

Manual : GlycoFragment

(Version 1.0 :17 March 2004)

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1 Introduction

Mass spectrometry is frequently used to analyze complex oligosaccharides and glycopeptides. The spectra of glycans can be complicated and difficult to interpret without reference data. Unfortunately, no libraries of suitably pure and homogeneous standards have so far been compiled. The web-based tool GLYCO-FRAGMENT allows the generation of all theoretically possible MS relevant fragments of oligosaccharides as defined using the extended IUPAC nomenclature. The main focus of GLYCO-FRAGMENT is to support the manual assignment of all peaks contained in mass spectra of complex carbohydrates. The service is provided by the Molecular Modeling Group of the Central Spectroscopic department of the German Cancer Research Center ([http://www.dkfz.de/spec/projekte/fragments/.](http://www.dkfz.de/spec/projekte/fragments/)) This work was supported by the German Research Council (URL: www.dfg.de) (Deutsche Forschungsgemeinschaft)

Publication:

Lohmann KK, von der Lieth CW

GLYCO-FRAGMENT: *A web tool to support the interpretation of mass spectra of complex carbohydrates.* Proteomics. **2003** Oct;3(10):2028-35.

The **purpose of GLYCO-FRAGMENT** is to calculate and display the main **fragments** (B- and C-, Z- and Y-, A- and X-ions) **of oligosaccharides** that should occur in **MS-spectra**. The extended ASCII character set as recommended by IUPAC is used to input the sequence of complex oligosaccharides.

This web application has been developed by the molecular modeling group of the central spectroscopic department of the German Cancer Research Center (Deutsche Krebsforschungszentrum). Should you find mistakes within the program, or should you have any suggestions about possible changes please contact:

Klaus Lohmann (k.lohmann@dkfz.de) or Willi von der Lieth (w.vonderlieth@dkfz.de)

Other glyco-related web application can be found at:

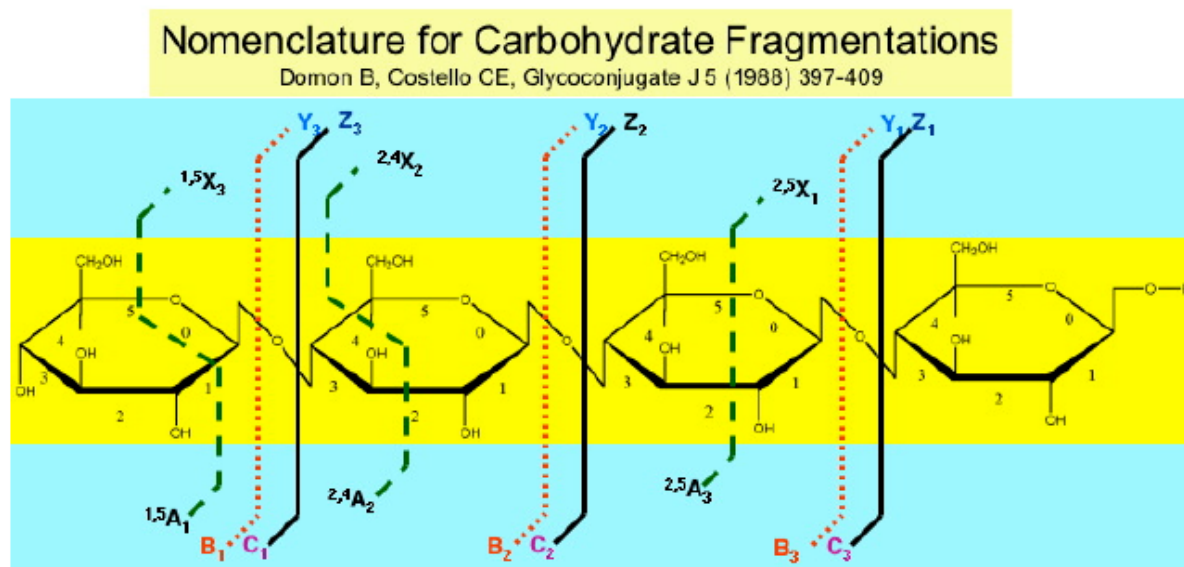
<http://www.dkfz.de/spec/> and <http://www.glycosciences.de>

2 Start

Start your browser (Internet Explorer, Netscape (4.xx) or Mozilla) and activate the following URL:

<http://www.dkfz.de/spec/lohmann/fragment.php4>

You will get the following page:



3 Structure Input Window

This is a simple ASCII input window where you can type in the sequence of your carbohydrate structure using the so-called extended description. The **extended ASCII character set** (see 3.2.) as recommended by IUPAC is used to input the sequence of complex oligosaccharides. However, some additional input rules have to be fulfilled (see 3.4.2.). If only the **topology and composition** of the oligosaccharide is known, a simpler way to input carbohydrate sequences is possible (see 3.1.2.). Since the hydroxyl groups of synthetic carbohydrates are often protected we have included a way to indicate if **sugar residue are persubstituted** (see 3.1.3.).

