

User Manual

GALAXY : Glycoanalysis by the three axes of MS and chromatography.

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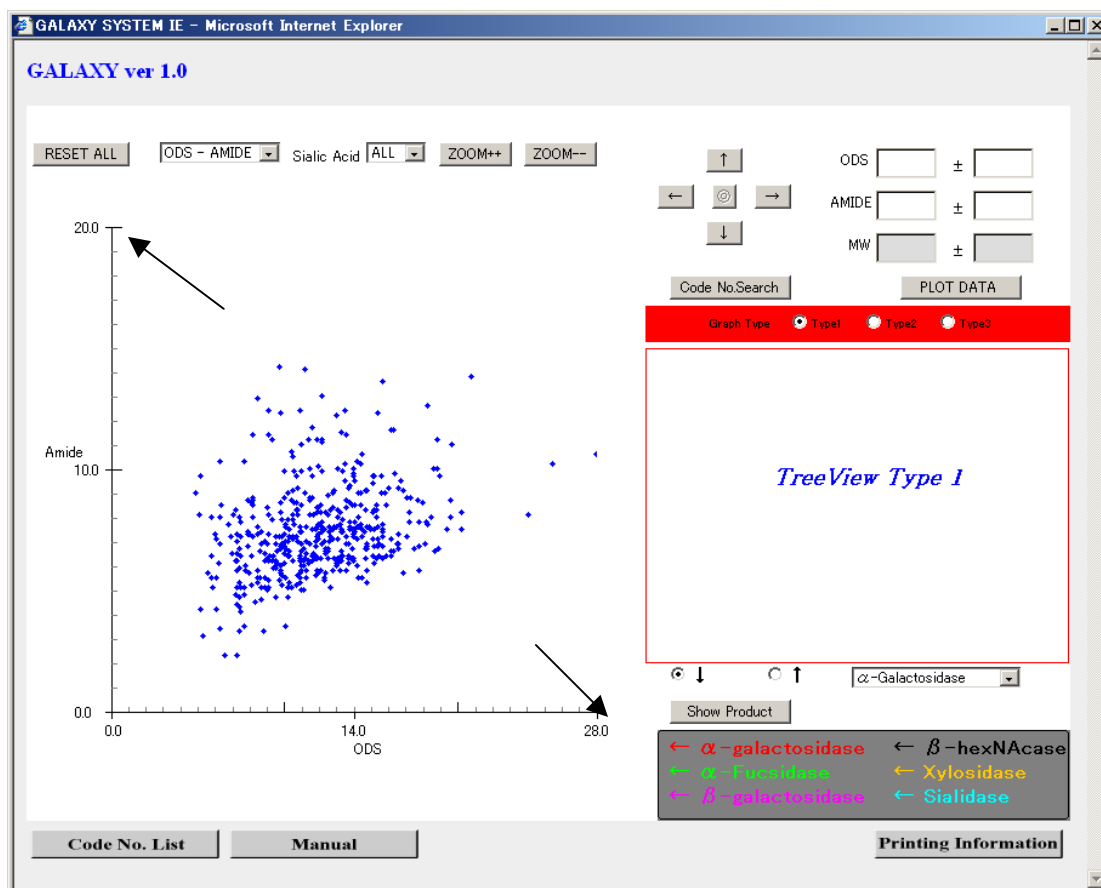
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1. Display

1.1 Start up Screen



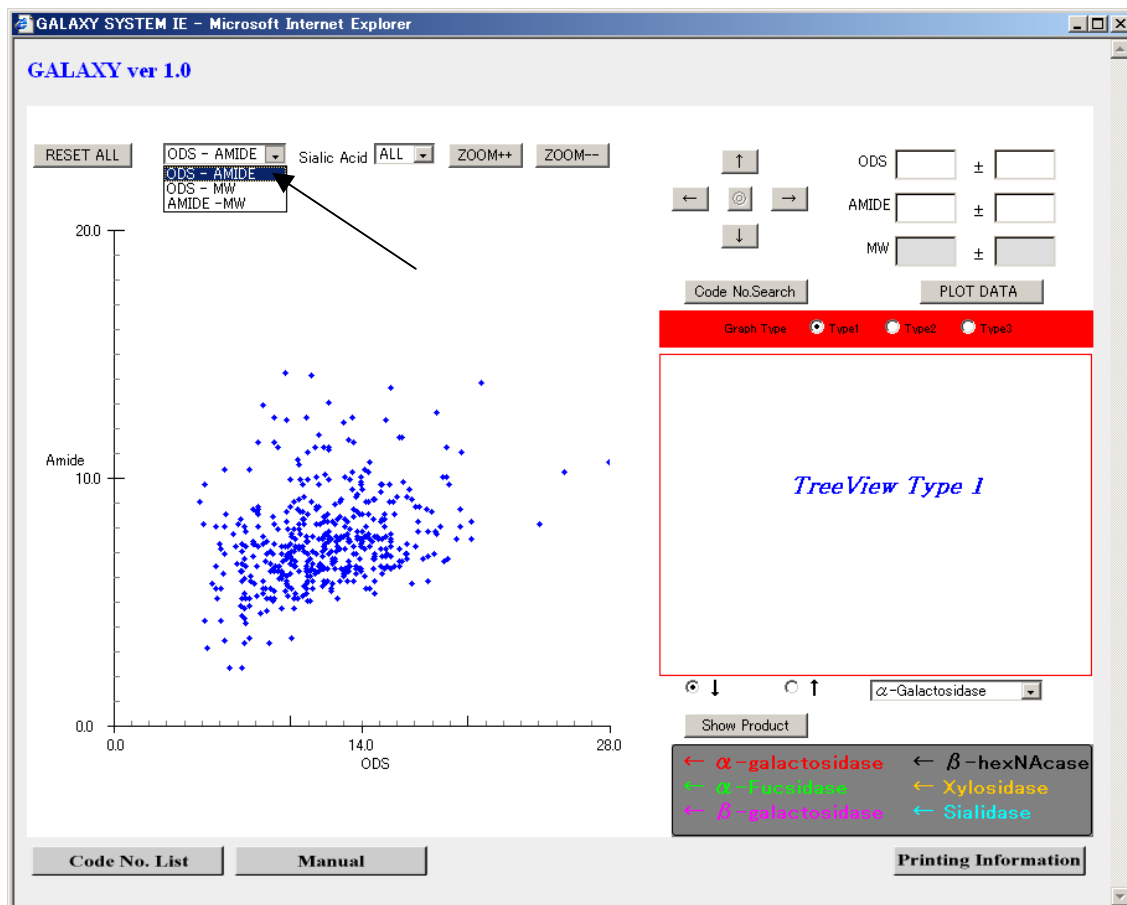
This screen is the basic view of the system displaying various tools available with this system. The system display consists of various text field, buttons, combo boxes and checkboxes for user to select different options and perform various functions.

