

CS-M14 Industrial Project User Manual

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25th May 2012

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1 Customer Web Application

1.1 Logging In

The application requires an active user session when browsing any section of the application. If one is not found the application will automatically take you to the login screen.

contact us.'" data-bbox="209 191 779 424"/>

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Login

Password

Login Change Password

If you do not have a login name and password and wish to apply to use the service, [contact us](#).

To begin a new user session log on to the system by entering your **Swan Code** and **Password** into the relevant fields on the login form. If correct you will be redirected to the samples page where all your samples can be viewed. However, if the details were incorrect the system will prompt you to re-enter your login details again.

1.2 Submitters

The submitters functionality of the application allows users to create multiple submitter identities using the same user account. This could be used, for example, if there are a number of post-graduates all submitting samples from within the same institution. By specifying who submitted a sample during the submission process it will be easier to view all the samples submitted by a specific individual.

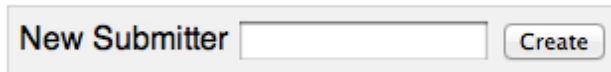
Managing submitters is done using the **Submitters** page which can be accessed using the menu found at the top of the each page.

Submitter Code	Submitter Name	Edit Submitter	Delete Submitter
SWATEST	Test Submitter	Edit	<input type="button" value="SWATEST"/>
SWAMJL	Matthew Lewis	Edit	<input type="button" value="SWAMJL"/>
SWAEXA	Example Submitter	Edit	<input type="button" value="SWAEXA"/>

1.2.1 Creating Submitters

1. Enter a code you wish to use to identify the submitter into the box and click 'New Submitter'. The code must be one that is not already assigned to a different submitter. If it is already

being used the system will prompt you to enter a different code.

A screenshot of a web form titled "New Submitter". It features a text input field for entering a unique code, followed by a "Create" button.

2. After entering an unique code, you will be taken to the 'Edit Submitter' page where it is possible to add the details about the submitter such as their name, email address and direct telephone number.
3. Once all data has been entered, click 'Save Changes' to save any changes and return to the submitter list.
4. To cancel any changes click 'Cancel Changes'.

1.2.2 Editing Submitter Details

1. From the submitter list click 'Edit' in the row of the submitter you wish to change.
2. You will be taken to the 'Edit Submitter' page where it is possible to edit the details about the submitter.
3. Once any changes have been made click 'Save Changes' to save any changes and return to the submitter list.
4. To cancel any changes click 'Cancel Changes'.

1.2.3 Removing Submitters

1. From the submitter list click the button in the 'Delete Column' that corresponds to the submitter you wish to delete.
2. The submitter will be removed from the system and will no longer be visible in the list of submitters.

1.3 Submitting Samples

Submitting a new sample is achieved using the 'Submit Samples' page which can be accessed using the menu at the top of each page.

The screenshot shows a web form for submitting samples, divided into several sections:

- Submitter Details:** Includes a dropdown menu for 'Submitter Code' (currently set to 'SWAMJL') and a 'Change' button. Below it, the 'Submitter Name' is displayed as 'Matthew Lewis'.
- Sample Details:** Contains input fields for 'Your Reference', 'Molecular Formula', 'Molecular Weight (Nominal mass; NO UNITS)', 'Melting Point (°C)', and 'Solvents'.
- Additional Information:** Features a dropdown for 'COSHH' (set to 'Low') and a text area for 'If High or Extreme please specify'.
- Special Requirements:** A large empty text area for additional notes.
- Services Required:** Includes checkboxes for 'Characterisation' (Let us decide, EICI, ESI, FAB, MALDI), 'Accurate Mass', and 'GC/MS' (Complete GC/MS Form).

At the bottom of the form are three buttons: 'Save Changes', 'Cancel Changes', and 'Submit Sample'. A yellow warning box at the top right states: 'You must save the sample before you can upload a structure file.'

1. Choose the submitter for the sample by selecting their submitter code from the drop-down menu labelled 'Submitter Code' and click 'Change'. Their name will be displayed allowing you to confirm you have chosen the correct submitter.

This close-up shows the 'Submitter Code' dropdown menu with the following options: 'SWATEST', 'SWAMJL' (which is selected and has a checkmark), and 'SWAPOT'. A mouse cursor is pointing at the 'SWAMJL' option. The 'Change' button is visible to the right of the dropdown.

