MSHelp: A PROGRAM FOR PROTEIN MASS SPECTROMETRY

Rolando Rodríguez.

Division of Physical Chemistry. Center for Genetic Engineering and Biotechnology, P.O. Box 6162, La Habana 6, Cuba.

SUMMARY

A new program for mass spectrometry analysis of proteins was written to upgrade the existing system, the new system is running on Microsoft Windows v3.1 and includes new graphic options.

RESULTS AND DISCUSSION

We have described before a computer program to the help on the characterization of proteins by mass spectrometry, such programs were running in MS-DOS, and covers the analysis of the sequences and of the mass spectrometric signals.

From this year we were working to have all the analysis programs in a common platform and we have chosen Microsoft Windows.

MSHelp is the first program of this series and contains all the options included in the previous programs, such as the calculation of the molecular mass and the atomic composition, the identification of posttranslational modification sites, the amino acid composition, cleavage with exo and endoproteinases and side chain modifications. This version also includes the calculation of the fragmentation series on Collisionally Activated Dissociation (CAD) experiments, observed in the B/E linked scan mode.

In the program, a protein sequence is defined as an object, containing the procedures for loading and basic calculations, as the protein is loaded we calculate the mass arrays and setup the cleavage sites if any enzyme is loaded, the user can configure the program to work with the entire sequence or with a defined fragment. For the calculation of the molecular mass we always use the monoisotopic and the average mass values arrays in parallel.

Up to now the program can load sequences in the SwissProt database and in free style text format.

The user can interact with the program using a main menu and dialog boxes for each of the options. The user interface has been redesigned to improve the data entry and validation procedure.

- *Molecular mass and atomic composition.*
- *Amino acid composition.*
- *Postranslational modification sites.*
- *Exopeptidase treatment and stepwise Edman degradation.*
- *Endoproteinase cleavage.*
- *Chemical treatments.*
- *Peptide search.*
- *Side chain modification.*
- *Peptide CAD fragmentation.*
- *Miscellaneous and configuration options.*

We are working now in other programs to conform a full package, including the calculation of the ion isotopic distribution, matching for unknown peaks, and fragmentation analysis. The program was written using Borland Pascal version 7 on Microsoft Windows 3.1.

REFERENCES

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