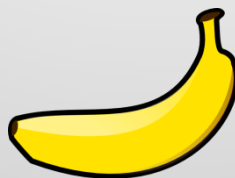


12.06.2013

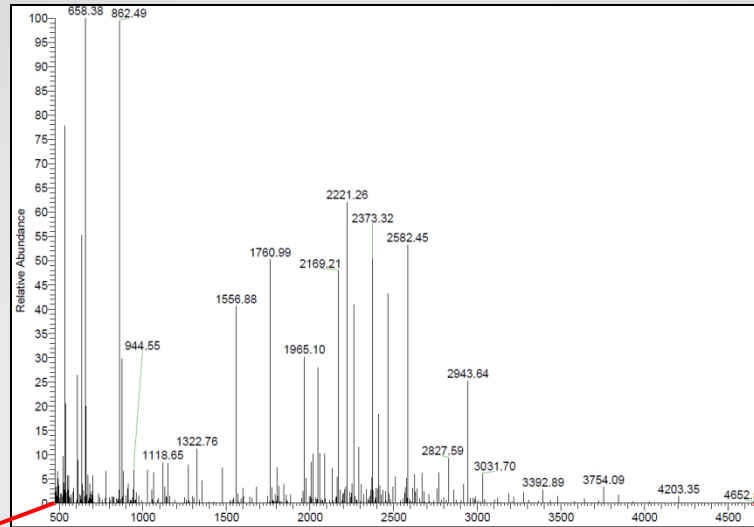
René Ranzinger  
3rd Beilstein Symposium on  
Glyco-Bioinformatics



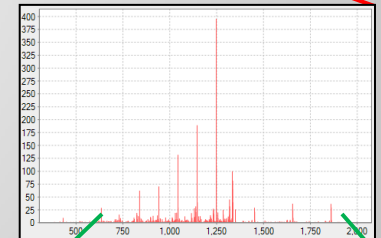
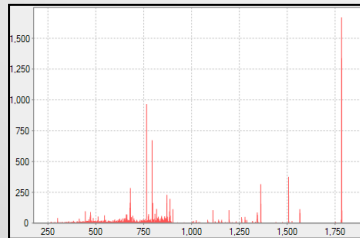
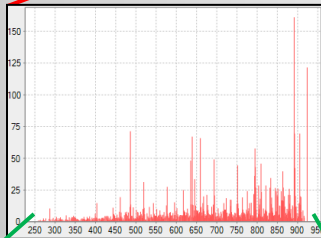
Simian Tools Demo



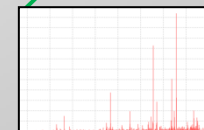
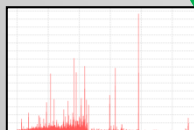
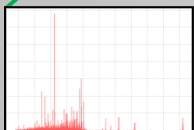
# MS<sup>n</sup> Data



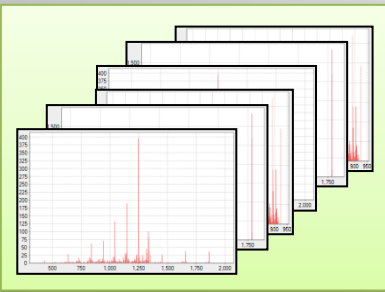
Up to several hundred MS<sup>2</sup>



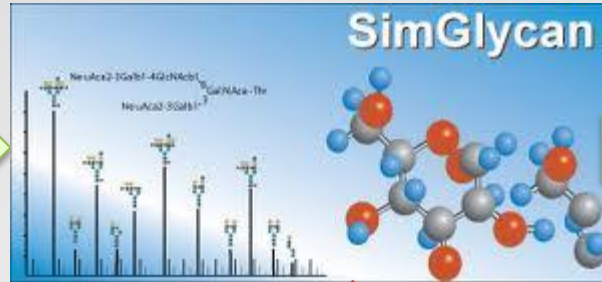
0 - several MS<sup>3</sup> per MS<sup>2</sup>



# SimGlycan



Data



Annotation

SimGlycan 2.0 software interface showing a table of glycan profiles and their associated information. The table lists MS/MS Data File, Glycan ID, Glycan S., Compos., Branching, and Glycan R. for several profiles. Below the table, the Glycan Information section provides details for a selected glycan, including Name, Sequence, Composition, Glycan Mass, Precursor Ion m/z, Class, Reaction, Pathway, Enzyme, and Other DB links.

