

Manual Version 2.1

From Biopolymer Mass Spectrometry

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Credits

A short manual created by **David Damerell** and **Kai Maass** for GlycoWorkbench version 2.1

GlycoWorkbench was developed by **Alessio Ceroni** (Division of Molecular Biosciences, Imperial College London, UK) assisted by **Kai Maaß** (Institute of Biochemistry, Faculty of Medicine, University of Giessen, Germany) as part of the EUROCarbDB project, a Research Infrastructure Design Study Funded by the 6th Research Framework Program of the European Union (Contract: RIDS Contract number 011952).

GlycoWorkbench is now developed by **David Damerell** (Division of Molecular Biosciences, Imperial College London, UK) funded by the Biotechnology and Biological Sciences Research Council (BBF0083091 to Prof Anne Dell and Dr Stuart Haslam) assisted by **Kai Maaß**, **Rene Ranzinger**, and **Matthew Campbell** (to name but a few)

Citation

If you are using *GlycoWorkbench* for preparing your articles, or if you employed the *GlycanBuilder* applet in your web interface, please cite:

A. Ceroni, K. Maass, H. Geyer, R. Geyer, A. Dell and S.M. Haslam,

***GlycoWorkbench: A Tool for the Computer-Assisted Annotation of Mass Spectra of Glycans*,**

[Journal of Proteome Research](#), 7 (4), 1650--1659, 2008, DOI: 10.1021/pr7008252

Support

If you have any questions regarding the installation or use of *GlycoWorkbench* or you have feature suggestions or have identified bugs - please email info@glycoworkbench.org (we try to respond the same day)

Introduction

GlycoWorkbench is a suite of software tools designed for the rapid drawing of glycan structures and for assisting the process of structure determination from mass spectrometry data. The graphical interface of GlycoWorkbench provides an environment in which structure models can be rapidly assembled, their masses can be computed, their fragments can be automatically matched with MSn data, the results can be compared to assess the best candidate, and, finally, the best match to the spectrum can be displayed graphically. GlycoWorkbench can greatly reduce the time needed for the interpretation and annotation of mass spectra of glycans. The aim of GlycoWorkbench is to offer complete support for the routine interpretation of MS data.

Download and Installation

System requirements

The tool has been tested under Windows, Linux and Mac OS X. In order to run the GlycoWorkbench tool, the Java Runtime Environment (JRE) version 6.0 update 20 or later must be installed on the computer. The latest release of the JRE 6.0 can be found on the Sun homepage ([\[1\]](#)) together with the installation guide and system requirements.

Download

The latest version of the GlycoWorkbench tool can be downloaded from the GlycoWorkbench homepage (<http://www.glycoworkbench.org>).

Installation

Windows

* Windows Installer (recommended) [winsetup_x86](#) or [winsetup_x86-64](#)

* Windows Archive [zip_archive_x86](#) or [zip_archive_x86-64](#)

Unless you are a Java developer it is highly unlikely that you have a 64bit version of Java installed (the Oracle web page defaults to 32bit for all Windows users) regardless of whether your OS is 64bit. It is therefore recommended that you try the 32bit packages first (x86 not x86-64). If GlycoWorkbench fails to launch it might mean that you have downloaded the wrong package for your system. When you launch GlycoWorkbench you might be met with a message saying something along the lines of "Java could not be found". This either means you don't have Java installed or you have tried to run a 32bit version of GlycoWorkbench when you have a 64bit version of Java installed (or the other way around).

If the installer doesn't work for you - download and extract the above ZIP archive to your directory of choice; GlycoWorkbench can be launched with the enclosed executable. Failing this please try the procedure below to launch GlycoWorkbench manually.

- Open a command prompt (Start->Accessories->Command prompt) (icon is a small black screen with a cursor icon)
- Next navigate to the folder you extracted GlycoWorkbench to

```
chdir C:\Users\<username>\<directory_you_extracted_glycoworkbench_to>\gwb\ (for Windows Vista and 7)
chdir C:\Documents and Settings\<username>\<directory_you_extracted_glycoworkbench_to>\gwb\ (for Windows XP)
```

- Finally launch GlycoWorkbench

```
java -jar eurocarb-glycoworkbench-1.0rc.jar
```

Finally if GlycoWorkbench still won't load for you email the following information to info@glycoworkbench.org

- List all versions of Java you can see in the Add/Remove programs dialog box (on Windows XP) or Uninstall a program dialog box (on Windows Vista and 7) which can be launched from the Control Panel
- Windows Version (if your not sure run the builtin program "winver", which can be launched either via the run command or within a command prompt, which will display the precise version of Windows you are running) - including if it's 64bit or not (indicated by either x86-64 or 64bit, note that some older 64bit versions of Windows do not display this information with the winver command).
- Stacktrace which you can obtain by manually launching GlycoWorkbench (as documented above) (optional, but without this we might not be able to offer much help)

Linux

* Linux Archive [zip_archive_x86](#) or [zip_archive_x86-64](#)

Software installation packages are not provided for Linux users, as they are for Windows users, this is primarily because of the diversity of Linux distributions that users may be using. Linux users should start by identifying whether they have a 64bit or 32bit version of Java installed, note that unlike Windows users, Linux users are far more likely to have a 64bit version of Java installed by default. The simplest method to check the version of Java you have installed is to run the command below.

```
java -version
```

Below is the output of a 64bit Oracle version of Java

```
java version "1.6.0_26"
Java(TM) SE Runtime Environment (build 1.6.0_26-b03)
Java HotSpot(TM) 64-Bit Server VM (build 20.1-b02, mixed mode)
```

And another for a 64bit OpenJDK version of Java

```
java version "1.6.0_22"
OpenJDK Runtime Environment (IcedTea6 1.10.2) (6b22-1.10.2-0ubuntu1~11.04.1)
OpenJDK 64-Bit Server VM (build 20.0-b11, mixed mode)
```

- Users with a 64bit version of Java should download the x86-64 Linux ZIP archive and users with a 32bit version of Java should download the x86 Linux ZIP archive.
- Once downloaded simply extract the ZIP archive to your directory of choice.

The method of running GlycoWorkbench varies between Linux distributions and desktop environments (i.e. Gnome versus KDE)

- Gnome users should start by opening the file manager on the directory GlycoWorkbench has been extracted to

First you need to enable execution of the main GlycoWorkbench jar

- Right-click on eurocarb-glycoworkbench-1.0rc.jar
- Left-click on Properties
- Left-click on the Permissions tab
- Tick Enable Execution.
- Left-click on close

Now launch GlycoWorkbench as follows

- Right-click on eurocarb-glycoworkbench-1.0rc.jar

This should display a list of Java virtual machines you have installed

- Left-click on Open with <java_version>

Alternatively you can launch GlycoWorkbench from the command line (this is also useful when GlycoWorkbench fails to launch as this method allows you to obtain a stack trace)

- Open a terminal
- Type the following

```
>cd <directory_you_installed_glycoworkbench_to>
>java -jar eurocarb-glycoworkbench-1.0rc.jar
```

If GlycoWorkbench won't launch please email info@glycoworkbench.org with the following information

- Linux distribution version (including if it is 64bit or not)
- Output of "java -version"
- Stack trace obtained by trying to launch GlycoWorkbench manually

Mac OSX

It is our aim to support GlycoWorkbench on Mac OSX - although it should be stressed that none of the developers has routine access to a machine running Mac OSX for testing and development purposes. For this reason the GlycoWorkbench website and this manual will always contain a link to the last version of GlycoWorkbench which was tested on Mac OSX - which is currently build [83](#). Of course the latest version of GlycoWorkbench may indeed run perfectly fine on Mac OSX machines - if you have any feedback on GlycoWorkbench running on Mac OSX (i.e. you know the latest version isn't running on Mac OSX) please send an email to info@glycoworkbench.org

Complexities of supporting a Java application on Mac OSX

With the release of GlycoWorkbench version 2.0 the minimum version of the Java language that the installed Java virtual machine needed to be compliant with was changed from version 5 to 6. For Windows and Linux users who only had a Java virtual machine installed that was compliant with version 5 of the Java language this simply required them to upgrade the Java virtual machine. Oracle and other companies have released Java virtual machines that are compliant with version 6 and greater of the Java language for virtually all versions of Windows (including Windows XP) and Linux.

Unfortunately the same can not be said for Mac OSX users - the basic rule appears to be that if you have Snow Leopard or newer installed you should be able to run GlycoWorkbench (although you may need to update the version of Java installed via the usual Apple update procedure). Lion users can visit this [link](#) to download the latest version of Java (which is not installed by default). It is also understanding that some Leopard users are able to update their Java virtual machine, via the normal Apple update procedure, to a version that can run GlycoWorkbench (this seems to depend on whether you are running an Intel x86/x86-64 or PowerPC processor)

Installing and running GlycoWorkbench

It is currently not clear to us which version of GlycoWorkbench different users of Mac OSX will need to download - principally because we have little experience with Mac OSX and can't find any definitive information online with regards to which Mac OSX models are 32bit or 64bit (and of these if a 64bit version of Java is always installed). It is probably a safe bet that the newer your Mac computer is the more likely you need the 64bit version of GlycoWorkbench (this is the first link below). The best advice we can give you is to try each version below in order until GlycoWorkbench launches correctly.

- * Mac Cocoa (64bit) Archive [zip_archive_cocoa_x86-64](#)
- * Mac Cocoa (32bit) Archive [zip_archive_cocoa_32](#)
- * Mac Carbon (32bit) Archive [zip_archive_carbon_32](#)

Run GlycoWorkbench by clicking on the GlycoWorkbench.jar file (you might need to click open afterwards).

You can run GlycoWorkbench manually by first opening a terminal and typing the following.

```
>cd <directory_you_extracted_glycoworkbench_to>
>java -jar GlycoWorkbench.jar
```

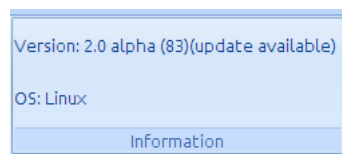
If you can't get GlycoWorkbench to launch please email as much of the following information as you can obtain to info@glycoworkbench.org

- * Output of "uname -a" (launch this command in a terminal)
- * Mac OSX version and whether it is 64bit or not
- * Processor type if you know it (although this is becoming less of an issue, as most people will be running on Intel processors by now)
- * Output of "java -version" (again launch this command in a terminal)

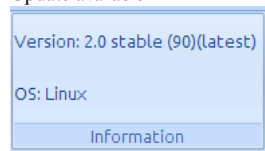
Finally we will continue to update this page, as we learn more about supporting GlycoWorkbench on Mac OSX

Updating

New versions of GlycoWorkbench are released fairly frequently so that users can benefit from new features and bug fixes as soon as possible. GlycoWorkbench checks the GlycoWorkbench web site every time it starts up to see what the latest build number is. If the latest build number is higher than what you have installed, GlycoWorkbench will notify you that an update is available in the information panel located on the "Home" ribbon - as shown in the first image below. Simply click the "update available" button which will launch a web browser inside GlycoWorkbench and direct you to the GlycoWorkbench download page.



Update available



Running latest version

Configuration files

GlycoWorkbench has a single configuration file that stores all global settings (i.e. settings that apply across GlycoWorkbench projects). The location of this configuration file was changed with the release of version 2.1 - this change was required to support new functionality in this version. See the table below for the previous and current locations of these settings files.

Version	OS	Location
1.x	All	<glycoworkbench_run_directory>/glycoworkbench.xml

- | | | |
|------------|---------|---|
| | Windows | AppData/GlycoWorkbench/glycoworkbench.xml |
| 2.0 | Linux | \$HOME/.glycoworkbench.xml |
| | Mac OSX | \$HOME/glycoworkbench.xml |
| | Windows | AppData/GlycoWorkbench/settings.xml |
| 2.1 | Linux | \$HOME/.GlycoWorkbench/settings.xml |
| | Mac OSX | \$HOME/.GlycoWorkbench/settings.xml |

The GlycoWorkbench settings file used to be stored in the same directory that GlycoWorkbench was installed into - this makes it difficult for Windows Vista and Windows 7 users to install GlycoWorkbench into the "Program Files" directory as GlycoWorkbench doesn't have write access to this directory. This also meant that unless you were careful you would also lose your settings when you downloaded a new version of GlycoWorkbench. The latest version of GlycoWorkbench stores all its settings in a hidden directory - which makes it easy for us to store files in a convenient location. Note that on Windows the AppData directory can be called different things depending on which language version of Windows you are running - this isn't an issue for GlycoWorkbench as the location of the "AppData" directory is determined at run time by asking the Java virtual machine for the correct location. Finally note that when you upgraded from version 2.0 to 2.1 your settings file was automatically moved to the new location.

