Battelle Pacific Northwest Division
as operator of Pacific Northwest National Laboratory (PNNL) for the DOE
Request for Proposal 746072 Amendment 1
Statement of Work
Automated Soil Analysis Platform
~~April 11, 2023~~June 8, 2023

LIST OF TERMS

AD	air dried
ASAP	automated soil analysis and processing system
EMSL	Environmental Molecular Science Laboratory
FTICR	Fourier transform ion cyclotron resonance
LIMS	laboratory information management system
MCE	mixed cellulose ester
NEXUS	Network for the Execution of User Science
OS	original soil
OMA	organic matter analysis
PNNL	Pacific Northwest National Laboratory
PES	polyethersulfone
SBS	Society for Biomolecular Screening
SOW	statement of work
SPE	Solid Phase Extraction
TOR2	Technical Oversight Representative-2
UPW	ultrapure water

STATEMENT OF WORK FOR THE AUTOMATED SOIL ANALYSIS AND PROCESSING (ASAP) SYSTEM

1.0 INTRODUCTION

Battelle Pacific Northwest Division, as operator of Pacific Northwest National Laboratory (PNNL), manages the Environmental Molecular Sciences Laboratory (EMSL) for the Department of Energy. This scope requires the development and provision of an automated soil analysis and processing (ASAP) system to support ongoing research at EMSL.

The completed automated system will replace the collection of spatially isolated, human-administered systems used to conduct the suite of analyses that comprise the organic matter capability. The ASAP system must add modularity, expandability, robotic liquid handling, robotic sample handling, sample tracking, remote monitoring and scheduling, and comprehensive metadata and data collection through integration of scheduling software with EMSL's Network for the Execution of User Science (NEXUS) laboratory information management system (LIMS).

This Statement of work requires designing and building a system that is capable of processing 32 samples per 8-hour workday when completed, but must possess the capability to expand and increase throughput to 80 samples per 8-hour workday. Throughout this document, the ASAP system that processes 32 samples per day is referred to as "Phase I". This system is the subject of this scope of work. The ASAP system that would process 80 samples per day is referred to as "Phase II" and is NOT the subject of this scope of work. The Phase II throughput is presented solely to assure that the Phase I system is designed with the ability to be expanded to handle 80 samples per day.

Note: throughput benchmarking shall apply to the "sandy loam" type model soil defined in section 9.3 with the understanding that due to natural variations in real soil samples, throughput will also vary.

The completed ASAP system must include components that perform the following five actions.

1. Aliquot and weigh: Receive soil samples, aliquot and weigh multiple subsamples into mixture of 50 mL and 15 mL tubes with the numbers selected by the user at runtime and move a subset of the samples to the solvent extractions step (Step 2, next) and the remainder to racks for processing off of the system.

2. Solvent extraction and filter: Conduct extractions on each soil sample, to include solvent addition, capping, rotating or gentle horizontal shaking, centrifugation, and extractant filtration through a 0.22 micron hydrophilic filter, e.g. mixed cellulose esters (MCE), polyethersulfone (PES), or similar.

3. Acidification: acidification with HCL, pH measurement, and adjustment if necessary (with final pH less than or equal to pH 2).

4. Solid-phase extraction: solid-phase extraction and movement to MicroSolv tubes, racking (mass spectrometer autosampler rack), and movement to a cooled storage unit.

5. Control software and LIMS integration: execute user-developed experimental designs, track samples in the system by barcode, collect process and related sample metadata, and

transfer/interface with EMSL's LIMS system, NEXUS. Thus, the completed ASAP system must include a software platform to schedule and implement the automated workflow (workflow scheduling and management software) and interact with NEXUS.

Technical performance specifications, throughput, and other requirements are described in detail in Section 4.0.

2.0 SCOPE OF WORK

Work under this statement of work (SOW) shall consist of the following tasks.

2.1 TASK 1: REQUIREMENTS REVIEW

Task 1 consists of (1) reviewing and receiving concurrence on a final set of ASAP system requirements. Performance requirements delineated in this statement of work (SOW) reflect Battelle's scientific and technical experience with the human-driven and off-the-shelf instrument aspects of the proposed workflow, but not the technical expertise in automation offered by the contractor.

- Contractor will review the site specifications provided in Attachment 9.1.1 and confirm that the site meets all requirements for the ASAP system or detail site changes that EMSL must implement before delivery of the ASAP system.
- Contractor will meet remotely with the EMSL ASAP system team to review and discuss all system and component technical requirements and potential system components identified in the SOW before the start of Task 2.2 (Design Acceptance). This includes the workflow control software. Requests for additional information will be made in writing, for example by email. A total of 8 hours of meeting time, across 2-4 meetings is expected to complete the review of all technical requirements.
- The total time to hand off a working system is not to exceed 12 months.