3.1 Examples of valid input structures

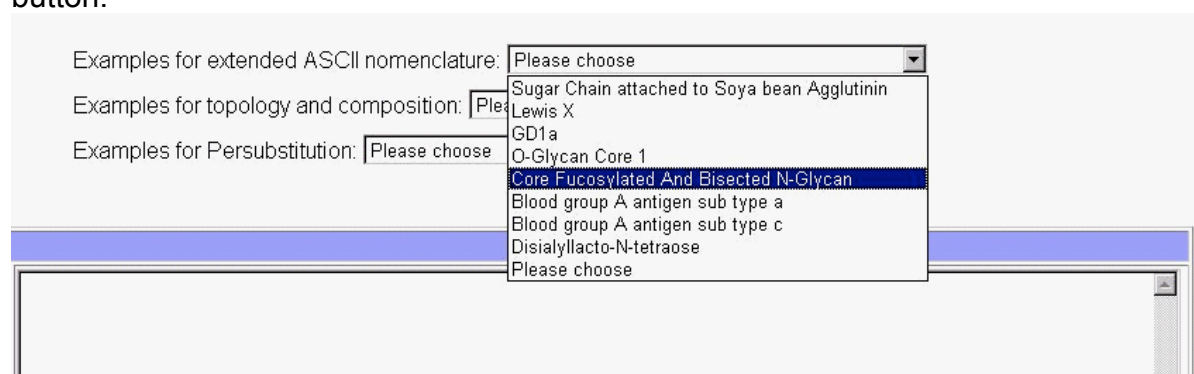
Activating the examples button above the structure input window you can chose between the three example sets:

Examples for extended ASCII nomenclature:

Examples for topology and composition:

Examples for Persubstitution:

A few typical glycan structures are listed when you activate the 'please choose' button.

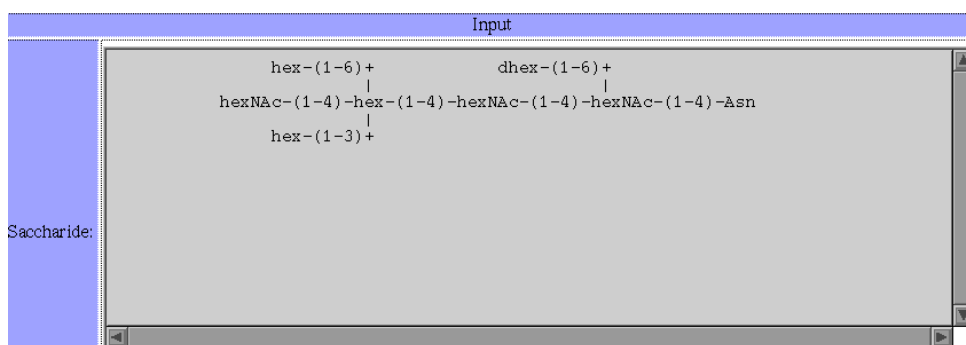


Selecting one of these structures will paste the glycan structure into the input window. The structure of a core fucosylated and bisected N-Glycan will be used throughout this manual as an example.

3.2 Extended ASCII character set

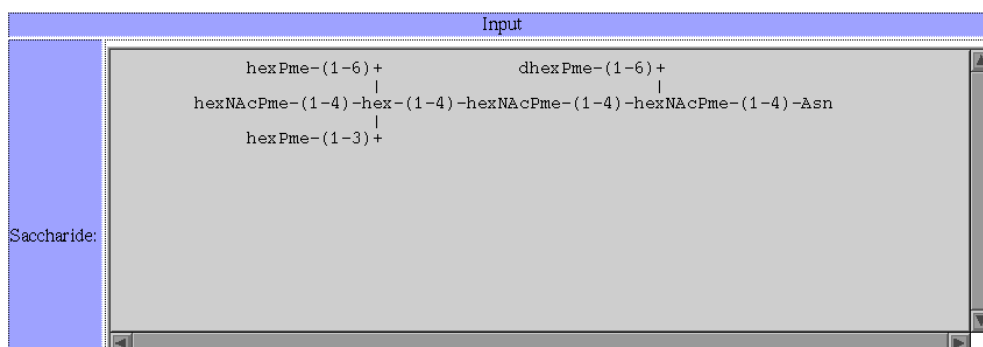
Input							
Saccharide:	$\begin{array}{c} \text{a-D-Manp-(1-6)+} \qquad \qquad \qquad \text{a-L-Fucp-(1-6)+} \\ \qquad \qquad \qquad \\ \text{b-D-GlcpNAc-(1-4)-b-D-Manp-(1-4)-b-D-GlcpNAc-(1-4)-b-D-GlcpNAc-(1-4)-Asn} \\ \\ \text{a-D-Manp-(1-3)+} \end{array}$						
	Ion: <input type="button" value="none"/> use <input type="button" value="monoisotopic mass"/>						
Mass of other Ion	<input type="text"/>						
Adducts:	<table border="1"><tr><td>H2O</td><td>18.2</td></tr><tr><td> </td><td> </td></tr><tr><td> </td><td> </td></tr></table> <input type="button" value="Clear"/>	H2O	18.2				
H2O	18.2						
Number of Saccharides	<input type="button" value="8"/>						
Output:	<input type="button" value="View as Structure"/> <input type="button" value="View B,Y-Ions"/> <input type="button" value="View B,C,Y,Z-Ions"/> <input type="button" value="View All Ions"/> <input type="button" value="Reset Form"/>						

