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Standard Guide for Laboratory ~~Information Management Systems (LIMS)~~Informatics[1]

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1. Scope

1.1 This guide helps describe the laboratory informatics landscape and covers issues commonly encountered at all stages in the life cycle of laboratory informatics from inception to retirement. It explains the evolution of laboratory informatics tools used in today's laboratories such as Laboratory Information Management Systems ~~from inception to retirement. The~~ (LIMS), Electronic Laboratory Notebooks (ELN), Scientific Data Management Systems (SDMS), and Chromatography Data Systems (CDS). It also covers the relationship (interactions) between these tools and the external systems in a given organization. The guide discusses supporting laboratory informatics tools and a wide variety of the issues commonly encountered at different stages in the life cycle. The sub-sections that follow describe details of scope of this document in specific areas.

1.2 ~~*High Level*~~ *High-Level Purpose*—The purpose of this guide includes: *(1)* ~~help~~helping educate new users of ~~Laboratory Information Management Systems (LIMS),~~ laboratory informatics tools, *(2)* provide a standard terminology that can be used by ~~LIMS~~different vendors and end users, *(3)* establish minimum requirements for ~~primary LIMS functions,~~ laboratory informatics, *(4)* provide guidance for the specification, evaluation, cost justification, implementation, project management, training, and ~~documentation,~~ documentation of the systems, and *(5)* provide ~~an example of a LIMS function checklist.~~function checklist examples for laboratory informatics systems that can be adopted within the laboratory and integrated with the existing systems.

1.3 ~~*LIMS*~~ *Laboratory Informatics Definition*—~~The term Laboratory~~ Laboratory informatics is the specialized application of information technology aimed at optimizing laboratory operations. It is a collection of informatics tools utilized within laboratory environments to collect, store, process, analyze, report, and archive data and information from the laboratory and supporting processes. Laboratory informatics includes the integration of systems, the electronic delivery of results to customers, and the supporting systems including training and policies. Examples of laboratory informatics include: Laboratory Information Management Systems ~~(LIMS) describes the class of computer systems designed to manage laboratory information.~~(LIMS), Electronic Laboratory Notebooks (ELNs), Chromatography Data Systems (CDS), and Scientific Data Management Systems (SDMS).

NOTE 1—Laboratory informatics scope encompasses multiple technical solutions or systems. The division between these system categories continues to soften as functionality continues to be added to each of them. LIMS were originally created to address the laboratories' need to manage laboratory operations and data, provide traceability for all laboratory samples and equipment, and ensure that laboratory procedures are followed. ELNs, on the other hand, were originally created to meet the scientists' need to document their experimental design, execution, and conclusions in an electronic format instead of in a paper notebook. SDMS was created to provide a repository of all scientific data files and results regardless of instrument type. The current definitions of each of these system categories are far more encompassing.

1.4 *Scope Considerations When Selecting and Implementing Laboratory Informatics Solutions*—Many laboratories have determined that they need to deploy multiple laboratory informatics systems to automate their laboratory process and manage their data. Selection of an informatics solution requires a detailed analysis of the laboratory's requirements rather than by choosing a product category. It is important to include representatives from Information Technology (IT) and Subject Matter Experts (SMEs), who understand the needs of the laboratory, to be involved in the selection and implementation of a laboratory informatics system to ensure that the needs of the laboratory are met and that IT can support it. Customers (internal and external) of laboratory information should also be included in the laboratory informatics solution design, to ensure there is full electronic integration between systems.

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1.5 ~~*Laboratory Categories*—~~The ~~spectrum of laboratories that employ LIMS is wide spread. The following break down provides an overview of the laboratory categories that use LIMS as well as examples of laboratories in each category.~~scope of this guide covers a wide range of laboratory types, industries, and sizes. Examples of laboratory types and industries are listed in the following:

1.5.1 *General Laboratories:*

1.5.1.1 Standards (ASTM, IEEE, ISO), and

1.5.1.2 Government (EPA, FDA, JPL, NASA, NRC, USDA, FERC).

1.5.2 *Environmental:*

1.5.2.1 Environmental Monitoring.

1.5.3 *Life Science Laboratories:*

1.5.3.1 Biotechnology, and

~~1.4.3.2 Diagnostic,~~

~~1.4.3.3 Healthcare Medical,~~

~~1.4.3.4 Devices, and~~

1.5.3.2 ~~Pharmaceuticals Vet/Animal.~~Diagnostic.

1.5.4 *Healthcare Medical:*

1.5.4.1 Devices,

1.5.4.2 Pharmaceuticals vet/animal,

1.5.4.3 Public health, and

1.5.4.4 Hospital LIS.

1.5.5 *Heavy Industry Laboratories:*

1.5.5.1 Energy ~~& Resources,~~and resources,

1.5.5.2 Manufacturing ~~& Construction,~~ and construction,

1.5.5.3 Materials ~~& Chemicals,~~and chemicals, and

1.5.5.4 Transportation ~~& Shipping.~~and shipping.

1.5.6 *Food ~~&~~and Beverage Laboratories:*

1.5.6.1 Agriculture,

1.5.6.2 Beverages,

1.5.6.3 Food, and

1.5.6.4 Food ~~Service & Hospitality.~~service and hospitality.

1.5.7 *Public Sector Laboratories:*

1.5.7.1 Law ~~Enforcement,~~enforcement,

1.5.7.2 State ~~& Local Government,~~and local government,

1.5.7.3 Education, and

1.5.7.4 Public ~~Utilities (Water, Electric, Waste Treatment).~~utilities (water, electric, waste treatment).

~~1.4.7 *Laboratory Size:*~~

~~1.4.7.1 This guide covers topics regarding LIMS for a range of laboratory sizes ranging from small with simple requirements to large multi-site/global laboratories with complex requirements. Although the guide addresses complex issues that impact primarily large LIMS implementations, laboratories of all sizes will find this guide useful. The implementation times and recommendations listed in this guide are directed at medium and large laboratories.~~

1.6 *Integration*—~~Integration between LIMS~~ The scope includes communication and meaningful data exchange between different laboratory informatics tools and other external systems (document management, chromatography data systems, laboratory instruments, ~~spectroscopic~~spectroscopy data systems, Enterprise Resource Planning (ERP), Manufacturing Execution Systems (MES), ~~Corrective Action and Preventative Action (CAPA), Electronic Laboratory Notebooks (ELNs) and data archive) provides~~ Investigations/Deviations and CAPA management systems), and other integrated business systems (for example, clinical or hospital environments) provide significant business benefits to any ~~laboratory. Integration between LIMS and other external systems~~ laboratory and is discussed at a high level in this ~~guide including data interchange and XML standards.~~guide.

1.7 ~~*Lifecycle*~~ *Life Cycle Phases*—The ~~LIMS lifecycle described in this guide includes the following phases:~~ scope of this guide ~~(1) project initiation, (2) requirements analysis, (3) design, (4) build/configure, (5) test and commission, (6) operation and maintenance, and (7) retirement. This guide~~ is intended to provide an understanding of ~~the LIMS system life cycle and good practices for each of the activities. It will help first time LIMS implementers~~ laboratory informatics tools' life cycle from project initiation point to retirement and absolution. This guide was designed to help newer audiences in understanding the complexity in the relationships between different laboratory informatics tools and how to plan and manage ~~their LIMS projects~~the implementation project, while seasoned ~~LIMS~~ users may use the ~~LIMS system~~ different life ~~cycle~~cycles to maintain existing ~~LIMS and prepare for the implementation of the next generation LIMS.~~laboratory informatics tools. Integrating additional tool(s) to the existing one(s) in today's evolving laboratory informatics world adds constraints that need to be considered. The lifecycle discussion includes both the laboratory informatics solution lifecycle as well as the project lifecycle, which describes steps to a laboratory informatics solution.