2.2 TASK 2: DESIGN REVIEW

Task 2 consists of a series of meetings/presentations/deliverables constituting a staged review of the component and system design culminating in final concurrence to build the system. Review will occur at logical milestones, for example at the 25%, 50%, 75%, and 100% conceptual design stages or at other more appropriate milestones proposed by the contractor and mutually agreed upon in Task 1. Design reviews will examine at least the following: (1) meets component/system requirements, (2) safety during operations, (3) applicability to soil types ranging from dry and sandy, to moist and clay-rich, but each having particles sizes no greater than the sieve size of 4mm (Example soils will be provided in bulk by EMSL), (4) throughput limitations, (5) expandability/modularity, (6) durability/maintenance needs, and (7) consumable use/recycling/costs.

- Contractor will propose a schedule for a staged review of the conceptual design of the overall system and system components.
- Contractor will present the design at each agreed-upon stage, with sufficient detail for Battelle to (1) determine if the design meets all design criteria/requirements, (2) identify safety and other potential

operational challenges, (3) assess applicability to the range of soil types described above, (4) identify any throughput limitations and assess the potential for expanding throughput and adding modules, (5) evaluate maintenance and operation costs, (6) assess facility needs and safe operations, and (7) assess computer, network, and information technology needs.

- Design shall include details related to chemical compatibility of components and mitigation & maintenance strategy to avoid damage/replace wear parts associated with the chemicals that will be used on the system as shown in section 9.2.
- Design shall include all necessary hardware access and software utilities so that PNNL staff or contractors can perform calibration and/or verification activities on balances, pH meters, and liquid handlers integrated in the system as needed in the future.
- Design shall include error recovery and tracking such as:
    - Software prompts to guide operators through common errors that can be recovered from during a run.
    - Error tracking in the log/exported data with the affected samples, e.g over/under fill and by how much, and processing time exceeded and by how much.

2.3 TASK 3: SOFTWARE INSTALLATION AND LIMS CONNECTION

Task 3 consists of installing workflow control software at PNNL, including connections to EMSL's LIMS, NEXUS, validation of the installation, and initial training in its use before the ASAP system is delivered. This task is to enable PNNL to complete integration of the software with its systems ahead of delivery of the ASAP system's physical components, train EMSL ASAP system team staff in its use, and pilot use of the software using non-automated workflows in preparation for delivery of the ASAP system.

- Contractor shall provide the software that connects from the ASAP system workflow control software and EMSL's LIMS, including troubleshooting, (with input from EMSL subject matter experts) and shall verify it meets operational and technical requirements.
- Contractor shall provide all documentation and software options necessary to establish a data connection between the ASAP system software and EMSL's LIMS in order to pull sample ID information from the LIMS to the system at the beginning of a run and send process metadata from the system to LIMS at the end of a run.
- Contractor shall provide a user-friendly software interface to run the capabilities which can be integrated with most of upstream and downstream products (commercial and custom) for facilitating closed-loop experimental planning and execution, and analytics into their planning. This capability package shall be successfully incorporated into existing EMSL data management packages (EMSL's Laboratory Information Management System (LIMS), NEXUS in consultation with experts in EMSL) for data transfer, manipulation, analysis, and storage.
- Contractor shall provide a complete set of industry standard training materials for the workflow control software.

- Contractor shall train EMSL staff on the use of the workflow control software for experimental design/set up, sample tracking, metadata collection, new device integration, trouble shooting, and EMSL's LIMS interactions.
- Contractor will deliver a report verifying that the workflow control software meets the subset of technical requirements detailed in this SOW.

2.4 TASK 4: OFF-SITE ASSEMBLY AND FACTORY ACCEPTANCE TESTING

Task 4 consists of component and materials purchases, off-site assembly, and factory acceptance testing of the full automated system. The contractor will assemble the complete workflow in their facility and verify with PNNL representatives on site that all design requirements and performance metrics are satisfied. Specifically:

- Contractor will complete assembly of the ASAP system in their facility and integrate the system with the workflow control software.
- Contractor will implement the automated soils processing protocol and verify its performance, e.g., all performance metrics and other specifications are met, with EMSL ASAP team representatives on site. This is referred to as factory acceptance testing. Specifically:
  - Throughput of the full process using the "sandy loam" soil type (see section 9.3) for weighing and aliquoting, and surrogates for all other reagents (See 9.2 for surrogates).
  - Demonstrating accurate weighing and aliquoting the "high clay content" and "sandy loam" soil types (see section 9.3).
  - Demonstration of other design requirements as outlined in section 2.2.
  - ~~Factory acceptance testing includes benchmarking the results of specific molecular analyses conducted by EMSL on soil extracts produced by the ASAP system on the contractor's site by implementing the processes defined in this SOW. Benchmarking would compare the analysis results of contractor's samples to those produced by the EMSL team. Analyses will be conducted by the EMSL ASAP team. Benchmarking would include:~~
    - ~~PNNL representatives from EMSL will select three soil samples (high clay content soil, agricultural soil, and peat~~ (section 9.3) ~~) and ship them to the contractor for processing into three replicates each for benchmarking. These will be referred to as "Contractor Samples." EMSL staff will process the same soil through conventional means at EMSL. These will be referred to as "Benchmark Samples." The products of these two processes will be compared on EMSL analytical instruments to verify the absence of process related contaminants and the quality and quantity of carbon in the samples. A common Quality Control (QC) sample (Suwanee River Fulvic Acid II, SRFA) will also be analyzed at EMSL. Process (solvent only) blanks will also be prepared and compared. All solvents and materials used will be of equivalent grade. The specific analyses and criteria are:~~
      - ~~Metal contaminants: Confirm the absence of process-related metals in all solvent blanks by inductively coupled mass spectrometry. Criteria: absence of process-related metals.~~

