Labsafe version 0.8, R.: 2023.06.22

Contents

Software, requirements and configuration

Software description

The software provides a web-based interface for:

- Emergency report regarding the safety hazards at any particular location with visual map interface helping to quickly locate adjacent locations. The report also shows any running experiments that are affected by the infrastructure failure, like power outage or other incidents
- Initiating purchase of chemicals from external suppliers through internal stores with steps of order authorisation, purchasing and delivery
- Material safety datasheet parsing for the most common suppliers. This is done to extract specific safety hazards for safety reports and storage analysis
- Manual chemical safety assessment that can be used in the system for the analysis of incompatible chemicals
- Tracking the chemicals internally using barcodes
- Purchasing chemicals and stationery/consumables from the internal stores
- Email alerts on order delivery and authorisation of purchase of categorised compounds
- Searching chemicals by name, sub/structure, CAS number inside the user locations or the whole database
- Controlling chemicals visibility – group/department/site
- Grant expenditure reports
- Internal stores stock control and reports
- Storage chemical compatibility analysis
- Location chemical auditing
- Storage content analysis for incompatible materials when transferring chemicals
- Chemical experiment planning – with currently running experiments showing up in the safety report for the location
- Experiment protocols describing the complete experimental procedure that can complement experiment plans

System requirements

Disk space: 50Gb for up to 500k records

Memory: 2Gb min

Environment and required software

Java virtual machine with JDK v 8 or later

MySQL database v 5.5 or later or PostgreSQL

Glassfish server open-source edition v4.1.2[1], Payara or Tomcat server

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[1] Note that a few files have to be updated for Glassfish server – jboss-logging.jar to a new version and manifest fixed for org.eclipse.persistence.moxy.jar; Payara server works out of the box

Apache webserver v 2.4 or later – optional for http/s access and routing. This will require mod_jk to be installed and configured to communicate to the Glassfish server.

Component configuration

MySQL database has to be preconfigured for the software to run; for this 3 database schemas have to be created:

- osadmin – this schema holds user and location related data
- oschemicals – the COSHH software and stores shop schema
- oslims – the laboratory information management schema
- osassets – the assets management schema
- osinspection – the asset inspections schema
- ostranslation – the translation schema

A limit on the packet size should be set in the configuration file to 16Mb and the case-insensitivity enforced using the following values under 'mysqld' section in the configuration file:

lower_case_table_names = 1
max_allowed_packet=16M

The access to these schemas should be given to the account specified in the {application folder}/WEB-INF/classes/hibernate.cfg.xml file using the 3 properties listed below:

```
<property name="hibernate.connection.url">
  jdbc:mysql://localhost:3306/?zeroDateTimeBehavior=convertToNull
</property>

<property name="hibernate.connection.username">
  oslims_admin
</property>

<property name="hibernate.connection.password">
  password
</property>
```

These values can be set externally using the following system variables:

LABSAFE_DB_URL, LABSAFE_DB_USERNAME and LABSAFE_DB_PASSWORD respectively.

Data file storage

As the system ages and accumulates various files (BLOBs), it is recommended to offload these files onto the hard disk and backup separately. The offload location can be setup under the "Site specific" settings and the storage analysed under in the "File storage" tool under the "System administration". The tool provides information about the size of the files on the hard disk as well as the size of BLOBs in the database.

Offloading BLOBs significantly shortens the time needed for the database backup.

Installation

The program installation is done by deploying the application archive to the applications folder. This could be achieved using a web interface to the Glassfish server or from an SSH connection by uploading the "war" archive to the autodeploy directory of the Glassfish server.

Setting up single sign-on

To set up the system to accept single sign-on at first the certificate and the private kay have to be generated:

openssl req -x509 -sha256 -nodes -days 7300 -newkey rsa:2048 -keyout sso.key -out sso.crt

The key then needs to be converted to the Labsafe supported format:

openssl pkcs8 -topk8 -nocrypt -inform PEM -outform DER -in sso.key -out sso.der

Make sure that the certificate file does not have the comments at the beginning and the end. Upload the generated file to the system, refresh the page and download the SSO service provided metadata.

Running the software

After the first installation, when the database is empty, the software will provide institution and user registration pages. The first registered user becomes the system administrator. Any consequent user registrations will require the account activation and authorisation by one of the existing accounts (a group leader or an administrator).

Application structure

Overview

The application provides multi-tiered access to the underlying data and provides clear role separation to perform specific tasks.

The administrative part relating physical locations and user account is shown in Diagram 1. Each user account can be associated with a set of groups and each group with a single institution and a set of locations. The locations can be shared by a set of group. Each of the locations shared with a group will be later referred to as 'Group's locations'.
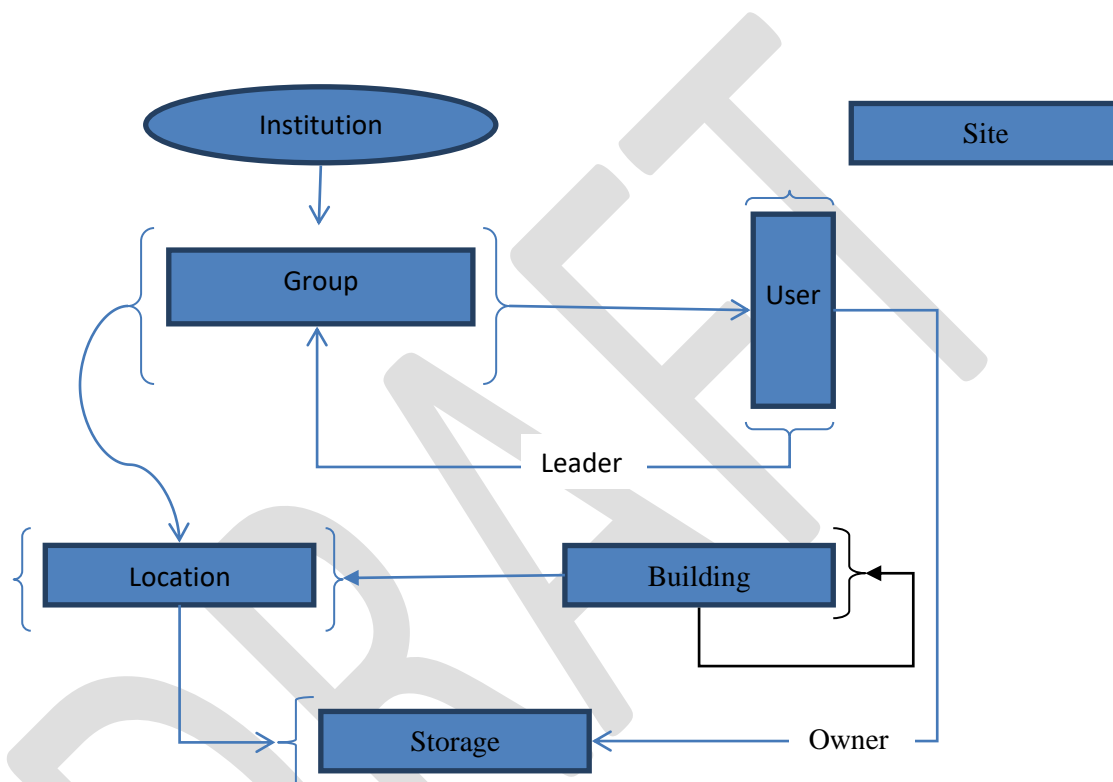
Diagram 1. Hierarchical view of the user account and locations

The chemicals are stored in cabinets ('Storage' in Diagram 1) which could be shared between the groups at the location or to be owned by groups of one of the PIs.