Customizing definition files

GlycoWorkbench uses a number of files which define...

- Residue types (i.e composition, fragmentation, etc.)
- Fragmentation patterns
- Builtin core structure types (i.e. those shown in the drop-down gallery, core, core-fucosylated, etc)
- Builtin terminal types (i.e. Blood group A antigen)
- Atoms (i.e. average mass, mono-isotopic mass)
- Isotopes (actual mass)

Starting with version 2.1 of GlycoWorkbench it is possible to customize all but the atom and isotope definition files (these will be customizable in the future, along with derivatization and reducing end types). GlycoWorkbench also uses files which define the different symbolic notations - again these can now be customized. The GlycanBuilder jar, which is located in the lib directory of GlycoWorkbench installations, contains the default versions of each of these files. To alter these resources you create new files that initially have the same content as the default definitions.

Be careful: At the moment it is possible to stop GlycoWorkbench launching by corrupting or deleting things you shouldn't (see [this section](#) for possible solutions). The guaranteed way of getting GlycoWorkbench to launch again is to delete your global configuration settings - see [this section](#) for details on locating this file

Compatibility warning

There are a number of issues that need to be pointed out that arise from allowing users to alter the definition files, which is directly related to how custom definitions are stored.

- Definition file locations are not stored in GlycoWorkbench project files
- Instead they are stored in the global GlycoWorkbench settings file (i.e. on Linux systems this file is ~/.glycoworkbench.xml)

This means that if a GlycoWorkbench project makes use of custom definition files you won't simply be able to give someone else your GlycoWorkbench project file and expect it just to work. In this case you must also provide the custom definition file and ask the user to update (possibly temporarily) where their instance of GlycoWorkbench looks for its definition files. In the future we may look at incorporating custom definitions directly in the GlycoWorkbench project file. That said please see the [Sharing custom definitions](#) section for further guidance.

As previously stated GlycoWorkbench will now let you alter any of the current symbolic notation formats - the main motive behind this was to allow users to assign symbols to residues that they add. Users are strongly encouraged to use this feature sparingly - especially if you are generating figures for publication. Remember that most of your readers will not be familiar with your new symbol and so you will obviously need to provide a key. In addition consider that if you are creating a new symbol that many people in your particular field are already familiar with it might be useful for others if you ask us to add this symbol to the default definition list.

Hopefully knowing what issues may arise - will help you to use this new feature correctly.

Definition file locations

By clicking the main application menu button followed by settings you will see the new GlycoWorkbench settings dialog box. If you scroll down to the section titled "Dictionaries and definition files" you will see the current list of definition files that you can customize and the current location of the corresponding definition file. By default each definition file location will be set to the default path - which is for a file located in the GlycanBuilder jar. You will notice that the edit button next to each definition file is disabled. You can only edit custom definition resources, not the default ones located within the GlycanBuilder jar.

A text box is provided for each definition file that allows you to set the definition file location - valid file locations are...

- Resources on the GlycoWorkbench class path (most users can ignore this)
- Resources on the local system (i.e. a local file)
- Resources located on a remote system (i.e. those on a web server).

Conflict warning

You might be tempted to store configuration files in a directory called "conf" which is located at the root of your file system - i.e. "/conf/residue_types" (which is equivalent to C:\conf\residue_types, for most Windows users). You might even think that is where GlycoWorkbench looks by default as the default location for all resources starts with "/conf". However at the moment you shouldn't do this, for the following reason...

- The default location is actually pointing to a file located on the root of the class path not the file system
- And by default GlycoWorkbench won't look for a resource on the local file system if it finds a matching resource on the class path

This issue is considered a bug (which probably won't affect anyone) but that requires a non-trivial fix - because of the way this new functionality interacts with legacy code.

Changing definition file path

GlycoWorkbench provides a few simple ways to change where it looks for a definition file - once GlycoWorkbench sees that you have pointed it to a custom definition file, the edit button will be automatically enabled.

1. Manually enter either a file location or URL into the corresponding text box (don't do this unless there's actually a real definition file located there)
2. Click "Create custom"
 1. This will ask you where you would like to save the new definition file
 2. This will copy the default definition contents to the new file
3. Click "Open" if you already have a local file that you would like to use
 1. You will be asked for the location of the file

Changing the location of all definition files

There are two ways of updating the location of all definition files...

1. Click "Customize all"
 1. This will ask you for a directory to save the new definitions files into
 2. A new definition file will be created for each resource with the contents of the default definition file
 3. The location of each definition file will be updated to point to the new definition
2. Click "Enter base URL"
 1. This will allow you to tell GlycoWorkbench to look for each resource in a particular directory of a remote resource (i.e. a web server) (for information on this technique see the [Sharing definition files section](#))
 2. You will be prompted for the base URL where all resources can be located
 3. The location of each definition file will be changed to a remote URL

Sharing custom definitions

If you are working in a group where you all need to change the GlycoWorkbench definitions in the same way (i.e. you all work with glycans with a particularly unusual sugar) - you will probably want to share your new definition files with the others in your group. GlycoWorkbench gives you a few choices...

1. Simply give the other members of your group the new definition files - and get them to update the relevant paths in GlycoWorkbench
2. Place the new definition files on a shared drive that you can all see - and point GlycoWorkbench at this location
3. Store the definition files on a web server
 1. Simply upload the definition files to a web server
 2. And ask the members of your group to point GlycoWorkbench to the web server (note that if you are uploading all of the definition files, GlycoWorkbench can point its self to the web server in one go if you click "Enter base URL" - you should enter the URL that all of your custom definition files are located at).

Obviously you can use the final option to make your custom definitions available to people outside of your group as well. If you feel that what you are changing in the default definitions should become part of the default GlycoWorkbench definitions, please email info@glycoworkbench.org with preferably either a link to your new definition files or the actual files attached along with a description of what you have changed.

Editing definition files

At the moment GlycoWorkbench doesn't provide a nice UI to guide you through the process of editing definition files - instead it simply provides you with a text editor when you click the "Edit" button. It is entirely possible for you to make it impossible for GlycoWorkbench to start if you make mistakes when editing these definition files. Until a nice UI is created please read the following carefully.

1. Never delete a residue from the residue_types file (this goes for pretty much all the definition files, unless you know what you are doing delete nothing)
2. Don't panic if GlycoWorkbench won't start there are a couple of simple solutions.
 1. The easiest is to locate the custom file using your file browser and undo what ever you just did
 2. If you don't mind losing everything you have changed you have two choices
 1. Delete your GlycoWorkbench global settings file (this is the easiest solution, but you will lose all saved settings)
 2. Edit the GlycoWorkbench global settings file and remove the XML element that specifies the custom definition file.

For reference see this section for information on locating the GlycoWorkbench [settings file](#)

If you can't fix the problem on your own, don't hesitate to [email us](#)

In future releases we will create a verification step that won't let you save changes until you have passed this test - and we will make sure GlycoWorkbench is able to start even if your definitions are corrupt (although this is again not trivial because of legacy code)

Adding a residue

Adding residues to GlycoWorkbench is a fairly simple procedure as long as it's carried out carefully.

Step one (Defining a new residue)

1. Start by navigating to the GlycoWorkbench settings (Main menu->Settings)
2. Now navigate to the section "Definition file locations" (for more information on customising file paths see [Definition file locations](#))
3. If you haven't already defined a file to store custom residues in click "Create custom" (Save the file where ever you want)
4. Now click "Edit"

You will be presented with a text editor showing you the default residue definitions (unless you have already made changes). Each residue is defined on a single line by 24 fields - don't let the number of fields put you off adding new residues, most are obvious and the default definitions contain plenty of examples. The simplest solution is to find a similar residue copy this to a new line and begin editing the new residue.

Field name	Field description
Name	residue name
	This field is used to classify residues - some GlycoWorkbench GUI components display residues clustered by their superclass. You are free to use whatever

SuperClass	classes you like - those currently used are; Pentose, Hexose, Hexosamine, Acidic sugar, Heptose, Reducing end, Substituent and Modification.
Class	More specific classification - e.g. ManA has a superclass of "Acidic sugar" and a class of "HexA"
Composition	The atomic composition of a residue, e.g. C ₆ H ₈ O ₆ , note that compositions can specify isotopes using the following notation format ATOM_NUMBER_^_ISOTOPE (e.g. C ¹³ H ₈ O ₆ - which is the same composition as before but we have specified Carbon 13 rather than Carbon 12).
Synonym	Another name for the residue
IUPAC	IUPAC name for a residue
AnomC	Position of anomeric Carbon atom
Chir	Chirality - valid values are ?,D or L
Ring	Valid values are ?,p or f
IsSacc	Is residue a saccharide, valid values are yes or no
IsCleav	Should the residue be cleaved, valid values are yes or no (see)
Labile	Valid values are yes or no
BarOrder	Valid values are yes or no
NoMe	Number of methyl groups that should be added when permethylated
DropMe	
NoAc	Number of acetyl groups that should be added when peracetylated
DropAc	
noLinks	Number of child linkages
LinkPos	Comma separated list of linkage positions
ChargePos	Position of charge
Alidtol	Valid values are yes or no
RedEnd	Is residue a reducing end, valid values are yes or no
Parent	Can residue have a parent, valid values are yes or no
Description	Residue description

Step two (Defining cross-ring fragmentation)

This step involves specifying how you would like your new residue to undergo *in silico* cross-ring cleavage - obviously you can skip this step if you don't want to generate cross-ring fragments from your new residue.

1. Start by creating a custom cross-ring fragment definition file (i.e. click "Create custom")
2. Next click the "Edit" button next to the cross-ring fragmentation file

The cross-ring fragmentation file is much simpler to edit than the residue definition file - with only 12 fields. Each line in this file specifies a single cross-ring fragment and the residues that it applies to.

Field name	Field Description
Residues	Comma separated list of residues that this fragment applies to
AnomC	Anomeric Carbon (Integer)
Ring	Ring type, valid values are p or f
Type	Cross-ring fragment type, valid values are X or A
First	Number of first Carbon
Last	Number of last Carbon
NoMe	Number of methyl groups to be added when derivitization is set to permethylation
NoAc	Number of acetyl groups to be added when derivitization is set to peracetylation
noLinks	Number of links
LinkPos	Linkage positions of parent residue that present in this fragment
ChargePos	Position of charge
Composition	Composition of fragment (remember that compositions can include isotope specification)

GlycoWorkbench supports the carbohydrate cross-ring fragments described in the original [Domon and Costello paper](#) - to clarify the Carbon specified by First is present in X fragments but not A and the Carbon specified by Last isn't present in X fragments but is in A.

Step three (Adding a new symbol)

By default GlycoWorkbench will display your new residue as a simple rectangle with the residue name centred inside. GlycoWorkbench supports six different symbolic notations; CFG, CFG black and white, CFG colour linkage, UOXF colour, UOXF black and white, and Text. Each of these is defined with three files; a styles file, linkage file, and placements file. In the same way that you can create custom residue and cross-ring fragmentation definition files you can create custom symbolic notation files. For each notation that you would like to customise the display of your new residue for, you will need to edit the corresponding styles file - obviously this means you will need to edit between one and six styles files.

1. Start by opening up the settings panel and locating the "Definition file locations" section
2. Next locate the style file for the notation you would like to edit
3. If you haven't already done so create a custom style file for this notation (click "Create custom")
4. Now click the "Edit" button next to the corresponding styles file.
5. Create a new line for your new residue and create the fields in the order shown in the table below.