2. Enter a unique reference for the sample. This could be the sample references used internally by your institution. The system will alert you if enter a non-unique reference.
3. Continue to complete the form filling in any data you have about the sample such as molecular weight, formula and melting point. It is possible to leave these fields empty if the values are not known.
4. Under 'Additional Information' it is possible to specify the COSSH level of the sample together with any specific information about it.

5. You can also specify any special requirements under the 'Special Requirements' heading.
6. Under the 'Services Required' heading use the checkboxes to specify which services you wish the lab to perform on the sample such as EICI, ESI and Accurate Mass.

Services Required

Characterisation	<input type="checkbox"/> Let us decide <input type="checkbox"/> EICI <input type="checkbox"/> ESI <input type="checkbox"/> FAB <input type="checkbox"/> MALDI
Accurate Mass	<input type="checkbox"/>
GC/MS	<input type="checkbox"/> Complete GC/MS Form

If at any point you need to save the details about a sample and submit at a later point in time, it is possible by clicking 'Save Changes' at the bottom of the form. The details will be saved on the system allowing you to resume the submission process by selecting the sample from the 'Unsubmitted' list of samples.

When you are ready to submit the sample click 'Submit Sample'. This will take you to a confirmation page so that you can double-check that all the correct details have been provided. If everything is correct click 'Submit' to finish the submission process.

1.3.1 Sample Structure

Together with the basic details about the sample it is also possible to provide the chemical structure of the sample. This can be achieved in two different ways - Uploading a structure file or using the built-in drawing tool.

Structure

File	<input type="button" value="Choose File"/> No file chosen
Draw	Built-in Drawing Tool

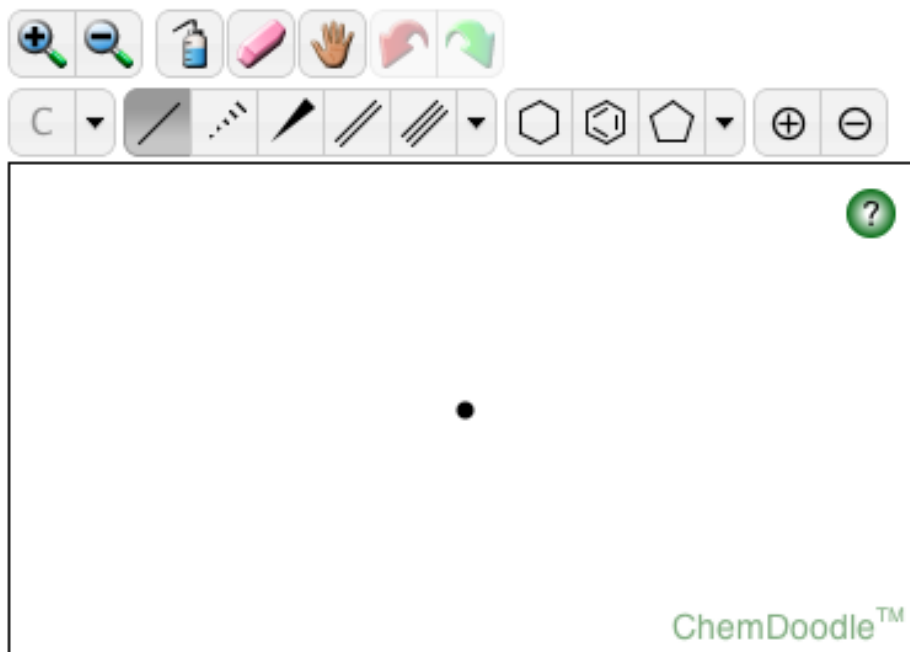
Upload Structure File

Currently the system only supports the upload of MOL structure files. To upload a MOL file for your sample:

1. Before a file can be uploaded the sample you must provide a unique reference for the sample and any details must be saved by clicking 'Save Changes'.
2. Under the 'Structure' heading click 'Choose File'. This will display a dialog allowing you to select a file stored on your local system.
3. After choosing a MOL file click 'Save Changes' again. This will upload the file to the system and the contents will be displayed graphically on the sample submission form.
4. If you need to change the structure file at any point it will still be possible to upload a different MOL file.