User interface elements

The main aspects of the system are listed in the software description section. The user interface is provided for all of the features described, but accessibility to each feature is controlled by the user roles as described below.

User roles

Standard user	- register or transfer a compound - place an order to stores - search for compounds by name/structure/substructure
Group leader	as above + roles of Groups and Location administrators
System administrator	- as above

	- administer users, locations, chemical suppliers, chemical lists, safety records, disposed compounds etc

User account statuses

Active	The only status when a user can interactively log in to the system
Inactive	The user whose role is undecided – typically a user who has just been registered and who has not yet activated the account through the email activation link. If the user was added by an administrator – they have to try to 'login in' in order to receive the activation link
Unauthorised	Users who activated their account, but who have not been confirmed by any of the group leaders or administrators
Expired	The account reached the expiration date
Blocked	The account is blocked

Associative user roles

These roles can be assigned to any user in a department.

Department administrator	This role allows the person to manage the administrative layout of the department
Building administrator	This role allows the user to manage the physical layout of the building. It is typically to be combined with the role of the department administrator
Safety coordinator	This role allows approving the student research projects and manages safety aspects of the system and training
User administrator	This role gives the user the access to other users' accounts to modify basic information and also to approve visitor records
Financial administrator	Deal with financial data and reports
Purchase manager	Process purchase orders
Order delivery manager	Accept goods and mark orders as delivered and collected. Users with this role can also cancel orders that have been processed automatically.
Stores manager	Deal with internal Stores stock management
Tutor	The user becomes a tutor when they are associated with any of the training course by system administrators or safety coordinators. The role implies making staff attending some training course
Room delivery manager	A person who gets notified when an order is ready to be delivered for the designated room
Inspector	The user becomes an inspector when there is any scheduled asset inspection to which they have been assigned.
Group administrator	Manage group users
Location administrator	Manage location storage cabinets

Populating the database

There are two ways to populate the database using the user interface.

Registering existing chemicals

 The first route to populate the database is to register a chemical. The process is initiated by uploading a MSDS or providing a CAS number. For existing safety records, the view will change according to the user role: the administrators will be allowed to <u>edit</u> the records, whereas the user will simply <u>see </u>the record details. If a CAS number does not exist – the system will generate one and provide the safety record editing form, regardless of the user role.

Purchasing new chemicals

The second method should be used for ongoing purchases and allows combining basic grant expenditure calculation alongside the COSHH management. The order is initiated by choosing the funding account, order destination and the chemicals supplier. Then order lines are created in a process very similar to the existing compound registration, with some extra input like the compound price and catalogue number. A similar method can also be used to place an order on the internal stores system.

For consistent results, when generating an order request, it is recommended to use prices exclusive of tax. The tax on the expenditure then will be available as a separate column.

Internal purchasing through the stores

The process of internal purchasing is somewhat simpler than purchasing of the chemicals externally since the system contains all the required information about the stock items and no extra user input is required. There are several 'shortcuts' can be implemented by system administrator/PI when performing the purchasing:

- the order gets automatically authorised when it contains items that require no authorisation and when it is under a certain amount (££) - set by PI
- the order gets automatically "completed" when the items are stored externally to the stores – e.g., liquid nitrogen or solvents

Interaction with external webservers

In order to aid users with the data input/search there are several functions that allow the user interacting with the CACTUS server to retrieve CAS number(s) for the diagrams and to resolve chemical name and chemical drawing from a CAS number.

Labsafe can interact other instance of Labsafe to update safety information. Both system administrators are required to exchange public RSA keys to establish a connection. There is fine-grained control over accessible endpoints.

The order flow

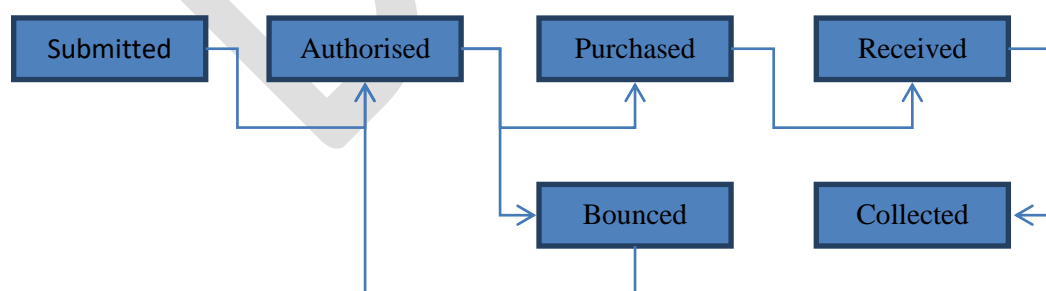Once the order is placed for approval it follows the process shown in Diagram 2.

Diagram 2. View of the chemical order flow

Each order has an available comment field to alert the person handling the chemicals (e.g. – 'on delivery place into the fridge') as well as the fact that the order may have attached files containing quotes or related documentation required to set up the purchase. Chemicals from orders having a

comment will be highlighted in the list of the expected in-coming chemicals. The order comment can be edited until the order is received at stores. Once the order has arrived in stores, an email notification will be sent to the user who placed the order, and the goods will be available for collection.

After the order is authorised, it can be either marked as purchased or bounced. If the order is bounced – the submitter/group leader/admin can cancel the order or review it and resubmit. Cancelled orders are not automatically removed from the system and can be seen when changing the Order table status filter to 'Cancelled' (they do not appear when the filter is set to 'All'). Cancelled orders still can be edited and re-submitted.

Any chemical that has been purchased is set a default expiry date 4 years after the purchase date. The default expiration time can be adjusted on per safety record basis and can be changed by the user for new safety records or by admins for the existing ones. The 'time expired' compounds are colour-coded in the chemical lists and can be quickly identified. These compounds can be either disposed of or a new expiry date set by the group leader/PI.

CAS entries and Safety Records

Each of the catalogue items must be associated with a CAS entry to mark it as a chemical. Each of the CAS entries may have several names identifying them (like methylbenzene and toluene) and this refers to the Safety Record which is typically based on an MSDS. The safety records contain a list if the GHS clauses that are typically extracted by the system automatically, but also these can be edited by the user for new records and the existing records can be edited by administrator. The relation between the catalogue item, CAS entry and Safety records is illustrated in Diagram 3.

Whenever the user purchases a chemical, the system looks up for a catalogue item or a CAS entry with the similar item name and offers a selection of items with similar name trying to identify the underlying safety record.
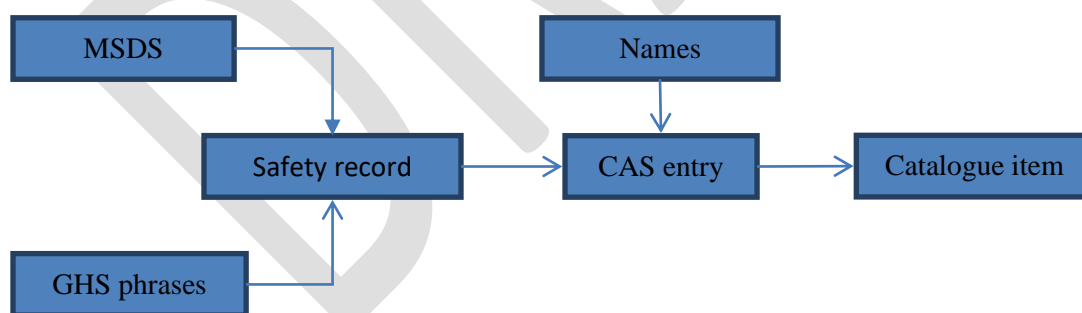
Diagram 3. An illustration of relation between safety record, CAS entries and the catalogue item.

