AQUALYSIS
waterlaboratorium

User requirements specification for Laboratory Information Management system (LIMS)

Version 1.0

HELDER IN WATERONDERZOEK

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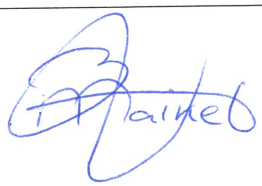
SME	Maikel Broekgerrits	 26-10-2022
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Version history

Version	Date	Description
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0.2	19-oct-2022	Updated after review
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1. Background

Aqualysis is an accredited laboratory for water research. We conduct hydrobiological, bacteriological and chemical research using modern analysis techniques. To manage the information workflow a Laboratory Information Management System (LIMS) is used. The current LIMS (QMA) application dates from 2007 and is no longer supported by updates/upgrades. This is a liability for the business continuity and the system is in need of replacement.

2. Purpose

The purpose of this document is to specify the user requirements for LIMS for use at the Aqualysis Facility.

The User Requirement Specification (URS) captures the business needs. It describes the features or capabilities needed to meet the business goals and objectives of the Laboratory information management system

This User Requirements Specification provides a basis for:

- Communicating the expectations of the solution to the vendor.
- Providing a platform for system design, configuration, build and testing; The URS is the basis for the functional specification that specifies how the required functionality is implanted.
- Identification of requirements subject to validation / qualification testing
- Contractual agreement between Aqualysis and the supplier.

3. Process Description

For a detailed process description refer to the document: "Processen en Functionaliteiten LIMS"

4. Abbreviations

Term	Definition
ELN	Electronic Laboratory Notebook
DTAP	Development, testing, acceptance and production
URS	User Requirement Specification
CoA	Certificate of analysis
SOP	Standard operating procedure
OOS	Out of Specification
OOL	Out of Limit
CLE	Confirmed Laboratory Error
CET	Central European Time
QMA	Quality Manager Aqua
SME	Subject Matter Expert
Aquo	The Aquo standard (Aquo) is a Dutch standard for the exchange of data within the water sector

5. Requirement Definitions

Below are the definitions for business priority designation

Priority	Meaning
H	Mandatory: critical business process requirement, regulatory requirement, direct impact on quality
M	Beneficial business process requirement, indirect impact on quality
L	Nice to have improvement

The supplier must adhere to the content of this document; any deviations proposed must be clearly identified and justified by the supplier. Compliance with the agreed contents is a contractual requirement of the purchase order and any costs associated with meeting the agreed requirements must be included in the purchase price.

6. System Requirements

Requirements are grouped per topic.

6.1 Regulatory Requirements (RE)

Req.No.	Description of the Requirement	Priority
RE001	The system must be fully compliant with NEN-EN-ISO/IEC 17025 requirements	H
RE002	Written procedures must be provided for the operation and maintenance of the computerised system	M
RE003	Audit trail records must be read only. They shall not be editable, and shall be protected from accidental or intentional deletion or modification.	H
RE004	Authorized user must be able to configure reporting templates according to Aquo rules, facilitating exchanging of data conforms Aquo standard.	H

6.2 General Requirements (GR)

Req.No.	Description of the Requirement	Priority
General		
GR001	The system must be Commercial of the Shelf (COTS)	H
GR002	The system must provide functionality to transfer newly developed functionality or static data from one environment to the other in a controlled manner (DTAP approach).	H
GR003	The system must provide a mechanism to allow a customer read-only access to stored data. (Customer is only able to see own data)	H
GR004	The system must be accessible through the network of Aqualysis	H
GR005	The system must be able to manage (import, export, reports or as an attachment) different file types (e.g. pdf, xlsx, CSV txt, or JPEG)	H
GR006	The system should contain functionality to automatically alert or notify users of required actions through email	M
GR007	An authorized user should be able to expand the standard statuses in the system with user-defined statuses that can be used in the configuration of the workflows	M
GR008	The system should contain the possibility of introducing an Electronic Laboratory Notebook (ELN) (or equivalent) functionality to facilitate paperless workflows in the future.	M
GR009	It should be possible to configure different workflows for different sample types. (e.g. Hydrobiologie, Chemie)	H
GR010	It should be possible for the system to validate user input in fields against configured (field) limits. (e.g. a pH measurement result entry cannot be lower than 1 or higher than 14)	L
GR011	The system must be installed using Dutch as the base language.	M
GR012	The system should provide Offline Mode functionality to address sampling areas that are not internet enabled	M
GR013	The system must be able to cope with different price units (Euro/Points)	H
GR014	Authorized user must be able change object status (e.g. project cancellation/reactivation)	H
GR015	It must not be possible to delete data from the system, it should only be possible to deactivate data by changed the status to: (e.g canceled, rejected, disable)	H
GR016	Authorized user must be able to manage access using role-based access control	H