The values displayed in the graph will always be limited to the black lines representing graph divisions.

Arrows in above figure indicate the maximum limit of ODS / Amide graph.

Each blue point shown in above graph represent sugar chain structures associated with that particular point.

1.2 Graph Selection



By clicking the choice box (indicated by an arrow), one of the three types of graphs can be selected. By default ODS - Amide graph is selected and the same graph is displayed on the screen but user can select ODS - Molecular weight or Amide - molecular weight graphs.

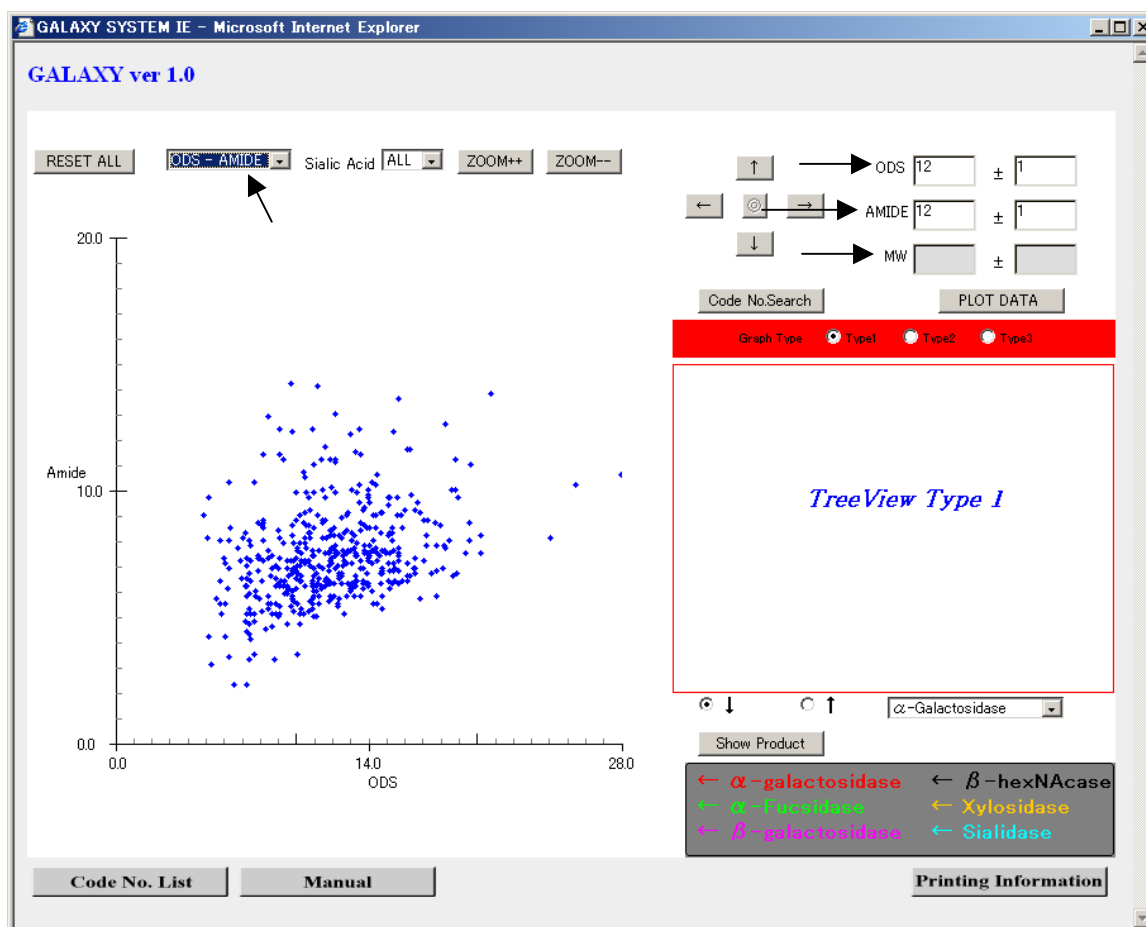
If the choice box selection is changed, X and Y axis values and limits also change according to the selected graph.

Similarly by clicking on the Sialic Acid choice box, one of the SIX(6) types of the Sialic Acid (ALL, 0, 1, 2, 3, 4) can be selected. By default "all" is selected and the graph is drawn according to this default selection.

If the Sialic selection is changed, PA - glycon`s represented by the selected Sialic acid are displayed. According to the Sialic selection, number of PA - glycons displayed change.

Molecular weight is referred as mw in this manual.