Field name	Field description

Name	Name of residue, should match that of the first column in the residues style file
Shape	Shape to draw, valid value;pentagon,-,star,triangle,hexagon,square,circle,diamond,hatdiamond,heptagon,rhatdiamond,end
ShapeColor	Colour of shape border colour, expressed as an RGB value in the format; Integer,Integer,Integer
Fill	Shape fill mode, valid values are; fill,empty,top,bottom,left,right,topright
FillNegative	Should the internal fill shape be reversed
FillColor	Colour of the internal shape, expressed as an RGB value in the format; Integer,Integer,Integer
Text	Text to centre in the text shape, use a hyphen "-" when you don't want any text in the shape
TextColor	Colour of the internal shape text

Example: Pentagon with a black border and white internal shape with the black text "2d"

```
2dPen    pentagon    0,0,0    full    no    255,255,255    2d    0,0,0
```

Although it is possible to edit the linkage and placement files for each symbolic notation - these files are not yet documented in this manual (most users shouldn't need to edit these files).

Adding base structure types to gallery

A gallery of basic glycan structure types are shown on the "Structure" ribbon band - clicking one of these structures copies it onto the glycan drawing canvas. The majority of users start drawing new glycan structures by first selecting one from this gallery. It is now possible for you to customize this gallery of structures to include whatever structures you like, classified however you like.

1. Start by opening up the GlycoWorkbench settings dialog box (Application Menu->Settings)
2. Next navigate to the section "Dictionaries and definition files"
3. Now locate the line for "coreTypesFile" and if you haven't already done so click "Create custom"
4. Finally click on the corresponding "Edit" button

You should be presented with a file editor that shows you the definitions for the default, basic glycan structure types (unless of course you have already edited them).

Field	Description
Name	Name of glycan
Super class	Glycan structures are shown classified by their superclass in the glycan structure gallery (you can use any class you like)
Structure	Structure in GlycoWorkbench sequence format
Description	Description of glycan structure

Example:

ncorefuc N-glycans freeEnd--?b1D-GlcNAc,p(--6a1L-Fuc,p)--4b1D-GlcNAc,p--4b1D-Man,p(--3a1D-Man,p)--6a1D-Man,p N-glycan fucosylated

Adding terminal structure types to gallery

A gallery of terminal structure types are shown on the "Structure" ribbon band - clicking one of these terminals copies it onto the glycan drawing canvas (or selected residue). It is now possible for you to customize this gallery of terminals to include whatever structures you like, classified however you like.

1. Start by opening up the GlycoWorkbench settings dialog box (Application Menu->Settings)
2. Next navigate to the section "Dictionaries and definition files"
3. Now locate the line for "terminalTypesFile" and if you haven't already done so click "Create custom"
4. Finally click on the corresponding "Edit" button

You should be presented with a file editor that shows you the definitions for the default, terminal structure types (unless of course you have already edited them).

Field	Description
Name	Name of glycan
Super class	Terminal structures are shown classified by their superclass in the terminal structure gallery (you can use any class you like)
Structure	Terminal structure in GlycoWorkbench sequence format
Description	Description of glycan structure

Example:

bga Antigen b1D-Gal,p(--2a1L-Fuc,p)--3a1D-GalNAc,p Blood group A antigen

Loading custom dictionary files (Developer API)

When you are designing software that uses the GlycanBuilder software library you can easily load custom dictionaries by providing a configuration file to the BuilderWorkspace constructor that you have previously configured to point to your custom dictionaries.

```
BuilderWorkspace workspace=new BuilderWorkspace("/home/david/glycoworkbench_test.xml", true, new GlycanRendererAWT());
```

Note that when the second argument to the constructor is set to true and the supplied configuration file doesn't yet exist, the constructor will create a file of the same name, with the default configuration. The default configuration is shown below. To change the file used to load residue definitions you would change the text value "/conf/residue_types" in the "residueTypesFile" element (<residueTypesFile>/conf/residue_types</residueTypesFile>) to the location of your custom residues types file.

```
<Configuration>
<dictionaries>
<uoxf_residueStylesFile>/conf/residue_styles_uoxf</uoxf_residueStylesFile>
<uoxfcol_residuePlacementsFile>/conf/residue_placements_uoxf</uoxfcol_residuePlacementsFile>
<uoxf_linkageStylesFile>/conf/linkage_styles_uoxf</uoxf_linkageStylesFile>
```



```
<crossRingFragmentTypesFile>/conf/cross_ring_fragment_types</crossRingFragmentTypesFile>
<uoxf_residuePlacementsFile>/conf/residue_placements_uoxf</uoxf_residuePlacementsFile>
<cfgLink_residueStylesFile>/conf/residue_styles_cfg</cfgLink_residueStylesFile>
<cfgBW_linkageStylesFile>/conf/linkage_styles_cfg</cfgBW_linkageStylesFile>
<residueTypesFile>/conf/residue_types</residueTypesFile>
<coreTypesFile>/conf/core_types</coreTypesFile>
<cfgBW_residueStylesFile>/conf/residue_styles_cfgbw</cfgBW_residueStylesFile>
<cfgBW_residuePlacementsFile>/conf/residue_placements_cfg</cfgBW_residuePlacementsFile>
<cfg_linkageStylesFile>/conf/linkage_styles_cfg</cfg_linkageStylesFile>
<uoxfcol_linkageStylesFile>/conf/linkage_styles_uoxf</uoxfcol_linkageStylesFile>
<text_residueStylesFile>/conf/residue_styles_text</text_residueStylesFile>
<cfgLink_linkageStylesFile>/conf/linkage_styles_cfglink</cfgLink_linkageStylesFile>
<uoxfcol_residueStylesFile>/conf/residue_styles_uoxfcol</uoxfcol_residueStylesFile>
<terminalTypesFile>/conf/terminal_types</terminalTypesFile>
<cfgLink_residuePlacementsFile>/conf/residue_placements_uoxf</cfgLink_residuePlacementsFile>
<text_linkageStylesFile>/conf/linkage_styles_cfg</text_linkageStylesFile>
<cfg_residuePlacementsFile>/conf/residue_placements_cfg</cfg_residuePlacementsFile>
<text_residuePlacementsFile>/conf/residue_placements_cfg</text_residuePlacementsFile>
<cfg_residueStylesFile>/conf/residue_styles_cfg</cfg_residueStylesFile>
</dictionaries>
<FileHistory>
<file_path3/>
<file_path2/>
<file_path1/>
<file_path0/>
<file_path7/>
<file_path6/>
<file_path5/>
<file_path4/>
<file_type1/>
<file_type2/>
<file_type3/>
<file_type4/>
<file_type0/>
<file_type5/>
<file_type6/>
<file_type7/>
</FileHistory>
<CompositionOptions>
<dpn>0</dpn>
<or1>0</or1>
<dhexa>0</dhexa>
<or2>0</or2>
<ddhex>0</ddhex>
<neu5aclac>0</neu5aclac>
<pyr>0</pyr>
<hexnac>0</hexnac>
<hex>0</hex>
<hep>0</hep>
<or1_mass>0.0</or1_mass>
<or3>0</or3>
<neu5gc>0</neu5gc>
<hexn>0</hexn>
<mur>0</mur>
<or3_mass>0.0</or3_mass>
<or2_mass>0.0</or2_mass>
<mehex>0</mehex>
<pen>0</pen>
<kdp>0</kdp>
<kdn>0</kdn>
<s>0</s>
<hexa>0</hexa>
<neu5ac>0</neu5ac>
<pc>0</pc>
<p>0</p>
<neu5gclac>0</neu5gclac>
<ac>0</ac>
<dhex>0</dhex>
</CompositionOptions>
<ResidueHistory>
<queue_size>0</queue_size>
</ResidueHistory>
<GraphicOptions>
<mass_text_font_face_custom>SansSerif.plain</mass_text_font_face_custom>
<collapse_multiple_antennae>true</collapse_multiple_antennae>
<node_font_size_custom>14</node_font_size_custom>
<mass_text_space_custom>15</mass_text_space_custom>
<node_space_custom>30</node_space_custom>
<show_masses>false</show_masses>
<linkage_info_size_custom>12</linkage_info_size_custom>
<node_size_custom>22</node_size_custom>
<show_info_custom>true</show_info_custom>
<node_font_face_custom>SansSerif.plain</node_font_face_custom>
<show_masses_canvas>true</show_masses_canvas>
<notation>cfg</notation>
<composition_font_size_custom>18</composition_font_size_custom>
<orientation>0</orientation>
<theme>org.pushingpixels.substance.api.skin.OfficeBlue2007Skin</theme>
<display>normalinfo</display>
<show_info>true</show_info>
<save_spectra>false</save_spectra>
<scale_canvas>1.0</scale_canvas>
<composition_font_face_custom>SansSerif.plain</composition_font_face_custom>
<mass_text_size_custom>14</mass_text_size_custom>
<node_sub_space_custom>1</node_sub_space_custom>
<linkage_info_font_face_custom>Serif.plain</linkage_info_font_face_custom>
<show_redend>false</show_redend>
```

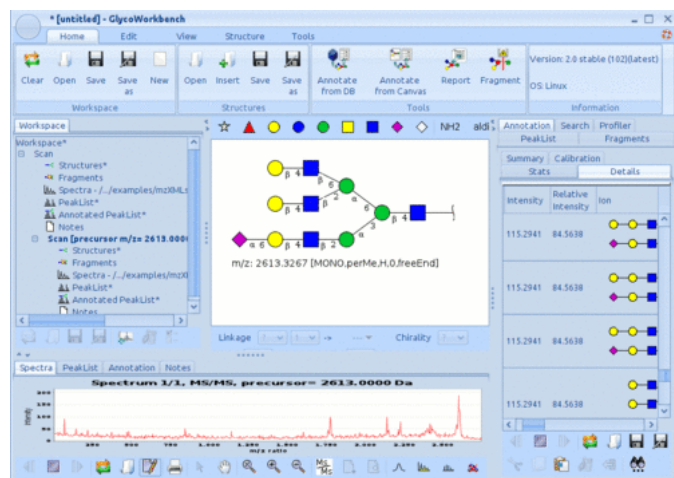
```

<structures_space_custom>40</structures_space_custom>
</GraphicOptions>
<MassOptions>
  <ion_cloud>Na</ion_cloud>
  <reducing_end_type>freeEnd</reducing_end_type>
  <derivatization>perMe</derivatization>
  <neutral_exchanges>0</neutral_exchanges>
  <isotope>MONO</isotope>
</MassOptions>
</Configuration>

```

Interface

Starting with version 2 of GlycoWorkbench a new interface was introduced that makes extensive use of the [Fleming library](#) - which is used to create ribbon style graphical interfaces. The graphical interface is broken up into a number of different panes - as described below.



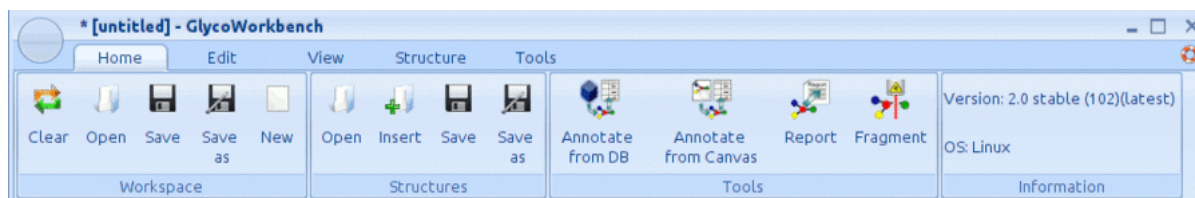
- Application main menu - Top left circular button
- Ribbon bands - Top horizontal pane
- Help button - Top far right life-ring icon
- Workspace explorer - Left center pane (left plugin pane)
- Glycan builder - Center pane (center plugin pane)
- Annotation/Peak list pane - Right center pane (right plugin pane)
- Spectrum pane/Notes pane - Bottom left pane (bottom left plugin pane)

In the same way as you can have multiple web sites open in different tabs in the same browser window - GlycoWorkbench panes can have multiple components open within them. For example the bottom left pane has a "Spectra tab", "PeakList tab", "Annotation tab" and "Notes tab". Note that plugins can be created for GlycoWorkbench (which are loaded at runtime) which can each have one tab open at a time in any of the tab container panes (i.e. left pane, center pane, right pane, and bottom left pane).