It is known that some chemicals have a number of CAS numbers and the system captures this. Some chemicals however do not have CAS numbers (like mixtures) and then the system generates an 'artificial' number that all are greater than 900000000000. It is important to check if the entry for any chemical/mixture without CAS number exists in the system before trying to create duplicate safety record although the system does allow the administrator to merge duplicated safety records afterwards.

Searching the database

The database (DB) may be searched in several ways. The most common is text-based search.

Text search

The database can be searched for chemical/catalogue item names as well as for CAS number and of course chemical barcodes. The latter are used to quickly locate the chemical record in the DB and always returns a single result for a valid barcode. Other barcodes (orders, assets etc) can be also used.

Structure and substructure search

The system can be searched for chemicals using a chemical drawing. This depends heavily on the structural information provided by the users when they register/purchase the chemicals and thus the users have to be encouraged to provide a chemical drawing for new entries or at least try to use the chemical drawing resolution from the CAS number using the CACTUS webservice link. The drawing can be provided with the embedded JSME[2] molecular editor that can accept SMILES and SMARTS strings.

Analysing the results

Once the chemical record is identified the user may perform one of the available actions – purchase (re-order), dispose, transfer, update amount/expiry date or swap the chemical visibility between site, department or group.

System safety features

Getting safety reports ready

The safety reports can be generated by any person who can log into the system. The reports can be generated for any particular location selected and consist of two parts – the combined safety report for the whole location and detailed reports for specific storage cabinets. Each of the reports has two sections – a section based on hazard pictograms and a section based on the safety unique clauses as demonstrated in Figure 1.

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[2] JSME: a free molecule editor in JavaScript, J. Cheminformatics 5:24 (2013)

Figure 1. View of a safety report

Each of the reports also provides a list of suitable and unsuitable fire extinguishing reagents as read from the material safety data sheets. Details of the chemicals included into each group can be also inspected by administrators.

The system will also show the list of any concurrent experiments at the given location.

There is an option to generate an offline version of the combined safety reports. This can be executed by administrators – the system will generate a combined report for each of the locations and allow downloading as a zip file. Group leaders and administrators can also generate reports for their location(s). The offline safety reports may be generated to overcome any potential problems with the access to the online system and the automatic generation can be scheduled to occur daily or weekly and will contains HTML-enabled visual maps of the locations. The offline report will also contain a printable Excel spreadsheet document containing summary hazards at each of the available locations suitable (critical incident report).

For easier readability of the reports – specific safety clauses can be highlighted in different colour. This can be done by the system administrator as the list has to be agreed between all of the departments.

Storage analysis function

The storage analysis tool can be accessed by system administrator for global storage analysis and by group administrators/PIs for the analysis of their own storage areas. An illustration of the analysis results is shown in Figure 2.

Storage		Highlight	
	Pictogram	Phrase	Amounts
		H228 : Flammable solid	0.51 kg / 0.00 l / 0.0
Cupboard 1.1B-CG001-Chemistry		H271 : May cause fire or explosion; strong oxidizer	0.01 kg / 0.00 l / 0.0
		H272 : May intensify fire; oxidizer	0.02 kg / 0.00 l / 0.0

Figure 2. View of the storage analysis results

The global analysis can be performed by the safety officers in order to identify any storage area with potential risk. The report is interactive and allows direct inspecting of the chemicals in the highlighted groups.

Storage compatibility analysis

A storage cabinet may be associated with a list of incompatible H-phrases, chemical classes and storage attributes (like being ventilated). When a user transfers some chemical into the cabinet, the phrases that marked as incompatible with the cabinet and the safety records of chemicals already in storage are analysed for compatibility with the safety record of the compound being transferred into that space. It also includes the analysis of the incompatibility of classes of chemicals already in the storage and any missing storage requirements. Any incompatibilities will be reported as shown in Figure 3.

Please confirm

You are transferring 1,3-Butadiene from
Safe 1-CG71-Chemistry

Storage content	
Pictogram	Amounts
	0.05 kg / 0.35 l / 0
	0.09 kg / 0.05 l / 0
	0.10 kg / 0.00 l / 0
	0.05 kg / 0.30 l / 0

Incompatible with the cabinet

Cabinet
H220: Extremely flammable gas

OK   Cancel

Figure 3. View of storage cabinet analysis that happens on chemical transfer.

More information regarding the chemical incompatibility is available in the "Chemical compatibility" section.

Storage inspections

The system provides an extra tool for routine storage inspections. It combines the automatic analysis compatibility of the storage chemicals as well as checks if the storage attributes match the chemicals' storage requirements. During the inspection notes can be added as well as notes from previous inspections are displayed for information. The storage properties also can be updated as required.
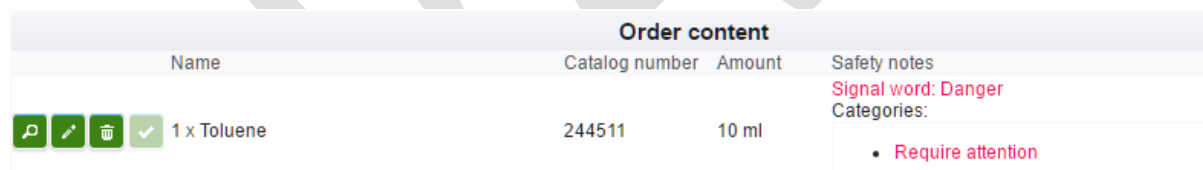
Dangerous/categorised chemicals control

Each of the safety records in the system may be associated with a particular list (e.g. categorised chemicals). When these chemical lists are created, they are associated with an email list. These lists can be used for quick locating of the chemicals on the list and to prepare downloadable reports describing the owners, location and amounts of these chemicals. Whenever a chemical on the list is purchased, a notification email is sent to the associated email list.

If a chemical is not one of the categorised ones but still needs some monitoring – email lists can be used. Several triggers like purchasing, use and disposal can be set, and when activated the system will notify only the email lists belonging to those departments that are located on the same premises as the item /chemical.

Purchasing categorised chemicals

When an order is placed that contains any of the categorised chemicals, that category is highlighted in the order details as well as on chemical details page, as shown in Figure 4 and Figure 5.

Order content			
Name	Catalog number	Amount	Safety notes
1 x Toluene	244511	10 ml	Signal word: Danger Categories: • Require attention

Figure 4. Order details highlighting the chemical categories.

