GSL-finder applications are described in:

Marko Rožman, Dragana Fabris, Tomislav Mrla, Željka Vukelić; Database and data analysis application for structural characterization of gangliosides and sulfated glycosphingolipids by negative ion mass spectrometry,

Installing and running:

Before you start ensure that you are using dot (.) as decimal mark. Windows -> Control Panel -> Region and Language -> Additional settings

GSL-finder MS

GSL-finder MS is created as standalone Windows based application for comparing MS data from imported reference list with database according to selected search criteria.

Installation:

1. The program utilizes a SQL CE for data storage and retrieval. So before starting GLS-finder-MS make sure that your computer has installed Microsoft SQL CE database driver and .NET Framework 4. Links for downloading SQL CE driver and .NET Framework are provided. Follow install instructions on provided links.

2. GSL-finder-MS can be run directly from its location. Copy entire GSL-finder-MS folder to desired location on your hard drive (e.g. D:\gangliosides\GLS\)

3. Start the application by clicking on GLS-finder-MS.exe. It takes half a minute for application to initialize, depending on system.

4. Start using GLS-finder-MS by importing test-list.csv or any of your search lists. The requirement for the candidate MS ion search list is that each ion (only *m/z* values) should be written in a separate line and stored as comma delimited (csv) file. Comma delimited files can be easily created in Excel.

5. Search results can be exported in csv format so that results can be stored in a readable form.

GSL-finder MSMS

GSL-finder MSMS is application written in Mathematica for correlating obtained tandem MS data with GSL database according to search criteria. The application requires Mathematica 8.0 or higher.

Creating MSMS ion search list:

At the moment program does not take into account ion intensities, accordingly the search list should contain only *m/z* values. MSMS ion search list should contain a precursor ion mass followed by the masses of its product ions in the same line. Next precursor ion together with the masses of its product ions should follow in a new line; e.g.;

1863.92   290.084   586.995   655.211   1053.752

2067.06   290.1   325.19 678.64 731.45 748.79

MSMS ion search list should be in txt format (example file test-GD1a.txt is provided), again easily created in Excel.

Running GSL-finder MSMS:

1. Open Mathematica notebook file GSL-finder MSMS.nb in Mathematica 8.0 or higher.

2. Click on Database Initialization, upon initialization click OK.

3. Use slider to set MS and MSMS tolerance. Click OK even if preset values suit you.

4. Click Import List

5. Some or all structural modifications e.g: fucosylation (Fuc), *O*-acetylation, de-*N*-acetylation etc. can be excluded from search. After defining inclusions/exclusions, press OK. Click OK even if you agree with preset option. More options included will result in higher search time.

6. Press search button.

7. Results can be displayed or saved by clicking appropriate buttons.