1.7.1 The product lifecycle encompasses a specific laboratory informatics system and the expected useful life of that system before it needs to be replaced or upgraded.

1.7.2 The project lifecycle encompasses the activities to acquire, implement, operate, and eventually retire a specific laboratory informatics system.

1.8 *Audience*—This guide has been created with the needs of the following stakeholders in mind: *(1)* end users of ~~LIMS,~~ laboratory informatics tools, *(2)* implementers of ~~LIMS,~~ laboratory informatics tools, *(3)* quality personnel, *(4)* information technology personnel, *(5)* ~~LIMS~~ laboratory informatics tools vendors, *(6)* instrument vendors, *(7)* individuals who ~~must approve LIMS~~ shall approve laboratory informatics tools funding, *(8)* ~~LIMS application~~ laboratory informatics applications support specialists, and *(9)* software test/validation ~~specialist.~~specialists. Information contained in this guide will benefit a broad audience of people who work or interact with a laboratory. New ~~LIMS~~ users can use this guide to understand the purpose and functions of ~~LIMS.~~ the wide varieties of laboratory informatics tools as well as the interactions between these tools with external systems. The guide can also help prospective ~~LIMS~~ users in understanding terminology, configurations, features, design, benefits and ~~costs.~~ costs of these different laboratory informatics tools. Individuals who are purchasing ~~a LIMS may~~ (a) specific tool(s) may also use this guide to identify functions that are recommended for specific laboratory environments. Research and ~~Development~~development staff of ~~commercial LIMS~~ different commercial laboratory informatics systems vendors may use the guide as a tool to evaluate, identify, and potentially improve the capabilities of their products. ~~LIMS vendor~~The vendors' sales staff may use the guide to represent functions of their ~~LIMS product~~ laboratory informatics products to prospective customers in more generic and product neutral terms.

1.9 *Out of Scope*—~~The full description and use of systems mentioned in this guide within the context of interfaces to LIMS are beyond the scope of this standard. Examples of these systems include Chromatography Data Systems (CDS), Electronic Laboratory Notebooks (ELN), Data Archive, Scientific Data Management Systems (SDMS), Enterprise Resource Planning (ERP), Manufacturing Execution Systems (MES) and Electronic Document Management Systems (EDMS).~~This guide does not attempt to define the boundaries, as they continue to evolve, between the different types of laboratory informatics but rather focuses on the functionality that is provided by laboratory informatics as a whole.

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E1340 Guide for Rapid Prototyping of Information Systems

~~E1947 Specification for Analytical Data Interchange Protocol for Chromatographic Data~~

~~E1948 Guide for Analytical Data Interchange Protocol for Chromatographic Data~~

E2066 Guide for Validation of Laboratory Information Management Systems

~~E2077 Specification for Analytical Data Interchange Protocol for Mass Spectrometric Data~~

~~E2078 Guide for Analytical Data Interchange Protocol for Mass Spectrometric Data~~

~~2.2 *ANSI Standards:*~~[3]

~~ANSI HL7 Arden Syntax for Medical Logic Systems~~

2.2 *EPA Data ~~Standards:~~Standard:*[3]

40 CFR 160 Code of Regulations, 54 FR 34067, August 17, 1989

~~40 CFR 792 Code of Regulations, 54 FR 34043, August 17, 1989~~

~~EPA 2185 Good Automated Laboratory Practices Principles and Guidance to Regulations For Ensuring Data Integrity In Automated Laboratory Operations with Implementation Guidance, 1995 Edition~~

2.3 *FDA ~~Regulations:~~Regulation:*[4]

FDA ~~21CFR~~ 21 CFR Part 11 ~~Code of Regulations, 57 FR 32185, July 21, 1992~~Electronic Records, Electronic Signatures Final Rule, 62 Federal Register 13464, March 20, 1997

2.4 *GAMP:*[5]

GAMP ~~4~~5 Good Automated Manufacturing Practice (GAMP) Guide for Validation of Automated Systems in Pharmaceutical Manufacture, ISPE, ~~December 2001~~2008

~~GAMP Good Practice Guide Validation of Laboratory Computerized Systems, April 2005 (this is a supplement to the GAMP 4 document)~~

[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[14] Available from International Health Terminology Standards Development Organisation (IHTSDO), Gammeltorv 4, 1., 1457 Copenhagen K, Denmark, http://www.ihtsdo.org

~~[3] Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, http://www.ansi.org.~~

[3] Available from United States Environmental Protection Agency (EPA), ~~Ariel Rios Bldg.,~~ 1200 Pennsylvania Ave., NW, Washington, DC 20460, http://www.epa.gov.

[4] Available from Food and Drug Administration (FDA), ~~5600 Fishers Ln., Rockville, MD 20857,~~10903 New Hampshire Ave., Silver Spring, MD 20993-0002, http://www.fda.gov.

[5] ~~Available from the~~ Registered trademark of and available from International Society for Pharmaceutical Engineering (ISPE), ~~3109 W. Dr. Martin Luther King, Jr. Blvd., Suite 250, Tampa, FL 33607-6240,~~600 N. Westshore Blvd., Suite 900, Tampa, FL 33609, http://www.ispe.org.

GAMP GPG IT Infrastructure Control and Compliance, ISPE, September 2005

2.5 *ICH Standard:*[6]

ICH Quality Guideline Q9 Quality Risk Management

2.6 *IEEE Standards:*[7]

IEEE 829 1998 1998 IEEE Standard for Software Test Documentation

IEEE 830 1998 1998IEEE Recommended Practice for Software Requirements Specifications

IEEE 1008 1987 1987 IEEE Standard for Software Unit Testing

IEEE 1012 2004 2004 IEEE Standard for Software Verification and Validation

IEEE 1028 1997 1997 IEEE Standard for Software Reviews

IEEE 1063 2001 2001 IEEE Standard for Software User Documentation

2.7 *Instrument Interface ISO Standards:*

AnIML (Analytical Information Markup Language) an emerging standard for laboratory instruments covering multiple analytical techniques. The E13.15 subcommittee is responsible for the development of this standard.[8]

NetCDF (Network Common Data Form) an interface for array-oriented data access and a library that provides an implementation of the interface. The netCDF library also defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data. Unidata Program Center at the University Corporation for Atmospheric Research (UCAR).[9]

Staged Electronic Data Deliverable (SEDD) EPA—eXtensible Markup Language (XML)—joint standard developed by US EPA Office of Superfund Remediation and Technology Innovation (OSRTI) Analytical Services Branch (ASB)and US Army Corps of Engineers (US ACE)[108]

ISO/IESISO/IEC 12207 Subcommittee for Electronic Data Standards (SEDS), reference spectroscopic databases sponsored by the International Union of Pure and Applied Chemistry (IUPAC) and standards related to the Joint Committee on Atomic and Molecular Physical Data (JCAMP) and JCAMP-DX (XML in the chemistry area) ISO Standards ISO/IEC 12207 Information technology—Software life cycle processes, as amended by ISO/IEC 12207 AMD2processes

ISO/HL7 27932:2009 Data Exchange Standards—HL7 Clinical Document Architecture, Release 2

2.8 *NRC Standards:*[9]

FDA CFR Pa rt 21Part 21 10 10 Code of Federal Regulations (CFR) Part 21.42 FR 28893, June 6, 1977

FDA CFR Part 50, Appendix B 10 10 Code of Federal Regulations (CFR) Part 50 Appendix B. 35 FR 10499, June 27, 1970, as amended at 36 FR 18301, Sept. 11, 1971; 40 FR 3210D, Jan. 20, 1975

FDA CFR Part 50, Appendix E 10 10 Code of Federal Regulations (CFR) Part 50 Appendix E. 45 FR 55410, Aug. 19, 1980Aug. 19, 1980, , et sequentia as amended

FDA CFR Part 50, Appendix K 10 10 Code of Federal Regulations (CFR) Part 50 Appendix K. 21 FR 355, Jan. 19, 1956Jan. 19, 1956, , unless otherwise noted

3. Terminology

3.1 This guide defines the majority of different terminology used in the LIMS field. Sectionlaboratory informatics tools 3.2 defines LIMS terms specific to this guide. field. Users of this documentguide should request a terminology list from each vendor with a cross reference to the terms used in this guide.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *CAPA, n*—acronym for corrective action, preventative action.