Structure Sketcher

The buttons presented on top of the sketcher provide functionality as described by the following list. It should also be noted, that in all states, you can use the mouse wheel to scale the sketcher rendering. You can also click and drag on the background, with nothing hovered, to move the entire molecule. If the shift key is held while dragging the background, the entire molecule will be rotated. Double-clicking on the background will center the molecule.



Zoom In Increases the rendering scale of the sketcher.

Zoom Out Decreases the rendering scale of the sketcher.

Erase Puts the sketcher into erase mode. Highlighting an atom and clicking will remove that atom and any small disconnected fragments, leaving the largest fragment remaining. Highlighting a bond and clicking will only have an effect if that bond is part of a ring, and in that case it will remove that bond.

Move Puts the sketcher into move mode. Highlighting an atom or bond and then pressing the mouse down and dragging will translate those objects.

Undo Undoes the last performed action.

Redo Redoes the last undone action.

Label After an element has been selected, hover an atom and click to change that atoms label to the selected element symbol.

Periodic Table Pops up a periodic table to select a symbol. After a symbol has been selected, hover an atom and click to change that atoms label to the selected element symbol. Press the Close button to close it.

Bonds After a bond type has been selected, hover an atom and press the mouse down to begin drawing a new bond of that type. Drag and place the preview to the preferred position and then release the mouse to place the bond. The optimize zone (blue circle) is provided to help place the bond in the optimal position when the mouse pointer is within the bounds of the circle. Hover a bond and click to change that bonds type to the selected type. The single bond tool is special and will add to bond orders instead of overriding them. Hold down the shift key to modify standard lengths and hold down the alt key to modify standard angles.

Rings After a ring type has been selected, hover an atom and press the mouse down to begin drawing a new ring of that type. Drag and place the preview to the preferred position and then release the mouse to place the ring. The optimize zone (blue circle) is provided to help place the ring in the optimal position when the mouse pointer is within the bounds of the circle. Hover a bond and press the mouse down to begin drawing a ring from that bond. Drag the preview to either side of the bond and then release the mouse to place the ring. Hold down the shift key to modify standard lengths and hold down the alt key to modify standard angles.

Charges After a charge sign has been selected, hover an atom and click the mouse to add or subtract from that atoms charge amount.

Lone Pairs After a lone pair icon has been selected, hover an atom and click the mouse to add or remove a lone pair from that atom.

1.4 Viewing Samples

The list of samples you have submitted can be viewed using the 'Samples' page available using the 'View Samples' option on the menu at the top of each page.

The system organises the samples into five lists, one for each stage and can be viewed by selecting the relevant tab on the page.



Unsubmitted Contains the list of all samples which you have provided some details for but have yet to submit.

Submitted All samples which have been submitted to the centre.

Received The list of samples that have been received by the lab and are ready for analysis.

In Progress The samples which are currently in the lab being analysed.

Completed All samples which have completed analysis and results processed.

Each list will contain the list of samples currently at that stage together with any identification data and the date at which it reached each stage. By default, the system displays 10 samples at a time and provides links so that each page can be accessed. However, it is possible to increase the number of samples per page by choosing an option next to 'Samples Per Page' and clicking 'Update'.

Unsubmitted (9)
Submitted (3)
Received (11)
In Progress (3)
Completed (10)

Displaying all samples
 Samples per page

Sample Reference	Submitter	Date Submitted	Date Received
Test10	SWATEST	2011-09-21 14:02:41	2011-09-26 16:31:23
Test11	SWATEST	2011-09-21 14:02:41	2011-09-26 16:31:20
Test12	SWATEST	2011-09-21 14:02:41	2011-10-09 11:39:23
Test14	SWATEST	2011-09-21 14:02:41	2011-09-26 19:03:58
Test15	SWATEST	2011-09-21 14:02:41	2011-10-09 11:39:26
Test18	SWATEST	2011-09-21 14:02:41	2012-04-27 15:08:00
Test19	SWATEST	2011-09-21 14:02:41	2012-04-27 15:08:02
Test20	SWATEST	2011-09-21 14:02:41	2012-04-27 15:08:04
Test21	SWATEST	2011-09-21 14:02:41	2012-05-01 15:38:56
roger1	SWATEST	2011-10-07 14:31:58	2012-04-27 16:18:52

To view the details of a specific sample click the 'Sample Reference' of the sample. This will take you to the page displaying the details of the form such as the structure and any data that was entered when the sample was submitted.

