

A. Correct Format of the MS Methods in the Library to be Imported

In order to import a Quanoptimize Compound Library into a Quanpedia database, the optimized MS Methods in the library must be correctly formatted, as described below. If any of the methods have a different format, none of the methods will be imported.

1. Only MRM or SIR function methods can be imported. Furthermore, the function type (MRM or SIR) must match the acquisition on mode that is selected in Quanpedia. Any other functions are ignored.
2. The methods must contain only one function and one channel. If any of the methods contain multiple functions, the following error message is displayed:



Import Failure Report

The reasons why the import failed are shown below. Fix the issues and retry.

Import files:

C:\CompoundsTest\MSMS_CYCLOBENZAPRINE_new.expC:\CompoundsTest\MSMS_test1.exp

Import mode: [MS method files]

Acquisition mode: [Multiple Reaction Monitoring (MRM)]

Error: Unable to import - Too many functions found in MS Method File

[C:\CompoundsTest\MSMS_test1.exp].

Only able to import MS Method files containing a single function

If any of the methods contain multiple channels, the following error message is displayed:

'Unable to Import - Compound Name Variation for Function 1 channel 0 in File xxxx.exp'.

3. The name of each MS method file in the library must have the format MSMS_[compoundname].exp. If the format is incorrect, the following error may be displayed:



Import Failure Report

The reasons why the import failed are shown below. Fix the issues and retry.

Import files:

C:\CompoundsTest\msms BUMETANIDE.exp C:\CompoundsTest\MSMS_CYCLOBENZAPRINE_new.exp

Import mode: [MS method files]

Acquisition mode: [Multiple Reaction Monitoring (MRM)]

Error: Unable to import - Invalid File

[C:\CompoundsTest\msms BUMETANIDE.exp].

Only able to import MS Method files with a prefix of [MSMS_]

4. The compound name must exactly match the compound name inside the MS Method. Even just an extra space after the compound name in the method is sufficient to prevent the import. Quanpedia displays an appropriate error messages if there is a mismatch between the compound name in the file name and the compound name inside the method:



Import Failure Report

The reasons why the import failed are shown below. Fix the issues and retry.

Import files:

```
C:\CompoundsTest\MSMS_ACETAMINOPHEN.expC:\CompoundsTest\MSMS_ACETAMINOPHEN_NEW.expC:\CompoundsTest
\MSMS_ACETAMINOPHEN_SAB.expC:\CompoundsTest\MSMS_ACETAMINOPHEN_TEST.expC:\CompoundsTest\MSMS_ALBENDAZOLE.expC:\CompoundsTest
\MSMS_ALPHA_NAPHTHOFLAVONE.expC:\CompoundsTest\MSMS_AMIODARONE.expC:\CompoundsTest\MSMS_Antipyrine.expC:\CompoundsTest
\MSMS_ATENOLOL.expC:\CompoundsTest\MSMS_BEK1.expC:\CompoundsTest\MSMS_BEK2.expC:\CompoundsTest\MSMS_BEK3.expC:\CompoundsTest
\MSMS_BISACODYL.expC:\CompoundsTest\MSMS BUMETANIDE.expC:\CompoundsTest\MSMS_CARBAMAZEPINE.expC:\CompoundsTest
\MSMS_CARBAMAZEPINEMDCK.expC:\CompoundsTest\MSMS_CYCLOBENZAPRINE_new.exp
```

Import mode: [MS method files]

Acquisition mode: [Multiple Reaction Monitoring (MRM)]

Error : Unable to import - Compound Name variation for Function[1] Channel[0]

File:[C:\CompoundsTest\MSMS_ALPHA_NAPHTHOFLAVONE.exp]

Compound Name[ALPHA-NAPHTHOFLAVONE] should be[ALPHA_NAPHTHOFLAVONE]

Error : Unable to import - Compound Name variation for Function[1] Channel[0]

File:[C:\CompoundsTest\MSMS_Antipyrine.exp]

Compound Name[Antipyrene] should be[Antipyrine]

'Unable to Import - Compound Name Variation for Function 1 channel 0 in File xxxx.exp'. In the first example, the file is called MSMS_alpha_Naphthoflavone.exp, but the compound name is alpha-Naphthoflavone.

5. If there are no valid methods found in the Compound Library, or if the specified acquisition mode does not match any of the methods, the Path field will be highlighted in red, as shown below:



Select QuanOptimize Library

Enter the name of the QuanOptimize library to import.

Path:

B. Upper Limit on the Number of Compounds in the Library that can be Imported

In addition to the formatting issues described above, there is an upper limit to the number of compounds that can be imported at the same time. For example, testing shows that using an M58 PC with Windows 7 and 2GB RAM, the upper limit was 460 compounds. Using a PC with more RAM did not allow more compounds to be imported.

If the upper limit is exceeded, Quanpedia may either crash with the error 'Quanopedia has stopped working', or the import fails but there are no error messages. In both cases, Quanpedia needs to be restarted.