3.2.1 *Chromatography Data System (CDS),chromatography data system, CDS, n*—computer system used to acquire, analyze, store, and report information from chromatography instruments.chromatographs.

3.2.2 *cloud computing, v*—term generally used to refer to software applications that are delivered as a software service through remote hosting using the public internet (public cloud) or within the users' network environment (private cloud).

[6] Available from International Conference on Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use (ICH), ICH Secretariat, c/o IFPMA, 15 ch. Louis-Dunant, P.O. Box 195, 1211 Geneva 20, Switzerland, http://www.ich.org.

[7] Available from Institute of Electrical and Electronics Engineers, Inc. (IEEE), 445 Hoes Ln., P.O. Box 1331, Piscataway, NJ 08854-1331,08854, http://www.ieee.org.

[8] Available from International Organization for Standardization (ISO), 1, ch. de la Voie-Creuse, CP 56, CH-1211 Geneva 20, Switzerland, http://www.iso.org.

[9] Available from U. S. Nuclear Regulatory Commission (NRC), One White Flint North, 11555 Rockville Pk., Rockville, MD 20852-2738, http://www.nrc.gov.

3.2.2.1 *Discussion*—

Essentially, the difference between cloud computing and a traditional application deployment is that the application users are not responsible for the installation and maintenance of the computing infrastructure and application software.

3.2.3 *corrective and preventative action, CAPA, n*—CAPA applications are used to collect information, analyze information, identify and investigate product and quality problems, and take appropriate and effective corrective or preventive or both action to prevent their recurrence.

3.2.3.1 *Discussion—*

Verifying or validating corrective and preventive actions, communicating corrective and preventive action activities to responsible people, providing relevant information for management review and documenting these activities are essential in dealing effectively with product and quality problems, preventing their recurrence, and preventing or minimizing device failures.[10]

3.2.4 *data exchange standardization, n*—as defined by the International Organization for Standardization (ISO) in ISO/HL7 27932, the process of agreeing on standards, which represent the common language that allows the exchange of data between disparate data systems.

[10] For additional information, visit http://www.fda.gov/ICECI/Inspections/InspectionGuides/ucm170612.htm#page1.

3.2.4.1 *Discussion—*

The goals of standardization are to achieve comparability, compatibility, and interoperability between independent systems, to ensure compatibility of data for comparative statistical purposes, and to reduce duplication of effort and redundancies. A data standard often includes data elements, data element definitions, and such agreements as formats, message structures, vocabulary. In the context of this paper, a standard is a specification or requirement and is not synonymous with a policy, procedure, guideline, framework, technique, or best practice. Adopting standards has the potential to improve interoperability and reduce costs by facilitating the ability of networked laboratories to coordinate activities during public health incidents where surge capacity may be required (for example, national response and readiness). Adopting standards may reduce the costs of LIMS implementation and vendor/developer support.

3.2.5 *electronic document management system, EDMS, n*—~~acronym for electronic document management system.~~used to store, catalog retrieve, view, and print digital documents.

3.2.5.1 *Discussion—*

Modern EDMS applications typically provide the ability to manage a document throughout its lifecycle with functions including document initiation, multiple levels of review, version controls, security and archive of historical versions of documents.

3.2.6 *electronic laboratory notebook, ELN, n*—~~acronym for electronic laboratory notebook. computer system~~ software program designed to replace paper laboratory notebooks. Defined by CENSA (Collaborative Electronic Notebook Systems Association) as "a system to create, store, retrieve, and share fully electronic records in ways that meet all legal, regulatory, technical and scientific requirements."

3.2.6.1 *Discussion—*

~~Lab~~Laboratory notebooks in general are used by ~~scientists~~ scientists, engineers, and technicians to document research, experiments, and procedures performed in a laboratory. A ~~lab~~laboratory notebook is often maintained to be a legal document and may be used in a court of law as evidence. Similar to an inventor's notebook, the ~~lab~~laboratory notebook is also often referred to in patent prosecution and intellectual property litigation. ~~Electronic laboratory notebooks enable electronic access to information including searching, data capture from instruments and collaboration between laboratory personnel and personnel outside the laboratory.~~

~~3.2.4.2 *Discussion—*~~

~~ELNs can be divided into two categories: specific ELNs contain features designed to work with specific applications, scientific instrumentation or data types. Refer to laboratory exectuion system (LES) as an example of a specific ELN. Cross-disciplinary ELNs or generic ELNs are designed to support access to all data and information that needs to be recorded in a lab notebook.~~

3.2.7 *enterprise resource planning, ERP, n*—~~acronym for enterprise resource planning.~~ERP system integrates different types of data such as inventory levels, product orders, accounting, manufacturing capacity, inspection results, and customer relationship management information from organizations within an enterprise (company) to facilitate the flow of information between various business functions across a company as well as with outside business partners.

3.2.8 ~~*GALP, good automated manufacturing practice forum, GAMP Forum, n*—the GALPs are a union of federal regulations, policies, and guidance documents. Several of the GALP provisions are embodied in EPA's Good Laboratory Practice Standards (GLPs). The GLPs are regulations that govern the management and conduct of most nonclinical laboratory studies submitted to EPA's office of Toxic Substances and its Office of Pesticide Programs. Reference EPA 2185.~~a volunteer group under the auspices of the International Society of Pharmaceutical Engineering (ISPE) for writing guidance for the validation of computerized systems used in the regulated portions of the pharmaceutical and allied industries. It is specifically designed to aid suppliers and users in the pharmaceutical industry.

3.2.9 *integration broker, n*—messaging application that can receive or extract data from a source system at the appropriate time, transform the data, and route the reformatted data to the target node.

3.2.9.1 *Discussion*—

An integration broker application can also provide a repository for archiving, searching, and retrieving these messages.

3.2.10 ~~*GAMP, laboratory information system, LIS, n*—acronym for good automated manufacturing practice.~~class of application software that supports clinical laboratories by helping technologists manage the quality and integrity of test samples; departmental workflow functions, result review processes, reporting of finalized results, interpretations, and diagnosis.

3.2.10.1 *Discussion*—

These systems often interface with instruments and other information systems such as hospital information systems (HIS). A LIS is a highly configurable application and often includes laboratory-specific electronic medical records; direct clinician access via secure web connections; billing modules for laboratories performing commercial testing; sophisticated interface engines for routing orders and results to external systems; and on-board image archival systems for pathology images. Patient confidentiality and HIPAA requirements define unique security functionality for a LIS. The College of American Pathologists (CAP) publishes LIS product guides[11] that list current LIS in the market.

3.2.11 *laboratory execution system, LES, n*—~~acronym for laboratory execution system. Computer system employed~~computer system used in the laboratory at the analyst work level to aid in step enforcement for laboratory test method execution.

[11] For additional information, visit http://www.captodayonline.com/productguides/software-systems.html

3.2.11.1 *Discussion*—

Laboratory execution systems (LES) ~~are a sub-class of electronic laboratory notebooks (ELNs) that~~ focus on step execution of defined laboratory test methods. The LES are typically ~~employed~~used in ~~Quality Control~~quality control laboratories that have defined test methods. The functionality of LES and LIMS overlap in the areas of result entry, instrument integration and specification flagging. Deployment options include LES and LIMS systems deployed as an integrated solution, LIMS only or LES only (for limited functions).