3.2.1 Topology and Composition



Currently supported compositions: Hex, dHex, HexNac, hexAc. Compositions and extended nomenclature can be mixed.

3.2.2 Persubstituted Sugar Residue



Currently supported persubstitutions: PMe and PAc. Persubstitutions are only possible for sugar compositions and cannot be used in combination with the extended nomenclature.

3.3 Copy/Paste your sequences from other sources

Alternatively you can copy/paste your sequences from predefined templates as discussed below or copy/paste sequences using your favourite editor. In case you copy your sequence from a word processing software like MS-WORD we strongly recommend you create your structure using a non-proportional font like Courier .

3.3.1 Predefined templates for various types of complex carbohydrates

can be found at

<http://www.dkfz-heidelberg.de/spec/sweet2/doc/sam/leftframe.html>

If you active for example Spingo lipids on the left hand side you get a list of often discussed Spingo lipids as display on the right hand side:

For example, if you select Spingo lipids on the left side you will get a list of common Spingo lipids on the right side.

[Sphingo lipids](#)

[GPI Anchor](#)

[LPS Anchor](#)

[LOS Anchor](#)

[O-Glycans](#)

[N-Glycans](#)

[Example \(SBA\)](#)

[Example \(N-Glycan\)](#)

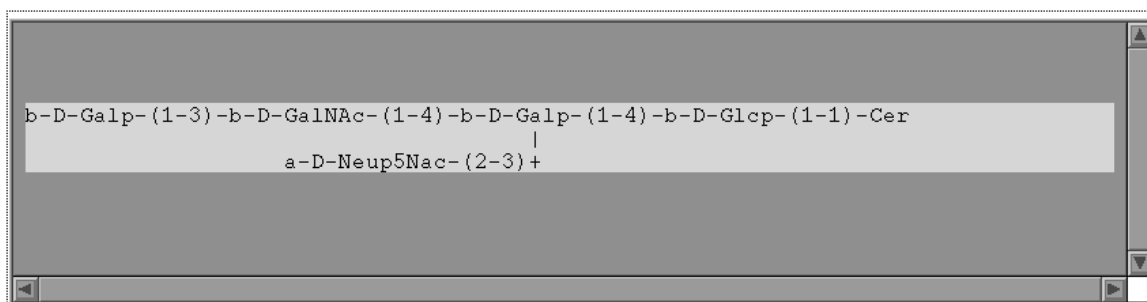
[Back](#)

Typical tumor-associated Globo Sphingo Lipids (GSL) antigens in human cancer:

Globo-series antigens:		Lacto-series (Type 1 chain) antigens:	
Gb3	Gal-Gb4	Le^c	Sialosyl-Le^c
Globo-H	Sialosyl Gal-Gb4	Sialosyl-Le^a	Dimeric Le^a
		Le^b-Le^a	Le^a-Le^x
Ganglio-series antigens:		Lacto-series (Type 2 chain) antigens:	
GD3	GD3-9-OAc	SLe^x-Le^x	Le^x
GD2	Fucosyl GM1	Le^y	Dimeric Le^x
Extended GM2		Le^y-Le^x	SLe^x

Gangliosides	
gm1	gd1a
gm2	gd1b
gm3	
asialo_GM1	
asialo_GM2	

Clicking on one of these items you receive the extended description of the corresponding molecule. The example below shows the structure of GM1.



With a copy/paste procedure you can directly copy this structure into the input window. The copy option works slightly different on different computers. Here the procedure for Windows is described.

- Indicate the structure you want to transfer as shown above (press left mouse button until the complete structure is highlighted)
- Call copy (kopieren) from the edit (bearbeiten) menu of your browser window.
- Click into the Structure input window
- Call paste (einfügen) from the edit (Bearbeiten) pulldownmenu of the input browser window

Please check that you copied the complete structure and that all vertical connections are at the right position (see Extended Description for Oligosaccharides; additional rules).

