

GRITS Toolbox 1.0

A freely available software suite for the processing and interpretation of glycomics MS/MS data

René Ranzinger, D. Brent Weatherly, Shahnawaz Khan, Sena Arpinar, Khalifeh AlJadda, Mindy Porterfield, Michael Tiemeyer and William S. York

Complex Carbohydrate Research Center, University of Georgia, Athens, GA, USA

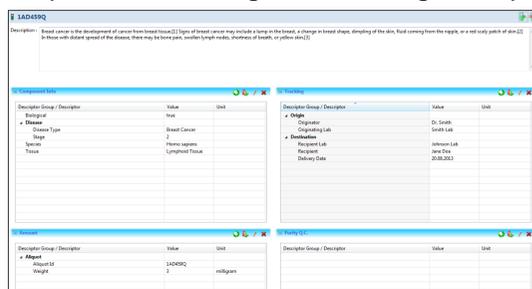
Ongoing technical advancements have made tandem mass spectrometry (MS/MS) the dominant experimental technique used to identify structures of purified glycans as well as complex mixtures of glycans extracted from biological samples. Currently, most interpretation of the generated high throughput MS/MS data are done manually, due to the lack of software support. The freely available tools and commercial systems that have been developed over the last decades are not suited for analysis of large datasets that include hundreds or thousands of MS/MS spectra. **GRITS toolbox is a freely available software suite for the processing and interpretation of these datasets.**

<http://www.grits-toolbox.org>



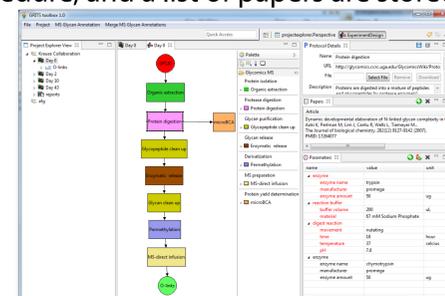
Sample Information

To allow a comprehensive overview of the processed data when exchanging GRITS projects with colleagues, the software can **store meta-data describing the analyzed sample** in the form of free text or using common vocabularies that are defined in broadly used namespaces or ontologies. Providing this optional data and using the vocabulary controlled terms simplifies data exchange and data submission to data repositories.



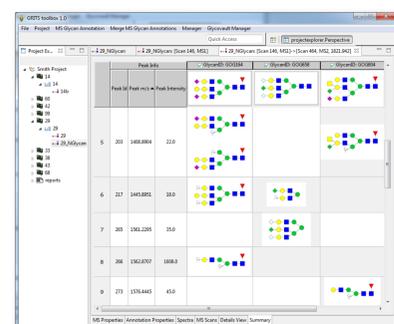
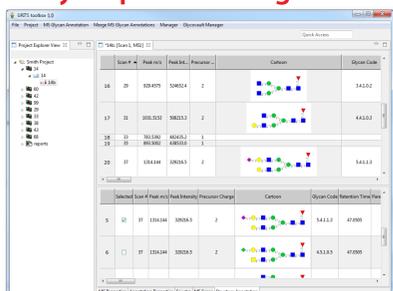
Experiment description

In addition to the description of the sample, GRITS can also **store the experimental workflow** used to process the sample material and to generate the experimental data. For each processing step a general description, a webpage or file describing the exact procedure, and a list of papers are stored to improve reproducibility and understandability of the experiment as well as facilitate data sharing. Sample information and experiment description can also be **exported to Word or PDF.**



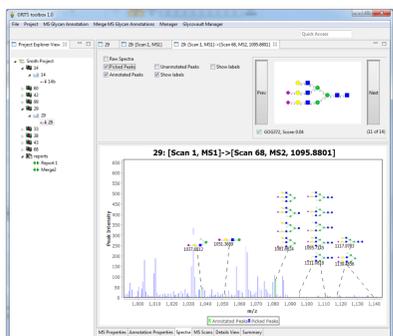
MS Annotation

After automatic annotation of the MS/MS data the annotation results can be **manually inspected using diverse display options.** The annotation overview shows all MS² precursor annotations of each sub spectrum in the top frame of the application and the different candidate structures for each peak in the bottom frame.



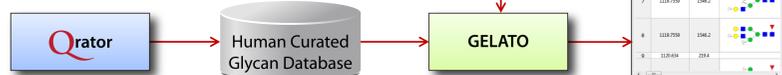
Double clicking the MS² precursor annotations, opens the fragment summary view to show all **candidate structures side by side** with the MS² fragment ions supporting each structure. The same procedure can be used to study MSⁿ annotations.

The annotation **spectrum viewer** shows the MS spectrum and highlights peaks that are annotated or are not annotated. In addition the viewer shows both the annotation of **MS¹ spectra with intact structures** and annotation of **MSⁿ spectra with fragment ions.**



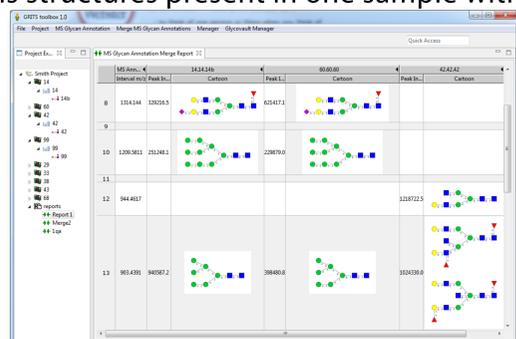
GELATO

The Glycomics Elucidation and Annotation Tool (GELATO) is the **integrated MS/MS annotation module** within GRITS, which associates spectral features in the MS/MS data sets with structures supplied by customizable databases. The default databases used by GRITS consist of sets of **human curated mammalian glycan structures**, which have been approved by experts using our curation tool - Qrator. (<http://glycomics.ccrcc.uga.edu/qrator/>)



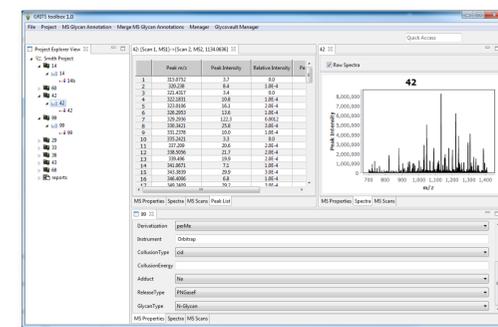
Comparative Glycomics

The MS annotation merge plugin provides a visual **side-by-side comparison** of the user curated **MS annotations of multiple samples** or MS runs. The plugin can be used to compare the glycans structures present in one sample with the glycans in other samples. Intensity values are provided alongside the structures, making it easy to find changes in the glycan expression level for different samples.



Mass Spectrometry Data

MS data can be loaded into GRITS toolbox in **mzXML format.** Thermo RAW file format is supported for files up to 10 MB as well. Uploaded files are copied and archived within the GRITS project to facilitate data storage and sharing of projects among collaboration partners. MS data can be displayed as **peak lists** or in a **spectral viewer.** Meta data about instrumentation and settings can be stored as well.



Extendable Software Platform

GRITS toolbox is a platform-independent software based on the Eclipse software framework (<https://www.eclipse.org>) and the Java programming language. Although the current version of GRITS is primarily focused on the processing, interpretation and storage of glycomics MS data, its **modular architecture based on plugins** facilitates **easy extension of the software** and thereby reduce development time while reusing existing program components.

