Poster G-8

Prediction system for chemical structures of glycolipids using MALDI-TOF MS and MS/MS data.

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Short Abstract: A preliminary study of the prediction system of chemical structures of glycolipids using MALDI-TOF MS and MS/MS data is reported. The high accuracy of our system was confirmed with some known chemical structures of the glycolipid which had a normal chain type or two divergence type.

Long Abstract:

- Introduction -

One of the important targets of glycomics is to find out the role of glycolipids common to the all multicellular organisms in the post genome era. That is, it is to discover the relationship between diversity of cell surface glycolipids and the construction of cellular society. However, we know that the chemical structures were various and variable from the history of carbohydrate research and the alteration of gene expression of glycosyltransferase and lipid synthetase affects not only the glycolipids directly biosynthesized, but also broadly the expression patterns of the glycolipid system.

Proteomics is a rapidly expanding research field in order to be able to use genome information as proteins are primary products from genes. On the other hand, glycomics and lipidomics is the research field that is hard to spread than proteomics because sugars and lipids are the secondary products from genes. Proteomics field enabled exhaustive analysis of genome-wide level by recent advances in, and novel applications of, matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF MS) and electrospray ionization mass spectrometry (ESI/MS). In glycomics field, the novel approaches, MALDI-TOF MS and ESI/MS, are used a lot of individual chemical structure analysis, but do not yet reach establishment of exhaustive analysis. In particular, in the glycolipid study, it is reality that obtained data from MALDI TOF MS or ESI/MS are still analyzed with eyes of a researcher. As the reason, the chemical structure analysis of glycolipids, which have a normal chain type and many divergence type chains, is more difficult than sequence analysis of proteins which have only normal chain type. Therefore, we aim at development of the system which predicts chemical structure of glycolipid from the MALDI-TOF MS and MS/MS data automatically.

- Materials and Methods -

there is many kind of matrices used for the MALDI-TOF MS analysis. Choice of a matrix is affected very much to the results of analysis and, in particular, is extremely important in our system aiming to automation. Therefore, two matrices, Coumarin 120 (7-amino-4-methyl-cumarin; Sigma) and DHBA (2,5-Dihydroxybenzoic acid; Wako), used by the measurement of conventional glycolipids are examined. The glycolipids of measurement object are three neutral glycolipids of the arhro- series (ceramide tri-, penta- and hexa-

saccharide) and a ceramide lactoside. MALDI-TOF MS and MS/MS analysis is performed using an Applied Biosystems/Voyager-DE STR TM Biospectrometry, operating in the positive-ion reflector mode and the positive-ion PSD mode. External mass calibration of MALDI TOF MS and MS/MS is provided by the [M+H]+ of angiotensin I (1296.68 Mass units; Sigma) and bradykinin, fragment 1-5 (Arg-Pro-Pro-Gly-Phe; 573.31 Mass units; Sigma), respectively.
In this poster, a preliminary study of the prediction system of chemical structures of glycolipids using MALDI-TOF MS and MS/MS data is reported. Our system consists of three programs as follows: (1) The noises are removed and important molecular weight peak and fragment peaks for prediction are extracted from MALDI-TOF MS and MS/MS data, respectively. (2) Combination of sugar and ceramide components are predicted using the molecular weight peak extracted from the MALDI-TOF MS data. (3) Chemical structure of the glycolipid is predicted using the fragment peaks extracted from the MALDI-TOF MS/MS data. Here, the environment on a computer is used by C language in Linux (Red Hat 7.3).

- Results -
The matrix of our system chose the Coumarin 120 by showing high peak resolution and the plasticity than DHBA. A preliminary study of our system intended for structure of the neutral glycolipid which was easy to comparatively ionize. Development status of three programs incorporated in our system is as follows: (1) The fragment automatic extraction program: The parameter of fragment extraction assumed it width and height of detection peaks. In addition, the optimization of a value of each parameter was performed with fragment data by known chemical structures of the glycolipid. (2) Prediction program of sugar and ceramide composition using molecular weight peak extracted from MALDI-TOF MS analysis data: A combination of sugar and ceramide composition was tested by artificial molecular weight, and an order charge account was performed by low order of the molecular weight error. (3) Prediction program of chemical structure of the glycolipid using fragment peak extracted from MALDI-TOF MS/MS analysis data: This program adopted the decision tree algorithm for each fragment peaks. The accuracy of our developed system was tested with some known chemical structures of the glycolipid which had a normal chain type or two divergence type. Our system showed high accuracy. In other words, all tested structures were included in predicted chemical structures by our developed system.

- Summary -
The presentation is a preliminary study on the prediction system of chemical structures of glycolipid using the decision tree algorithm. The basic idea is to utilize the molecular weight peak extracted from MALDI-TOF MS data and fragment peaks from extracted MALDI-TOF MS/MS data, automatically. In the future, this system will be expanded in an available system to acid glycolipids and mixture glycolipid samples.