

# **Operations** Manual





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# **EMSL Operations Manual**

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Pacific Northwest National Laboratory Richland, Washington 99352

# Acronyms and Abbreviations

BAM	Budget Allocation Committee
BER	DOE Office of Science, Office of Biological and Environmental Research
CAM	Computing, Analytics, and Modeling
CDO	Chief Data Officer
СМ	Commercialization Manager
COO	Chief Operations Officer
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
GRID	Global Research Identifier Database
HBCUs	Historically black colleges and universities
HDI	PNNL's How Do I instruction system
IRP	Integrated Research Platform(s)
INSI	International Standard Name Identifier
JGI	Joint Genome Institute
LOI	Letter of Intent
LPM	Lead Project Manager
MOA	Memorandum of Agreement
NMR	Nuclear magnetic resonance
NPUA	Non-Proprietary User Agreement
OSTI	DOE Office of Scientific and Technical Information
PC	Project Coordinator
PI	Principal Investigator
PM	Project Manager
PNNL	Pacific Northwest National Laboratory
PNSO	Pacific Northwest Site Office

PRP	Proposal Review Panel
PUA	Proprietary User Agreement
ROR	Research Organization Registry
SAL	Science Area Leader(s)
STAC	Science and Technology Advisory Committee
SC	DOE Office of Science
TDO	PNNL's Office of Technology Deployment and Outreach
UEC	User Executive Committee
UI	Underserved Institutions
UPS	User Program Services

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# 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, experiment with computing and simulation, and our user program proposal calls with other user facilities demonstrates 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 organization (ISNI ID: 0000 0004 0373 6523). ISNI acts as a bridge identifier across multiple domains, including Ringgold Inc. (124574), Research Organization Registry (<u>https://ror.org/04rc0xn13</u>), Global Research Identifier Database (<u>grid.436923.9</u>), 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 22.0. 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 multi-modal molecular science instruments, data analytics, production computing, and multi-scale 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

The vision that directed the development of the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) has led to significant scientific progress. 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. The science areas were developed in collaboration with the scientific community and DOE's Office of Biological and Environmental Research (BER) leadership. EMSL's three science areas are Functional and Systems Biology, Environmental Transformations and Interactions, and Computing, Analytics, and Modeling. More information on each area is provided in the next three sections.

Although each science area focuses on drivers important to that field of science, there are significant overlapping and linked areas of common 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. Each science area is led by a Science Area Leader (SAL).

# 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 improved 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 integrated research platforms (IRPs) support FSB scientific research:

- The Structural Biology IRP seeks 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 investigates 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 reveals dynamic interactions and trafficking of molecular signals between cells, populations, and communities to understand complex inter-relationships between organisms in response to their environment.

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# 3.3 Environmental Transformations and Interactions

The **Environmental Transformations and Interactions (ETI)** science area seeks to understand molecular transformation and transport across scales to predict ecosystem response. It focuses on the mechanistic and predictive understanding of environmental (physiochemical, hydrological, biogeochemical), microbial, plant, and ecological processes in above- and belowground ecosystems, the atmosphere, and their interfaces. EMSL provides the experimental, computational, and simulation expertise to investigate and model cycling, transformation, and transport of critical nutrients, elements, contaminants, and atmospheric aerosols. Experiment and modeling approaches, joint with the Computing, Analytics, and Modeling group, accelerates 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 investigates the biochemical, physical, and microbial interactions that impact chemical speciation, transport, and transformation of critical nutrients, contaminants, and compounds within the environment.
- The Terrestrial-Atmospheric Processes IRP addresses the emission mechanisms of aerosols and gases from plants and soil into the atmosphere and will develop molecular-level understandings of the multiphase interfacial chemistry and aging processes occurring near Earth's surface and extending up to the atmospheric boundary layer.
- The Rhizosphere Functions IRP dissects molecular and microscale interactions between roots, the soil, and microbes to understand the impacts and mechanisms of root-controlled processes on plant resilience and biogeochemical cycling of carbon, nutrients, and mineral elements.

# 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. This cohesive approach to integrating experimental and computational methods 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, nutrients, and contaminants) in the environment.

Currently, two IRPs support CAM scientific research:

- The Systems Modeling IRP focuses on delivering state-of-the-art modeling approaches to accelerate 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 integration of modeling and EMSL's experiments through advances in AI/ML.
- The Data Transformations IRP delivers state-of-the-art data science capabilities for exploratory data analysis and data integration, and curating and preparing datasets for release to the data science community to accelerate data science research in directions relevant to BER.

4

# 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 <a href="http://science.energy.gov/user-facilities/">http://science.energy.gov/user-facilities/</a>. For 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:

- **Onsite 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 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 to download EMSL data.

**User Counts:** An individual is counted as a user only once per fiscal year 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 Onsite 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 DOE program managers 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 each proposal type. However, only distinct users are included when reporting the total number of users per fiscal year. 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.

EMSL

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

# **User and Proposal Statistics**

Start Period: October 01, 2021 End Period: September 30, 2022

Proposals by Proposal Type						FY2022	Year End FY2021
	Call Responders	Capacity (Regular)	Limited Scope	Scientific Partner		Distinct P	roposals
Total Active Proposals	162	52	26	4		244	270

Users by Proposal Type						
Total Users	529	236	37	5		
Onsite Users	106	63	5	2		
Remote Users	423	173	32	3		
Data Users	0	0	0	0		

<b>User Institution</b>	ns by Proposal	Туре			Distinct Inst
Academic	262	44	30	0	330
DOE Laboratory (Other)	55	4	2	0	60
Foreign	46	0	1	0	47
PNNL	153	187	3	3	290
Industry	3	1	0	2	6
Other	10	0	1	0	11

244	270			
Distinct Users				
744 801				
174	199			

570

0

602

0

Distinct Users by Institution			
330	388		
60	72		
47	45		
290 280			
6	6		
11	10		

# 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 non-proprietary with results shared with the scientific community through publications in open literature or conference presentations and papers.

### 5.1.1 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 of 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 the Facilities Integrating Collaborations for User Science program, or FICUS), or team with EMSL scientists on larger projects (Research Campaigns). Projects typically have an award duration of up to 24 months.
- 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 fiscal-year 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 <u>User Portal</u> (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. Proposals are valid for two years.
- **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 (Facilities Integrating Collaborations for User Science), which was initially developed by user facilities stewarded by the Department of Energy Office of Biological and Environmental Research. 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 a letter of intent, 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 <u>EMSL's science areas</u>. With proposal review panel (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.

To maintain consistency across calls, the proposal score under this cycle must meet or exceed the minimum established for proposals that were accepted in the winter award cycle. This minimum or "cut-off score" can vary year to year and is established by the PRP based on the lowest score of proposals recommended for acceptance in that award cycle.

**Special Calls for Proposals.** On occasion, researchers may have opportunities to request access through special science calls that are announced outside of 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 of 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 multi-resource 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 of 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. If approved, the entire scope of the project must be completed within a 90-day EMSL access window.

- Contracted Time. Requests to use contracted time on instruments that are 100% 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 scientists, 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 PNNL to access the instruments and fund instrument scientist 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 U.S. Department of Energy 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 a 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 <u>EMSL User Portal</u>, 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 CDO. For full details of this program, see <u>section</u> 7.0.

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Table 5.1 User Proposal Types Available					
Proposal Type	Call / Submission Dates		Research Focus	Duration	Merit Review
Large-Scale EMSL Research*			PI-initiated scope based on call topics in EMSL science areas	24 months	
FICUS Research*	Calls open December	Due dates vary by Call	PI-initiated scope based on call topics defined jointly with multiple facilities	24-30 months	
Research Campaign*			EMSL-initiated scope for larger campaigns to advance strategic science	Defined in Call	External Reviewers
Exploratory Research*	Call opens June	Due dates may vary, but usually mid- summert	PI-initiated scope on calls to targeted user communities	9 months	
Scientific Partner*			PI-initiated scope for capability development.	Negotiated	
Limited Scope	- Any Time			90 days	
Contracted Time			PI-initiated research scope	Up to 1 fiscal year	Internal Reviewers
Proprietary*			PI-initiated research scope not intended for public dissemination	Up to 1 calendar year	

Table 5 1	User	Proposal	Type	s Available
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\*Proposal type requires a Letter of Intent

#### 5.1.2 **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 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, the team leader or group leader. As well as internal health, safety and environmental reviews as required. For more details, see section 8.0.

**EMSL Intramural Program Proposals.** These proposals are submitted under a competitive intramural program for directed research and development 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 <u>User Portal</u> 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 <u>section 9.0</u>.

# 5.2 Submitting a Proposal

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

### 5.2.1 Proposal Screening and Technical Review

Proposals are screened by User Program Services to determine if the required information is present and the proposal package adheres to the published guidance for page length and formatting. If the proposal passes screening, it is assigned to a primary IRP leader, based on the scope of work, as well as a project manager (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 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.