Chemical details

🖶 Barcode	000000238007	
Name	Toluene	
Formula	C7H8	
✎ CAS Number	108-88-3	
Catalogue number	244511 / Amazon	
Amount	10 / 10 ml	
Notes		
Location	Unallocated	
Delivery date	Not delivered	
Expiry date	01-04-2020	Download SDS
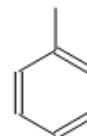
Hazards and Precautions

- H225: Highly flammable liquid and vapor
- H304: May be fatal if swallowed and enters airways
- H315: Causes skin irritation
- H336: May cause drowsiness or dizziness
- H361: Suspected of damaging the unborn child
- H373: May cause damage to organs through prolonged or repeated exposure if inhaled
- P210: Keep away from heat/sparks/open flames/hot surfaces. - No smoking
- P260: Do not breathe dust/fume/gas/mist/vapors/spray
- P281: Use personal protective equipment as required
- P301+P310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
- P302+P352: IF ON SKIN: Wash with plenty of soap and water
- P304+P340: IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing

Compound category	• Require attention
Signal word(s)	Danger
Incompatible meterials	Strong oxidizing agents. Strong acids.
Suitable extinguishing media	
Unsuitable extinguishing media	

Figure 5. Chemical details showing the chemical category.

When the order has been authorised, the email is sent to the email list associated with that specific chemical category.

Downloading categorised chemical reports

The system provides two reports – the report regarding the actual amounts of the chemicals and the stock take in the given period of time. It worth noting that the reports may not always be accurate if there locations/storage cabinets shared between different departments and reports are done for each as the chemicals in shared locations will be accounted for in either report – so a care should be taken that there is an unambiguous ownership of these chemicals. Also if a chemical is stored at a location that has no groups – it will not be accounted for. In order to identify the institution to which the chemical belongs the system will try to locate the owner of the storage cabinet and then uses the owner's groups to identify the institution; If the storage cabinet owner is not set – then the system will check for the groups at the location of the storage cabinets.

The stock take report currently is based on the number of the chemicals that have been disposed in the given period of time.

Chemical experiment planning

The system provides a simple interface to plan a chemical experiment and provide responses for typical incidents like spillage or electricity outage. It also allows control of the chemicals' stock, as the amounts of those chemicals to be used, are automatically updated.

A typical procedure involved identifying chemicals participating in the reaction; specify their amounts and their role in the reaction and to complete a list of incident responses that may affect the experiment.

Any of the chemical experiments running at any one time and any that will require a special procedure for incidents that might affect the facility globally, like a power outage or water stoppage, can then be located easily and dealt with rapidly.

User safety training and research projects

The system provides tools to monitor and review user safety training and the progress of the undertaken research projects. There are three main areas which describe research projects: training courses, safety topics to discuss with the supervisor as well as any declarations that need to be signed.

The supervisor can edit a user account record and create a research project by filling in the project title and description, specifying the project start and end dates and by specifying any materials used during the project. By default, the next project review is automatically scheduled for a year since the project start date, but this can be altered. Whenever a review is added the project becomes available for approval by the researcher. There project can be approved only if all compulsory safety topics are marked as discussed with the supervisor and any outstanding declarations have been signed.

Once the project (project review) is initiated by the supervisor and approved by the researched it falls into hands of the Department Safety Coordinator (DSC). The DSC then can either approve the project and provide any relevant comments or ask the supervisor/researcher to update the description and safety aspects. *For as long as the project is not approved by the DSC, its description can be modified. The system only keeps the approved project description.*

If there are any outstanding training/safety topics to be completed there will be a noticeable red-text link at the top of the user's home page. The training details of the user can be accessed through the Training review item in the User menu of the main toolbar.

Important notes regarding editing safety training aspects of the system

Since the system hold references to the objects rather their copies, it worth noting that editing should be used to ONLY fix any typos or incorrect information – if the scope of the item changes the obsolete one should be marked as inactive and a new one should be created. This will ensure that the user signatures stay under the correct items.

Training courses

The list of the training courses is available to System and Department administrators as well as to the DSC. For the administrators this is accessible through the 'Departments' section of

'Administration' menu – each of the department will have the 'Training courses' menu. DSC can use their designated "DSC" menu. Training courses have 'Active' status, which can be set to indicate if they can be available to the supervisors when updating user training.

The courses can be associated with one or more tutors and have a scheduled date and time for the user records. Once a user is set as a tutor, on the next logging into the system they will get 'Training courses' item in the User menu. They can follow that item to access the list of courses they designated to run and mark users as attended the course. For any particular training course they will be asked once to provide the course date. Their signature will then appear on the user account review page.

Safety topics

These are accessed through a similar way to 'Training courses' using the 'Safety topics' item instead. As well as the training courses these are department specific and can be edited or removed if unused. In addition to standard title and description safety topics have the 'default' status which simplifies specifying the safety topics that have to be discussed by the researcher – the supervisor can use 'Add all default' button rather than picking the topics one by one. Some of the topics can also be marked as 'compulsory' which means that the researcher cannot approve the project without first discussing the topic with the supervisor.

Safety training and chemicals' visibility

Training aspects of the system may be used to control chemicals people see on their home screens or in the department-wide shared location. For example if there is a cabinet for some toxic chemicals in the department – it contents can be set to be visible only to people who has had particular discussions with their supervisor and/or performed some particular training course in handling those chemicals.

Project materials/procedures

These are accessible similar to the training courses and safety topics through 'View project materials/procedures' and describe what materials and procedures the project will use and involve. These items are managed in a similar manner to the others with one distinction is that any of the procedures can be associated with a designated safety coordinator who has to validate and approve them.

Document templates

Document templates are designed managing fixed format forms that require user input and signatures. They are accessible from the DSC menu->View Document templates.

The document templates associated with a particular department can be created by a DSC. System administrators can create templates that are shared between all of the departments (or share any of the existing document templates).

A typical document template consists of title, a detailed description and content – header, sections and footer. It is possible to specify a DSC that has to sign the document for it to be completed.

Each section requires some user input. The section number is used for sorting the sections if there is a need to change the sections order. The title is used for navigating the document structure but not

for the final document, so the section content should have the complete section title as it should appear in the document.

When training is enabled in the system, the users can instantiate a shared or designated to their department document template from the Chemicals->View documents menu. After the completion the document has to be signed and submitted for the approval. If the document is created by a group leader, they can specify their group's people who participate in any described work and have to sign the document. If the document template specifies that it has to be signed by a DSC – they will be able to sign it after it has been signed by all of the users. Document instances can be partly populated and saved before the submission.

Chemical compatibility

When transferring chemicals to different locations, the system will notify the user whether there are acceptable conditions in the location to store their chemical. To do this, the system will compare specific requirements for the chemical and the conditions of the destination, which include specific chemical classes of the chemical and any storage attributes, as well as any specified incompatibilities with other chemicals. The system will warn the user about these clashes before proceeding with the transfer.

For each chemical there is a safety record that beside of the information extracted from MSDS also contains a list chemical specific incompatibility. The administrator can set up the system in such a way that whenever the system extract information from an MSDS in can automatically set up the chemical class and storage requirements when any particular GHS phrases is encountered.

The system also checks for clashes with individual chemicals through the comparison of the individual SDS for each chemical. This lets the user know which chemicals cannot be stored together and a warning message will be given if this is the case.

