent EMSL call for the Science Area under review and the BER mission.	State-of-the-art resources are requested or use of EMSL resources would significantly enhance the results, and the amount of the request is well aligned with the scope of the call.	Highly recommend this proposal; ranks within the top 25% of proposals reviewed.
3 Good	Not groundbreaking but likely to produce useful results. Some weaknesses identified in the research plan or approach, or lacks a plan for predictive understanding.	Does not have a strong fit to the focused topics outlined in the most recent EMSL call but will advance one or more of the broader goals for the Science Area under review and the BER mission.	Resources requested are not state-of-the-art, well integrated, or not justified in the research plan, and the amount of the request is marginally aligned with the scope of the call.	Recommend this proposal, if resources available or identified concerns are revised; ranks within the top 50% of proposals reviewed.
2 Fundamentally Sound	Routine study in a well-worked area of research; incremental results. Major flaw(s) identified in the research plan or approach would limit success.	Does not address the focused topics outlined in the most recent EMSL call and will have minimal impact to the broader goals of the Science Area under review and the BER mission.	EMSL capabilities marginally enhance results; similar results could be achieved with broadly available instrumentation and expertise, and the amount of the request is not well aligned with the scope of the call.	Does not advance EMSL goals or have a strong argument for the use of EMSL resources. Ranks below 50% of proposals reviewed.
1 Questionable Impact	Serious doubts regarding feasibility or potential impact. Several major flaw(s) identified in the research plan would significantly limit success.	Is not responsive to the most recent EMSL call or does not address the goals of the Science Area under review and the BER mission.	There is no evident need for, or unique impact from, the use of EMSL's suite of resources, and the amount of the request is unreasonable based on the scope of the call.	Decline to provide a recommendation for award.

6.0 Appeals

For Large-Scale and Exploratory Research calls, proposal authors may submit an appeal letter only if the letter (1) describes the factual flaws in the review process for the application in question, (2) explains the reasons for the appeal, and (3) is based on one or more of the following issues related to the process of the initial peer review:

- direct evidence of bias on the part of one or more of the reviewers
- direct evidence of a conflict of interest on the part of one or more of the reviewers
- direct factual error(s) made by one or more reviewers that substantially altered the outcome of the initial peer review.

Appeals to reverse management decisions that are related solely to resource availability and funding will not be considered.

Overturning the results of the peer review panel is a very serious matter, and the standard of proof for a successful appeal is exceptionally high.

To submit an appeal, the proposal author should email UPS with a concise (2–3 paragraphs only) summary of facts directly related to the criteria listed above. Authors do not need to resubmit extension summaries or project descriptions. Appeals must be submitted within 30 days from the date on the award decision notice.

For the FICUS proposal calls, the decision of the review panel is final.

The Appeals Committee is appointed by the EMSL director. The committee reviews and makes recommendations to the EMSL director. All decisions by the EMSL director are final. UPS will coordinate with the committee and notify the user of the decision within eight weeks from the receipt of the appeal on proposals submitted against the annual call for proposals.

7.0 EMSL Scientific Partner Program

7.1 Definition

The scientific partner program supports R&D to improve an existing capability or develop and build unique new capabilities that enhance EMSL's user program. The research must be conducted by a team comprising individual(s) from a non-EMSL organization and individual(s) from EMSL. Both parties must contribute resources (for example, staff time, instruments, methods, samples) to the project. Either party may submit the partner proposal. Proposals may be in response to a specific call or submitted at any time. Capability development efforts that utilize collaborative multidisciplinary teams, pooled or leveraged resources, unique operating environments, or other resources that may be beyond those available to individual researchers or teams are encouraged. Scientific partner proposals are intended to leverage the combined resources, expertise, and capabilities of the partner institution to maximize impact for EMSL, the partner, and future EMSL users. Proposals must be aligned with and supportive of goals, outcomes and milestones that are updated annually. The EMSL PI, SALs, IRP leaders, and CSO are expected to work with the external partner to assess alignment with these goals or provide help aligning the work with these goals. This would happen in the early stages of the collaboration or in the white paper stage. In return for co-development, EMSL's scientific partner users may have priority access to the new capability for a negotiated and specified period. The award and timing of EMSL scientific partner projects are contingent upon EMSL strategic needs and the availability of EMSL resources. The LOI review process is detailed in Section 7.3.

7.2 Proposal Process

The partner organization or EMSL PI submits an LOI for the partnership to EMSL's CSO by email to initiate a dialog on suitability, interest, and strategic need for the capability. The CSO leads the review and approval process. A scientific partner author is encouraged to work with appropriate EMSL IRP leaders or other technical contacts in preparing the LOI, which should be no more than two pages and include short descriptions of the significance, impact, outcome, approach, resources, EMSL and scientific partner contributions, and the team. The advantage of the partnership should be clearly stated.

Successful investigators will be invited to develop full proposals using a supplied template. The proposed partnership must meet criteria including (1) the development of high-impact capabilities with strategic alignment to EMSL and BER science and (2) being supportive of the EMSL user program. Proposals are submitted for review via the User Portal. The proposal review process is detailed in Section 7.4.

Approved projects will provide regular written or verbal progress updates at times determined by the CSO. Summaries must include a brief introduction of the project; a description of the results to date; a list of any publications, awards, or recognition resulting from the project; and (for multiple-year projects) a detailed justification for any changes to the project plan, outcome, or resources allocated as outlined in the original proposal. Periodic reviews of scientific partner projects are also required, and reviews will be done at least annually for each project; the CSO will schedule and lead such reviews.

7.3 Review Process – Letters of Intent

LOIs are submitted by either the partner organization or EMSL PI. They are reviewed by a panel convened by the CSO. The review panel will include some or all of the following: the CSO, the CDO, relevant IRPLs and SALs, subject matter

experts, the COO if facility space is needed, and the EMSL director. Review criteria for LOIs will generally follow those used for the EMSL Intramural Program, to include strategic alignment, user/scientific impact and need, and resource and time requirements. Interaction, deliberation, and refinement of concepts with the review panel and/or EMSL staff should be expected during the LOI review process. Upon review and approval, the CSO or delegate will contact the scientific partner investigators and request a full proposal, provide review comments, and if necessary, provide additional guidance to proposers.

7.4 Review Process – Full Proposals

Full proposals are to be submitted by the partner organization investigator or EMSL PI via the EMSL User Portal (https://nexus.emsl.pnnl.gov/Portal/) using a template provided by the CSO. Proposals will be reviewed by a panel selected by the CSO to include when appropriate: the CSO, CDO, COO, relevant IRPLs and SALs, and other ad hoc subject matter experts as may be required for technical evaluation. Proposals will also be reviewed by select members of EMSL's advisory committees. Review criteria will include innovation, significance and impact, relevance to EMSL roadmaps/users/BER science, the advantage brought by the partnership, and the adequacy of resources and timing.

7.5 Notification Process

The CSO will be responsible for communicating the final decisions to the proposal team. Letters for accepted proposals will document the details of the agreement, including, at a minimum, the agreed-upon schedule and deliverables, the requirements for interim and final progress reports, and the negotiated terms of access to the deployed capability. Extensions of the original agreement may be made by the CSO but will be informed by a review of progress, feasibility, and resources conducted by a review panel assembled by the CSO. The CSO will be responsible for communicating extension decisions and details to the scientific partner investigator.

Projects may be closed at any time for cause by the EMSL director.

8.0 EMSL Staff Time Policy

This document formalizes the procedures for submission, review, approval, implementation, and utilization of EMSL Staff Time projects. The EMSL Utilization Policy states the following:

> *Up to 10% of the available instrument time is open to Environmental Molecular Sciences Division (EMSD) staff members to help advance their scientific careers through independent or collaborative research. This research is expected to result in EMSL staff publications or externally funded programs. Another 10% is available to EMSL staff and others at the EMSL director's discretion to help advance EMSL's strategic goals.*

This policy was developed to provide an opportunity for EMSL line staff to pursue and develop their own research programs outside their roles as scientific consultants for users. EMSL staff submit proposals to utilize EMSL resources using the EMSL Staff Time proposal mechanism. These proposals are subject to internal safety and management reviews only, and participants on EMSL Staff Time proposals will not be counted as users. Staff time proposals are valid for up to three FYs. This mechanism does not replace user proposals by PNNL staff who pay EMSL staff to run the experiments on their behalf (Contracted Time Proposals).

The EMSL Staff Time proposal mechanism can also be used by active joint appointees in the EMSD. Staff Time projects are subject to EMSL's data management policy detailed in Section 12.0.

Although up to 20% of available instrument time is set aside for EMSL staff time utilization, EMSL staff will make a reasonable effort to rearrange schedules to accommodate external users' needs with the assumption that on-site staff and users can more easily adjust their schedules if needed.

The following submission and review procedures will be followed:

- EMSL staff submit requests via EMSL's User Portal, selecting the "EMSL Staff Time" proposal type. Submission guidance for EMSL Staff Time proposals is found on EMSL's internal SharePoint site. Prior to submitting an external grant proposal, EMSL staff are responsible for making sure they do not propose work that cannot be performed at EMSL. The following type of work cannot be done at EMSL and will not be accepted:
    - work requiring biosafety level 3
    - samples or materials with radiation levels exceeding EMSL capabilities
    - work that might require instrument or facility modifications.
- The proposal is reviewed by the appropriate IRP leader(s) for technical feasibility and instrument availability.
- The proposal will also route through additional internal health, safety, and environmental reviews as required.
- **All usage** on EMSL Staff Time projects for tracked instruments **must** be recorded in EMSL's management system.
- Use by EMSL Staff Time projects will be reported in the usage breakdown (pie chart) and utilization reports as *EMSL Staff Time, Planned* or *EMSL Staff Time, Unplanned*, following the definitions in Usage Types (Section 11.0).

9.0 EMSL Intramural Science and Technology (S&T) Program

The objective of this program is to create new capabilities for the BER research community by advancing the goals laid out in EMSL's S&T roadmap presented in the 2021 EMSL Strategic Science Plan, the FY 2023 addendums that clarify some aspects of the 2021 strategy, the December 2023 Strategic Science Objectives concrete outcomes, and the supporting Research Area Roadmaps. Projects funded by the Intramural S&T Program should develop new scientific research areas and capabilities for the broader scientific community that are aligned with EMSL's roadmap, will further the impact of EMSL's user program, and should drive progress in achieving BER objectives. The program prioritizes and selects proposals through a scientific and technical peer review process to provide both instrument time and operations funding to achieve the specific aims of intramural S&T projects. Intramural S&T Program funding is not available to support collaborators external to PNNL.

9.1 Intramural S&T Proposal Types and Review Process

Proposals to the intramural program are managed through the EMSL User Portal and are organized in two tiers according to the scope of work proposed, duration, and funding level.

- Dash proposals: work scope should be accomplished within 6 months and not exceed $60K.
- Developer proposals: work scope should be accomplished within 24 months and not exceed $250K per year.

Dash proposals may be submitted in response to calls published approximately three times a year. Concepts are screened by the CSO, SALs, and IRPLs, and invitations for full proposals issued. Full proposals are reviewed internally and selected for funding by the CSO and the relevant SALs and IRPLs.

Developer proposals must be submitted in response to an annual call for proposals that outlines focused topics designed to advance EMSL's S&T roadmap as presented in the 2021 EMSL Strategic Science Plan, the FY 2023 addendums that clarify some aspects of the strategy, the December 2023 Strategic Science Objectives concrete outcomes, and the supporting Research Area Roadmaps. The annual call will consist of two review phases to first screen one-page white papers, followed by peer review of full proposals. White papers will be screened by the CSO and the SALs for relevance to the EMSL roadmap and responsiveness to the call topics. The PIs for selected white papers will be invited to submit full proposals that will be evaluated for technical approach by the IRPLs and peer-reviewed by a panel composed of PNNL staff and EMSL's Science & Technology Advisory Committee (STAC), using the Intramural S&T Program review criteria. The review panel's written comments and scores will be reviewed by the CSO and SALs, and final decisions will be made based on scientific and technical merit, prioritization related to the goals and timelines of the EMSL S&T roadmap (with revisions noted above), and the need to support a balanced portfolio of projects to advance each element of the roadmap. The timeline for Developer proposals will typically be a call for proposals issued each spring, with accepted projects starting in early October. Proposals are submitted to NEXUS and archived.

White papers and proposals must follow proscribed format and length requirements using templates made available on EMSL's SharePoint site. The requested funding support should allocate sufficient resources for sharing the results, including open literature publication, intellectual property commercialization activities, etc. and may include equipment purchases up to $140K.

9.2 Peer Review Criteria

Evaluation of the white papers that are precursors for Developer proposals will focus on relevance to EMSL's roadmap and responsiveness to the call topics. Full proposals will be evaluated for innovation, impact, and relevance to assess opportunity and on the approach and milestones, qualifications of the research team, use of resources, and funding requested to assess feasibility. To be considered for support, proposals should rank highly in one or both categories (opportunity or feasibility).

Opportunity criteria

Criterion 1: Innovation

Does the approach/technology challenge current research paradigms by utilizing novel theoretical concepts, approaches or methodologies, or instrumentation? Are the concepts, approaches or methodologies, or instrumentation novel to one field of research or novel in a broad sense? What is the likelihood for the project to make an important scientific contribution to the research field(s)? How does the proposed project compare with other work in its field, both in terms of scientific and/or technical merit and originality?

Criterion 2: Significance and Impact

Does the project address an important problem or a critical barrier to progress in the field? If the objectives of the project are achieved, how will scientific knowledge or technical capability be improved, and would the proposed work deliver high impact products—will the research be publishable? How might the results of the proposed project impact the direction, progress, and thinking in relevant scientific fields of research? Does the project plan represent a unique application or an increase in throughput or performance that will be valuable to EMSL and its user community and significantly impact their productivity?

Criterion 3: Relevance to EMSL Roadmap and Call Topics

Does the project advance EMSL's strategic goals? Does the proposal identify which EMSL strategic goal(s) or DOE-BER strategic goal(s) are advanced by this research? If successful, would the proposed work deliver new capabilities for the EMSL user program or enhance an existing high-demand capability? Does the project significantly advance EMSL IRPs? Does the project include a strategy to make the approach (technology) available to EMSL users?

Feasibility criteria

Criterion 1: Feasibility of the Proposed Approach and Achievable Milestones

Are the strategy, method, and analyses well-justified and appropriate to accomplish the goals of the proposal? If appropriate, is the approach scalable? Is there previous work that supports the described experimental and computational approach? If there is a software development component, is long-term maintenance sustainable in proportion to the labor or cost involved in the development of the software? Does EMSL have the existing infrastructure to support deployment of the proposed technology? Does the proposal identify the risks and include mitigation plans? Are the milestones sufficiently defined with objective criteria to measure progress? Milestones are measurable outcomes that serve to mark project progress. They need to have clearly defined, objective criteria that will inform go/no-go decisions regarding project continuation. Proposals that include software development must provide a software sustainability plan.

Criterion 2: Competency and Availability of Proposal Team

Does the team have the appropriate experimental and/or computational experience and skills to accomplish the proposed work? Are the project team roles and responsibilities defined and appropriate to effectively manage a milestone-driven project? Does the project lead have appropriate experience, or an identified mentor, to ensure successful project execution? Does the project team have a prior record of working together successfully?

Criterion 3: Adequacy of Proposed Resources

Are the proposed resources, equipment, and infrastructure (space, instrument time, compute cycles, data repository needs) adequate and available (or readily obtainable)? Will the project employ the unique features of the EMSL environment?

Criterion 4: Funding and Timing

Are the budget and the requested period of support fully justified and reasonable in relation to the proposed work?

9.3 Project Reviews

The progress of ongoing projects is reviewed by the CSO and SALs throughout the year and at least semiannually for each project. These reviews enable the evaluation of the project progress, the identification of barriers, and the redirection of the approach if needed to ensure progress. At each review, the continuation of projects and funding depends upon progress toward the completion of milestones and the funds available. A project summary is due annually, typically in September, and should be uploaded to the NEXUS User Portal. Summaries should describe progress toward the completion of milestones and, for continuing projects, should also include a summary of planned work for the upcoming year.

10.0 EMSL Utilization Policy

10.1 Overview

The user program is housed primarily within the EMSL building, a 240,000 square-foot research facility that is funded by BER, although it may also include experimental and computational instrumentation (resources) housed in other PNNL facilities. The EMSL utilization policy covers all resources purchased or co-purchased by the user program and all resources located in space that EMSL maintains or manages.

The policy for using EMSL user program resources is focused on maximizing the benefit to the user program. All research performed in EMSL or utilizing EMSL resources must provide benefit to the user program and must be managed by an active user or staff project in EMSL's management system. A set of resources, as defined by EMSL management, is tracked and reported to the EMSL management at least annually and on request. Analyses of these data are used to determine the level of continued support and schedule for the divesting of resources as part of life-cycle management. Lab space supported by the EMSL user program is subject to the EMSL Space Policy as detailed in Section 16.0.

10.2 Funding and Ownership of Research Resources

EMSL's research resources are funded from a variety of sources. Most of the resources are 100% purchased and supported by the EMSL user program. Some resources are purchased using non-user-program funding, and these are owned by PNNL or other research programs. Resources can also be supplied by a partner as part of a scientific partner proposal. Its usage is governed by the terms in the accepted proposal (see Section 7.0). Additionally, some resources are co-purchased by the user program and PNNL or other research programs. The EMSL user program participates in copurchasing research resources and allows other programs to place resources within EMSL-supported space only when benefit to the user program is clearly demonstrated and approved by EMSL's COO. The COO will consult with the EMSL operations manager, CSO, or EMSL director as needed.

Regardless of ownership, the user program provides significant support to all research performed in EMSL spaces and may include the following:

- EMSL infrastructure support
    - computer and network support
    - machine shop access
    - waste management costs
    - ESS&H support
- laboratory space and associated costs
- support by EMSL scientific consultants through the EMSL user program.

To maximize the benefit of this support to the user community, available time on all resources is open to users according to the percentage of EMSL's ownership by resource, as defined by funding source. Available time is defined as all time that the equipment is normally scheduled for operation and is not undergoing maintenance, upgrades, repair, or capability development.

Costs associated with space, maintenance, operation, and supplies of any resource located in EMSL-supported space are paid by the respective programs according to the percentage of ownership or as detailed within a formal Memorandum of Agreement (MOA) between EMSL management and the system owner or delegate, as detailed below.

10.3 Memoranda of Agreement (MOAs)

Occasionally, an MOA will be established to document utilization arrangements for user program resources that are shared with or transferred to other research programs or organizations within PNNL.

The MOA will identify the subject EMSL instrument or system of instruments, the utilization agreement time period, the principal points of contact in the EMSL organization and in the other PNNL organization or research program, the scope of activities or purpose for which the agreement is being established, and the percentage of time that it will be made available to each of the parties, and will detail the respective responsibilities of EMSL and the PNNL organization or program.

Each MOA must be approved by the EMSL director, the appropriate PNNL division director, the BER program manager for EMSL, and if applicable, a program manager from any other affected Office of Science program.

New MOAs can be established at any time and will have a standard duration of two years. MOAs with a term longer than two years must be reviewed and reapproved every two years by the EMSL director, and the appropriate PNNL division director. If changes are made to the terms of the MOA during this process, the MOA must also be reapproved by the same original approvers. This reapproval process must also be followed whenever a major upgrade or change in the value of the instrument(s) occurs.

All MOAs will be documented in EMSL's management system by instrument (or system of instruments) and stored in EMSL's project record file (FLD-00179.-8.22860) within ERecords, PNNL's electronic records management application system. ERecords is certified to meet federal standards for electronic record keeping and enables PNNL to meet its record requirements for corporate information in any form.

10.4 Utilization Policy

10.4.1 100% User Program Purchased Research Resources

At least 80% of the available annual time is open to users through EMSL's user proposal review and selection process. Up to 20% of the available annual instrument time is open to EMSL staff members and others via the director's discretion. Requests will be submitted as Staff Time proposals through the EMSL User Portal for internal review and tracking purposes.

- Up to 10% is available to help advance the scientific careers of EMSL staff through independent or collaborative research. This research is expected to result in EMSL staff publications or externally funded programs.
- Another 10% is available to EMSL staff and others at the EMSL director's discretion to help advance EMSL's strategic goals.
- On an exception basis, EMSL may negotiate MOAs between EMSL and PNNL or other research programs on a specific EMSL resource when it benefits the user program and advances EMSL's mission and vision.

- Each agreement will be approved by the EMSL director, the appropriate PNNL division director, the BER program manager for EMSL, and if applicable, a program manager from any other affected Office of Science program.
- The agreement will be documented (1) in a formal MOA and (2) in EMSL's management system by instrument (or system of instruments).
- The MOA will identify the subject EMSL capability, the utilization agreement time period, the principal points of contact in the EMSL organization and in the other PNNL organization or research program for carrying out the agreement, the scope of activities or purpose for which the agreement is being established, and the percentage of time that it will be made available to each of the parties and will detail the respective responsibilities of EMSL and the PNNL organization or program.

10.4.2 100% Other Program Purchased Research Resources

- Twenty percent (20%) of the available time will be open to users through the user proposal process unless a separate agreement is developed and documented in an MOA. Utilization of the resource by EMSL users must be tracked thought the EMSL User Portal and data stored according to EMSL's data policy.
- The balance of the time is dedicated to the program that purchased the system. An individual will be identified to serve as the "Resource Owner" for the capability to help manage the percentage of time utilized by the other program. Resource owners do not have to submit a proposal to use their instruments, but utilization must be tracked in the reservation tool under the resource owner usage type. It is the responsibility of the resource owner to keep EMSL's UPS apprised of any changes to the equipment status, particularly if the resource is removed from EMSL. The data management on resource owner projects is the responsibility of the resource owner.

10.4.3 Co-purchased Research Resources

- A minimum of 20% or the percentage purchased by the EMSL user program, whichever is greater, will be open to users through the user proposal process. For example, if the user program paid 10% of the cost of the system, then 20% of the access is open to users. If the user program paid 50% of the cost of the system, then 50% of the access is open to users.
- Of this user portion, up to 20% of the available instrument time is open to EMSL staff members and others via the director's discretion. Requests will be submitted as Staff Time proposals through the EMSL User Portal for internal review and tracking purposes.
    - Up to 10% is available to help advance the scientific careers of EMSL staff through independent or collaborative research. This research is expected to result in EMSL staff publications or externally funded programs.
    - Another 10% is available to EMSL staff and others at the EMSL director's discretion to help advance EMSL's strategic goals.
    - The remaining time will be allocated to the program that co-purchased the research capabilities and tracked via resource owner usage type (no proposal required).
- The utilization agreement for co-purchased research capabilities can be documented in an MOA, detailing the percentage of ownership and shared costs for managing the instrument and space.

10.4.4 Transferred User Program Purchased Research Resources

- In cases where a capability has gone through the divestment process (see Section 17.4), EMSL may transfer ownership of the capability to another program or organization within PNNL.
- EMSL may elect to negotiate a percentage of time on the capability for EMSL users through the user proposal process.
- Of this user portion, up to 20% of the available instrument time is open to EMSL staff members and others via the director's discretion. Requests will be submitted as a Staff Time proposal though the EMSL User Portal for internal review and tracking purposes.
    - Up to 10% is available to help advance the scientific careers of EMSL staff through independent or collaborative research. This research is expected to result in EMSL staff publications or externally funded programs.
    - Another 10% is available to EMSL staff and others at the EMSL director's discretion to help advance EMSL's strategic goals.
- If necessary, the utilization agreement for transferred research capabilities will be documented in an MOA and in EMSL's management system by instrument (or system of instruments) and will detail the percentage of ownership and shared costs for managing the instrument and space.