        - ~~Metal contaminants: Confirm the absence of process-related metals from soils by inductively coupled mass spectrometry. Criteria: same mean and standard deviation for metal concentrations as those measured in EMSL-processed soils.~~
        - ~~Total organic carbon: Confirm similar efficiency of extraction: Criteria: 90–110% of the EMSL benchmark sample(s).~~
        - ~~Organic and inorganic contaminants: confirm the absence of organic and inorganic process-related contaminants by Fourier transform ion cyclotron resonance mass spectrometry (FTICR MS) and liquid-state nuclear magnetic resonance for all solvent blanks and test soil samples. Criteria: subject matter expert assessment of minimal new peaks related to plastic contamination (peak patterns associated with plastic polymer contamination), including that no process-related contaminants preclude conventional analysis due to signal overlap or ionization suppression.~~
        - ~~Organic matter: Confirm that the total number of FTICR MS peaks/features detected and assigned. Criteria: the number of peaks, number of feature assignments, and their ratio should be within 20% of the corresponding EMSL benchmark sample(s).~~
    - Contractor will provide the PNNL EMSL ASAP team with a formal report detailing the factory acceptance testing before executing Task 5.

2.5 TASK 5: DELIVERY, INSTALLATION, AND SOFTWARE/LIMS INTEGRATION

Task 5 consists of the delivery of all system components to EMSL, their installation on site, their physical integration, individual system testing, and integration with the workflow control software.

- Contractor will coordinate delivery of all system components to PNNL and their placement in the ASAP system laboratory in coordination with the EMSL ASAP team.
- Working with PNNL's Technical Oversight Representative (TOR) and Subject Matter Expert, the contractor will complete the re-assembly/installation and integration of the physical system components.
- Working with PNNL's Technical Oversight Representative (TOR) and Subject Matter Expert, the contractor will complete integration of the physical system with the workflow control software.
- Working with PNNL's Technical Oversight Representative (TOR) and Subject Matter Expert, the contractor will complete integration of the system with EMSL's LIMS system and assure the LIMS, workflow control, and physical systems function together and meet all appropriate performance requirements.

2.6 TASK 6: SYSTEM COMMISSIONING AND SITE ACCEPTANCE TESTING

Task 6 involves the final commissioning of the ASAP system. This is referred to as site acceptance testing. The task will involve verification that the fully installed and operating system meets all system performance and other requirements specified in this SOW. These requirements would have been a part of the factory acceptance testing conducted in Task 4. A key requirement at this stage is that EMSL staff can operate, troubleshoot, and maintain the ASAP system over time. Training in operations, troubleshooting, and maintenance is therefore a part of Task 6.

- Contractor will establish that the ASAP system meets all system performance and other requirements specified in SOW Task 4 (factory acceptance testing).
- Training for up to 4 EMSL staff shall include, at a minimum:
    - How to safely operate the system and perform user-maintenance tasks.
    - How to adjust the process variables that may be necessary to change during performance validation.
    - How to resolve common errors that can be safely resolved by users.
- Contractor will provide the EMSL ASAP team with a formal report detailing the outcome of the site~~factory~~ acceptance testing and training.

2.7 TASK 7: TECHNICAL SUPPORT

Task 7 involves providing remote and/or on-site technical support for 1 year after installation and commissioning of the ASAP system to address technical or software issues that arise during operations and to provide additional training as needed.

- Contractor must provide 1 year of technical support and training.
- Contractor must provide applications support while EMSL ASAP team performs process validation post-installation.

3.0 (RESERVED)

4.0 TECHNICAL REQUIREMENTS

4.1 OVERALL SYSTEM PERFORMANCE SPECIFICATION AND REQUIREMENTS

The completed ASAP system must include components that perform the following five actions. (1) Aliquot and weigh: Receive 32 soil samples ranging from 500–700 g, aliquot and weigh up to 17 subsamples into 50 and 15 mL tubes with the exact numbers entered by the user at runtime, and move up to 6 (exact number provided by the user at runtime) of the weighed samples to the solvent extractions step (Step 2, next) and the remainder to racks for the user to remove from the system. (2) Solvent extraction and filter: Conduct extractions on each soil sample, to include solvent addition, capping, rotating or gentle horizontal shaking, centrifugation, and extractant filtration through a 0.22 micron hydrophilic filter, e.g. MCE, PES, or similar. (3) Acidification: acidification with HCL, pH measurement, and adjustment if necessary (less than or equal to pH 2). (4) Solid-phase extraction: solid-phase extraction and movement to microSolve tubes, racking (mass spectrometer autosampler rack), and movement to a cooled storage unit. (5) Control software and LIMS integration: execute user-developed experimental designs, track samples in the system by barcode, collect process and related sample metadata, and transfer/interface with EMSL's LIMS system, NEXUS. Thus, the completed ASAP system must include a software platform to schedule and implement the automated workflow (workflow scheduling and management software) and interact with NEXUS.

