

Supplementary Information for GlycoGenius: a streamlined high-throughput glycan composition identification tool

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Supplementary Figure 1. The data visualizations modules in GlycoGenius, File Editor and GlycoGenius Draw. a, Two-dimensional heat map, where the x-axis represents RT/MT and the y-axis the m/z values. Peak intensity is displayed in a color scale of the heatmap cell, from dark red (most intense) to white (less intense), in logarithmic scale. Blue markings indicate peaks chosen for fragmentation in MS1 spectra. b, Maximum Intensity Spectrum (MIS), which is a composite spectrum constructed from the maximum MS1 intensity of m/z values in the LC-/CE-MS. A quick analysis can be performed on this spectrum to quickly assess the presence of glycan compositions, depicted on the left side panel. c, GlycoGenius File Editor, depicting the calibration module. A list of calibrants is composed by the user based on the top options (m/z, standard or from glycans library) and searched within the sample. After adjusting the hits, the file is calibrated, generating a report. d, The Glycan Browser window allows the user to filter out choices and select the glycan cartoon that best matches the putative glycan or remove it altogether.