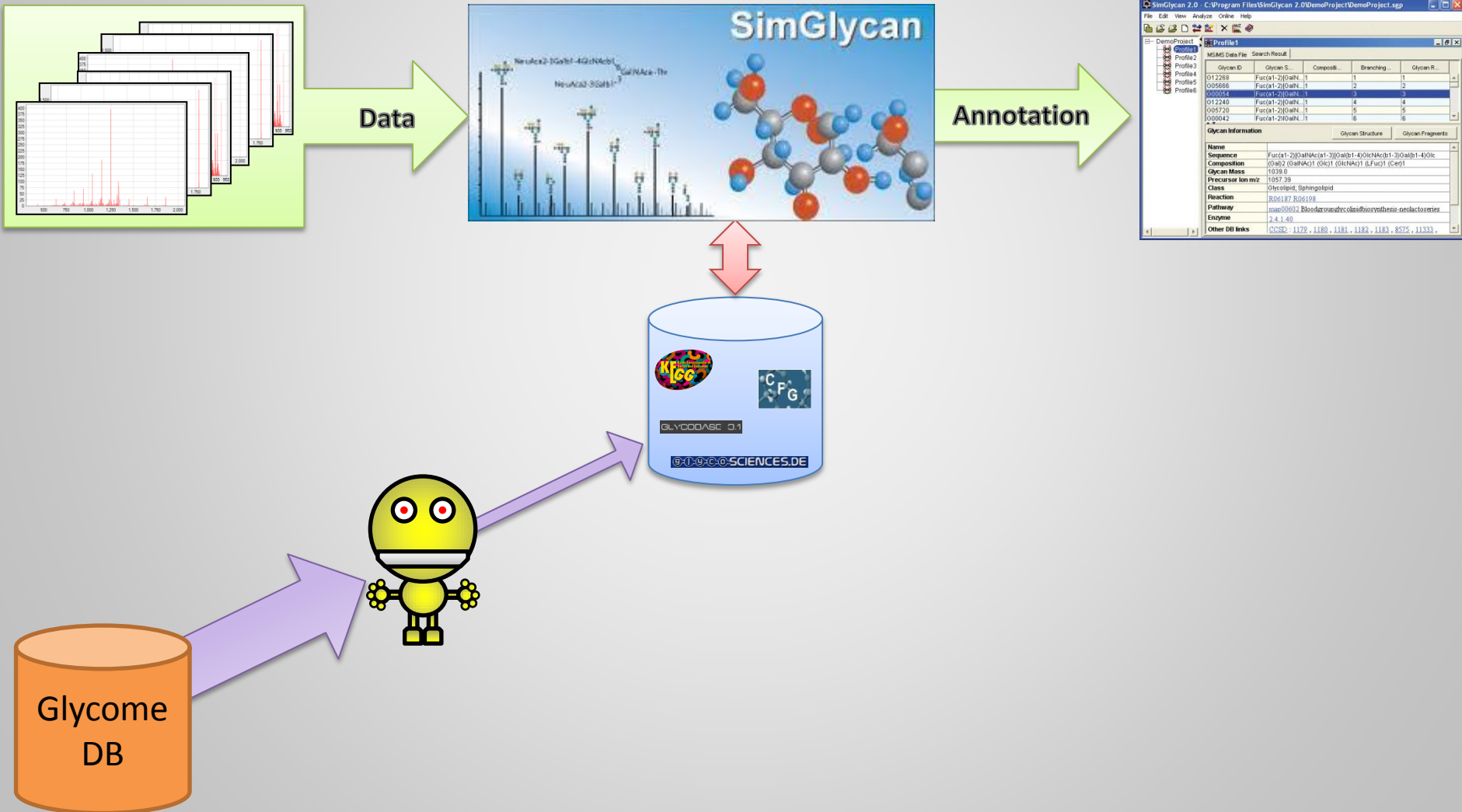
| MS/MS Data File | Glycan ID | Glycan S.          | Compos. | Branching | Glycan R. |
|-----------------|-----------|--------------------|---------|-----------|-----------|
| Profile1        | G12386    | Fuc(1-2)GalNAc1-11 | 1       | 1         | 1         |
| Profile2        | 005686    | Fuc(1-2)GalNAc1-11 | 2       | 2         | 2         |
| Profile3        | 000044    | Fuc(1-2)GalNAc1-11 | 3       | 3         | 3         |
| Profile4        | 012440    | Fuc(1-2)GalNAc1-11 | 4       | 4         | 4         |
| Profile5        | 005720    | Fuc(1-2)GalNAc1-11 | 5       | 5         | 5         |
| Profile6        | 000042    | Fuc(1-2)GalNAc1-11 | 6       | 6         | 6         |