The technical specifications are provided in the following six sections: Aliquot and Weigh (Section 4.2), Solvent Extraction (Section 4.3), Acidification (Section 4.4), Solid-Phase Extraction (Section 4.5), and Control Software and LIMS Integration (Section 4.6). Section 4.7 covers requirements for technical support. Key performance parameters are presented in Table 4.1. Usually, the requirements are embedded in a description of the laboratory method—as it stands at this point in development—to provide the vendor experimental and scientific context.

In addition to the device-specific requirements listed below, individual devices must meet the following requirements:

- Capable of being loaded by a robotic arm.
- Capable of being controlled via external software e.g. via an API.
- Ensures operator safety by including appropriate engineering controls, signage, training, and documentation.
- Reprogrammable to enable new protocols with existing hardware, and able to be upgraded with new hardware.
- Reliable—Downtime or sample loss of not more than 5% on a 4 week rolling average.
- Easy access for user maintenance activities.

4.1.1 Planning for future expansion

In the materials below, Phase I refers to the ASAP system built to meet the requirements of this SOW. Phase II refers to a later expansion of the ASAP system which will include one or more of the following:

- The same process run at higher throughput of 80 samples per 8 hour workday.
- Similar processes run with different parameters, e.g. different volumes, numbers of aliquots, different types of labware for processing and/or output, etc.
- Different processes that can be run with the same hardware or with minor upgrades.

Though these expansions are not part of this SOW, the proposed system must demonstrate that it has the capability (from a space and component expansion standpoint) be able to be upgraded. To allow for future expansion, the design required by this SOW must identify any extra space, software hooks, hardware access, etc. as necessary.

Table 4.1: Key performance parameters for the ASAP system

Key Performance Parameter	System Expectations
Modularity and Expandability	Key instruments and devices can be added to the workflow in the future. Liquid handling or other devices added to increase throughput.
Connectivity to Unique Instruments	Driver development and connectivity through APIs is straightforward through developer kits. No software or

	hardware-specific barriers to integration with uncommon or newly engineered instruments exist. Connectivity to non-benchtop instruments possible.
Software Connectivity and Security	Workflow management software can support user authentication, connect with EMSL's LIMS system, and be operated securely and remotely. Software can accept the design of experiment/sample structure information from the LIMS system.
Sample Labeling and Tracking	System registers samples at multiple steps in the workflow by reading barcodes.
Data and Metadata Capture and Transfer	System collects instrument performance metrics, sample treatments, and analytics results and transfers the information to EMSL's LIMS system compatible with EMSL metadata schema and protocols.
Integration with Machine Learning Algorithms	Scheduling software can interface with analytic software to support real-time decisions regarding sample processing or analyses.
Data and Systems Security	Application and network security includes role-based access control and/or integration with existing PNNL user management systems. API, web API, RPC, and other network communications support encryption. Applications support logging for auditing purposes.
Sample Platforms	Supports multiple tube formats: 15 mL, 50 mL, MicroSolv tubes, and modest changes in the dimensions of those tube formats.

4.2 ALIQUOT AND WEIGH COMPONENT

This component shall meet the following performance requirements:

- Scheduling and workflow control software received information from the NEXUS LIMS on the number and identity (barcodes) of samples and subsamples below.
- System receives and processes 32 pre-sieved (4 mm screen) soil samples ranging from 500–700 g per day. These are called original soil (OS) samples.
    - Technicians will load the system with samples in to-be-determined containers.
        - The contractor should recommend or design the sample containers in order to minimize the number of sample transfers between containers, i.e. operators will fill the container in the sample prep lab, transport them to the automation lab and load them directly into the system.
        - Containers can be off-the-shelf or customized, but must be reusable and washable at 100 °C without causing leaching of container material.
        - Containers must be sealable, e.g. with a tight-fitting cap so they can be transported between labs without risk of spilling/cross contamination, but the caps could be removed manually when samples are loaded into the system if cross contamination can be avoided.

        - Each sample must fit within a single container, i.e. no splitting samples across multiple small containers.
        - The samples have different densities and thus take up different volumes at the same mass. The largest volume will require ~1000 mL containers.
    - The system must be designed to allow expansion to receive and process up to 80 samples per day in a Phase II effort, which is NOT a part of this SOW. The design must demonstrate that there is enough physical space available on the system so future ~~moducles~~modules can be connected to expand the capacity by allowing samples to be passed between modules. In addition, the software and electronics should be ready to connect to and interface with future modules. Examples include but are not limited to demonstration of how future modules would be connected, expansion ports for electrical or other connection, etc.
    - The system must keep samples cool (4 °C) if residence times before processing will exceed 1 hour.
        - Samples placed in cold storage shall be capped/sealed to prevent evaporation.