The same procedure has to be applied if you have created your carbohydrate structures using your favourite editor. We strongly recommend you use Courier to create your input structures.

Additionally you have to input the number of residues contained in the sequence you input. In case this number and the number of residues identified by the program are not identical, you get a warning.

```
Wrong number of residues found! I have found 5 residue(s).
Should have found 3 Residue(s).
Structural data is not correct!
```

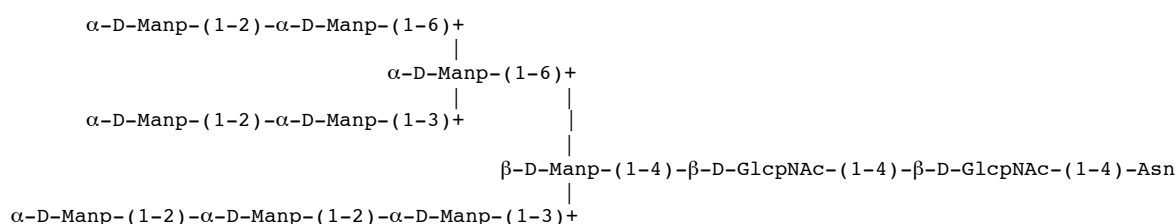
Normally this warning indicates that your input sequence was not correct. Most frequently the vertical alignment of monosaccharides in different lines is incorrect. See (2.3.2.) for more details.

3.4 Extended Description for Oligosaccharides

To input your carbohydrate structure, the so-called extended form is used to describe Oligosaccharides . The definition can be found at

<http://www.chem.qmw.ac.uk/iupac/2carb/38.html>

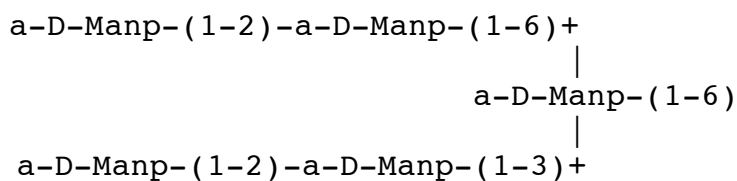
3.4.1 Example of a N-Glycan structure



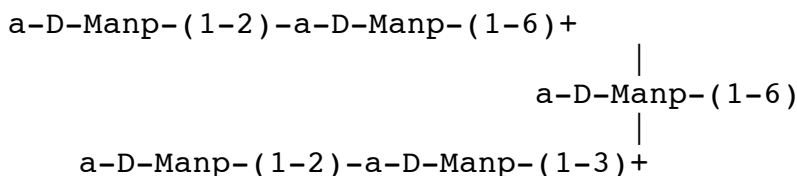
Using the input window a few special input rules have to be fulfilled; these are discussed for the N-Glycan structure given above.

3.4.2 Additional Input rules

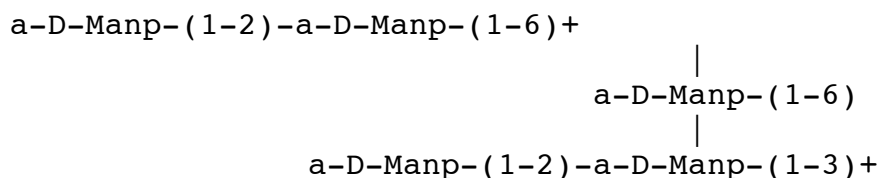
- a,b have to used instead of α,β .
- the ring configuration (D or L) has to be given always.
- a hyphen before and after the linkage information is required $-(1-3)-$
- Furanoses and Pyranoses have to be indicated.
- A '+'-sign is required to indicate continuation of the structure in an upper of lower line of the editor.
- To indicate the vertical connections the '+', '|' and the connection to the corresponding monosaccharide have to be in one vertical line. This requirement often causes problems when inputting structures by the copy/paste option when a proportional fond (like Arial or Times) is used.



Incorrect input:



Incorrect input:



4 Representations of the Fragmentation Scheme

Three different representation of the fragmentation scheme are currently available.

4.1 Ordered list

Press the **“view B,C,Y,Z Ions” button** at the bottom of the input window to activate this option.

