An Integrated Concept of Automated Instrument Control, Quality Assurance and Data Reporting for Dioxin/Furan Analysis

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The identification and quantitation of chlorinated/brominated dibenzodioxins/dibenzofurans in a wide range of matrices continue to present imposeing challenges to the analyst. A growing number of samples have to be evaluated for ever lower concentrations of these compounds. HRGC/HRMS is a proven and well accepted technique which offers the required selectivity and sensitivity. But the lack of automation was the bottleneck for high sample throughput and made quality assurance and quality control very time consuming.

The present paper describes the application of a newly designed instrument control language for automation of a HRGC/HRMS system tailored for dioxin/furan analysis (Fig. 1). Mouse bottom selectable routines guide the user through the MS-setup. They start complete autotune for high resolution at full and decreased acceleration voltage as well as algorithms for magnetic and electric calibration. Automatic multiplier gain selection for optimal detection limits is documented in a quality control chart as well as instrument resolution and other important performance parameters.

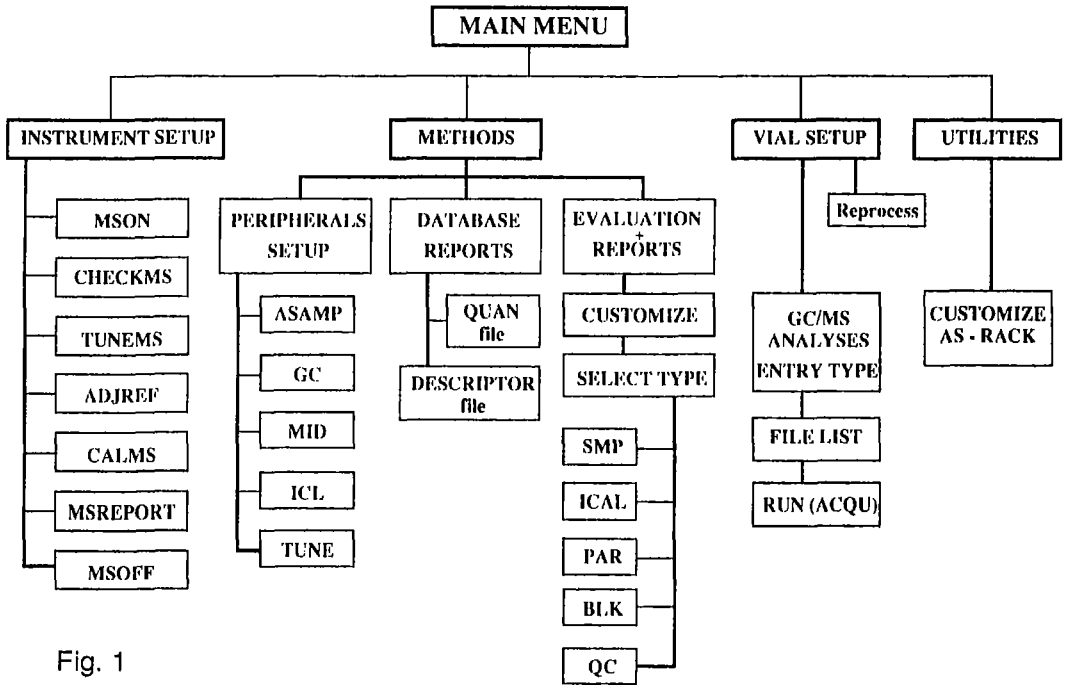

Fig. 1

A novel target compound analysis program is used to customize methodes which adjust labority standard working procedures to the system. This fully integrates peripherals like the GC and the Autosampler and gives access to the MS-setup calling predefined MID-descriptors and instrument control procedures. This also ensures proper and flexible data evaluation and reporting for different sample types like precision and recovery standards, blanks, samples, etc. Various quality control parameters like isotope ratios, retention time tolerances and the recovery of standards are included. Precision and recovery charts are permanently updated.

A vial setup menue allows to load the autosampler rack for unattended overnight operation and specifies the sample type for each individual vial entry. The specified method for data evaluation and reporting guarantees complete quality control documentation. Feedback from the data evaluation program ensures that samples are not wasted if specified quality criteria don't fit.