Conversational Mass Spectral Search System and Its Application

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Abstract

This paper describes a conversational mass spectral search system which is suitable for microcomputer or minicomputer and runs on PDP-11/34A computer. It permits user to set up a special mass spectral library for various organic compounds. The software consists of a library generation program and a library search program. These programs were written by PDP-11 FORTRAN IV-PLUS language, and is easy to transfer to other computers. The library generation program is used to produce a data file for simplified mass spectra and a index file for searching. In order to keep integrity of a library, the program was designed to have some additional functions, such as inserting, modifying, deleting, examining etc. The library search program used immediate and dual searching techniques and had seven pattens for searching. The search system was applied to identify some special toxic and volatile compounds in food, the results were satisfactory.



QP-1000质谱计用户协作组成立

中国科学院科学仪器厂和日本岛津公司于1986年10月24日在北京举办了QP-1000A GC/MS技术讲座,50余位来自全国的质谱界人士参加。科仪厂介绍了四极质谱的基本原理、组装岛津QP-1000A GC/MS的特征,并用实际仪器示范了各种操作程序。岛津公司北京分析中心的村田武博士报告了高质量数高沸点样品在QP-1000A上作GC/MS分析。

国内12家已有QP-1000的用户在会上成立了用户协作组,推选北京市劳动保护研究所赵子璋同志为负责人,并立即和岛津公司进行了有关仪器维修方式的座谈,一致同意每年召开一次用户协作会议,以促进该仪器的使用效率。

(野 渡)