- First set of aliquots: for each received OS sample, weigh and aliquot the following subsamples into pre-labeled (barcodes and text) tubes.
    - Six replicates of 0.25 grams of each OS sample placed in 15 mL tubes OR (selectable) 1.0 grams each placed into 50 mL tubes. Accuracy and precision are important (up to +10% is acceptable). Record weights for probable system use (determines extraction solvent volume). These six replicates will be referred to as organic matter analysis (OMA) samples. Process consideration: the OMA samples should move directly into the extraction workflow or be moved to chilled storage (4 °C) if the time to solvent addition is > 1 hour. Throughput: In Phase I of development, PNNL anticipates that the 32 OS samples per day will be processed into 192 OMA samples at this stage.
- Second set of aliquots: In any order, for each received OS sample, weigh and aliquot the following subsamples into pre-labeled (barcodes and text) tubes. In all cases, the actual amount of soil in each aliquot must equal or exceed the value below, but accuracy and precision can be low (+20% is acceptable). Record weights. Cap samples. Each sample type will be accumulated in a rack to be collected by a technician (leaves system for other uses). Cool samples (4 °C) if residence times before processing exceed 1 hour.
    - One replicate of 10 grams in a 50 mL tube. Referred to as the DNA sample.
    - One replicate of 1.5 grams in a 15 mL tube. Referred to as the RNA sample.
    - Three replicates of 8 grams each in 15 mL tubes. Referred to as Microbial Biomass samples.
    - Three replicates of 4 grams each in 15 mL tubes. Referred to as Inorganic Phosphorous samples.
    - Three replicates of 10 grams each in 50 mL tubes. Referred to as Water Content samples.

- (User Selected at Run Time) Two replicates of 30 grams each in 50 mL tubes. Referred to as Respiration samples. Note: in the future, we may need to aliquot the Respiration samples from the OS samples rather than the AD samples.

- System also receives and processes 32 pre-sieved (4 mm screen) and air-dried (AD) soil samples ranging from 200–400 g (referred to as AD soil samples) per day.
  - Technicians will load the system with samples in containers matching the criteria listed in the OS sample section above.
  - Throughput: 32 (Phase I) to 80 (Phase II) AD samples received and processed per day.
  - These samples do not require cooling.
- Third set of aliquots: For each received AD sample, weigh and aliquot the following subsamples into pre-labeled (barcodes and text). In all cases, the actual amount of soil in each aliquot must equal or exceed the value below, but accuracy and precision can be low (+20% is acceptable). Record weights. Cap samples. Each sample type should accumulate in a rack to be collected by a technician (leaves system for other uses).
  - Two replicates of 30 grams each in 50 mL tubes. Referred to as Respiration samples.
  - Two replicates of 30 grams each in 50 mL tubes. Referred to as Texture samples.
  - Two replicates of 30 grams each in 50 mL tubes. Referred to as Outsource samples.

4.3 SOIL SOLVENT EXTRACTIONS AND FILTRATION COMPONENT

This part of the workflow starts with moving the six replicates that contain 0.25–0.30 grams of each OS sample placed in 15 mL tubes OR (selectable) 1.0–1.1 grams each of OS samples placed into a 50 mL tube created during the Aliquot and Weigh Component. Each of the 6 OS replicates undergo the same extraction process, but with a different solvent. Two replicates are extracted with ultrapure water (UPW), and one each is extracted with HCl (0.5 M), hydroxylamine (0.25 M), dithionite (0.05 M), and sodium pyrophosphate (0.1 M). One of the water extractions may be swapped with oxalate (0.2 M).

The performance requirements include the following protocol steps:

- Receive and register (barcode read) OS samples either directly from the Aliquot and Weigh Component or from a cooled storage unit.
- De-cap if necessary.
- Add solvent where the volume = 40 times the weight in grams of soil (from the Aliquot and Weigh Component). This is ~10 mL for the 15 mL tubes and 40 mL for the 50 mL tube sample.
- Cap the tube tight enough to form a leak-free seal.
- Gently rock or rotate the tubes to mix the soil and solvent for 1 hour.
- Centrifuge tubes (10 min at 4,000 rpm).

- Pass supernatant through a 22-micron hydrophilic filter, e.g., MCE, PES, or similar. These come in 24- and 96-well formats. Note: filters must be pre-conditioned by passing through 10 mL of ultrapure water to wash out contaminants.
- Aliquot 1–5 ml of each filtered extract to new 15 mL bar-coded tubes, capped, racked, and move to chilled storage. These are the inductively coupled plasma samples and total organic carbon samples.

4.4 ACIDIFICATION AND PH MEASUREMENT COMPONENT

This part of the workflow starts with the samples from the Soil Extractions Component.

The performance requirements are to complete the following protocol steps:

- Add HCl (~ 2 µl of 37% HCl per 5 mL of sample is the current protocol) to reach a target pH of < 2.0.
- Measure and verify that pH < 2.
- Repeat HCl addition and pH verification as needed (once is typically enough).

Move the samples to the Solid-Phase Extractions Component.

4.5 SOLID-PHASE EXTRACTIONS COMPONENT

This part of the workflow starts with the samples from the Acidification and pH Measurement Component. PNNL solid-phase extractions workflow is currently done in tube-based format using Agilent Bond Elut PPL (Priority PolLutant) Solid Phase Extraction (SPE) in a cartridge format. This is a proprietary nonpolar styrene divinylbenzene that also comes in a 96-well format (same sorbent mass, 1.8 mL volume. The workflow for PNNL's current SPE process is provided here, but may be adapted for automation—for example, one large wash instead of six 9-milliliter washes.