**Glycan Information**

Name: [Empty]  
Sequence: Fuc(1-2)GalNAc(1-3)Gal(1-4)GlcNAc(1-7)Gal(1-4)Glc  
Composition: C48H78O48N11O13S1 (GlcNAc)1 (Gal)1 (Fuc)1 (Glc)  
Glycan Mass: 1039.0  
Precursor Ion m/z: 1057.39  
Class: OHexose, Sphingolipid  
Reaction: R06187.R06198  
Pathway: map00602.Bloodserumglycolipidbiosynthesis-neolactoseries  
Enzyme: 2.4.1.40  
Other DB links: CCSID: 1179, 1180, 1181, 1182, 1183, 1185, 8572, 11333.



# SimGlycanDatabaseBot



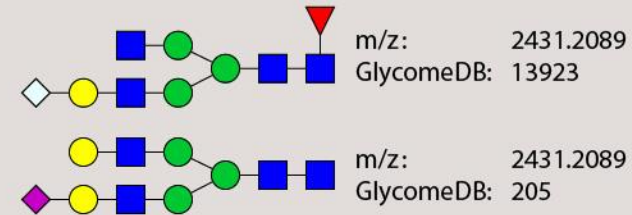
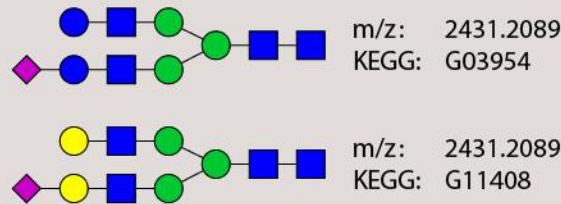
# Benefits of customized databases

m/z

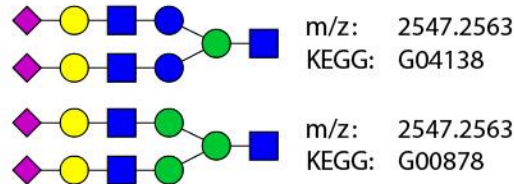
SimGlycan™ database

Customized database

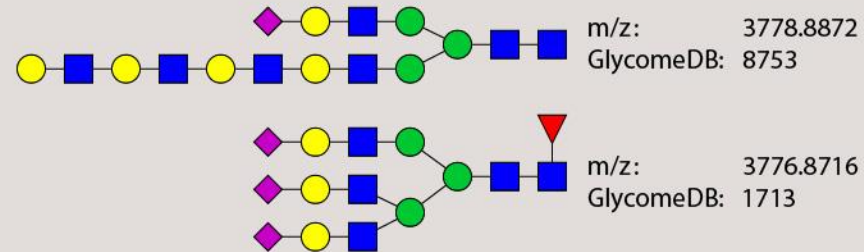
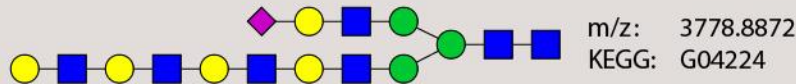
2431.22