Input							
Saccharide:	$ \begin{array}{c} \text{a-D-Manp-(1-6)+} \qquad \qquad \qquad \text{a-L-Fucp-(1-6)+} \\ \text{b-D-GlcpNAc-(1-4)-b-D-Manp-(1-4)-b-D-GlcpNAc-(1-4)-b-D-GlcpNAc-(1-4)-Asn} \\ \\ \text{a-D-Manp-(1-3)+} \end{array} $						
	Ion: <input type="text" value="none"/> use <input type="text" value="monoisotopic mass"/> Mass of other Ion <input type="text"/>						
Adducts:	<table border="1"> <tr> <td>H2O</td> <td>18.2</td> </tr> <tr> <td> </td> <td> </td> </tr> <tr> <td> </td> <td> </td> </tr> </table> <input type="button" value="Clear"/>	H2O	18.2				
H2O	18.2						
Number of Saccharides	<input type="text" value="8"/>						
Output:	<input type="button" value="View as Structure"/> <input type="button" value="View B,Y-Ions"/> <input type="button" value="View B,C,Y,Z-Ions"/> <input type="button" value="View All Ions"/> <input type="button" value="Reset Form"/>						

In the first column the fragments are ordered according their increasing mass. The type of ion is given in the second column. The identification of a fragment in carbohydrate sequence is given through the linkage path information. The core

fucosylated N-Glycan structure given above contains two a-D-Manp residues. Linkage path information is used to tell the user which of the two residues is specified. Starting from the reducing end of the molecule (right side) and counting only the connections on the reducing side the linkage path 4,4,4,6 indicates the a-D-Manp residue at the top/left. The other a-D-Manp has the linkage path information 4,4,4,3.

View with A and X Ions

Total Mass: 1357.5130 M[+]; 1358.5208 M[Na+]; 1380.5020 M[K+]; 1396.6110		
Mass in amu	Ion	Linkage-Path
99.0558	Z(1)-Ion	4
115.0507	Y(1)-Ion	4
147.0657	B(1)-Ion	4, 6
163.0606	C(1)-Ion	4, 6
163.0606	B(4)-Ion	4, 4, 4, 3
	B(2)-Ion	4, 4, 4, 6
179.0556	C(4)-Ion	4, 4, 4, 3
	C(2)-Ion	4, 4, 4, 6
204.0872	B(3)-Ion	4, 4, 4, 4
220.0821	C(3)-Ion	4, 4, 4, 4
448.1931	Z(2)-Ion	4, 4
464.1880	Y(2)-Ion	4, 4
651.2725	Z(3)-Ion	4, 4, 4
667.2674	Y(3)-Ion	4, 4, 4
690.2456	B(5)-Ion	4, 4, 4
706.2406	C(5)-Ion	4, 4, 4
893.3250	B(6)-Ion	4, 4
909.3199	C(6)-Ion	4, 4
1137.4309	Z(5)-Ion	4, 4, 4, 4
1153.4258	Y(5)-Ion	4, 4, 4, 4
1178.4575	Z(4)-Ion	4, 4, 4, 3
	Z(6)-Ion	4, 4, 4, 6
1194.4524	Y(4)-Ion	4, 4, 4, 3
	Y(6)-Ion	4, 4, 4, 6
1194.4524	Z(7)-Ion	4, 6
1210.4473	Y(7)-Ion	4, 6
1242.4623	B(7)-Ion	4
1258.4572	C(7)-Ion	4

Activating the '**view with A- and X- Ions**'-button displays an ordered list of all possible Y-,Z-,B-,C- and A Ions, which is normally rather long. Here only the possible assignment of the first five smallest fragments (left) and a cut out of some fragments with higher masses (right) are given. The complete list of fragments and their assignments can be output using the print option of the browser.

View without A and X Ions

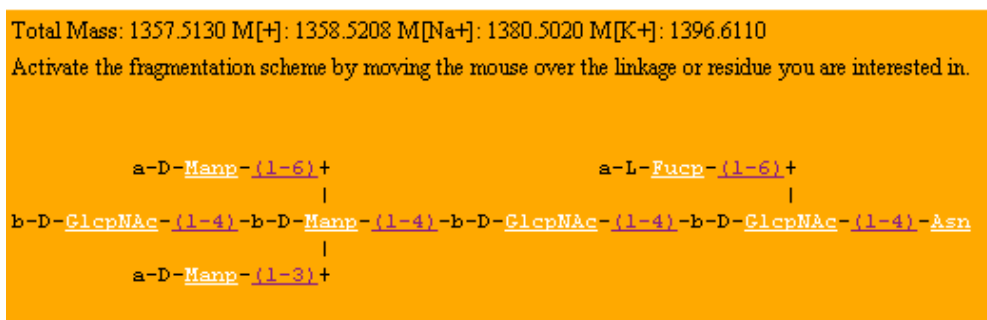
Total Mass: 1357.5130 M[+]: 1358.5208 M[Na+]: 1380.5020 M[K+]: 1396.6110