11.0 Usage Type Definitions

11.1 EMSL Management System

EMSL's management system captures resource use. EMSL management uses the data for evaluating proposal use as well as for making budget decisions regarding enhancements, acquisitions, consolidation of capabilities, and strategic direction for capability growth.

Staff members are designated in the management system as Instrument Custodians/Authorized Reservers by their respective IRP leaders. Only those designated as such on an instrument can create a reservation/booking and record usage. The management system schedule tool is to be used to create reservations on instruments. Nonstaff (e.g., users, collaborators) are not eligible to serve as Instrument Custodians/Authorized Reservers.

Instruments are evaluated each year on the unique or state-of-the-art characteristics, purchase or replacement costs, user community interest, and productivity. Usage data must be entered into the management system for all tracked instruments. UPS annually sends a list of instruments that require utilization tracking to Instrument Custodians.

Instrument Custodians/Authorized Reservers are required to record usage data by Friday of each week and by the last day of the month for the final week. The UPS data analyst reviews the data for anomalies prior to data archival for reporting purposes at the end of the fifth day following month end. Changes needed after the archive date are not reflected in subsequent reports or statistical analyses unless arrangements have been made with the Lead Project Manager.

Core hours for instruments have been established to help manage the Utilization Policy for the 20% of instrument time made available for EMSL staff research and for managing contracted time utilization. For instruments that operate 10 hours a day, 5 days a week, core hours are considered 8 a.m.–6 p.m., Monday–Friday, excluding official laboratory holidays and planned outages. For instruments that operate 24 hours a day, 7 days a week, core hours are 12 a.m.–12 a.m., excluding official laboratory holidays and planned outages. Other core hours may be established based on factors such as past user utilization.

Instrument time is reported under four different categories: (1) In Use; (2) Out of Service, Planned; (3) Out of Service, Unplanned; and (4) Available. Definitions for the types of use to be recorded within each category are provided below.

In Use

- **On-site Usage** – Use by any individual who is a member of an approved research team and is physically present using an EMSL capability to conduct research at any time during the reservation.
- **Remote Usage** – Use by any individual who is a member of an approved research team and has been granted authority by the PI to participate remotely in experimental planning (including remote operation of instrumentation/computing hardware or engaging with EMSL staff on sample submission/delivery), execution, and data analysis.
    - *Note: For reporting purposes, selecting remote usage will automatically include all team members who qualify under the user definition.*
- **Resource Owner Usage –** Organizations that own a percentage of an instrument that resides in EMSL may authorize scientists to utilize their portion of available time. No proposal is necessary to access the instrument in

this manner, but this type of usage needs to be documented under the "Resource Owner" category in the reservation tool.

- **Capability Development** – Time allocated on a resource to develop a new capability or enhance an existing capability. Capability development activities may require extended booking of the instrument.
- **EMSL Staff Time, Planned** – Use during instrument core hours by any individual under an EMSL Staff Time project in NEXUS.
    - *Note: Participants recording use on EMSL Staff Time projects will not be counted as users.*
- **EMSL Staff Time, Unplanned** – Use outside instrument core hours or when the instrument is idle during core hours because of late cancellation or unscheduled time by users.
    - *Note: The time recorded will be included in the "In Use" totals but will not go against the percentage of time allocated to staff under the Utilization Policy.*

Out of Service, Planned

- **Maintenance** – Resource is not available because periodic maintenance or modification of a facility or equipment is being performed to keep the laboratory or resources at peak performance and readied for users. Includes calibration runs, vendor visits for periodic maintenance, and ***planned*** power outages or ***planned*** operational restrictions by Facility and Operations, including instrument moves, chiller outages, etc. ***Comments to clarify this designation are required.***
- **Upgrade** – Resource is not available because an upgrade is being installed.
- **Unavailable, Staffing** – Resource is not available because staff are not available to operate the equipment. Includes vacation, holidays, travel, personal illness, or other business commitments. Personal information, such as staff member names or reasons for medical appointments, business travel, etc., should ***not*** be included in the comments.
- **Unavailable, Other** – Resource is not available for any other ***planned*** reason. This may include a time when, for instance, a sample must be contained in vacuum, but no experiment is on-going; thus, no one else can use the resource. ***Comments to explain this booking are required.***

Out of Service, Unplanned

- **Broken/Out of Service** – Resource is not available because it is broken or damaged to the point that it cannot be used until fixed or because it is out of service because of unforeseen events ***such as a PNNL closure (e.g., poor air quality, snow day, etc.) or an unplanned power failure, fire alarm, lacking essential supplies for operating the instrument, etc***. ***Comments to explain this booking are required.***

Unused, Available – Any time not captured under any other Usage Type.

11.2 Selecting the User on a Booking – Guidance and Examples

This section provides general guidance with examples to help determine which of the proposal team members (a.k.a. participants) are to be entered as "user(s)" in the EMSL management system when PNNL staff are working on the EMSL user project.

General Guidance:

The program funding the PNNL staff member's time determines if the staff member is considered a consultant or a participant on the user project. If the EMSL user program is paying for a PNNL staff member to work with one of the participants on the user project, then the staff member is considered a consultant and the team member being helped is designated as the "user" on the booking. If any other program/project is paying for the PNNL staff member's time, then the PNNL staff member is a "user" and should be selected on the booking, along with anyone else associated with that use.

Examples:

1. The EMSL user program pays Joe (a PNNL staff member) to work with Sarah (a team member) on an EMSL user project. Joe is considered a *consultant* on the project, so Sarah would be considered the "user" on the booking. The usage type for the booking (e.g., remote or on-site) follows the definitions for "In Use" above. For example, if Sarah is teleconferencing with Joe from her home institution during the booked use, she would be a remote user. If she is at PNNL and working with Joe, who is running the instrument, she would be an on-site user.
2. Chuck pays Joe (a PNNL staff member) from his Basic Energy Sciences project to work on Chuck's user project. Joe is considered a *team member* on the user project and is selected as an "on-site user" on the booking. If other team members on the project are at PNNL and working with Joe at the same time, they also are selected as "on-site users" on the booking. Participants who are not physically present at PNNL will be recorded as "remote users" following the description above.

12.0 EMSL Data Management Policy

EMSL's Public Data Release policy applies to all nonproprietary user projects and is subject to change without notice under the Terms and Conditions for EMSL use.

The EMSL Data Management Policy details the resources available to EMSL users and facility staff for managing data associated with research using EMSL resources. This policy is provided to help users and staff understand the data resources available at EMSL, including storage and retrieval capabilities, data definitions, data release requirements, and the data management responsibilities of EMSL's instrument custodians and computational scientists. EMSL's policy is based on the guiding principles summarized below from the DOE, DOE Office of Science (DOE-SC), and BER. It also provides information necessary to assist researchers in developing a data management plan to meet funding agency requirements.

To promote the efficient delivery of scientific discoveries and effective use of government resources, DOE and DOE-SC have mandated that data management planning be an integral element of research planning.[1,2] Data preservation and sharing facilitate the validation and reproducibility of scientific results and broaden the applicability of data products beyond the scope of individual research projects. Therefore, it is the intent of DOE-SC that scientific data generated at scientific user facilities such as EMSL be made available to the scientific community, industry, and the public to the greatest extent possible. In particular, SC policy requires that "all research data displayed in publications resulting from [SC-sponsored] research be open, machine-readable, and digitally accessible to the public at the time of publication." Additional information on data and publication sharing requirements and guidelines is provided in DOE's Public Access Plan[3].

BER, EMSL's sponsor, provides further guidance regarding digital data management for some of its research programs, and a compilation of data management policies at all SC user facilities is also available[4].

12.1 Data Management Resources

EMSL currently provides the ability to store all data generated at EMSL (including numerical simulation outputs) in a hierarchal storage archive, which provides short-term disk storage of recently used data combined with long-term archival of infrequently used data on lower-cost tape resources. The EMSL data archive system, known as Aurora, currently has the capacity to store tens of petabytes (PB) of data and is readily expandable. This archive serves as the foundation for the metadata-based data repository that is currently accessible to EMSL staff members and is connected to all major EMSL instruments. Authorized EMSL users and facility staff can electronically access their nonproprietary data in the repository through the Get Data tab of the applicable project in the User Portal.

To facilitate resource planning, researchers expecting to generate 250 terabytes of data or more on a single user project should include this in their proposal package request for resources. If projects generate more data than originally anticipated in the proposal process, researchers should discuss this with their project manager who will request additional resources.

[1] https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management
[2] https://science.osti.gov/Funding-Opportunities/Digital-Data-Management
[3] https://www.energy.gov/downloads/doe-public-access-plan
[4] https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management-resources

12.2 EMSL Data Access Policy for User Project Team Members

Under this policy, data are released to EMSL user project team members as follows:

- For projects producing data at EMSL and one or more non-DOE user facilities, immediate access and release of data generated on an approved user project are granted to all team members (aka participants) listed on the project by the PI. All team members on the project will have full access to their data both during the project period and in perpetuity after the project ends. EMSL staff are granted access to the data but are not authorized to release the data in any form.
- For collaborative projects utilizing EMSL and one or more user facilities, the data generated at EMSL will be released to the team members as described above. Data generated at other user facilities will be released by those facilities in accordance with their respective data management policies.

Project team members who are unable to find and download project data through the User Portal should contact their project manager or UPS. They will work with the team member to create a data package from the repository and transmit the data by appropriate means.

12.3 EMSL Open Access Data Release Policy

EMSL's Open Access Data Release Policy applies ***only*** to ***nonproprietary data*** collected under the user program. The purpose of this policy is to balance the need to make data openly accessible to the scientific community and the public as soon as possible with the reasonable expectation that project teams are afforded time to analyze the data, evaluate the results, and prepare publications on their conclusions, while easing fear of preemption. Data, for purposes of this policy, refer to the sample metadata, raw instrument data, associated experiment metadata and processed data and will be released to the public on EMSL's open access data portal.

To support making data openly accessible, tracking data use for SC, and encouraging proper citation of the researchers who generated the data, EMSL's data portal requires the creation of a user account and provides Digital Object Identifier (DOI) minting services. DOIs may be minted in association with specific data packages, including (1) data packages associated with scientific publications, (2) unique data packages developed by EMSL users and/or staff, and (3) data packages requested through the data portal. An award DOI is also generated by EMSL for every user project for inclusion in publication acknowledgements. These data and award DOIs provide an avenue for data reuse with appropriate citation and attribution of EMSL and the generating PI or team members.

Under this policy, the data will be released to the public as follows:

- **Specific data** will be released immediately upon upload to EMSL's repository:
    - data generated under EMSL's Strategic Science Objectives, including but not limited to the 1000 Soils Research Pilot and MONet
    - **field sensor data**.
- **All other resource data** will be released as follows:
    - All nonproprietary data uploaded to the repository on an approved user project will become openly accessible at the time a data DOI is minted, at the time of publication of the associated scientific results, or within one year after data generation and upload to the EMSL repository, whichever comes first.

- Prior to the open access release date, data can be released only by the user project PI or team member to other entities (people, publishers as supplementary materials in a manuscript submission, institutions, etc.).

- For **collaborative projects** utilizing EMSL and additional user facilities, the data generated at EMSL will be released as described above. Data generated at other user facilities will be released by those facilities in accordance with their respective data management policies.

12.4 Repository Management

Nonproprietary project data that are from EMSL resources must be uploaded to the repository; data stored outside EMSL's repository does not meet the requirements of this policy. All data uploaded to the repository will be stored permanently to ensure long-term accessibility. Legacy data (data collected prior to the availability of the repository and stored elsewhere) are being evaluated by EMSL staff, and all legacy data that meet the requirements below and for which required metadata can be established will be uploaded to the repository and become available per the policies below.

Data uploads are regularly monitored using reporting tools that are linked to instrument usage records in EMSL's management system to evaluate compliance with this policy. For purposes of this policy, EMSL's instrument custodians and computational scientists are expected to use the following guidance to determine which data will be uploaded to the data repository.

12.4.1 Data Included in the Repository

Essentially all nonproprietary data should be uploaded, except data that fall under Section 12.4.2. Data that fall into the exception category can be uploaded in some cases but are not required. EMSL instrument custodians and computational scientists should direct any questions they have regarding the type of data collected to the EMSL IRPL responsible for the instrument or computing system being used. All sample metadata, raw instrument data, simulation outputs, processed data, and associated experiment metadata collected from experiments or computations that are expected to be delivered to EMSL users as part of an approved project must be uploaded to the repository. EMSL instrument custodians and computational scientists should upload the data as soon as practicable, but *no later than* the end of each month for raw data and associated metadata and *no later than* the end of the quarter for processed data. A command line uploader has been provided for computational resources and should be used to store computational outputs in the same manner as for experimental data.

Data definitions should conform to relevant community standards for data and metadata when they exist. All data uploaded to the repository conform to the Dublin Core bibliographic metadata standard (bibliographic metadata are automatically extracted from project text stored in EMSL's management system), which facilitates linkage to the DOE Office of Scientific and Technical Information (OSTI) where all EMSL publications are archived. Other standards are domain-specific, such as the Human Proteome Organization (HUPO) proteomics standards initiative that guides metadata collected and stored by both EMSL and the PNNL proteomics data management systems. In cases where there are no clear community standards, data in a form that allows unbiased interpretation by the relevant scientific community should be uploaded. Note that a single experiment or simulation run could require more than one dataset to be uploaded; the original data may be uploaded initially and processed data subsequently. The time stamps for upload of each dataset determine its date of release to the public.

12.4.2 Data Not Required to be Uploaded to the Repository

As an exception to the requirements in Section 12.4.1, some data are not required to be uploaded to the repository. These are data that will not form the basis of publishable research findings or are not associated with an EMSL project. These include data from experiments known to be faulty in some regard, e.g., through mishap or due to a flawed experimental design, data from preliminary experiments that are not intended to be delivered to EMSL users, calibration runs for which results are not needed to interpret legitimate project data, and data generated to verify successful operation of the instrument or demonstrate capability to prospective users.

12.4.3 Blocking Released Data

In the rare case where users or staff have identified faulty data that have been released to the project team or made openly accessible to the scientific community, the instrument custodian should contact the appropriate IRPL and CDO in writing, providing sufficient detail and justification for requesting that the released data be blocked. If approved, the CDO will forward the email to UPS who will flag the appropriate dataset(s) and document both the request and approval in the applicable project records.

12.4.4 Data Repository Management

The archive size is maintained to ensure at least 48 months of headspace at any time (based on extrapolation of recent data upload rates). Disk storage comprises approximately 15% of the archive, with the remainder being tape storage. As data are uploaded, two permanent copies of the data are stored to tape (for data redundancy and integrity). The data are also maintained on disk to facilitate rapid access, but as data age they may be removed from disk storage. Selected data may also be “locked” to disk by system operations staff. The disk archive is actively managed by automated processes that purge data once the disk usage reaches 90% of its capacity; files are purged in order of longest time since last access until 80% capacity is achieved. Thereby the disk storage is continually maintained at 80% to 90% usage of its capacity, with only the most recently accessed files retained on disk. At any point, a file can be retrieved from tape to the disk if requested.

13.0 EMSL Software Development and Sustainability Policy

As a scientific user facility, EMSL adheres to the mandate to release as quickly as possible any scientific and technical information (STI) produced in part or in whole with EMSL resources. As defined by DOE, STI includes scientific and technical computer software, in addition to a range of products such as technical reports, conference papers and presentations, theses and dissertations, journal articles, workshop reports, patents, and publicly available scientific research datasets. DOE recognizes the important role played by scientific software to advance their missions in basic and applied scientific research for innovative clean energy and environmental discoveries and technologies and that open-source software accelerates progress by ensuring use and adoption by industry, academia, government, and other national laboratories. Thus, software developed by staff at scientific user facilities is expected to be made open-source, whereby the source code is released under a license that grants users the rights to study, change, and distribute the software to anyone and for any purpose. To support the collection, preservation, and dissemination of scientific software, the DOE OSTI maintains DOE CODE (https://www.osti.gov/doecode), a software service platform and search tool that provides functionality for collaboration, archiving, and discovery of scientific and business software.

This EMSL Software Development and Sustainability Policy details the expectations and procedures for software development efforts supported by EMSL user program funding and the procedures necessary to adhere to the software release policy. Exceptions to this policy must be reviewed and approved by both the EMSL CDO and CAM SAL. In reviewing requests for exceptions, considerations are given to factors such as (1) the nature of the software (application; library, module, or package; scripts, workflows, or pipelines; or container definitions); (2) the role of the software in the project (e.g., a primary deliverable, a secondary deliverable, or incidental); (3) the type of EMSL effort supporting the development (e.g., a user call project, a staff-time project, or an S&T intramural project); and (4) the expected and possible impacts on BER science, including the contributions of the software results towards publications or data resources.

13.1 Software Development

Staff developing software supported by EMSL funding must develop a plan describing the software engineering best practices to be used that will ensure software quality, sustainability, and interoperability[5,6]. The software development plan will be provided to the EMSL CAM SAL and CDO prior to initiating development efforts.

The software plan should include the following elements:

1. the identification of clear roles and responsibilities of development team members
2. a description of software requirement specifications and design documentation, including whether the software will be offered as a service requiring user authentication
3. project control tracking and task management (using tools such as JIRA or GitLab)
4. software configuration management and version control (using tools such as Bitbucket or GitLab)
5. plans for eventual public release of software under an open-source license on EMSL GitHub

[5] https://github.com/betterscientificsoftware/PSIP-Tools/blob/master/PSIP-Overview.md
[6] https://confluence.pnnl.gov/confluence/display/DC/Welcome+to+Developer+Central

6. a comprehensive software unit testing plan and continuous integration process, including automated execution of unit tests whenever a software change is committed
    a. If the software will make significant use of scientific software developed by others (third-party software), the plan should include how the third-party software will be tested (verified and validated) and describe the risk mitigation plan in the event that the third-party software fails or becomes unavailable.
7. the process for user testing, feedback, and modification prior to production release
8. thorough documentation of software including underlying theory, code implementation, user guide, and tutorials with links on the code repository, preferably hosted on EMSL GitHub (https://github.com/EMSL-Computing/).

The expectation is that software development efforts will use tools available through PNNL Developer Central to document software design (Confluence), track software development tasks (JIRA), and support version control (EMSL GitLab).

13.2 Release Policy

DOE policy states that software is a form of data and is therefore subject to the EMSL data release policy (see Section 12.0 for details).

Procedures and Responsibilities

1. The lead developer must file a software invention disclosure with PNNL's Office of Technology Deployment and Outreach (TDO) and include the EMSL CAM SAL and CDO as witnesses.
2. As directed, the lead developer will work with a commercialization manager (CM) from TDO to obtain an open-source license and copyright.
3. The EMSL CAM SAL and CDO will contact EMSL's sponsor to seek concurrence on the licensing and copyright strategy.
4. The PNNL CM will seek permission from the DOE Patent Counsel office to assert copyright.
5. The lead developer will implement software release on EMSL's GitHub (preferably at https://github.com/EMSL-Computing/).
6. The CM TDO will register the software at DOE CODE.

13.3 Contributions to Open-Source Community Codes

Staff must be an authorized contributor before contributing patches, modifications, or additions to open-source codes. Staff should first determine whether PNNL has an existing Contributor License Agreement (CLA)[4] with the applicable community. In cases where PNNL has a CLA, staff should speak with the lead contributor to be added to the contributor list prior to contributing to the community. When a CLA has not yet been established, staff should contact PNNL's TDO to start the process of establishing a CLA prior to contributing to the community.

13.4 Software Retirement

The operations involved in retiring software applications include identifying the reasons for the discontinuation, planning and communicating the decision to stakeholders, and implementing a plan to decommission the software to minimize

disruption to users and the organization. This will involve data migration, archiving, or transfer to an alternative system and communication and support to users during the transition period. Several critical activities are engaged during the sunsetting of a software application. Such activities will be finalized based on individual software. One important activity is data management, which involves identifying, categorizing, and migrating the data associated with the software to a new system or archiving it for future reference. Another essential activity is ensuring that all licenses and agreements related to the software are terminated or transferred to a new system. This may involve working with vendors or legal teams to ensure compliance with licensing terms and conditions. Additionally, retiring software applications may include updating or reconfiguring other systems or applications integrated with the retired software. Finally, communication and training activities are also critical to ensure that users know the sunsetting process, understand any new systems or processes that will replace the old software, and have the necessary training to use the new systems effectively.

14.0 User Agreements

To facilitate having a safe, healthy, and inclusive environment, EMSL has developed a code of conduct for our staff, users, and visitors. Tracking and archiving of the acknowledged code of conduct will be managed through our user portal and ERecords in accordance with EMSL's Records Management Plan for users and visitors and via PNNL enterprise training for EMSL staff.

As a designated federal user facility for the Department of Energy, requests to use EMSL requires acceptance of a Non-Proprietary User Agreement (NPUA) by the home institution(s) of the proposal author and any participants listed on the proposal. The NPUA must be signed by a representative of the institution (e.g., dean, vice provost, director, sponsored programs officer, legal office, etc.) who is authorized to sign on behalf of and legally bind the institution. With approval by PNNL, DOE, and the Pacific Northwest Site Office (PNSO), the execution of the NPUA was fully automated in FY 2010. In accordance with the approved electronic process, signed institutional agreements will have a unique NPUA ID and are stored in EMSL's management system with the REPRESENTATIVE'S certification, signature date, and name and the name and signature date of the EMSL COO. The NPUA ID in effect at the time of active projects is stored in the project record for each user, and a printable version of the signed agreement is stored in ERecords in accordance with EMSL's Records Management Plan. Approval for the use of the electronic signature process can be found in ERecords.

14.1 EMSL Code of Conduct

The Environmental Molecular Sciences Laboratory (EMSL), a Department of Energy (DOE) Office of Science (SC) User Facility, is committed to providing a safe and healthy work environment for all staff, users, and visitors and, as stated in the DOE-SC Statement of Commitment (https://science.osti.gov/SW-DEI/SC-Statement-of-Commitment), "…does not tolerate discrimination or harassment of any kind, including sexual harassment, discrimination, bullying, intimidation, violence, threats of violence, retaliation, or other disruptive behavior in the workplace." EMSL is committed to providing training to ensure a safe and harassment-free working environment and expects EMSL staff, users, and visitors to conduct themselves and their activities in a safe, professional, and ethical manner. Treating everyone with respect and dignity sets the right environment to support collaboration and success for all EMSL staff, users, and visitors. While EMSL staff have internal trainings that are mandatory and adhere to Battelle's and Pacific Northwest National Laboratory's (PNNL's) code of conduct, this document outlines EMSL's expectations for EMSL staff, users, and visitors who access EMSL resources, either on-site or online. Specific expectations are detailed below.

1. **Ensure the safety and protection of the work environment, the external environment, others, and you. This includes but is not limited to the following:**
    - Conduct work within the scope of the work plan.
    - Complete, in a timely manner, all necessary trainings to safely access resources and spaces.
    - Wear personal protective equipment (PPE) when mandated. On-site users should contact their host to arrange for PPE.
    - Report ALL injuries, chemical spills, and unsafe work environment conditions, regardless of perceived magnitude, to your host.
    - Stop work immediately if you feel unsafe and report to your host or User Program Services (UPS) office staff. Seek help and ask questions when you are unsure of processes and procedures.
    - When on-site, comply with campus and Washington state traffic laws.

- Wear at least the following minimum attire in laboratories where hazardous chemicals, machinery, electrical hazards, etc. are used:
    i. full length pants (or equivalent) that cover the legs
    ii. a shirt or top that covers the torso and upper arms
    iii. closed toe shoes.