Filtering Samples

It is also possible to filter down the list of samples by providing a date range from which you want to view samples. This can be done in two ways.

Search for sample reference

Show samples from the

From:
To:

- Select a time period from the drop down menu to automatically display samples from within the last one, three, six or twelve months.
- Enter both dates from the beginning and end of the period you wish to filter. The date must be in the format DD/MM/YYYY.

1.4.1 Retrieving Results

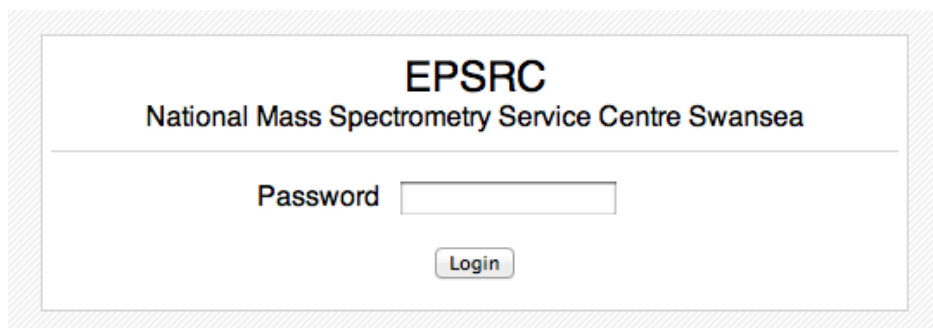
Throughout analysis of a sample the various techniques will produce a number of different result files. To provide these to yourself in an efficient manner, all files are added to a compressed Zip file.

1. Only samples that have reached the 'Completed' will have result files available.
2. Using the tabs, view the 'Completed' samples.
3. The 'Results' column of the list will indicate if a sample has a result file attached to it. If there is a file, the column will contain a link allowing you to download the results.
4. Click the 'Download' link. This will automatically download the Zip file containing any results produced by analysis of the sample.

2 Administration Web Application

2.1 Logging In

The administration area of the system requires a password to access the site. The system will automatically direct you to the login page if there is not an active session.



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Password

To log in to the system enter the administrator password into the field and click Logon. If correct you will be taken to the sample lists. The system will alert you if the password was incorrect.

2.2 Samples

The list of samples that have submitted can be viewed using the 'Samples' page available using the 'View Samples' option on the menu at the top of each page.

The system organises the samples into five lists, one for each stage and can be viewed by selecting the relevant tab on the page.



Unsubmitted (8)	Submitted (5)	Received (11)	In Progress (1)	Completed (6)
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Unsubmitted Contains the list of all samples that the user has provided some details for but have yet to submit.

Submitted All samples which have been submitted to the centre.

Received The list of samples that have been received by the lab and are ready for analysis.

In Progress The samples which are currently in the lab being analysed.

Completed All samples which have completed analysis and results processed.

Each list will contain the list of samples currently at that stage together with any identification data and the date at which it reached each stage. By default, the system displays 10 samples at a time and provides links so that each page can be accessed. However, it is possible to increase the number of samples per page by choosing an option next to 'Samples Per Page' and clicking 'Update'.

To view the details of a specific sample click the 'Sample Reference' of the sample. This will take you to the page displaying the details of the form such as the structure and any data that was entered when the sample was submitted.

2.2.1 Filtering Samples

The screenshot shows a blue filter box. On the left, there is a section titled 'Filter by Swansea Code' with an input field and 'Filter' and 'Clear' buttons. On the right, there is a section titled 'Show samples from the' with a dropdown menu set to 'Last Month' and a 'Filter' button. Below this, there are 'From:' and 'To:' input fields with a 'Filter' button.

While browsing the sample lists it is possible to filter by a Swan code so that only samples submitted by that institution are displayed.