Application menu



Home ribbon

**Workspace band**

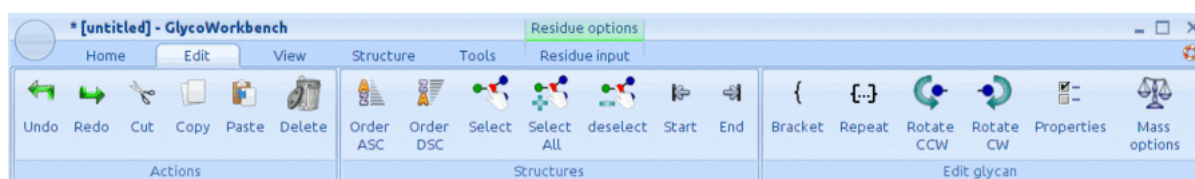
	Clear workspace
	Open a workspace file
	Save workspace
	Save workspace as
	Create new workspace

Structures band

	Open a canvas structure file
	Insert structure onto canvas
	Save canvas structures to file
	Save canvas structures as

Tools band

	Annotate peak list from database
	Annotate peak list with structures from canvas
	Generate an annotation report
	Fragment all structures or selected structures from canvas

Edit ribbon**Actions**

	Undo last action
	Redo last action
	Cut selected
	Copy selected
	Paste clipboard contents
	Delete selected

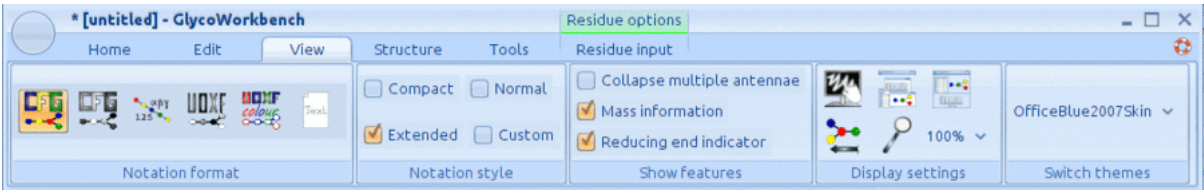
Structures







	Order structures on canvas in ascending mass order
	Order structures on canvas in descending mass order
	Select structure
	Select all structures
	Unselect all structures
	Scroll canvas view to first structure
	Scroll canvas view to last structure






Edit glycan

	Add a bracket to the selected residues
	Create a repeating block for the selected structures
	Rotate selected residues counter-clockwise
	Rotate selected residues clockwise
	Show residue properties
	Show mass options of selected structure

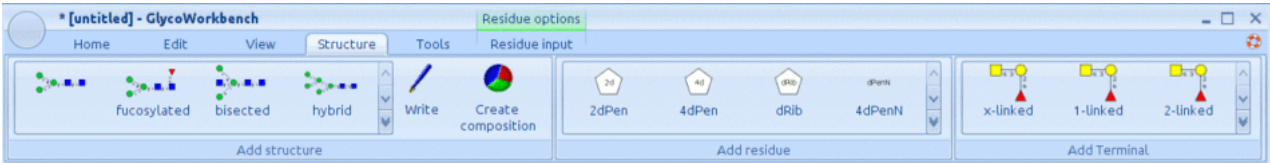
View ribbon



Notation format	Notation style	Show features
 CFG colour	<input type="checkbox"/> Compact Compact	<input type="checkbox"/> Collapse multiple antennae Hide multiple antennae
 CFG black and white	<input type="checkbox"/> Normal Normal	<input checked="" type="checkbox"/> Mass information Show mass information
 CFG colour with linkage	<input checked="" type="checkbox"/> Extended Extended	<input checked="" type="checkbox"/> Reducing end indicator Show reducing end indicator
 UOXF black and white	<input type="checkbox"/> Custom Custom	
 UOXG colour		
 Text		

Display settings
 Edit font family and size
 Detach all panes
 Reattach all panes
 Change glycan orientation
 Restore zoom level to 100%
100% ▾ Set zoom level
OfficeBlue2007Skin ▾ Change the theme (requires restart)

Structure ribbon



Tools ribbon

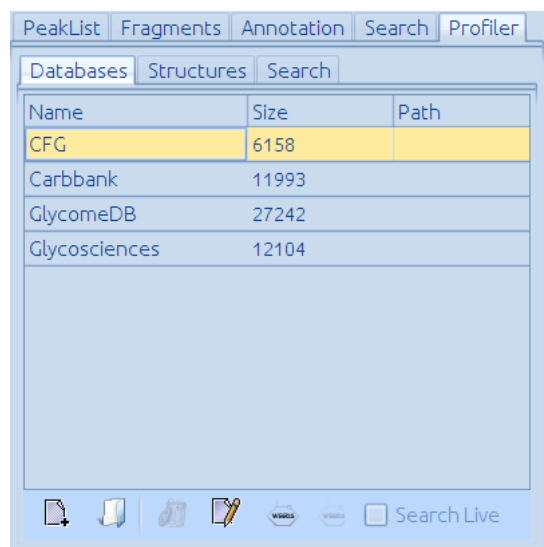


Structure databases (searching and annotation)

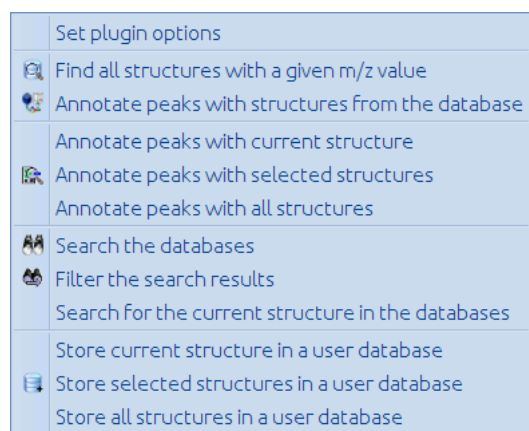
GlycoWorkbench is packaged with four structure databases that can be searched or used to annotate peak lists.

Database name	Number of entries	URL
CFG (Consortium for Functional Glycomics)	6,159	www.functionalglycomics.org
CarbBank	11,993	http://www.genome.jp/dbget-bin/www_bfind?carbbank
GlycomeDB	27,242	www.glycome-db.org
Glycosciences	12,104	www.glycosciences.de

Profiler plugin



The profiler plugin provides the database search and peak annotation functionality - it is docked in the right pane under the tab with the header "Profiler". This plugin also has an extended menu that can be found in the "Tools" ribbon - simply click on the "Profiler" icon.



Creating your own database

Structures that you have drawn using GlycoWorkbench can be saved to your own custom database.

- Start by navigating to the profiler plugin component (Right pane->Profiler->Database)
- Now click the "New" icon located in the bottom left corner
- Enter a name for your database
- Finally select a file to save the database to.

Now draw some structures on the glycan canvas

- Select the structure(s) you would like to copy
- Right-click on one of the selected structures
- Click "Copy"

Now go to the database editor panel (Right-pane->Profiler->Structures)

- Select your new database from the drop down menu
- Finally click the paste icon (clipboard)

Sharing databases

After you have created a custom database you might decide that it would be useful to share it with other people. All you need to do is send people the file you told GlycoWorkbench to save the custom structure database to (see above, for a reminder) and ask them to click the "Open" button (second icon at the bottom of Right pane->Profiler->Database) to open your custom database.

Syncing built-in databases

Some of the databases that are packaged with GlycoWorkbench are (or will be in the future) associated with WGGDS web services (see, [proxy databases](#)). This makes it possible for you to update a database without waiting for a new release of GlycoWorkbench - simply right-click on the database and left-click on "Sync" (for more information on syncing a WGGDS proxy database see, [syncing databases](#)). Note that once you have synced a built-in database it will no longer be updated when you install a newer version of GlycoWorkbench (this issue might be resolved in latter releases, but should nevertheless not cause you any issues). To restore a built-in database to the state that it was in when you installed GlycoWorkbench - simply right-click on the corresponding database and left-click on restore.

Working Group on Glycomics Data(base) Standards (WGGDS) proxy databases

The WGGDS (<http://wggds.org/>) has created a web service API ([specification](#)) which all the main glycan-structure databases are implementing. Starting with version 2.1 GlycoWorkbench supports "WGGDS proxy" databases - which you can either search live or sync periodically to a local file. Each database in the profiler database manager (right pane->Profiler->Databases) can be associated with a URL which corresponds to a WGGDS web service.

Assigning a WGGDS URL to a database

- Right-click on the chosen database
- Left-click on "Edit WGGDS URL"
- Enter the WGGDS URL

Live searching

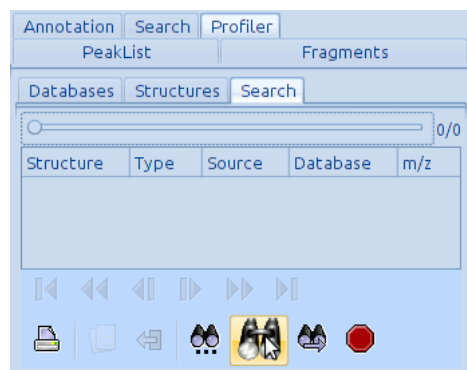
To tell GlycoWorkbench to perform live searches against a WGGDS web service you must enable the "Live search" option on the corresponding database

- Right-click on the chosen database
- Tick "Live search"

Syncing

Performing substructure searches live against a WGGDS service is probably not going to be the fastest method of performing a substructure search. It is therefore possible to store a local copy of all sequences stored on the corresponding database, and search this local copy instead. Every database is associated with a local file - weather you have added any structures or not. To save a copy of all sequences held by the WGGDS associated database, simply right-click on your chosen database and left-click on "Sync". This might take some time depending upon your network bandwidth and the load on the remote WGGDS service. You must un-tick "Live search" (see, [Live searching](#)) otherwise GlycoWorkbench will still perform substructure searches against the remote WGGDS web service.

Database substructure search

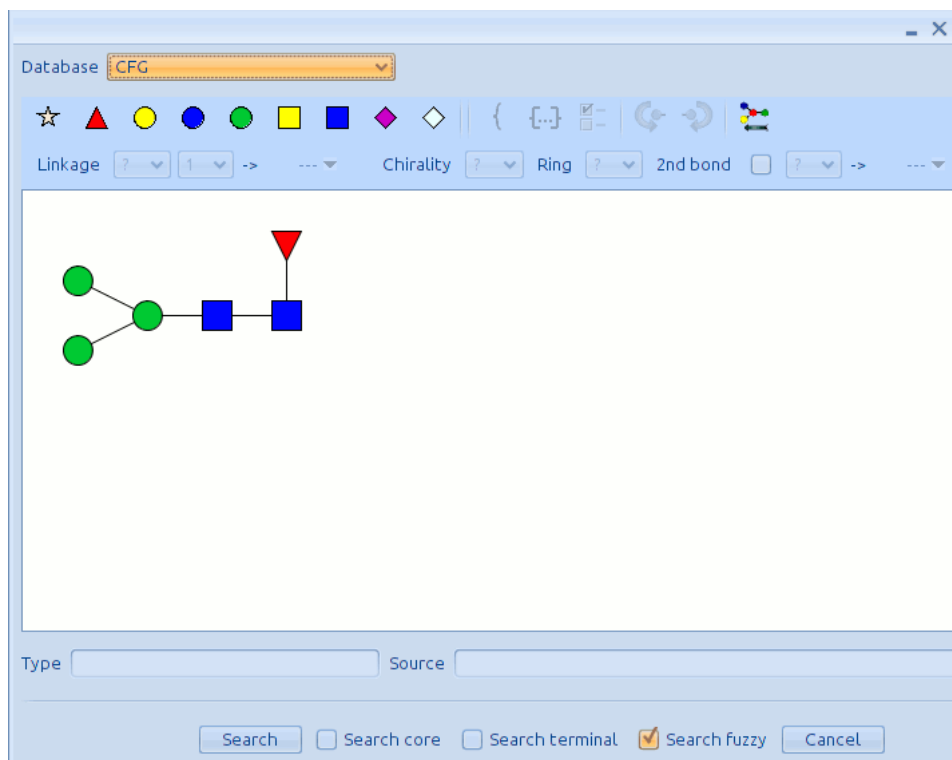


You can perform substructure searches against the builtin and custom databases as well as WGGDS proxy databases