2. **Ensure the security & integrity of the work environment, the external environment, others, and you. This includes, but is not limited to the following:**

- Always wear your ID badge when on-site. Control your access card, provided to you based on your training. Do not share your card.
- Do not attempt to access space/resources for which you do not have authorization.
- Do not alter equipment/technology and/or safety devices/procedures.
- Data access and training: The user understands that browsing through multiple users' data files on PNNL computers connected to any instrument violates PNNL policy and will result in loss of network account privileges. This does not include EMSL and PNNL staff in the normal execution of their official duties.
- Handle, store, and dispose of chemicals and hazardous materials following PNNL's procedures. Contact your host if you are unsure.
- Comply with warning signs, construction barriers, and access postings including areas posted as Controlled.
- Be respectful of staff and office equipment in shared office spaces.
- Do not remove equipment, supplies, or chemicals from EMSL.
- Do not be under the influence alcohol or controlled substances while on campus.
- Do not engage in any form of physical or verbal abuse of any person on-site, including but not limited to, harassment, stalking, bullying, or hazing of any kind, whether the behavior is carried out verbally, physically, electronically, or in written form.
    i. Do not engage in conduct that is offensive, indecent, obscene, or disorderly, such as wearing clothing that has offensive images/words.

3. **Prohibited activities on PNNL premises**

- trespassing/loitering
- gambling
- being under the influence of illegal drugs (including marijuana), alcohol, and any other item prohibited by law
- unauthorized soliciting, vending, and/or debt collection
- posting, affixing, or distributing unauthorized material in writing or electronically
- bringing animals on campus; excluding service animals for disabled persons.

4. **Reporting**
    - For emergencies and security issues: 509-375-2400
    - Where complaints and unresolved issues can be lodged:
        i. Gert Patello, Chief Operations Officer, gert.patello@pnnl.gov

5. **Be familiar with and abide by the following:**
    - Terms and conditions of EMSL Use: https://www.emsl.pnnl.gov/terms-conditions
    - Acknowledging EMSL and Terms of Use: https://www.emsl.pnnl.gov/acknowledging-emsl-and-terms-use
    - Data Management Policy: https://www.emsl.pnnl.gov/data-management-policy
    - EMSL User Agreements: https://www.emsl.pnnl.gov/user-program/emsl-user-agreements

6. **Photography/videos**
    - Ask your EMSL UPS project manager or host about any patent-pending/proprietary technologies or areas that should not be photographed or recorded. Photography or videos of anything that could jeopardize unpublished research is not permitted.
    - Photography or videos taken secretly and without the consent of individuals in the immediate area are not permitted.
    - Provide a verbal announcement to fellow researchers in the room or area where you are taking photographs or recording videos so they can decide if they are comfortable being featured in these visuals.
    - Staff or visitor badges cannot be visible in photos or videos.
    - PNNL/EMSL laboratory PPE requirements must be reflected in photos and videos.
    - Be mindful that certain laboratories are noisy and may be difficult for recording videos.
    - Special permission must be obtained to use the name or identifying characteristics (e.g., logos) of Battelle, PNNL, or DOE.

7. **Consequences of violation**

    EMSL reserves the right to take actions against individuals who are found violating the code of conduct. Refusal to comply or repeat violations will be considered when determining consequences. Consequences can include suspension of site/resource access, removal from site and/or cancellation of future site access, separation of individuals, and reporting the incident to the violator's home institutions or relevant authorities. Depending on the severity or repeat offender status, revocation of access to EMSL and participation in the EMSL User program can also be enacted.

I acknowledge that I have received, reviewed, and will comply with this Code of Conduct.

_____ _____

Name Date

14.2 NPUA – Non-Proprietary User Agreement

The Department of Energy has opted to utilize the following agreement for Designated Non-Proprietary User Facilities transactions. Because these transactions are widespread across Departmental facilities, uniformity in agreement terms is desirable. Except for the *** provisions, minor modifications to the terms of this agreement may be made by CONTRACTOR, but any changes to the *** provisions or substantive changes to the non *** provisions will require approval by the DOE Contracting Officer, WHICH WILL LIKELY DELAY YOUR ACCESS TO THE USER FACILITY. In instances where DOE Contracting Officer approval for substantive changes cannot be obtained, Strategic Partnership Projects (SPPs) and Cooperative Research and Development Agreements (CRADAs) may be more appropriate due to the increased flexibility such agreements afford. Where this Agreement is to be used as an umbrella agreement for multiple transactions it may be modified to reflect such usage.

Non-Proprietary User Agreement

No. [insert NPUA number here]

BETWEEN

Battelle Memorial Institute, Pacific Northwest Division
(hereinafter "CONTRACTOR")
Operator of Pacific Northwest National Laboratory (hereinafter "Laboratory")
under U.S. Department of Energy (hereinafter "DOE")
Contract No. DE-AC05-76RL01830

AND

_____
("USER")

(Collectively, "the Parties")

The obligations of the above-identified CONTRACTOR may be transferred to and shall apply to any successor in interest to said CONTRACTOR continuing the operation of the DOE Non-Proprietary User Facility involved in this User Agreement (hereinafter "Agreement").

ARTICLE I. FACILITIES AND SCOPE OF WORK

CONTRACTOR will make available to employees, consultants and representatives of USER (hereinafter called "Participants") certain Laboratory Non-Proprietary User facilities, which may include equipment, services, information and other material, with or without Laboratory scientist collaboration, for purposes as described in the research proposal accepted by CONTRACTOR and conducted by Participants at the designated Non-Proprietary User Facility during the effective period of this Agreement. Additional future research proposals referencing this Agreement may be submitted by USER for identified User Facilities and purposes during the term of this Agreement (see Article II). Such additional research proposals will be considered to be part of this Agreement upon acceptance by CONTRACTOR. Each accepted and approved research proposal shall set forth the Technical Scope of Work of a specific project, including deliverables, to be performed pursuant to this Agreement. The scope of work shall not be considered proprietary information and shall

be publicly releasable. The Parties agree that an initial abstract of the work to be performed shall be a deliverable under this Agreement.

ARTICLE II. TERM OF THE AGREEMENT

This Agreement shall have a term of five (5) years from the effective date. The term of this Agreement shall be effective as of the date on which it is signed by the last of the Parties. Unless terminated in accordance with the terms herein, this Agreement shall automatically renew on a year-to-year basis after the initial five year term.

ARTICLE III. COST

Each Party will bear its own costs and expenses associated with this Agreement. No money will be transferred to or from either Party as consideration, in whole or in part, for this Agreement.

ARTICLE IV. ADMISSION REQUIREMENTS

USERs and Participants are subject to the administrative and technical supervision and control of CONTRACTOR; and will comply with all applicable rules of CONTRACTOR and DOE with regard to admission to and use of the User Facility, including safety, operating and health-physics procedures, environment protection, access to information, hours of work, and conduct. Participants shall execute any and all documents required by CONTRACTOR acknowledging and agreeing to comply with such applicable rules of CONTRACTOR. Participants will not be considered employees of CONTRACTOR for any purpose.

ARTICLE V. PROPERTY AND MATERIALS*

USER may be permitted by CONTRACTOR to furnish equipment, tooling, test apparatus, or materials necessary to assist in the performance of its experiment(s) at the User Facility. Such items shall remain the property of USER. Unless the Parties otherwise agree, all such property furnished by USER or equipment and test apparatus provided by USER will be removed by USER within sixty (60) days of termination or expiration of this Agreement or will be disposed of as directed by USER at USER's expense. Any equipment that becomes integrated into the User Facility shall be the property of the Government. USER acknowledges that any material supplied by USER may be damaged, consumed or lost. Materials (including residues and/or other contaminated material) remaining after performance of the work or analysis will be removed in their then condition by USER at USER's expense. USER will return User Facilities and equipment utilized in their original condition except for normal wear and tear.

CONTRACTOR shall have no responsibility for USER's property in CONTRACTOR's possession other than loss or damage caused by willful misconduct or gross negligence of CONTRACTOR or its employees.

Personal property produced or acquired during the course of this Agreement shall be disposed of as directed by the owner at the owner's expense.

ARTICLE VI. SCHEDULING*

USER understands that CONTRACTOR will have sole responsibility and discretion for allocating and scheduling usage of the User Facilities and equipment needed for or involved under this Agreement.

ARTICLE VII. INDEMNITY AND LIABILITY*

A. Personnel Relationships - USER shall be responsible for the acts or omissions of Participants.

B. Product Liability - To the extent permitted by U.S. and U.S. State law, if USER utilizes the work derived from this Agreement in the making, using, or selling of a product, process or service, then USER hereby agrees to hold harmless and indemnify CONTRACTOR and the United States Government, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, as a result of or arising out of such utilization of the work by or on behalf of USER, its assignees or licensees.

C. General Indemnity - To the extent permitted by U.S. and U.S. State law, USER hereby agrees to indemnify and hold harmless CONTRACTOR and the United States Government, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, to the extent such liability, claims, or damages is caused by or contributed to the negligence or intentional misconduct of USER or its employees or representatives during the performance of the work under this Agreement.

D. Patent and Copyright Indemnity—Limited - To the extent permitted by U.S. and U.S. State law, USER shall fully indemnify the Government and CONTRACTOR and their officers, agents, and employees for infringement of any United States patent or copyright arising out of any acts required or directed or performed by USER under this Agreement to the extent such acts are not normally performed at the User Facility.

E. The liability and indemnity provisions in paragraphs B, C and D above shall not apply unless USER shall have been informed as soon as practicable by CONTRACTOR or the Government of the suit or action alleging such infringement, and such indemnity shall not apply to a claimed infringement that is settled without the consent of USER unless required by a court of competent jurisdiction.

F. General Disclaimer -

THE GOVERNMENT AND CONTRACTOR MAKE NO EXPRESS OR IMPLIED WARRANTY AS TO THE CONDITIONS OF THE USER FACILITY FURNISHED HEREUNDER. IN ADDITION, THE GOVERNMENT, CONTRACTOR AND USER MAKE NO EXPRESS OR IMPLIED WARRANTY AS TO THE RESEARCH OR ANY INTELLECTUAL PROPERTY, GENERATED INFORMATION, OR PRODUCT MADE OR DEVELOPED UNDER THIS AGREEMENT, OR THE OWNERSHIP, MERCHANTABILITY, OR FITNESS FOR A PARTICULAR PURPOSE OF THE RESEARCH OR RESULTING PRODUCT; THAT THE GOODS, SERVICES, MATERIALS, PRODUCTS, PROCESSES, INFORMATION, OR DATA TO BE FURNISHED HEREUNDER WILL ACCOMPLISH INTENDED RESULTS OR ARE SAFE FOR ANY PURPOSE INCLUDING THE INTENDED PURPOSE; OR THAT ANY OF THE ABOVE WILL NOT INTERFERE WITH PRIVATELY OWNED RIGHTS OF OTHERS. THE GOVERNMENT, CONTRACTOR AND/OR USER SHALL NOT BE LIABLE FOR SPECIAL, CONSEQUENTIAL, OR INCIDENTAL DAMAGES ATTRIBUTED TO USE OF SUCH FACILITIES, RESEARCH OR RESULTING PRODUCT, INTELLECTUAL PROPERTY, GENERATED INFORMATION, OR PRODUCT MADE OR DELIVERED UNDER THIS AGREEMENT.

ARTICLE VIII. PATENT RIGHTS***

A. Definitions

1. “Subject Invention” means any invention or discovery conceived or first actually reduced to practice in the course of or under this Agreement.
2. “USER Invention” means any Subject Invention of USER.
3. “CONTRACTOR Invention” means any Subject Invention of CONTRACTOR.
4. “Patent Counsel” means the DOE Counsel for Intellectual Property assisting the DOE Contracting activity.

B. Subject Inventions

CONTRACTOR and USER agree to disclose their Subject Inventions, which includes any inventions of their Participants, to each other, concurrent with reporting such Subject Inventions to DOE.

C. CONTRACTOR's Rights

Except as provided below in the case of joint inventions, CONTRACTOR Inventions will be governed by the provisions of CONTRACTOR's Prime Contract for operation of the User Facility.

D. USER's Rights

Subject to the provisions herein, USER may elect title to any USER Invention and in any resulting patent secured by USER within one year of reporting the Subject Invention to DOE. The USER shall file a U.S. patent application within a reasonable period of time. Where appropriate, the filing of patent applications by USER is subject to DOE security regulations and requirements.

E. Joint Inventions

For Subject Inventions conceived or first actually reduced to practice under this Agreement that are joint Subject Inventions made by CONTRACTOR and USER, each Party shall have the option to elect and retain title to its undivided rights in such joint Subject Inventions.

F. Rights of Government

1. USER agrees to timely assign to the Government, if requested, the entire right, title, and interest in any country to each USER Invention where USER:

   a. Does not elect to retain such rights; or

   b. Fails to timely have a patent application filed in that country on the USER Invention or decides not to continue prosecution or not to pay the maintenance fees covering the Invention; or

   c. At any time, no longer desires to retain title.

2. USER shall provide the Government a copy of any patent application filed by USER promptly after such application is filed, including its serial number and filing date.

3. USER hereby grants to the Government a nonexclusive, nontransferable, irrevocable, paid-up license to practice or have practiced for or on behalf of the United States the USER Invention made under said project throughout the world.

4. USER acknowledges that the DOE has certain March-in Rights to any USER Inventions elected by the USER in accordance with 48 C.F.R. 27.304-1(g) and that the USER is subject to the requirements with respect to preference for U.S. industry pursuant to 35 U.S.C. § 204 to any USER Inventions elected by the USER.

5. The USER agrees to include, within the specification of any U.S. patent applications and any patent issuing thereon covering a USER Invention, the following statement: "The Government has rights in this invention pursuant to a USER Agreement (specify number) between (USER name) and Battelle Memorial Institute, Pacific Northwest Division, which manages and operates the Pacific Northwest National Laboratory for the U.S. Department of Energy."

6. USER agrees to submit on request periodic reports to DOE no more frequently than annually on the utilization of USER Inventions or on efforts to obtain such utilization that are being made by USER or its licensees or assignees.

7. Facilities License: USER agrees to and does hereby grant to the Government a nonexclusive, nontransferable, irrevocable, paid-up license in and to any inventions or discoveries, regardless of when conceived or actually reduced to practice or acquired by USER, which are incorporated in the User Facility as a result of this Agreement to such an extent that the User Facility is not restored to the condition existing prior to the Agreement (1) to practice or to have practiced by or for the Government at the User Facility, and (2) to transfer such licenses with the transfer of that User Facility. The acceptance or exercise by the Government of the aforesaid rights and license shall not prevent the Government at any time from contesting the enforceability, validity or scope of, or title to, any rights or patents herein licensed.

G. Invention Report and Election

USER shall furnish the Patent Counsel a written report concerning each USER Invention within six months after conception or first actual reduction to practice, whichever occurs first. If USER wishes to elect title to the USER Invention, a notice of election should be submitted with the report or within one year of such date of reporting.

ARTICLE IX. RIGHTS IN TECHNICAL DATA***

A. Definitions:

1. "Technical Data" means recorded information regardless of form or characteristic, of a scientific or technical nature. Technical Data as used herein does not include financial reports, costs analyses, and other information incidental to Agreement administration.

2. "Proprietary Data" means Technical Data which embody trade secrets developed at private expense, outside of this Agreement, such as design procedures or techniques, chemical composition of materials, or manufacturing methods, processes, or treatments, including minor modifications thereof, provided that such data:

   a. Are not generally known or available from other sources without obligation concerning their confidentiality.

   b. Have not been made available by the owner to others without obligation concerning their confidentiality, and

   c. Are not already available to the CONTRACTOR or the Government without obligation concerning their confidentiality.

   d. Are marked as "Proprietary Data."

3. "Unlimited Rights" means right to use, duplicate, or disclose Technical Data, in whole or in part, in any manner and for any purpose whatsoever, and to permit others to do so.

B. Allocation of Rights

1. The Government shall have Unlimited Rights in Technical Data first produced or specifically used in the performance of this Agreement except as otherwise provided in this Agreement.

2. USER shall have the right to use for its private purposes, subject to patent, security or other provisions of this Agreement, Technical Data it first produces in the performance of this Agreement provided the data delivery requirements of this Agreement have been met as of the date of the private use of such data; and Technical Data first produced by CONTRACTOR, if any, under this Agreement. USER agrees that to the extent it receives or is given access to Proprietary Data or other technical, business or financial data in the form of recorded information from DOE or a DOE contractor or subcontractor, USER shall treat such data in accordance with any restrictive legend contained thereon, unless use is specifically authorized by prior written approval of the Contracting Officer.

C. Deliverables

1. USER agrees to furnish to DOE or CONTRACTOR those data, if any, which are (a) specified to be delivered in the research proposal, (b) essential to the performance of work by CONTRACTOR personnel or (c) necessary for the health and safety of such personnel in the performance of the work. Any data furnished to DOE or CONTRACTOR shall be deemed to have been delivered with unlimited rights unless marked as "Proprietary Data" of USER.

2. Upon completion or termination of the project, USER agrees to deliver to DOE and CONTRACTOR a nonproprietary report describing the work performed under this Agreement.

D. Legal Notice

The following legal notice shall be affixed to each report or publication resulting from this Agreement which may be distributed by USER:

DISCLAIMER NOTICE

This document was prepared by (USER name) as a result of research conducted at the U.S. Department of Energy (DOE) Environmental Molecular Sciences Laboratory (EMSL), which is located at the Pacific Northwest National Laboratory and managed by Battelle Memorial Institute, Pacific Northwest Division, acting under Contract No. DE-AC05-76RL01830. EMSL is a DOE Office of Science User Facility and is sponsored by the Office of Biological and Environmental Research. Neither Battelle Memorial Institute, Pacific Northwest Division, DOE, the U.S. Government, nor any person acting on their behalf: (a) make any warranty or representation, express or implied, with respect to the information contained in this document; or (b) assume any liabilities with respect to the use of, or damages resulting from the use of any information contained in this document.

E. Copyrighted Material

1. USER agrees to, and does hereby grant to the Government, and to its officers, agents, servants and employees acting within the scope of their duties:

   a. A royalty-free, nonexclusive, irrevocable license to reproduce, translate, publish, use, and dispose of and to authorize others so to do, all copyrightable material first produced or composed in the performance of this Agreement by USER, its employees or any individual or concern specifically employed or assigned to originate and prepare such material; and

   b. A license as aforesaid under any and all copyrighted or copyrightable works not first produced or composed by USER in the performance of this Agreement but which are incorporated in the material furnished or delivered under this Agreement, provided that such license shall be only to the extent USER now has, or prior to completion or final settlement of this Agreement may acquire, the right to grant such license without becoming liable to pay compensation to others solely because of such grant.

2. USER agrees that it will not knowingly include any copyrightable material furnished or delivered under this Agreement without a license as provided for in subparagraph 1(b) hereof, or without the consent of the copyright owner, unless it obtains specific written approval of the DOE Contracting Officer for the inclusion of such copyrighted materials.

F. Disclosure of Proprietary Data

All Proprietary Data shall be protected from disclosure for a period of three years from the date of execution of this Agreement or three years from CONTRACTOR acceptance of future research proposals where Proprietary Data is received under such future research proposals.

ARTICLE X. LABORATORY SITE ACCESS, SAFETY AND HEALTH***

As a precondition to using CONTRACTOR User Facility, Participants must complete all CONTRACTOR Site Access documents and requirements. USER and Participant shall take all reasonable precautions in activities carried out under this Agreement to protect the safety and health of others and to protect the environment. Participants must comply with all applicable safety, health, access to information, security and environmental regulations and the requirements of the DOE and CONTRACTOR, including the specific requirements of the User Facility covered by this Agreement. In the event that USER or Participant fails to comply with said regulations and requirements, CONTRACTOR may, without prejudice to any other legal or contractual rights, issue and order stopping all or any part of USER's activities at the User Facility.

ARTICLE XI. PERSONNEL RELATIONSHIPS***

Participants will remain employees or representatives of the USER at all times during their participation in the work under this Agreement, and shall not be considered employees of CONTRACTOR or DOE for any purpose. Participants shall be subject to the administrative and technical supervision and control of CONTRACTOR during and in connection with the Participant's activities under this Agreement.

ARTICLE XII. EXPORT CONTROLS***

USER acknowledges that the export of goods or Technical Data may require some form of export control license from the U.S. Government and that failure to obtain such export control license may result in criminal liability under the laws of the United States.

ARTICLE XIII. PUBLICATIONS***

A. USER and CONTRACTOR will provide each other copies of articles of any publication of information generated pursuant to this Agreement for review and comment 14 days prior to publication.

B. USER will not use the name of CONTRACTOR or the United States Government or their employees in any promotional activity, such as advertisements, with reference to any product or service resulting from this Agreement, without prior written approval of the Government and CONTRACTOR.

ARTICLE XIV. DISPUTES***

The Parties will attempt to jointly resolve all disputes arising under this Agreement. If the Parties are unable to jointly resolve a dispute within a reasonable period of time, either Party may contact the Laboratory's Technology Transfer Ombudsman (TTO) to provide assistance. The TTO may work directly to resolve the dispute or, upon mutual agreement of the Parties, contact a third party neutral mediator to assist the Parties in coming to a resolution. The costs of the mediator's services will be shared equally by the Parties. In the event that an agreement is not reached with the aid of the TTO or mediator, the Parties may agree to have the dispute addressed by neutral evaluation. The decision rendered by the neutral evaluator shall be nonbinding on the Parties, and any costs incurred there from shall be divided equally between the Parties. Upon mutual agreement, the Parties may request a final decision by the DOE Contracting Officer. Absent resolution, either Party may seek relief in a court of competent jurisdiction.

ARTICLE XV. CONFLICT OF TERMS***

This Agreement constitutes the primary document which governs the work described in the research proposal. In the event of any conflict between the terms of this document and any other document issued by either Party, the terms of this document shall prevail.

ARTICLE XVI. TERMINATION***

Either Party may terminate this Agreement for any reason at any time by giving not less than thirty (30) days prior written notice to the other Party. Notice will be deemed made as of the day of receipt. The obligations of any clause of this Agreement, which by their nature extend beyond its termination, shall remain in full force and effect until fulfilled.

FOR THE CONTRACTOR:

BY:

TITLE: EMSL Chief Operations Officer

ADDRESS: EMSL, PO Box 999, K8-86, Richland, WA 99352

DATE:

TELEPHONE: 509/371-6003

FOR THE USER:

BY:

TITLE:

ADDRESS:

DATE:

TELEPHONE:

14.3 PUA – Proprietary User Agreement - Advance Option

The Department of Energy has opted to utilize the following agreement for Designated Proprietary User Facilities transactions. Because these transactions are widespread across Departmental facilities, uniformity in agreement terms is desirable. Except for the *** provisions, minor modifications to the terms of this agreement may be made by CONTRACTOR, but any changes to the *** provisions or substantive changes to the non *** provisions will require approval by the DOE Contracting Officer, WHICH WILL LIKELY DELAY YOUR ACCESS TO THE USER FACILITY. In instances where DOE Contracting Officer approval for substantive changes cannot be obtained, Strategic Partnership Projects (SPPs) and Cooperative Research and Development Agreements (CRADAs) may be more appropriate due to the increased flexibility such agreements afford. Where this Agreement is to be used as an umbrella agreement for multiple transactions it may be modified to reflect such usage.

Proprietary User Agreement

No. [insert PUA number here]

BETWEEN

Battelle Memorial Institute, Pacific Northwest Division
(hereinafter "CONTRACTOR")
Operator of Pacific Northwest National Laboratory (hereinafter "Laboratory")
under U.S. Department of Energy (hereinafter "DOE")
Contract No. DE-AC05-76RL01830

AND

_____
(hereinafter "USER")

(Collectively, "the Parties")

The obligations of the CONTRACTOR may be transferred and shall apply to any successor in interest to said CONTRACTOR continuing the operation of the DOE User Facility involved in this Proprietary User Agreement (hereinafter "Agreement").