### 5.2.2.1 Internal Management and ESS&H Review

Once the proposal has passed the screening and technical review, concurrent internal management reviews occur. All proposals 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 CRADA or subcontract. For details regarding the DOE user agreements, see <u>section 14.0</u>. Proprietary work is assessed for appropriate cost reimbursement, etc.
- Environment, Safety, Security, and Health: 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.

### 5.2.2.2 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 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 <u>8.0</u> and <u>9.0</u>.

### 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 comprises the Science Area Leader (SAL) and 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 scientific merit, team qualifications, mission, and science area relevance. The starting score for the fifth criterion (resource request) is provided to the PRP by the IRP leaders based on a formula that takes into account instrument time, staffing support costs, and the scientific merit score provided by the assigned reviewers. 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 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 Lead Project Manager (LPM).

• **Special Independent Reviews.** Due to 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 <u>section 7.0</u> for further details.

### 5.2.3 Allocation of Resources

At the beginning of each fiscal year, 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 for the first year 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, User Program Services (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), science area leaders, 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, BER PIs and by institution (PNNL vs. external). The science area leaders 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 User Program Services to issue decision notifications. The final decision to conduct work on an accepted project, however, is dependent on approval by the Department of Energy if the PI is not a US 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.

### 5.2.4 Notification and Appeals

User Program Services issues decisions to the applicants for approved proposals and brief reasons for denied proposals. Peer reviewer comments, as well as the composite score and relative ranking (top 25%, top 50%, and bottom 50%) for all user proposals, are made available to the applicants in the <u>EMSL User Portal</u>.

Appeals may be submitted following the process outlined in  $\underline{\text{section } 6.0}$ .

### 5.2.5 Project Team Access and Project Closure

Team members on approved proposals work through the assigned project manager or User Program Services 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 that are open for only 90 days, 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 User Program Services 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

Reviewers are asked to score each user proposal based on five criteria to ensure the proposed research is of high quality and an appropriate use of EMSL's resources. Each criterion is scored from 1 to 5, with 5 being the highest. 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 5.4 for additional calibration.

### Criterion 1. Scientific merit and quality of the proposed research

**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?

# <u>Criterion 2.</u> Qualifications of the proposed research team to achieve proposal goals and contribute to high-impact science

*Potential considerations:* Does the proposal team, combined with relevant EMSL staff expertise, possess the appropriate breadth of skill/knowledge to successfully perform the proposed research and drive progress in this science area? If successful, would the proposed research deliver high-impact products (for example, be publishable in high-impact journals)?

Note: Impact factors are a measure of the average number of citations per published articles. Journals with higher impact factors reflect a higher average of citations per article and are considered more influential within their scientific field.

### Criterion 3. Relevance of the proposed research to EMSL's mission

EMSL's mission as a national scientific user facility is to provide access to premier multi-modal molecular science instruments, data analytics, production computing, and multi-scale 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 supports the mission of the Biological and Environmental Research (BER) program in the Department of Energy 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.

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.

*Note:* Projects with direct relevance in these areas will have the best chance for selection. Other projects of scientific significance also are welcomed, but the applicant should clearly outline how the project will further a DOE mission or other areas with economic or societal impact.

**Potential considerations:** What is the relationship of the proposed research to EMSL's mission? Does the research project significantly advance the mission goals? How well does the project plan represent a unique or innovative application or development of EMSL capabilities?

### Criterion 4. Impact of the proposed research on one or more EMSL Science Areas

**Potential considerations:** Will the proposed research advance scientific and/or technological understanding of issues pertaining to one or more EMSL science areas? To what extent does the proposed research suggest and explore creative and original concepts related to one or more EMSL science areas? How strongly does the proposal relate to the science area's focused topics as outlined in the most recent call for proposals? How well will it advance EMSL along the directions specifically outlined in the focused topics?

# <u>Criterion 5.</u> Appropriateness and reasonableness of the requested EMSL resources for the proposed research

**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?

# 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.

Score	Science Merit	Team Qualifications	Mission Impact	Science Area Relevance	Resource Use	Reviewer Calibration Summary
	50%	10%	10%	20%	10%	Summary
5 Outstanding	Highly innovative research; will launch new direction or have exceptional impact on existing problems in the research field. No flaws in research plan; includes approach or plan for predictive understanding.	Outstanding track record in research field; considered expert(s) in area of study; results expected to have high impact in top- tier journals.	Direct relevance to BER mission; strongly supports DOE mission or will have significant economic or societal impact; unique or innovative applications of EMSL capabilities; exceptionally strong plan for developing predictive understanding.	Outstanding fit to focused topics outlined in most recent EMSL Call for the science area under review.	State-of-the-art resources are requested and are essential to perform this research.	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 research field. Minor flaw(s) in research plan; includes approach or plan for predictive understanding.	Very strong track record in research field; results likely to have high impact.	Broadly addresses BER mission, but directly addresses DOE mission; excellent applications of EMSL capabilities; well-designed plan for developing predictive understanding.	Strong fit to the focused topics outlined in the most recent EMSL call for the science area under review.	State-of-the-art resources are requested or use of EMSL resources would significantly enhance the results.	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.	Solid track record; results likely to have some impact in domain-specific journals.	Does not directly address BER mission, but broadly supports DOE or economic or societal needs.	Does not have 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.	Resources requested are not state-of-the- art, well integrated, or not justified in the research plan.	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 well- worked area of research; incremental results. Major flaw(s) identified in research plan or approach would limit success.	Some expertise but not a strong record in the field; likely to have minimum impact in domain-specific journals.	Minimum impact to DOE missions, but broadly supports other economic or societal needs.	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.	EMSL capabilities marginally enhance results; similar results could be achieved with broadly available instrumentation and expertise.	Does not advance EMSL goals or have a strong argument for 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 research plan would significantly limit success.	Does not have a strong record and doubtful that results would have publishable impact.	Does not support DOE missions and questionable impact on economic or societal needs.	Is not responsive to the most recent EMSL call or does not address the goals of the science area under review.	There is no evident need for, or unique impact from, the use of EMSL's suite of resources.	Decline to provide a recommendation for award.

Table 5.4 Large Scale Research Review Criteria, Relative Weight, and Scoring Descriptions

# 6.0 Appeals

Proposal authors may submit appeals regarding the decisions made on new proposals if they have substantive evidence to show that reviewers made a serious error or there was some flaw in the review process. Appeals of denied proposal extensions may be made if decisions appear to have been based on inadequate or incorrect information or if there are extenuating circumstances not noted in the progress summary or resource request. Appeals to reverse management decisions that were based on limited resources and funding will not be considered.

To submit an appeal, the proposal author must email User Program Services (<u>emsl@pnnl.gov</u>) with a concise (2-3 paragraphs) summary of concerns as well as any supporting arguments for reversing the decision. Authors should not include extension summaries or project descriptions, as these will be provided to the Appeals Committee as part of the appeals package. *Appeals must be submitted within 30 days from the date on the award decision notice*.

The Appeals Committee, appointed by the director, reviews and makes recommendations to the EMSL director. All decisions by the EMSL director are considered final. User Program Services will coordinate with the committee and notify the user of the committee's decision within 1) eight weeks from receipt of the appeal on proposals submitted against the annual Call for Proposals, or 2) within four weeks from receipt of the appeal for other proposals.

# 7.0 EMSL Scientific Partner Proposals

# 7.1 Definition

Scientific partner proposals are submitted 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 science and user programs. 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 should be aligned with and strategically supportive of EMSL and BER missions. 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 submits a letter of intent (LOI) to EMSL's chief science officer (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 integrated research platform (IRPL) 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 development of high-impact capabilities with strategic alignment to EMSL and BER science and supporting 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 the partner organization investigator and will be reviewed by a panel convened by the CSO. The review panel will include some or all of the following: the CSO, the CDO, relevant IRP and science area leaders, subject matter experts, the chief operation officer (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 investigator 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 via the EMSL User Portal (<u>https://nexus.emsl.pnnl.gov/Portal/</u>) 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 IRP and science area leaders, 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 author. Letters for accepted proposals will document details of the agreement, including at a minimum the agreed-upon schedule and deliverables, 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:

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 of 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 fiscal years. 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 Environmental Molecular Sciences Division. Staff Time projects are subject to EMSL's data management policy detailed in <u>section 12</u>.

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 onsite 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.
  - $\circ$  Samples or materials with radiation levels exceeding EMSL capabilities.
  - Work that might require instrument or facility modifications.
- After the proposal is reviewed by the appropriate IRP leader(s) for technical feasibility and instrument availability, the team leader or group leader will be assigned as an internal reviewer.
- 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
   <u>11.0</u>).

Point of Contact: Rick Washburn, Lead Project Manager

# 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 science and technology roadmap presented in the 2021 EMSL Strategic Science Plan and FY 2023 addendums that clarify some aspects of the strategy and present new IRPs and Research Areas. 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 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. Instrument hours allocated for this program will be based on the instrument's total operating hours minus time scheduled for maintenance, upgrades, or repair. Any time remaining will be made available to the user program for user or Staff Time projects.