Chemical classes

These are used to class chemicals into groups to check for incompatibility. The classes can be changed and edited by selecting the 'Chemicals' section and choosing 'Administration'. A list of the existing classes will appear which can be edited, removed and added to. Each class also has a list of the classes that it is incompatible with. Any particular storage cabinet can be associated with the list of incompatible chemical classes. It is also important to note that if a particular safety phrase in a given SDS for a chemical, is associated with a class then the class can be filled in automatically. By default, the system provides basic set of chemical classes shown in Table 1, but it can be extended:

	Alkalis and Bases	Flammable Liquids	Inorganic Acids	Organic Acids	Oxidising Chemicals
Alkalis and Bases	✓	✗	✗	✗	✓
Flammable Liquids	✗	✓	✗	✓	✗
Inorganic Acids	✗	✗	✓	✗	✓
Organic Acids	✗	✓	✗	✓	✗
Oxidising Chemicals	✓	✗	✓	✗	✓

Table 1. Default chemical classes compatibility ✓- compatible   ✗ - incompatible

Storage attributes

Similar to chemical classes any storage can also be associated with a list of attributes. These will be checked against the chemical storage requirement to highlight any conflicts.

Safety Phrases

Beside of the more generic chemical classes, the system can use any particular GHS safety phrases to specify incompatibility either between the chemicals having particular phrases in MSDS or the storage cabinet and any particular safety phrase. Safety phrases can also be assigned some declarations that the users have to sing when purchasing the chemicals. This way the training aspects of the users can be ensured when handling dangerous chemicals..

Safety/user declarations

As mentioned previously, declarations are used when purchasing different chemicals. The user must agree that they have understood these declarations before the chemical can be ordered. These can be viewed in the 'Department' section of 'Administration'. Here they can be edited, deleted (only if unused) and added. They also have an 'Active' field which is automatically given as 'True' unless stated otherwise, meaning they are effective immediately.

System setup

The system must be pre-set to operate properly. The setting up involves creating administrative site layout (departments and groups) and physical layout (buildings, rooms and storage cabinets).

Site specific settings

There are a few site-specific settings which have to be initialised in order for the system to operate properly. These are:

- Administrator emails. The first email will be used as the email messages 'sent from' reference and therefore should be 'local' to the server to prevent email filters from automatically discarding the system generated emails. Any following emails should be separated by semicolon.
- Catch all email. This is useful for system testing when all system generated emails are forwarded to the specified email address. Leave this empty to disable the email forwarding.

- Google Advertisement ID. This can be used along with Google analytics to analyse the site usage and gather usage statistics.
- Stock reorder email(s). This is the email where the messages regarding low stores stock are sent. If more than one email address is specified – they should be separated by semicolon.
- Weekly safety report email – each week the system will generate a summarised safety report and sent it to this address.
- Printer queues. This is a list of the printer queues available.

Email template can also be customised to fit the system's purpose.

Administrative layout setup

The administrative setting up is carried out in Administration, Departments.

There is always going to be at least one department registered in the system. Using departments allows compartmentalisation of department data and utilisation of department administrator role. The system administrator can create a department using the '+' icon. During the setup a department administrator(s) can be added – these people will then be able to perform further administrative job on the department. The user list can be populated by department/system administrators or by people themselves when first registering in the system. To create a group a group leader account has to be created at first. As noted in Overview, groups are essential for identifying the ownership of items and shifting the responsibility for group user and storage management to the group leader and group administrators.

In order to process any 'order' through the system, the users have to be associated with specific funding account(s) on which they can purchase and also with a physical location.

For group leader accounts the system provides a convenient wizard dialog available through 'Authorise PI' user menu. In this dialog any information that is needed to set up the account can be provided and, if missing, - created. Without using this tool the user group has to be created first, then any missing funding accounts and locations created and linked to the user (funding accounts) or the group (locations).

Physical layout setup

The top level of the physical layout is a site. Site contains buildings. Buildings have locations (rooms) and locations have storage cabinets. Whenever an order is placed, the destination room has to be identified and when registering or transferring chemicals, the storage cabinet must be specified. Some locations can be shared between groups and cabinets may be either shared by those groups or owned exclusively by one group. If a location is shared and there is a shared storage, the storage content will be available and visible on the system to all groups at that location; however when the storage is owned by a group – its content is only available [visible] to group members associated with that group leader.

The system provides mapping utilities to associate buildings with a site map and locations with the building maps and storage within the location map. These maps are later available from the online safety reports for closer inspection of any possible risks which may arise from adjacent locations.

Funding accounts

Each of the departments has its own list of funding accounts. Funding accounts are essential to use the system for populating the chemicals database through the ordering sequence and to perform basic accountancy.

A funding account may be time limited and only currently active accounts will be available to users. The group leaders/administrators can see their funding accounts' expenditure and instantly generate expenditure reports for a particular time period. The System/Department/Financial administrators can carry out the same tasks on the complete list of accounts.

There is also a special kind of 'generic' accounts that are available to all group leaders (assuming that they have some other, personalised account). An example of such an account could be a shared funding for computer equipment.

Another special funding account type is 'shared' account that is similar to the generic one besides that the list of people who have access to can be controlled. Orders placed on the shared accounts are typically authorised by the supervisor of the person placing the order (even if they are not on the list). If the supervisor does not want to receive the authorisation requests – they can be added to the account and their authorisation role removed.

In order to authorise orders, the account should have a user that have authorisation permission. If there is a case that the funding account does not have anyone to authorise – a user with financial administrator rights can be added to it and that user will be able to see the order authorisation requests and authorise those orders.

Dangerous/categorised chemical control

The chemical lists may differ from department to department and can be edited by system/department administrators as required from the "Departments" page. Once a list is created any of the CAS/Safety records can be associated with it.

Inventory, assets and inspections

The main inventory consists of items that could be associated with a safety records ('chemicals') or not (stationary, consumables etc). Assets are similar to non-chemical items but provide more information regarding them – the user can associate an asset with pictures, notes and any asset related documentation, like maintenance and inspection reports. Assets module also helps with performing routine inspections.

Tasks

Tasks are recurring or one-off list of particular steps that may include a choice of options, user input and confirmations. On completions the tasks are timestamped and archived.

Chemical tasks

Safety entries can be associated with 'Goods in' and 'Disposal' task. The chemical disposal task will be executed when a chemical is disposed by the user. The default task simply asks for a comment that can be left empty. For some chemicals the standard disposal procedure might be not sufficient

or the users may need to be reminded to perform a particular procedure. This task must be executed before the chemical can be disposed of. The 'Goods in' task created when a chemical is marked as 'delivered' on the purchase order page. The task is added to the user's tasks list and has to be completed within a week time (?).

Storage and location tasks

Storage and locations can also be associated with some tasks like annual inspection. These tasks have to be recurring and associated with a list of people for the system to inform them periodically about the task.

Barcodes

The system provides the barcode-based item identification and also provides some 'action' barcode that instruct the system to perform some action (see Automating stock control). The item identifying barcodes contain information regarding the items and have human-readable information like room number and the CAS number and, if the item was purchased through the system – the owner's name.

General concept

The system generates a system unique identifier (Id) for each item registered in the system. This Id can be used to locate items rapidly and is the source information for the barcodes. The barcodes can be printed at any point when viewing the item details, registering an item, or processing an order. There is a program (Printer.jar) that has to be run locally to the printer in order to print barcodes. When the program is run, it is provided with the 'printing queue' name to pull data from and the 'printer to use', for printing the barcodes. Although by default the program requires the user to login to the system, there is a way to create a batch file that can automatically create a user printing session with a user name and a queue password, pre-set by an administrator. The list of required parameters is printed by the program in the Command Prompt when no arguments are provided.