1. In the blue filter box enter the Swan code into the field under 'Filter by Swansea Code' and click 'Filter'
2. The lists will now update to show only those samples from the Swansea code you specified.
3. To remove the filter and re-display all samples click 'Clear' in the blue filter box.

It is also possible to filter down the list of samples by providing a date range from which you want to view samples. This can be done in two ways.

- Select a time period from the drop down menu to automatically display samples from within the last one, three, six or twelve months.
- Enter both dates from the beginning and end of the period you wish to filter. The date must be in the format DD/MM/YYYY.

2.2.2 Booking In Samples

Booking in samples to the system in a semi-automatic process.

You can now book in samples for SWAMJL. The next sample code is **SWAMJL026**.

Sample Reference	Sample Code	Swan Code	Submitted	Book in	Unsubmit
Sample50		SWAMJL	2012-05-01 15:32:01	Received	Unsubmit
Reference1		SWAMJL	2012-05-01 15:35:50	Received	Unsubmit
Ref20		SWAMJL	2012-05-01 15:54:38	Received	Unsubmit

1. Filter the samples by a the Swan code of the samples you wish to book in.
2. Ensure that the 'Submitted' list of samples is selected using the tabs.
3. The system will automatically calculate the next sample code for you allowing you to click the 'Received' button in the 'Book In' column that corresponds to the sample you are booking in.
4. The sample will be assigned the sample code and the next sample code will be calculated.

2.2.3 Unsubmitting Samples

If at any point you need to unsubmit a sample due to data being missing or by request of the submitter, each sample has a 'Unsubmit' link next to it in the sample lists. Clicking this will move the sample back to the 'Unsubmitted' stage and will allow the submitter to edit the details and resubmit. However, the sample code that was assigned to the sample will remain so that the updated sample data can be matched up against the physical sample.

2.2.4 Deleting Samples

If at any point you need to remove a sample from the system, each sample in the 'Un-submitted' stage has a 'Delete' link next to it in the sample list. Clicking this will remove the sample and will no longer be displayed in the sample lists.

2.2.5 Sample Analysis Data

Analysis Details

	EICI	ESI	FAB	MALDI	GC	LS
LR	<input type="text" value="0"/>	<input type="text" value="2"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
HR	<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>

During the 'In Progress' stage it is possible to specify data about which techniques have been performed on the sample.

1. Navigate the sample detail page of the sample.
2. Under 'Analysis Details' there will be a number of fields for each technique that can be performed on the sample.
3. The fields represent a count of which techniques have been used. Increase the value in each field after each analysis.

2.2.6 Attaching Results

Attaching results is performed when a sample is at the 'In Progress' stage.

Sample Results

SWAMJL017_a.pdf	<input type="checkbox"/>
SWAMJL017_b.pdf	<input type="checkbox"/>
SWAMJL017_c.pdf	<input type="checkbox"/>

1. View the sample details page of the sample you wish to attach results to.

2. The system will automatically identify any result files for the sample and list them.
3. Use the checkboxes to identify which ones you want to attach.
4. Click 'Attach Results'. This will attach the files to the sample and move it into the completed stage.

2.3 Settings

Change Administrator Password	
Current Password	<input type="text"/>
New Password	<input type="text"/>
<input type="button" value="Change Password"/>	

Change Year Code	
Current Year Code	YM
New Year Code	<input type="text"/>
<input type="button" value="Change Year Code"/>	

2.3.1 Changing Year Code

The 'Year Code' functionality of the system allows the samples to be organised into different year codes. This groups all samples that have been analysed within the same year code together. Changing the year code will allow you to view samples from previous year codes and also begin a new year code.

1. Access the settings page using the 'Settings' option on the menu at the top of each page.
2. Under 'Change Year Code' heading, enter the new year code into the field and click 'Change Year Code'. The current year code will be updated and will be displayed.

The year code filtering only applies to samples that have been booked in during a specific year code. All other samples that have not reached this stage will be visible regardless of the year code.

2.3.2 System Password

The administration application uses a single password to control access for all members of staff at the centre. To change the password:

1. Access the settings page using the 'Settings' option on the menu at the top of each page.
2. Under 'Change Administration Password' heading, enter the current password and the new password into the relevant fields.
3. Clicking 'Change Password' will update the password and will be required when logging into the system in the future.