# 9.1 Intramural S&T Proposal Types and Review Process

Proposals to the intramural program are managed through the EMSL <u>User Portal</u> 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 \$50K.
- 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 3 times a year. Concepts are screened by the CSO, SAL's and IRPL's and invitations for full proposals issued. Full proposals and are reviewed internally and selected for funding by the chief science officer (CSO) and the relevant science area and integrated research platform (IRP) leaders.

Developer proposals must be submitted in response to an annual call for proposals that outlines focused topics designed to advance EMSL's science and technology roadmap as presented in the 2021 EMSL Strategic Science Plan and the supporting Research Area Roadmaps. The annual call will consist of two review phases to first screen one-page whitepapers, followed by peer review of full proposals. Whitepapers will be screened by the CSO and the science area leaders for relevance to the EMSL roadmap and responsiveness to the call topics. The PIs for selected whitepapers will be invited to submit full proposals that will be evaluated for technical approach by the IRP leaders 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 science area leaders, and final decisions will be made based on scientific and technical merit, prioritization related to the goals and timelines of the EMSL science and technology roadmap, 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.

Whitepapers and proposals must follow a proscribed format and length requirement 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 \$50K.

Point of Contact: Justin Teeguarden, Chief Science Officer

# 9.2 Peer Review Criteria

Evaluation of the whitepapers 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 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 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 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

Progress of ongoing projects is reviewed by the CSO and the science area leaders throughout the year and at least semiannually for each project. These reviews enable evaluation of the project progress, identification of barriers, and redirection of the approach if needed to ensure progress. At each review, continuation of projects and funding depends upon progress toward completion of milestones and 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 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 divesting of resources as part of lifecycle management. Lab space supported by the EMSL user program is subject to the EMSL Space Policy as detailed in <u>section 16.0</u>.

# 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 co-purchasing 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:

- EMSL infrastructure support
  - Computer and network support
  - Machine shop access
  - Waste management costs
  - ES&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 percent 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 percent 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 Agreements (MOAs)

As needed, MOAs 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.

An 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 standard durations of up to 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 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, 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.
- While a new MOA can be established at any time, all MOAs will be reviewed and reapproved annually at the beginning of each fiscal year 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, and whenever a major upgrade or change in the value of the instrument(s) occurs.

### 10.4.2 100% Other Program Purchased Research Resources

- 20% of the available time will be open to users through the user proposal process unless a separate agreement is developed and documented in a on 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. It is the responsibility of the resource owner to keep EMSL's User Program Services 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 percent 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 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 a 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 18.0), 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 director's discretion. Requests will be submitted as 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.
- The utilization agreement for transferred research capabilities will be documented in a 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 Scientists by their respective integrated research platform (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. Non-staff (e.g., users, collaborators) are not eligible to serve as Instrument Scientists.

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 User Program Services annually sends a list of instruments that require utilization tracking to Instrument Scientists.

Instrument Scientists are required to record usage data by Friday of each week and by the last day of the month for the final week. The data analyst on the User Program Services team 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. (24 hours a day), seven days a week, excluding official laboratory holidays and planned outages. Other core hours are 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

- **Onsite 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 principal investigator 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.
- **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 of instrument core hours or when the instrument is idle during core hours due to 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 percent of time allocated to staff under the Utilization Policy.

#### Out of Service, Planned

- Maintenance Resource is not available because periodic maintenance or modification of 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, *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 under 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 due to 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:**

- 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 onsite) 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 onsite 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 "onsite 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 "onsite 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 non-proprietary 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 and computational scientists. EMSL's policy is based on the guiding principles summarized below from the Department of Energy (DOE), DOE Office of Science (DOE-SC) and the Office of Biological and Environmental Research (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.<sup>1,2</sup> Data preservation and sharing facilitates validation and reproducibility of scientific results and broadens 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<sup>3</sup>.

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<sup>4</sup>.

## 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 non-proprietary data in the repository through the Get Data tab of the applicable project in the <u>User Portal</u>.

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.

<sup>2</sup> https://science.osti.gov/Funding-Opportunities/Digital-Data-Management

<sup>&</sup>lt;sup>1</sup> <u>https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management</u>

<sup>&</sup>lt;sup>3</sup> https://www.energy.gov/downloads/doe-public-access-plan

<sup>&</sup>lt;sup>4</sup> <u>https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management-resources</u>

# 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:

- Immediate access and release of data generated on an approved user project is granted to all team members (aka participants) listed on the project by the principal investigator (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 additional 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 User Program Services. 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 *non-proprietary 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, refers 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 <u>data portal</u>.

To support making data openly accessible, tracking data use for the Office of Science, and encouraging proper citation of the researchers who generated the data, EMSL's data portal requires 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 the EMSL's repository:
  - Data generated under EMSL's Strategic Science Objectives, including but not limited to the 1000 Soils Research Pilot and the Molecular Observation Network (MONet)
  - Field sensor data
- All other resource data will be released as follows:
  - All non-proprietary 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

Non-proprietary project data that are from EMSL resources must be uploaded to the repository; data stored outside of 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 availability of the repository and stored elsewhere) are being evaluated by EMSL staff, and all legacy data that meets 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 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 non-proprietary data should be uploaded, except data that fall under <u>section 12.4.2</u> below. Data that fall into the exception category can be uploaded in some cases but are not required. EMSL instrument and computational scientists should direct any questions they have regarding the type of data collected to the EMSL IRP leader 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 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 conforms 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 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 data set to be uploaded; the original data may be uploaded initially and processed data subsequently. The time stamps for upload of each data set 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 <u>section 12.4.1</u>, some data are not required to be uploaded to the repository. These are data that will not form the basis of publishable research findings nor are 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 has been released to the project team or made openly accessible to the scientific community, the instrument scientist should contact the appropriate IRP leader and chief data officer (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 User Program Services who will flag the appropriate data set(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 the 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 Office of Scientific and Technical Information (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 chief data officer (CDO) and Computing, Analytics, and Modeling Science Area Leader (CAM SAL).

## 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<sup>5,6</sup>. 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. Identification of clear roles and responsibilities of development team members.
- 2. Description of software requirements 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.
- 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.

<sup>&</sup>lt;sup>5</sup> https://github.com/betterscientificsoftware/PSIP-Tools/blob/master/PSIP-Overview.md

<sup>&</sup>lt;sup>6</sup> https://confluence.pnnl.gov/confluence/display/DC/Welcome+to+Developer+Central

- 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 (<u>Confluence</u>), track software development tasks (<u>JIRA</u>) and support version control (EMSL <u>GitLab</u>).

# 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 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 opensource 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 <u>https://github.com/EMSL-Computing/</u>).
- 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)<sup>4</sup> 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 office 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. There are several critical activities 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**

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 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 Chief Operations Officer. 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 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, Work for Others (WFOs) 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. <u>SCHEDULING\*\*\*</u>

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. <u>PATENT RIGHTS\*\*\*</u>

## 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. <u>RIGHTS IN TECHNICAL DATA\*\*\*</u>

## 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. <u>DISPUTES\*\*\*</u>

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:** 

## 14.2 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, Work for Others (WFOs) 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 <a href="https://nexus.emsl.pnnl.gov/Portal/">https://nexus.emsl.pnnl.gov/Portal/</a>. 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 costs 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			
<u>Statements</u> .	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:

## **Operations Manual**

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. <u>RESERVED</u>

## 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. <u>SCHEDULING\*\*\*</u>

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

Point of Contact: Rick Washburn, Lead Project Manager

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. <u>DISPUTES\*\*\*</u>

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: ADDRESS: DATE: TELEPHONE:

#### FOR THE USER:

BY:
TITLE:
ADDRESS:
DATE:
TELEPHONE:

## 14.3 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, Work for Others (WFOs) 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 <a href="https://nexus.emsl.pnnl.gov/Portal/">https://nexus.emsl.pnnl.gov/Portal/</a>. 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 costs 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. <u>SCHEDULING\*\*\*</u>

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. <u>RIGHTS IN TECHNICAL DATA\*\*\*</u>

## 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:

ADDRESS:

DATE:

**TELEPHONE:** 

## FOR THE USER:

BY:

TITLE:

ADDRESS:

DATE:

TELEPHONE:

# 14.4 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, WFOA 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:

FOR CONTRACTOR B:

BY:	BY:
TITLE:	TITLE:
DATE:	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 non-proprietary 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. However, on-site users are treated differently than remote users. Onsite users may be charged for some support where remote users generally are not.

EMSL defines a user in <u>section 4.0</u> of this manual.

The Department of Energy's Office of Biological and Environmental Research provides programmatic funding for the operation and maintenance of EMSL as a user facility, frequently referred to as the EMSL operations budget. Users located at the PNNL campus are always considered onsite users for charging purposes.