ARTICLE I. FACILITIES AND SCOPE OF WORK

Employee(s), consultant(s), and representative(s) of USER (hereinafter "Participant(s)") shall be permitted to use Laboratory facilities for the purpose described in Proposal No. [insert Proposal No. here] (hereinafter "Proposal") submitted by USER and approved by CONTRACTOR via the EMSL User Portal at https://nexus.emsl.pnnl.gov/Portal/. Said Proposal is hereby incorporated into this Agreement by reference. This Proprietary User Agreement shall be incorporated by reference and apply to all such experiments authorized for performance at Laboratory facilities which are totally funded by USER. CONTRACTOR will retain its employees assigned to this work on its payroll and will be reimbursed by USER for the account of DOE in accordance with DOE's pricing policy, which provides for full cost recovery.

User Facility: Environmental Molecular Sciences Laboratory (EMSL)

Scope of Work: As described in Proposal No. [insert Proposal No. here]

ARTICLE II. TERM OF THE AGREEMENT

This Agreement shall have a term that is coextensive with the active date corresponding to the Proposal. However, this Agreement shall not have a term that exceeds one calendar year from the effective date of this Agreement. The term of this Agreement shall be effective as of the latter date of (1) the date the Proposal is approved by the CONTRACTOR, (2) the date on which this Agreement is executed by the last of the Parties, or (3) the receipt of any advance payment required under Article III.

ARTICLE III. BILLING AND PAYMENT OF EXPENSES

A. The estimated cost of the work, described in Article I above is $_____.

Full cost recovery rates are established at the beginning of each fiscal year and are subject to revision to reflect changing cost factors during the fiscal year. The minimum unit of charge at the User Facility is an 8 hour shift.

No work can begin until this advance payment is received by CONTRACTOR.

B. USER shall pay CONTRACTOR the following advance payment:

Advance Payment. USER shall advance the following amount at the time shown:

Amount Due	Date Due
$_____.__	00/00/00

This is a full advance for the estimated cost.

All advance payments must be made in U.S. dollars. For foreign wire transfers, please add $30 to the invoice amount to cover payment charges levied by USER's banking institution.

Monthly Expense Statements. When work commences, monthly expense statements showing actual costs incurred for the month and the balance remaining in the account are mailed to USER for information only. The expense statements are not requests for payment.

If the estimated cost is increased during the project or the project is expected to be renewed, an additional advance may be requested of USER. CONTRACTOR is not obligated to continue the work unless it is holding an adequate advance.

Upon completion of the project there will be a reconciliation of the total costs incurred to total payments received and a final expense statement along with any remaining advance will be returned to USER.

Expense statements shall be sent to: (this information is mandatory)

USER Reference No. if applicable: _____

Contact Name: _____

Street Address: _____

City, State, Zip Code: _____

Country: _____

Telephone with area code: _____

Email: _____

Tax ID Number (TIN): _____

C. All costs of Experiments will be in accordance with DOE Order O 522.1, "Pricing of Departmental Materials and Services.

ARTICLE IV. RESERVED

ARTICLE V. PROPERTY AND MATERIALS***

USER may be permitted by the CONTRACTOR to furnish equipment, tooling, test apparatus, or materials necessary to assist in the performance of its experiment(s) at the User Facility. Such items shall remain the property of USER. Unless the Parties otherwise agree, all such property furnished by USER or equipment and test apparatus provided by USER will be removed by USER within sixty (60) days of termination or expiration of this Agreement or will be disposed of as directed by USER at USER's expense. Any equipment that becomes integrated into the User Facility shall be the property of the Government. USER acknowledges that any material supplied by USER may be damaged, consumed or lost. Materials (including residues and/or other contaminated material) remaining after performance of the work or analysis will be removed in their then condition by USER at USER's expense. USER will return User Facilities and equipment utilized in their original condition except for normal wear and tear.

CONTRACTOR shall have no responsibility for USER's property at the User Facility other than loss or damage caused by willful misconduct or gross negligence of CONTRACTOR or its employees.

Personal property produced or acquired during the course of this Agreement shall be disposed of as directed by the owner at the owner's expense.

ARTICLE VI. SCHEDULING***

USER understands that CONTRACTOR will have sole responsibility and discretion for allocating and scheduling usage of the User Facilities and equipment needed for or involved under this Agreement.

ARTICLE VII. INDEMNITY AND LIABILITY***

A. Personnel Relationships - USER shall be responsible for the acts or omissions of Participants.

B. Product Liability - To the extent permitted by U.S. and U.S. State law, if USER utilizes the work derived from this Agreement in the making, using, or selling of a product, process or service, then USER hereby agrees to hold harmless and indemnify CONTRACTOR and the United States Government, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, as a result of or arising out of such utilization of the work by or on behalf of USER, its assignees or licensees.

C. General Indemnity - To the extent permitted by U.S. and U.S. State law, USER hereby agrees to indemnify and hold harmless CONTRACTOR and the United States Government, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, arising out of the performance of this Agreement or arising out of the use of the services

performed, materials supplied or information given hereunder by any persons including the USER, and not directly resulting from the fault or negligence of the CONTRACTOR or the United States Government, or persons acting on their behalf.

D. Patent and Copyright Indemnity—Limited - To the extent permitted by U.S. and U.S. State law, USER shall fully indemnify the Government and CONTRACTOR and their officers, agents, and employees for infringement of any United States patent or copyright arising out of any acts required or directed or performed by USER under this Agreement to the extent such acts are not normally performed at the Facility.

E. The liability and indemnity provisions in paragraphs B, C and D above shall not apply unless USER shall have been informed as soon as practicable by CONTRACTOR or the Government of the suit or action alleging such liability or infringement, and such indemnity shall not apply to a claimed liability or infringement that is settled without the consent of USER unless required by a court of competent jurisdiction.

F. General Disclaimer -

THE GOVERNMENT AND CONTRACTOR MAKE NO EXPRESS OR IMPLIED WARRANTY AS TO THE CONDITIONS OF THE FACILITY FURNISHED HEREUNDER. IN ADDITION, THE GOVERNMENT, CONTRACTOR AND USER MAKE NO EXPRESS OR IMPLIED WARRANTY AS TO THE RESEARCH OR ANY INTELLECTUAL PROPERTY, GENERATED INFORMATION, OR PRODUCT MADE OR DEVELOPED UNDER THIS AGREEMENT, OR THE OWNERSHIP, MERCHANTABILITY, OR FITNESS FOR A PARTICULAR PURPOSE OF THE RESEARCH OR RESULTING PRODUCT; THAT THE GOODS, SERVICES, MATERIALS, PRODUCTS, PROCESSES, INFORMATION, OR DATA TO BE FURNISHED HEREUNDER WILL ACCOMPLISH INTENDED RESULTS OR ARE SAFE FOR ANY PURPOSE INCLUDING THE INTENDED PURPOSE; OR THAT ANY OF THE ABOVE WILL NOT INTERFERE WITH PRIVATELY OWNED RIGHTS OF OTHERS. THE GOVERNMENT, CONTRACTOR AND/OR USER SHALL NOT BE LIABLE FOR SPECIAL, CONSEQUENTIAL, OR INCIDENTAL DAMAGES ATTRIBUTED TO USE OF SUCH FACILITIES, RESEARCH OR RESULTING PRODUCT, INTELLECTUAL PROPERTY, GENERATED INFORMATION, OR PRODUCT MADE OR DELIVERED UNDER THIS AGREEMENT.

G. Notice and Assistance Regarding Patent and Copyright Infringement

1. USER shall report to the Government, promptly and in reasonable written detail, each notice or claim of patent or copyright infringement based on the performance of this Agreement of which USER has knowledge.

2. In the event of any claim or suit against the Government on account of any alleged patent or copyright infringement arising out of the performance of this Agreement or out of the use of any supplies furnished or work or services performed hereunder, USER shall furnish to the Government when requested by the Government, all evidence and information in possession of USER pertaining to such suit or claim. Such evidence and information shall be furnished at the expense of the Government except where USER has agreed to indemnify the Government.

ARTICLE VIII. PATENT RIGHTS***

A. Definitions

1. “Subject Invention” means any invention or discovery of USER conceived or first actually reduced to practice in the course of or under this Agreement.

2. “Patent Counsel” means the DOE Patent Counsel assisting the CONTRACTOR.

B. Rights of USER – Election to Retain Rights

With respect to any USER Subject Invention, which includes inventions of any Participants, reported and elected in accordance with paragraph (C) of this clause, USER may elect to obtain the entire right, title and interest in any patent application filed in any country on a Subject Invention and in any resulting patent secured by USER. Where appropriate, the filing of any patent application by USER is subject to DOE security regulations and requirements.

C. Invention Identification, Disclosures, and Reports

USER shall furnish the Patent Counsel a written report concerning each USER Subject Invention, which includes inventions of any Participants, within six months after conception or first actual reduction to practice, whichever occurs first. If USER wishes to elect title to the Subject Invention, a notice of election to the Subject Invention should be submitted with the report or within one year of such date of reporting of the Subject Invention.

D. Facilities License

USER agrees to and does hereby grant to the Government an irrevocable, nonexclusive paid-up license in and to any inventions or discoveries, regardless of when conceived or actually reduced to practice or acquired by USER, which at any time through completion of this Agreement are owned or controlled by USER and are incorporated in the Facility as a result of this Agreement to such an extent that the Facility is not restored to the condition existing prior to the Agreement (1) to practice or to have practiced by or for the Government at the Facility, and (2) to transfer such licenses with the transfer of that Facility. The acceptance or exercise by the Government of the aforesaid rights and license shall not prevent the Government at any time from contesting the enforceability, validity or scope of, or title to, any rights or patents herein licensed

ARTICLE IX. RIGHTS IN TECHNICAL DATA***

A. Definitions

1. "Technical Data" means recorded information, regardless of form or characteristic, of a scientific or technical nature. Technical data as used herein does not include financial reports, cost analyses, and other information incidental to Agreement administration.
2. "Proprietary Data" means technical data which embody trade secrets, developed at private expense, such as design procedures or techniques, chemical composition of materials, or manufacturing methods, processes or treatments, including minor modifications thereof, provided that such data:

   a. are not generally known or available from other sources without obligation concerning their confidentiality,

   b. have not been made available by the owner to others without obligation concerning their confidentiality,

   c. are not already available to the Government without obligation concerning their confidentiality, and

   d. are marked as "Proprietary Data."
3. "Unlimited Rights" means rights to use, duplicate or disclose technical data, in whole or in part, in any manner and for any purpose whatsoever, and to permit others to do so.

B. USER agrees to furnish to DOE or CONTRACTOR those data, if any, which are (1) essential to the performance of work by DOE or CONTRACTOR personnel or (2) necessary for the health and safety of such personnel in the performance of the work. Any data furnished to DOE or CONTRACTOR shall be deemed to have been delivered with unlimited rights unless marked as "Proprietary Data" of USER.

C. USER agrees that it shall have the sole responsibility for identifying and marking all documents containing Proprietary Data which are furnished by USER or produced under this Agreement. USER further agrees to mark each such document by or before termination of this Agreement by placing on the cover page thereof a legend identifying the

document as Proprietary Data of USER and identifying each page and portion thereof to which the marking applies. The Government and CONTRACTOR shall not disclose properly marked Proprietary Data of USER outside the Government and CONTRACTOR. The Government and CONTRACTOR reserve the right to challenge the proprietary nature of any markings on data.

D. USER is solely responsible for the removal of all of its Proprietary Data from the User Facility by or before termination of this Agreement. The Government shall have unlimited rights in any Technical Data (including Proprietary Data) which are not removed from the User Facility by or before termination of this Agreement. The Government shall have unlimited rights in any Technical Data (including Proprietary Data) which are incorporated into the User Facility under this Agreement to such extent that the User Facility or equipment is not restored to the condition existing prior to such incorporation.

E. Upon completion or termination of the project, USER agrees to deliver to DOE and CONTRACTOR a non-proprietary report describing the work performed under this Agreement.

ARTICLE X. LABORATORY SITE ACCESS, SAFETY AND HEALTH***

As a precondition to using CONTRACTOR User Facility, Participants must complete all CONTRACTOR Site Access documents and requirements. USER and Participants shall take all reasonable precautions in activities carried out under this Agreement to protect the safety and health of others and to protect the environment. Participants must comply with all applicable rules of CONTRACTOR and DOE with regard to admission to and use of the User Facility, including safety, health, operating and health-physics procedures, access to information, security and environmental regulations, procedures, and the requirements of the DOE and CONTRACTOR, including the specific requirements of the User Facility covered by this Agreement. Participants shall execute any and all documents required by CONTRACTOR acknowledging and agreeing to comply with such applicable rules of CONTRACTOR. In the event that USER or Participant fails to comply with said regulations, procedures, and requirements, CONTRACTOR may, without prejudice to any other legal or contractual rights, issue and order stopping all or any part of USER's or Participant's activities at the Designated Proprietary User Facility.

ARTICLE XI. PERSONNEL RELATIONSHIPS***

Participants will remain employees or representatives of USER at all times during their participation in the work under this Agreement, and shall not be considered employees of CONTRACTOR or DOE for any purpose. Participants shall be subject to the administrative and technical supervision and control of CONTRACTOR during and in connection with the Participants' activities under this Agreement.

ARTICLE XII. EXPORT CONTROLS***

USER acknowledges that the export of goods or Technical Data may require some form of export control license from the U.S. Government and that failure to obtain such export control license may result in criminal liability under the laws of the United States.

ARTICLE XIII. THIRD-PARTY CONTRACTS

Contracts between USER and third parties for work on CONTRACTOR premises including, but not limited to, construction, installation, maintenance, and repair, will be subject to prior approval by the DOE and CONTRACTOR. The DOE and CONTRACTOR may require the insertion of specific terms and conditions into such contracts.

ARTICLE XIV. DISPUTES***

The Parties will attempt to jointly resolve all disputes arising under this Agreement. If the Parties are unable to jointly resolve a dispute within a reasonable period of time, either Party may contact the Laboratory's Technology Transfer Ombudsman (TTO) to provide assistance. The TTO may work directly to resolve the dispute or, upon mutual agreement of the Parties, contact a third party neutral mediator to assist the Parties in coming to a resolution. The costs of the mediator's services will be shared equally by the Parties. In the event that an agreement is not reached with the aid of the TTO or mediator, the Parties may agree to have the dispute addressed by neutral evaluation. The decision rendered by the neutral evaluator shall be nonbinding on the Parties, and any costs incurred there from shall be divided equally between the Parties. Upon mutual agreement, the Parties may request a final decision by the DOE Contracting Officer. Absent resolution, either Party may seek relief in a court of competent jurisdiction.

ARTICLE XV. CONFLICT OF TERMS***

In the event of any conflict between the terms of this document and any other document issued by either Party, the terms of this document shall prevail.

ARTICLE XVI. TERMINATION***

Either Party may terminate this Agreement for any reason at any time by giving not less than thirty (30) days prior written notice to the other Party, provided that CONTRACTOR shall recover payment for the costs incurred by CONTRACTOR on behalf of USER prior to termination and for termination costs.

In witness whereof, the Parties hereto have executed this Agreement:

FOR THE CONTRACTOR:

BY:
TITLE: EMSL Chief Operations Officer
ADDRESS: EMSL, PO Box 999, K8-86, Richland, WA 99352
DATE:
TELEPHONE:

FOR THE USER:

BY:
TITLE:
ADDRESS:
DATE:
TELEPHONE:

14.4 PUA – Proprietary User Agreement – Partial Advance Option

The Department of Energy has opted to utilize the following agreement for Designated Proprietary User Facilities transactions. Because these transactions are widespread across Departmental facilities, uniformity in agreement terms is desirable. Except for the *** provisions, minor modifications to the terms of this agreement may be made by CONTRACTOR, but any changes to the *** provisions or substantive changes to the non *** provisions will require approval by the DOE Contracting Officer, WHICH WILL LIKELY DELAY YOUR ACCESS TO THE USER FACILITY. In instances where DOE Contracting Officer approval for substantive changes cannot be obtained, Strategic Partnership Projects (SPPs) and Cooperative Research and Development Agreements (CRADAs) may be more appropriate due to the increased flexibility such agreements afford. Where this Agreement is to be used as an umbrella agreement for multiple transactions it may be modified to reflect such usage.

Proprietary User Agreement

No. [insert PUA number here]

BETWEEN

Battelle Memorial Institute, Pacific Northwest Division
(hereinafter "CONTRACTOR")
Operator of Pacific Northwest National Laboratory (hereinafter "Laboratory")
under U.S. Department of Energy (hereinafter "DOE")
Contract No. DE-AC05-76RL01830

AND

_____
(hereinafter "USER")

(Collectively, "the Parties")

The obligations of the CONTRACTOR may be transferred and shall apply to any successor in interest to said CONTRACTOR continuing the operation of the DOE User Facility involved in this Proprietary User Agreement (hereinafter "Agreement").

ARTICLE I. FACILITIES AND SCOPE OF WORK

Employee(s), consultant(s), and representative(s) of USER (hereinafter "Participant(s)") shall be permitted to use Laboratory facilities for the purpose described in Proposal No. [insert Proposal No. here] (hereinafter "Proposal") submitted by USER and approved by CONTRACTOR via the EMSL User Portal at https://nexus.emsl.pnnl.gov/Portal/. Said Proposal is hereby incorporated into this Agreement by reference. This Proprietary User Agreement shall be incorporated by reference and apply to all such experiments authorized for performance at Laboratory facilities which are totally funded by USER. CONTRACTOR will retain its employees assigned to this work on its payroll and will be reimbursed by USER for the account of DOE in accordance with DOE's pricing policy, which provides for full cost recovery.

User Facility: Environmental Molecular Sciences Laboratory (EMSL)

Scope of Work: As described in Proposal No. [insert Proposal No. here]

ARTICLE II. TERM OF THE AGREEMENT

This Agreement shall have a term that is coextensive with the active date corresponding to the Proposal. However, this Agreement shall not have a term that exceeds one calendar year from the effective date of this Agreement. The term of this Agreement shall be effective as of the latter date of (1) the date the Proposal is approved by the CONTRACTOR, (2) the date on which this Agreement is executed by the last of the Parties, or (3) the receipt of any advance payment required under Article III.

ARTICLE III. BILLING AND PAYMENT OF EXPENSES

A. The estimated cost of the work, described in Article I above is $_____.

Full cost recovery rates are established at the beginning of each fiscal year and are subject to revision to reflect changing cost factors during the fiscal year. The minimum unit of charge at the User Facility is an 8 hour shift.

No work can begin until this advance payment is received by CONTRACTOR.

B. USER shall pay CONTRACTOR the following advance payment and monthly invoice payments:

Advance Payment. USER shall advance the following amount at the time shown:

Amount Due	Date Due
$_____.__	00/00/00

This is a partial advance for the estimated cost. Once received, this advance will be held to pay for approximately the last four months of incurred costs on the project (or until the amounts on the month invoices plus the advance payment equals the contractual cost limitation level authorized under this Agreement).

All advance payments must be made in U.S. dollars. For foreign wire transfers, please add $30 to the invoice amount to cover payment charges levied by USER's banking institution.

Monthly Invoice Payments. Once each month during the Agreement term CONTRACTOR shall invoice USER for costs incurred in the previous month. Payment for such costs shall be due upon receipt of the invoice.

CONTRACTOR is not obligated to continue the work unless it is holding an adequate advance and may stop work if the monthly invoices are not paid on a timely basis.

When the advance payment plus the amounts paid in response to the monthly invoices equals the contractual cost limitation, the advance payment will be applied to pay for the remaining costs incurred on the Agreement. From that time forth, monthly Expense Statements showing actual costs incurred for the month and the balance remaining in the Agreement are mailed to USER for information only. The expense statements are not requests for payment.

Upon completion of the project there will be a reconciliation of the total costs incurred to total payments received and a final expense statement along with any remaining advance will be returned to USER.

USER shall provide its Purchase Order number if applicable and the name, address, and other contact information, of the person or department who will be making the invoice payments. This information is mandatory.

USER Reference No. if applicable: _____

Contact Name: _____

Street Address: _____

City, State, Zip Code: _____

Country: _____

Telephone with area code: _____

Email: _____

Tax ID Number (TIN): _____

C. All costs of Experiments will be in accordance with DOE Order O 522.1, "Pricing of Departmental Materials and Services.

ARTICLE IV. RESERVED

ARTICLE V. PROPERTY AND MATERIALS***

USER may be permitted by the CONTRACTOR to furnish equipment, tooling, test apparatus, or materials necessary to assist in the performance of its experiment(s) at the User Facility. Such items shall remain the property of USER. Unless the Parties otherwise agree, all such property furnished by USER or equipment and test apparatus provided by USER will be removed by USER within sixty (60) days of termination or expiration of this Agreement or will be disposed of as directed by USER at USER's expense. Any equipment that becomes integrated into the User Facility shall be the property of the Government. USER acknowledges that any material supplied by USER may be damaged, consumed or lost. Materials (including residues and/or other contaminated material) remaining after performance of the work or analysis will be removed in their then condition by USER at USER's expense. USER will return User Facilities and equipment utilized in their original condition except for normal wear and tear.

CONTRACTOR shall have no responsibility for USER's property at the User Facility other than loss or damage caused by willful misconduct or gross negligence of CONTRACTOR or its employees.

Personal property produced or acquired during the course of this Agreement shall be disposed of as directed by the owner at the owner's expense.

ARTICLE VI. SCHEDULING***

USER understands that CONTRACTOR will have sole responsibility and discretion for allocating and scheduling usage of the User Facilities and equipment needed for or involved under this Agreement.

ARTICLE VII. INDEMNITY AND LIABILITY***

A. Personnel Relationships - USER shall be responsible for the acts or omissions of Participants.

B. Product Liability - To the extent permitted by U.S. and U.S. State law, if USER utilizes the work derived from this Agreement in the making, using, or selling of a product, process or service, then USER hereby agrees to hold harmless

and indemnify CONTRACTOR and the United States Government, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, as a result of or arising out of such utilization of the work by or on behalf of USER, its assignees or licensees.

C. General Indemnity - To the extent permitted by U.S. and U.S. State law, USER hereby agrees to indemnify and hold harmless CONTRACTOR and the United States Government, their officers, agents and employees from any and all liability, claims, damages, costs and expenses, including attorney fees, for injury to or death of persons, or damage to or destruction of property, arising out of the performance of this Agreement or arising out of the use of the services performed, materials supplied or information given hereunder by any persons including the USER, and not directly resulting from the fault or negligence of the CONTRACTOR or the United States Government, or persons acting on their behalf.

D. Patent and Copyright Indemnity—Limited - To the extent permitted by U.S. and U.S. State law, USER shall fully indemnify the Government and CONTRACTOR and their officers, agents, and employees for infringement of any United States patent or copyright arising out of any acts required or directed or performed by USER under this Agreement to the extent such acts are not normally performed at the Facility.

E. The liability and indemnity provisions in paragraphs B, C and D above shall not apply unless USER shall have been informed as soon as practicable by CONTRACTOR or the Government of the suit or action alleging such liability or infringement, and such indemnity shall not apply to a claimed liability or infringement that is settled without the consent of USER unless required by a court of competent jurisdiction.