3.2.12 *laboratory informatics, n*—term used to describe the specialized application of information technology aimed at optimizing laboratory operations and it is a collection of informatics tools utilized within laboratory environments to collect, store, process, analyze, report, and archive data and information from the laboratory and supporting processes.

3.2.12.1 *Discussion*—

Laboratory informatics includes the integration of systems, the electronic delivery of results to customers, and the supporting systems including training and policies. Examples of laboratory informatics include: Laboratory Information Management Systems (LIMS), Electronic Laboratory Notebooks (ELNs), Chromatography Data Systems (CDS) and Scientific Data Management Systems (SDMS).

3.2.13 *laboratory informatics tools configuration, n*—refers to the process of changing the functions of any of the laboratory informatics tools to match the business process used in a particular laboratory. It does not involve the use of writing software code either via a recognized software language or a language provided by the informatics application supplier. This is a GAMP 4 software category.

3.2.13.1 *Discussion*—

It typically involves using an interface provided by the vendor to enter information that describes the types of samples, analytical methods, specifications, and so forth used in the laboratory.

3.2.14 *laboratory informatics tools customization, n*—refers to the process of changing the functions of any of the laboratory informatics tools to match the business process used in a particular laboratory. It involves the writing software code either via a recognized software language or a language provided by the informatics application supplier. This is a GAMP 5 software category.

3.2.14.1 *Discussion*—

It typically involves adding tables, modifying table structures and writing code or programs to alter the behavior of any of the laboratory informatics tools.

3.2.15 ~~*Laboratory Information Management System (LIMS),*~~*laboratory information management system, LIMS, n—(1)* ~~acronym for laboratory information management System. Computer~~ computer application(s) software and hardware that can acquire, analyze, report, and manage data and information in the laboratory; *(2)* computer software that is used in the laboratory for the management of samples, test results, laboratory users, instruments, standards, and other laboratory functions such as invoicing, plate management, product/material stability ~~LIMS,~~ programs, and work flow automation; and *(3)* a class of application software which handles storing and managing of information generated by laboratory processes. ~~These systems are used to manage laboratory processes including defining master data, sample management and chain of custody, work assignment, instrument and equipment management, standard and reagent management, scheduled sample collection and testing, result entry, result review, reporting, trending and business rule enforcement. These systems interface with laboratory instruments (for example, chromatography data systems (CDS), spectrophotometers and balances) and other information systems such enterprise resource planning (ERP), manufacturing execution systems (MES), or health care based laboratory information systems). A LIMS is a highly flexible application, which can be configured or customized to facilitate a wide variety of laboratory workflow models.~~

3.2.15.1 *Discussion*—

These systems are used to manage laboratory processes including defining master data, sample management and chain of custody, work assignment, instrument and equipment management, standard and reagent management, scheduled sample collection and testing, result entry, result review, reporting, trending and business rule enforcement. These systems interface with laboratory instruments (for example, chromatography data systems (CDS), and other information systems such enterprise resource planning (ERP), manufacturing execution systems (MES), or health care based laboratory information systems (LIS)). A LIMS is a highly flexible application, which can be configured or customized to facilitate a wide variety of laboratory workflow models.

3.2.16 ~~*LIMS configuration,*~~*lean laboratory, n*—~~refers to the process of preparing the LIMS for use in a particular laboratory. It typically involves using an interface provided by the vendor to enter information that describes the types of samples, analytical methods, specifications, etc. used in the laboratory.~~set of management and organizational processes derived from lean manufacturing and the Toyota Production System (TPS) and the goal of a lean laboratory is to use less effort, fewer resources, and less time to test incoming samples.

3.2.17 ~~*LIMS customization,*~~*mapping tools, n*—~~refers to the process of modifying the LIMS to meet the requirements of a particular laboratory. It typically involves adding tables, modifying table structures and writing code or programs to alter the behavior of the LIMS.~~graphical data mapping, conversion, and integration applications that map data between any combination of XML, database, flat file, EDI, Excel (OOXML), XBRL, and/or web service, then transforms data or autogenerates data integration code for the execution of recurrent conversions.

3.2.18 *metadata, n—(1)* data about ~~data;~~data and *(2)* information that describes another set of data.

3.2.18.1 *Discussion*—

Metadata in ~~the LIMS~~ any laboratory informatics tools context typically includes all data that supports a test result that is recorded in ~~a LIMS.~~this tool. Examples include for a pH test, a pH result can be supported by metadata including what instrument was used, what is the calibration date of the instrument, what standard buffer solutions (reagents) were used to calibrate the pH probe ~~sensor and~~ sensor, the expiration dates for the standard ~~solutions. sample~~solutions and the temperature of the solution at time of measurement.

3.2.19 *sample registration, n*—~~the~~ process of ~~registering samples in a LIMS.~~recording incoming sample information in a given laboratory informatics tool.

3.2.20 *scientific data management system, SDMS, n*—~~acronym for scientific data management system.~~used to capture, centrally store, catalog, and manage data generated in a laboratory environment.

3.2.20.1 *Discussion—*

These data are then available for re-use and integration with other laboratory informatics systems. An example of an SDMS is an electronic repository for reports from laboratory informatics systems.

3.2.21 *spectroscopic data systems, n*—computer ~~system~~systems used to collect, process, visualize, interpret, store, and report information from spectroscopic ~~and non-chromatographic~~ instruments.

~~3.2.16 *static tables, n*—descriptive LIMS database tables where templates, tests, calculations, specifications, and related information are defined and stored (commonly found in "look up/reference/dictionary" tables).~~

~~3.2.16.1 *Discussion*—~~

~~LIMS stores look up information to speed sample registration and test assignments. Generally prior to sample registration the static tables need to be configured. Some LIMS implementations can enter static table information directly from the sample registration step. Synonyms of static tables include master data and configuration data.~~

4. Significance and Use

4.1 *Relevance*—This guide is intended to educate those in the intended audience on many aspects of ~~LIMS.~~ laboratory informatics. Specifically, the guide may:

4.1.1 Help educate new users of ~~LIMS;~~laboratory informatics;

4.1.2 Help educate general audiences in laboratories and other organizations that use ~~LIMS;~~laboratory informatics;

4.1.3 Help educate instrument manufactures and producers of other commonly interfaced systems;

4.1.4 Provide standard terminology that can be used by ~~LIMS~~ laboratory informatics vendors and end users;

4.1.5 Establish a minimum set of requirements for primary ~~LIMS~~ laboratory informatics functions;

4.1.6 Provide guidance on the tasks performed and documentation created in the specification, evaluation, cost justification, implementation, project management, training, and documentation of ~~LIMS;~~ laboratory informatics; and

4.1.7 Provide high-level guidance for the integration of ~~LIMS with the most commonly integrated systems such as laboratory instruments, CDS, ERP, ELN, SDMS and so forth.~~laboratory informatics.

4.2 *How Used*—This guide is intended to be used by all stakeholders involved in any aspect of ~~LIMS implementation~~ laboratory informatics implementation, use or maintenance.

4.2.1 It is intended to be used throughout the ~~LIMS~~ laboratory informatics life cycle by individuals or groups responsible for ~~LIMS~~ laboratory informatics including specification, build/configuration, validation, use, upgrades, retirement/decommissioning.