# **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) integrated research platform (IRP) leader 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 capability or improve current capability), which are 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, including IRP leader labor, for processing users to access EMSL and its resources; user training; and assisting users during experiments (e.g., in preparing samples); assembling, configuring, and disassembling equipment; 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 EMSL operations budget, when they are asked for technical support by a user who is—or whose team members are—qualified to operate the instrument independently or to perform any other support that does not qualify for operations project funding as outlined above. Staff support on resources that require specialized training for which a user is unqualified will be provided by EMSL operations funding up to the amount of time allocated in the BAM.

Examples of activities that shall be charged to the user's project:

• On-site user requests for EMSL staff to run samples, perform analyses, or contribute to a report that the user is able to perform but chooses not to do.

*Note: On-site user is defined as being on the PNNL campus, or in certain cases where EMSL-owned equipment is taken to a remote location for field work.* 

• EMSL staff travel to a conference at the user's request to present information specific to non-EMSL projects (i.e., other programmatic funded research), and the conference provides limited outreach opportunity or EMSL capability discussions (i.e., it primarily benefits the programmatic-funded research).

#### 15.2.2 Proprietary Proposals

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

### 15.2.3 Utilization Policy

EMSL houses resources that were not fully purchased with the 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 the 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. User Program Services maintains the agreements for all resources documenting the percentage of the instrument that is EMSL owned. A full description of the EMSL Utilization Policy can be found in <u>section 10.0</u>.

#### 15.2.4 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.

# 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

As per the guidance above, 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 who operate the equipment themselves, and equipment maintenance. In turn, all non-proprietary EMSL users are expected to pay for their own labor, travel, and EMSL scientific consultant support in cases when they are able but choose not to operate or participate in operation of EMSL equipment in the conduct of their own research work. EMSL's philosophy is to support projects that plan to use EMSL equipment and personnel when the experiment is conducted onsite (within identified EMSL spaces on the PNNL campus).

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

- preparation time to mobilize and demobilize equipment (disassembly, pack, set up, receive back and unpack, 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 funds for the 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 non-proprietary 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, 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. (<u>https://www.directives.doe.gov/directives-documents/500-series/0522.1-BOrder</u>).
- Cost Accounting Standard (CAS) 418 9904.418-40 (i.e., Allocation of Direct and Indirect Costs) has provision for exclusion of special purpose facilities which would apply in this extension to the EMSL National User Facility (<u>http://www.ecfr.gov/cgi-bin/retrieveECFR?gp=&SID=ece9696a1a8b58cb7d9c139138479c58&mc=true&n=pt48.7.9904&r=PART&ty=H</u> TML#se48.7.9904 1418 640)
- PNNL Finance Manual, Section 5.1, EMSL User Facility policy (<u>https://business.pnl.gov/documentManual/FinOps/documentType/837</u>).

# **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 Office of Biological and Environmental Research 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. Due to the unique nature of this facility, priority must be given to those capabilities and individuals that significantly support the EMSL 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. 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.

Priority for laboratory space is based on the level of support the individual or capability brings to the EMSL 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?
- 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 chief operations officer (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.

Point of Contact: Gert Patello, Chief Operations Officer

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 the 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 <u>10.0</u> and <u>16.0</u>) and any Memorandums of Agreement (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 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 <u>Executing a Lab Move</u> 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 post-doctoral researchers and students.
- **Priority 2:** Non-PNNL staff members (external users) who have an active user project for using EMSL research capabilities onsite.
- **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.

Point of Contact: Gert Patello, Chief Operations Officer

### 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:

- identify space outside of 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 Lifecycle Management**

The Environmental Molecular Sciences Laboratory (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 enables 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 chief operations officer (COO) in partnership with the Integrated Research Platform leaders (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 provided 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 current strategic needs identified in the 2021 EMSL Five-Year Strategic Science Plan and science and technology (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 chief science officer (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 not tracked nor is an EMSL user proposal needed for the other owner. 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 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 the procurement. Depending on the complexity of the instrument, vendor installation and commission is included in the procurement contract. Any facility modifications are also initiated. Pacific Northwest National Laboratory's processes are followed for procurement and facility modifications. If installation and commissioning is not performed by a vendor, it is completed by the instrument scientist as part of core Integrated Research Platform (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 scientist 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 NMRs, 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 project 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 is 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 not tracked, nor is an EMSL user proposal 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 is managed per EMSL's data management policy. The usage by the owning organization or project does not need to be scheduled or recorded in NEXUS, nor is an EMSL user proposal 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 scientist. Factors that are considered are (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 scientist before renewal, who consider the factors above, as well as the age and obsolescence of the instrument. The EMSL instrument scientist is responsible for maintaining the instrument in working order and arranging for appropriate preventive maintenance. The instrument scientist annually estimates how much instrument downtime is needed during the year and provides that information to the project manager assigned to the IRP the instrument is associated with.

Point of Contact: Gert Patello, Chief Operations Officer

### **17.4 Instrument Divestment**

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 fiscal year. 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 IRPLs. The IRPL 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 IRPL 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, the IRPL follows the process defined in the New Instrument Planning section (17.1). For instruments that are strategic but expensive to maintain and for which newer technology is available, the IRPL also follows the process in the New Instrument Planning chapter 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. EMSL then is no longer responsible for 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 the Office of Science or in support of PNNL reporting requirements to DOE Management. Table 19-1 outlines these reports and interactions.

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	Quarterly (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 2 <sup>nd</sup> and 4 <sup>th</sup> quarter end)
Resource Summary Report	BER, PNSO	UPS Lead Project Manager	Biannually (21 days after 2 <sup>nd</sup> and 4 <sup>th</sup> 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)

### Table 19-1. Formal Reports Provided to DOE and PNNL

# **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 in 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 research and development 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 UEC (Section 20.0 below) 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 science and technology, 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 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 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 1<sup>st</sup> 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, as well as 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 pre-meeting 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 the 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 User Executive Committee (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 fiscal year or in either of the two preceding fiscal years), 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 the 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 proposal review panels.
- 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 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 chief operations officer, who serves as 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 post-doctoral user, with special emphasis on selecting one from underserved institutions. The post-doctoral 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 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 the 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 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 fiscal years and 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 science and technology, education, government policy, and industry that are relevant to the EMSL user facility mission, the U.S. Department of Energy, 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 conflict of interest (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 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 are one-year terms each. 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 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 Science and Technology Advisory Committee. 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 onsite. If deemed necessary by the UEC chair and the EMSL director, additional meetings may be called and held onsite, 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	Owner
Entire Book	9/18/2023 08/20/2021	<ul> <li>Updated terminology throughout to refer to new staff titles. Updated footers with review dates and new POCs. EMSLUO changed to EMSL user community.</li> <li>Updated terminology throughout to refer to new staff titles.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	06/25/2019	<ul> <li>Updated footers with review dates and new POCs.</li> <li>Updated terminology throughout to refer to new staff titles.</li> <li>Removed references to individual ERecord numbers for each section.</li> </ul>	
	03/08/2018	Updated footers with new POCs.	
	10/23/2017	<ul> <li>Updated footers with review dates and new POCs.</li> </ul>	
	08/15/2016	<ul> <li>Updated footers with review dates and new POCs.</li> </ul>	
	10/01/2013	<ul><li>POC changed from Foster-Mills to Law.</li><li>Updated footers with review dates and new POCs.</li></ul>	
	02/09/2011	<ul> <li>Updated Review Dates on sections that did not require updates.</li> <li>Changed "Capability Steward" to "Capability Lead" (in chapters, not in CCR).</li> <li>Changed POC in Sections 17, 18, and 19 from West to Baer.</li> <li>Updated Nancy Foster-Mills' title to "Product Line Manager."</li> <li>Updated Don Baer's title to "Interim Lead Scientist."</li> </ul>	
	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	09/18/2023 08/20/2021	<ul> <li>Added references for Research Organization Registry and Global Research Identifier Database.</li> <li>Minor wording changes to spell out acronyms.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	08/12/2020	<ul> <li>Minor update to include EMSL's Research Organization Registry (ROR) ID.</li> </ul>	
	06/25/2019	<ul> <li>Updated sentence referring to BER mission to match Mission criterion changes in section 5.3.</li> <li>Updated to include EMSL's unique identifiers.</li> <li>Updated last paragraph to include schedule for updating the Operations Manual (note: legal review not required as their original text was not changed).</li> </ul>	
	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	<ul> <li>Original document = EMSL Operations Manual Rev 3 (PNNL-15828). Note – this requires legal review. Do not edit this section without legal review.</li> </ul>	