F. General Disclaimer -

THE GOVERNMENT AND CONTRACTOR MAKE NO EXPRESS OR IMPLIED WARRANTY AS TO THE CONDITIONS OF THE FACILITY FURNISHED HEREUNDER. IN ADDITION, THE GOVERNMENT, CONTRACTOR AND USER MAKE NO EXPRESS OR IMPLIED WARRANTY AS TO THE RESEARCH OR ANY INTELLECTUAL PROPERTY, GENERATED INFORMATION, OR PRODUCT MADE OR DEVELOPED UNDER THIS AGREEMENT, OR THE OWNERSHIP, MERCHANTABILITY, OR FITNESS FOR A PARTICULAR PURPOSE OF THE RESEARCH OR RESULTING PRODUCT; THAT THE GOODS, SERVICES, MATERIALS, PRODUCTS, PROCESSES, INFORMATION, OR DATA TO BE FURNISHED HEREUNDER WILL ACCOMPLISH INTENDED RESULTS OR ARE SAFE FOR ANY PURPOSE INCLUDING THE INTENDED PURPOSE; OR THAT ANY OF THE ABOVE WILL NOT INTERFERE WITH PRIVATELY OWNED RIGHTS OF OTHERS. THE GOVERNMENT, CONTRACTOR AND/OR USER SHALL NOT BE LIABLE FOR SPECIAL, CONSEQUENTIAL, OR INCIDENTAL DAMAGES ATTRIBUTED TO USE OF SUCH FACILITIES, RESEARCH OR RESULTING PRODUCT, INTELLECTUAL PROPERTY, GENERATED INFORMATION, OR PRODUCT MADE OR DELIVERED UNDER THIS AGREEMENT.

G. Notice and Assistance Regarding Patent and Copyright Infringement

1. USER shall report to the Government, promptly and in reasonable written detail, each notice or claim of patent or copyright infringement based on the performance of this Agreement of which USER has knowledge.

2. In the event of any claim or suit against the Government on account of any alleged patent or copyright infringement arising out of the performance of this Agreement or out of the use of any supplies furnished or work or services performed hereunder, USER shall furnish to the Government when requested by the Government, all evidence and information in possession of USER pertaining to such suit or claim. Such evidence and information shall be furnished at the expense of the Government except where USER has agreed to indemnify the Government.

ARTICLE VIII. PATENT RIGHTS***

A. Definitions

1. "Subject Invention" means any invention or discovery of USER conceived or first actually reduced to practice in the course of or under this Agreement.

2. "Patent Counsel" means the DOE Patent Counsel assisting the CONTRACTOR.

B. Rights of USER – Election to Retain Rights

With respect to any USER Subject Invention, which includes inventions of any Participants, reported and elected in accordance with paragraph (C) of this clause, USER may elect to obtain the entire right, title and interest in any patent application filed in any country on a Subject Invention and in any resulting patent secured by USER. Where appropriate, the filing of any patent application by USER is subject to DOE security regulations and requirements.

C. Invention Identification, Disclosures, and Reports

USER shall furnish the Patent Counsel a written report concerning each USER Subject Invention, which includes inventions of any Participants, within six months after conception or first actual reduction to practice, whichever occurs first. If USER wishes to elect title to the Subject Invention, a notice of election to the Subject Invention should be submitted with the report or within one year of such date of reporting of the Subject Invention.

D. Facilities License

USER agrees to and does hereby grant to the Government an irrevocable, nonexclusive paid-up license in and to any inventions or discoveries, regardless of when conceived or actually reduced to practice or acquired by USER, which at any time through completion of this Agreement are owned or controlled by USER and are incorporated in the Facility as a result of this Agreement to such an extent that the Facility is not restored to the condition existing prior to the Agreement (1) to practice or to have practiced by or for the Government at the Facility, and (2) to transfer such licenses with the transfer of that Facility. The acceptance or exercise by the Government of the aforesaid rights and license shall not prevent the Government at any time from contesting the enforceability, validity or scope of, or title to, any rights or patents herein licensed

ARTICLE IX. RIGHTS IN TECHNICAL DATA***

A. Definitions

1. "Technical Data" means recorded information, regardless of form or characteristic, of a scientific or technical nature. Technical data as used herein does not include financial reports, cost analyses, and other information incidental to Agreement administration.

2. "Proprietary Data" means technical data which embody trade secrets, developed at private expense, such as design procedures or techniques, chemical composition of materials, or manufacturing methods, processes or treatments, including minor modifications thereof, provided that such data:

   a. are not generally known or available from other sources without obligation concerning their confidentiality,

   b. have not been made available by the owner to others without obligation concerning their confidentiality,

   c. are not already available to the Government without obligation concerning their confidentiality, and

   d. are marked as "Proprietary Data."

3. "Unlimited Rights" means rights to use, duplicate or disclose technical data, in whole or in part, in any manner and for any purpose whatsoever, and to permit others to do so.

B. USER agrees to furnish to DOE or CONTRACTOR those data, if any, which are (1) essential to the performance of work by DOE or CONTRACTOR personnel or (2) necessary for the health and safety of such personnel in the performance of the work. Any data furnished to DOE or CONTRACTOR shall be deemed to have been delivered with unlimited rights unless marked as "Proprietary Data" of USER.

C. USER agrees that it shall have the sole responsibility for identifying and marking all documents containing Proprietary Data which are furnished by USER or produced under this Agreement. USER further agrees to mark each such document by or before termination of this Agreement by placing on the cover page thereof a legend identifying the document as Proprietary Data of USER and identifying each page and portion thereof to which the marking applies. The Government and CONTRACTOR shall not disclose properly marked Proprietary Data of USER outside the Government and CONTRACTOR. The Government and CONTRACTOR reserve the right to challenge the proprietary nature of any markings on data.

D. USER is solely responsible for the removal of all of its Proprietary Data from the User Facility by or before termination of this Agreement. The Government shall have unlimited rights in any Technical Data (including Proprietary Data) which are not removed from the User Facility by or before termination of this Agreement. The Government shall have unlimited rights in any Technical Data (including Proprietary Data) which are incorporated into the User Facility under this Agreement to such extent that the User Facility or equipment is not restored to the condition existing prior to such incorporation.

E. Upon completion or termination of the project, USER agrees to deliver to DOE and CONTRACTOR a non-proprietary report describing the work performed under this Agreement.

ARTICLE X. LABORATORY SITE ACCESS, SAFETY AND HEALTH***

As a precondition to using CONTRACTOR User Facility, Participants must complete all CONTRACTOR Site Access documents and requirements. USER and Participants shall take all reasonable precautions in activities carried out under this Agreement to protect the safety and health of others and to protect the environment. Participants must comply with all applicable rules of CONTRACTOR and DOE with regard to admission to and use of the User Facility, including safety, health, operating and health-physics procedures, access to information, security and environmental regulations, procedures, and the requirements of the DOE and CONTRACTOR, including the specific requirements of the User Facility covered by this Agreement. Participants shall execute any and all documents required by CONTRACTOR acknowledging and agreeing to comply with such applicable rules of CONTRACTOR. In the event that USER or Participant fails to comply with said regulations, procedures, and requirements, CONTRACTOR may, without prejudice to any other legal or contractual rights, issue and order stopping all or any part of USER's or Participant's activities at the Designated Proprietary User Facility.

ARTICLE XI. PERSONNEL RELATIONSHIPS***

Participants will remain employees or representatives of USER at all times during their participation in the work under this Agreement, and shall not be considered employees of CONTRACTOR or DOE for any purpose. Participants shall be subject to the administrative and technical supervision and control of CONTRACTOR during and in connection with the Participants' activities under this Agreement.

ARTICLE XII. EXPORT CONTROLS***

USER acknowledges that the export of goods or Technical Data may require some form of export control license from the U.S. Government and that failure to obtain such export control license may result in criminal liability under the laws of the United States.

ARTICLE XIII. THIRD-PARTY CONTRACTS

Contracts between USER and third parties for work on CONTRACTOR premises including, but not limited to, construction, installation, maintenance, and repair, will be subject to prior approval by the DOE and CONTRACTOR. The DOE and CONTRACTOR may require the insertion of specific terms and conditions into such contracts.

ARTICLE XIV. DISPUTES***

The Parties will attempt to jointly resolve all disputes arising under this Agreement. If the Parties are unable to jointly resolve a dispute within a reasonable period of time, either Party may contact the Laboratory's Technology Transfer Ombudsman (TTO) to provide assistance. The TTO may work directly to resolve the dispute or, upon mutual agreement of the Parties, contact a third party neutral mediator to assist the Parties in coming to a resolution. The costs of the mediator's services will be shared equally by the Parties. In the event that an agreement is not reached with the aid of the TTO or mediator, the Parties may agree to have the dispute addressed by neutral evaluation. The decision rendered by the neutral evaluator shall be nonbinding on the Parties, and any costs incurred there from shall be divided equally between the Parties. Upon mutual agreement, the Parties may request a final decision by the DOE Contracting Officer. Absent resolution, either Party may seek relief in a court of competent jurisdiction.

ARTICLE XV. CONFLICT OF TERMS***

In the event of any conflict between the terms of this document and any other document issued by either Party, the terms of this document shall prevail.

ARTICLE XVI. TERMINATION***

Either Party may terminate this Agreement for any reason at any time by giving not less than thirty (30) days prior written notice to the other Party, provided that CONTRACTOR shall recover payment for the costs incurred by CONTRACTOR on behalf of USER prior to termination and for termination costs.

In witness whereof, the Parties hereto have executed this Agreement:

FOR THE CONTRACTOR:

BY:

TITLE: EMSL Chief Operations Officer

ADDRESS: EMSL, PO Box 999, K8-86, Richland, WA 99352

DATE:

TELEPHONE:

FOR THE USER:

BY:

TITLE:

ADDRESS:

DATE:

TELEPHONE:

14.5 Bilateral DOE Laboratory Utilization Agreement

Bilateral DOE Laboratory Utilization Agreement

No. _____

BETWEEN

Battelle Memorial Institute, Pacific Northwest Division ("CONTRACTOR A")
Facility Operator of **Pacific Northwest National Laboratory**
under U.S. Department of Energy (hereinafter "DOE")
Contract No. DE-AC05-76RL01830

AND

_____("CONTRACTOR B")
Facility Operator of _____Laboratory
under DOE Prime Contract No. DE-AC _____
(Collectively, "the Parties")

ARTICLE I. FACILITIES AND SCOPE OF WORK

A Contractor's facilities (including equipment, services, information and other materials--(hereinafter "Host Facility")) will be made available to employees and consultants (hereinafter "Participants") of the other Party solely for carrying out the Prime Contracts of the Parties. An additional funding agreement (e.g., an Integrated Contractor Order) for funding transfer may be necessary if goods and services are provided by one Party at cost to the other Party.

ARTICLE II. TERM OF THE AGREEMENT

This Agreement shall have a term of five (5) years from the effective date. The term of this Agreement shall be effective as of the date on which it is signed by the last of the Parties. Unless terminated in accordance with the terms herein, this Agreement shall automatically renew on a year-to-year basis after the initial five-year term.

ARTICLE III. INTELLECTUAL PROPERTY RIGHTS

With regard to patent and technical data rights, Participants will follow their Party's Prime Contract when working at a Host Facility. However, if the work performed by a Participant at the Host Facility is subject to an agreement with a third party (for example, SPP or CRADA), the intellectual property provisions of that third party agreement shall supersede this section.

ARTICLE IV. LABORATORY SITE ACCESS, SAFETY AND HEALTH

As a precondition to using a Host Facility, Participants must complete all of the Host Facility's Site Access documents and requirements. Participants shall take all reasonable precautions in activities carried out under this Agreement to protect the safety and health of others and to protect the environment. Participants must comply, or risk immediate

expulsion, with all applicable safety, health, access to information, security and environmental regulations and the requirements of the DOE and Host Facility.

FOR CONTRACTOR A:

BY: _____

TITLE: _____

DATE: _____

FOR CONTRACTOR B:

BY: _____

TITLE: _____

DATE: _____

15.0 Charging Guidance for EMSL User Facility Staff

This section provides EMSL staff and other PNNL staff supporting the EMSL user project with information for determining when to charge nonproprietary work to the EMSL operations budget and when to charge to other projects that are using EMSL resources. A guiding principle is that users are treated equitably with respect to charging. Charging user support activities to the EMSL operations budget (see below) will apply the same logic whether the user is from PNNL or is an external (non-PNNL) user.

EMSL defines a user in Section 4.0 of this manual.

The DOE's BER provides programmatic funding for the operation and maintenance of EMSL as a user facility, frequently referred to as the EMSL operations budget.

15.1 Support Activities Charged to the EMSL Project

The EMSL operations budget is managed through a work breakdown structure (WBS), which captures costs in a consistent manner across the EMSL user facility. This section provides guidance on appropriate charging within the EMSL operations project's WBS.

- **Management** (Work that crosscuts individual proposals and/or supports the EMSL mission at large) — IRPL labor when providing management and oversight for the IRP and to support proposal calls, proposal reviews, and user outreach.
- **Core/Maintenance** (Work to keep the equipment/facility in a ready-to-use status) — Equipment maintenance agreements, consumables, performing routine maintenance, instrument calibration, and managing laboratory space. IRP capability development (work to create new capabilities or improve current capabilities), which is approved through proposals to IRPLs and PMs.
- **User Support** (Anything that is specifically addressing a single or limited group of user projects) — All administrative processing for granting users access to EMSL and its resources; user training; assisting users during or before experiments (e.g., preparing samples); assembling, configuring, disassembling equipment; and evaluating and monitoring the progress of user research.

15.2 Support Activities Charged to Other Projects

15.2.1 Staff Charging

EMSL staff should charge to the benefiting project or pool, other than the EMSL operations budget, when they are asked for technical support to perform any function that does not qualify for operations project funding.

15.2.2 Proprietary Proposals

Support for approved proprietary proposals requires full cost recovery and, as such, are charged accordingly.

15.2.3 Contracted Time Proposals

EMSL offers scientific analysis on a contract basis. Scientist labor, consumables, and a nominal per hour fee to recover instrument maintenance costs are the responsibility of the contracting party.

15.2.4 Utilization Policy

EMSL houses resources that were not fully purchased with EMSL operations funding. In these cases, a minimum of 20% of this resource is made available to the user community or the percentage purchased by EMSL operations funding, whichever is larger. Research performed on the percentage of these resources not owned or made available to EMSL users is not supported by EMSL operations funding. UPS maintains documentation regarding the percentage of ownership for resources in EMSL. A full description of the EMSL Utilization Policy can be found in Section 10.0.

15.2.5 EMSL NMR Instrument in Building 331

EMSL and the Biological Sciences Division of the Earth and Biological Sciences Directorate (EBSD) jointly occupy and formed a scientific collaboration in the 331 building, where large magnets are stored. EMSL and EBSD each pay one-half of the space charge for lab 130 within the 331 building.

15.3 Deployment of EMSL Capabilities

15.3.1 Background

EMSL commonly receives proposals from users who intend to make use of EMSL's capabilities at EMSL and, less commonly, proposals from users who would like to remove one or more of EMSL's capabilities from the EMSL building or other related EMSL-supported satellite labs at PNNL and use it/them for field work (termed a "field campaign"). A field campaign proposal not only involves removing one or more EMSL capabilities from the building to an off-site location, but often, one or more EMSL scientists/support staff are required to conduct the scope of work outlined in the proposal.

15.3.2 Charging Guidance

Regardless of whether a user intends to make use of the EMSL equipment on-site or for a field campaign, EMSL's operating budget is used to pay for managing the user proposal review process, training users, providing technical support

to users related to EMSL work, and equipment maintenance. In turn, all nonproprietary EMSL users are expected to pay for their own labor and travel. EMSL's philosophy is to support projects that further DOE-BER science through scientific experimentation, data analysis, and publication.

Field campaign proposals, however, incur costs that are above-standard and require special consideration and support. Above-standard costs typically include the following:

- preparation time to mobilize and demobilize equipment (disassembly, pack, set up, and return to normal configuration)
- equipment shipping costs
- travel and per diem expenses for support staff, including recorded staff labor during travel between EMSL and the off-site location
- labor costs incurred by support staff at the off-site location for the field campaign
- any other incremental costs that arise from the field campaign (e.g., minor equipment damage or destabilization of the capability within EMSL).

15.3.3 External Deployment of EMSL Capabilities

For user projects that require field campaigns, the requesting user will be expected to provide funding for above-standard costs. The above-standard costs are summarized below:

- EMSL staff effort above-standard – 100%
- Equipment shipping and preparation – 100%
- EMSL staff travel and per diem – 100%
- Additional above-standard activities – 100%

Exceptions to this policy can occur if EMSL defines and issues a call for proposals around a specified scope for a field campaign.

Scheduled use of the equipment requested in a field campaign will be entered into EMSL's management system to ensure its use does not conflict with other approved research in the facility.

This guidance only applies to nonproprietary work where the user has agreed to disclose and disseminate information and results associated with work performed in EMSL (as defined in the EMSL User Facility policy 5.7 in PNNL's Finance Manual). In the case of proprietary work, the full cost is charged to the user (as described in DOE Order 522.1, Pricing of Departmental Materials and Services).

References

- DOE Order 522.1 pg. 7 11-3-04, under k. Use of Facilities, l. Office of Science User Facilities, (3) "When facilities are operated for special circumstances, such as running the facility outside the normal operating mode or schedule, the user will be charged a fee that recovers the incremental costs." (https://www.directives.doe.gov/directives-documents/500-series/0522.1-BOrder).

- DOE Order 522.1, Pricing of Departmental Materials and Services. (https://www.directives.doe.gov/directives-documents/500-series/0522.1-BOrder).
- Cost Accounting Standard (CAS) 418 - 9904.418-40 (e.g., Allocation of Direct and Indirect Costs) has a provision for the exclusion of special-purpose facilities that would apply in this extension to the EMSL National User Facility (http://www.ecfr.gov/cgi-bin/retrieveECFR?gp=&SID=ece9696a1a8b58cb7d9c139138479c58&mc=true&n=pt48.7.9904&r=PART&ty=HTML#se48.7.9904_1418_640).

16.0 EMSL Space Policy

An assumption in the formulation of EMSL's Space Policy is that all facility space, regardless of space chargeback designation, is owned by the DOE-BER and managed by the EMSL director's office and that all space allocation is governed by the policies below.

EMSL, as a national user facility, is funded and operated to provide state-of-the-art scientific capabilities to the national and international user community in EMSL's Science Areas. Because of the unique nature of this facility, priority must be given to those capabilities and individuals that significantly support EMSL's mission. Likewise, those capabilities and individuals that currently occupy the facility and are determined to not directly and significantly support EMSL's mission may be directed to relocate to other PNNL facilities. The costs associated with moving existing occupants are the responsibility of the occupant's organization. (This requirement is appropriate as long as the EMSL operations budget pays for half of the space chargeback of all laboratory-type space in the EMSL building.)

16.1 Laboratory Space

To be eligible for EMSL laboratory space, an individual and/or capability must be engaged in research that reflects the primary mission of EMSL:

> *EMSL's mission as a national scientific user facility is to provide access to premier multimodal molecular science instruments, data analytics, production computing, and multiscale modeling to enable researchers to study biotic and abiotic processes and understand their function in a systems context for energy and environmental security and infrastructure resilience.*

The priority for laboratory space is based on the level of support the individual or capability brings to EMSL's mission. The following criteria are used to measure the level of support:

- Is the individual's research or capability in demand by EMSL users? (Capabilities that are in minimal demand by external users will not rank as highly in priority as those in more demand.)
- Has the individual's research or capability resulted, or does it have the potential to result, in high-impact publications, awards, and other external recognition related to BER?
- Is the individual's research or capability aligned with EMSL Science Areas?
- Is a capability being developed that has direct benefit to the user community?

Any equipment proposed to be brought into EMSL must be approved by the EMSL COO and must comply with EMSL's equipment use policy.

The following criteria are used to prioritize capabilities when new requests for laboratory space are submitted:

- **Priority 1:** Capabilities that are owned by EMSL and directly support EMSL's user program and Science Areas.
- **Priority 2:** Capabilities that are in high demand for supporting EMSL's user program and Science Areas, but that are not owned by EMSL.

Any capabilities (and staff) in EMSL who do not meet one of these two criteria will be requested to move from the building, when space needs dictate. Should this be necessary, EMSL's COO will work with the COOs of the other organizations to establish a timeline for vacating the space(s).

16.1.1 Requesting EMSL Laboratory Space

Laboratory space requests are submitted to the EMSL research operations manager, who works with the space point of contact for the requesting research group to identify acceptable space. The requesting group must demonstrate how the individual's research or capability supports EMSL's mission and Science Areas and that it effectively and efficiently uses any existing EMSL space in relation to the activities and equipment in that space. The EMSL COO approves all laboratory space allocations in writing, documenting any timelines or expectations for instrument moves into and out of the EMSL space(s).

If approved, the occupying organization will pay a portion of the space chargeback, based on the EMSL Utilization and Space policies (Sections 10.0 and 16.0) and any MOAs. If the majority of equipment/capability located in an EMSL space was purchased with "other program funding" or the occupying organization is currently the custodian/steward of the equipment, the occupying organization's research operations officer (ROO) pays 50% of the space chargeback to utilize the space; the remaining 50% will be paid by the EMSL program unless a separate agreement is developed with the EMSL director.

The occupying organization must follow PNNL's HDI guidance for Executing a Lab Move and will be responsible for all costs associated with moving instruments into and out of EMSL, as well as the costs for all modifications to the space needed to house the instrument(s) and all costs associated with returning the lab to the condition prior to moving in the instruments.

16.2 Office Space

To be eligible for EMSL office space, an individual must be engaged in EMSL's mission. Priority for office space will be given as follows:

- **Priority 1:** Staff members in the EMSD organization and their postdoctoral researchers and students.
- **Priority 2:** Non-PNNL staff members (external users) who have an active user project for using EMSL research capabilities on-site.
- **Priority 3:** Non-EMSD staff and their students who occupy primary lab space or are directly supporting a lab space in EMSL.
- **Priority 4:** Matrixed staff who support the infrastructure of EMSL in support of its mission, including staff from PNNL's Operational Systems Directorate; Environment, Health, Safety and Security; Communications; and Business Systems and other PNNL support organizations.

PNNL staff who do not meet any of these criteria will be directed to move from the building, when office and/or laboratory space needs dictate, with all move-related costs paid by the occupant's organization, unless approved otherwise by the COO and research operations manager.

16.2.1 Requesting EMSL Office Space

Office space requests are submitted to the EMSL research operations manager, who works with the space point of contact for the requesting research group to identify acceptable space. The first solution is to place the occupant in space for which the requesting group already pays the space charge.

The requesting group must demonstrate that they effectively and efficiently use any existing EMSL space in relation to the activities and equipment in that space and the EMSL building.

If the requested space is already filled and other appropriate space cannot be identified, the requesting group can do the following:

- identify space outside EMSL for the new occupant or move existing staff out of the building so that the new occupant can assume the space
- request space from another EMSL group through the EMSL research operations manager.

Office space is paid for by the occupying organization unless a separate agreement is developed with the EMSL COO. The EMSL COO approves all office space allocations.

17.0 Instrument Life Cycle Management

EMSL houses state-of-the-art instruments and advanced platforms in support of its mission to provide access to premier multimodal molecular science analyses, data analytics, production computing, and multiscale modeling to enable researchers to study biotic and abiotic processes and understand their function in the context of energy and environmental security and infrastructure resilience. EMSL's mission acknowledges the institution's unique role of providing a continually improving suite of premier science instrumentation, data storage, analytics, and high-performance computing, which enable users to employ a ModEx approach to their research. Many of these capabilities are the products of technological innovations produced by EMSL staff and its other research partners. Maximizing the lifespan of instruments, optimizing life-cycle ends, and managing the transition to the next generation of instruments are critical for maintaining research productivity and access for users.

