Mass++ : A platform for mass spectrometry to construct suitable software to achieve user's own purposes

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1. Introduction

Mass++(Ver.2) is freely available software for mass spectrometric data analysis which is developed and maintained by Shimadzu and Eisai under First ms3d project(a Japanese national foundation). Mass++(Ver.2) can be Downloaded from the below website; http://www.first-ms3d.jp/english/.

Its' characteristics are;
(1) A wide range of vendors' data file formats are supported
(2) Essential functionalities for biological MS are implemented
(3) The plug-in structure makes it possible to add or remove functions

Data analysis

Mass spectrometers

Mass++(Ver.2)

Development & support   **Development & support**

Shimadzu   **Eisai**

FIRST ms3d project
(Japanese national foundation)

Contact

Vendor A
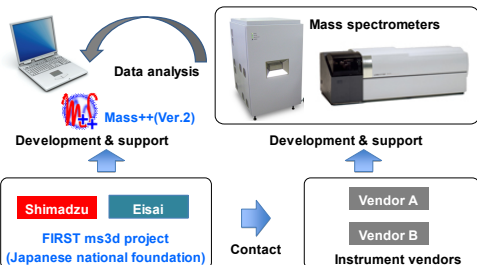**Vendor B**
Instrument vendors

Fig. 1 Mass++ development and multi vendor support

Mass++ successive objective taken over since 2006 first edition by Eisai is to provide a software whose functions cannot be supplied with commercial software attached to Instruments. Although it was not so easy to create new functions on Mass++ indeed.

In this poster, we will show the recent improvements on Mass++ to help developers and the examples of developed plug-ins of our own which are necessary to our ms3d project. Then we'll also make a discussion about the role of the Mass++ as a platform.

2. Method

2-1. Plug-in development assistance tools

We have prepared the Mass++ plug-in wizards for C++ and C# to help developers. The wizards will take the duty to provide a suitable environment to start the development to assist developers.

2-2. Script language programming function

However the plug-in development becomes to be easier than before, it is still difficult for chemists, biologists or medical scientists to develop plug-ins using C++ or C.
In order to extend the Mass++ developers to those, we have prepared the "Script Console" function which provides a script language programming environment. The employed script language is well known IronPython. The programming is much easier especially for those other than software engineers or programmers.

3. Results

3-1. Plug-in development with the wizards

The starting process which was time consuming and sometimes caused confusions is now automated by the Mass++ plug-in wizard as shown in fig.2. The processes are much simplified.
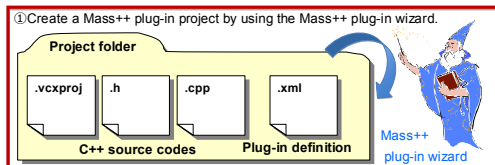
①Create a Mass++ plug-in project by using the Mass++ plug-in wizard.

Project folder
.vcxproj   .h   .cpp   .xml
C++ source codes   **Plug-in definition**

Mass++ plug-in wizard

②Set plug-in types, handlers, and parameters on the plug-in definition file.
③Implement functions on the C++ source codes to build dlls (dynamic link libraries).
④Put the plug-in folder which contains the plug-in definition and dll to the predetermined Mass++ plug-in folder

Fig. 2 Whole working processes to develop a Mass++ plug-in

3-2. Programming with the script console

Users can write the programming codes directly on the "Script Console" dialog and run it immediately as shown in fig.3. The process is much easier compared to fig.2, we surely expect that more users will be encouraged to develop their own functions by themselves.
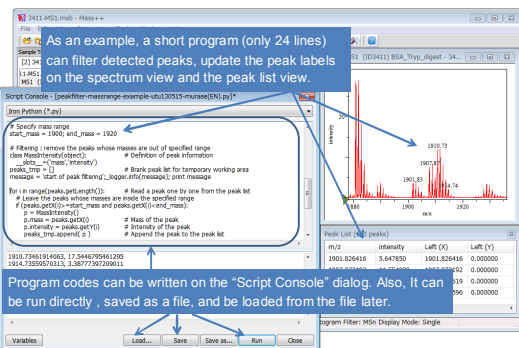
As an example, a short program (only 24 lines) can filter detected peaks, update the peak labels on the spectrum view and the peak list view.

Program codes can be written on the "Script Console" dialog. Also, It can be run directly , saved as a file, and be loaded from the file later.

