

GC and GC/MS Calculations using Spreadsheet Macro Programming

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An Excel macro system was developed by our lab for greater flexibility, control and consistency in doing GC and GC-MS calculations. Excel was chosen for its spreadsheet features, programmability and familiarity. The process for GC-MS calculations will be covered but it is largely the same for GC. Macros are computer programs which can be grouped for a specific application. The macro code for this application has survived different versions of Excel, instrument & operating system software and it has been validated by successful use in proficiency testing.

The code is a mixture of old Excel programming language and the newer Visual Basic. It runs across a network and operates as an accessory or add-in to Excel. Instrument software is used to integrate chromatograms and generate text-based peak response files. The macros are used interactively following integration of all chromatograms for a sequence of runs. Calibration table building, analyte peak selection and sample quantitation are done by using the macros and an Excel template file. Once the calibration table is completed, Sample & Spike quantitation are done with a few mouse clicks and brief data entry. The user activates and interacts with macros through a custom menu and dialog boxes. The code is easily loaded into Excel like any other file. Once loaded, the code cannot be seen viewed or edited by the user. An Excel template file is used to receive calibration and sample data and to hold formulas for quantitation. A custom dialog box is used for tracking important information such as retention time window, file locations and instrument ID. The macro system is set up for target analyte analysis using external or internal calibration. The macro code can easily be adapted to different instrument software and has been used with the following systems: HP 5970, 5971 & 5973 GC-MS with UNIX, DOS & Windows; Finnigan GCQ Ion Trap GC-MS; HP 5890 GC-ECD/FID; Varian 3400 GC-FID with Star Workstation.

The process for using the macros begins by loading the macro file into Excel and the user setting parameters for calculations. A peak response file for a calibration standard is loaded and the peak data is parsed. Analyte peaks are selected, labeled and calibration info is provided by the user. The calibration info is transferred by the macros to the calculation template file. A peak response file for a bracketing calibration standard is loaded and its analyte peak data is added to the template file. A peak response file for a sample is loaded and the sample is quantitated using sample info provided by the user. The last step is repeated for all samples governed by current calibration table.