Section	Date	Change	Owner
2.0 Mission and	08/20/2021	Complete revision of EMSL's mission and vision to reflect current practices.	Douglas
Vision*	06/25/2019	POC changed from Bolton to Mans.	Mans
	03/08/2018	POC changed from Liang to Bolton.	
	08/15/2016	<ul> <li>POC changed from Campbell to Liang.</li> <li>Updated to match approved Strategy Plan verbiage and add vision.</li> <li>Changed section heading.</li> </ul>	
	04/15/2010	• Level 1 approval changed from formal correspondence to informal email. Footnote added.	
	08/23/2005	<ul> <li>Same policy – new TRIM # created for future updates</li> </ul>	
	08/23/2005	<ul> <li>Original document = EMSL Action Plan 2005: WBS 1.03.01; EMSL Mission Statement.</li> </ul>	
3.0 EMSL Science Areas*	09/18/2023 08/20/2021	<ul> <li>Updated introduction to sciences areas, updated description of ETI, added new DT IRP to CAM. POC changed from Hess to Bargar.</li> <li>Complete revision, taking place of the Science Theme descriptions.</li> <li>Added Baker and Bardhan as additional POCs.</li> </ul>	John Bargar / Scott Baker / Jay Bardhan
	06/25/2019	POC changed from Bolton to Hess.	
	03/08/2018	POC changed from Liang to Bolton.	
	10/23/2017	<ul> <li>POC changed from Paša-Tolić to Liang.</li> </ul>	
	08/15/2016	<ul> <li>POC changed from Mueller to Paša-Tolić.</li> <li>Minor wording changes to introductory paragraph to reference approved 2014 Strategy Plan.</li> <li>Updated science theme descriptions to reference more current focus areas.</li> <li>Changed EMP science theme description to Molecular Transformations (MT).</li> <li>Replaced previous graphic with one that includes MT.</li> </ul>	
	07/21/2014	<ul> <li>POC changed from Cady to Mueller.</li> <li>Updated number and description of Science Themes, including a new figure, to reflect changes as of the latest strategic planning process.</li> </ul>	
	10/01/2013	POC changed from Baer to Cady.	
	04/15/2010	<ul> <li>Level 1 approval changed from formal correspondence to informal email. Footnote added.</li> </ul>	
	02/19/2010	Updated Science Themes.	
	10/23/2009	Changed POC from Felmy to Baer.	
	03/10/2008	<ul> <li>Science Themes were last updated before the 2008 Call for Proposals.</li> </ul>	
	12/28/2005	<ul> <li>Original document = EMSL Action Plan 2005: WBS 1.02.02; Science Themes.</li> </ul>	
4.0 Definition of an EMSL User*	09/18/2023 08/20/2021	<ul> <li>Updated User and Proposal Statistics table.</li> <li>Minor update to include a current example of EMSL's user and proposal statistics.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	08/12/2020	<ul> <li>Updated/clarified the definition of an Onsite user</li> <li>Updated counting method for Remote users to include all approved team members with signed user agreements.</li> <li>Revised the definition of a Data user.</li> <li>Removed Resource Owners from user counts.</li> </ul>	
	10/01/2013	<ul> <li>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.</li> </ul>	
	08/11/2010	Clarified REMOTE User	

Section	Date	Change	Owner
	08/16/2010	<ul> <li>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.</li> </ul>	
	04/15/2010	Level 1 approval changed from formal correspondence to informal email.	
	09/27/2006	<ul> <li>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".</li> </ul>	
	10/03/2005	<ul> <li>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."</li> <li>Note – through FY05, all participants on active proposals were counted as users.</li> </ul>	
5.0 EMSL Proposal Types, Review Process, and Peer Review Criteria* (Note: the * only applies to the Peer Review Criteria)	09/18/2023	<ul> <li>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.</li> <li>Clarified differences in winter and summer cycles.</li> <li>Updated FICUS Research duration and clarified General proposal durations.</li> <li>Updated summer cycle call dates.</li> <li>Updated table 5.1 with clarified due dates and durations.</li> <li>Updated titles.</li> <li>Clarified allocation process.</li> <li>Added section to address project team access and project closure.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	06/25/2019	<ul> <li>Significant revision of proposal opportunities, names, and descriptions to more clearly distinguish annual calls vs. general proposal opportunities.</li> <li>Updated wording for Scientific Partner and EMSL Staff Proposals for clarification.</li> <li>Updated table 5.1 describing proposal types available.</li> <li>Updated wording throughout section 5.2 for clarification of processes.</li> <li>Updated mission criterion wording in section 5.3 based on Strategic Plan.</li> </ul>	
	01/30/2019	<ul> <li>Revised Rating Description Table in section 5.4 for better calibration among reviewers.</li> </ul>	
	03/08/2018	<ul> <li>Revised description of Criterion 3 in section 5.3 to align with BER's and EMSL's current mission.</li> </ul>	
	10/23/2017	<ul> <li>Minor wording changes for clarification of processes.</li> <li>EMSL Staff Time proposal duration changed from "up to one year" to "up to three years."</li> </ul>	
	08/15/2016	<ul> <li>Updated wording for Annual Call Proposals and introduced "FICUS" terminology.</li> <li>Updated information about General Proposal Cycles and changed frequency from twice to once per year.</li> <li>Added text to EMSL Staff Time Proposals section to call out additional 10% made available at the EMSL director's discretion.</li> <li>Updated wording for peer review criteria.</li> <li>Clarified wording in the rating descriptions table (Table 5.4).</li> </ul>	
	07/21/2014	<ul> <li>Updated Science Themes, per latest strategic planning process. Number of themes went from three to four with subsequent name changes and new descriptions.</li> <li>Updated figure showing overlap of the four themes.</li> </ul>	
	10/01/2013	<ul> <li>Restructured proposal types to simplify process for users.</li> <li>Restructured General proposals to utilize Proposal Review Panels and review cycles.</li> <li>Revised review criteria descriptions for improved calibration by review panels.</li> <li>Changed title of Science Panels to Proposal Review Panels for consistency with other user facilities.</li> </ul>	

Section	Date	Change	Owner
	03/15/2012	<ul> <li>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.</li> </ul>	
	01/27/2012	Updated Section 5.3, Criterion 2, Potential Considerations.	
	09/06/2011	<ul> <li>Changed title changed 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.</li> </ul>	
	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	<ul> <li>Changed title to reflect new proposal type.</li> <li>Added new section title: EMSL Proposal Evaluation Process.</li> <li>Replaced current criteria (1-5) and rating levels (Excellent – Poor) with revised verbiage and ratings for improved calibration and consistency among reviewers.</li> </ul>	
	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	<ul> <li>Same Review Criteria – new TRIM # created for future updates</li> </ul>	
	04/14/2006	<ul> <li>As of 4/14/2006, in general, all proposals started going through peer review using the 5 review criteria questions.</li> </ul>	
	10/06/2005	<ul> <li>Original document = EMSL Action Plan 2005: WBS 1.02.04; User Proposal Review Criteria.</li> </ul>	
6.0 Appeals	08/20/2021	<ul> <li>Minor wording changes to update titles and clarify process.</li> <li>POC changed from Law to Hatt.</li> </ul>	Alison Hatt
	06/25/2019	<ul> <li>Minor wording change in second paragraph for clarification.</li> </ul>	
	10/23/2017	<ul> <li>Minor wording change to remove reference to CSO.</li> </ul>	
	10/01/2013	<ul> <li>Section changed from 15.0 to 6.0.</li> <li>Minor revisions to clean up language referring to the different types of proposals.</li> <li>Updated USO email address.</li> </ul>	
	11/12/2009	<ul> <li>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.</li> <li>Established a deadline for submitting appeals.</li> <li>Clarified that Appeals Committee makes recommendation to EMSL director.</li> <li>Added that USO will coordinate appeals with committee.</li> </ul>	
	03/17/2009	<ul> <li>Revised text – increased the number of paragraphs (from 1-2 to 2-3), and decreased the response time (from 8 to 4 weeks).</li> </ul>	
	05/27/2008	Original – as posted on website	

Section	Date	Change	Owner
7.0 EMSL Scientific Partner Proposals	09/18/2023 08/20/2021	<ul> <li>Removed references to CDO and DoUS.</li> <li>Updated titles.</li> <li>Updated process to include CDO in the review and approval.</li> <li>Clarified requirements for LOI submission and removed page limit for full proposals.</li> <li>Updated lists of potential review panel members for both LOIs and full proposals.</li> <li>Clarified that progress updates may be written or verbal.</li> <li>Updated the extension process to specify that extensions will be made by the CSO and CDO.</li> <li>POC changed from Paša-Tolić to Teeguarden.</li> </ul>	Justin Teeguarden
	06/25/2019	<ul> <li>POC changed from Kelly to Paša-Tolić.</li> <li>Updated wording to refer to the EMSL Science &amp; Technology Committee (ESTC) as part of the proposal review.</li> <li>Other minor wording changes.</li> </ul>	
	10/23/2017	<ul> <li>POC changed from Koppenaal to Kelly.</li> <li>Wording changes to clarify process, update terminology, and remove reference to CSO.</li> </ul>	
	08/15/2016	<ul> <li>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.</li> </ul>	
	07/21/2014	<ul> <li>Minor wording changes to reflect alignment with EMSL and BER missions and clarify the requirement of progress reports.</li> </ul>	
	10/01/2013	<ul> <li>Section changed from 16.0 to 7.0.</li> </ul>	
	07/18/2011	<ul> <li>Updated members of review Panels to include Associate Director for Molecular Science Computing.</li> </ul>	
	04/07/2011	<ul> <li>Minor updates to change requirement from "2" to "1-2" pages.</li> <li>Added info regarding periodic reviews.</li> <li>Clarified proposal requirements.</li> </ul>	
	02/18/2010	<ul> <li>Changed title of "Partner Proposals" to "Scientific Partner Proposals" per PNNL Legal request. Added requirements for annual progress reports. Minor edits.</li> </ul>	
	03/04/2009	Original.	
8.0 EMSL Staff Time Policy	09/18/2023 08/20/2021	<ul> <li>Changed Capacity to Contracted Time and updated language about recording instrument usage. POC changes from Hatt to Washburn.</li> <li>Updated titles.</li> <li>Clarified submission and review procedures.</li> <li>Updated wording to specify that Staff Time proposals are for Environmental Molecular Sciences Division (EMSD) staff and joint appointees.</li> <li>Updated wording to clarify that EMSL will make a reasonable effort to rearrange schedules to accommodate external users' needs.</li> <li>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.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	06/25/2019	<ul><li>Removed outdated reference to Wiley Visiting Scientists.</li><li>Updated terminology for new position titles.</li></ul>	
	10/23/2017	<ul> <li>Minor wording change to remove reference to CSO.</li> </ul>	
	08/15/2016	<ul> <li>Updated policy to include additional 10% available to EMSL staff and others at the Director's discretion.</li> <li>Updated section references.</li> </ul>	