Printer queues

The printer queues are set by the system administrator on the 'Site specific settings' page and the users are allocated a printing queue on request[3]. The users can specify their printing queue from the User settings menu located in the right top corner ('Logged in as…'). It is important to set up the correct printer queue matching the printing program settings.

The user set printing queue is used as a default one, but some tools do provide a selection of the printing queues. An example is the item registration and barcode 'translation' tools.

There is a way to set a default printing queue on a specific computer and to override the user's settings on that particular PC. This is useful for a centralised computer where people can log in and print some barcodes. This can be done by system administrators when viewing the list of printing queues.

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[3] All printing queues available to the group leader are automatically available to the group members so only the group leader account should be updated.

Stock control

There are several ways the user can control the stock. The manual stock control involves registering chemicals and disposing them and updating the remaining amount when needed and registering chemical transfers from one location to another. It is also possible to highlight some stock items that require a review or disposing using the chemicals expiry date. The stock items can be sorted by the expiry date; also the expired items are highlighted in the lists.

Automating stock control

For chemicals that are purchased regularly the system provides the concept of 'reusable' containers – for any chemical that is regularly re-ordered a special 'action' barcode can be generated that instructs the system to dispose the previously associated chemicals and on order collection to transfer the new one into the same storage as the old one. This significantly simplifies re-ordering and managing stock for bulk solvents and other bulk-consumed chemicals.

The experiment planning also helps with automatic stock control by updating the remaining amounts of the chemicals and disposing chemicals when needed.

Local shop items can be marked as 'Auto-dispose' which means when a user purchases the item all other items will be automatically disposed from the destination location. This is in particular useful for consumables and other non-chemical items.

Batch processing of chemicals

There is a tool for processing chemicals (disposal or transferring) in a batch mode. The user can prepare a list of chemicals that either have to be disposed or transferred to one of the storage cabinets.

When the list of selected chemicals is empty – clicking on the transfer button will show the chemicals the user has to transfer. This is a convenient way to transfer a number of items into the same storage cabinet.

The user can enter /scan a series of barcodes, type a part of the chemical name and use the '+' button or the return key. If the entered value is a part of the name an there is more than one chemical found – the system will display the dialog where the user can select the chemical of interest. Once the list of chemicals is populated – they can be either disposed or transferred.

Chemicals' audit

A lab space manager can initiate a chemicals' audit. Under My group(s), 'Audit the chemicals'. To start expand the 'Start and finish here' panel and click on the 'Start' button. This will reset the chemicals 'last audited' timestamp for all chemicals where the timestamp is older than 4 weeks. You may need to refresh the page to update the list of chemicals. Then you can either supply the tool with the barcodes for the chemicals or pick them from the list and choose one of the 3 actions:

- Transfer
- Dispose
- OK – to confirm that the chemical in the right place

After the action has been chosen - the chemical will disappear from the list. Once all of the chemicals have been processed, you may need to dispose the rest on the 'Start and finish here' panel – but be careful as this action cannot be undone.

Generating and managing order requests

The system provides a straightforward way to generate order requests.

Generating the order request

The user starts the order request generation from selecting the supplier followed by choosing the funding account and the order destination. The supplier field provides auto-completion, so just type a few letters [4] in the supplier name and wait for it to show available names, if needed - provide more letters to restrict the result list. Note that if the required supplier is not in the list you can specify 'New supplier' (follow your department instructions; there could be few suppliers for different currencies) to instruct the person dealing with the order to add new supplier to the list – in this case the information regarding the supplier should be added to the order comments. Although this may look like a complication it actually helps with keeping a curated list of the suppliers.

After the supplier, funding account and destination are selected - an order line can be added. The order line 'Name' field also provides auto-completing functionality. It will try to complete entered sequence (at least 2 characters) with any of the available catalogue items, CAS entry name or alternative name (like acetone and propan-2-on).

If the name auto-complete list shows the required item – simply choose it. The system then will extract and display the information available in the system. In the case the item is a chemical – the safety record will also be displayed. It is possible that there are several catalogue items with the same name – look at the catalogue number drop-down list to see if the required item catalogue number is in the list. If it is not – simply provide the required information – catalogue number, container size and the price. To purchase a few items – specify the 'number of containers'. There is also an option to purchase multi-pack items. This option should really be used only when each of the items in the container requires its barcode and an entry in the database.

When the item is not in the database, you will need to provide information about its catalogue number, container size and price. For consistent results please user prices exclusive of tax as this will give more control over the expenditure reports later on. When you click on 'Add the item' button the system will ask you to confirm if the purchased item is a chemical (like requiring and MSDS) or not. If the purchased item is not a chemical – it is simply added to the order; otherwise the material safety record has to be completed.

The material safety record consist of few items – the CAS number (if known or available), the GHS safety clauses and information regarding the incompatible chemicals, extinguishing media, disposal procedure and the chemical diagram. The system can extract most of this information from an uploaded PDF form of MSDS. If the system does not recognise the supplier or the information is incorrect – it has to be edited manually. It is important to provide correct information regarding the GHS clauses as they are used to automatically generate reports. Similar is the chemical diagram that is used in the structure and substructure searches.

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[4] Labsafe uses whitespace to anchor string ends. For example ' sig' specifies a string that should start with 'sig', similarly 'sig ' – the ending must match 'sig' and ' sig ' – the searched value is 'sig' exactly.

Order and item details

The user can provide extra information regarding the order – like any details about handling the delivery as well as to attach quotes and other relevant information. Any of the order lines can also have comments – like what to do with the items on delivery. If needed - the delivery charge can also be accounted separately.

Orders are also associated with a list of messages where people involved into the order placement and handling can exchange messages with e-mail notifications – an example would be to notify the user about the partial order delivery.

Handling the order

Choosing the financial team

When an order is placed, the user can choose the financial team that has to handle the order. By default the system uses the financial team associated with user's department. But when the user works in a department that occupies several building – the system offers to choose from all financial teams located in those buildings. The orders placed for handling by a specific team generally will **not be visible** to the other teams – keep this in mind.

Private orders

The user placing or authorising the order can mark it as 'private. This means that although people who have access to the same not-shared grant code will see it in their lists – they will not be able to view the order details. This could be important for confidentiality of orders involving external companies.

The process

Depending on circumstance, after the order is placed it may require authorisation. In this case an e-mail will be sent to the person responsible for the authorisation (typically the PI or a group admin) with the authorisation request. Once the order is reviewed and authorised it appears on the list of the 'Stores' staff and is ready for processing. The Stores staff can review the order (change any relevant information if needed), place the purchase and supply the system with the requisition number. In the case when the order requires significant changes it can be bounced with the comment – in this case the order originator will receive an e-mail regarding the need to review the order. This will place the corresponding message to the order messages. If the order clarification is needed – messages can be sent to people involved in the order processing.

Avoiding duplicate purchases

Although the system displays people currently looking at the order - the person who want to handle the order should first try to lock the order for processing to make sure that they get exclusive access to the order and to avoid duplicate purchases. This only works if everyone follows the same procedure – trying to lock the order before processing it. In the recent update there is an extra check – the order is time-stamped and if somebody has an outdated copy – they will not be able to update the order without reloading it.

Orders with split cost

Sometimes for accurate accounting it is needed to draw funds from several accounts or the same account by different people. The system allows provides the necessary tools to the person processing the order and uses that information when generating various reports.