The instrument life cycle is managed by the EMSL COO in partnership with IRPLs, who are responsible for instrument purchasing and development planning following the EMSL strategy. Toward that end, EMSL employs operational processes to manage instruments from planning and purchase through maintenance and final divestment of retired instrumentation (Figure 1). Success here is measured by (1) minimal instrument downtime; (2) high instrument usage by EMSL users; (3) regular purchase of high-impact, state-of-the-art, or unique instrumentation per our capital and expense instrument strategies; and (4) effective divestment of aging instruments to provide space for improved instrumentation. A future is envisioned where instrument lifespans and obsolescence are understood, and more holistic planning occurs to assure funding is in place when instruments exceed their lifespan or become obsolete.

The following sections of this chapter provide additional detail related to each stage of the instrument life cycle (Figure 1).

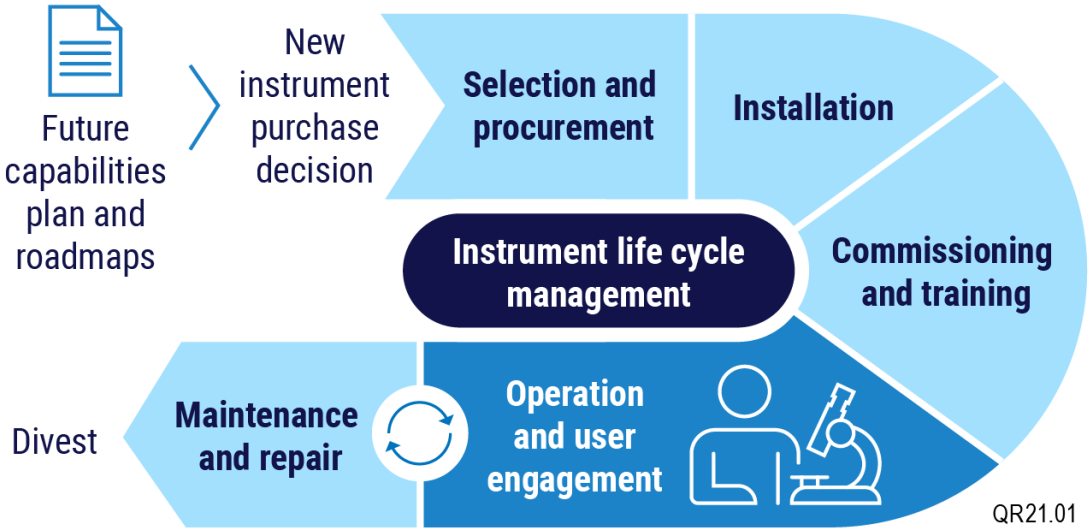

Figure 1. EMSL's instrument life-cycle management will enable proactive planning for instrument investments and instrument tracking through each life-cycle phase and will provide input for divestment decisions.

17.1 New Instrument Planning

New instruments can be purchased using (1) EMSL operations/capital funding, (2) a combination of EMSL and other project funding, or (3) non-EMSL funding sources. The cost of the instrument also factors into purchase planning. Instruments costing less than $500,000 are considered "Expense" instruments and can be purchased with any of the mechanisms listed above. Instruments costing $500,000 or more are considered "Capital" and must be purchased with funding that is specifically designated for capital purchases. More detail is provided in the sections below on planning instrument purchasing. Annually, the expense and capital equipment budgets are established by the EMSL director in concert with the Biological and Environmental Research (BER) program manager.

17.1.1 EMSL Instrument Planning

EMSL, at a minimum, annually reviews and revises both its expense and capital instrument purchasing plans. Instruments may be added or removed from the plan as a result of the review. These decisions are based on criteria including the current strategic needs identified in the 2021 EMSL Five-Year Strategic Science Plan and S&T roadmaps, instrument obsolescence risk (i.e., no longer state-of-the-art), or usage-driven needs to increase capacity for the user program.

Figure 2 shows the process for the annual review and refreshment of instrument purchasing plans. In response to a call from EMSL's CSO and COO, staff provide requests for equipment. These requests are reviewed by EMSL's S&T leadership and COO according to the criteria above. At this time, the requests are also divided into capital and expense equipment lists. For the top five to six items on the lists, additional information and justification are developed in the form of a quad chart, and initial decisions are made by EMSL's S&T leadership and COO. At this time, any additional information may be requested, and quad charts may be refined. Based on the budget available, the EMSL leadership team determines which items to approve for purchase. Results of the decision are then communicated to EMSL staff. As additional funding becomes available during the year, the lists may be refreshed or used for the purpose of making additional funding decisions.

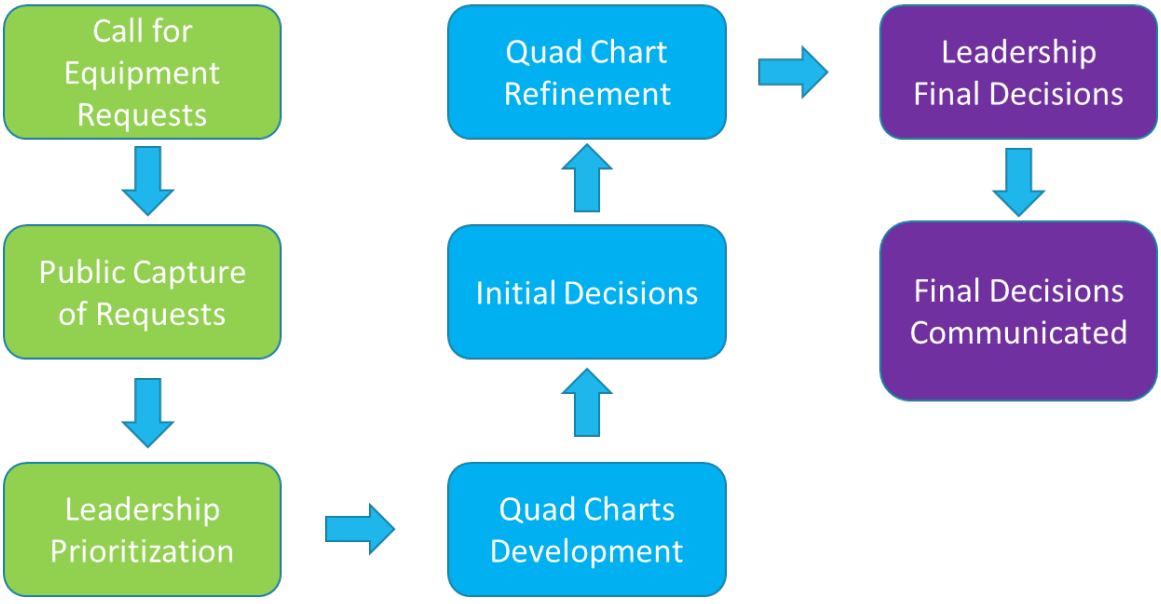

Figure 2. Annual instrument planning cycle.

Additionally, computational needs for new capital and expense instruments need to be identified so that appropriate resources can be planned. Staff who recommend an instrument purchase are tasked with determining whether specialized hardware or software are required to interface with the instrument, estimating data generation volume to inform the network bandwidth and disk storage requirements for data movement and archiving, and identifying the data processing and analysis needs, which could range from purchasing commercial software licenses to investing in custom software development within EMSL.

17.1.2 Shared Purchases (EMSL +Other Projects) – Additional Considerations

When there is an opportunity to share the costs of an instrument with other projects, EMSL will still make decisions based on the criteria described in the section above. These opportunities are more carefully scrutinized by the EMSL leadership team because access to the instrument is allocated based on the percentage of the funding contribution. Additionally, it needs to be determined whether the opportunity is in EMSL's best interest. It is expected that maintenance costs are also split accordingly. These instruments are entered into NEXUS, and their usage for the EMSL user program is tracked. Usage by the other owner is tracked as resource owner usage, however, an EMSL user proposal is not needed. EMSL is not responsible for managing the other owner's data.

17.1.3 Non-EMSL Funded Instruments

Instruments may be brought into EMSL where its purchase was funded by other funding sources such as Laboratory Directed Research and Development, overhead, or other projects. In some cases, this is general equipment that broadly supports multiple organizations or programs, including EMSL. Examples of these types of purchases in the past have been ancillary equipment for EMSL's machine shop, freezers for sample storage, or autoclaves. The usage of these types of equipment is not entered or tracked in NEXUS. In other cases, projects or other organizations may bring in analytical instruments such as mass spectrometers, nuclear magnetic resonance (NMR) spectrometers, or electron microscopes into EMSL. EMSL may elect to request up to 20% usage on these instruments. More information on this is provided in Section 17.3.1.

17.1.4 Instrument Location Planning

Regardless of funding source and as part of the instrument planning process, a location for the instrument needs to be identified, and the EMSL COO needs to approve the location. This assures that there is adequate space, utilities/services are available in the intended location, and the addition of the new instrument does not cause or exacerbate laboratory environment issues such as overheating. When possible, heat-generating components are located in service corridors rather than in laboratories. Additionally, the COO will review to assure the placement is aligned with future space usage strategies.

17.2 Instrument Procurement, Installation, and Commissioning

Once an instrument is approved for purchase, the IRPL works with the EMSL project coordinators to establish a work package number and to identify a technical oversight representative for procurement. Depending on the complexity of the instrument, vendor installation and commission are included in the procurement contract. Any facility modifications are also initiated. PNNL's processes are followed for procurement and facility modifications. If installation and commissioning are not performed by a vendor, they are completed by the instrument custodian as part of core IRP funding.

17.3 Instrument Operations and Maintenance

17.3.1 Instrument Operations

For EMSL-owned instruments, once an instrument is commissioned, it is available for use through the user program. It is entered into NEXUS to enable scheduling for use in user projects. Operating hours are established for the instrument by the instrument custodian in consultation with the IRPL based on the usage anticipated. Operating hours are standardly 24 hours daily/7 days a week or 10 hours daily/5 days per week, but other operating hours can be established. Examples of instruments that operate 24/7 are NMR spectrometers, which have high usage, and instruments with autosamplers that are typically loaded during normal business hours.

As part of operations, instrument use is scheduled using the NEXUS scheduling tool. Usage is also recorded per the usage policy in Section 11.1. Data generated by instruments for user projects or BER-sponsored projects must be uploaded for archiving per EMSL's data management policy.

For partially owned EMSL instruments, the operating time is based on the percentage of EMSL ownership but is not less than 20%. The instrument is entered into NEXUS, where EMSL usage is scheduled and tracked, and the data are managed per EMSL's data management policy. The total operating hours of the instrument for the user program are prorated based on the percentage of EMSL ownership. The other owner's usage is tracked as resource owner usage; however, an EMSL user proposal is not required. EMSL is not responsible for managing the other owner's data.

For non-EMSL-owned instruments that are located within the EMSL facility, EMSL may elect to require 20% of the instrument time for the user program. The operating hours are based on 20% of the instrument's normal operating hours. EMSL also shares 20% of the maintenance costs and provides supplies related to usage. The usage of these instruments by the user program is entered into NEXUS, and the data are managed per EMSL's data management policy. The usage by the owning organization or project also needs to be scheduled or recorded in NEXUS; however, an EMSL user proposal is not needed. If EMSL elects not to require 20% usage, the instrument is not entered into NEXUS and is not tracked. The decision on whether to request 20% time on a non-EMSL-owned instrument is based on the value of the instrument to the EMSL user program and is made by the appropriate IRPL. The IRPL considers whether (1) the instrument would add capacity to the user program, (2) it provides a unique capability to users, and (3) it aligns with EMSL's strategy. If a decision is made that EMSL does not need 20% time on a non-EMSL-owned instrument, the decision can be revisited in the future if a need for the instrument arises.

17.3.2 Instrument Maintenance

Most newly purchased instruments receive a 1-year warranty. At the time of contracting, an extended warranty can be included in the request for proposal. After the warranty duration is completed, annual service contracts can be purchased. The decision to purchase a service contract is made by the IRPL with recommendations from the instrument custodian. Factors that are considered are the (1) complexity of the instrument, (2) cost of the contract, and (3) availability of in-house maintenance and repair expertise. The need to continue the service contract is annually evaluated by the IRPL and instrument custodian before renewal, who consider the factors above, as well as the age and obsolescence of the instrument. The EMSL instrument custodian is responsible for maintaining the instrument in working order and arranging for appropriate preventive maintenance.

17.4 Instrument Divestment

The divestment of instruments is an important part of instrument life-cycle management. Removing instruments that have low use rates, are no longer state-of-the-art, no longer align to BER missions, and are costly to maintain or cannot be repaired makes space and resources available for new capabilities that are strategically aligned and attractive to users.

Instrument usage for the purpose of making divestment decisions is evaluated annually. The user program services office provides a report of the past 3 years of instrument usage to the IRPLs, the EMSL COO, and EMSL project managers typically in the first quarter of the FY. The instrument usage is compared to a set of utilization minimums that trigger the instrument to be flagged for further evaluation. Initially, instruments that are used less than 30% of the time will be reviewed by PMs. The PMs with input from IRPLs will consider instruments for divestment based on criteria such as utilization, strategic alignment, distinctiveness, availability of new technology, cost of operation/maintenance, and operational status. Based on the strategic importance or uniqueness of the instrument, the PMs may elect to decrease this trigger value. Instruments that are inoperable with no intention to repair are divested and excessed without the need for approval. If the instrument is strategic and needs to be replaced, either the PM or IRPL follows the process defined in Section 17.1 on new instrument planning. For instruments that are strategic but expensive to maintain and for which newer technology is available, the PM or IRPL also follows the process in Section 17.1 to plan for a replacement. Once the instrument is replaced, the old instrument is divested without the need for approval. Instruments that are no longer aligned with EMSL or BER missions will be recommended for placement on a divestment list. The list is submitted to the EMSL COO, who reviews and makes recommendations to EMSL's leadership team and the EMSL director for final decisions. The EMSL director vets the list with the BER program manager for approval. Figure 3 below represents the decision process for the divestment of instruments.

An instrument that is approved for divestment may be excessed or transferred to another project or organization. Then, EMSL is no longer responsible for the maintenance or supplies associated with the instrument. If the instrument remains in the EMSL facility, EMSL may elect to claim 20% access. However, this would be rare because the process for divesting verifies that the instrument is not useful to the EMSL user program.

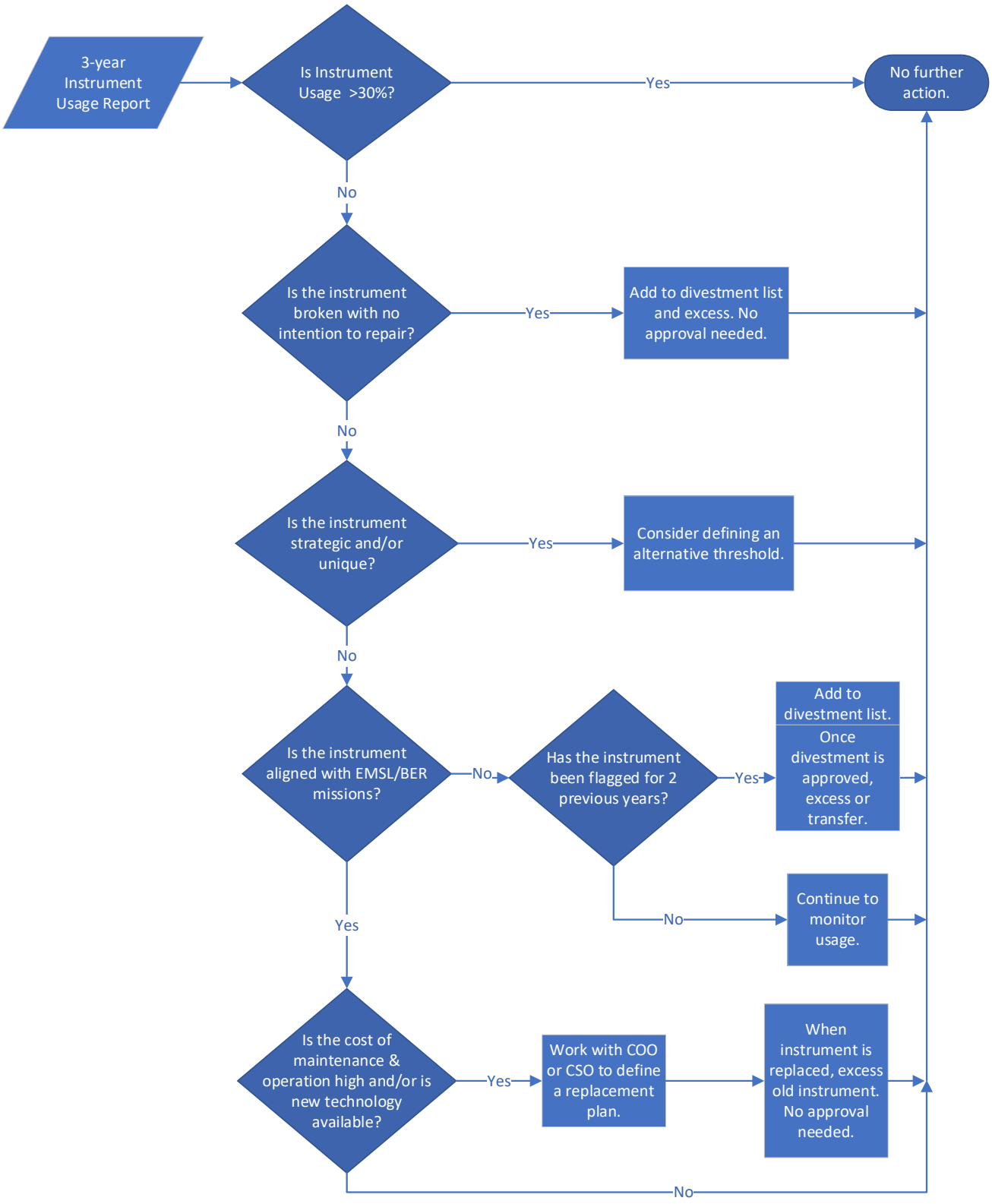

Figure 3. Several conditions are considered in making the decision to divest an EMSL instrument.

18.0 Engagement with DOE and Laboratory Management

EMSL management works closely with PNNL, BER, and PNSO staff to ensure that the user facility is meeting performance expectations and to address issues and future opportunities.

In addition to teleconferences and visits to and from BER, EMSL management provides, at BER's request, various reports either monthly, quarterly, or annually. EMSL also provides user demographics to SC or in support of PNNL reporting requirements to DOE management. Table 3 outlines these reports and interactions.

Table 3. Formal Reports Provided to DOE and PNNL

Report	Requestor	Responsible Person	Due Date
Operating Hours	BER, PNSO, Battelle EVP for Global Laboratory Operations	UPS Lead Project Manager	Quarterly
Proposal and User Statistics	BER, PNSO	UPS Lead Project Manager	1st and 3rd quarter *(21 days after quarter end)*
EMSL Dashboard	BER, PNSO	UPS Lead Project Manager	Quarterly *(21 days after quarter end)*
EMSL User Facility Financial Profile	BER, PNSO	EMSD Business Manager	Biannually *(within 1 month after 2nd and 4th quarter end)*
Resource Summary Report	BER, PNSO	UPS Lead Project Manager	Biannually *(21 days after 2nd and 4th quarter end)*
Additional Protocol (AP) Compliance	PNNL	UPS Lead Project Manager	Annually *(October 14)*
List of Major Resources	BER, PNSO	UPS Lead Project Manager	Annually *(November 30)*
User Demographics for Office of Science Projects-Experiments Database	DOE	UPS Lead Project Manager	Annually *(typically, by November 30)*
DOE Technology Transfer by Laboratory	DOE	UPS Lead Project Manager	Annually *(December 31)*
User Survey Summary	BER, PNSO	UPS Lead Project Manager	Annually *(January 15)*
Capital and Operations Field Work Proposal	BER, PNSO	Chief Operations Officer	Annually *(determined by DOE)*
Facilities Research Field Work Proposal	BER, PNSO	Chief Science Officer	Annually *(determined by DOE)*

19.0 Science and Technology Advisory Committee Charter

19.1 Committee Functions and Objectives

The Science and Technology Advisory Committee (Committee or STAC) of EMSL is chartered by and reports to the EMSL director. The STAC is chartered to render advice, guidance, and counsel on the strategy and scientific objectives of EMSL. The STAC serves as the EMSL director's key external advisory committee and advocate on EMSL strategy, scientific relevance, and quality. The STAC neither performs management and operation functions nor directs the EMSL director or his/her management team on how to operate and manage EMSL. Input, guidance, and counsel from the STAC is taken into consideration with strategic planning exercises as part of the annual capital investment plans, internal S&T R&D focus and priorities, and incorporation into EMSL's Large-Scale Research, FICUS, and Exploratory proposal calls.

19.2 Membership

19.2.1 Size of Committee and Selection Process

The EMSL director will appoint members. The membership will consist of at least eight (8) external (non-PNNL/non-Battelle) advisors with knowledge of and influence in the major R&D areas that EMSL serves. No more than one (1) member of the full Committee may be a Battelle/PNNL employee. Members of the Committee may propose nominees for consideration at any time by submitting names and supporting information to the EMSL director. The chair of the EMSL User Executive Committee (UEC; Section 20.0) is a standing ex officio member of the EMSL STAC, rotating off at the conclusion of the UEC chair period of service.

19.2.2 Qualifications

Members of the Committee must possess the highest personal and professional ethics, integrity, and values and be committed to representing the long-term interests of EMSL and the EMSL mission. They must also have an inquisitive and objective perspective, practical wisdom, and mature judgment. The Committee should have diverse experience in S&T, government, and education and in areas that are relevant to EMSL's mission and national and international activities.

Members must be willing to devote sufficient time to carry out their duties and responsibilities effectively and should be committed to serve on the Committee for the entire term. Members should offer their resignation in the event of any significant change in their personal circumstances, including a change in their principal job responsibilities that would result in a conflict of interest (COI) in continuing to service on the STAC. A COI would arise when a potential or current member has a financial interest, personal activity, or relationship that could impair that individual's ability to act impartially and in the best interest of EMSL or its sponsor. COIs may also include relationships with an individual or entity that has influence or authority over EMSL project work, funding, or employment status. The EMSL director may remove members from the Committee for cause.

19.2.3 Terms of Service

Committee members serve a minimum of a three (3)-year term or at the discretion of the EMSL director. The EMSL director will appoint a chair from the Committee's external membership. The annual cycle for all terms of STAC membership, including the position of chair, will be from April 1 to March 31.

19.3 Committee Activities and Duties

19.3.1 Duties

The major duties of the Committee are to provide advice, guidance, and counsel on the strategy and scientific objectives of EMSL. As such, the Director and/or EMSL CSO will seek input from the Committee during the annual on-site science strategy meeting as well as via email requests or conference calls.

19.3.2 Frequency of Meetings

The Committee will minimally meet annually at EMSL or virtually when conditions require. In addition, video conference calls may be scheduled as needed. Efforts will be made to hold the annual meeting on or around the 1st of April to coincide with terms of service.

19.3.3 Quorum

The Committee may conduct business where a quorum of its members is present; such a quorum must consist of at least fifty (50) percent of the members and must include the Committee chair. During each scheduled meeting, the Committee must review and discuss reports by management on the scientific performance of EMSL, its plans and prospects, and immediate issues facing EMSL. Committee members are expected to prepare for and attend the scheduled meeting of the Committee. Delegates are not permitted.

19.3.4 Setting the Committee Agenda

Prior to each Committee meeting, the EMSL director and EMSL CSO will discuss the planned agenda items for the meeting with the Committee's chair. The EMSL director and EMSL CSO will determine the nature and extent of information that will be provided to the members in advance of each scheduled Committee meeting. Members are urged to make suggestions for agenda items or additional premeeting materials to the EMSL director, CSO, or the Committee chair at any time.

19.3.5 Reimbursement for Committee Members

Travel to EMSL for meetings will be fully reimbursed under PNNL business rules.