The performance requirements of this component are to complete the following protocol steps for SPE samples.

- Condition with 3 mL methanol.
- Equilibrate with 3 mL of 10mM HCL.
- Load sample.
- Wash with 9 mL HCL solution (10 mM HCl).
- Wash with 9 mL HCL solution (10 mM HCl).
- Wash with 9 mL HCL solution (10 mM HCl).
- Wash with 9 mL HCL solution (10 mM HCl).
- Wash with 9 mL HCL solution (10 mM HCl).
- Wash with 9 mL HCL solution (10 mM HCl).

- Dry under nitrogen gas, 10 mL (20 mL/minute, likely flexible).
- Elute with 1.5 mL of methanol into 2 mL glass MicroSolv tubes or into a matching 2 mL collection plate available from Agilent, and then move to MicroSolv tubes.
- Cap and rack MicroSolv tubes into the Thermo Fisher FTICR autoloader rack (Society for Biomolecular Screening (SBS) Format, Fisher Scientific Product Code 15580775). Capping can be done with screw or snap caps designed for use with the MicroSolv tubes. Capping may have to be done by humans.
- Tubes moved to cooled storage by robot unless capped by humans.
- The tubes are designated as FTICR samples as described in Section 4.2.

4.6 WORKFLOW CONTROL SOFTWARE AND LIMS CONNECTION

Workflow control software refers to software that schedules specific devices to perform certain functions at a designated time to meet scientific requirements. In some cases, the software will accommodate "virtual cells," which are operations managed by humans. The workflow control software will also interface between the work cell execution software and EMSL's LIMS system for overall workflow operations scheduling, management, and data generation. Vendor workflow control software must support connection to the EMSL and PNNL secure networks and EMSL's LIMS. Table 4.1 provides key performance parameters for the workflow control software and its connection to the LIMS.

4.6.1 Data and Metadata Capture Needs

~~EMSL's LIMS captures data from analytical instrumentation and provides secure access to the data for EMSL staff and external collaborators. The automated system shall support or manage capture of instrument performance, analytical procedures, and results (pH readings) in real-time or near real-time. The system shall have the demonstrated ability to support capturing and managing data from new instruments and sensors if they are added after system delivery, including instrument calibration and quality control information.~~

EMSL's LIMS tracks sample IDs, connects them to data collected from analytical instrumentation, and provides secure access to the data for EMSL staff and external collaborators. The automated system shall provide a means to connect the sample being run with the sample ID in the LIMS, and at the end of the run it will send data collected during the run to the LIMS. Vendor will work with EMSL LIMS team to create the necessary data connection, e.g. by providing an API. Data to be collected includes times/dates of run, barcodes of aliquots, weights of aliquots, pH, deviations (e.g. errors that occurred during a run), i.e. data generated by the ASAP system that may be needed for tracking purposes and downstream experiments/data analysis. Exact details to be finalized during Task 1 and 2, but it will not include data collected by downstream analytical instruments.

4.7 TECHNICAL SUPPORT

The requirements for technical support are that the contractor provides remote and on-site technical support for 1 year after installation and commissioning of the ASAP system to address technical or software issues that arise during operations and to provide additional training as needed. At a minimum:

- Contractor will act as a single point of contact for support. If support is needed for a 3rd party component, e.g. an integrated liquid handler, contractor will coordinate support with the 3rd party vendor.

- Support shall be available via phone, email, ticket portal, etc. during normal PST business hours 8 AM PST – 5 PM PST, Monday through Friday.

- Contractor will respond to support requests within 24 hours if request is sent during the support hours listed above, otherwise within 24 hours of the start of the next business day.

- If the problem cannot be resolved remotely within 72 hours, contractor will travel to the site to resolve the problem unless the 72-hour mark falls on a weekend day, then arrival is expected the following Monday.

    - Exceptions include situations where the problem is not resolved and Battelle unilaterally approves on a path to resolution, e.g. a part is being shipped and the local support team will install it.

- Contractor will be responsible for performing any preventive maintenance that occurs quarterly or less frequently, with one annual onsite preventive maintenance visit to be included in the first year after installation.

- Contractor will provide work instructions for any user maintenance tasks that the users are expected to perform.

5.0 DELIVERABLES

The deliverables associated with the tasks in Section 2.0 include those described in the following sections.

5.1 TASK 1: REQUIREMENTS REVIEW

- Contractor shall complete each Task 1 subtask, ending with submission of a report describing final system performance, technical requirements, and a schedule of timelines and milestones.

5.2 TASK 2: DESIGN REVIEW

- Contractor shall complete each Task 2 subtask, ending with submission of a report and supporting materials detailing the final ASAP system design for concurrence by PNNL's Technical Oversight Representative (TOR) and Subject Matter Expert.