Mass in amu	Ion	Linkage-Path
13.0078	A(7)0,1-Ion	4
	A(6)0,1-Ion	4, 4
	A(5)0,1-Ion	4, 4, 4
	A(4)0,1-Ion	4, 4, 4, 3
	A(3)0,1-Ion	4, 4, 4, 4
	A(2)0,1-Ion	4, 4, 4, 6
	A(1)0,1-Ion	4, 6
25.0078	X(1)4,5-Ion	4
	X(2)4,5-Ion	4, 4
	X(3)4,5-Ion	4, 4, 4
	X(4)4,5-Ion	4, 4, 4, 3
	X(5)4,5-Ion	4, 4, 4, 4
	X(6)4,5-Ion	4, 4, 4, 6
	X(7)4,5-Ion	4, 6
27.0109	X(1)1,2-Ion	4
	X(2)1,2-Ion	4, 4
	X(5)1,2-Ion	4, 4, 4, 4
28.0313	A(1)4,5-Ion	4, 6
29.0027	X(1)2,3-Ion	4
	X(1)3,4-Ion	4
	X(2)2,3-Ion	4, 4
	X(2)3,4-Ion	4, 4
	X(3)1,2-Ion	4, 4, 4
	X(3)2,3-Ion	4, 4, 4
	X(3)3,4-Ion	4, 4, 4
	X(4)1,2-Ion	4, 4, 4, 3
	X(4)2,3-Ion	4, 4, 4, 3
	X(4)3,4-Ion	4, 4, 4, 3
	X(5)2,3-Ion	4, 4, 4, 4
	X(5)3,4-Ion	4, 4, 4, 4
	X(6)1,2-Ion	4, 4, 4, 6
	X(6)2,3-Ion	4, 4, 4, 6

952.3383	A(7)2,4-Ion	4
1023.3754	A(7)1,4-Ion	4
1036.3832	A(7)0,4-Ion	4
1112.4119	A(7)3,5-Ion	4
1137.4309	Z(5)-Ion	4, 4, 4, 4
1142.4224	A(7)2,5-Ion	4
1153.4258	Y(5)-Ion	4, 4, 4, 4
1166.4337	X(5)0,1-Ion	4, 4, 4, 4
1178.4575	Z(4)-Ion	4, 4, 4, 3
	Z(6)-Ion	4, 4, 4, 6
1193.4446	X(5)0,2-Ion	4, 4, 4, 4
1194.4524	Y(4)-Ion	4, 4, 4, 3
	Y(6)-Ion	4, 4, 4, 6
1194.4524	Z(7)-Ion	4, 6
1207.4602	X(4)0,1-Ion	4, 4, 4, 3
1207.4602	X(6)0,1-Ion	4, 4, 4, 6
1210.4473	Y(7)-Ion	4, 6
1213.4595	A(7)1,5-Ion	4
1222.4473	X(5)0,3-Ion	4, 4, 4, 4
1223.4551	X(7)0,1-Ion	4, 6
1226.4674	A(7)0,5-Ion	4
1236.4629	X(4)0,2-Ion	4, 4, 4, 3
1236.4629	X(6)0,2-Ion	4, 4, 4, 6
1242.4623	B(7)-Ion	4
1251.4500	X(5)0,4-Ion	4, 4, 4, 4
1252.4579	X(7)0,2-Ion	4, 6
1258.4572	C(7)-Ion	4
1265.4657	X(4)0,3-Ion	4, 4, 4, 3
1265.4657	X(6)0,3-Ion	4, 4, 4, 6
1276.4579	X(5)0,5-Ion	4, 4, 4, 4
1281.4606	X(7)0,3-Ion	4, 6
1294.4684	X(4)0,4-Ion	4, 4, 4, 3
1294.4684	X(6)0,4-Ion	4, 4, 4, 6
1310.4633	X(7)0,4-Ion	4, 6
1319.4762	X(4)0,5-Ion	4, 4, 4, 3

4.2 View as structure

Press the **“view as structure”** button at the bottom of the input window to activate this option.



When moving the mouse over the linkage of interest (indicated in magenta), the masses of corresponding B- and C-Ions as well as the masses of Z-,Y-Ions will be presented in a small popup window

Total Mass: 1357.5130 M[+]: 1358.5208 M[Na+]: 1380.5020 M[K+]: 1396.6110

Activate the fragmentation scheme by moving the mouse over the linkage or residue you are interested in.

a-D-Mannp-(1-6)+

|

b-D-GlcpNAc-(1-4)-b-D-Mannp-(1-4)-b-D-GlcpNAc-(1-4)-b-D-GlcpNAc-(1-4)-Asn

|

a-D-Mannp-(1-3)+

a-L-

B-Ion =	Z-Ion =
893.3250	448.1931
C-Ion =	Y-Ion =
909.3199	464.1880

When moving the mouse over the residue of interest (indicated in white), the masses of corresponding A- and X-Ions will be presented in a popup window. The indices following the ion indicate the type of fragmentation. (A(0,4)) means that the bond between the ring oxygen/C1 and the bond between C4 / C5 are broken.