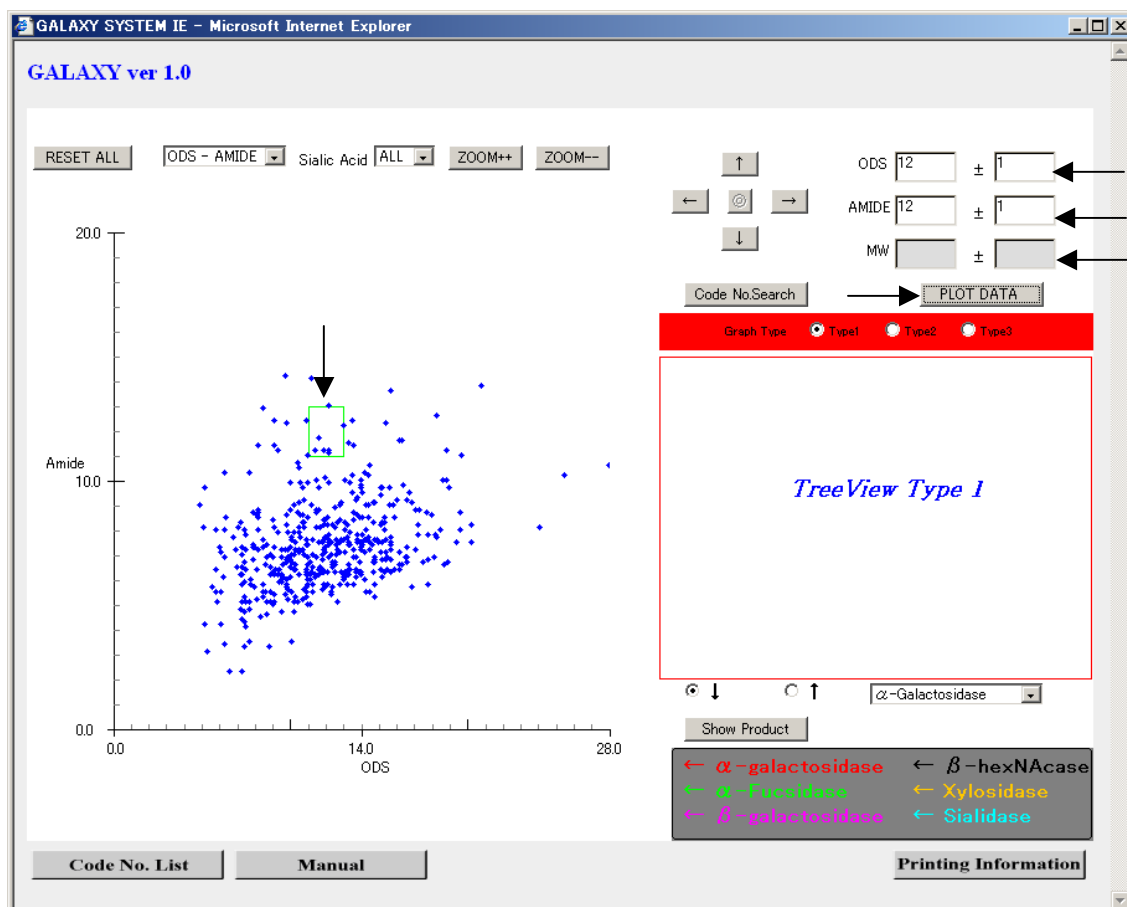
1.3 Text Fields



TextFields are provided with this system to input the data manually. Text Fields representing the X and Y entities of the graph have white background and the Text Fields, which does not represent either of the selected graph type, have gray background.

Background color is changed to indicate the selected graph type, but data can be entered in the gray background textfields.

1.4 Manually inserted Data Display



To display the Text Field data in the current graph click mouse on “PLOT DATA” button. According to the values entered in the Text Field various shapes are created. Text Fields are set 2 in a row and parallel to each other. Text Fields on the right side of the +/- sign are error fields. These error fields are used to insert error factors related to the experiment data.

According to the values entered in the Text Fields various shapes are drawn on the screen as explained below –

Example: - ODS(x axis) – Amide(y axis)

1. ODS (x axis) values are inputted

A green line is drawn parallel to Y-axis at the ODS (x axis) value.

