

How To : Tips for GC-MS data annotation

Aim: How to “cheat” with GC-MS annotation tool

- ➔ First run GC-MS preprocessing tools until you’ve got peakspectra.msp file (or any *.msp spectra file)
- ➔ Then open Golm Metabolome Database search spectrum tool

The screenshot shows the Galaxy web interface for the 'Golm Metabolome Database search spectrum' tool. The left sidebar lists various tools under 'GC-MS', with 'Preprocessing' selected. The main panel shows the tool's configuration form. The 'File of masses (format: msp)' field is filled with '257: peakspectra.msp'. Under the 'Column' section, 'VAR5' is selected. Two input fields, 'Alkane Retention Index' and 'Retention Index Window', both contain the value '2500' and are highlighted with red rectangular boxes. The interface also shows a search bar and a list of tools on the left.

Fig1 : Screen shot of W4M Golm Metabolome Database search spectrum tool with first parameters. In red we’ve set Alkane Retention Index to 1500 and the “trick” is to use a very large Retention Index Window to be able to launch database search on all spectra available in the *.msp file rather than one by one.

- ➔ Just press Execute and wait for Golm results

Note: You can use that procedure even if you don’t have Retention Index in *.msp file, in that case Retention Time will be used

Important: You can also use *.msp file with your usual NIST MSSearch software see http://application.sb-roscoff.fr/download/w4m/howto/w4m_HowToUseNIST_V01.pdf