4.2.2 It is also intended to provide an example of a ~~LIMS function~~ laboratory informatics functions checklist.

5. ~~LIMS~~ Laboratory Informatics Concept Model—Graphic Picture of Systems and Functionality

~~NOTE 1—The LIMS primary functions, integration points, life cycle and industry segments are described in Fig. 1.~~

5.1 ~~*LIMS Concept Model—High Level*—~~*Laboratory Informatics Systems Evolution*—~~The~~Fig. 1 ~~core LIMS functions cover a wide range of laboratory workflows, information management and integration with other enterprise computer systems. These core LIMS functions are illustrated in the LIMS box. Integration with LIMS and a number of external systems, instruments, reporting tools and automated test tools are illustrated by the boxes above and below the LIMS box in~~ shows a timeline for the development of software products designed to meet the needs of the laboratory community. Over time additional software tools entered the laboratory and existing software products added functionality. The expanding breadth of software tools available illustrates the increased functionality and complexity of laboratory informatics solutions. The laboratory informatics solutions/tools illustrated in this figure are examples and do not imply these are the only tools available.~~Fig. 1~~.

5.2 *Laboratory Informatics Systems Integration Concept Model*—Laboratory informatics systems, the possible overlaps between them, and their potential integration with business and enterprise computer systems both within organizations and with customers of laboratory information are illustrated in Fig. 2.

5.3 ~~*LIMS Concept Model—Mid Level*—~~*Laboratory Informatics Functions*—~~The LIMS functions and their relationship with external systems, extended LIMS functions and future LIMS functions is~~ Laboratory informatics core and extended functions are illustrated in Fig. ~~2~~3. The ~~diagram~~figure defines:

5.3.1 Core ~~LIMS functions (LC) with sub-divisions of LC-1.X Operations and LC-2.X Support;~~laboratory functions are described by items listed in boxes labeled with C-x;

5.3.2 Extended ~~LIMS~~laboratory functions are described by items listed in boxes ~~LE-X;~~labeled with E-x;

5.3.3 ~~Systems external to LIMS are illustrated with boxes coded with E;~~Functions related to system configuration, administration and validation are shown with boxes labeled with S-x; and

5.3.4 ~~Future LIMS~~Document support functions are described in boxes ~~coded~~labeled with ~~LF.~~D-x.

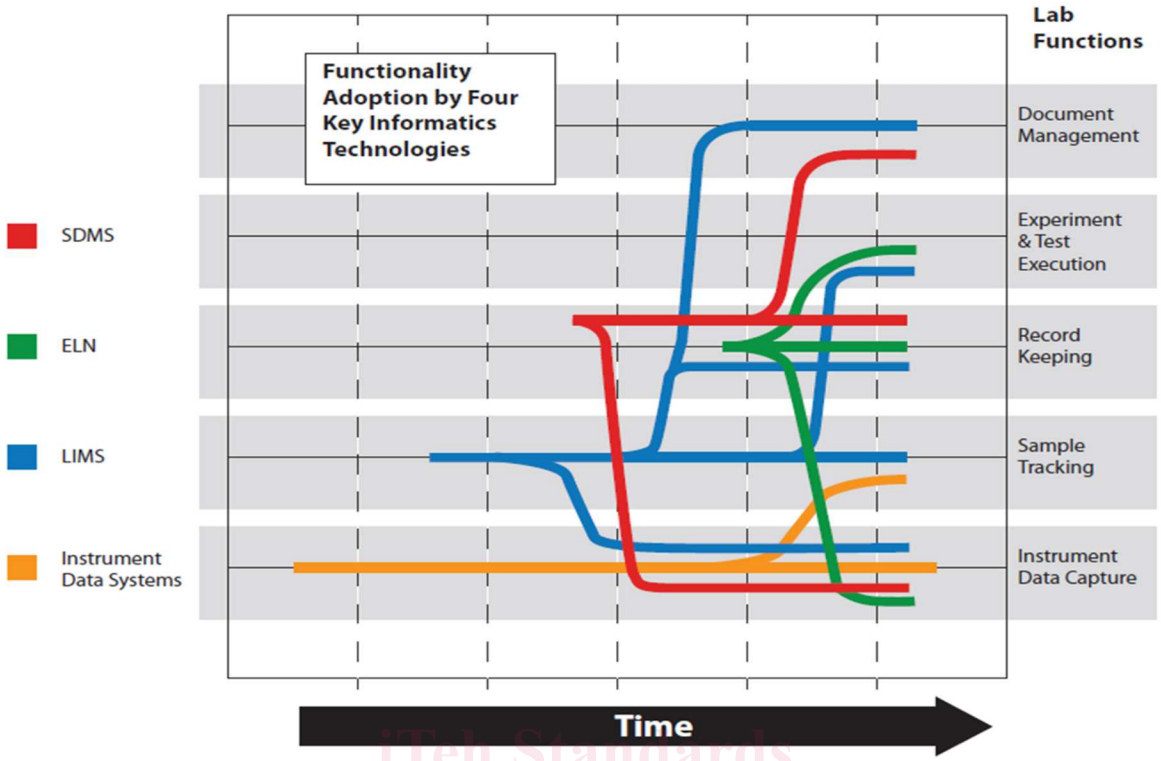

FIG. 1 ~~LIMS Concept Model—High Level~~Laboratory Informatics Systems Evolution

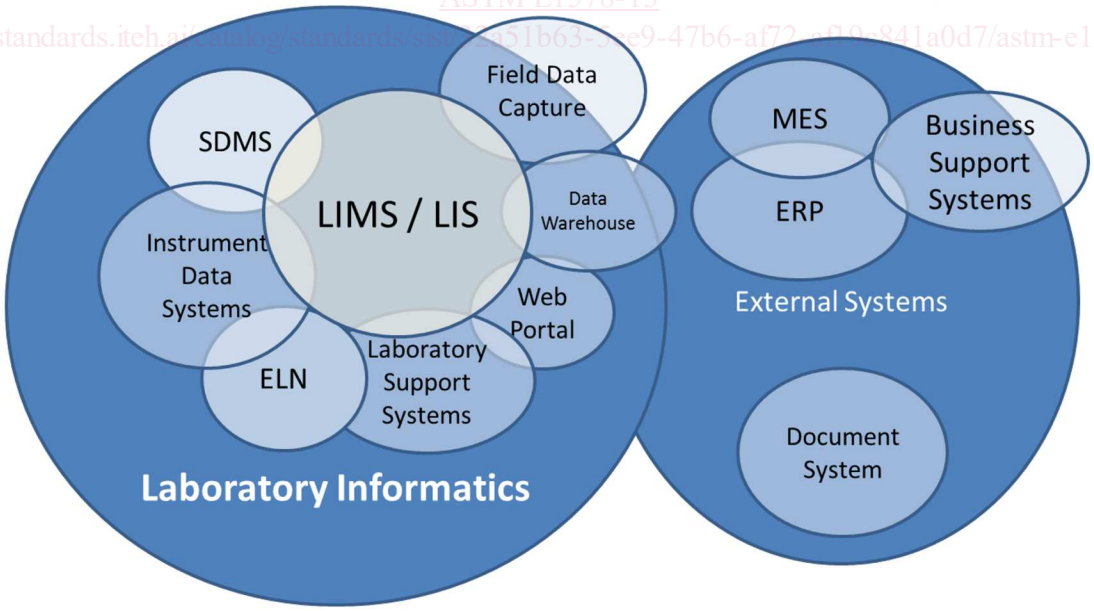

FIG. 2 ~~LIMS Concept Model—Mid~~ Laboratory Informatics Systems Integration Concept Model ~~Level—Requirements Structure~~

