

GCMS Data Wrangler Software is able to rapidly parse large numbers of Gas Chromatography-Mass Spectrometry (GC-MS) data sets, and outputs the parsed data into an interface that allows scientists to make rapid and accurate decisions about their samples. Using advanced multivariate analysis tools, GCMS Data Wrangler parses GC-MS data into pure mass spectra, without the need for users to tinker with complicated fit parameters – including peak width estimates and background subtraction – that are a difficult and tedious part of GC-MS data analysis with other tools. The program displays parsed data in a series of auto-generated and auto-formatted tables that allows users to search, filter, and save results – saving countless hours versus assembling those graphs by cutting-and-pasting. The user-friendly interface also gives analysts access to powerful machine learning tools that can automatically cluster data sets with similar chemical fingerprints, allowing users to instantly attach meaning to complicated chemical reports. GCMS Data Wrangler identifies the chemical species in parsed data sets through automated processing with the NIST mass spectral database, saving time and money versus manually entering in mass spectra. GCMS Data Wrangler is compiled as a fully deployable executable from its native Matlab language, meaning no installation of Matlab (and no Matlab licensing fee) is necessary to run the program.

TECHNICAL BENEFITS

- Rapid and automated parsing of large numbers of GC-MS data sets
- Data set deconvolution without users fine tuning fit parameters
- Useful tables and graphs automatically generated and formatted
- Machine learning tools allow rapid decisions about samples

INDUSTRIES & APPLICATIONS

- Pollution Monitoring and Source Attribution
- Fire and Explosives Investigation
- National Security
- Medical/Pharmaceutical
- Drug/Law Enforcement