Managing tax

Although the people placing the order do not see the tax incurred by the items/delivery, the person handling the order should make sure that the numbers on the order details page correspond to those on the supplier's invoice – this will insure that the final expenditure reports represent trustworthy figures.

The system provides the "global" tax rate that is set by a System administrator – this tax rate is automatically applied to any new catalogue items. Each of the existing catalogue items also carries the default tax rate associated with it – in the case the default tax rate changes - they have to be updated through the Catalogues tool.

When managing the order – the tax rates can be adjusted by clicking on the "Total Tax" link in the order summary. The adjustment tool allows changing the global tax rate (by using the Apply' button) as well as tax on any particular item. For convenience this tool can also be used to subtract the tax if it was mistakenly added into the order line/delivery price by the user – simply use the negative tax rate to update item/deliver price to the tax-free value. There also shortcut buttons – to remove the tax all together and to add and to subtract the default tax rates.

Handling bounced order

Any bounced order can be edited and resubmitted. This however does not allow adding extra lines to the order or changing the number of order line items (for chemicals); but it is possible to remove order lines and to change any other relevant information regarding order lines (prices, catalogue numbers amounts, etc) and the order itself – changing the supplier, funding accounts, attaching quotes and so on. After the order is reviewed it can be resubmitted.

Post-delivery order management

After the order items have been delivered, the order is marked as 'Received' or 'Collected'. At this point the purchaser may decide to return some of the order lines or cancel the order. Cancelled orders can be viewed when setting the orders table Status filter to 'Cancelled'. Cancelled orders can be resubmitted later. In the case some of the items are returned, the record of the purchase of these items kept in the system.

For partly delivered orders the system provides a one-click action to notify the user that some items have been delivered and can be collected. It is also possible to part-deliver order lines. For non-chemical order lines the line is split into two with one marked as delivered. For chemical this happens slightly differently as the order lines are pre-expended into the chemicals inventory items – each of the delivered items has to be marked as delivered to print the barcodes and the there are no new order lines generated – so with the following up deliveries, the same order line has to be updated.

Once the order is delivered and all order lines are marked as delivered – the system automatically sends 'order delivered' notification to the user who placed the order and all users at the order

destination location who have the role of the 'delivery manager'. Similar message can be sent manually for partly-delivered orders.

Reverting order status

Typically the order status changes automatically as action performed – like from getting authorised (submitted to Stores) to purchased, delivered and finally collected. But sometimes mistakes happen and the order gets an invalid status like – collected while it is still in the delivery room. The system allows to undo the order change – so the order status can be change in reverse – from collected to delivered, purchased, submitted and to require authorisation.

Labsafe and external web services

Before any of the functionality described below can be used, the system has to be set up with the private key as described in this section – "Setting up single sign-on".

MSDS information synchronisation

Labsafe provides functionality to synchronise MSDS information between different instances. In order for this to operate the one needs to register their instance in another Labsafe. Once the access to the MSDS service is granted in the other Labsafe, the system administrator can synchronise MSDS using the "Synchronisation" tool in the "Administration->Safety" section. The tool only synchronises entries that have not been synchronised within a month.

When Labsafe is paired with another instance – it also tries to download missing safety records when the user creates an order.

Integration with ELN

There is a basic interface provided by Labsafe and documented under "Site URL/oslims/swagger-ui".

Importing users from Labsafe

Once a group leader gets an account in the ELN and their account is linked to Labsafe – they can import and link all of their group members from Labsafe using /service/group/link.

How to...?

This section describes typical uses cases.

Administrative setup

The administrative setup starts from populating the database with departments, groups and people. There is a small catch that a group can only be created if there is a group leader already in the system.

Add a department

Only system administrators can create departments. After a department is created the responsibility to populate it with group leaders, groups and users can be given to a department admin. In order to add a department, follow to Administration menu, Departments and use the '+' button. You need to provide the basic department information and possibly to specify the department administrators (they have to be registered in the system).

After the department is created, you need to create group leader accounts and/or funding accounts. Funding accounts, unlike groups do not require an explicit owner but can be used to specify the user funding accounts when creating a user. Group leader accounts are just a standard user accounts that you can later assign as group leader. Note the 'group leader' role is evaluated implicitly from the fact that the user is some group's leader rather than explicitly – so the role will not be visible in the user lists as such.

Add user

A user can be added to the system in three ways - self-registration and registration by an administrator and using batch account import. Note that there could be only one active account that

has the same e-mail address. If the user changes their supervisor or their status - the previous account should be marked as expired and the new one should be created– this will allow to keep the accounts activity separated. There is an option to "Create new identity" to streamline the process.

Self-registration

The user can follow to the application website and choose to register. Then they can provide their personal information and selects a research group(s). If the user does not have a group or is a group leader, the group has to be created by the department/system administrator. The self-registration process sends an activation e-mail to the e-mail specified by the user. Once the user activates their account - an e-mail will be sent to their group leaders (if any are chosen) or to the system administrator asking them to authorise the account. The person responsible for the account authorisation has to check the information provided by the user and update information regarding the user's funding accounts and account expiration date (if any) and to change the user's role from Unauthorised to 'User'.

Manual registration

Follow Administration, Departments, click on any department's 'Choose action…' button and select 'View people'. The list of existing department's people will be displayed. Use the '+' button to create a new user account. Please provide mandatory fields, specify a valid user role and set random strong password or leave it empty (as the system does not allow these and the password reset will be required) – after this you can inform the user that they can rest their password with their e-mail address. Once the user has a valid account, they can use either their e-mail or user name to login.

Batch account creation

This tool is available to System administrators on the 'Users' page and allows to create and set up multiple accounts in one go. The import is performed from a CSV text file containing the following columns:

Title	First name	Middle name	Last name	Email	Start date	End date	Supervisor email	Funding
Mr	Anthony	S	Smith	a.smith@smw.ac.uk	26/12/2023	26/11/2024	sprv1@smw.ac.uk	GCF1;GCF2:1000
Dr	Clair	N	West	c.west@smw.ac.uk		30/12/2025	sprv1@smw.ac.uk	GCF3

Once the CSV file is uploaded – a dialog box appears that allows to review the data. The already existing accounts will be highlighted – for this account only the start/end dates and the financial information will be updated. For the new accounts – all the provide information will be used. Note that supervisors should already be registered in the system for this tool to work correctly. The Funding is consists of grant code separated by ';'. To impose an expenditure limit on any of the grant codes – add the it with ':' to the grant code like in 'GCF2:1000' which limits the expenditure on GCF2 to 1000 (default system currency).

Once the imported data has been processed – the supervisors for new accounts will receive account authorisation notifications.

Add a group

There is a convenient way to authorise PI accounts using the 'Authorise PI' tool in the user's' list and that is described in Administrative layout setup, but there is also a step-by step way.

After a group leader's account is created, the group can be created. Follow to Administration, Departments, and choose any department's 'Choose action…' button and select 'View groups'. Use the '+' button to create a new group. Give the group a name (typically as group leader's surname group like 'Peterson's group') and choose the group leader. If you have already created some physical locations – you can add them at this stage, otherwise – you can add groups to the locations when creating ones.

User groups and locations

When a user is added to a group, the group's locations are automatically added to the list of locations "visible" to the user. However, if the user is should not see some of the group's location chemicals by on their home page – these locations can be removed from the list. Please note that when location's groups are edited– those the user locations **are** not automatically updated, instead edit the group's locations and use the '+' button to add that location to all group members. However, if one or more of the group locations are removed or a group is removed from a location – the group user's locations are updated accordingly automatically.