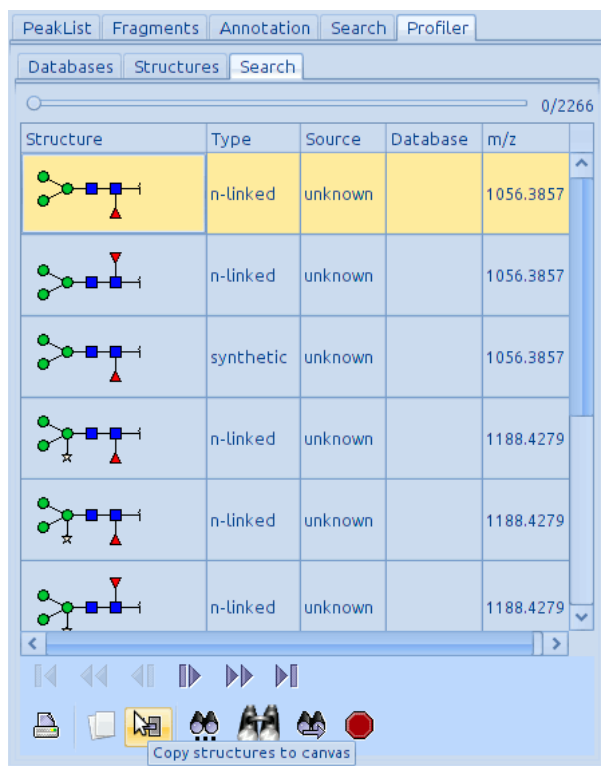
- Start by launching the substructure search dialog box (Right-pane->Profiler->Search->Third button from the end)
- Select the database that you wish to search from the drop down menu
- Draw the structure that you wish to search for
- Select search options
- Click "Search"

Search options

- Type (i.e. n-linked)
- Source (i.e. *Mus musculus*)
- Search core, structure must be found at the reducing end
- Search terminal, structure must be found at the non-reducing end
- Search fuzzy, fuzzy match bonds, fuzzy match chirality, fuzzy match residues by superclass (e.g. Glucose matchers Hexose)



To perform a structure search rather than a substructure search, select both "Search core" and "Search terminal" - an exact structure search can be performed if "Search fuzzy" is additionally deselected. At the moment the "Type" and "Source" entry boxes are disabled when a WGGDS proxy database is selected (hopefully in the future the WGGDS web service API will support searching with both of these concepts).



Results

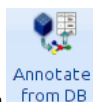
Matching structures are shown in the Profiler Search pane (right-pane->Profiler->Search). Note that you can scroll through the results using either the scroll bar at the top of the pane or the buttons located at the bottom of the pane.

- To perform a substructure search confined to the correct result set click, this icon
- To copy matched structures to the glycan canvas, first select the structures in the results viewer and click this icon
- Multiple structures can be selected by holding down the shift key, during selection.
- Search results can be printed by clicking on this icon

Annotate peaks with database structures

GlycoWorkbench allows you to annotate peaks with structures from any of the databases that are listed in the profiler database management panel.

- Start by defining your peak list (see [Defining peak lists](#))



- Next click on Home->Tools->Annotate from DB, represented by this icon

This will display the Profiler database annotation dialog box. Select the database you wish to search as well as the derivatization and reducing end that each glycan in the database should be modified with. Finally select the charge state that you wish to set each glycan too. Annotation results are shown using the [Annotation plugin](#).

Glycan structure mass options

Each glycan that you draw on the glycan canvas is associated with a series of mass parameters which are used to calculate the m/z value of the corresponding structure. The mass options dialog box can be brought up by either clicking "Edit->Edit glycan->Mass options" or right-clicking a selected structure (on the glycan canvas) and left-clicking on "Mass options of selected structures"

Parameter list

- Calculation type [Mono-isotopic or average isotopic]
- Derivatization
- Reducing end, to customize see [Adding residues](#)
- Charge state
- Neutral exchanges

Note that the mass calculation supports both positively and negatively charged ions. It's not currently possible to customize the list of possible ions (please email info@glycoworkbench.org to request additions).

Derivatization list

- perMeth (Permethylation)
- perDMeth
- perMeth(C¹³) (Heavy methylation)
- perAc (Peracetylation)
- perDAc

The derivatization list also can't be customized at present, please send requests for new derivatizations to info@glycoworkbench.org

File formats

GlycoWorkbench – Fileformats

File type	Extension	Description	How to read / write
Annotation	.gwa	Calculated annotations for a peak list can be separately saved as an annotated peak list file containing all information presented in the annotation panel of the tools section.	Annotated peak list files can be loaded / saved via the tool bar of the annotation panel.
Dictionary	.gwd	Dictionary files contain user defined databases with structure entries.	Dictionary files can be loaded / saved via the tool bar of the profiler panel.
Fragment	.gwf	Fragment files contain all fragments of a single or the selected glycans from a structure section presented in the fragments panel of the tools section. Fragments calculated in the editors' sub sections cannot be stored.	Dictionary files can be loaded / saved via the tool bar of the fragments panel.
Report	.gwr	Report files contain a generated report based on a pre calculated annotation. Once a report was generated it is an independent object. Changing the annotation it is originally based on does not change the report automatically.	Report files can be loaded and saved via the tools/reporting menu and form the menu and toolbar of the report window.
Structure	.gws	Structure files can be loaded and saved via the file menu, from the second group of buttons in the upper tool bar or from the tool bar in the workspace section.	
Workspace	.gwp	A workspace file contains all data organised in the workspace section including the; drawn structures, the calculated fragments, spectra, peak lists, annotated peak lists, reports and notes.	Workspace files can be loaded / saved via the file menu, from the left handed buttons in the upper tool bar or from the tool bar in the workspace section.

Supported graphical formats

Structure plots and reports can be exported to various graphic file formats:

- Bitmap (*.bmp)
- Encapsulated postscript (*.eps)
- JPEG file interchange format (*.jpg)
- Portable document format (*.pdf)
- Portable network graphics (*.png)
- postscript (*.ps)
- scalable vector graphics (*.svg)

Supported sequence formats

Glycan sequence information can be imported and exported from/to:

Sequence format	Import filter	Export filter
BSCDB sequence encoding	X	
Carbbank encoding	X	
GlycoMindes encoding	X	
GlycoCT condensed	X	X
GlycoCT XML	X	X
Glycominds	X	X
Linucs	X	
IUPAC condensed	X	
IUPAC short ver.1	X	
IUPAC short ver.2	X	
LINUCS encoding	X	X
OGBI motif encoding	X	
Glyde II	X	

Supported spectrum formats

Spectra can be uploaded from various formats:

- ACSII spectra files (*.txt)
- xml spectra formats (*.xml, *.mzxml, *.mzdata)
- ABI 400 series spectra files (*.t2d)

Additionally, users of Bruker machines can import raw data after installing the CompassXport program, which can be downloaded from Bruker homepage. For installation copy files CompassXport.exe and CompassXport.dll into folder c:\program Files\Common Files\Bruker Daltonik\AIDA\export. This tool converts Bruker raw data files into either .mzxml or .mzdata files.

Supported peak list formats

A peak list can be imported and exported as follows:

Peak list file format	Import filter	Export filter
Mascot generic peak list file format (*.mgf)	X	X
Bruker peak list files (*.xml)	X	X
Cartoonist peak list files (*.msa)	X	X
Cartoonist centroid files (*.ctd)	X	X
Comma separated peak list files (*.txt, *.csv)	X	X

Other supported file formats

Annotated peak lists can be additionally imported or exported in Cartoonist annotated peak list format (*.msa)

Examples

The installation file contains a folder named examples where you can find some sample files which you can use to test the annotation features of the tool with. In each sub-folder you will find sample structures together with their fragment peak lists. To test the annotation process just open a workspace file (*.gwp) inside GlycoWorkbench and load its corresponding raw data inside the spectrum section of the program.

Set 1

The structures and peak lists contained in this set have been retrieved from:

Y. Mechref and M.V. Novotny,

Structural Characterization of Oligosaccharides Using Maldi-TOF/TOF Tandem Mass Spectrometry.

Analytical Chemistry, Volume 75, Issue 18, 4895 - 4903, 2003.

The peak lists have been obtained by running the underivatized structures through a MALDI-TOF/TOF equipment. To obtain the same mass values the options "underivatized" and "Na+" ion must be selected in the *Mass options* dialog.

Set 2

The structures and peak lists contained in this set have been retrieved from:

E. Spina, L. Sturiale, D. Romeo, et al,

New fragmentation mechanisms in matrix-assisted laser desorption/ionization time-of-flight/time-of-flight tandem mass spectrometry of carbohydrates,

Rapid Communications in Mass Spectrometry, Volume 18, Issue 4, Pages 392-398, 2004.

Set 3

This set contains various structure files that show the display of different types of structures.

GAGs

This folder contains a workspace file showing the complete assignment of mass spectrometry data for a heparin oligosaccharide. A sample containing a mixture of dp10 oligosaccharide has been analysed by MS and MS/MS both in norharmane and ionic liquid. Further details regarding the experimental setup can be found in here:

B. Tissot, N. Gasiunas, A.K. Powell, et al,

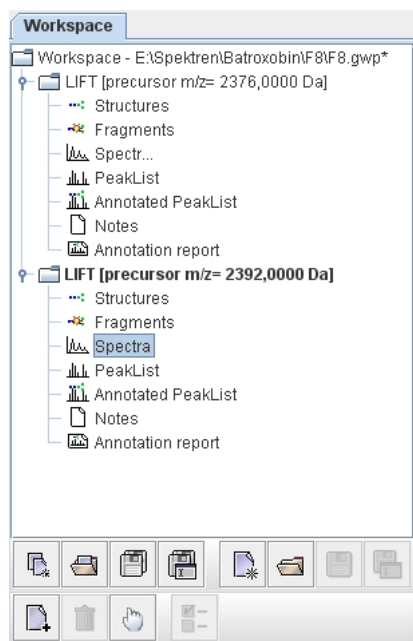
Towards GAG glycomics: Analysis of highly sulfated heparins by MALDI-TOF mass spectrometry,

Glycobiology Volume 17, Pages 972-982, 2007.

Workspace

The organisation of all data objects which are needed to run the annotation process can be managed via the "Workspace" panel. The acquired spectra and the associated documents are organized in a tree like structure that can map a complete MSⁿ run.

The workspace allows for the grouping of all documents needed to annotate a spectrum. More than one dataset can be



organised in a tree-like structure to model a complete MSⁿ run.

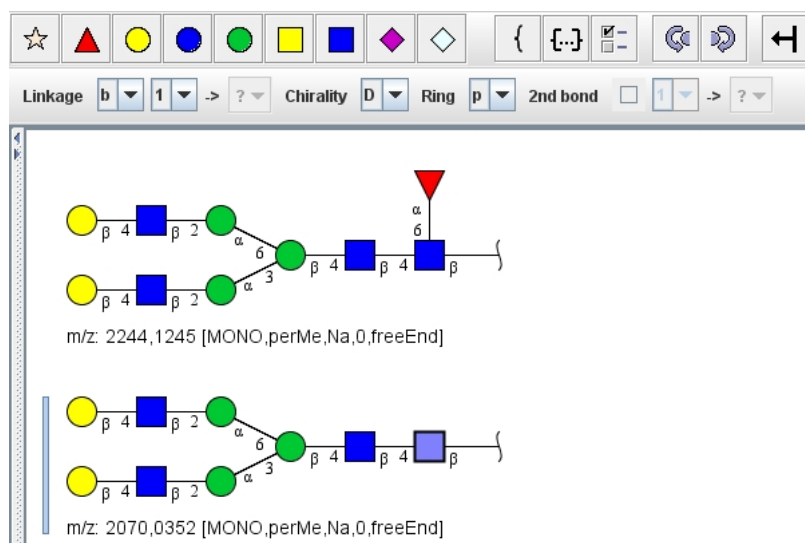
A complete dataset contains:

- a "Structures" panel,
- a "Fragments" section,
- a "Spectrum",
- a "Peak list",
- a "Annotated Peak list",
- a "Notes" document, and
- a minimum of one "Annotation report".