5.3 TASK 3: SOFTWARE INSTALLATION AND LIMS CONNECTION

- Contractor shall complete each Task 3 subtask and deliver a report verifying that the workflow control software meets the subset of technical requirements detailed in this SOW. Contractor shall provide all documentation and software options necessary to establish a data connection between the

ASAP system software and EMSL's LIMS. Contractor will work with the EMSL subject matter experts to integrate with EMSL's data policy, metadata standards, and Archival systems for data storage. Further information related to EMSL's data policy can be found at https://www.emsl.pnnl.gov/basic/data-management-policy/1243.

5.4 TASK 4: OFF-SITE ASSEMBLY AND FACTORY ACCEPTANCE TESTING

- Contractor shall complete each Task 4 subtask and deliver a report verifying that the ASAP system meets the subset of technical requirements detailed in this SOW.

5.5 TASK 5: DELIVERY, INSTALLATION, AND SOFTWARE/LIMS INTEGRATION

- Contractor shall complete each Task 5 subtask.

5.6 TASK 6: SYSTEM COMMISSIONING AND SITE ACCEPTANCE TESTING

- Contractor shall complete all tasks and subtasks presented in Task 6.
- Contractor shall provide Battelle with a formal report detailing the outcome of the factory acceptance testing and training and receive agreement that the system meets all requirements, and that training is complete.

5.7 TASK 7: TECHNICAL SUPPORT

- Contractor shall complete each Task 7 subtask.

6.0 SCHEDULE

- Contractor shall provide a revised and final project timeline and milestones if necessitated by design changes emerging from the requirements review in Task 1. The timeline will include a schedule for the staged review of the conceptual design. The schedule shall include the duration of each task, proposed milestones, and total elapsed time.
- At a minimum, updates to the schedule shall address the deliverables in Section 5.0 of this SOW.

Table 6.1. Proposed Project Schedule

Deliverable	Activity	Completion Date
Task 1	Requirements Review	Award +1 month
Task 2	Design Review	Award + 2 months
Task 3	Software Installation	Completion of Task 2 + 1 month
Task 4	Off-Site Assembly and Testing	Completion of Task 2 + 9 months
Task 5	Delivery, Installation, and Software/LIMS connection	Completion of Task 2 + 11 months
Task 6	System Commissioning and Site Acceptance	Completion of Task 2 + 12 months
Task 7	Technical Support	Completion of Task 6 + 12 months

The schedule shall be updated upon contract award, after which status shall be provided to PNNL on a monthly basis.

7.0 (RESERVED)

8.0 REFERENCES

9.0 ATTACHMENTS

9.1 SCHEDULING AND WORKFLOW CONTROL SOFTWARE REQUIREMENTS

- Must be able to manage full operations of the ASAP system including manual, semi-automated, and fully automated processes.
- Has graphical user interface for visualization of location and status of samples within the ASAP system.
- Support parameterization of method steps to allow user-specified parameters at run time Accepts data during process execution and follows the appropriate logic path according to the data received.
- Manages requests from users or external software.
- Has native programming/coding capabilities to build custom functions and connections to LIMS databases or third-party software—must describe which scripting languages are supported within the platform, RESTful services, APIs, and network interfaces.
- Supports integration of components necessary for Phase II expansion.
- Has an agnostic device and system control capability.
- Has an API for interfacing with external software for the programmatic creation/manipulation of workflows, orders, and data tracking. Please provide API documentation.
- Supports concurrent processing of multiple orders and processes at once with a goal of interleaving samples (but not necessarily protocols) to minimize bottlenecks and maximize the system throughput.
- Supports remote access to manage system and devices in normal and error recovery modes.
- Supports monitoring of critical assay timings to ensure assay integrity is maintained.
- Supports run-time changes to protocols in the event of failure to reassign work or to allow step changes to recover from errors.
- Has protocol versioning and user authentication capabilities.
- Supports inventory scanning such that the labware on the system can be tracked at all times. Inventory should be queryable through the API.
- Must manage workflows where workflows are a series of linked protocols. The workflow may have different decision nodes or parameters based on data events within protocols.

- Has error-handling protocols and error communication protocols, for example, and collects and reports error information (especially from integrated devices/software) via messages, email notification, external audible alarms, automatic or manual recovery options, error logs, etc.

9.2 CHEMICAL COMPATIBLITY TABLE

Chemical	Concentration	Pipetting Characteristics (Viscous/Volatile/Water-like)	Surrogate
Hydrochloric Acid	0.5 M	Water-like	Water
Hydrochloric Acid	37%	Water-like	Water
Hydrochloric Acid	10 mM	Water-like	Water
Hydroxylamine hydrochloride, 99%	0.25 M	Water-like	Water
Sodium dithionite	0.05 M	Water-like	Water
Sodium pyrophosphate, 98%	0.1 M	Water-like	Water
4:3 ammonium oxalate:oxalic acid solution	0.2 M	Water-like	Water
Methanol	100%	Volatile	≥ 99.8% Methanol

9.3 SOIL SAMPLES FOR TESTING

Soil Type	Description	Example
High clay content	Clay-rich terrarium substrate mixed with water per package instructions	https://zoomed.com/excavator-clay-burrowing-substrate/
Sandy loam	A non-USDA-regulated sandy loam from Prosser, Washington	To be provided by EMSL
Peat	Sphagnum peat moss	https://www.homedepot.com/p/3-cu-ft-Peat-Moss-3001-CFC003P/205883917

Soil samples will be passed through a 4mm sieve (for example: https://www.globalgilson.com/200mm-sieve-all-stainless-full-height-4mm) before being loaded onto the system.