6.3 Operational and Functional Requirements (FU)

Req.No.	Description of the Requirement	Priority
Customer		
FU001	Authorized user must be able to create a customer	H
FU002	A customer must contain (but not limited to) the following customer information: • Customer name • Customer description • Status • Customer group • Billing information like: - Taxes information - Debtor account number	H
FU003	The system should contain customer portal functionality to facilitate: - Project planning initiation from the customer site - Project reporting like: o Project progress report o Project annual reports	M
Project		
FU004	Authorized user must be able to create a project	H
FU005	Authorized user must be able to create a sub project	H
FU006	A project must contain (but not limited to) the following project information: • Project code • Project description • Status • Project type (Parent/Child) • Contacts • Project attributes like: - Project start date - Project end date - Client - Fixed project price - Project reduction (%) - Project raise (%) - Project priority - Samples delivered by • Billing information: - Price per Point - Price UOM - Transportation costs - Invoice Reference - invoice frequency - invoice validity period - Taxes information • Reporting information: - When to report - Reporting methods	H

Req.No.	Description of the Requirement	Priority
Planning		
FU007	The system must contain planning module or have equivalent functionality	H
FU008	Authorized user must be able to import planning data into the system by direct import of (data) file types: e.g. excel, CSV, txt, xml.	H
	The system must have the ability to generate an daily, weekly, or monthly planning data, including sampling ranges based on existing object data, like (but not limited to): - Client - Project code - Sampling frequency - Sample-code - Description - Sampling location - Coordination (WGS84) (x y) - Sampling date and time - Sampled by AQL (YES/NO) - Sample priority - Sample start date and time - Sample end date and time	L
FU009	It should be possible for authorized users to adjust the plan period	M
FU010	The system must have the ability to generate status for the data sent to the planning tool (ServiceWare) used by AQL	M
Sample reception		
FU011	The system must be able to use the barcode on a label to trigger automatic actions in the system. For example, sample receival by scanning a barcode.	H
FU012	Authorized user must be able to change the priority of a sample	H
FU013	Authorized user must be able to change the priority of a analysis	H
FU014	Authorized user must be able to import data/information/results into the system by direct import of (data) file types, e.g. excel, pdf, CSV, txt, xml.	H
FU015	It should be possible for a user to generate an automatically filled request letter for an external lab when a sample or analysis for an external lab is received.	M
FU016	The system should be able to provide a comprehensive view of all projects, samples and analysis in the system, using a color-coded status view of the current and scheduled samples through user-configurable templates, all without requiring additional programming.	M
FU017	The system should be able to generate an incremental lab-number when sample is received	M
Analysis		

