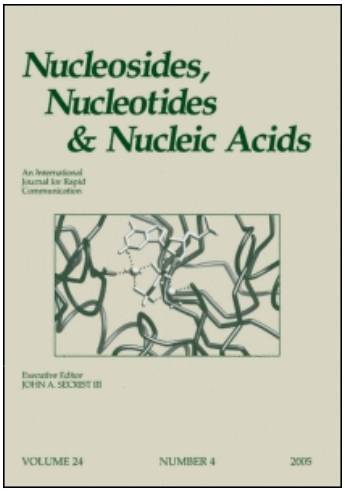

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Computerized Interpretation of the Electron Ionization Mass Spectra of Nucleoside TMS Derivatives

Thomas D. McClure[a]; Karl H. Schram[a]
[a] College of Pharmacy, University of Arizona, Tucson, Arizona

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COMPUTERIZED INTERPRETATION OF THE ELECTRON IONIZATION MASS SPECTRA OF NUCLEOSIDE TMS DERIVATIVES

Thomas D. McClure and Karl H. Schram*
College of Pharmacy, University of Arizona,
Tucson, Arizona 85721

ABSTRACT

A computer program has been developed for the automated interpretation of mass spectra of TMS derivatives of nucleosides found in human urine. The m/z values in the unknown spectrum are compared to m/z values of 3 different ion series commonly observed in the mass spectra of nucleoside TMS derivatives.[1] If a correlation exists, the unknown spectra are marked with color according to the scheme: 1) blue - molecular ion series, 2) red - base ion series and 3) yellow - sugar ion series. The program suggests a structural assignment for each of the marked ions and calculates a series related ion current. The calculated ion current is used to assign the of sugar contained in the unknown nucleoside.

INTRODUCTION

Urinary nucleosides have been studied as possible indicators for the presence of cancer.[2] The rationale for such work is the high catabolism of t-RNA in cancer cells compared with normal cells. In addition to quantitative changes in known urinary nucleoside levels, novel modified nucleosides have been identified in human urine. In some instances correlations with cancer are suggested.[3]

A computer program has been developed to scan through large numbers of mass spectra from the TMS derivatives of urinary extracts and suggest modifications in the sugar portion of possible nucleosides.

MATERIALS AND METHODS

Sample preparation, derivatization and instrumental conditions for the analysis of urinary nucleosides have been described elsewhere.[4] The data was acquired using a Micro VIP computer (DEC PDP 11/73 clone, US Designs, Palo Alto, CA). Following acquisition, the data was transferred to a PS/2 model 50 computer (IBM, New York, NY) with 1 MByte of memory and an optical disk drive with 200 Mbytes of storage. Transfer was accomplished using Kermit error free protocol software (Cornell University, Ithica, NY) on the Micro VIP and Smart Term software (Persoft, Madison, WI) with a kermit

emulator on the PS/2. The analysis software was written using Microsoft C version 5.0 (Microsoft Corp, Redmond, WA).

DISCUSSION

The program calculates the molecular ion, base ion and sugar ion series after the molecular weight of the nucleoside (represented by the mass spectrum) has been determined. The mass spectrum is then compared with the calculated series of ions, appropriate structural assignments are made and the ion series marked with colors (red - base ion series, yellow - sugar ion series and blue - molecular ion series). Any nominal mass overlap between series are flagged with combinations of colors [i.e. orange = red (base) + yellow (sugar)]. Following assignment and marking, a reconstructed ion current for each sugar modified class of nucleoside is determined. Two recently discovered novel urinary nucleosides, 5'-deoxyxanthosine and 5'-deoxy-5'-methylthioguanosine, have been successfully analyzed by the program correctly identifying modifications in the sugar portion of the molecule. In each case the calculated RIC for the correct choice was 2 to 3 times greater than for the other possibilities.

CONCLUSION

Software has been developed which will aid in interpretation of GC/MS data from the analysis of complex mixtures of TMS derivatives of nucleosides.

The software has been written in modular form such that other sugar modified nucleoside classes can be added very easily.

Work is proceeding on the next generation of this software which will include similar algorithms to identify the classes of base modification.

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