LIMS Implementation Checklists

This document contains supplemental information for the manuscript titled "*MaRDA FAIR Materials Microscopy and LIMS Data Working Groups' Recommendations*" by Joshua A. Taillon, Edward S. Barnard, Laura M. Bartolo, Maria K. Y. Chan, Eric A. Stach, Mitra L. Taheri, L. Catherine Brinson, and Peter W. Voorhees.

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Introduction

As discussed in the primary manuscript, Laboratory Information Management Systems (LIMS) are an essential component of modern laboratory operations, providing the digital infrastructure that supports data management, sample tracking, result reporting, and more. Their implementation however, is not a simple task and requires considerable planning and preparation.

This document provides three succinct checklists to help guide an organization in the planning of a LIMS implementation:

1. *LIMS Profile of Roles and Activities*: what activities related to research data management should be considered when research projects use a LIMS
2. *Organizational Prerequisites*: what functionality an organization should ideally have in place before deciding to deploy a LIMS
3. *LIMS Capabilities*: what functionality should the new LIMS include to provide maximum utility and to support FAIR Data Principles

A LIMS can be implemented at different levels within an organization. For example, this could be an individual laboratory, a group of laboratories or research facilities, or coordinated at the highest level of an entire organization in academia, government, or industry. The checklists below reflect those multiple organizational types and levels by using the generic term "organization" while bringing out what is needed for the successful deployment of a LIMS at the specific organizational level in terms of roles, prerequisites, and capabilities.

Like the recommendations of the primary manuscript, these checklists are not intended to mandate but rather to recommend. Topics covered will include system requirements, infrastructure readiness, data management, human resources, change management strategies, budget considerations, and vendor selection. Whether the task at hand involves the inaugural implementation of a LIMS or the upgrading of an existing system, this document aims to serve as an evolving and community-based foundational reference for facilitating a seamless and efficient transition to enhanced laboratory data management. The overarching objective is to prepare research groups and organizations' laboratories for the integration of a potent tool, capable of augmenting workflows, enhancing data integrity, ensuring adherence to pertinent regulatory standards, and, consequently, fostering an overall improvement in laboratory practices and performance.

General Information

Note that in the three checklists below we are discussing a range of sizes and types of organizations as well as roles and responsibilities within organizations (as opposed to specific job titles or formal positions as the latter may vary between different types and sizes of organizations – academic, government, industry, etc). In **Checklist 1**, *LIMS Profile of Roles and Activities*, the role of a facility manager subsumes the role of an instrument manager, the role(s) of a "researcher" includes principal investigators, graduate students, and lab technicians at all levels of involvement in a research project. In **Checklist 2**, *Organizational Prerequisites*, the institutional classification is meant to solely help identify the institutional target audience of this document and assist with institution-specific requirements and adaptations. **Checklist 3**, *LIMS Capabilities*, is organized in descending order of what most people with specific roles and responsibilities related to operating a LIMS are going to perform frequently, most likely on a day-to-day basis. The intent is

to define specific tasks and to help identify the people involved to encourage interactions and ways of sharing responsibilities for best results.

The discussion and checklists presented in this document are intended to be downloaded, adapted, and extended by interested parties in the materials community to meet current and future laboratory related needs and interests. The document will be freely available as a community resource for download and implementation on the MaRDA website (https://www.marda-alliance.org/). The use of this document and its checklists by the materials community will help research groups successfully implement FAIR-compliant LIMS to manage their data now. Suggestions for updates to this document by community members to reflect future advances in technology and research approaches in the materials community are welcomed and encouraged to ensure that the document will evolve to best serve the community.

Checklist 1: *LIMS Profile of Roles and Activities*

Introduction:
For the purpose of discussing requirements and preconditions of a LIMS, this rubric defines a "custom profile" (in the terminology of the NIST RDaF [1]), which outlines the roles and responsibilities of those directly involved with implementing and managing the LIMS. As not every member of a LIMS project team will be concerned with every topic, the profile is organized into "Activities" on the left, which represent relevant tasks or duties within the planning or operation of a LIMS, and "Roles" on the right, which indicate what roles within an organization will likely have either a primary (★) or secondary (○) responsibility for that activity. The purpose of this profile is to allow an organization to conduct a self-assessment of what topics need attention, and to identify individuals that may be able to serve in the various roles, with the goal of implementing a maximally FAIR data management system [2].

References:
[1] R. J. Hanisch, D. L. Kaiser, A. Yuan, A. Medina-Smith, B. C. Carroll, and E. M. Campo, “NIST Research Data Framework (RDaF): Version 1.5,” National Institute of Standards and Technology (U.S.), Gaithersburg, MD, NIST SP 1500-18r1, May 2023. doi: 10.6028/NIST.SP.1500-18r1.
[2] A. Jacobsen et al., “FAIR Principles: Interpretations and Implementation Considerations,” Data Intelligence, vol. 2, no. 1–2, pp. 10–29, Jan. 2020, doi: 10.1162/dint_r_00024.