19.3.6 Access to EMSL Management

Committee members are encouraged to contact senior managers of EMSL as necessary to fulfill their duties. Meetings should be coordinated through the EMSL director's office or the Committee's EMSL CSO Administrative Assistant.

20.0 User Executive Committee Charter

This charter defines the membership, responsibilities, and structure of the EMSL UEC.

20.1 User Executive Committee

The EMSL UEC is charged with providing objective, timely advice and recommendations to the EMSL director and leadership team related to matters affecting the EMSL user community (a user is defined as every named investigator or participant on an approved EMSL user project in the current FY or in either of the two preceding FYs), such as operating policies, operating hours for specific instruments, and needs for facilities, infrastructure, and instrumentation. It is also charged with facilitating discussions among facility users, the broader research community, and EMSL management on matters important to the users. The UEC is expected to serve as an advocacy group for the EMSL user community and for the EMSL user facility and to promote and encourage research at EMSL by providing forums for organized discussions among facility users.

20.1.1 UEC Responsibilities

The **committee** must carry out the following functions and procedures in a manner that reflects the sentiment of the EMSL user community:

a. Make recommendations to EMSL management on matters affecting the user community, such as operating policies, operating hours for specific instruments, and needs for facilities, infrastructure, and instrumentation.

b. Make recommendations to EMSL management for persons to serve on PRPs.

c. Provide timely reports to the EMSL user community throughout the year as appropriate.

d. Provide advice on other matters affecting EMSL at the request of the EMSL director.

e. Form, as appropriate, ad hoc committees to deal with the special needs of EMSL management or the EMSL user community as identified by the UEC. Ad hoc committee members will consist of EMSL user community members.

f. Meet as needed with the EMSL COO, who serves as an ombudsperson for user concerns, during an executive session at the annual UEC meeting to mutually discuss interactions between users and staff.

20.1.2 UEC Membership and Terms of Service

The UEC must have at least nine members, including a chair, vice chair, and ex officio past chair. Additionally, no two members may be from the same institution. Members must represent research areas included within the scientific focus of EMSL's user program. During the 3-year membership cycle, a reasonable attempt will be made to recruit nominations on the annual election ballot for (i) an industry representative and (ii) an individual with experience at other DOE user facilities. UEC membership will include a postdoctoral user, with special emphasis on selecting one from historically black colleges and universities (HBCUs) and/or minority serving institutions (MSIs). The postdoctoral membership position will be filled via a direct invite-only process by EMSL Leadership. The EMSL director or UEC chair with concurrence of the EMSL director may appoint additional nonvoting "member-at-large" positions as needed.

General members will typically serve a three-year term and cannot serve more than two terms. A member elected to a second term is eligible for vice chair only in the first year of the second term so that the total length of their service does

not exceed six years. The vice chair, chair, and past chair will serve from the time they were first elected to the UEC until they have completed service as past chair.

Terms for UEC members commence and end on the date of the annual UEC meeting. Newly elected members will assume their UEC positions at the annual meeting in October following the spring voting period for new members as per the guidelines delineated below. Likewise, for members rotating off the UEC, terms end after completion of the third year's annual UEC meeting.

20.1.3 UEC Membership Qualifications

All UEC members must be an EMSL user at the time of their election or within either of the two preceding FYs; possess the highest personal and professional ethics, integrity, and values; and be committed to representing the long-term interests of the EMSL user community and the EMSL user facility mission and vision. UEC members must also have an inquisitive and objective perspective, practical wisdom, and mature judgment. The committee must have diverse experience in areas of S&T, education, government policy, and industry that are relevant to the EMSL user facility mission, DOE, and national and international activities.

Members must be willing to devote enough time to fulfill their duties and responsibilities effectively, and they are expected to serve on the committee for the entire term. Members should offer their resignation immediately in the event of any significant change in their personal circumstances or principal job responsibilities that would interfere with their UEC responsibilities leading to a potential or actual COI. A COI would arise when a potential or current member has a financial interest, personal activity, or relationship that could impair that individual's ability to act impartially and in the best interest of EMSL or its sponsor. COIs may also include relationships with an individual or entity that has influence or authority over EMSL project work, funding, or employment status. Replacement of elected members will follow the steps outlined in Section 20.1.4 (UEC Elections).

Members may be removed from the committee for cause by the EMSL director.

20.1.4 UEC Elections

Elections to select new members will be held every year in late winter/spring. The election cycle will begin with a formal call for nominations to the EMSL user community by the UEC chair. The chair will work with the committee members to review and select the final slate of nominees, ensuring broad representation across the capabilities and scientific focus of EMSL's user program. The EMSL user community will vote for the best candidates using an electronic ballot or other method as deemed appropriate by the UEC, but the UEC chair and EMSL director will make the final selections of new members to ensure a balance of scientific expertise and representation across the committee.

20.1.5 UEC Leadership Terms and Responsibilities

The UEC chair will serve a one-year term and is expected to moderate UEC meetings during their term. A new UEC vice chair will be selected each year at the annual meeting of the UEC from among its members. The chair, vice chair, and ex officio positions each have one-year terms. Upon the completion of the annual UEC meeting, the ex officio will rotate off the UEC, the chair will move to ex officio, the vice chair will assume the chair, and the newly elected vice chair will serve in that position until the end of the following annual UEC meeting. The vice chair and chair work closely together to preserve continuity once the chair moves to ex officio.

The ex officio position of the past chair provides advice and guidance to the current committee.

The UEC chair is responsible for preparing the agenda for all UEC meetings in collaboration with the EMSL COO, including UEC-sponsored public outreach/information meetings or telecons, and facilitating the meeting schedule and discussion. The UEC chair is also responsible for managing the annual election cycle. In addition, the chair, or vice chair in the event the chair cannot attend, will serve as an ex officio member of the EMSL STAC. The UEC chair is also responsible for ensuring that the UEC is represented by one or more UEC members at events involved in promoting public awareness of the benefits and significance of national user facilities as well as at the EMSL User Meeting.

If the UEC vice chair becomes vacant prior to the annual meeting, the committee will select a new vice chair from among its members via email. If the chair becomes vacant prior to the annual meeting, the past chair will resume the position of chair for the remainder of the term. If other elected members step down, the positions will remain vacant until the next election.

20.2 Meetings and Agendas

All meetings of the UEC will be organized or facilitated by the UEC chair, with at least one annual meeting per year. Activities and discussions will be documented, and the reports will be made available to all members of the EMSL user community and to EMSL management.

20.2.1 EMSL User Community Meetings

Special meetings of the EMSL user community may be called as needed by a majority of the UEC or a majority of the EMSL user community members.

20.2.2 UEC Meetings

The annual UEC meeting is to be held in October during the same week as the annual EMSL User Meeting. As a standing agenda item, the first order of business at the annual UEC meeting is to elect a new vice chair who will assume the role at the completion of the annual UEC meeting.

The committee may conduct business where a quorum of its members is present, either in person or via teleconference; such a quorum must consist of at least fifty (50) percent of the UEC members and include the committee chair or vice chair. It is expected that committee members make every effort to attend scheduled committee meetings in person.

Once per year, the committee will meet, with reasonable travel reimbursement provided by EMSL based on established PNNL business rules if the meeting is held on-site. If deemed necessary by the UEC chair and the EMSL director, additional meetings may be called and held on-site, at a remote location, or via teleconference.

Prior to each committee meeting, the UEC chair will draft the agenda items for the meeting in discussion with the UEC members and EMSL director and/or the EMSL COO. The UEC chair will also work with the committee to determine the nature and extent of information that will be provided to the members in advance of each scheduled committee meeting.

20.3 Role of EMSL Director and Management

EMSL management will partner with the UEC to investigate user concerns, evaluate operational recommendations, and respond to requests for information in a timely manner. However, the operations and management of EMSL are vested in the EMSL director and the EMSL management team. The management team is responsible for assuring that the objectives

of EMSL are accomplished within the policies, DOE prime contract, and legal environment within which PNNL operates. The management team is responsible for assuring that the assets of PNNL and DOE are protected.

21.0 Change Control

The following documents the changes that have been made to the EMSL Operations Manual since it was published in 2006. The entire Operations Manual will be updated in ERecords with each revision, and all change control forms will be saved with copies of the modifications made under EREC.369907. Whole sections that have been deleted can be found under Section 21.2.

21.1 Change Control Record of Current Sections

Section	Date	Change
Entire Book	05/29/2024 9/18/2023 08/20/2021	• POC of Section 6 Appeals, Section 10 EMSL Utilization Policy changed from Allison Hatt to Rick Washburn. Section 10 also added "EMSL" in front of Utilization Policy. • POC of Section 12 EMSL Data Management Policy changed from Lee Ann McCue, Alison Hatt to Ratna Saripalli, Rick Washburn. • Deleted Work for Others (WFO) and replaced with Strategic Partnership Project (SPP). • Changed Instrument Scientist to Instrument Custodian. • Updated terminology throughout to refer to new staff titles. Updated footers with review dates and new POCs. EMSLUO changed to EMSL user community. • Updated terminology throughout to refer to new staff titles. • POC changed from Law to Hatt.
	06/25/2019	• Updated footers with review dates and new POCs. • Updated terminology throughout to refer to new staff titles. • Removed references to individual ERecord numbers for each section.
	03/08/2018	• Updated footers with new POCs.
	10/23/2017	• Updated footers with review dates and new POCs.
	08/15/2016	• Updated footers with review dates and new POCs.
	10/01/2013	• POC changed from Foster-Mills to Law. • Updated footers with review dates and new POCs.
	02/09/2011	• Updated Review Dates on sections that did not require updates. • Changed "Capability Steward" to "Capability Lead" (in chapters, not in CCR). • Changed POC in Sections 17, 18, and 19 from West to Baer. • Updated Nancy Foster-Mills' title to "Product Line Manager." • Updated Don Baer's title to "Interim Lead Scientist."
	04/14/2010	• Level 1 document changes will be reviewed and approved informally via e-mail to BER and PNSO as opposed to sending hard-copy letters through the formal correspondence process. Agreements saved in ERecords under EREC.693680 and EREC.693987.
1.0 Introduction	05/29/2024 09/18/2023 08/20/2021	• Resolved typo. • Added references for Research Organization Registry and Global Research Identifier Database. • Minor wording changes to spell out acronyms. • POC changed from Law to Hatt.
	08/12/2020	• Minor update to include EMSL's Research Organization Registry (ROR) ID.
	06/25/2019	• Updated sentence referring to BER mission to match Mission criterion changes in section 5.3. • Updated to include EMSL's unique identifiers. • Updated last paragraph to include schedule for updating the Operations Manual (note: legal review not required as their original text was not changed).

Section	Date	Change
	08/15/2016	• Text updated to provide a fuller description of EMSL. Introduction previously was primarily the mission and vision, which are part of section 2.0.
	10/01/2013	• POC changed from Foster-Mills to Law.
	10/21/2009	• Operations Manual v4.4.
	06/2006	• Original document = EMSL Operations Manual Rev 3 (PNNL-15828). Note – this requires legal review. Do not edit this section without legal review.
2.0 Mission and Vision*	08/20/2021	• Complete revision of EMSL's mission and vision to reflect current practices.
	06/25/2019	• POC changed from Bolton to Mans.
	03/08/2018	• POC changed from Liang to Bolton.
	08/15/2016	• POC changed from Campbell to Liang. • Updated to match approved Strategy Plan verbiage and add vision. • Changed section heading.
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email. Footnote added.
	08/23/2005	• Same policy – new TRIM # created for future updates.
	08/23/2005	• Original document = EMSL Action Plan 2005: WBS 1.03.01; EMSL Mission Statement.
3.0 EMSL Science Areas*	05/29/2024 09/18/2023 08/20/2021	• Updated introduction to Science Areas in 1st and 2nd paragraph, updated FSB, ETI, and CAM descriptions. • Updated introduction to Sciences Areas, updated description of ETI, added new DT IRP to CAM. POC changed from Hess to Bargar. • Complete revision, taking place of the Science Theme descriptions. • Added Baker and Bardhan as additional POCs.
	06/25/2019	• POC changed from Bolton to Hess.
	03/08/2018	• POC changed from Liang to Bolton.
	10/23/2017	• POC changed from Paša-Tolić to Liang.
	08/15/2016	• POC changed from Mueller to Paša-Tolić. • Minor wording changes to introductory paragraph to reference approved 2014 Strategy Plan. • Updated science theme descriptions to reference more current focus areas. • Changed EMP science theme description to Molecular Transformations (MT). • Replaced previous graphic with one that includes MT.
	07/21/2014	• POC changed from Cady to Mueller. • Updated number and description of Science Themes, including a new figure, to reflect changes as of the latest strategic planning process.
	10/01/2013	• POC changed from Baer to Cady.
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email. Footnote added.
	02/19/2010	• Updated Science Themes.
	10/23/2009	• Changed POC from Felmy to Baer.
	03/10/2008	• Science Themes were last updated before the 2008 Call for Proposals.
	12/28/2005	• Original document = EMSL Action Plan 2005: WBS 1.02.02; Science Themes.

Section	Date	Change
4.0 Definition of an EMSL User*	05/29/2024	• Minor language update to "Reporting: guidelines. • Updated User and Proposal table to reflect FY 23 statistics. • Added definition of Call Responders.
	09/18/2023	• Updated User and Proposal Statistics table.
	08/20/2021	• Minor update to include a current example of EMSL's user and proposal statistics. • POC changed from Law to Hatt.
	08/12/2020	• Updated/clarified the definition of an Onsite user. • Updated counting method for Remote users to include all approved team members with signed user agreements. • Revised the definition of a Data user. • Removed Resource Owners from user counts.
	10/01/2013	• Updated definition used by Office of Science; clarified all EMSL resources regardless of building/location and included reporting specifics for BER quarterly reports to BER.
	08/11/2010	• Clarified REMOTE User.
	08/16/2010	• Added "user" in front of "facility" to clarify that the definition doesn't refer to just the EMSL building, but wherever EMSL user operations take place.
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email.
	09/27/2006	• Starting in FY07, the definition was changed to "An individual who makes use of the facility as part of an active user proposal in the EMSL Usage System is considered an EMSL user."
	10/03/2005	• Original document = EMSL Action Plan 2005: WBS 1.02.074; User Definition. Thus in FY06, the definition was changed to "Any individual not in the EMSL line organization who makes use of the facility as part of an active user proposal in the EUS, the EMSL user proposal system is considered an EMSL user." • Note – through FY05, all participants on active proposals were counted as users.
5.0 EMSL Proposal Types, Review Process, and Peer Review Criteria* *(Note: the * only applies to the Peer Review Criteria)*	05/29/2024	• Added year-2 internal review process and total duration of winter cycle proposals. • Deleted obsolete funding guidance for Exploratory proposals. • Added guidance language for Limited Scope proposals. • Minor grammar corrections. • Edited process change adopted for internal approvals during proposal review. • Inserted "external" to indicate PRP panel nature. • Edited notifications and appeal language to reflect information provided to applicants post-peer review. • Peer review criteria changes. • Table 5.4 edited to reflect new peer review criteria.
	09/18/2023	• Updated user proposal types with new contracting time and timelines. Minor updates to Merit Review, updated allocation process and extensions. Added language about dual anonymous to rating descriptions. POC changed from Hatt to Washburn.
	08/20/2021	• Clarified differences in winter and summer cycles. • Updated FICUS Research duration and clarified General proposal durations. • Updated summer cycle call dates. • Updated table 5.1 with clarified due dates and durations. • Updated intramural program details. • Updated titles. • Clarified allocation process. • Added section to address project team access and project closure. • POC changed from Law to Hatt.

Section	Date	Change
	06/25/2019	• Significant revision of proposal opportunities, names, and descriptions to more clearly distinguish annual calls vs. general proposal opportunities. • Updated wording for Scientific Partner and EMSL Staff Proposals for clarification. • Updated table 5.1 describing proposal types available. • Updated wording throughout section 5.2 for clarification of processes. • Updated mission criterion wording in section 5.3 based on Strategic Plan.
	01/30/2019	• Revised Rating Description Table in section 5.4 for better calibration among reviewers.
	03/08/2018	• Revised description of Criterion 3 in section 5.3 to align with BER's and EMSL's current mission.
	10/23/2017	• Minor wording changes for clarification of processes. • EMSL Staff Time proposal duration changed from "up to one year" to "up to three years."
	08/15/2016	• Updated wording for Annual Call Proposals and introduced "FICUS" terminology. • Updated information about General Proposal Cycles and changed frequency from twice to once per year. • Added text to EMSL Staff Time Proposals section to call out additional 10% made available at the EMSL director's discretion. • Updated wording for peer review criteria. • Clarified wording in the rating descriptions table (Table 5.4).
	07/21/2014	• Updated Science Themes, per latest strategic planning process. Number of themes went from three to four with subsequent name changes and new descriptions. • Updated figure showing overlap of the four themes.
	10/01/2013	• Restructured proposal types to simplify process for users. • Restructured General proposals to utilize Proposal Review Panels and review cycles. • Revised review criteria descriptions for improved calibration by review panels. • Changed title of Science Panels to Proposal Review Panels for consistency with other user facilities.
	03/15/2012	• Separated Rating Descriptions from section 5.3, Peer Review Criteria, to clearly delineate the Level 1 document, and revised language under Rating Descriptions to provide better guidance to reviewers regarding review scores.
	01/27/2012	• Updated Section 5.3, Criterion 2, Potential Considerations.
	09/06/2011	• Changed title to "5.0 EMSL Proposal Types, Review Process, and Peer Review Criteria." The current section records primarily the 3-step review of science theme proposals. Revised the review section (which is not part of the Level 1 document) to include descriptions of all proposal types with their respective review processes. Moved peer review criteria and descriptions (Level 1 document) to the end (Section 5.3) for better flow of information; wording wasn't changed except for the section heading of "Overall Rating Descriptions." Since reviewers are no longer asked for an "overall" rating, it was removed from the section title.
	08/19/2011	• Revised to include descriptions of all proposal types and their review process (not part of the Level 1 document for peer review criteria). Moved the peer review criteria and descriptions (which are a Level 1 document) to the end for better flow of information.
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email.
	02/12/2010	• Changed title to reflect new proposal type. • Added new section title: EMSL Proposal Evaluation Process. • Replaced current criteria (1-5) and rating levels (Excellent – Poor) with revised verbiage and ratings for improved calibration and consistency among reviewers.

Section	Date	Change
	01/21/2009	• BER was notified that the external proposal evaluation process will change. External reviewers will respond to 2 criteria. The remaining 3 criteria will be scored by an internal Science Review Panel. No change was made to the criteria verbiage, although they were renumbered. The potential considerations were slightly modified. Note: only the criteria (questions) are a Level 1 document.
	01/21/2009	• Same Review Criteria – new TRIM # created for future updates.
	04/14/2006	• As of 4/14/2006, in general, all proposals started going through peer review using the 5 review criteria questions.
	10/06/2005	• Original document = EMSL Action Plan 2005: WBS 1.02.04; User Proposal Review Criteria.
6.0 Appeals	05/29/2024	• Edited Appeals criteria.
	08/20/2021	• Minor wording changes to update titles and clarify process. • POC changed from Law to Hatt.
	06/25/2019	• Minor wording change in second paragraph for clarification.
	10/23/2017	• Minor wording change to remove reference to CSO.
	10/01/2013	• Section changed from 15.0 to 6.0. • Minor revisions to clean up language referring to the different types of proposals. • Updated USO email address.
	11/12/2009	• Clarified that appeals are to address errors submitted in original documentation or respond to reviewer comments, not to restate how much a user needs access. • Established a deadline for submitting appeals. • Clarified that Appeals Committee makes recommendation to EMSL director. • Added that USO will coordinate appeals with committee.
	03/17/2009	• Revised text – increased the number of paragraphs (from 1-2 to 2-3), and decreased the response time (from 8 to 4 weeks).
	05/27/2008	• Original – as posted on website.
7.0 EMSL Scientific Partner Program	05/29/2024	• Updated “proposal” to program. • Edited definition of the program. • Updated proposal submission, review, and notification process.
	09/18/2023 08/20/2021	• Removed references to CDO and DoUS. • Updated titles. • Updated process to include CDO in the review and approval. • Clarified requirements for LOI submission and removed page limit for full proposals. • Updated lists of potential review panel members for both LOIs and full proposals. • Clarified that progress updates may be written or verbal. • Updated the extension process to specify that extensions will be made by the CSO and CDO. • POC changed from Paša-Tolić to Teeguarden.
	06/25/2019	• POC changed from Kelly to Paša-Tolić. • Updated wording to refer to the EMSL Science & Technology Committee (ESTC) as part of the proposal review. • Other minor wording changes.
	10/23/2017	• POC changed from Koppenaal to Kelly. • Wording changes to clarify process, update terminology, and remove reference to CSO.
	08/15/2016	• Updated wording to (1) clarify requirement that Scientific Partners have regular project status meetings or submit summaries of their work, and (2) specify that full proposals should include a detailed list of funds, equipment, and other in-kind contributions they will provide.

Section	Date	Change
	07/21/2014	• Minor wording changes to reflect alignment with EMSL and BER missions and clarify the requirement of progress reports.
	10/01/2013	• Section changed from 16.0 to 7.0.
	07/18/2011	• Updated members of review Panels to include Associate Director for Molecular Science Computing.
	04/07/2011	• Minor updates to change requirement from “2” to “1-2” pages. • Added info regarding periodic reviews. • Clarified proposal requirements.
	02/18/2010	• Changed title of “Partner Proposals” to “Scientific Partner Proposals” per PNNL Legal request. Added requirements for annual progress reports. Minor edits.
	03/04/2009	• Original.
8.0 EMSL Staff Time Policy	05/29/2024 09/18/2023 08/20/2021	• Edited Staff Time proposal review process. • Changed Capacity to Contracted Time and updated language about recording instrument usage. POC changes from Hatt to Washburn. • Updated titles. • Clarified submission and review procedures. • Updated wording to specify that Staff Time proposals are for Environmental Molecular Sciences Division (EMSD) staff and joint appointees. • Updated wording to clarify that EMSL will make a reasonable effort to rearrange schedules to accommodate external users’ needs. • Updated review criteria. • Updated submission and review procedures to state that Staff Time proposals must be fully approved before committing to work via subcontracts or submitting funding agency proposals. • POC changed from Law to Hatt.
	06/25/2019	• Removed outdated reference to Wiley Visiting Scientists. • Updated terminology for new position titles.
	10/23/2017	• Minor wording change to remove reference to CSO.
	08/15/2016	• Updated policy to include additional 10% available to EMSL staff and others at the Director’s discretion. • Updated section references.
	10/01/2013	• Section changed from 14.0 to 8.0. • Modified to refer to proposals as “EMSL Staff Time” instead of “EMSL Staff 5%.” • Modified to include all Wiley investigators. • Modified to include EMSL director and CSO as internal peer reviewers. • Clarified that participants on Staff Time proposals and Intramural proposals are counted against staff usage totals. • Clarified new usage types for “EMSL Staff Time, Planned” and “EMSL Staff Time, Unplanned.”
	08/15/2011	• Revised purpose of proposals to remove limiting language that staff must be PIs or co-Pis and instead allow independent or collaborative research. • Updated review process to match new workflow of proposals. • Added Wiley Research Fellows to the EMSL Staff 5% policy to document their ability to use the proposal category to request “special time allocations” as listed under 18.3 Benefits section of the Research Fellow program.
	02/24/2009	• Original document.