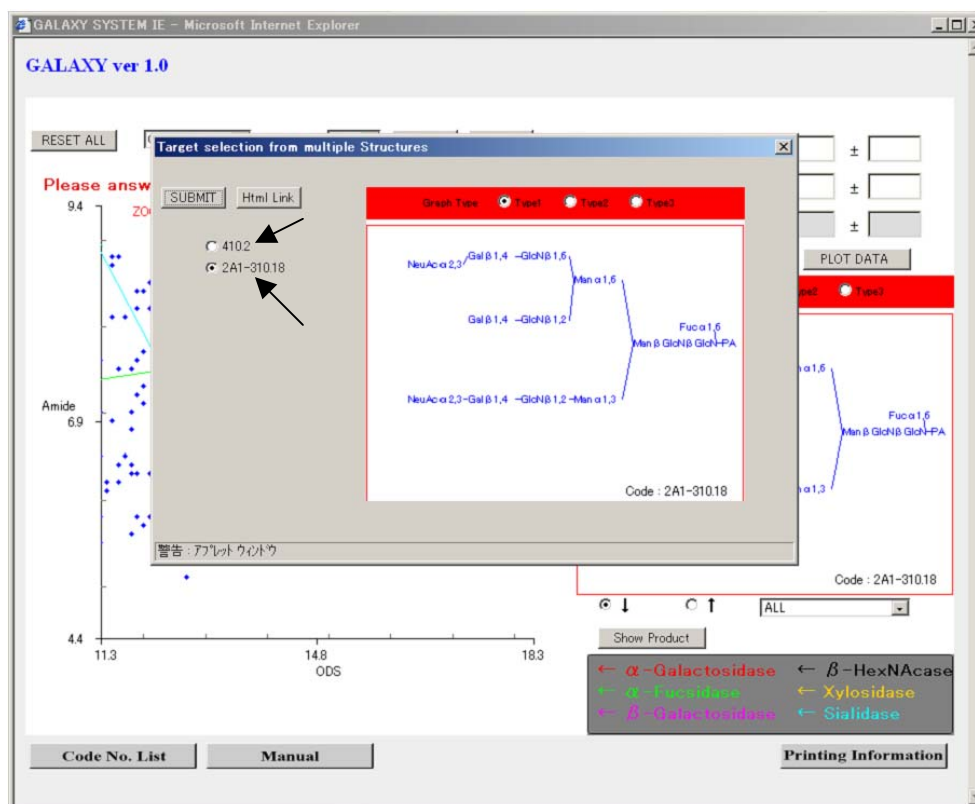
2. Amide (y axis) values are inputted

A green line is drawn parallel to X axis at the Amide (y axis) value.

- 3. ODS (x axis) and Amide(y axis) values are inputted.**
A plus sign is drawn at ODS (x axis) and Amide(y axis) values. If this point has a sugar chain, that point is selected. (Refer User Manual 1.5)
- 4. ODS (x axis) and ODS error are inputted**
A green line is drawn parallel to Y axis at ODS (x axis) value along with 2 green lines drawn parallel to Y axis at (ODS (x axis) + error) and ODS (x axis) – error).
- 5. Amide (Y axis) and Amide error are inputted**
A green line is drawn parallel to X axis at Amide (Y axis) value along with 2 green lines drawn parallel to X axis at (Amide (Y axis) + error) and Amide (Y axis) – error).
- 6. ODS (X axis), Amide (Y axis) and Amide error are inputted**
A green line is drawn with ODS (X axis) and Amide (Y axis) as base (center) from (Amide (Y axis) + error) to (Amide (Y axis) – error).
- 7. ODS (X axis), Amide (Y axis) and ODS error are inputted**
A green line is drawn with ODS (X axis) and Amide (Y axis) as base (center) from (ODS (X axis) + error) to (ODS (X axis) – error).
- 8. ODS (X axis), Amide (Y axis), ODS error, Amide error are inputted**
ODS (X axis) +/- error and Amide (Y axis) +/- error are set as 4 points of the square and a green square is drawn.

In case of ODS (X axis) - Mw (Y axis) and Amide (X axis) – Mw (Y axis) also above 8 rules are used to draw various combinations according to the values entered by the user.

1.5 Mouse Click



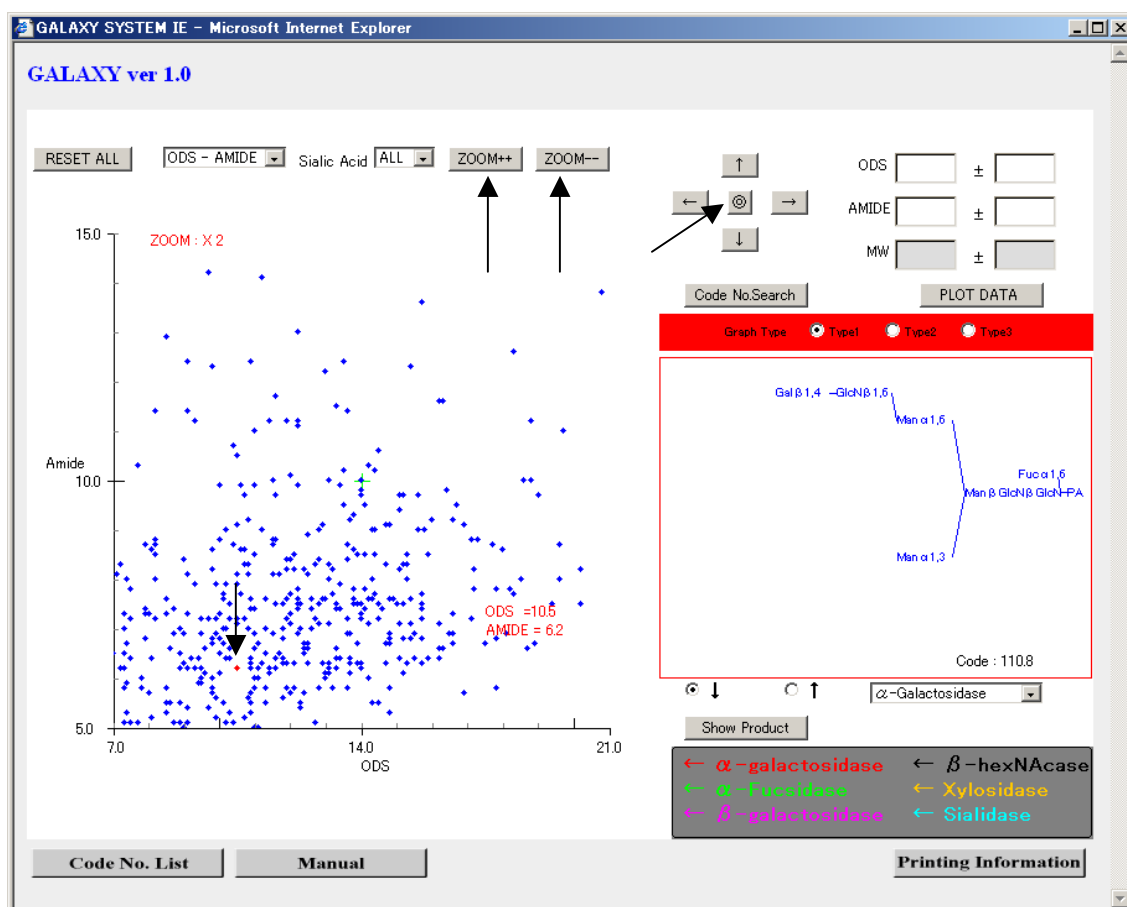
If mouse is clicked within the graph limits on a PA-glycon, Sugar chain related to that point is displayed on the right of the screen. If the mouse is clicked within the graph limits, a mark is drawn according to the click position.