~~9.2~~9.4 LAB LAYOUT AND AVAILABLE SPACE

- The area reserved for the ASAP system is a rectangle 18’-11 ¼” by 13’-6” with one of the shorter sides against a wall.

- The entire system must fit within the footprint of the reserved area.

  - The system should be as compact as practical to allow for other activities in the lab as much as possible.

    - Include details about what will be required to scale up the system for the Phase 2 capacity so we can understand what the future space requirements will be.

- There are cable trays and utilities 7'-0" above the floor in the area, but they can be moved or removed if necessary.

- The ceiling is 11'-0", but we need to maintain an 18" distance between the top of the instrument and the ceiling to conform to fire codes.

- Utilities in the reserved area:

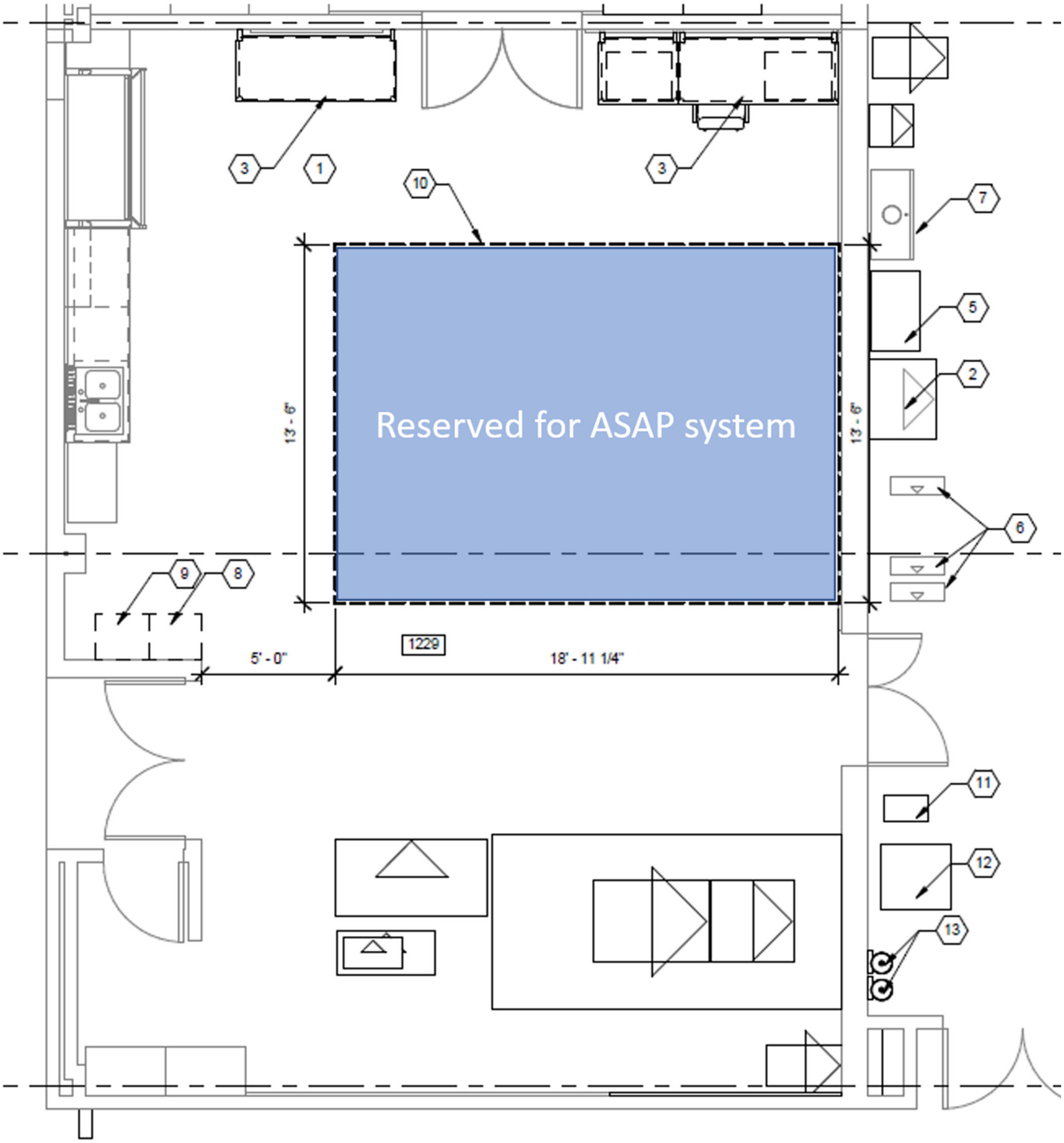
    - 120V power outlets

    - Ethernet ports

    - Clean Dry Air (CDA)

    - Vacuum

    - Exhaust


3
1
10
3
7
5
2
6
13' - 6"
Reserved for ASAP system
13' - 6"
9
8
5' - 0"
1229
18' - 11 1/4"
11
12
13