Section	Date	Change	Owner
	10/01/2013	<ul> <li>Section changed from 14.0 to 8.0.</li> <li>Modified to refer to proposals as "EMSL Staff Time" instead of "EMSL Staff 5%".</li> <li>Modified to include all Wiley investigators.</li> <li>Modified to include EMSL director and CSO as internal peer reviewers.</li> <li>Clarified that participants on Staff Time proposals and Intramural proposals are counted against staff usage totals.</li> <li>Clarified new usage types for "EMSL Staff Time, Planned" and "EMSL Staff Time, Unplanned".</li> </ul>	
	08/15/2011	<ul> <li>Revised purpose of proposals to remove limiting language that staff must be Pls or co-Pls and instead allow independent or collaborative research.</li> <li>Updated review process to match new workflow of proposals.</li> <li>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.</li> </ul>	
	02/24/2009	Original document.	
9.0 EMSL	09/18/2023	Updated program titled. Added information about FY23 addendums. Removed	Justin
Intramural Program	08/20/2021	<ul><li>references to CDO.</li><li>Complete revision to capture tiered proposal process and new review criteria.</li><li>POC changed from Hess to Teeguarden.</li></ul>	Teeguarden
	06/25/2019	<ul><li>POC changed from Bolton to Hess.</li><li>Updated terminology for new position titles.</li></ul>	
	03/08/2018	<ul> <li>POC changed from Liang to Bolton.</li> </ul>	
	10/23/2017	<ul> <li>POC changed from Koppenaal to Liang.</li> <li>Updated process for this program, including review and selection processes.</li> <li>Removed details of proposal requirements, as these can change yearly.</li> <li>Added review criteria specific to this program.</li> </ul>	
	06/29/2016	<ul> <li>POC changed from Mueller to Koppenaal.</li> <li>Revised to include new types of Intramural proposals and updated process for reviews, selection, and renewals.</li> </ul>	
	07/21/2014	<ul><li>POC changed from Cady to Mueller.</li><li>Minor wording change to clarify the duration of funding for Intramural proposals.</li></ul>	
	10/01/2013	<ul> <li>POC changed from Baer to Cady.</li> <li>Section changed from 23.0 to 9.0.</li> <li>Minor wording changes.</li> <li>Updated dates to reflect new start dates and due dates of proposals.</li> </ul>	
	08/20/2010	New section.	
10.0 Utilization Policy*	09/18/2023 08/20/2021	<ul> <li>Updated reporting to EMSL management. Responsibility for research resources changed to COO from director. Removed MOAs.</li> <li>Wording changes to clarify or update current processes and titles.</li> <li>Added text to allow other organizations' delegates to sign MOAs.</li> <li>Clarified that MOAs for co-purchased instruments will detail each organization's costs, including space chargeback.</li> <li>POC changed from Law to Hatt.</li> </ul>	Alison Hatt
	06/25/2019	Updated terminology for new position titles.	
	10/23/2017	<ul> <li>Minor wording change to remove reference to CSO.</li> </ul>	
	08/15/2016	<ul> <li>Minor wording changes to include "staff" proposals and PNNL's new records management system.</li> <li>Changed percent of time available for staff research, per increase approved in 2015 to 20%.</li> </ul>	

Section	Date	Change	Owner
	10/01/2013	<ul> <li>POC changed from Teller to Law.</li> <li>Section changed from 6.0 to 10.0.</li> <li>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".</li> <li>Rearranged layout to simplify references to MOA purchases.</li> </ul>	
	09/06/2011	<ul> <li>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.</li> </ul>	
	06/23/2010	<ul> <li>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.</li> </ul>	
	04/15/2010	<ul> <li>Level 1 approval changed from formal correspondence to informal email</li> </ul>	
	12/28/2005	<ul> <li>Original document = EMSL Action Plan 2005: WBS 1.02.02; EMSL Utilization Plan.</li> </ul>	
11.0 Usage Type Definitions	09/18/2023 08/20/2021	<ul> <li>Added information about scheduling tool, how usage data is reviewed, and contracting time. POC changed from Hatt to Washburn.</li> <li>Clarified deadlines for recording instrument usage.</li> <li>Clarified that core hours include planned outages.</li> <li>Clarified when "EMSL Staff Time, Unplanned" should be recorded.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	08/12/2020	<ul> <li>Updated usage type definitions and examples to match the changes to the user definition in section 4.0.</li> </ul>	
	10/23/2017	<ul> <li>Minor wording changes to add in review process prior to archival and to clarify some of the usage categories.</li> </ul>	
	08/15/2016	<ul> <li>Minor wording changes to update when data is archived and to match the Utilization Policy for amount of time available for staff.</li> <li>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.</li> </ul>	
	10/01/2013	<ul> <li>Section changed from 12.0 to 11.0.</li> <li>Shortened title.</li> <li>Added reporting details for major and non-major instruments.</li> <li>Changed "Instrument Custodian" to "Instrument Scientist".</li> <li>Expanded charging examples.</li> <li>Added description of Core hours.</li> <li>Changed "EMSL Staff 5%" to "EMSL Staff Time".</li> <li>Added new booking types ("EMSL Staff Time, Planned", "EMSL Staff Time, Unplanned", "Unavailable, Cancellation").</li> </ul>	
	02/09/2011	<ul> <li>Updated Usage Type Definitions to reflect reduced categories and requirements for comments.</li> <li>Reformatted section to mimic the appearance of categories on the Usage Breakdown report. Moved Section 11 to 12.2 and updated it.</li> </ul>	
	02/24/2009	<ul> <li>Revised to show EMSL 5% as new usage type. Note: Participants selecting EMSL 5% will not be counted as users as of FY09.</li> </ul>	
	10/31/2006	<ul> <li>Revised to clarify and give examples.</li> </ul>	
	06/2006	Original document in June 2006 Operations Manual	
<u>12.0 Data</u> <u>Management Policy</u>	08/20/2021	<ul> <li>Updated the open access data release policy and captured immediate release of field sensor data</li> <li>Updated links and titles.</li> <li>Second POC changed from Law to Hatt.</li> </ul>	Lee Ann McCue, Alison Hatt

Section	Date	Change	Owner
	02/28/2020	Minor changes to clarify the public release of data.	
	06/25/2019	<ul> <li>Almost full revision of section to update terminology, policies for open access data, and repository management.</li> </ul>	
	10/23/2017	<ul><li>Second POC changed from Cowley to McCue.</li><li>Full revision of section.</li></ul>	
	08/15/2016	<ul> <li>Wording changes to reflect the current state of development of MyEMSL and the open data repository.</li> </ul>	
	10/01/2013	New section.	
13.0 EMSL Software Development and Sustainability Policy	09/18/2023 08/20/2021	<ul> <li>Added CAM SAL to share responsibilities. Added section about software retirement. POC changed from McCue to Saripalli.</li> <li>Updated titles.</li> <li>Minor wording changes to clarify what should be included in the software plans and where documentation should be stored.</li> </ul>	Ratna Saripalli
	06/25/2019	New section.	
14.0 User Agreements	09/18/2023 08/20/2021	<ul> <li>Changed EMSL signatory to COO. POC changed from Hatt to Washburn.</li> <li>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.</li> <li>Updated title of the signatory for the contractor on the NPUA.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn
	06/25/2019	Section changed from 13.0 to 14.0.	
	07/21/2014	<ul> <li>Minor wording change under Article IX, paragraph D, to include SC requirement for "DOE Office of Science User Facility" in acknowledgment.</li> </ul>	
	03/21/2011	<ul> <li>New subsection added Section 13.4: Bilateral DOE Laboratory Utilization Agreement</li> </ul>	
	02/19/2010	<ul> <li>Changed section title from "non-proprietary use agreements and appendices" to "User Agreements". Section now includes NPUA, PUA – Full Advance, and PUA – Partial Advance.</li> <li>Added intro to document roll-out of electronic signature process.</li> <li>Replaced previous NPUA form with new User Agreement approved for use by DOE in FY2009 and mandatory by March 31, 2010.</li> <li>In FY2009, DOE implemented new user agreements, including one that can be used for proprietary research requests (PUAs).</li> </ul>	
	07/12/2006	<ul> <li>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.</li> </ul>	
	10/01/1999	Appendix A	
	10/01/1998	<ul> <li>NPUA</li> <li>Appendix C</li> </ul>	
15.0 Charging Guidance for EMSL User Facility Staff	09/18/2023 08/20/2021	<ul> <li>Clarification added to Suport Activities. POC changed from Haulk to Johns.</li> <li>Wording changes to clarify the support activities charged to the EMSL project and to update titles.</li> <li>Removed section referring to resources in building 3410 (RadEMSL).</li> <li>POC changed from Swan to Haulk.</li> </ul>	Audrey Johns
	06/25/2019	<ul> <li>Updating charging guidance for Limited Scope projects.</li> <li>Updated section referring to per diem rates to reference the GSA per diem website vs. yearly update of rates within document.</li> <li>Section changed from 14.0 to 15.0.</li> </ul>	