 Also note that if the user groups are in different departments – the account has to be associated with the default department as that will control various resource access rules.

Move group chemicals to a new location

When a group is moved to a new location you can also move the chemicals that have been purchased by that group. To do this the new location **should not** be associated with the group. A department/system administrator can choose this option from 'Actions' in the list of groups. Note that only purchased chemicals will be moved, any manually registered chemicals will have to be moved manually. When moving the chemicals a record in the chemical's flow will be created. The system then will replicate the cabinets from the source location and add '-moved' to their names.

Alternatively whole cabinets can be moved to the new location. For this a building/system administrator needs to edit the source location, find the storage cabinet to move and then choose 'Move chemicals' from 'Actions' menu. This will move the cabinet to the newly selected location, create chemical relocation records.

Add funding account

Funding accounts are required if the purchases are to be placed through the system. If a group leader has a funding account (that could be shared between many groups) they can see all the orders originated on that account and authorise them.

The funding account list is available in the same 'Action' menu for any of the departments. The list of the funding account displays the account information and the total grant expenditure. A new account can be added in a similar manner by using the '+' button. The accounts that are outside the start and ends dates will not be available to people with non-admin accounts. The account can be associated with a list of existing people as well as user accounts can be associated with the list of funding accounts.

Funding account tools

There are a few tools that allow analysing and downloading a list of transaction on any of the funding account for the whole period or some specific period. For example, when clicking on the

button with magnifying glass icon the list of all orders placed on that account can be displayed. The view of that list can be switched between orders and the particular items and the view can be downloaded as Excel spreadsheet.

Using the '£' toolbar button a report regarding purchases in a particular period of time can be generated. This report will split the expenditure into purchase categories but will also allow viewing the individual items purchased for any of the accounts by clicking on the account name. The combined and detailed reports can be downloaded using the 'Download' buttons.

Note that by default the generated reports will contain only records for funding accounts for the departments of the user using the tool. Sometimes there is a need to do recharges to other departments – like for internal shops. This can be managed by setting up 'Report department' for any particular supplier (like an internal workshop) – then all of the grant codes used by that supplier will also become visible to the user who is from the reporting department.

Add sites, buildings and locations

There are four identifiable levels of storage organisation in the system – sites, buildings, locations and storage cabinets. If the locations are used for placing orders and storage – to transfer items, sites and buildings are mostly used for mapping purposes.

In order to add a site or a building follow to Administration, Buildings and use the '+' button. Adding a building requires specifying the site to which it belongs and its name. If the site has an associated map – the building map reference can be added. Building maps can also be added and generate the building locations using a list of html map like entries for example:

<area shape="rect" coords="98,14,332,263" alt="MC201" nohref="nohref" />
<area shape="rect" coords="335,13,585,263" alt="MC202" nohref="nohref" />

Note that the location name is stored in the 'alt' attribute and the location coordinates – in the 'coords' attribute. The free software like GIMP can be used to create and edit these entries visually. Once these entries are placed along the map file, the system will generate (or update if exists) the names of locations and will associate them with the provided coordinates – these can be late used to locate rooms (locations) on the interactive maps when investigating emergency reports.

Add storage cabinets

Storage cabinets are the final destination for chemicals and other items. They have to be created in order to transfer or register chemicals. The storage management can be delegated to the group leader or a person who the group leader can nominate as a location admin. The system/department admins can also manage the storage.

The storage cabinets can be created in an automated way from html-like image map in a manner similar to batch creating building locations.

The storage cabinets can be shared between all groups at any given location or have a single owner. The storage ownership only affects the chemicals list in the front page or when searching chemicals by substructure and forcing the system to show group's chemicals only. Also you can specify what chemicals are not compatible with the storage using the list of hazard phrases and specify the storage limits.

Add department-wide shared storage

Sometimes there is a need to make a storage cabinet available to everyone in one or more departments. This can be used as a centralised disposal location or a 'chemicals' bank for undesired chemicals. Although people can always search for chemicals that are shared – some people may prefer to clean-up the list of chemicals they see in their inventory and transfer undesired chemicals to those locations.

These 'functional' storage cabinets are available to everyone to transfer chemicals to and also to see the list of chemicals stored there. Note that on transfer the chemical's visibility will be set to 'Site' to make it accessible to everyone.

Any existing storage cabinet can be turned into a 'functional' storage by administrators. Follow to the storage properties and choose the 'Special storage' tab; add any departments that need to have access to this storage.

Create site/building/room maps

Once you have a suitable picture for the map (make sure it has enough details but not too big as operating with it may become clumsy) you will need to create the coordinates for building on the site map, rooms on building maps and storage cabinets on the room (location) maps.

One of the ways of doing it is using the free GIMP software (https://www.gimp.org/). Load you picture through the file menu. Then follow to "Filters/Web/Image Map". This will display the picture and provide a set of tools to map rectangles and polygons on the left-hand side.

As mentioned in Add sites, buildings and locations section For building maps Labsafe provides an easy way to create locations using the generated file (just remove heading and the footer). For buildings and storage cabinets the coordinates must be specified on one-to-one basis but for storage cabinets this can be done by each of the research groups themselves.

Adding a supplier

A supplier is required to perform chemical registration or purchasing. Follow to Chemicals, Chemical suppliers to see the list of current suppliers and to add a new one – use the '+' button. You need to specify the supplier's name and the currency (as a single char, £, $ or a 3 letter abbreviation like CAD, NZD). You can also provide the supplier information such as the address or any other relevant information.

If there are special procedures for placing orders with any specific supplier – the warning/instructions message can be added to the supplied which will be displayed once the used has picked up the supplier.

Having set up user accounts, groups, locations, funding accounts and chemical suppliers the system is ready to be used.[5]

When users place an order but the supplier is not registered in the system – you can provide them with special 'New supplier' option that also will have a relevant currency associated. When users place an order for a '*New supplier*' they are asked to provide the supplier details. The person who

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[5] You also need to set some printing queues to enable the barcodes to be printed

processed the order will them be asked to add the supplier to the system. Note that in this case the order comment is copied to the supplier details field and need to be edited to leave only relevant information.

The option of the 'Report department' allows to make reports for purchases from this supplier by the specified department's financial team disregarding of the funding account's department.

Populating the database

As mentioned before the database can be populated by registering chemicals or by generating the purchase orders.

Registering chemicals

In order to register a chemical make sure the chemical supplier is in the list and that the storage cabinet where the chemical is, is also in the system.

1. Specify the chemical provider in the lookup list – start typing the name until the full supplier name is shown in the drop down list – chose the name from the drop down list
2. A. Start typing the chemical name in the Name box – if the chemical is in the system, the drop down list will be populated – if there is a matching name or CAS number – select the one
   B. If you have an MSDS – drag and drop it (or click on 'Choose' to pick the file) onto the 'Choose' button. If the system is able to parse the supplied MSDS – the extracted information will appear on screen (not that only administrators will be able to edit information for already existing chemicals)
3. Specify the container content amount and the original container content amount (leave the second one empty if matches the first one). If there are several containers to register – specify the number
4. If printing labels – choose the label printing queue. Once the 'Register' button is pressed – the label(s) will be printed

Purchasing chemicals and other items

It is very similar to registering and is discussed in detail in the "Generating the order request" section.