Red Point – If sugar chain is available with the clicked point.

Red Plus sign – If clicked point doesn't have sugar chain.

It is also the case that clicked point has more than one structures associated with it. In this case a dialog as shown in the figure is displayed. User can determine the sugar chain of his interest and selected sugar chain will be displayed for further reference. If a red point is displayed at the clicked position, Sugar chain related to that point is displayed on the Structure panel. (right side of the screen).

1.6 ZOOM++ / ZOOM--

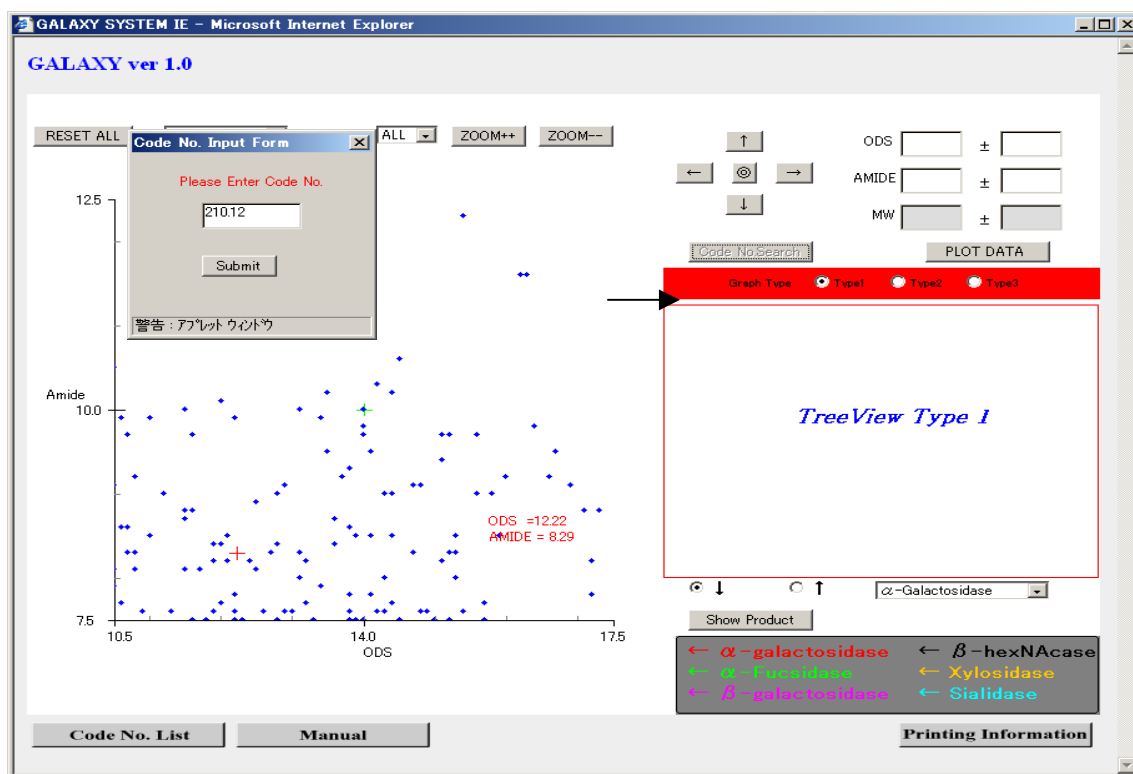


Graph can be zoomed or compressed by pressing the Zoom++ / Zoom-- button. Zoom and compression is always carried out with reference to the center of the graph.

Example: In the image shown above **RED POINT** represents the point selected by the user. In above case the zooming will be done according to y (amide) = 10.0 and x (ODS) = 14.0. Zooming can be done upto X8. The limit for compression is X1.

Tip: To zoom (compress) with respect to the selected point, select the point and press Center button((Circle in circle)). This will bring the selected point to the center of the graph. Then press the ZOOM++ (ZOOM--) button.