Section	Date	Change	Owner
	01/30/2019	Updated per diem rates for current fiscal year.	
	10/23/2017	<ul><li>POC changed from Bettinson to Swan.</li><li>Updated fiscal year reference for per diem rates.</li></ul>	
	08/15/2016	<ul> <li>POC changed from Avery to Bettinson.</li> <li>Added section 14.2.5 to reflect that EMSL is sharing space cost for NMR lab in 331.</li> <li>Clarified that users are required to pay for "above-standard" costs for EMSL staff effort in section 14.3.3.</li> <li>Updated per diem rates for FY16.</li> <li>Minor wording change to indicate meal costs for local interview candidates are unallowable.</li> <li>Updated reference links.</li> </ul>	
	10/01/2013	<ul> <li>POC changed from Smith to Avery.</li> <li>Section changed from 9.0 to 14.0.</li> <li>Updated per diem year and rates so policy reflects current rates published by GSA.</li> </ul>	
	08/11/2011	Removed redundancy of User Definition.	
	07/07/2011	<ul> <li>Changed Capability Steward to Capability Lead.</li> <li>Changed Instrument Time Allocation Committee to Resource Allocation Committee (RAC).</li> <li>Added the EMSL and EED joint occupancy and collaboration in PSF 3410 building.</li> <li>Added EMSL unallowable charging guidance.</li> </ul>	
	06/01/2009	<ul> <li>Minor update to change "facility" to "capability" and "facility lead" to "capability steward"; deleted sentence; corrected the definition of user.</li> </ul>	
	02/28/2007	Significantly updated.	
	10/06/2005	<ul> <li>Original document = Appendix C of the 2006 Operations Manual</li> </ul>	
16.0 EMSL Space Policy	09/18/2023 08/20/2021	<ul> <li>Updated language describing EMSL mission. Added HDI link.</li> <li>Wording changes to update titles and clarify that the COO is the approver of lab and office space allocations.</li> <li>Updated details for requesting lab space to outline space chargeback.</li> <li>POC changed from Hartzell to Patello.</li> </ul>	Gert Patello
	06/25/2019	<ul> <li>Revised Mission statement in section 15.1 to match revised Mission statement in section 2.0.</li> <li>Section changed from 15.0 to 16.0</li> </ul>	
	10/23/2017	<ul><li>Minor wording changes.</li><li>Updated EMSL mission in section 15.1.</li></ul>	
	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	<ul> <li>Last updated for the Operations Manual (Feb 2009). No significant changes, mainly updating terminology.</li> </ul>	
	05/2006	Original document = Staff Resource Guide May 2006.	
19.0 Engagement with DOE and Laboratory Management	09/18/2023 08/20/2021	<ul> <li>POC chnaged from Hatt to Washburn.</li> <li>Updated list of reports to reflect current owners.</li> <li>Removed planned operating hour report.</li> <li>POC changed from Law to Hatt.</li> </ul>	Rick Washburn

Section	Date	Change	Owner
	02/28/2020	<ul> <li>Updated list to include additional requirement for reporting EMSL's quarterly operating hours to Battelle.</li> </ul>	
	06/25/2019	<ul> <li>Section changed from 18.0 to 19.0.</li> <li>Updated list of formal reports provided to BER and PNNL.</li> <li>Updated due date for quarterly reports.</li> </ul>	
	10/23/2017	<ul> <li>POC changed from Tingey to Law.</li> <li>Updated "Responsible Person" in table for Operating Hours, EMSL Dashboard, and Planned Operating Hours.</li> </ul>	
	08/15/2016	<ul> <li>Changed section heading.</li> <li>Minor wording changes in description of what is sent and to whom.</li> <li>Updated table 18.1 to include all major reports sent to BER, DOE, PNSO, and PNNL, along with the due date for each.</li> </ul>	
	07/21/2014	<ul> <li>Removed duplicate report listed in table 22-1.</li> <li>Removed report that is no longer provided annually.</li> <li>Minor wording changes for clarification.</li> </ul>	
	10/01/2013	<ul><li>POC changed from Foster-Mills to Tingey.</li><li>Section changed from 22.0 to 18.0.</li></ul>	
	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.	
20.0 Science and	09/18/2021	Added information about involvement of UEC chair, term length, virtual meetings,	Douglas
Technology Advisory Committee Charter*	08/20/2021	<ul><li>and role of CSO.</li><li>New section to outline the roles and responsibilities of new advisory committee.</li></ul>	Mans
21.0 User Organization and <u>User Executive</u> <u>Committee Charter*</u>	09/18/2023 08/20/2021	<ul> <li>Changed section title. Removed User Organization section. Updated description of UEC, responsibilities, membership, and elections. Updated meeting information.</li> <li>Section changed from 20.0 to 21.0.</li> <li>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.</li> <li>Added new section to better outline the UEC leadership responsibilities of the chair and vice chair.</li> <li>Removed the responsibility of overseeing the MT Thomas Award.</li> <li>Removed the users' forum as part of the annual Integration Meeting.</li> <li>Added language regarding conflicts of interest on the committee.</li> <li>Wording updates for clarification and to update titles.</li> </ul>	Douglas Mans
	06/25/2019	POC changed from Bolton to Mans.	
	03/08/2018	POC changed from Liang to Bolton.	
	10/23/2017	<ul> <li>Almost complete re-write of Charter, including         <ul> <li>Term limits imposed</li> <li>Vice Chair responsibilities added</li> <li>Committee responsibilities revised</li> </ul> </li> </ul>	
	08/15/2016	<ul><li>POC changed from Campbell to Liang.</li><li>Minor wording change to remove "ex officio" seat on SAC.</li></ul>	
	07/21/2014	<ul> <li>Changed representation of the UEC to "science theme" instead of "capability".</li> <li>Removed duplicative sentence regarding the chair and vice chair.</li> <li>Added industry representation</li> </ul>	
	10/01/2013	• Section changed from 8.0 to 20.0.	

Section	Date	Change	Owner
	03/31/2011	<ul> <li>Changed title from "User Advisory Committee Charter" to "User Executive Committee Charter".</li> <li>Updating to "at least 14 members".</li> <li>All parties subscribed to EMSL's listserve will be eligible to vote.</li> <li>All members are expected to members w/in the last 5 years.</li> <li>The Chair and EMSL director may appoint members directly if gaps in expertise are identified following election results.</li> </ul>	
	05/10/2010	<ul> <li>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.</li> </ul>	
	04/15/2010	<ul> <li>Level 1 approval changed from formal correspondence to informal email.</li> </ul>	
	10/06/2005	<ul> <li>Original document = EMSL Action Plan 2005: WBS 1.02.04; Charters and Committees.</li> </ul>	
Change Control	08/20/2021	Updated titles of signatories.	Courtney
<u>Request Form</u>	06/25/2019	<ul> <li>Updated terminology.</li> <li>Removed line for HPRM (ERecords) number – individual sections are not tracked separately in official records.</li> </ul>	Carpenter
	08/15/2016	<ul> <li>Updated form to change "TRIM" to "HPRM."</li> </ul>	
	10/01/2013	<ul> <li>POC changed from Foster-Mills to Carpenter.</li> <li>Updated form to simplify information needed and to require electronic signatures.</li> </ul>	
	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 08/20/2021 06/25/2019 10/23/2017 08/15/2016 07/21/2014 10/01/2013 01/25/2012	<ul> <li>Section deleted. Now included in Instrument Lifecycle section.</li> <li>Wording changes to update titles and to reflect current practices for transferred instrument ownership.</li> <li>POC changed from Paša-Tolić to Patello.</li> <li>POC changed from Kelly to Paša-Tolić.</li> <li>Updated section wording with new terminology.</li> <li>Minor wording changes to clarify process.</li> <li>Section changed from 17.0 to 18.0.</li> <li>POC changed from Koppenaal to Kelly.</li> <li>Removed reference to CSO and updated terminology for CTO ("Lead Technologist").</li> <li>Minor wording to clarify the definition of divestment or "sunsetting."</li> <li>Updated wording to clarify "divestment or 'sunsetting" and clarify EMSL's divestment process.</li> <li>Section changed from 24.0 to 17.0.</li> <li>Minor changes and updates to Divestiture terminology and procedures.</li> <li>New section.</li> </ul>	Removed in Rev. 10

