INSTRUCTIONS: MaSC mass spectral electronic submission tool

Address: http://research.ng-london.org.uk/scientific/masc/

Thank you for using this tool to submit your mass spectra to MaSC. With your help we aim to construct a library of mass spectra relevant to the cultural heritage community.

The process for submitting spectra is outlined in more detail below, but the main steps are;

- **Initiation:** Select/Make a profile and upload data file.
- **JCAMP file editing:** The uploaded mass spectral data is combined with information from the profile to create a JCAMP template which is then edited by the user to include sample specific information.
- **Submission:** The complete file is submitted to the MaSC database, where it will be checked by the MaSC committee and (hopefully) accepted.

Each of these steps is fully explained below:

Login and creating a profile

You will need a username and password that can be used to login via the tab at the top right of the homepage. If you have not yet been sent this information, please email spectra@mascgroup.org.

If you wish to change your password, click on the Edit user details tab on the left hand 'User Options' panel. Here you can also change personal information, such as your email address or job title. You can also select your institution from a drop-down menu. If your current institution is not on this list, then please email spectra@mascgroup.org, requesting the institution to be added.

Once you have edited your details, pressing update (or cancel) will take you back to the front page. You are now ready to create a profile. To do this you can click the yellow [+] button next to the 'Select a profile' field. This takes you to the Default profiles page, also accessible by clicking on the Default profile(s) tab on the User Options pane on the left. If you clicked on the default profile(s) tab, you will now have to click New to get a blank profile. You can create as many profiles as you like, so if several different systems are routinely used in your laboratory, you could create a profile for each of them.

You must now give your profile a name (all required fields are marked with a *). The analyst field is a drop-down menu which is limited to MaSC members within your institution. This is to ensure that submitted spectra are always linked to a MaSC member.

The following field is for the derivatisation method. Although this might change from sample to sample, it is worth remembering that everything that is entered in the profile can be edited at a later stage, so it would be best to select the method used most routinely. To ensure consistency, only the MaSC committee can add derivatisation methods to this list, so if your method isn't there, select '(Other: Defined in additional information)'. You should also notice a yellow information tab to the left of the derivatisation field. Clicking this will provide a pop-up box with more information about the respective field and what kind of information is expected.

The next section contains information related to the inlet/mass spectrometer system. The inlet, spectrometer and spectrometer type fields must all be selected from a defined list to ensure consistency across submitted spectra. If your system is not on this list, please email spectra@mascgroup.org, requesting it to be added.

The instrumental parameter field is a free text field where you can enter relevant inlet information, e.g. for a GC inlet method, you might include the column, pressure/flow control, temperature program, carrier gas, etc.

The Ionisation mode in the acquisition conditions section must be selected from a drop-down menu. Once again, if your ionisation mode is not listed, please email spectra@mascgroup.org, requesting it to be added. The source temperature and ionisation energy are both required fields. If a soft ionisation technique is being used, please write N/A in the ionisation energy field. If the scan rate, resolution and threshold of your mass spectrometer are known, please enter these into their respective fields, including the units.

Once you have completed as many fields as you can, press continue. If all the required fields have not been filled, the system will not let you proceed. Otherwise, a blank profile will be displayed and you will see that your new profile now appears in the 'current profile(s)' drop-down box at the top of the page. Your profile can be edited at any time and remember, you can create as many profiles as you like.

You are now ready to upload some mass spectral data, so click the upload new file tab on the 'User Options' tab at the left hand side of the page and select your profile from the drop-down menu. Now click browse to select a file to upload.

Any ASCII based file can be uploaded i.e. .txt; .csv; .JCAMP-DX. For information about how to export spectra into an ASCII based format on different mass spectrometer systems, please see the MaSC website (http://www.mascgroup.org/datasubmission.html). If there is an upload error and the file is not recognised, check that it conforms to one of the acceptable layouts by clicking on the 'Example file layouts' tab on the 'Extra Options' pane on the left of the page. If you are still having problems, please email spectra@mascgroup.org, attaching the problematic file to your email.

JCAMP file editing

Upon successfully uploading your file, click continue. All JCAMP-DX fields are now visible, including the information previously entered into the profile. If for any reason you had to stop at this moment, you could press the cancel button at the bottom of the page. This takes you to a list of your uploaded files (also accessible via the 'List user files' tab on the 'User Options' pane to the left of the page) where the file you have just uploaded (and any previously uploaded files) should be visible. The file status should read 'Uploaded'.