Fig. 3 A programming example with the Mass++ script console

4. Discussion

4-1. Examples of developed plug-ins

We are working in research and development of mass spectrometry data analysis, then some outcomes have been implemented as Mass++ plug-ins and become to be freely available on Mass++. Those are the de novo sequencing method[1], the search method for MSn data[2] [4], the peak detection algorithm[3], the tools for statistic analysis[5], and so on.

Besides, we've developed some unique plug-ins which are required by chemists or biologists in our project.
Fig.4 shows an example of those plug-ins which works for the Glycan analysis using the specific labelling[4][6]. It can show the structure candidates predicted by the specified conditions and displays annotations of each peak on the spectrum view. These kinds of functions are not necessary to general users, so instrument vendors will never support generally. Mass++ plays an important role in these cases.
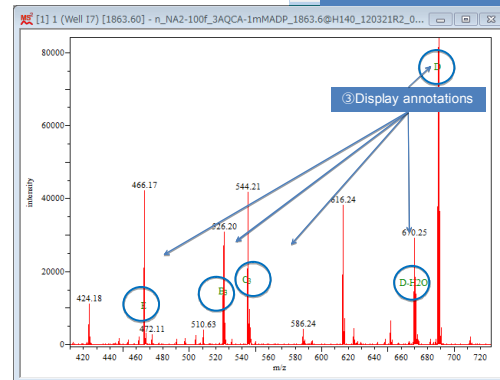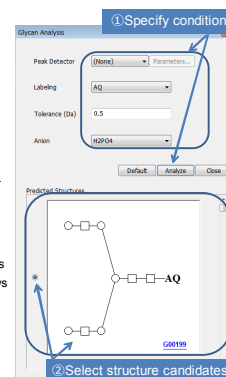
①Specify conditions
②Select structure candidates
③Display annotations

Fig.4 The plug-in for labelled glycan analysis[4][6]

4-2. Roles of the platform

Mass++ consists of three parts as shown in Fig.5 .
(1)The platform provides a simple viewer which can open data files and display those.
(2)Plug-ins developed by ms3d are available if necessary.
(3)Plug-ins developed by users can be add and run on Mass++.

Plug-in [developed by ms3d]
Glycan analysis   MSn Search
Peak detection   Statistical analysis

Plug-in [developed by users]
User1 Application   User2 Application

Data display   Core Functions   Data file read
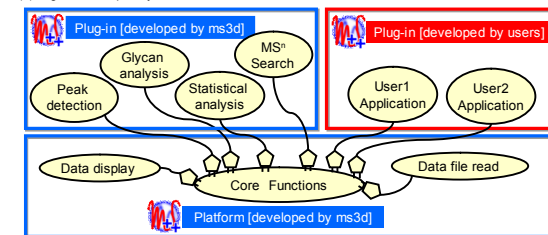
Platform [developed by ms3d]

Fig.5 Software structure of Mass++(Ver.2)

In current ms3d project, Mass++ plays a role to distribute the outcomes of the public project open to public. Now, we will suggest its' roles and availabilities as a public platform software as below.
(1)The platform provides a simple viewer. It seems to be worth as a commonly available tool to visualize mass spectrometry data stored in public databases or shared between collaborators.
(2)The software structure allows additional functions developed by anyone. Mass++ seems to be useful as a common platform to evince or demonstrate developed software or algorithms.
(3)According to the Mass++(Ver.2) license, users have right to sell, distribute, lend, or transfer the plug-ins which are developed by themselves at their own risk and account same as Shimadzu and Eisai. This may encourage some kinds of users to develop Mass++ plug-ins.

5. Conclusions

・ The Mass++ plug-in development was simplified with the recently added wizards for C++ and C#.
・ The new "Script Console" function provides an easier way to develop use's own function, so the users with small programming experiences will be able to participate in developing functions by themselves.
・ Outcomes of ms3d project are implemented as Mass++ plug-ins and distributed freely .
・ Mass++ has possibilities to play unique roles as a common viewer or a platform.

Mass++ can be downloaded from the ms3d project website http://www.first-ms3d.jp/english/. Suggestions or requests are much appreciated. You can post them on the same website, thank you.

References.

[1] Murase, M. ; et. al., ASMS(2010), TP148
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[5] Fujita, Y.; et. al., ASMS (2013), MP18-359
[6] Nishikaze, T.; et. al., Anal. Chem.2012, 84, pp9453