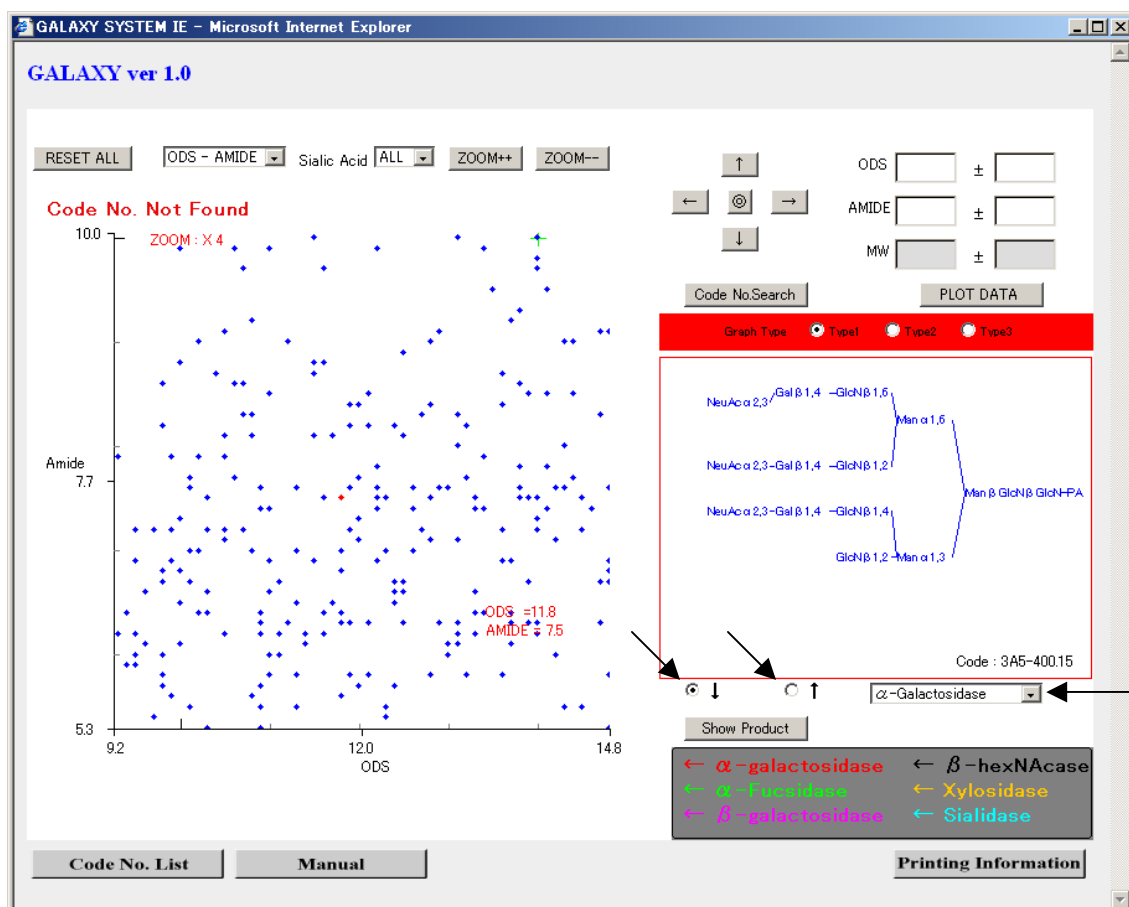
1.7 Code No. Search



This button is used to search the PA-glycan according to code number associated with that PA-glycan. On pressing this button, new dialog will pop up as shown in the figure. User can enter the Code to be searched, in the text field of the popped up dialog and click submit button or press Enter. If the code entered by the user is available in the data, the product representing that code will be selected (that point will become red) else error message will be displayed. **The user input is case insensitive.**

Once this button is pressed a dialog box will pop up and **THE BUTTON WILL BE DISABLED UNTIL USER CLEARS THE POPPED UP DIALOG.**

1.8 Product / Precursor Selection

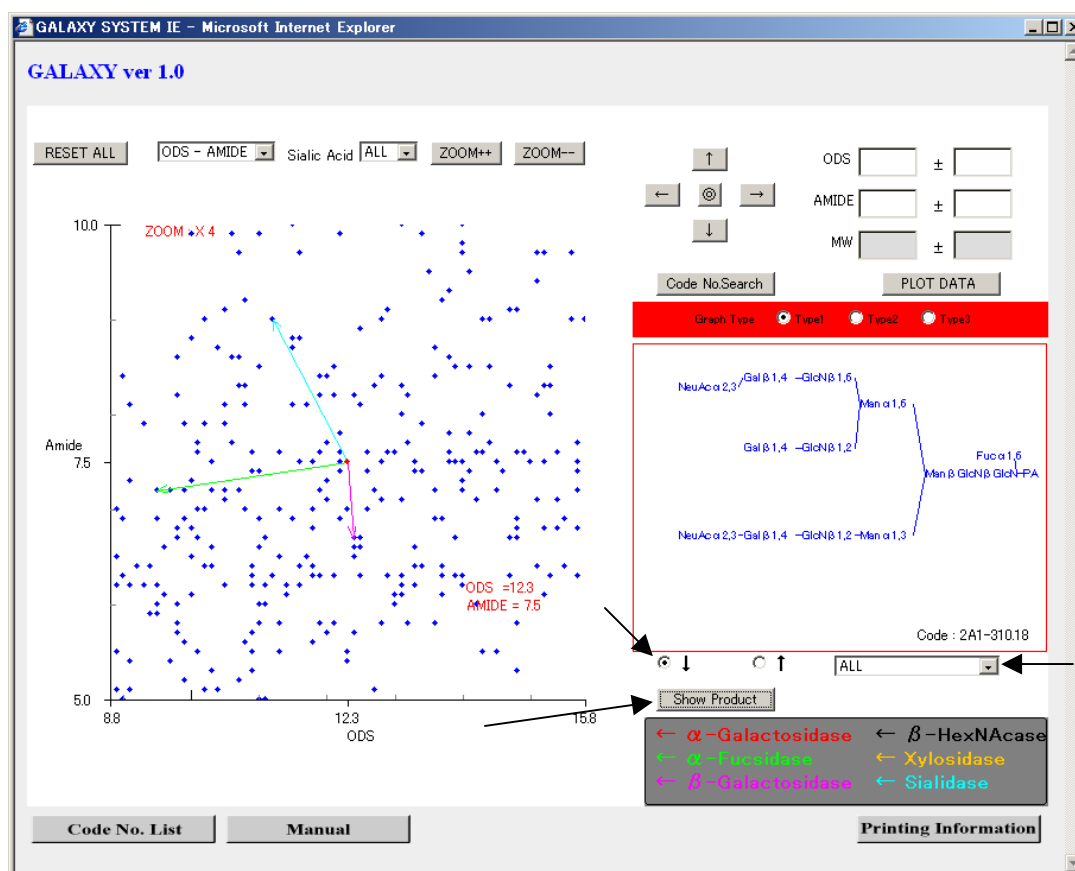


These checkboxes are used for the product and Precursor selection. The default selection is **SHOW PRODUCT** (downward arrow). For Precursor simply click the other checkbox and select the precise enzyme. Then press Precursor button.