Once an annotation report has been generated it is independent from the stored annotation. Therefore, several "Annotation Reports" can be generated.

GlycanBuilder

The main component of *GlycoWorkbench* is *GlycanBuilder*, a rapid and flexible visual editor of glycan structures. Carbohydrates mostly present as tree-like non-sequential structures, and their constituents exhibit great diversity. Therefore, the input of a structure in a computer readable format is not as straightforward as writing a sequence of characters, as for DNA, RNA and peptide sequences. Additionally, numerous alternative notations are commonly adopted to graphically represent glycan structures. Finally, the more powerful formats for computer encoding of glycan structures (like Glyco-CT or Glyde-II) are difficult to produce manually. The *GlycanBuilder* addresses all these issues: the user can rapidly specify a glycan structure by simply selecting the points of attachment of the residues, the growing structure is displayed using one of the available symbolic notations and the output is a computer encoding of the structure in Glyco-CT format. The popular notations for glycan representation from the Consortium for Functional Glycomics (CFG) and the Oxford Glycobiology Institute are available.



The list of structural constituents comprises an exhaustive collection of saccharides, substituents, reducing-end markers and saccharide modifications. All the stereo-chemical information about a saccharide, like anomeric conformation, chirality, ring configuration and linkage position, can be specified. The display of a glycan is dependent only on its structure and the chosen notation: the appearance and the spatial placement of the residues are automatically determined according to a set of rules specified by the given notation. The software always knows how to represent a structure, and a new notation can be applied without the need for user intervention. Therefore, the tool can be used both as an editor for drawing structures and as an automated component for generating pictorial representations of computer encoded glycans. The *GlycanBuilder* component will be used in the EUROCarbDB interface to specify structures or sub-structures for insertion or searching in the database, and to display the glycans in the various web pages and reports.

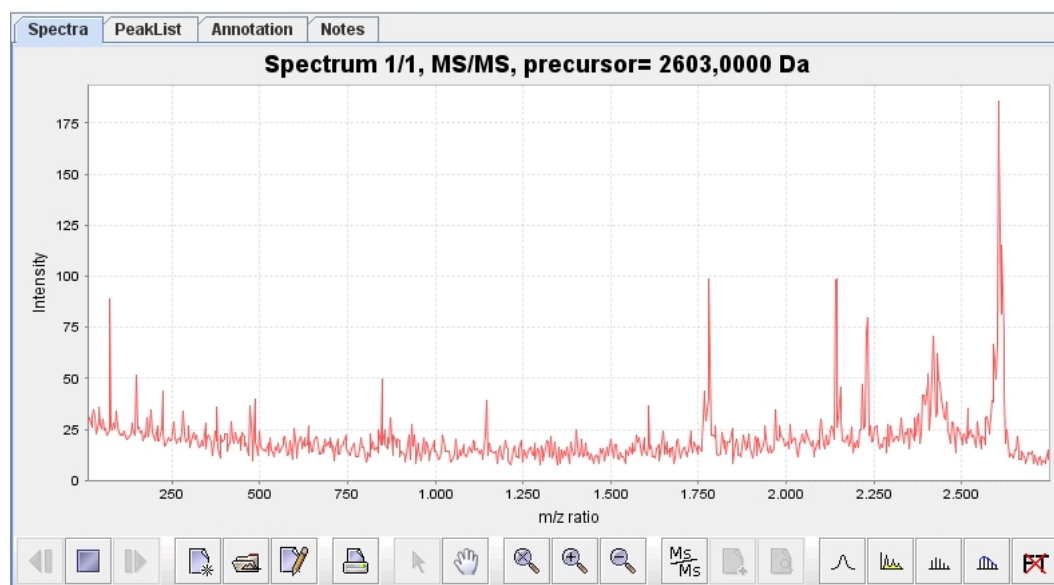
Spectra Viewer section

The "Spectra Viewer" section contains four tab sheets for visualising spectral data; peak lists, statistics about the annotation, and the notes for the currently active scan.

Spectrum viewer

The "real" spectrum viewer is designed to make it easy to view raw recorded data. Spectral data can be read from; ASCII files, MS XML formatted (mzxml and mzdata) files, and directly from ABI 4000 series spectra files (.t2d). Additional proprietary formats are supported via vendor supplied libraries and software (see section 3.2.1.4 Supported

spectrum formats).



A tool bar is provided below the spectrum viewer, as shown above, which can be used for the manipulation of the spectrum.

Symbol	Function
	Navigation through the spectrum file. In case the raw data file contains more than one spectrum, the buttons allow navigate between different spectra or to selectively close the active spectrum.
	Clear the spectrum viewer
	Open a new raw data file
	Edit scan data View or change parameters which are extracted from a raw data file. (see 4.4.1.1 Edit scan data).
	Print the spectrum
	Activate manual zoom A selected section of the spectrum will automatically be enlarged to fill the complete spectrum window.
	Activate move With the mouse clicked on any point of the spectrum the mass region which is shown can be changed. The intensity axis remains in auto scale mode.
	Zoom options: reset, zoom in and zoom out.
	Change current scan level. Triggers options for selected peaks (see 4.4.1.2 Change current scan level)
	Add selected peaks to list Peaks can be selected by clicking with left mouse button (multi selection of peaks by ctrl + left mouse button). The selected peaks will be added to the peak list.
	Find possible annotation for selected peaks.
	Filter noise in current spectrum
	Baseline correction of current spectrum




Compute peak centroids

Automatic computation of isotopic distribution active / inactive



FTICR mode active / inactive

Edit scan data

While uploading a raw data file characteristic parameters for each spectrum are extracted and can be viewed and edited latter on. The corresponding window can be entered by clicking the  icon in the tool bar of the spectrum viewer.

The following parameters are read from raw data files:

MS-level: MS exponent of the actual spectrum

Precursor m/z: mass to charge ratio of precursor (MS/MS mode only)

Charge: charge state of precursor

(MS/MS mode only)

Base peak: peak with maximum intensity

Intensity: Intensity of base peak

Start m/z: lowest m/z value

(used only when raw contains raw data and peak list)

End m/z: highest m/z value

(used only when raw contains raw data and peak list)

Low m/z: lowest m/z value

High m/z: highest m/z value

Retention time: (optional) given when raw spectrum is part of LC run

TIC: (optional) total ion count

Positive mode: ion polarity

Centroided: raw data or peak list

Deisotoped: (for peak list only) isotopic pattern eliminated Deconvoluted: artificial spectrum or peak list recalculated to only singly charged ions

Change current scan level

With this option users can switch data processing options between those for either profile spectra or fragmentation spectra.

After a peak selection (Peaks can be selected by clicking with left mouse button (multi selection of peaks by ctrl + left mouse button)) clicking the right mouse button opens a popup window with spectrum type specific options:

The same options can be selected from the annotations menu not only for the selected peaks but for the complete peak list.

MS mode:


MS/MS mode:


In MS mode there are three options for the annotation of the selected peaks:

- Search a selected database for matching structures (see profiler from tools menu)
- Find structure compositions matching the peaks (see *Glyco-Peakfinder* from tools menu)
- Find all GAG structures matching the peaks (see GAGs from tools menu)


In MS/MS mode two options are available:


- Find all fragments of the selected structures matching the peaks (see annotation from the tools menu)
- Find fragment compositions matching the peaks (see *Glyco-Peakfinder* from tools menu)


 Add selected peaks to list

☒  Find all fragments of the selected structures matching the peaks

☐ Find fragments compositions matching the peaks

 Reset zoom

 Zoom in

 Zoom out

Tools section

The tools menu contains 5 main headers, each of which is further subdivided.







- I
- Peak list
- II
- Fragments
- III
- Annotation
- IV
- Search
- V
- Profiler






Peak list


Peak lists are displayed in a simple tabular form; with individual peaks represented by rows. Mass-to-charge and intensity values are shown for each peak. In addition a third column is included which contains the relative intensity; calculated by setting the intensity of the base peak to 100.

Peak lists can be imported into GWB in four different ways; a) uploaded from a file, b) copied and pasted with data from another program, c) entered manually, and finally d) picked by selecting peaks within the spectrum viewer.

PeakList	Fragments	Annotation	Search	Profiler
Mass to charge	Intensity	Relative Intensity		
73,0674	86,1765	46,3608		
73,4229	80,8497	43,4951		
147,3783	45,8497	24,6660		
148,0809	51,4379	27,6723		
189,5175	34,7059	18,6709		
222,9338	43,7255	23,5232		
376,1011	36,1765	19,4620		
471,8419	28,5294	15,3481		
472,3637	36,4379	19,6027		
486,2221	38,4967	20,7103		
486,6152	35,0327	18,8467		
847,3063	47,4837	25,5450		
847,9631	49,4118	26,5823		
1145,6368	38,8562	20,9037		
1606,8364	36,3726	19,5675		
1766,8752	41,4706	22,3101		
1779,0477	57,5490	30,9599		
1780,7996	98,4314	52,9536		
1969,1726	34,8039	18,7236		
2010,2904	27,1242	14,5921		
2056,0764	24,6405	13,2560		
2058,1409	24,3137	13,0802		





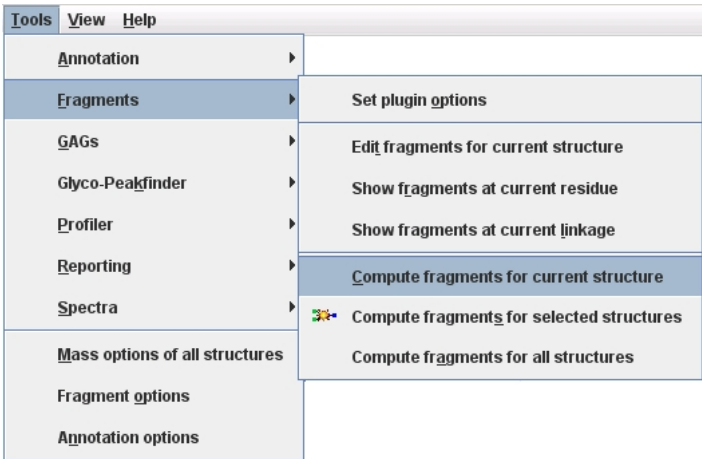
Ms

Fragments

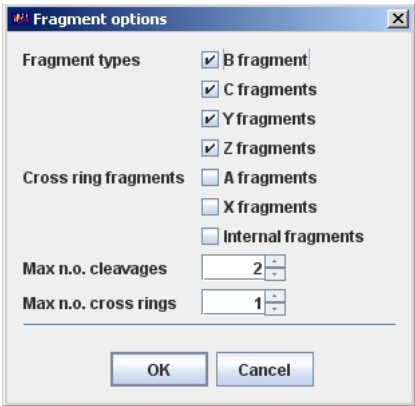
The *insilico* fragmentation of a selected structure in the *GlycanBuilder* section is displayed in the fragments section. This section is composed of three tabs.

Details tab

This view can be initialized via the tools menu:



Which provides a dialog box allowing for the specification of fragmentation options.



Based on the selected fragmentation options an Insilco fragmentation is performed and the results displayed in tabular form. This table contains a list of all predicted fragments and all the parameters calculated for each one. Such parameters include; fragment type, attached charged ion, neutral exchanges, and finally the exact calculated fragment mass.

Different fragments with the same exact mass are represented separately within the details table.

PeakList Fragments Annotation Search Profiler

Details Summary Editor

m/z: 2605,2981 [MONO,perMe,Na,0,freeEnd]

Fragment	Type	m/z	Ions	Neutral Exchanges	Fragment Mass
	YY	939,4520	Na	0	916,4628
	BZ	1019,4782	Na	0	996,4890
	B	1021,4938	Na	0	998,5046
	BY	1037,4888	Na	0	1014,4995

Navigation icons: back, forward, search, save, print, etc.

Summary

The summary tab contains a condensed form of the information present within the detail tab. Unlike the detail tab, the summary tab groups fragments with the same exact mass value into one entry. The additional parameters shown for each fragment within the detail tab are omitted from this tab.