Req.No.	Description of the Requirement	Priority
FU018	The system should be able to give an automated warning to pre-defined users when all samples of a specific project have been taken. (Not yet received)	M
FU019	The system should be able to give an automated warning to pre-defined users when all samples of a specific project have been analysed and are approved	M
FU020	It should be possible for users to get an overview of unperformed analysis, and an overview of performed analysis, pending or approval, sorted by due date and priority.	H
FU021	The system must automatically generate a report containing results of analysis according to a pre-determined template. (CoA, not containing all analysis of the sample, but only pre-defined analysis).	H
FU022	It should be possible for an analyst to generate a configurable structured list of work ("analytical batch") to perform.	M
FU023	Authorized user must be able to initiate a repeat or re-analysis of an analytical batch or an individual analysis when the analysis has failed internal controls (invalid analysis).	H
FU024	The analytical batch must contain standard and reference samples (Control samples / Blanco's) if so configured.	H
FU025	The sequence of the samples, standard and reference samples should be defined in an configurable template for the analytical batch.	H
FU026	Authorized user must be able to remove or add a sample or analysis from an analytical batch.	H
FU027	Result fields must allow at minimum the following: - numerical, alpha-numerical, or pre-set values.	H
FU028	Authorized user must be able to configure rounding rules on result fields. The non-rounded input must be retained as well for calculation purpose	H
FU029	Authorized user must be able to configure different conservation date for different sample types.	H
FU030	Authorized user must be able to configure different conservation date for different analysis	H
FU031	When a user has entered a result, it should be possible to automatically round to a pre-configured number of significant numbers.	M
FU032	Authorized user must be able to re-enter results. Both the old and the new version must be retained. A justification for the change must be mandatory	H
FU033	Out of trend rules should be configurable by authorized users.	H
FU034	The detection limit should be configurable by authorized users.	H
FU035	It should be possible for the system to automatically add an analysis to a sample based on a result from another analysis.	L
FU036	It should be possible to generate a report listing all samples to be discarded	M
FU037	It should be possible for users to assign a storage location to samples.	L
FU038	It should be possible to configure groups of analysis and assign the group to a sample.	M
FU039	It should be possible for authorized users to add extra analysis to a sample.	H
FU040	It should be possible to configure a sequence of analysis, making sure that one analysis is performed before another.	L
FU041	Authorized users must be able to change or add extra information to a sample or analysis. (e.g. comments, or attachments)	H
FU042	It should be possible to select default pre-programmed comments and add to a sample or analysis.	M
FU043	It should be possible to add internal comments to a sample or analysis which is not visible for users with visitor (read-only access) role.	M
FU044	Authorized user must be able to configure a workflow for ad-hoc analysis	M
FU045	The system should be able to group ad-hoc analysis requests based on extra information like a project/ description number so that it is visible in the system that they belong to the same request, project.	L
FU046	The system must indicate the volume or quantity that needs to be sampled for each analysis	H
FU047	It should be possible to add the necessary packaging to an analysis	M
FU048	The system should indicate the storage condition for the sample. And max hold time if needed	M

Req.No.	Description of the Requirement	Priority
FU049	It should be possible for users to assign priority levels to, samples and analysis that need to be performed.	M
FU050	It should be possible in the system to split samples into pre-configured sub samples.	M
FU051	It should be possible to link different samples together, whereby reporting only follows when all samples have been approved by the supervisor.	M
FU052	User-input fields must be set to read-only after approval workflow steps have been performed.	H
FU053	Authorized user must be able to change the status of a sample (e.g. from approved to online or from online to pending)	H
FU054	Authorized user must be able to change the status of a analysis (e.g. from approved to online or from online to pending)	H
FU055	It must be possible to specify if the analysis is performed by an external lab	H
Specifications		
FU056	The system must visually signal out of spec and out of limit results on analysis and component level.	H
FU057	The system should be able to send notifications to specific users when out of specification or out of limit results are found.	M
FU058	It should be possible to configure a value that is displayed by the system when an entered result is outside of a detection limit (for example '<20' when the limit is 20 and the entered result 18)	M
FU059	It should be possible for the system to automatically check results against "out of trend" situations and visually signal the end-user that an out of trend has occurred.	M
FU060	The system should automatically check against detection limits when a result is saved.	M
Trending		
FU061	The system must automatically process control sample results into a configurable Control chart.	H
FU062	The system must be able to apply control chart rules, (NEN6603) with associated statistical calculations such as F and T testing and uncontrolled quality.	H
FU063	The system should be able to apply Z-control chart rules according to: NEN6603	M
FU064	It must be possible to configure automatic actions when an out of control is detected by the system.	H
FU065	It should be possible to classify out of control results as systematic or incidental. In addition the option to include or exclude results from the statistics.	M
Sample management		
FU066	The system should provide functionality for inventory and management of chemicals, reagents and other consumables.	M
FU067	The system should provide functionality for inventory and management of standards and control samples.	M
FU068	Standards and control samples should not be selectable for use in the system without warnings if their expiry date has passed.	M
FU069	The system should be able to automatically warns if the expiry date has passed for Reagents and chemicals	M
FU070	The system should be able to automatically warns specified users when inventory counts reach a definable threshold and either prompt for or process a reorder	L
FU071	The system should include comprehensive scheduling, tracking, and flow management of samples	M
FU072	The system must be able to determine whether the preservation period has been exceeded on the basis of the date of sampling and date in progress and make a comment on the report.	M
Instrument management		