Activities		Roles				
		Data Manager	**Facility Manager**	**IT Manager**	**Instrument Vendor/ Product Manager**	**Researcher**
Planning and Implementation		★ *Primary Responsibility*			○ *Secondary Responsibility*	
	Data Management Expertise and Training	★	○	○	○	
Data	Criteria for selection	○				★
	Nature of data required	○			○	★
	Intended extent of FAIRness Open as possible/closed as necessary	○	○	○	○	★
	Methods to capture, transfer & store	○	★	○	★	★
Metadata	Criteria for selection	★				○
	Nature of Metadata required	★				○
	Intended extent of FAIRness	★	○	○	○	○
	Methods to capture, transfer & store	★			★	
	Metadata schema	★			○	○
Data Generation						
Experimental Data	Consideration of research study	○				★
	Instruments & tools specifications				○	★
	Parameters for instruments & tools					★
	Methods, protocols & calibrations		○	○	○	★
	Provenance capture methods	○	★		○	★
	Reproducibility		○		○	★
Community Standards	General vs Domain specific	★	○		○	○
	Data format & file structure			○	○	★
	Metadata format & file structure	★			○	○
	Vocabulary & Ontology	★	○	○	○	○
Acquisition Software	Open source & Proprietary		○		○	★
	LIMS		★		○	
	Instrument control		○		○	★
	Electronic laboratory notebook		○		○	
Data Processing and Analysis						
	Managing access	○	★	○		○
	Manage instrument outputs	○	★		○	○
	Design & program data analysis tools				○	★
	Perform data analysis					★

Checklist 2: *Organizational Prerequisites*

Introduction:
This document puts forward what an organization should have in place prior to implementing a LIMS. For more information, see the primary manuscript text and Ref. 3. As shown below, while the types of prerequisites do not change substantially between organization types, the scale of the resulting deployment will (*e.g.* instrument scheduling software could be a simple shared calendar for an individual research group, but that would not scale to a facility-wide implementation). Items marked with (★) are recommended to have in place (or have a plan for) before a LIMS implementation proceeds.

References:
[3] G. Greene et al., "A Roadmap for LIMS at NIST Material Measurement Laboratory," National Institute of Standards and Technology (U.S.), Gaithersburg, MD, NIST TN 2216, Apr. 2022. doi: 10.6028/NIST.TN.2216.

Prerequisite Functionality	Organization Type			
	Individual Research Group	**University Research Facility**	**Industry Research Facility**	**Government Laboratory**
Planning Process				
A project team with representatives from all relevant departments and stakeholders (see Checklist 1)	★	★	★	★
LIMS implementation: Clear definition of goals & objectives	★	★	★	★
A thorough understanding of the laboratory's workflows and processes	★	★	★	★
A comprehensive inventory of all laboratory equipment, instruments, and software	★	★	★	★
Data migration and data backup plan from existing systems to the new LIMS including disaster recovery		★	★	★
A plan for system validation and testing		★	★	★
A defined user training and support plan	★	★	★	★
A plan for ongoing maintenance and system updates	★	★	★	★
Detailed project plan: Includes timelines, milestones, and resource allocation.	★	★	★	★
Technical capabilities				
A facility management/instrument scheduling strategy or system	★	★	★	★
Network connected instruments (can be a segregated "research equipment network")	★	★	★	★
Centralized data storage location (network-attached storage)	★	★	★	★
Electronic laboratory notebook software	★	★	★	★

Checklist 3: *LIMS Capabilities*

Introduction:
As in Ref. [3], the working group considers LIMS to be best described as a *system* of interconnected components providing a range of capabilities related to research data management throughout the data lifecycle. This document describes the capabilities a LIMS promoting the collection and management of FAIR data should include for various organization types. This checklist can help organizations as they are evaluating "off-the-shelf" LIMS offerings or planning for a custom implementation. Items marked with (★) are recommended capabilities for each organization type. Those items without a mark may still be worth considering however, depending on an organization's individual needs.

References:
[3] G. Greene et al., "A Roadmap for LIMS at NIST Material Measurement Laboratory," National Institute of Standards and Technology (U.S.), Gaithersburg, MD, NIST TN 2216, Apr. 2022. doi: 10.6028/NIST.TN.2216.

Capability	Organization Type			
	Individual Research Group	**University Research Facility**	**Industry Research Facility**	**Government Laboratory**
Core capabilities				
Centralized automated collection and permanent storage ("repository") of research data and metadata	★	★	★	★
Access rights control to limit access to centralized research data as necessary		★	★	★
Use of persistent identifiers (PIDs) wherever possible within the LIMS (e.g Handles, Ark IDs, DOIs, IGSNs, etc.)	★	★	★	★
Data and metadata within the LIMS are searchable for later retrieval and analysis	★	★	★	★
Interfaces with instrument scheduling and laboratory facility management software (if present)		★	★	★
All components of the LIMS provide and can consume data via well-documented application programming interfaces (APIs)	★	★	★	★
Compliance with FAIR principles of open research data (Findable, Accessible, Interoperable, Reusable)	★	★	★	★
Useful recommended capabilities				
Data and metadata collection integrates with and supports research workflows and project management		★	★	★
Experimental data is stored in, or system provides automatic conversion to, open data formats	★	★	★	★
Data and metadata follow recommended standardized models/schemas		★	★	★
Supports creation of derivatives and metrics, either directly within the LIMS, or by integration with visualization, analysis, and data evaluation tools		★	★	★
Integrates or supports external data publication		★		★
Interoperability with other laboratories and LIMS systems on data and metadata levels using open and well-documented API layers		★		★