PeakList	Fragments	Annotation	Search	Profiler
Details	Summary	Editor		
Mass to charge				
209,0784				
211,0941				
227,0890				
229,1046				
241,1046				

Editor Tab

This tab allows for the manual fragmentation of a selected structure; in contrast to the automated fragmentation process previously discussed. The selected structure is displayed in the editor and can be fragmented by clicking on either a bond or a residue (forming cross-ring fragments instead of glycosidic cleavages).

PeakList
Fragments
Annotation
Search
Profiler

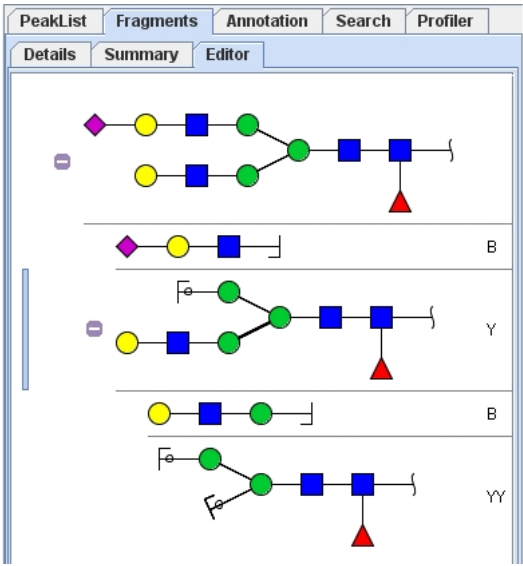
Details
Summary
Editor

B/Y fragments
C/Z fragments
B fragment
Y fragment
C fragment
Z fragment
All fragments

Right clicking on a bond allows for the selection of the fragment type which will be generated..

The similar options for cross ring fragments will be available by clicking on a residue instead of a bond. Cross ring fragments can only be calculated if all bonds attaching the selected residue are completely defined.

Multiple cleavages can be calculated in a step by step process clicking on a remaining bond or residue in a previously generated fragment.



Annotation

In the annotation section results of matching a peak list with the in silico fragmentation of one or more structure candidates are displayed. Four different views allow comparison of the obtained results.

The automatic annotation process can be started via the tools menu:

Tools	View	Help
Annotation		Set plugin options
Fragments		Find all fragments of the current structure with a given m/z value
GAGs		Find all fragments of the selected structures with a given m/z value
Glyco-Peakfinder		Find all fragments of all the structures with a given m/z value
Profiler		Annotate peaks with fragments from current structure
Reporting		Annotate peaks with fragments from selected structures
Spectra		Annotate peaks with fragments from all structures
Mass options of all structures		Place uncertain antennae in current structure using the peak list
Fragment options		
Annotation options		

In an additional dialog box further annotation options can be selected:

The upper section allows specification of the fragments to be calculated for the annotation of the mass list.

Each fragmentation type (either glycosidic or cross-ring) can be selected separately.

Fragment options

Fragment options

Fragment types

☒ B fragments

☒ C fragments

☒ Y fragments

☒ Z fragments

Cross ring fragments

☐ A fragments

☐ X fragments

☐ Internal fragments

Max n.o. cleavages

2

Max n.o. cross rings

1

Mass options

Negative mode

☐

Neutral exchanges

☐

Max # H ions

1

Max # Na ions

0

Max # Li ions

0

Max # K ions

0

Max # charges

1

Max ex. Na ions

Max ex. Li ions

Max ex. K ions

☐ Derive options from parent ion

Accuracy

200

ppm

OK

Cancel

For calculation of internal fragments the number of cleavages needs to be raised to values greater than one.

These options refer to the mass spectrometric technique used.

Further options can be set in the lower section, referring again to the mass spectrometric technique used and the preparation of the sample.

Details

Within this view detailed information is provided on the calculated annotation. Fragments which match the mass signals within the peak list are displayed here. Each fragment generates a separate entry in the table. The dataset for each entry comprises additional information about the; fragment type, the absolute and relative mass accuracy, the calculated m/z value, and the attached charged ions and neutral exchanges.

PeakListFragmentsAnnotationSearchProfiler

StatsDetailsSummaryCalibration

m/z: 2605,2981 [MDND,perMe,Na,0,freeEnd]

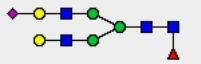

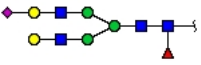
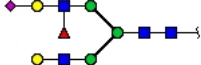
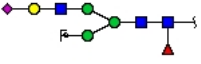
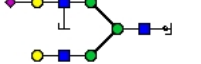
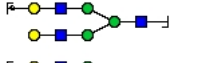

Mass to charge	Intensity	Relative Intensity	Ion	Type	Score	Accuracy	Accuracy PPM	Ion m/z	Charges	Neutral Exchanges
2604,0981	185,8824	100,0000			0,0000	0,0000	0,0000	0,0000	0	0
2143,4136	98,7255	53,1118		ZZ	0,0000	-2,3388	-1091,1614	2141,0748	H	0
1780,7996	98,4314	52,9536		ZZ	0,0000	-0,8985	-504,5281	1779,9011	H	0
2142,0686	95,6863	51,4768		ZZ	0,0000	-0,9938	-463,9625	2141,0748	H	0

The listed entries in the annotation table can be sorted either by mass or intensity -allowing the user to get a detailed overview of the quality of the annotation.

Summary

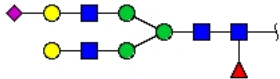
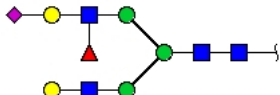
A more condensed view to the calculated annotation comprises the summary view. The details for each calculated fragment are omitted and different fragments matching the same mass signal are summarized to one entry for the corresponding m/z value.

Nevertheless this view is of great importance for the annotation process because it allows the comparison of the annotations with different structure candidates. Sorting by intensity is especially insightful for comparing the quality of more than one annotation.

PeakList	Fragments	Annotation	Search	Profiler
Stats	Details	Summary	Calibration	
Mass to charge	Intensity	Relative intensity		
2604,0981	185,8824	100,0000		
2143,4136	98,7255	53,1118		
1780,7996	98,4314	52,9536		

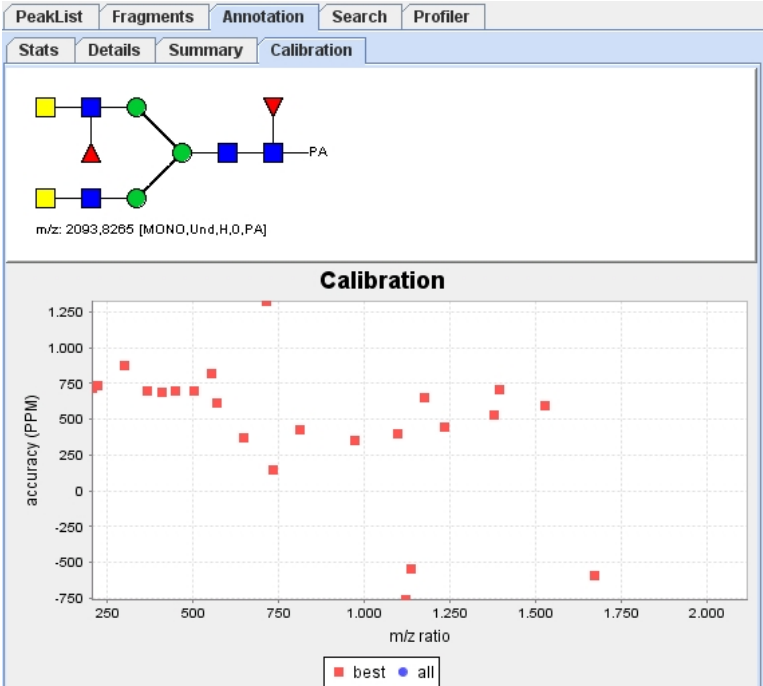
Stats

The most compact display is the stats view; which allows for a fast overview regarding the calculated annotation from all structure candidates. The calculated parameters "coverage" and "assigned" refer to the percentage of explained intensity and the number of assigned signals from the mass list, respectively. Additionally, the parameters ">10% assigned" and ">5% assigned" should help to verify if all major signals are annotated.

PeakList	Fragments	Annotation	Search	Profiler			
Stats	Details	Summary	Calibration				
Structure	Coverage	RMSD	RMSD PPM	Assigned	>10% assigned	>5% assigned	
	62,6508	2,1024	3919,6835	24/43 (55,81%)	24/43 (55,81%)	24/43 (55,81%)	
	61,6060	2,1906	3877,0611	26/43 (60,47%)	26/43 (60,47%)	26/43 (60,47%)	

Calibration

The Calibration view is an additional control page for the annotation of the peak list with the fragments from the structure candidates. Following the idea that spectra show a more or less constant relative deviation from the exact mass values, the annotation of each peak in the spectrum should reflect this fact.



* Best, uses only the most accurate annotation for each peak
* All, uses all annotations for each peak

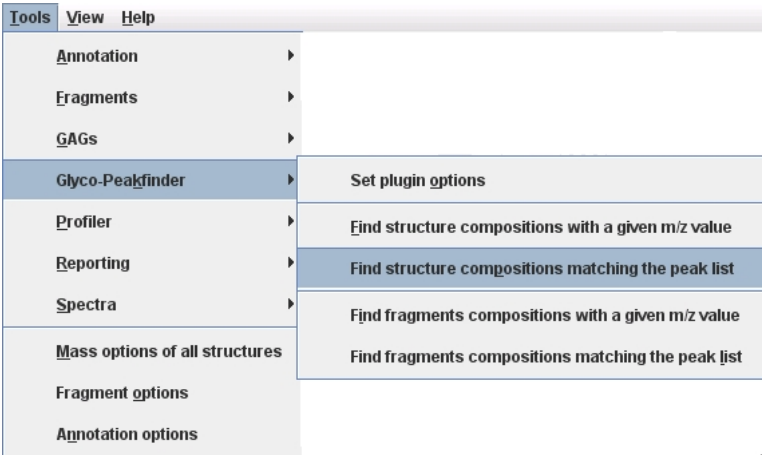
Search

The Search view of the tools section can be activated by using *Glyco-Peakfinder* for composition analysis of either profile spectra or fragment spectra alternatively the Profiler option can be used for searching the database for structures with a given m/z value.

Glyco-Peakfinder

The *Glyco-Peakfinder* plugin can be started via the tools menu and allows for either the calculation of structure compositions matching the peak list of a profile, or for calculating the fragment compositions matching an MS/MS spectrum.

This de novo calculation is often used as long as no structure candidates have be postulated.



Further settings for the calculation are available from two consecutive displayed windows. The first one refers to the monosaccharides and modifications to be expected for the analysed structures. The second form refers to the fragmentation options reflecting the technique used (see 4.5.3 Annotation).

[[Image:]]

The results are displayed in tabular form in the "details" view showing the calculated compositions matching the mass list:

PeakList	Fragments	Annotation	Search	Profiler						
Details		Summary								
Mass to charge	Intensity	Relative Intensity	Ion	Type	Score	Accuracy	Accuracy PPM	Ion m/z	Charges	
2091,4193	6816,0885	100,0000	Hex ₈ HexNAC ₂ NeuAc ₁ -PA		0,0000	-0,6665	-318,6900	2090,7528	H	
2091,4193	6816,0885	100,0000	Hex ₈ HexNAC ₂ dHex ₂ -PA		0,0000	0,3539	169,2089	2091,7732	H	
1540,4402	3111,1478	45,6442	Hex ₈ dHex ₁ -PA		0,0000	-0,8837	-573,6821	1539,5565	H	
1540,4402	3111,1478	45,6442	Hex ₁ HexNAC ₂ NeuAc ₂ dHex ₂ -PA		0,0000	-0,8460	-549,1937	1539,5942	H	

Again a more condensed form is available in the summary view:

PeakList	Fragments	Annotation	Search	Profiler
Details		Summary		
Mass to charge	Intensity	Relative intensity		
2091,4193	6816,0885	100,0000	Hex ₈ HexNAC ₂ NeuAc ₁ -PA Hex ₈ HexNAC ₂ dHex ₂ -PA	
1540,4402	3111,1478	45,6442	Hex ₈ dHex ₁ -PA Hex ₁ HexNAC ₂ NeuAc ₂ dHex ₂ -PA	

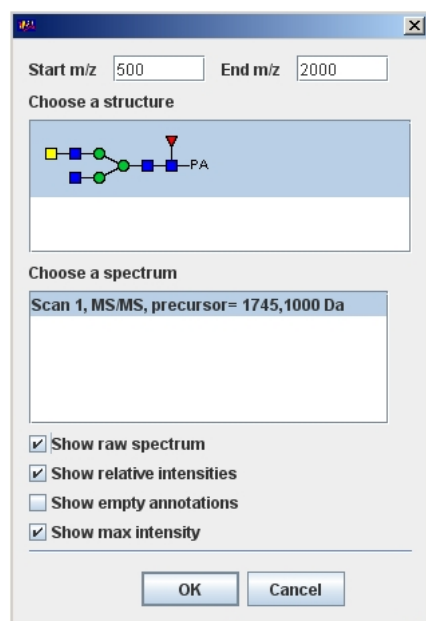
Reports

Final step in the annotation process is the generation of reports. Report files contain either a raw spectrum or an artificially generated line spectrum from the peak list with attached cartoons representing the annotation.