Downward arrow (Product) – default selection

Upward arrow (Precursor) – user can make this selection.

1.9 Product / Precursor Display



This button is used to draw product and Precursor arrows according to the selection of checkboxes. If the product checkbox (downward arrow) is selected this button will read as **Show Product**. If Precursor checkbox is selected (downward arrow), this button will read as **Precursor**. Select the appropriate checkbox. Select appropriate enzyme type and press this button.

Product: -

In **Show Product** case if the product is available with the selected enzyme, an arrow will be drawn else error message will be displayed. If selected Oligosaccharide has a cut site but the product is unknown, a Dialog box will pop up asking whether to display unknown data or not. If the user selects to display data, an arrow (dotted line in this case) will be drawn to the product and as the product is unknown, a **black point** will be displayed as the product. User can select this product (black point) by clicking mouse on it but can not

draw an arrow from this unknown product. User can double click the unknown point to see the Structure associated with this unknown product. If the unknown structure is a multiple point, Multiple point selection dialog will pop up and user can select from the Multiple products (known / unknown).

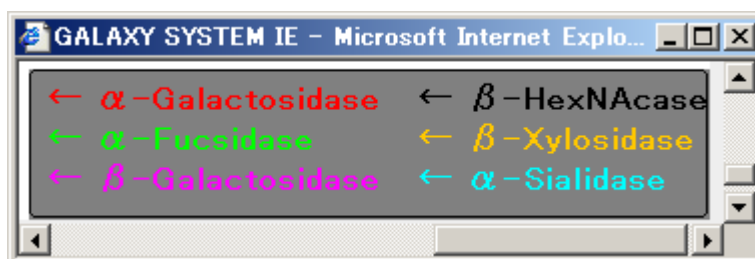
If from enzyme choicebox **ALL** option is selected and arrow button is pressed all the products related to all enzyme types are displayed.

If any of the enzyme type product has unknown data dialog will pop up. All the unknown products are shown if the user presses yes button on the dialog window else if the user presses no button none of the unknown products are shown but all the known products are shown.

Precursor: -

For displaying the precursor, select an appropriate enzyme from the choice box and press Precursor button. All the precursor products are displayed. **Red** lines indicate an **unknown product** and **Black** lines indicate **known products**. Here Known product means the products currently available with this system.

1.10 Color palette



The color of an arrow drawn represents the particular enzyme. The panel shown just below the Product / Precursor button explains the color scheme used with respect to enzyme.

Red – alpha galactosidase

Green – alpha Fucosidase

Magenta – beta galactosidase

Black – beta hexNAcase

Orange – beta Xylosidase

Cyan – alpha Sialidase

In case of Precursor: -

Red – unknown

Black - known

1.11 Graph movement



These buttons, except center button (circle in circle), are used to move the graph i.e. graph co-ordinates to left and right (x co-ordinates) or up and down (y co-ordinates).

Center button is used to bring the selected point to the center of the graph. Center button (circle in circle) is disabled when this applet is downloaded.

When user clicks in the graph limits or plots data from text fields, or plots the point according to Code no., this button is enabled and user can set the selected point at the center of the graph.

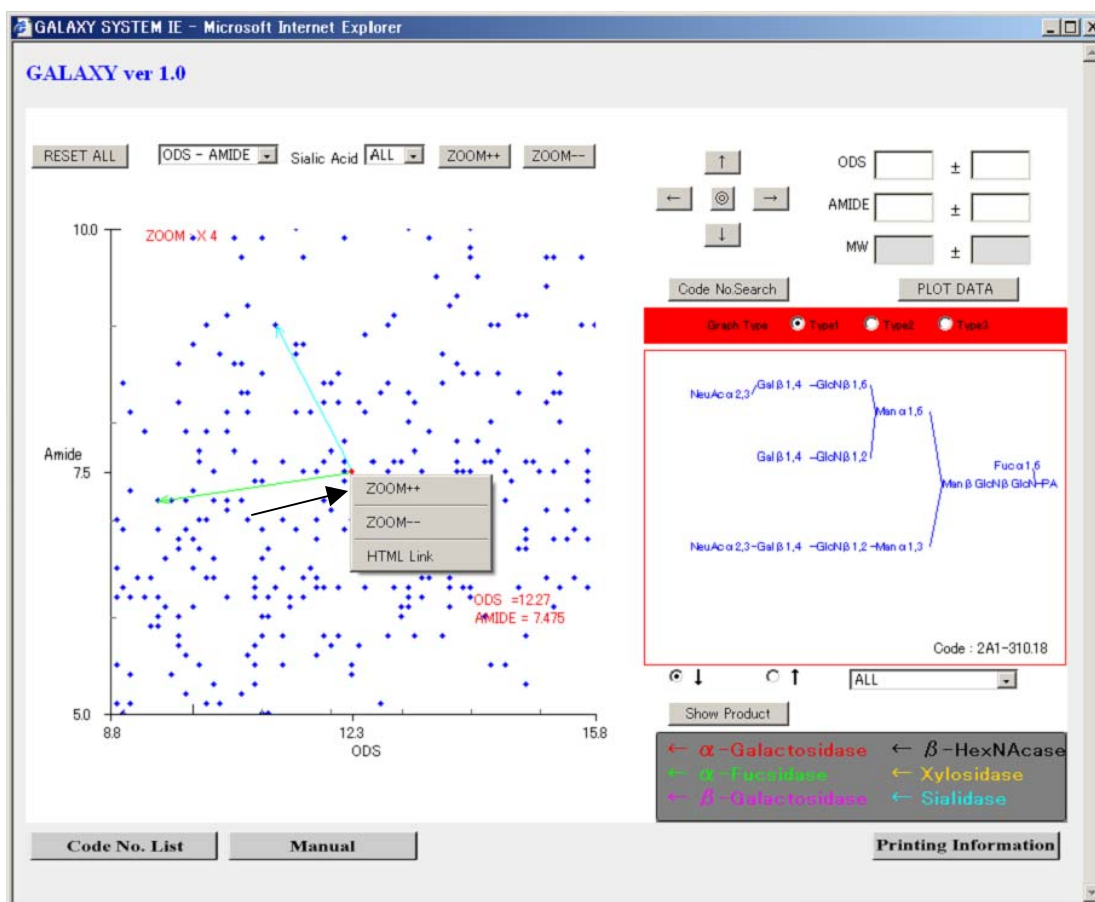
Rest of the buttons are basically used to locate an arrow head location if its not in graph limits.