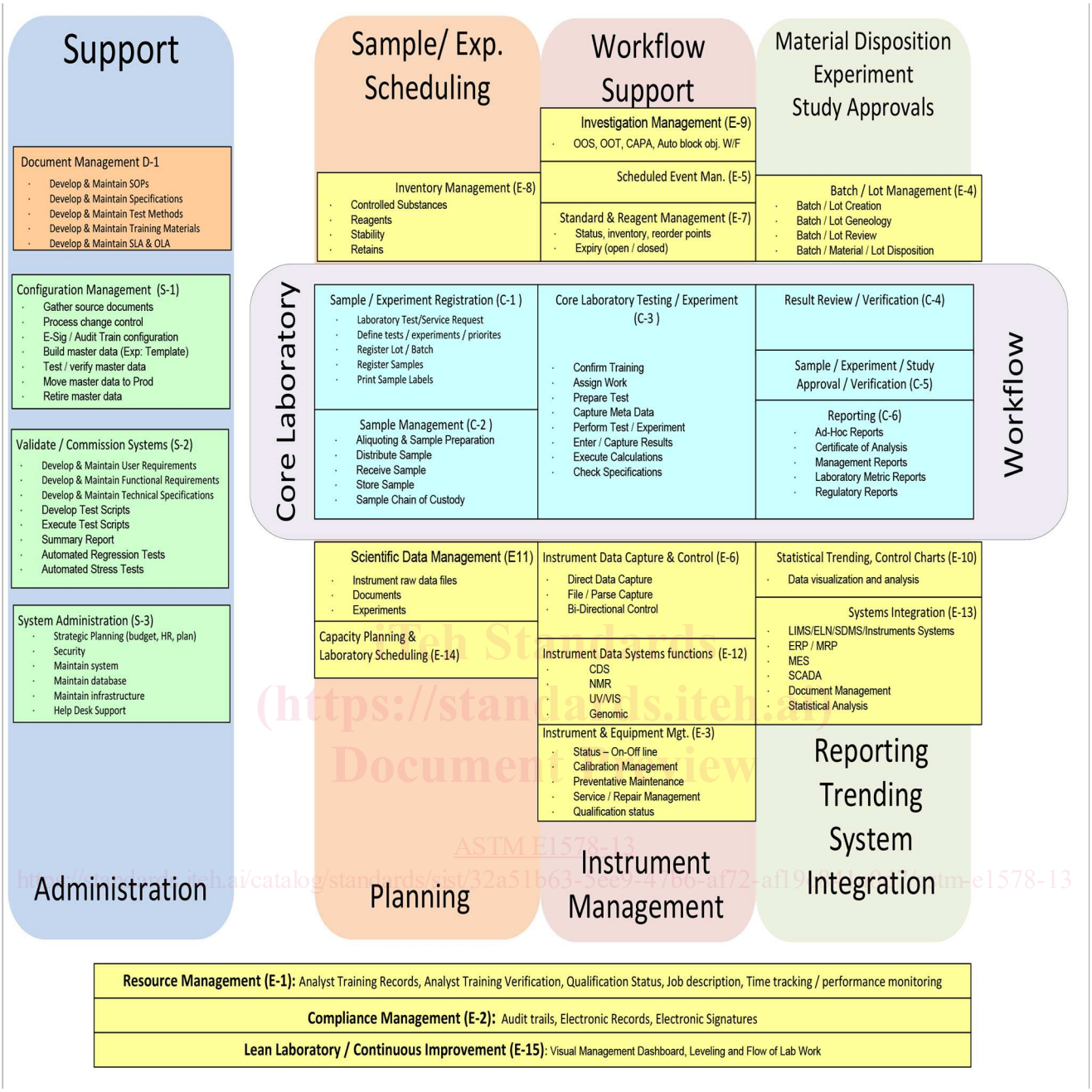

FIG. 3 Laboratory Informatics Functions

5.4 ~~*LIMS*~~ *Laboratory Informatics Systems Life Cycle Phases*—Fig. ~~3~~4 defines the ~~high level LIMS~~ high-level system life cycle phases ~~of~~of: *(1)* initial ~~LIMS~~system implementation, *(2)* ~~LIMS~~system operations, and *(3)* system maintenance. Each of these primary phases is further decomposed into primary functions. The numbering scheme ~~use~~used matches the ~~mid level~~ definitions in Fig. ~~2~~3 and also ~~tie~~ties to the requirements section located in Appendix X1.

5.5 ~~*LIMS Concept Model—Industry Segments—*~~*Laboratory Informatics Additional Functional Requirements by Laboratory Type*—All analytical laboratories require a basic ~~LIMS~~ work flow including sample or experiment registration, assignment of tests, entry of results, review and approval and reporting. Laboratories in various industries may require additional functionality to meet ~~special~~additional workflow requirements. An environmental laboratory, for example, may require tracking of sample containers, processing of samples in batches with control samples, instrument ~~integration to address the number of components reported, and~~ integration, multiple levels of ~~review. There also may be~~ review, and specific reporting requirements. Some laboratory informatics systems vendors gear their solutions towards a particular industry segment, while others attempt to meet the needs of many laboratory types. Fig. ~~4~~5 illustrates some of the additional functions that may be required to address the needs of ~~laboratories in~~

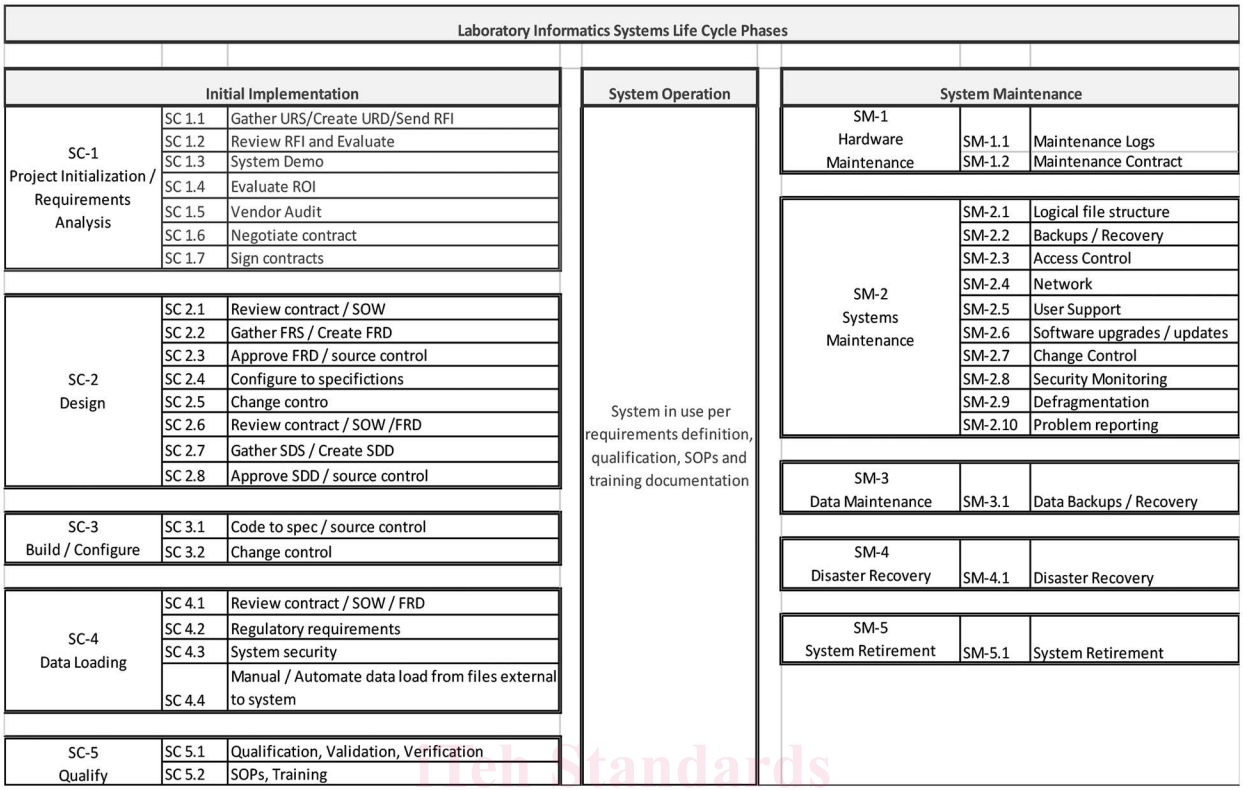

FIG. 34 ~~LIMS~~ Laboratory Informatics Systems Life Cycle Phases

~~particular industry segments.~~particular laboratory types. The functions illustrated ~~would be~~ are over and above the basic laboratory ~~workflow.~~workflow and are by no means an exhaustive list, but merely examples of possible additional functionalities.