Once the file is uploaded, it can be opened for editing at any time by the user who uploaded it. Once the correct information has been entered into the fields, the file can be submitted by pressing the submit button at the bottom of the page. The status of the file now changes to 'Submitted'.

The file will now be checked by a member of the MaSC committee. If it meets the review criteria, the status will change to 'Accepted'. You can see a list of all accepted files by clicking on the 'List all accepted files' tab in the 'Extra Options' pane on the left hand side. In summary a file status can be Uploaded (editable by user), Submitted (locked, editable by MaSC) or Accepted (locked). If you submit an incomplete file by accident, please email spectra@mascgroup.org who will unlock the file for you.

Before entering the relevant information in the sample specific fields (and checking the profile fields) you might want to take a look at the spectrum (re-scaled automatically during upload). You can do this by clicking the View spectrum tab at the top right hand side of the page.

In the JCAMP DX file variables page, you will notice that the spectrum 'Title' comprises a MaSC number, followed by a blank box. The MaSC number cannot be altered, but the common or trivial name of the compound should be entered in this field. The following three fields cannot be altered by the user, so are greyed-out.

The 'Analyst & Sample' section again has a mixture of user alterable and fixed fields. The 'Analyst' field utilizes information from your profile and institution, but can be altered if required. The 'Copyright' field is generally the year the spectrum was submitted as well as the institution's name (the submitting institution retains copyright over the spectrum) but can be altered if required. The 'license' statement field is not user alterable, but the 'original filename' field can be changed to allow the correct filename to be entered. The 'Derivatisation' field has been taken from the applied profile, but can be changed if not correct for this particular sample.

If '(Other: Defined in additional information)' was selected in the 'Derivatisation' or 'Spectrometer' field, details should be provided in the 'Additional Information' field, together with reaction times, solvents etc. In addition, the 'Sample Description' field allows information about the composition or origin of the sample, for example, linseed oil/mastic, painted out on a glass plate at the National Gallery, 1958. If the spectrum that you are uploading has been published, please indicate this and include the relevant citation in the Comment field at the bottom of the form. The date uploaded field is non-adjustable.

All fields in the 'Inlet / mass spectrometer system' section are taken from the applied profile, but can be altered for this sample if required. A significant number of the fields in the 'Acquisition conditions' section are also taken from the applied profile, but again are alterable if they were changed when acquiring the uploaded spectrum. The 'Scan

number', 'Retention time' and 'Kovats index' fields are not required, but the information is valuable and should be entered if known.

Please enter any information you are able to provide in the 'Compound Details' section. Even if the exact compound name is not known, general information e.g. dehydroabietic acid related (probably oxidation product), would be useful. The first two fields in the 'Spectrum' section are calculated from the uploaded spectrum, so are non-alterable. If the relative ion count is known, please enter in the appropriate field. Most importantly, if any data processing (including averaging and background subtraction) have been applied to the submitted spectrum, please put this in the 'Data processing' field. As mentioned above, the 'Comment' field could be used for bibliographic information on a previously published spectrum or for any additional comments you may have.

Submission

Once you are happy with the information in all the fields, the complete file can be submitted to the MaSC database by clicking 'Submit' at the bottom of the page. Clicking Cancel will lose any changes that have been made and the file will revert back to its 'uploaded' state.

Once submitted the status of the spectrum will change from 'Uploaded' to 'Submitted' and it will be checked by the MaSC committee. If it meets the review criteria, it will be accepted, upon which its status will then change from 'Submitted' to 'Accepted'. All files accepted by the MaSC committee can be viewed by clicking on the 'List All Accepted Files' tab in the 'Extra Options' pane at the left hand side of the page.

Clicking on the text of any of the files in this list (or in the list of your uploaded files, accessible via the "List user files" tab in the "User Options" pane to the left of the page) will bring up the JCAMP-DX file variables form. However, if you want to obtain the JCAMP-DX file, click on the notepad icon in the list of uploaded/accepted files (it will open in a new window/tab). If you want to compare this spectrum to one of yours and can't wait for the next release of the compiled MaSC library, you can also save it as a JCAMP-DX file. You should now be able to import this spectrum into your own system.
If you have any questions or queries about the process outlined above, please contact MaSC.

Thank you for contributing to this resource!