Req.No.	Description of the Requirement	Priority
FU073	The system should contain configurable instrument inventory and management functionality	M
FU074	The instrument inventory should support a hierarchical structure of instruments with different parts, configuration items or priority	L
FU075	It should be possible for authorized users to configure the instruments with different parts or configuration items with their own calibration and maintenance dates.	M
FU076	The system should provide functionality for maintaining an electronic logbook for the instrument.	M
FU077	It should be possible for authorized users to configure and schedule other actions than maintenance and calibration. For example, periodic review	L
FU078	It should be possible for authorized users to configure extra information fields in the instrument/computerized system inventories.	L
FU079	It should be possible to display a forecast of scheduled actions for all instruments per time period (for example in the next month).	M
FU080	Scheduled equipment actions that have not been performed should be visible in the system.	M
FU081	It should be possible to configure a reference between equipment and the analysis it is used for.	M
FU082	It should be possible for users to execute actions like calibration and qualification directly from the instrument management functionality	L
FU083	The system should be able to track and report on the usage of attached laboratory instruments.	M
Deviations		
FU084	It should be possible to configure LIMS deviation records of different types to facilitate different workflows. Types should include OOS/OOL and CLE (confirmed laboratory error).	L
Calculations		
FU085	Authorized user must be able to configure calculations that use all data fields ("Inter-analysis calculation")	H
FU086	The system permits user-generated and modifiable (for authorized user) calculations to be applied to analysis if required	M
Analyst Qualifications		
FU087	Authorized user must be able to grant authorization to analyst to perform particular analyses (e.g. based on gained qualifications)	H
FU088	Analyst qualifications should be updatable according to configurable business rules.	M
FU089	Records containing analyst authorisation history in the system should be available and maintained	M
Invoicing		
FU090	The system should be able to automatically generate invoice when analysis is finalized. (analysis are completed and COA (Analyse rapport) is sent)	M
FU091	The system should be able to automatically generate E-invoice when analysis is finalized. (Analysis are completed and COA (Analyse rapport) is sent)	M
FU092	Authorized user must be able to manually generate invoice when analysis is finalized. (analysis are completed and COA (Analyse rapport) is sent)	M
FU093	Authorized user must be able to configure invoicing rules for different projects.	M

6.4 Data Migration Requirements (DM)

Req.No.	Description of the Requirement	Priority
DM001	It should be possible to migrate existing static data to the new system	M
DM002	It should be possible to migrate existing dynamic and static data through validated tools facilitating a mass data load.	M

6.5 Audit Trail Requirements (AU)

Req.No.	Description of the Requirement	Priority
AU001	The electronic audit trail must be generated automatically	H
AU002	The audit trail must be human readable.	H
AU003	The audit trail must record the identity of the operator, the action that creates, modifies or deletes electronic records, including any changed values (old and new), justification or reason and the date and time of the action.	M
AU004	Audit trail entries must be protected against change or deletion by any individual.	H
AU005	The system must have the ability to generate accurate and complete copies of audit trail records in both human readable (printable) and electronic form	H
AU006	Time of the audit trail must be related to a predefined time standard used on the (application/database) server.	M
AU007	The audit trail must be readily available for inspection (review).	M
AU008	The system should record all login attempts whether successful of not.	M
AU009	There should be functions available to make queries on the audit trail to be able to provide the exact filtered information needed.	H
AU010	The audit trail should contain all changes to master data with user stamp and timestamp	H

6.6 Human Interface Requirements (HU)

Req.No.	Description of the Requirement	Priority
HU001	The system should be configurable to only show those menus, functions and data that are required for the user role(s) of the user that is logged in to the system.	H
HU002	The system should be able to automatically retain entered information in an individual field after the press of the "enter/return" button.	L
HU003	Entered information on a page is committed to the database after a press of a "save" button.	M