Section	Date	Change	Deleted Info
Policy for Requesting EMSL Capital Equipment Funds (previously section 18.0)	09/18/2023	<ul> <li>Section deleted. Information now included under Instrument Lifecycle Management</li> </ul>	Removed in Rev. 10
	08/20/2021	<ul> <li>Updated requirements to include new quad chart used to request capital equipment.</li> </ul>	
	06/25/2019	<ul> <li>Updated process for reviewing requests and the parties involved.</li> <li>Updated process used if additional funds are required.</li> <li>Removed the Capital Equipment Request Form, which is no longer used.</li> <li>POC changed from Paša-Tolić to Teeguarden.</li> <li>POC changed from Kelly to Paša-Tolić.</li> <li>Updated section wording and Capital Equipment Request form with new terminology.</li> <li>Minor wording changes to clarify process.</li> <li>Section changed from 16.0 to 17.0.</li> </ul>	
	10/23/2017	<ul> <li>POC changed from Koppenaal to Kelly.</li> <li>Removed reference to CSO and updated terminology for CTO ("Lead</li> </ul>	
	08/15/2016	Technologist"). <ul> <li>Minor change to remove EMSL Chief Operating Officer from the capital committee</li> </ul>	
	07/21/2014	list. • Minor wording changes. • Updated Capital Equipment Request form.	
	10/01/2013	<ul> <li>Section changed from 21.0 to 16.0.</li> <li>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.</li> </ul>	
	05/03/2012	Updated form (removed reviewers and changed approvers to CTO, and COO.	
	03/20/2012	Minor changes to clarify text.	
	07/22/2011	Updated form	
	03/01/2011	<ul> <li>Made minor changes to clarify text. Added EMSL Business Manager to committee list.</li> </ul>	
	02/21/2011	Updated form.	
	07/29/2010	Updated form.	
	03/04/2010	Updated form.	
	10/21/2009	Original.	
Wiley Visiting Scientist Program (previously section 21.0)	10/01/2018	<ul> <li>Section deleted. Complete revision of the program, policy, and requirements; removing old guidance and replacing with new program in Section 21.</li> </ul>	Removed in Rev. 6.04
	10/23/2017	<ul><li>POC changed from Paša-Tolić to Bolton.</li><li>Removed reference to CSO.</li></ul>	0.04
	08/15/2016	<ul> <li>POC changed from Mueller to Paša-Tolić.</li> <li>Updated minimum duration for long-term visits from 6 weeks to 6 months.</li> <li>Added communication platforms in which partnerships will be acknowledged.</li> <li>Clarified that evaluations will be made by the EMSL Leadership Team and requires EMSL director approval.</li> </ul>	
	07/21/2014	POC changed from Cady to Mueller.	

Section	Date	Change	Deleted Info
	10/01/2013	<ul> <li>POC changed from Baer to Cady.</li> <li>Section changed from 17.0 to 21.0.</li> <li>Minor wording changes.</li> </ul>	
	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	<ul> <li>Original – as posted on EMSL website.</li> </ul>	
Wiley Research Fellow Program	10/01/2018	<ul> <li>Section deleted. Complete revision of the program, policy, and requirements; removing old guidance and replacing with new program in Section 21.</li> </ul>	Removed in Rev. 6.04
(previously section 22.0)	10/23/2017	<ul><li>POC changed from Paša-Tolić to Bolton.</li><li>Removed reference to CSO.</li></ul>	0.04
	08/15/2016	<ul> <li>POC changed from Mueller to Paša-Tolić.</li> <li>Added communication platforms in which partnerships will be acknowledged.</li> <li>Clarified that evaluations will be made by the EMSL Leadership Team and requires EMSL director approval.</li> </ul>	
	07/21/2014	POC changed from Cady to Mueller.	
	10/01/2013	<ul><li>POC changed from Baer to Cady.</li><li>Section changed from 18.0 to 22.0.</li><li>Minor wording changes.</li></ul>	
	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	<ul> <li>Original – as posted on EMSL website.</li> </ul>	
Science Advisory	06/24/2019	Removed section for now, as this committee does not currently exist.	Removed
Committee Charter* (previously section	03/08/2018	POC changed from Liang to Bolton	in Rev. 7.00
19.0)	10/01/2013	<ul> <li>Section changed from 7.0 to 19.0.</li> <li>Updated "Terms of Service".</li> <li>Removed "Self-Assessment" section.</li> <li>Updated wording referring to UEC.</li> </ul>	
	04/15/2010	<ul> <li>Level 1 approval changed from formal correspondence to informal email.</li> </ul>	
	12/30/2005	<ul> <li>Original document = EMSL Action Plan 2005: WBS 1.02.04; Charters and Committees.</li> </ul>	
William R. Wiley	08/20/2021	Section deleted; program will be re-evaluated.	Removed
Research Fellow Program (previously section	06/25/2019	POC changed from Bolton to Hess.	in Rev 8.00
21.0)	01/30/2019	Complete revision of the Wiley program, policy, and requirements.	
Wiley Postdoctoral	08/20/2021	Section deleted; program will be re-evaluated.	Removed
Fellowship (previously section	06/25/2019	POC changed from Bolton to Hess.	in Rev. 8.00
22.0)	01/30/2019	Section changed from 23.0 to 22.0.	
	10/23/2017	<ul><li>POC changed from Paša-Tolić to Bolton.</li><li>Minor wording changes.</li></ul>	
	08/15/2016	<ul> <li>POC changed from Mueller to Paša-Tolić.</li> <li>Minor wording change to update with call for applications opens each year.</li> </ul>	

Section	Date	Change	Deleted Info
	07/21/2014	POC changed from Cady to Mueller.	
	10/01/2013	<ul> <li>POC changed from Teller to Cady.</li> <li>Section changed from 19.0 to 23.0.</li> <li>Updated salary section to reflect current practices.</li> </ul>	
	06/17/2011	• Slight change in 1 <sup>st</sup> paragraph.	
	02/09/2011	Changed dates to be generic for any given year.	
	10/06/2009	Updated for FY10 Call.	
	04/27/2009	<ul> <li>Original – as posted on EMSL website.</li> </ul>	
MT Thomas Award	08/20/2021	Section deleted. Other opportunities will be explored in the future.	Removed in Rev. 8.00
for Outstanding Postdoctoral	02/28/2020	Complete revision of section.	
Achievement (previously section	06/25/2019	POC changed from Bolton to Mans.	
23.0)	01/30/2019	Section changed from 24.0 to 23.0.	
	03/19/2018	<ul> <li>Updated evaluation process to revise the selection committee. Nominations will be reviewed by EMSL's User Executive Committee.</li> </ul>	
	10/23/2017	<ul><li>POC changed from Paša-Tolić to Bolton.</li><li>Updates to nature, rules, and eligibility of award.</li></ul>	
	08/15/2016	<ul> <li>POC changed from Mueller to Paša-Tolić.</li> <li>Minor wording changes to keep Selection Committee Chair generic and remove Robby Robinson.</li> </ul>	
	07/21/2014	POC changed from Cady to Mueller.	
	10/01/2013	<ul> <li>POC changed from Baer to Cady.</li> <li>Section changed from 20.0 to 24.0.</li> <li>Updated MT Thomas language and dates to reflect a universal process instead of having to update yearly.</li> <li>Corrected grammatical errors.</li> </ul>	
	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	<ul> <li>Original – as posted on EMSL website.</li> </ul>	

# 21.3 EMSL Policy Change Request Form

EMSL OPERATIONS MANUAL Change Request Form		020
1. Change Request Number (filled in by Ops. Manual Steward)	4. Impact	
	Correction	
2. Request Date	Update/revision	
	Create new section	
3. Requestor	Delete section	
	Other:	
5. Title of Affected Section (if new, provide title)		
		_
6. Brief description of change and reason for change		
7. File name(s)		
8. EMSL Approvals		
By entering your name in the field below, you are indicating your approval of the	e changes listed above.	
EMSL Chief Operating Officer Date EMSL	Director Date	
9. Client Approvals		
Is DOE/PNSO approval required?  Yes No Date of the second	of DOE/PNSO approval:	
10. Disposition (filled in by Ops. Manual Steward)		
Version of Ops. Manual affected: Date	e new version posted:	_2
Version of new Ops. Manual: Da	ate email sent to staff:	-