Section	Date	Change
9.0 EMSL Intramural Program	05/29/2024	• Edited introductory language. • Modified budget of Dash proposals and equipment purchase value of Developer proposals. • Added language to reflect call responsiveness.
	09/18/2023 08/20/2021	• Updated program title. Added information about FY 23 addendums. Removed references to CDO. • Complete revision to capture tiered proposal process and new review criteria. • POC changed from Hess to Teeguarden.
	06/25/2019	• POC changed from Bolton to Hess. • Updated terminology for new position titles.
	03/08/2018	• POC changed from Liang to Bolton.
	10/23/2017	• POC changed from Koppenaal to Liang. • Updated process for this program, including review and selection processes. • Removed details of proposal requirements, as these can change yearly. • Added review criteria specific to this program.
	06/29/2016	• POC changed from Mueller to Koppenaal. • Revised to include new types of Intramural proposals and updated process for reviews, selection, and renewals.
	07/21/2014	• POC changed from Cady to Mueller. • Minor wording change to clarify the duration of funding for Intramural proposals.
	10/01/2013	• POC changed from Baer to Cady. • Section changed from 23.0 to 9.0. • Minor wording changes. • Updated dates to reflect new start dates and due dates of proposals.
	08/20/2010	• New section.
10.0 EMSL Utilization Policy*	05/29/2024	• Minor language edit in MOA. • Changed standard duration of MOA to two years. • Deleted repetitive content between sections. • Updated Resource Owner utilization tracking policy. • Updated need-based transfer of utilization agreement for transferred research capabilities.
	09/18/2023 08/20/2021	• Updated reporting to EMSL management. Responsibility for research resources changed to COO from director. Removed MOAs. • Wording changes to clarify or update current processes and titles. • Added text to allow other organizations' delegates to sign MOAs. • Clarified that MOAs for co-purchased instruments will detail each organization's costs, including space chargeback. • POC changed from Law to Hatt.
	06/25/2019	• Updated terminology for new position titles.
	10/23/2017	• Minor wording change to remove reference to CSO.
	08/15/2016	• Minor wording changes to include "staff" proposals and PNNL's new records management system. • Changed percent of time available for staff research, per increase approved in 2015 to 20%.
	10/01/2013	• POC changed from Teller to Law. • Section changed from 6.0 to 10.0. • Revised percent available to users on co-purchased instruments to "a minimum of 20% or the percent purchased by the EMSL User Program, whichever is greater." • Rearranged layout to simplify references to MOA purchases.

Section	Date	Change
	09/06/2011	• Added ability to negotiate special utilization agreements with EMSL-owned resources when it benefits the User Program by sharing space or adding sought-after capabilities not currently available to the User Program.
	06/23/2010	• Revised to (1) expand use of the 5% available instrument time to include collaborative work in addition to EMSL staff member's projects as PI or co-PI and (2) update EMSL staff 5% proposal approvals to include any EMSL Associate Director.
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email.
	12/28/2005	• Original document = EMSL Action Plan 2005: WBS 1.02.02; EMSL Utilization Plan.
11.0 Usage Type Definitions	05/29/2024	• Edited role of instrument custodians/authorized reservers. • Added Resource Owner as usage type.
	09/18/2023	• Added information about scheduling tool, how usage data are reviewed, and contracting time. POC changed from Hatt to Washburn.
	08/20/2021	• Clarified deadlines for recording instrument usage. • Clarified that core hours include planned outages. • Clarified when “EMSL Staff Time, Unplanned” should be recorded. • POC changed from Law to Hatt.
	08/12/2020	• Updated usage type definitions and examples to match the changes to the user definition in section 4.0.
	10/23/2017	• Minor wording changes to add in review process prior to archival and to clarify some of the usage categories.
	08/15/2016	• Minor wording changes to update when data are archived and to match the Utilization Policy for amount of time available for staff. • Updated description of Remote Usage to clarify that teams with both onsite and remote users should be coded as onsite and include only users who were physically present.
	10/01/2013	• Section changed from 12.0 to 11.0. • Shortened title. • Added reporting details for major and non-major instruments. • Changed “Instrument Custodian” to “Instrument Scientist.” • Expanded charging examples. • Added description of Core hours. • Changed “EMSL Staff 5%” to “EMSL Staff Time.” • Added new booking types (“EMSL Staff Time, Planned”; “EMSL Staff Time, Unplanned”; “Unavailable, Cancellation”).
	02/09/2011	• Updated Usage Type Definitions to reflect reduced categories and requirements for comments. • Reformatted section to mimic the appearance of categories on the Usage Breakdown report. Moved Section 11 to 12.2 and updated it.
	02/24/2009	• Revised to show EMSL 5% as new usage type. Note: Participants selecting EMSL 5% will not be counted as users as of FY 09.
	10/31/2006	• Revised to clarify and give examples.
	06/2006	• Original document in June 2006 Operations Manual.
12.0 Data Management Policy	05/29/2024	• Added to EMSL Data Use Policy for off-site non-user facility work.
	08/20/2021	• Updated the open access data release policy and captured immediate release of field sensor data. • Updated links and titles. • Second POC changed from Law to Hatt.
	02/28/2020	• Minor changes to clarify the public release of data.

Section	Date	Change
	06/25/2019	• Almost full revision of section to update terminology, policies for open access data, and repository management.
	10/23/2017	• Second POC changed from Cowley to McCue. • Full revision of section.
	08/15/2016	• Wording changes to reflect the current state of development of MyEMSL and the open data repository.
	10/01/2013	• New section.
13.0 EMSL Software Development and Sustainability Policy	05/29/2024	• Added detailed criteria for reviewing exceptions to software development effort requests.
	09/18/2023	• Added CAM SAL to share responsibilities. Added section about software retirement. POC changed from McCue to Saripalli.
	08/20/2021	• Updated titles. • Minor wording changes to clarify what should be included in the software plans and where documentation should be stored.
	06/25/2019	• New section.
14.0 User Agreements	05/29/2024	• Added EMSL Code of Conduct. • Deleted “Work for Others” and replaced with “Strategic Partnership Program.” • Added contact information of EMSL in Proprietary User Agreement.
	09/18/2023	• Changed EMSL signatory to COO. POC changed from Hatt to Washburn.
	08/20/2021	• Updated introductory paragraph with additional examples of authorized representatives, clarified that agreements have unique IDs and are stored in EMSL’s management system, and updated titles. • Updated title of the signatory for the contractor on the NPUA. • POC changed from Law to Hatt.
	06/25/2019	• Section changed from 13.0 to 14.0.
	07/21/2014	• Minor wording change under Article IX, paragraph D, to include SC requirement for “DOE Office of Science User Facility” in acknowledgment.
	03/21/2011	• New subsection added, Section 13.4: Bilateral DOE Laboratory Utilization Agreement.
	02/19/2010	• Changed section title from “non-proprietary use agreements and appendices” to “User Agreements.” Section now includes NPUA, PUA – Full Advance, and PUA – Partial Advance. • Added intro to document roll-out of electronic signature process. • Replaced previous NPUA form with new User Agreement approved for use by DOE in FY 2009 and mandatory by March 31, 2010. • In FY 2009, DOE implemented new user agreements, including one that can be used for proprietary research requests (PUAs).
	07/12/2006	• Appendix B – updated to include “PNNL/EMSL research staff are often listed as co-authors on publications resulting from User research performed in EMSL due to their significant scientific contribution. If PNNL/EMSL staff are listed as co-authors, you are required to notify the staff member prior to submission so that the publication can be reviewed and processed through PNNL's clearance system” in Section 6.
	10/01/1999	• Appendix A.
	10/01/1998	• NPUA. • Appendix C.

Section	Date	Change
15.0 Charging Guidance for EMSL User Facility Staff	05/29/2024	• Edited charging guidelines to accurately reflect charging to EMSL operations budget and support activities to other projects. • Edited location of lab 130 to indicate that it is in Building 331. • Added reference links to DOE charging guidance, pricing of materials and services, and Cost Accounting Standard defining allocation for direct and indirect costs.
	09/18/2023	• Clarification added to Support Activities. POC changed from Haulk to Johns.
	08/20/2021	• Wording changes to clarify the support activities charged to the EMSL project and to update titles. • Removed section referring to resources in building 3410 (RadEMSL). • POC changed from Swan to Haulk.
	06/25/2019	• Updating charging guidance for Limited Scope projects. • Updated section referring to per diem rates to reference the GSA per diem website vs. yearly update of rates within document. • Section changed from 14.0 to 15.0.
	01/30/2019	• Updated per diem rates for current fiscal year.
	10/23/2017	• POC changed from Bettinson to Swan. • Updated fiscal year reference for per diem rates.
	08/15/2016	• POC changed from Avery to Bettinson. • Added section 14.2.5 to reflect that EMSL is sharing space cost for NMR lab in 331. • Clarified that users are required to pay for “above-standard” costs for EMSL staff effort in section 14.3.3. • Updated per diem rates for FY 16. • Minor wording change to indicate meal costs for local interview candidates are unallowable. • Updated reference links.
	10/01/2013	• POC changed from Smith to Avery. • Section changed from 9.0 to 14.0. • Updated per diem year and rates so policy reflects current rates published by GSA.
	08/11/2011	• Removed redundancy of User Definition.
	07/07/2011	• Changed Capability Steward to Capability Lead. • Changed Instrument Time Allocation Committee to Resource Allocation Committee (RAC). • Added the EMSL and EED joint occupancy and collaboration in PSF 3410 building. • Added EMSL unallowable charging guidance.
	06/01/2009	• Minor update to change “facility” to “capability” and “facility lead” to “capability steward”; deleted sentence; corrected the definition of user.
	02/28/2007	• Significantly updated.
	10/06/2005	• Original document = Appendix C of the 2006 Operations Manual.
16.0 EMSL Space Policy	05/29/2024	• Added BER relevance to criteria determining laboratory space.
	09/18/2023	• Updated language describing EMSL mission. Added HDI link.
	08/20/2021	• Wording changes to update titles and clarify that the COO is the approver of lab and office space allocations. • Updated details for requesting lab space to outline space chargeback. • POC changed from Hartzell to Patello.

Section	Date	Change
	06/25/2019	• Revised Mission statement in section 15.1 to match revised Mission statement in section 2.0. • Section changed from 15.0 to 16.0.
	10/23/2017	• Minor wording changes. • Updated EMSL mission in section 15.1.
	07/21/2014	• POC changed from Knutson to Hartzell.
	10/01/2013	• Section changed from 10.0 to 15.0.
	11/28/2011	• Added information on space charging.
	06/03/2010	• Updated Policy and terminology.
	02/03/2009	• Last updated for the Operations Manual (Feb 2009). No significant changes, mainly updating terminology.
	05/2006	• Original document = Staff Resource Guide May 2006.
17.0 Instrument Life Cycle Management	05/29/204	• Edited Resource Owner usage guidance as part of Shared Purchases and Instrument Operations and Maintenance. • Added role of PMs in instrument divestment exercise.
18.0 Engagement with DOE and Laboratory Management	05/29/2024	• Updated Proposal and User Statistics report delivery frequency to DOE and PNNL.
	09/18/2023	• POC changed from Hatt to Washburn.
	08/20/2021	• Updated list of reports to reflect current owners. • Removed planned operating hour report. • POC changed from Law to Hatt.
	02/28/2020	• Updated list to include additional requirement for reporting EMSL's quarterly operating hours to Battelle.
	06/25/2019	• Section changed from 18.0 to 19.0. • Updated list of formal reports provided to BER and PNNL. • Updated due date for quarterly reports.
	10/23/2017	• POC changed from Tingey to Law. • Updated "Responsible Person" in table for Operating Hours, EMSL Dashboard, and Planned Operating Hours.
	08/15/2016	• Changed section heading. • Minor wording changes in description of what is sent and to whom. • Updated table 18.1 to include all major reports sent to BER, DOE, PNSO, and PNNL, along with the due date for each.
	07/21/2014	• Removed duplicate report listed in table 22-1. • Removed report that is no longer provided annually. • Minor wording changes for clarification.
	10/01/2013	• POC changed from Foster-Mills to Tingey. • Section changed from 22.0 to 18.0.
	08/08/2011	• Updated Table 22-1.
	02/16/2011	• Updated Table 22-1.
	07/29/2010	• Fixed error in Table 22-1.
	10/20/2009	• Original.

Section	Date	Change
19.0 Science and Technology Advisory Committee Charter*	05/29/2024	• Added role of EMSL Chief Science Officer to guide the committee. • Edited meeting frequency of committee.
	09/18/2021	• Added information about involvement of UEC chair, term length, virtual meetings, and role of CSO.
	08/20/2021	• New section to outline the roles and responsibilities of new advisory committee.
20.0 User Executive Committee Charter*	05/29/2024	• Added recommendation from UEC to select postdoctoral member from HBCUs/MSIs.
	09/18/2023	• Changed section title. Removed User Organization section. Updated description of UEC, responsibilities, membership, and elections. Updated meeting information.
	08/20/2021	• Section changed from 20.0 to 21.0. • Updated the membership and terms of service to remove the requirement that neither the chair nor vice chair may be a Battelle employee and to clarify the membership term. • Added new section to better outline the UEC leadership responsibilities of the chair and vice chair. • Removed the responsibility of overseeing the MT Thomas Award. • Removed the users' forum as part of the annual Integration Meeting. • Added language regarding conflicts of interest on the committee. • Wording updates for clarification and to update titles.
	06/25/2019	• POC changed from Bolton to Mans.
	03/08/2018	• POC changed from Liang to Bolton.

	10/23/2017	• Almost complete re-write of Charter, including
		  ○ Term limits imposed
		  ○ Vice Chair responsibilities added
		  ○ Committee responsibilities revised

	08/15/2016	• POC changed from Campbell to Liang. • Minor wording change to remove "ex officio" seat on SAC.
	07/21/2014	• Changed representation of the UEC to "science theme" instead of "capability". • Removed duplicative sentence regarding the chair and vice chair. • Added industry representation
	10/01/2013	• Section changed from 8.0 to 20.0.
	03/31/2011	• Changed title from "User Advisory Committee Charter" to "User Executive Committee Charter." • Updating to "at least 14 members." • All parties subscribed to EMSL's listserve will be eligible to vote. • All members are expected to be members w/in the last 5 years. • The Chair and EMSL director may appoint members directly if gaps in expertise are identified following election results.
	05/10/2010	• Moving from a specific number of committee members to a minimum number; changing facilities to capabilities; adding a focus of giving advice on capital investments and strategy.
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email.
	10/06/2005	• Original document = EMSL Action Plan 2005: WBS 1.02.04; Charters and Committees.
Change Control Request Form	05/29/2024	• Created editable form, updated title of signatories.
	08/20/2021	• Updated titles of signatories.

Section	Date	Change
	06/25/2019	• Updated terminology. • Removed line for HPRM (ERecords) number—individual sections are not tracked separately in official records.
	08/15/2016	• Updated form to change “TRIM” to “HPRM.”
	10/01/2013	• POC changed from Foster-Mills to Carpenter. • Updated form to simplify information needed and to require electronic signatures.
	05/03/2012	• Updated form (removed some signatures).
	03/17/2009	• Original form.

21.2 Deleted Sections

Section	Date	Change	Deleted Info
Divesting or "Sunsetting" of Instruments and Scientific Capabilities (previously section 19.0)	09/18/2023	• Section deleted. Now included in Instrument Lifecycle section.	Removed in Rev. 10
	08/20/2021	• Wording changes to update titles and to reflect current practices for transferred instrument ownership. • POC changed from Paša-Tolić to Patello.	
	06/25/2019	• POC changed from Kelly to Paša-Tolić. • Updated section wording with new terminology. • Minor wording changes to clarify process. • Section changed from 17.0 to 18.0.	
	10/23/2017	• POC changed from Koppenaal to Kelly. • Removed reference to CSO and updated terminology for CTO (“Lead Technologist”).	
	08/15/2016	• Minor wording change to clarify the definition of divestment or “sunsetting.”	
	07/21/2014	• Updated wording to clarify “divestment or ‘sunsetting’” and clarify EMSL’s divestment process.	
	10/01/2013	• Section changed from 24.0 to 17.0. • Minor changes and updates to Divestiture terminology and procedures.	
	01/25/2012	• New section.	

Section	Date	Change	Deleted Info
Policy for Requesting EMSL Capital Equipment Funds (previously section 18.0)	09/18/2023 08/20/2021 06/25/2019 10/23/2017 08/15/2016 07/21/2014 10/01/2013 05/03/2012 03/20/2012 07/22/2011 03/01/2011 02/21/2011 07/29/2010 03/04/2010 10/21/2009	• Section deleted. Information now included under Instrument Lifecycle Management. • Updated requirements to include new quad chart used to request capital equipment. • Updated process for reviewing requests and the parties involved. • Updated process used if additional funds are required. • Removed the Capital Equipment Request Form, which is no longer used. • POC changed from Paša-Tolić to Teeguarden. • POC changed from Kelly to Paša-Tolić. • Updated section wording and Capital Equipment Request form with new terminology. • Minor wording changes to clarify process. • Section changed from 16.0 to 17.0. • POC changed from Koppenaal to Kelly. • Removed reference to CSO and updated terminology for CTO (“Lead Technologist”). • Minor change to remove EMSL Chief Operating Officer from the capital committee list. • Minor wording changes. • Updated Capital Equipment Request form. • Section changed from 21.0 to 16.0. • Minor changes to clarify approval policy, departure of EMSL Capital Coordinator (N. Foster-Mills), and addition of policy statement against negotiated use of unspent authorized funds from a capital authorization. • Updated form (removed reviewers and changed approvers to CTO and COO). • Minor changes to clarify text. • Updated form. • Made minor changes to clarify text. Added EMSL Business Manager to committee list. • Updated form. • Updated form. • Updated form. • Original.	Removed in Rev. 10
Wiley Visiting Scientist Program *(previously section 21.0)*	10/01/2018 10/23/2017 08/15/2016 07/21/2014	• Section deleted. Complete revision of the program, policy, and requirements; removing old guidance and replacing with new program in Section 21. • POC changed from Paša-Tolić to Bolton. • Removed reference to CSO. • POC changed from Mueller to Paša-Tolić. • Updated minimum duration for long-term visits from 6 weeks to 6 months. • Added communication platforms in which partnerships will be acknowledged. • Clarified that evaluations will be made by the EMSL Leadership Team and requires EMSL director approval. • POC changed from Cady to Mueller.	Removed in Rev. 6.04

Section	Date	Change	Deleted Info
	10/01/2013	• POC changed from Baer to Cady. • Section changed from 17.0 to 21.0. • Minor wording changes.	
	02/08/2011	• Changed POC from West to Baer.	
	03/04/2010	• Changed POC from Showalter to West.	
	10/23/2009	• Changed POC from Felmy to Showalter.	
	04/23/2009	• Original – as posted on EMSL website.	
Wiley Research Fellow Program *(previously section 22.0)*	10/01/2018	• Section deleted. Complete revision of the program, policy, and requirements; removing old guidance and replacing with new program in Section 21.	Removed in Rev. 6.04
	10/23/2017	• POC changed from Paša-Tolić to Bolton. • Removed reference to CSO.	
	08/15/2016	• POC changed from Mueller to Paša-Tolić. • Added communication platforms in which partnerships will be acknowledged. • Clarified that evaluations will be made by the EMSL Leadership Team and requires EMSL director approval.	
	07/21/2014	• POC changed from Cady to Mueller.	
	10/01/2013	• POC changed from Baer to Cady. • Section changed from 18.0 to 22.0. • Minor wording changes.	
	02/08/2011	• Changed POC from West to Baer.	
	03/04/2010	• Changed POC from Showalter to West.	
	10/23/2009	• Changed POC from Felmy to Showalter.	
	04/23/2009	• Original – as posted on EMSL website.	
Science Advisory Committee Charter* *(previously section 19.0)*	06/24/2019	• Removed section for now, as this committee does not currently exist.	Removed in Rev. 7.00
	03/08/2018	• POC changed from Liang to Bolton.	
	10/01/2013	• Section changed from 7.0 to 19.0. • Updated “Terms of Service.” • Removed “Self-Assessment” section. • Updated wording referring to UEC.	
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email.	
	12/30/2005	• Original document = EMSL Action Plan 2005: WBS 1.02.04; Charters and Committees.	
William R. Wiley Research Fellow Program *(previously section 21.0)*	08/20/2021	• Section deleted; program will be re-evaluated.	Removed in Rev 8.00
	06/25/2019	• POC changed from Bolton to Hess.	
	01/30/2019	• Complete revision of the Wiley program, policy, and requirements.	
Wiley Postdoctoral Fellowship *(previously section 22.0)*	08/20/2021	• Section deleted; program will be re-evaluated.	Removed in Rev. 8.00
	06/25/2019	• POC changed from Bolton to Hess.	
	01/30/2019	• Section changed from 23.0 to 22.0.	
	10/23/2017	• POC changed from Paša-Tolić to Bolton. • Minor wording changes.	
	08/15/2016	• POC changed from Mueller to Paša-Tolić. • Minor wording change to update with call for applications opens each year.	

Section	Date	Change	Deleted Info
	07/21/2014	• POC changed from Cady to Mueller.	
	10/01/2013	• POC changed from Teller to Cady. • Section changed from 19.0 to 23.0. • Updated salary section to reflect current practices.	
	06/17/2011	• Slight change in 1st paragraph.	
	02/09/2011	• Changed dates to be generic for any given year.	
	10/06/2009	• Updated for FY 10 Call.	
	04/27/2009	• Original – as posted on EMSL website.	
MT Thomas Award for Outstanding Postdoctoral Achievement *(previously section 23.0)*	08/20/2021	• Section deleted. Other opportunities will be explored in the future.	Removed in Rev. 8.00
	02/28/2020	• Complete revision of section.	
	06/25/2019	• POC changed from Bolton to Mans.	
	01/30/2019	• Section changed from 24.0 to 23.0.	
	03/19/2018	• Updated evaluation process to revise the selection committee. Nominations will be reviewed by EMSL's User Executive Committee.	
	10/23/2017	• POC changed from Paša-Tolić to Bolton. • Updates to nature, rules, and eligibility of award.	
	08/15/2016	• POC changed from Mueller to Paša-Tolić. • Minor wording changes to keep Selection Committee Chair generic and remove Robby Robinson.	
	07/21/2014	• POC changed from Cady to Mueller.	
	10/01/2013	• POC changed from Baer to Cady. • Section changed from 20.0 to 24.0. • Updated MT Thomas language and dates to reflect a universal process instead of having to update yearly. • Corrected grammatical errors.	
	03/16/2012	• Updated Rules and Eligibility.	
	02/08/2011	• Changed POC from West to Baer.	
	03/04/2010	• Changed POC from Showalter to West.	
	01/11/2010	• Updated dates.	
	10/23/2009	• Changed POC from Felmy to Showalter.	
	04/28/2009	• Original – as posted on EMSL website.	

21.3 EMSL Policy Change Request Form

EMSL OPERATIONS MANUAL
Change Request Form
V3.1
02/16/2024

1. Change Request Number *(filled in by Ops Manual Steward)*	**4. Impact**
2024-1	☐ Correction
2. Request Date	☒ Update/revision
July 17, 2024	☐ Create new section
3. Requestor	☐ Delete section
Rick Washburn, Lead Project Manager	☐ Other: _____

5. Title of Affected Section *(if new, provide title)*

Please see section 21.1 for details.

6. Brief Description of Change and Reason for Change

Periodic review and update of Ops Manual

7. File Name(s)

EMSL Operations Manual 11

8. EMSL Approvals
By entering your name in the field below, you are indicating your approval of the changes listed above.

Rick Washburn,	July 17, 2024	Douglas Mans	July 18 2024
EMSL Lead Project Manager	*Date*	*EMSL Director*	*Date*

9. Client Approvals

Is DOE/PNSO approval required? ☒ Yes ☐ No Date of DOE/PNSO approval: April 24, 2024

10. Disposition *(filled in by Ops Manual Steward)*

Version of Ops Manual Affected: Version 10	Date New Version Posted: _____
Version of New Ops Manual: Version 11	Date Email Sent to Staff: _____