Workflow4metabolomics

How To : Tips for GC-MS data annotation

Aim: How t o “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

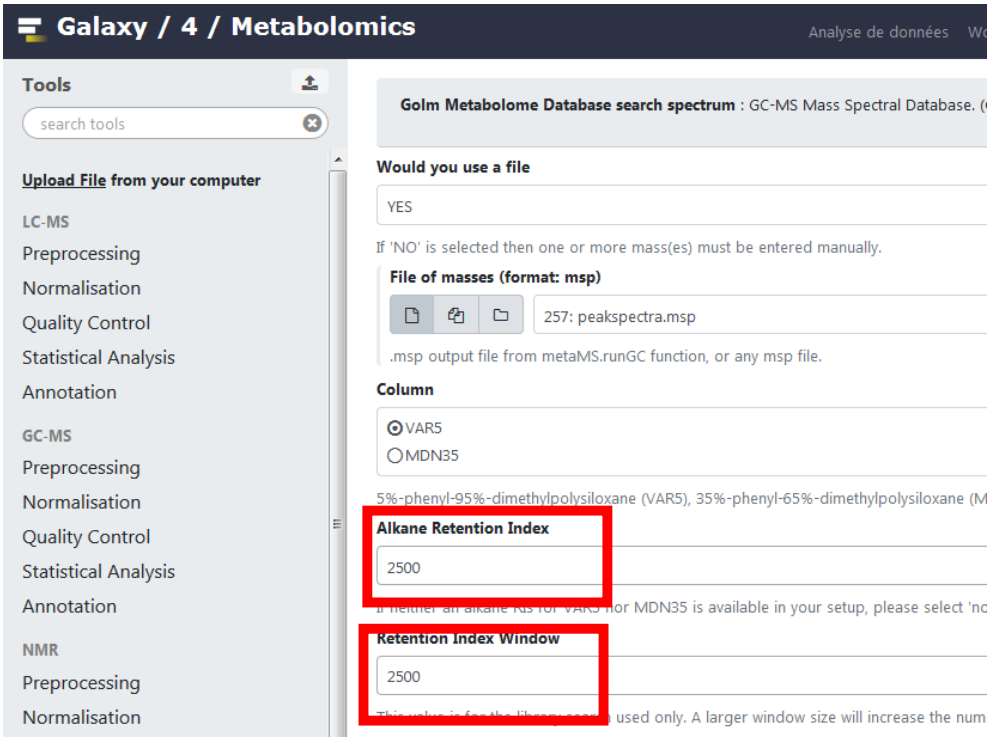

*Fig1 : Screen shot of W4M Golm Metabolome Database search spectrum tool with first parameters. In **red** we’ve set Alkane Retention Index to 1500 and the “trick” is to use a very large Retention Index Window to be able to launch database search on all spectra available in the *.msp file rather than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