6.7 Reporting Requirements (RE)

Req.No.	Description of the Requirement	Priority
RE001	Authorized user must be able to configure templates for standard reports, Invoice, Certificate of analysis or labels.	H
RE002	Authorized user must be able to configure reporting rules for different projects.	H
RE003	It should be possible for authorized users to configure templates for analysis results reporting.	M
RE004	It should be possible for authorized users to configure templates for ad-hoc reporting.	L
RE005	It should be possible for authorized users to configure KPI's and dashboard with (management) information within the application interface.	M
RE006	The data accessible for building reports, KPI's and dashboards should at minimum be the same as the data accessible for end-users.	L
RE007	It should be possible for a report to contain attached documents for example the underlying raw data.	L
RE008	It should be possible to obtain clear printed copies of electronically stored data..	M
RE009	It should be possible to automatically or manually print reports.	M
RE010	It should be possible to export reports to file formats (secure) e.g. pdf, docx, xlsx. Txt. HTML	M
RE011	It should be possible to automatically email reports to a distribution list defined in the project profile	M
RE012	It must be possible for reports to be versioned. One version can be printed multiple times, but regenerating the report changes the version.	H
RE013	The regenerated report must contain the following: - Reason of regeneration - Version number	H
RE014	It should be possible for end-users to use templates with predefined queries and filters to search for and select data in the system.	M
RE015	It should be possible to export the result from a search to a file.	M
RE016	It should be possible to generate graphical (trend) representations (graphs or charts) from selected data.	L
RE017	It should be possible to drill down in to underlying data by clicking on data point in graphs generated by the system.	L
RE018	It should be possible to automatically or manually generate labels containing user-configurable information, during every part of the workflow.	M
RE019	A trained LIMS administrator/key-user must be able to create templates, custom fields and user-role-based user-interfaces in the system.	H
RE020	A trained LIMS administrator/key-user must be able to create reports in the system.	H
RE021	The system must be able to generate concept reports (for not yet finalized projects, samples or analysis)	M

6.8 Security, Electronic Record and Electronic Signature Requirements (ES)

Req.No.	Description of the Requirement	Priority
ES001	The system must restrict access to authorised individuals.	H
ES002	Records containing information about which users have access to the system must be available and maintained	H
ES003	Users must access the system through a unique personal user account.	H
ES004	When a user account has multiple roles, it should be possible to automatically assign all roles.	M
ES005	Printouts should show all current and valid electronic signatures on paper copies of the signed record.	M
ES006	Authorized user must be able to revoke or disable users authorizations.	H
ES007	Record changes must not obscure previously recorded information.	H
ES008	It should be possible to configure mandatory input of a reason for changes to data.	M
ES009	It must be possible to secure PDF exports against editing after they have been generated.	L
ES010	Data must be secured by both physical and electronic means against damage.	H
ES011	Stored data must be checked for accessibility, readability and accuracy.	H
ES012	Access to data must be ensured throughout the retention period.	H

6.9 System Interface Requirements (IN)

Req.No.	Description of the Requirement	Priority
IN001	It should be possible to import results from an external lab in an electronic format.	M
IN002	The system should be able to interface with a third-party reporting application. e.g. Crystal Reports	M
IN003	The system must be able to bilaterally interface with analytical instruments and related software.	H
IN004	Computerised systems exchanging data electronically with other systems must include appropriate built-in checks for the correct and secure entry and processing of data, in order to minimize the risks.	M

6.10 IT (Infrastructure) Requirements (IT)

Req.No.	Description of the Requirement	Priority
IT001	The system must support multiple printers and be configured in such a way that users can choose the printer to print	H
IT002	It should be possible to configure a maximum idle time after which the current user session is automatically closed.	M
IT003	A backup and restore procedure must be in place.	H
IT004	Security monitoring must be in place to log failed signature / identification authentication.	H
IT005	Security logs must be retained in such a way that they are readily available for review.	H
IT006	The system should have the option of Two factor authentication.	M
IT007	The system must be able to integrate with Aqualysis site Active Directory (AD)	H

7. Scope of Supply (SC)

Req.No.	Description of the Requirement	Priority
SC001	The supplier must provide system installation and qualification services. All testing of critical items carried out by the supplier must be carried out following pre-approved protocols and test sheets witnessed by Aqualysis (where appropriate).	H
SC002	Training and education programs must be made available to understand the full functionality of the system (including e.g., software, on-line help and tutorials). Vendor will provide training of Aqualysis personnel in: • Technical (IT) training • LIMS Administrator training • Master data management training • User training Training certificates must be provided to all Aqualysis participants	H
SC003	The supplier must provide at least one user and administration manual along with the system	H
SC004	Supplier maintenance contract should be in place offering telephone support during office hours (CET)	H
SC005	The supplier should provide a method for periodic preventive maintenance scheduled with intervals and a manual.	M
SC006	The warranty must be at least 12 months long after documented final acceptancy of fully functional system by Aqualysis (maintenance agreement).	H

8. Related & Referenced Documents

The following documents were used as a basis for developing this User Requirements Specification.

Document Title
Processen en Functionaliteiten LIMS V1.0
Rapportage LabInfoScan Aqualysis V2.0
Projectplan Aanloopfase QM-AquaLims V1.0

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