Total Mass: 1357.5130 M[+]: 1358.5208 M[Na+]: 1380.5020 M[K+]: 1396.6110

Activate the fragmentation scheme by moving the mouse over the linkage or residue you are interest

a-D-Mannp-(1-6)+

|

b-D-GlcpNAc-(1-4)-b-D-Mannp-(1-4)-b-D-GlcpNAc-

|

a-D-Mannp-(1-3)+

A	13.0078	X	477.1958
(0,1)		(0,1)	
a-A	84.0449	X	504.2067
(0,2)		(0,2)	
A	114.0555	X	533.2095
(0,3)		(0,3)	
A	833.3039	X	562.2122
(0,4)		(0,4)	
A	877.3301	X	587.2200
(0,5)		(0,5)	
A	71.0371	X	27.0109
(1,2)		(1,2)	
A	101.0477	X	56.0136
(1,3)		(1,3)	
A	820.2961	X	85.0164
(1,4)		(1,4)	
A	864.3223	X	110.0242
(1,5)		(1,5)	
A	30.0106	X	29.0027
(2,3)		(2,3)	
A	749.2589	X	58.0055
(2,4)		(2,4)	
A	793.2852	X	83.0133
(2,5)		(2,5)	
A	719.2484	X	29.0027
(3,4)		(3,4)	
A	763.2746	X	54.0106
(3,5)		(3,5)	
A	44.0262	X	25.0078
(4,5)		(4,5)	

4.3 Ion mode and adducts

4.3.1 Input of ions

The user may enter the masses as neutral ions, positive ions, or as negative ions. Examples of these are [M], [M+H]⁺, [M+Na]⁺, [M+K]⁺

The screenshot shows a web-based input form titled "Input". The main text area contains a glycan structure: a-D-Manp-(1-6)+ a-L-Fucp-(1-6)+ h-D-GlcpNAc-(1-4)-h-D-Manp-(1-4)-h-D-GlcpNAc-(1-4)-h-D-GlcpNAc-(1-4)-Asn a-D-Manp-(1-3)+. Below the text area, there is a dropdown menu for "Ion:" set to "Na", a dropdown for "use" set to "monoisotopic mass", and a "Clear" button. Further down, there is a dropdown for "Number of Saccharides" set to "8". At the bottom, there are five buttons: "View as Structure", "View B,Y-Ions", "View B,C,Y,Z-Ions", "View All Ions", and "Reset Form".

The resulting output (given here as an ordered list) will look like this:

Mass in amu	Ion
[M-H] ⁻ : 1356.5060	Mass: 1357.5130
[M+H] ⁺ : 1358.5208	[M+Na] ⁺ : 1380.5020
[M+K] ⁺ : 1396.6110	
139.0483	Y ₄ + Na ⁺
169.0477	B _{4,6} + Na ⁺
185.0426	B _{4,4,4,3} + Na ⁺
	B _{4,4,4,6} + Na ⁺
226.0691	B _{4,4,4,4} + Na ⁺
488.1856	Y _{4,4} + Na ⁺
691.2650	Y _{4,4,4} + Na ⁺
712.2276	B _{4,4,4} + Na ⁺
915.3069	B _{4,4} + Na ⁺
1177.4234	Y _{4,4,4,4} + Na ⁺
1218.4500	Y _{4,4,4,3} + Na ⁺
	Y _{4,4,4,6} + Na ⁺
1234.4449	Y _{4,6} + Na ⁺
1264.4442	B ₄ + Na ⁺

4.3.2 Input of adducts

The user has the option of specifying any kind of adducts by giving the name of an adduct and the mass associated with this adduct. There is no restriction on the names which may be used for adducts.

Input

Saccharide: a-D-Manp-(1-6)+ a-L-Fucp-(1-6)+
 b-D-GlcpNAc-(1-4)-b-D-Manp-(1-4)-b-D-GlcpNAc-(1-4)-b-D-GlcpNAc-(1-4)-Asn
 a-D-Manp-(1-3)+

Ion: Na+ use monoisotopic mass

Mass: CH3COO-
 H-
 H2O none 18.2
 H+ 59.0
 N(C)
 Li+
 Na+
 K+
 Cs+

Adducts:

Number of Saccharides: 8

Output: View as Structure View B,Y-Ions View B,C,Y,Z-Ions View All Ions Reset Form

The result is an ordered list of masses. The mass of the adducts is added to each fragment of the oligosaccharide.