The report options can be accessed via the reporting entry of the tools menu:

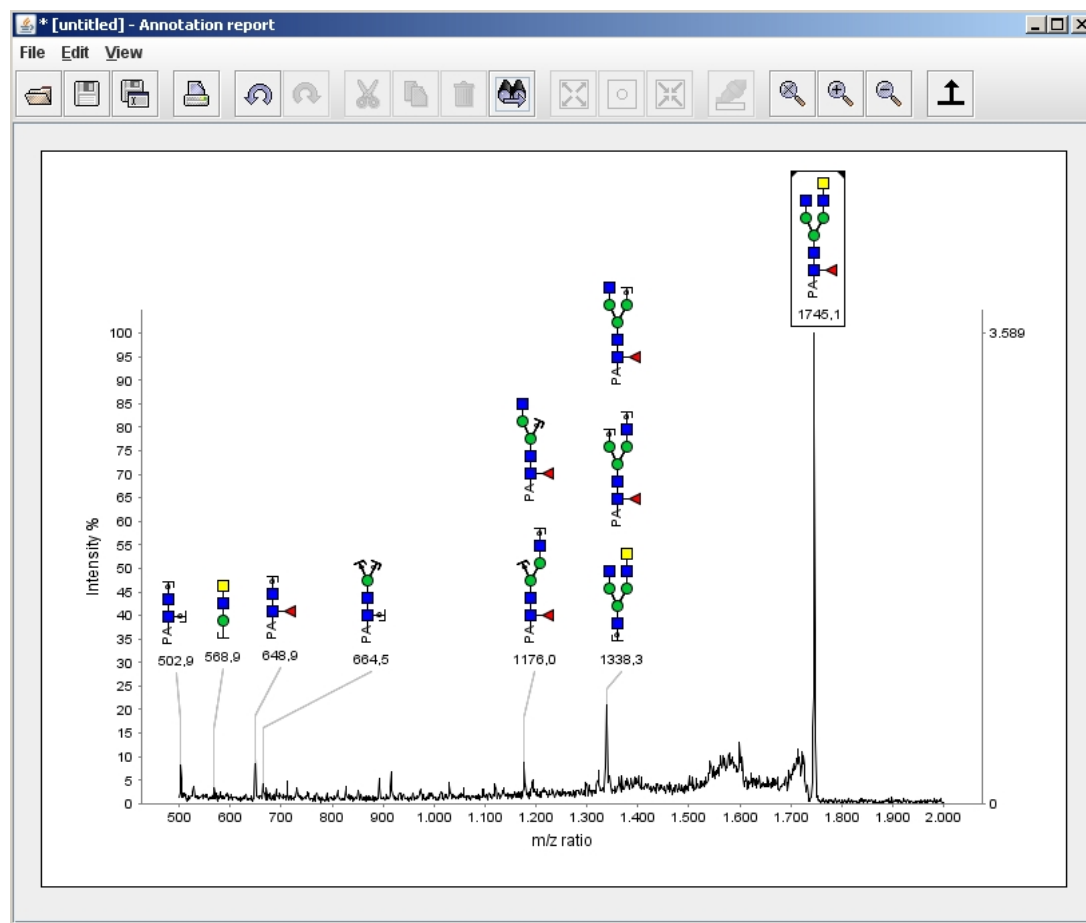
Tools	View	Help
Annotation		
Fragments		
GAGs		
Glyco-Peakfinder		
Profiler		
Reporting		Create a report of the annotations
Spectra		Open a previous annotations report
Mass options of all structures		Deisotope the annotated peaklist using the annotations
Fragment options		Create a report comparing different profiles
Annotation options		

The following menu allows selection of spectrum, and structure:



Additionally to the raw spectrum a mass range to be displayed in the report can be selected.

The report is generated in a separate editor window. Position and orientation of structure plots can be rearranged to create the optimal view for each annotation.



Once a report file is created it is independent from the originating annotation. Annotation reports therefore represent snapshots of the underlying annotation as it was when the report was generated.

Report files can be saved in independent files (.gpr).

Drawing structures

The structure building panel is designed to handle multiple structures at the same time. Initially the structure panel is empty. The user can start building a structure from a common core motif selected from the "File -> New" menu. To add subsequent structures using one of the core motifs the user can choose from the "Structure -> Add structure" menu.

Only tree-like glycan structures can be built. The residues are always added to the last selected residue. If no residue is selected a new structure is created and the residue is added to it. The substituents are treated as residues. A new residue is added by choosing from the "Structure -> Add residue" menu. Common terminal motifs can be added by choosing from the "Structure -> Add terminal" menu. A residue can be inserted before the current selection by clicking on "Structure -> insert residue before".

The properties of a residue (such as anomeric state, chirality and anomeric atom) and the position of the linkage to its predecessor can be set using the dialog box, activated by the command "Structure -> Residue properties". The type of the reducing end of the selected structure can be changed by clicking on "Structure -> change reducing end type". In this way labels and markers can be added to the structure. The mass of the marker is added to the total mass of the structure.

Fuzzy structures with uncertain antennae positions can be created by adding a bracket to a selected structure with the "Structure -> Add bracket" command. The antennae can then be added to the structure by selecting the bracket and adding the desired residues.

Export to file

The content of the structure panel can be saved to file, using the internal string format, for later retrieval. Otherwise, the structure drawings can be exported into a file in several graphical formats (PS, EPS, PDF, SVG, JPG, BMP, PNG, GIF) using the command "File -> Export to graphical formats".

Selection and Navigation

A single residue is selected by clicking the leftmouse button on it. If the <ctrl> button is pressed, the residues that are already selected will remain in the same state, otherwise they will be deselected. If the <shift> button is pressed all the residues on the path connecting the last selection and the current one will be selected as well. By pressing the mouse left button outside of any residues and dragging it, the rectangle selection tool will be activated. When the mouse button is released all the residues in the rectangle area will be selected. If the <ctrl> button is pressed, the residues that are already selected will remain in the same state, otherwise they will be deselected. To select all residues of all structures just press <ctrl+A> or go to "Edit -> Select all". The currently selected structure is the one containing the last selected residue.

By clicking <ctrl> plus one of the arrow buttons the selection is moved from the last selected residue to the nearest residue in the direction indicated by the arrow. If no residue is selected, the selection is placed on the reducing end of the first or the last structure (depending on the arrow button).

Cut and Copy

All the usual cut/copy/paste operations are implemented in the *GlycoWorkbench* application. The selected residues can be cut and copied from a location and then pasted in a different location in the same window. If no residues are selected when performing the "paste" action a new structure will be created, otherwise the content of the clipboard will be added to the last selected residue. The selection can also be pasted in a different window of the *GlycoWorkbench* application. Finally, the copied residues can be pasted as an image in a graphics editor or placed into a Word document.

Drag and Drop

By pressing the left mouse button on a single residue or a group of selected residues, the drag and drop mode is activated. The selected residues can be dragged to any part of the drawing canvas. When the mouse button is released the dragged residues will be moved to the final location. If the button is released upon an existing residue, the selection will be added to it - otherwise a new structure will be created containing the selected residues. If the <ctrl> button is pressed the selection will be copied from the original location to its destination, otherwise the selected residues will be deleted from the original location. The selection cannot be dragged outside the current drawing canvas.

Visualization Options

The orientation of the drawn structure can be changed from right-to-left to left-to-right, to bottom-to-top to top-to-bottom, by clicking on "Structure -> change orientation". The orientation will also affect the way fragments are drawn in the fragment panel. The cartoon notation used to represent structures can be changed from the menu "View". Currently, three notations are supported: CFG standard, CFG black and white, Oxford. The visualization of linkage information is controlled with the "View -> show linkage info" command. In the same menu with the command "View -> show masses when exporting" it is possible to activate/deactivate the display of mass information in the exported/printed structure drawings.

Insilico fragmentation

After a set of structures has been created with the **GlycanBuilder**, the remaining components of *GlycoWorkbench* can be used to derive their fragments, compute the fragment masses, build a peak-list and annotate it. Computation of fragments and their masses from the intact structure is a central step for the annotation of MSⁿ spectra. The "fragmentation tool" creates all topologically possible fragmentations of the precursor molecular ion, applying both multiple glycosidic cleavages and cross-ring fragmentations. Given a fragment structure, m/z values can be calculated both for native and derivatized structures (permethylated/ peracetylated) taking into account several types and quantities of charges. A visual editor of glycan fragments is also available, where the user can specify which positions the cleavages are occurring on the displayed structure in order to reproduce an already known fragment molecule. The fragment editor will be used in the database interface to manually specify fragmented glycans during the insertion of annotated peak lists or during the search for specific annotations in the database.

Automatic data interpretation

The next step in the annotation process is the definition of a peak list. In **GlycoWorkbench** a peak list can either be loaded from a tab-separated text file, thus allowing for import from peak-picking software, or it can be created by typing mass and intensity values directly into the application. Alternatively, the whole spectrum can be loaded from several standard XML or vendor specific data formats (supported through the use of the ProteomeCommons-IO library). The raw mass spectrum is displayed and can be panned or zoomed as in a normal spectrum viewer. The user can select m/z values directly from the curve and add them to the peak-list. Once the peak-list is complete, the fragmentation tool is used to generate all the possible fragments of each input structure and their m/z values are matched against every peak with the desired accuracy. The resulting annotated peak-list can be viewed using various panels that show its different aspects. Each panel is based around a spreadsheet-like table view, whose cell values can be sorted by each column, and can be copied into spreadsheet software. The detailed view lets the user check a comprehensive list of fragment-peak matches for each of the

structures, showing the fragment structure, mass, m/z value, distribution of charges and annotation accuracy. The annotation can also be reviewed by removing the matches that are not satisfactory. The summary view lets the user compare the annotations for the different structures back-to-back in the same table. The matching fragments from different structures are shown in adjacent columns, with each row corresponding to a single peak. In this way, signals that clearly distinguish the correct annotation from the other hypothetical models can be identified. The statistics view lets the user perform a quantitative comparison between the annotations, by showing the number of assigned peaks at different thresholds of relative peak intensity, the root mean square deviation between peak and fragment m/z values and the average intensity of assigned peaks. Finally, a calibration graph shows the annotation accuracies at the various m/z values, allowing the user to check the correct calibration of the mass spectra.

The annotated peak-list can be exported to file using an XML format specifically designed by EUROCarbDB for the storage and exchange of annotated MS experiments. This format will be used to upload annotated data to the database. The fragmentation and annotation tools will also be used as part of the database interface to propose a list of annotations to the user during the insertion of experimental data. The user of EUROCarbDB will thus be offered several choices for the insertion of annotated data in the database: on one hand, they could use **GlycoWorkbench** for the interpretation of new experimental data, specify the annotations on their computer, store the results on a file and upload the data into the database; on the other hand, they could use the annotation tool on-line either for the interpretation of new data or to automatically specify the annotations, they will only need to review the proposed annotations to match their knowledge; finally, they could use the web version of the fragment editor to specify the annotations in a complete manual mode.

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