2547.30

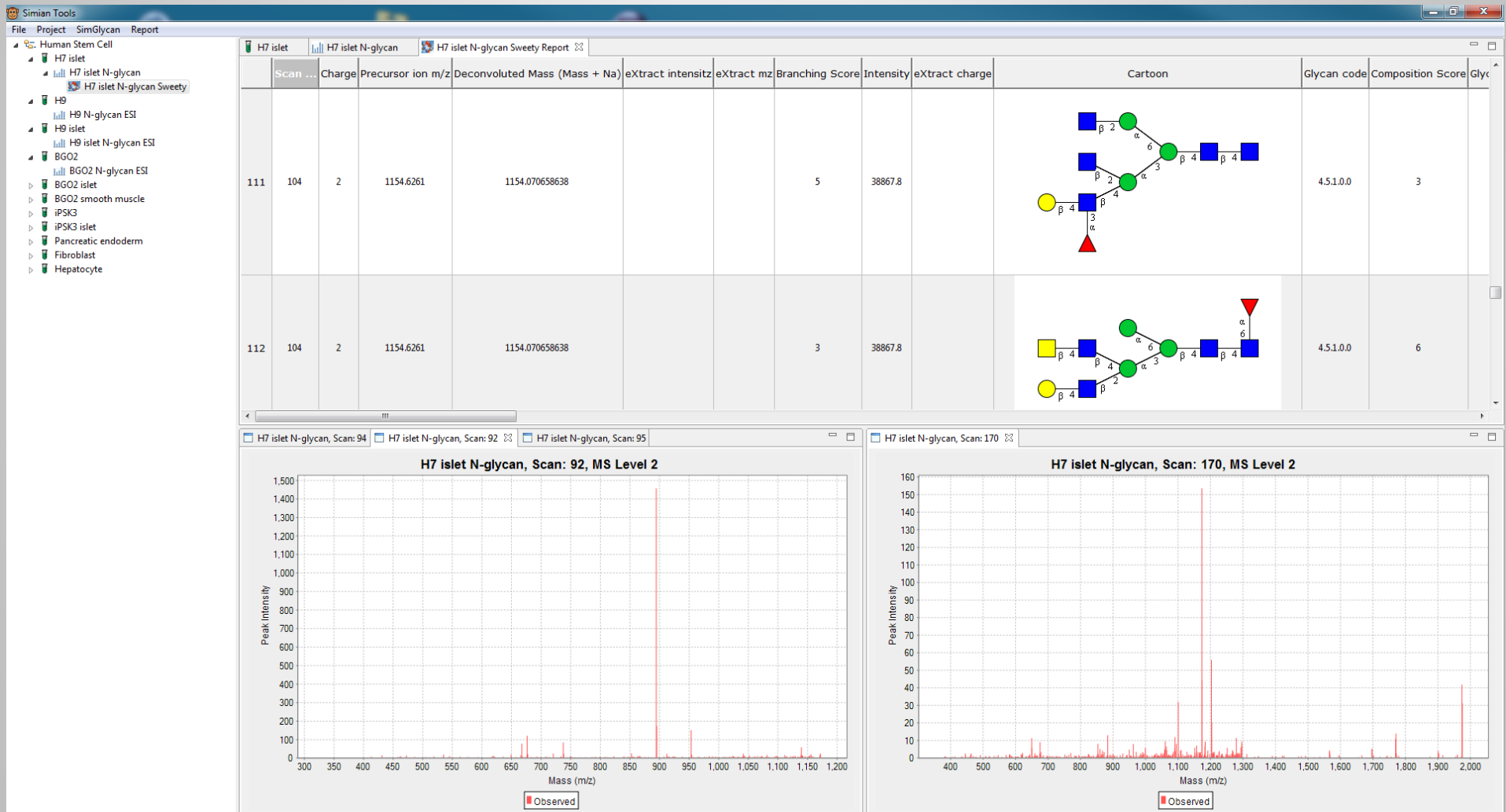
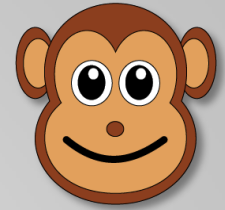


3777.95





# SimianTools Demo





**Will York**

**Michael Tiemeyer**



Project management  
Software design  
Software development



**René Ranzinger**



Software design  
Testing  
Sales

**Mindy Porterfield**



# SimianTools

**Brent Weatherly**

Software development  
GUI development



**Ki Tae Myoung**

Software development  
GUI development