Mass in amu			
[M-H]- 1356.5060	Mass: 1357.5130	[M+H]+: 1358.5208	[M+Na+]: 1380.5020
[M+K+]: 1396.6110			
30.0483	Y ₄ - N(CH ₃) ₃ + Na+	691.2650	Y _{4,4,4} + Na+
110.0477	B _{4,6} - N(CH ₃) ₃ + Na+	694.0276	B _{4,4,4} - H ₂ O + Na+
126.0426	B _{4,4,4,2} - N(CH ₃) ₃ + Na+	712.2276	B _{4,4,4} + Na+
	B _{4,4,4,6} - N(CH ₃) ₃ + Na+	856.3069	B _{4,4} - N(CH ₃) ₃ + Na+
139.0483	Y ₄ + Na+	897.1069	B _{4,4} - H ₂ O + Na+
150.8477	B _{4,6} - H ₂ O + Na+	915.3069	B _{4,4} + Na+
166.8426	B _{4,4,4,3} - H ₂ O + Na+	1118.4234	Y _{4,4,4,4} - N(CH ₃) ₃ + Na+
	B _{4,4,4,6} - H ₂ O + Na+	1159.4500	Y _{4,4,4,3} - N(CH ₃) ₃ + Na+
167.0691	B _{4,4,4,4} - N(CH ₃) ₃ + Na+		Y _{4,4,4,6} - N(CH ₃) ₃ + Na+
169.0477	B _{4,6} + Na+	1175.4449	Y _{4,6} - N(CH ₃) ₃ + Na+
185.0426	B _{4,4,4,3} + Na+	1177.4234	Y _{4,4,4,4} + Na+
	B _{4,4,4,6} + Na+	1205.4442	B ₄ - N(CH ₃) ₃ + Na+
207.8691	B _{4,4,4,4} - H ₂ O + Na+	1218.4500	Y _{4,4,4,3} + Na+
226.0691	B _{4,4,4,4} + Na+		Y _{4,4,4,6} + Na+
429.1856	Y _{4,4} - N(CH ₃) ₃ + Na+	1234.4449	Y _{4,6} + Na+
488.1856	Y _{4,4} + Na+	1246.2442	B ₄ - H ₂ O + Na+
532.2650	Y _{4,4,4} - N(CH ₃) ₃ + Na+	1264.4442	B ₄ + Na+
553.2276	B _{4,4,4} - N(CH ₃) ₃ + Na+		

5 Appendix:

5.1 How to Input Substitutions of Sugar Residues

5.1.1 Examples:

5.1.2 Extended Description for Oligosaccharides

The numbers following the monosaccharide description indicate the location of the substitution at the corresponding C-Atom of the sugar.

a-D-Galp2OMe, a-D-Galp2OAc3OAc, a-Galp2OMe3OMe4OMe6Ome

Currently supported substitutions: Me, Ac, OMe, OAc, NAc, SO3, PO4, Cl

Substituent	Input
cPCH	cPCH
PCH	PCH
PEA	PEA
n-SO3	NSO3
Phosphate	PO4
Schwefelrest	OSO3
Schwefelrest	SO3
NAC	NAc
NAC	OAc
OMe	OMe
Wasser	H2O
CH	CH
EA	EA
Pyridin	Py
Methyl	Me
Acetate	Ac
Glycolsaeure	Gc
Schwefelwasserstoff	SH
Amine	N

5.2 Composition of Oligosaccharides

Currently supported compositions: Hex, dHex, HexNac, HexAc. Compositions and extended nomenclature can be mixed.

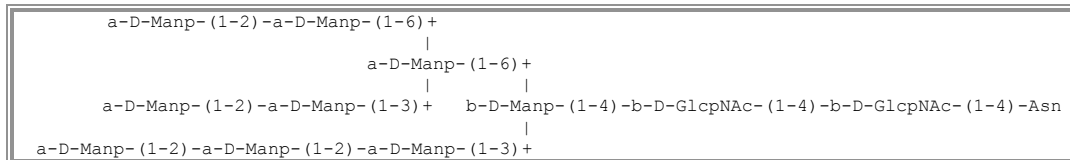
5.3 Persubstitutions of Oligosaccharides

Currently supported persubstitutions: PMe and PAc. Persubstitutions are only possible for sugar compositions and cannot be used in combination with the extended nomenclature.

5.4 How to handle secondary fragmentations

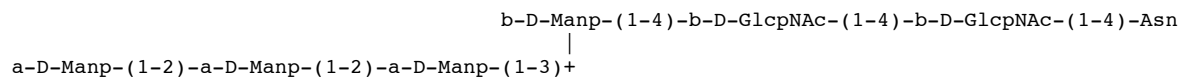
To identify the peaks which may result from secondary fragmentations of the complete glycan, the sequences resulting from this fragmentation have to be analyzed separately.

In case you have the following carbohydrate sequence

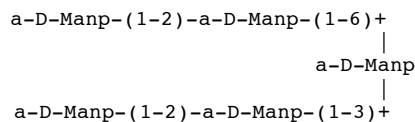


And you have the impression that some secondary fragmentation takes place than you have to input the sequence of the fragments which remains when the secondary fragmentation takes place. Assuming a fragmentation occurs at the 4,4,4,6 Linkage the following two fragments would result:

Fragment A:



Fragment B



Both carbohydrate sequences have to be analyzed separately as shown above. The input of the (sub)sequences can be easily accomplished using copy/paste options.