MASS SPECTRA AND NMR SPECTRA OF GANGLIOSIDES CONTAINING FUCOSE

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SUMMARY

Two gangliosides containing fucose, prepared from minipig posterior root ganglion, were analyzed as methylated, methylated-reduced and methylated-reduced-trimethylsilylated derivatives by mass spectrometry and NMR spectroscopy and shown to have the following structures:

\[ \text{Fuc}\alpha_1\text{Hex}\beta_1\text{HexNAc}(\text{NeuAc})\beta_1\text{Hex}\beta_1\text{Hex}-1\text{Ceramide} \]

\[ \text{Fuc-Hex-HexNAc(NeuGc)-Hex-Ceramide} \]

INTRODUCTION

The present status of structural fingerprinting of glycoconjugates by mass spectrometry has recently been reviewed (KARLSSON, 1977) and is also the subject of a paper by Karlsson in this monograph.

Mass spectra of pure methylated derivatives of gangliosides containing fucose were first presented in 1977 (KARLSSON et al., 1977; OHASHI and YAMAKAWA, 1977). Recently, mass spectrometry of the methylated-reduced-trimethylsilylated derivative was used in the structural characterization of an earlier unknown fucoganglioside containing 10 sugars in a branched carbohydrate chain (WATANABE et al., 1978). The present report will show the use of mass spectrometry in the structural characterization of two fucogangliosides prepared from minipig posterior root ganglion.
An improved micromethod of NMR spectroscopy of glycolipids using the same type of derivatives has recently been reported (FALK et al., 1979). With this method it has been possible to assign all anomeric protons in glycolipids with up to 8 sugars. This improved method is now applied for the first time on gangliosides.

MASS SPECTRA

Mass spectra of the methylated-reduced-trimethylsilylated derivatives of the two gangliosides are shown in Figs. 1 and 2.

Fig. 1. Mass spectrum of the methylated-reduced-trimethylsilylated fucoganglioside containing N-acetyleneuraminic acid. The simplified formula corresponds to the major molecular species found. NANA = N-acetyleneuraminic acid. The conditions of analysis were: electron energy 75 eV, trap current 500 microA, acceleration voltage 4 kV, ion source temperature 300°C, probe temperature 280°C.