6. ~~LIMS~~ Laboratory Informatics Workflow and Sample ~~Lifecycle~~ Life Cycle

6.1 ~~*LIMS*~~ *Laboratory Informatics Workflow Introduction*—The ~~LIMS~~ laboratory informatics workflow model (see Fig. ~~5~~6) provides a generic representation of the process flow in a typical analytical laboratory. The purpose of the work flow diagram is to elucidate the ~~LIMS~~ laboratory informatics functions and interaction points with typical laboratory work processes ~~(processing~~ (that is, processing of samples, analysis, and reporting). Specific laboratory ~~requirements will~~ workflow requirements and test definition may vary widely from one laboratory to ~~another. The definition and composition of a sample or collection of samples will also be specific to an individual's laboratory, and will change significantly from industry to industry. The individual's own laboratory workflow and sample definition should be defined as part of the LIMS life cycle.~~ another, as well as from one industry to another. However, before implementing a laboratory informatics solution, care should be taken to completely define ~~Fig. 5 explains the basic LIMS functions and workflow interactions. The numbers in the parentheses~~ and document the unique requirements and data model for the laboratory in ~~6.2 refer to specific workflow processes (bubbles) in~~question. To achieve a successful deployment and use ~~Fig. 5, which in turn relate to the areas shown in the LIMS concepts models~~ (of a laboratory informatics solution, it shall be properly configured before deployment. The relatively stable information about personnel, customers, tests, reports, and the like, shall be entered into the static data. Once configured,~~Figs. 1-4) in Section 5. To provide clear examples of what may be performed in each of the work flow model functions, items from all levels of the LIMS concept model are used. The description in 6.2 does not include every concept model function and is not limited to a particular level.~~the laboratory informatics solution is able to facilitate the sample lifecycle process. The boundaries of the laboratory informatics solution should be established during the data model design phase.

6.2 ~~*Generic LIMS Workflow—*~~*Laboratory Informatics Data Model*—~~Fig. 5 shows both the logical dataflow through the LIMS process in combination with the corresponding physical sample processes. Each box~~ Defining the correct data model for the laboratory is essential to a successful laboratory informatics implementation and deployment. Many laboratories opt for data models that are procedure centric (that is, test methods are defined from approved external procedures and SOPs) where the requestor selects the appropriate laboratory informatics methods based on a knowledge of which procedures are appropriate for the sample in question. This model relies on the experience of the user and has great flexibility for the R&D laboratory or laboratories where a wide variety of samples are submitted. Other models are sample or product specific (that is, a suite of "approved" tests are bundled together and typically always applied to one sample type), as is typically the case for a QA laboratory

Additional Functions Required by Laboratory Types		Laboratory Functional Area					
		Sample / Experiment Management	**Lab Testing**	**Review, Verification Approval**	**System Integration**	**Reporting and Trending**	**Other Functions**
Laboratory Type	**General Laboratories**	Chain of custody	Batch Processing of Samples including QA		ELN, SDMS, instrument integration	Electronic Reporting of QC Results	
	Environmental	Container management, Chain of custody, regulatory compliance - significant auxiliary data	Batch Processing of Samples including QA	Multiple levels of review and approval	GIS integration	Electronic Reporting of QC Results by batch	Method QA/QC, Calculation validation, electronic data delivery
	Public Health Sector- (clinical microbiology and chemical)	Chain of custody, electronic test ordering, Emergency response, public health surveillance	Batch Processing of Samples including QA, agent regulations	Multiple levels of review and approval, CLIA certification	Emphasis on surveillance at multiple state and federal levels	Electronic Reporting multiple data formats, vocabulary, and secure transport	Clinical and non-clinical, sample centric and patient centric
	Life Sciences	Controlled substances Stability samples	Uniformity Calculations Product Specifications	Multiple levels of review and approval	ERP integration	SPC and Process variability analysis	Instrument maintenanc e and calibration tracking
	Food and Beverage	Lot geneology	Product Specifications		MES and ERP integration	SPC and Process variability analysis	Exception Reporting
	Heavy Industry	Automatic scheduling, Lot Management	Product Specifications		Process Control / PM integration	SPC and Process variability analysis	
	R&D	Experiment sharing	Method versioning		ELN, SDMS, instrument integration	Experiment Conclusions, Technical Reports	Expanded Search capability
	Medical Laboratory	Embedded LIS Standalone LIS Niche LIS Patient centric			interface engines to external systems	Unique functions Diagnostic and Surveillance	electronic medical records; direct clinician access, billing modules

FIG. 45 ~~LIMS Needs by Industry Segment~~Laboratory Informatics Additional Functional Requirements by Laboratory Type

in ~~Fig. 5 is uniquely numbered (cross reference~~ charge of product release. This model removes the dependency upon the requestor to~~Fig. 2 and described in detail in subsequent sections.~~select the appropriate tests when submitting the sample for analysis and improve compliance to testing plans.

6.2.1 *Types of Data*—The technology used by a laboratory informatics solution varies with each vendor and platform. However, laboratory informatics databases are typically divided into two broad areas: *(1)* static data where descriptive information is defined (for example, users, locations, profiles, tests, calculations, specifications, and related information; commonly found in "look up/reference/dictionary" tables) and *(2)* dynamic data where sample and result/determination information is stored as samples are logged and results are entered. The terms static and dynamic represent a general characterization of laboratory informatics data, reflecting the frequency of change. The laboratory informatics implementation team shall assess the current laboratory information

