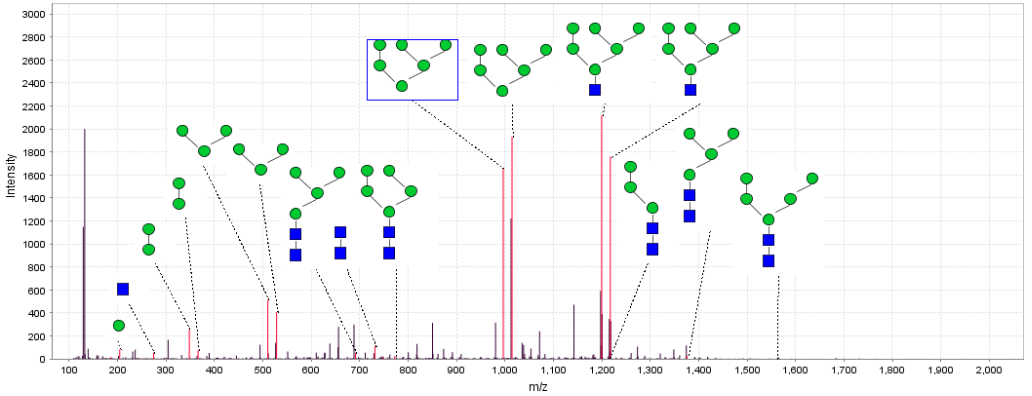
SimGlycan®

A high throughput software solution for Qualitative and Quantitative MALDI-, LC-, ESI-MS/MS Glycomic Analysis of Biological Samples

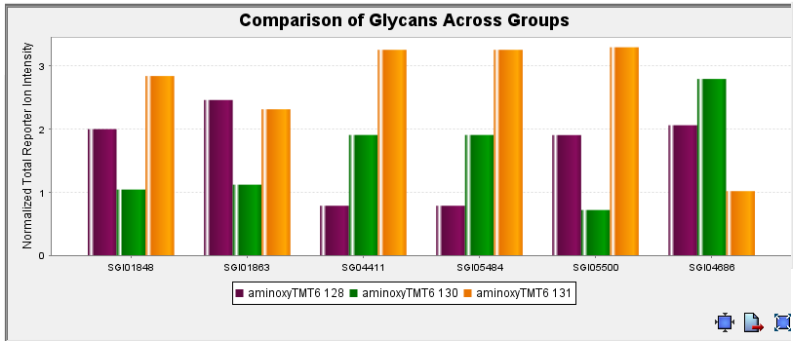
Key features:

1. Read raw data from
    1. Standard formats- mzXML, mzData, mzML
    2. Vendors' native file formats –
        i. .raw (Thermo Fisher)
        ii. .wiff, and .t2d (SCIEX)
        iii. .CEF (Agilent)
        iv. .baf, .yep, and .fid (Bruker), and
        v. .raw (Waters)
2. Fast LC-MS data pre-processing – peak detection, molecular feature finding, and precursor m/z corrections
3. Glycan structural elucidation using exact mass, retention times, and MS/MS data in batch mode
4. Reporter ion quantitation
5. Create LC-MS templates – create custom databases; store glycan structures along with retention times, column names, etc.
6. Automated annotation of MS/MS spectra
7. Portable reports: export results into MS excel files

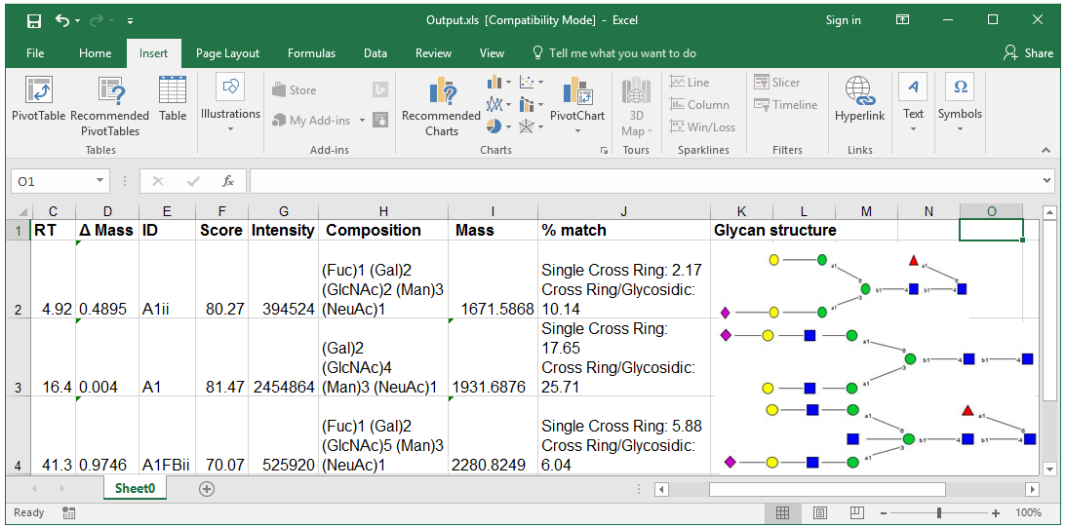
MS/MS Spectrum: Peaks Annotated with Glycan Fragments



Reporter Ion Quantitation: Bar Char



Export Results into MS Excel Files



	RT	Δ Mass	ID	Score	Intensity	Composition	Mass	% match	Glycan structure
2	4.92	0.4895	A1ii	80.27	394524	(Fuc)1 (Gal)2 (GlcNAc)2 (Man)3 (NeuAc)1	1671.5868	Single Cross Ring: 2.17 Cross Ring/Glycosidic: 10.14	
3	16.4	0.004	A1	81.47	2454864	(Gal)2 (GlcNAc)4 (Man)3 (NeuAc)1	1931.6876	Single Cross Ring: 17.65 Cross Ring/Glycosidic: 25.71	
4	41.3	0.9746	A1FBii	70.07	525920	(Fuc)1 (Gal)2 (GlcNAc)5 (Man)3 (NeuAc)1	2280.8249	Single Cross Ring: 5.88 Cross Ring/Glycosidic: 6.04	