1.12 Mouse Double Click

This option is used to open the “Information Page” (Html link page) of the selected product. Simply select the product and double click on the selected product, it will open a new HTML page which contains detailed information about the selected product.

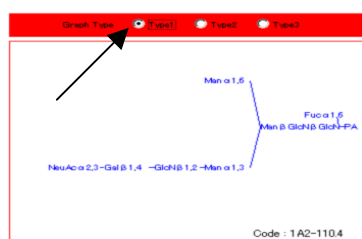
Tip: In case, if the selected product has multiple points, double click linking is not possible. As soon as such point is clicked it will pop up a dialog to select from the available products representing the same point. In this case to see the “Information Page”(Html link), click mouse’s right button on the point of multiple products (right click on that point), menu bar will pop up. Select Html Link from this Menu Bar. It will open all the Html pages depending on the number of products selected point represents. For example if the point represents 3 products, 3 Html pages, each related to the corresponding structure are displayed.

1.13 Right Click Menu

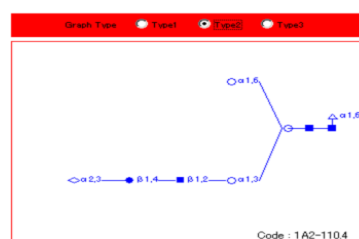


If user right clicks on the selected product, as shown in above figure, a menu bar will pop up. This menu bar has 3 menu items viz. 'ZOOM++', 'ZOOM--', 'HTML Link'. To select any of these menu options, simply click on the desired menu. These menu options will work same as the buttons representing these functions.

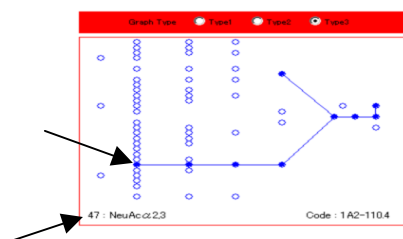
1.14 TreeDraw



(a) type1



(b) type2



(c) type3

Structure shown at the right lower corner of the System is called TreeDraw. TreeDraw represents the Structure of the selected PA-glycan. 3 Types of structure presentations are available with this system. User can select any one type at a time by selecting radio button at the top of the tree draw.

Type 1 - Textual representation

Type 2 - Symbolic representation

Type 3 - Complete sugar chain illustration

In type 2 and 3 user can click on the **Unit** to see the information related to that unit.

2 . Information Page

The screenshot shows a web browser window with the address bar displaying `http://k.kimera.enkaku.co.jp/webtest/Demo-final/OligoHTML0/1A1-301.8.html`. The page content includes:

- RESET /
- Oligosaccharide
- <Code. No> : 1A1-301.8
- <ODS> : 15.3
- <Amide> : 8.3
- <Molecular Weight> : 2579.42
- Amide 6.9
- DATA CONNECTED ENZYME -
- β -Galactosidase
 - β -HexNAcase
 - Sialidase
- Enzyme dropdown menu
- Legend: Black : Known Structure, Red : Predicted Structure
- 4.4
- <References>
- 1. Takahashi, N., Khoo, K.H., Suzuki, N., Johnson, J.R. & Lee, Y. C. (2001) N-glycan structures from the major glycoproteins of pigeon egg white : predominance of terminal Galalpha(1)Gal, *J Biol Chem.* 276, 23230-9. [PubMed]
- ページが表示されました
- インターネット

The diagram shows an oligosaccharide structure with the following components and enzymes:

- Gal β 1,4 - GlcNAc β 1,2 - Man α 1,6
- Gal β 1,4 - GlcNAc β 1,4 - GlcNAc β 1,4 - Man α 1,6
- Man α 1,3 - GlcNAc β 1,2 - Gal β 1,4 - NeuAc α 2,6
- Enzymes: Gal β 1,4 (black), GlcNAc β 1,2 (black), Man α 1,6 (black), GlcNAc β 1,4 (black), NeuAc α 2,6 (black), Man α 1,3 (red), Man α 1,6 (red), GlcNAc β 1,4 (red), and Man α 1,6 (red).

The link related to the particular product is as shown in the above figure. This link is called as “Information page”. This page contains detailed information about the selected product.

ODS, Amide, MW values are displayed along with product code number. It also provides the information about the data connected enzyme.

The data connected enzyme list is displayed. User can select the displayed enzyme from the choice box. The connected structure is displayed according to the selected enzyme.

Enzyme displayed in **RED** color have unknown data and enzymes displayed in black color have known products.

3. Customer Support:

In case of System assistance please contact us on +81-6-4792-6088 or Fax at 06-4792-6089.

E - mail us at info@primmune.com

For bug reports please mail at info@primmune.com

If you need more information about this product, download user manual or contact SystemInfo.

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