Application Note

CD-0021

Program of [JWMVS-529 CD multivariate SSE analysis]

Introduction

The structure of protein or peptide is closely related with its function, and CD measurement method is widely used for structural analysis of those molecules in the field of protein or peptide applied to the drug medicine. CD spectra show the shape reflecting the abundance ratio of secondary structure of protein or peptide, and secondary structural analysis using CD spectra is to analyze the abundance ratio of the secondary structure of protein or peptide from CD spectra.

JWSSE-513 protein secondary structural analysis program is the program by using Classical Least Squares (CLS) method, including the reference spectra of Yang[1] and Reed[2]. Yang's reference spectra are extracted from CD spectra of protein, and best suited to protein secondary structural analysis. On the other hand, Reed's reference spectra are extracted from CD spectra of peptide, and suitable to the secondary structural analysis of peptide because of less effect by CD derived from side chain of aromatic amino acid often seen in protein. In case of secondary structural analysis of peptide, JWSSE-513 protein secondary structural analysis program with Reed's reference spectra is effective.

In addition, JASCO added JWMVS-529 CD multivariate SSE analysis program as a new lineup. This program includes CD spectra (176 - 260 nm) of 26 proteins, which were created by JASCO and also calibration model based on those spectra. In this program Partial Least Squares (PLS) method which is the latest multivariate analysis method and Principal Component Regression (PCR) method are adopted. In PLS and PCR method, the spectra are compressed to a few potential factors, and the concentration is indicated based on such potential factors. Then abundance ratio of secondary structure is calculated so that the residual error of the concentration may be the minimum. This enables the improvement of the analysis accuracy of β-sheet structure which has no specific strong CD peaks.

Some functions for validating the analysis result and verification function of created calibration model are also included.

Keywords: Secondary structural analysis, PLS/PCR method, Validation of analysis result

Features

- PLS and PCR methods which are much more precise multivariate analysis methods as compared with CLS method that has been used for traditional protein secondary structural analysis
- Possible to verify the calibration model by cross validation
- Possible to edit the ratio of secondary structure and also reference spectra
- Possible to validate the analysis result by F-test
- Verification of recalculation and result of calculation (GLP/GMP compliant)
- CFR Part11 compliant
- CD spectra (176 – 260 nm) of 26 proteins and calibration model based on those spectra

Results of the cross validation for 26 proteins are shown in Fig. 1.

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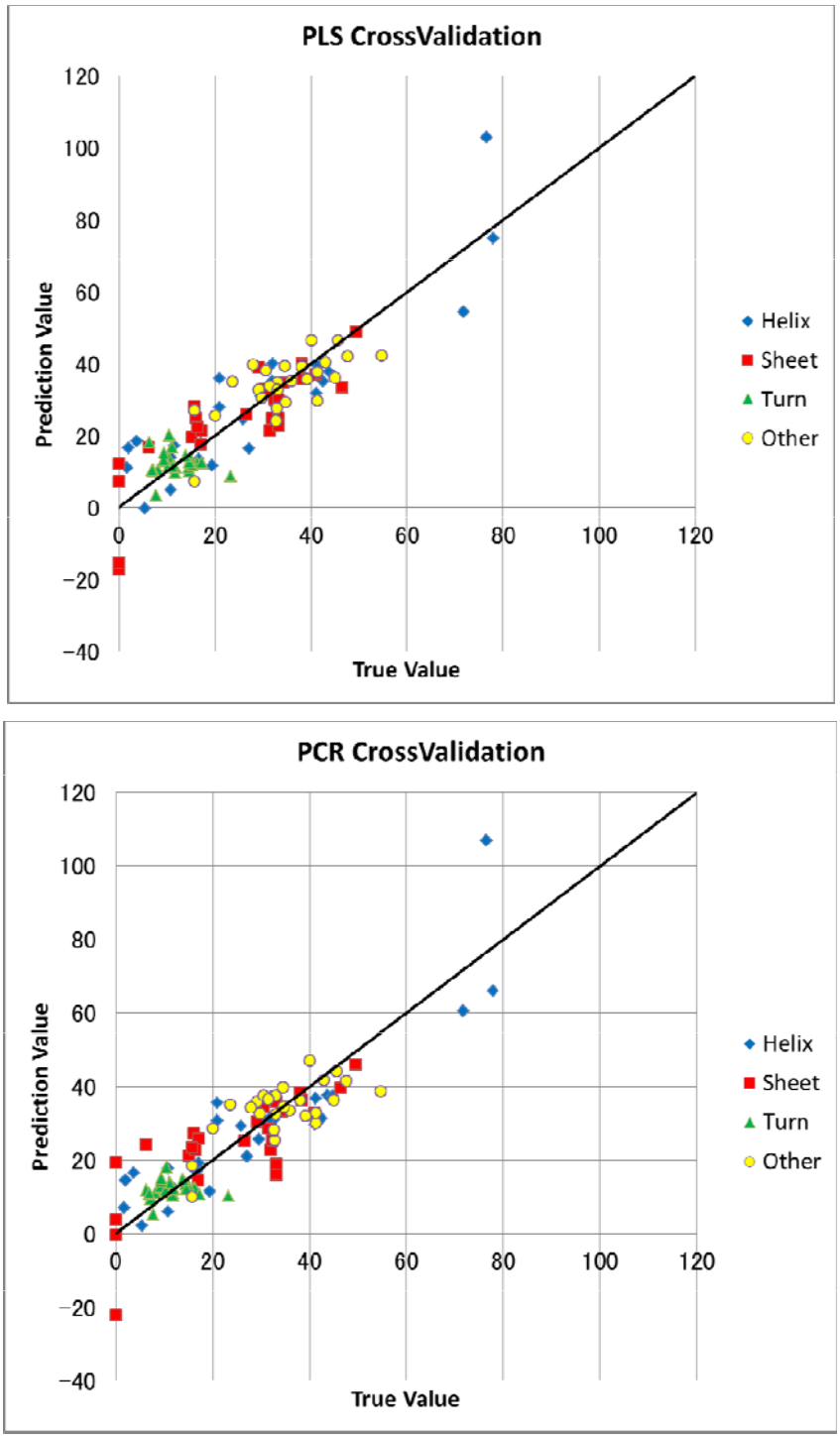

Fig. 1 Results of cross validation by PLS method and PCR method

<Reference>
(1) Jen Tsi Yang, Chuen-Shang C. Wu, and Hugo M. Martinez, *Methods in Enzymology*, **130**, 208-269, (1986)
(2) J. Reed, and T. A. Reed, *Anal. Biochem.* **254**, 36-40, (1997)

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