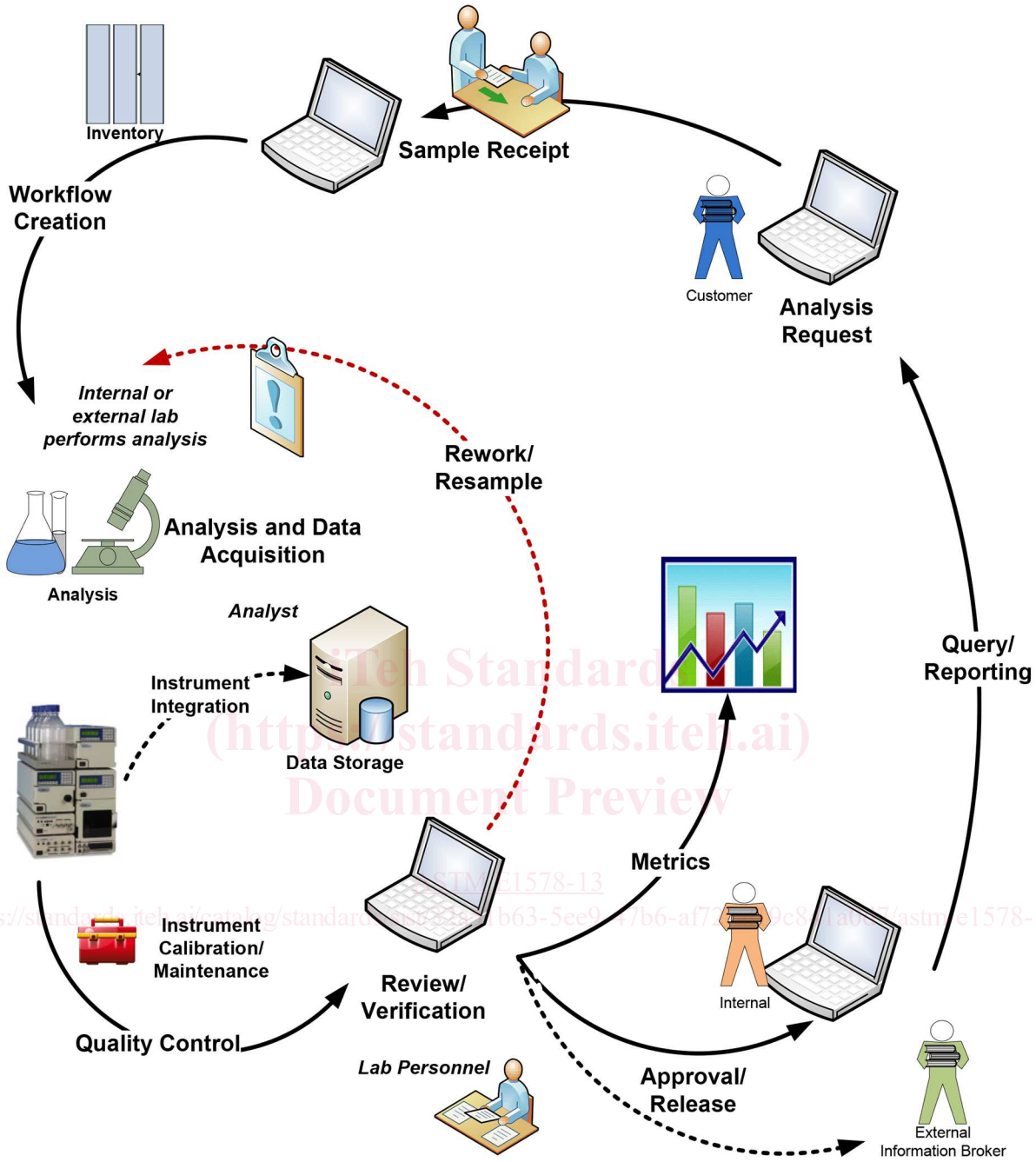

FIG. 56 ~~Generic LIMS~~Laboratory Informatics Workflow Model

organization and workflow in order to match the two database areas (static and dynamic) to the information/data collected, generated or required by the laboratory in order to conduct their laboratory processes, whether that be in processing samples or in general laboratory experiments.

6.2.2 *Statuses*—Laboratory informatics solutions are generally capable of maintaining information on the status of various items, for example, but not limited to: experiments, samples, individual tests/determinations, comparison of results to specifications, verification of results, approval of samples/orders, workflows, and much more. Status values provide the insight with the laboratory informatics solution to track the item's progress in its workflow (that is, active, complete, reviewed, and so forth) and may provide context on the evaluated result (that is, pass/fail). Other status information may be updated as each laboratory informatics transaction takes place. Individual functions/workflows may be configured to have an associated status value. Examples of sample/order statuses include, but are not limited to (and should be reflective of the laboratory's unique workflow): unavailable, available, received in the laboratory, testing in progress, suspended, complete, approved, and rejected. Examples of test/determination statuses include: available, active, complete, approved, out of specification.

6.2.3 *Data Load and Migration*—A laboratory informatics solution is capable of maintaining information for a broad range of business and laboratory data required for the effective operation of the laboratory. Laboratory informatics contains data that not only reflects the current operation state of the laboratory but also historical information on past performance and events. When implementing a laboratory informatics solution in a previously manual environment or replacing an outdated electronic version, it shall be determined how much and of what type (if any) historical data should be carried forward (that is, loaded, "migrated," or re-entered) into the new laboratory informatics solution to provide the base configuration. Static data are generally always loaded into the laboratory informatics solution as part of the deployment lifecycle. The decision on how to deal with historical dynamic data should be evaluated on the basis of risk. Appropriate strategies for dealing with this data include migration, preservation and archival. In cases in which a new solution is replacing an existing laboratory informatics solution, it may be possible to migrate data from the source laboratory informatics solution to the new target deployment. Migration of data needs to be carefully analyzed and planned. The plan should include processes to verify that the data are successfully migrated to the new database.

6.3 ~~*LIMS Functional Areas—*~~*Sample Management and Life Cycle:* ~~The following section describes the generic LIMS workflow steps as outlined in Fig. 5. Each step is described with a cross reference to Fig. 2. The index number show in parentheses refers to both Fig. 2 and the Appendix X1.~~

6.3.1 *Sample Registration*—Sample registration may precede or follow physical sample collection. The laboratory informatics sample registration function should be a simple, straightforward process with an intuitive and efficient user interface. The initiation of a request for testing/sampling generally starts the sample workflow process. Sample requests may include manual forms, electronic forms, phone requests, web requests, process-driven requests, time or calendar-based requests, ad-hoc requests, and system-generated requests. Information obtained from the sample request should include biographical, client, requested test(s), and safety information. Some laboratory informatics solutions allow the laboratory to pre-log or post-log samples or the client to pre-log samples through a web portal.

6.3.1.1 *Store/Retrieve Sample*—An often overlooked benefit of utilizing a laboratory informatics solution is the ability to manage inventories for reference samples, laboratories reagents, standards, QC samples, time-based samples (shelf-life stability), and laboratory equipment/instruments, in addition to normal samples. Inventory functions may provide critical business information with respect to resource and consumables management as well. This could include such information as expiration dates, vendor information, restock quantities, as well as, in the case of instruments; calibration status, maintenance history, and so forth.

6.3.2 *Sample ~~Registration (LC-1.1):~~ Identification—*

~~6.3.1.1 The initiation of a request for testing/sampling starts the process. Examples of sample requests include manual forms, electronic forms, phone requests, web requests, process-driven requests, time or calendar-based requests, ad-hoc requests, and LIMS-generated requests. Information obtained from the sample request includes biographical, client, requested test(s), and safety information. Some LIMS implementations allow the laboratory to pre-log or post-log samples or the client to pre-log samples through a web portal.~~The laboratory informatics solution should assign a unique number to each sample registered (that is, submitted for testing). The unique number can be a system generated sequential integer or a user-defined sequence. Multiple samples, submitted together for registration should be logically "linked" in the laboratory informatics solution (for example, all samples for a particular lot). The system will normally provide functionality to capture descriptive information about the sample(s) such as who submitted the sample(s), costs, sample description, and what tests are to be performed on the sample. Other information may also be important, such as the priority of the tests, what level of accuracy and precision of testing needed, what hazards the sample might present to the laboratory personnel, what approximate levels of components are expected, and what should be done with the sample when analysis is complete.

~~6.3.1.2 The LIMS must first be properly configured and the relatively fixed information about personnel, customers, tests, reports, and the like must be entered into the static tables. After the LIMS is configured, the process begins with a sample registration. The LIMS assigns a unique number to each sample that is registered. The unique number can be a sequential integer or a user-defined sequence. Multiple samples that are submitted together for registration can be logically linked in the LIMS. For example, all samples for a particular customer. The system will normally provide functionality to capture descriptive information about the sample(s) such as who submitted the sample(s), costs, sample description, and what tests are to be performed on the sample. Other information may also be important, such as the priority of the tests, what level of accuracy and precision of testing is needed, what hazards the sample might present to the laboratory personnel, what approximate levels of components are expected, and what should be done with the sample when analysis is complete. Sample registration can precede or follow physical sample collection. The LIMS sample registration function should be a simple, straightforward process with an intuitive and efficient user interface.~~

6.3.2.1 A confirmation report is often issued ~~to ensure users~~ (sometimes emailed) to assure requestors that the system accepted the sample ~~order. LIMS~~ request and may accompany the physical samples as they are delivered to the testing laboratory. Often, laboratory informatics solution statuses are updated for the ~~sample/order. The system needs~~ sample/order and may be used to record the fact that an order was made (for keeping operational metrics) and when it was made so the system can track the time intervals for the remaining steps of the process. This will also allow laboratory management to determine turnaround time, sample status and various overdue conditions.