



High estimation accuracy for a wide range of proteins including  $\beta$ -structure-rich -proteins such as antibodies.



Providing eight types of secondary structure information



Compatible with GxP and satisfying CSV, ER/ES and DI for practicing ALCOA+ principle.

## Secondary structure

### Helix 1 – regular $\alpha$ -helix

The middle part of  $\alpha$ -helices

### Helix 2 – distorted $\alpha$ -helix

2-2 residues at the ends of  $\alpha$ -helices

### Anti 1 – left-twisted $\beta$ -strand

Left-hand twisted antiparallel  $\beta$ -sheet

### Anti 2 – relaxed $\beta$ -strand

Relaxed (slightly right-hand twisted) antiparallel  $\beta$ -sheet

### Anti 3 – right-twisted $\beta$ -strand

Right-hand twisted antiparallel  $\beta$ -sheet

### Parallel $\beta$ -strand

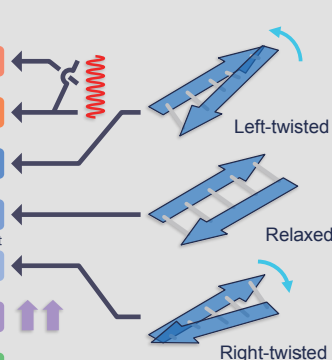
Parallel  $\beta$ -sheet

### Turn

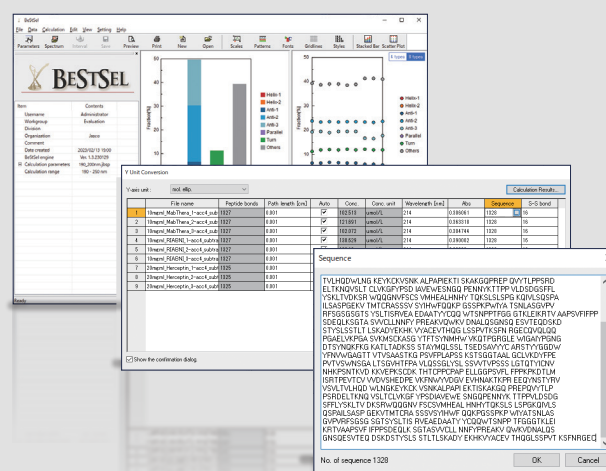
Turn, as defined by DSSP

### Others

3,10-helix,  $\pi$ -helix,  $\beta$ -bridge, bend, loop/irregular and invisible regions of the structure



Secondary structure information obtained by BeStSel algorithm



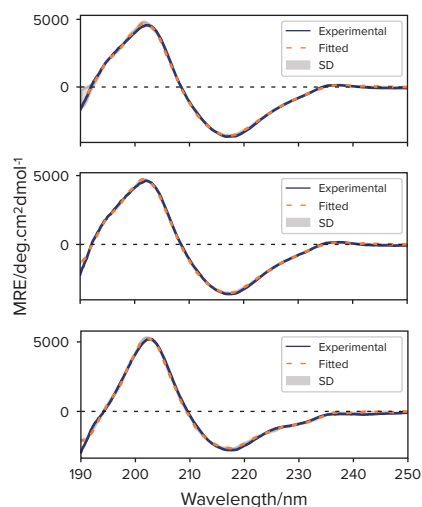
Automatic Y-axis conversion and concentration calculation by amino acid sequence and absorption

## APPLICATION

## Secondary structure prediction of therapeutic antibodies

### CD spectra of antibodies

### Secondary structure prediction



### MabThera®

NRMSD = 0.02



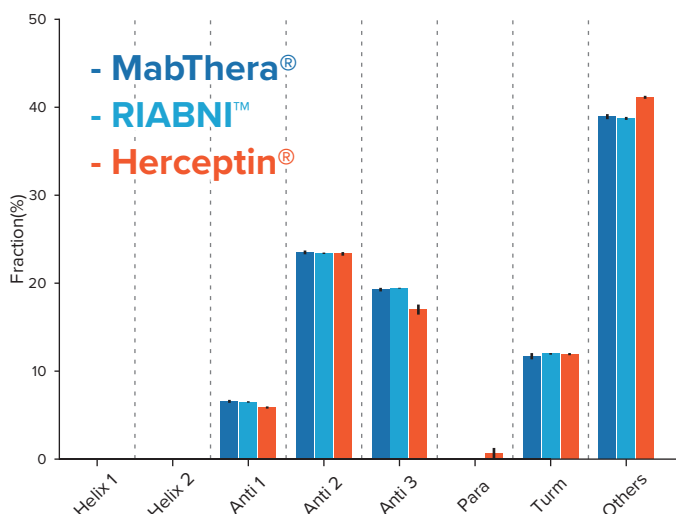
### RIABNI™

NRMSD = 0.01



### Herceptin®

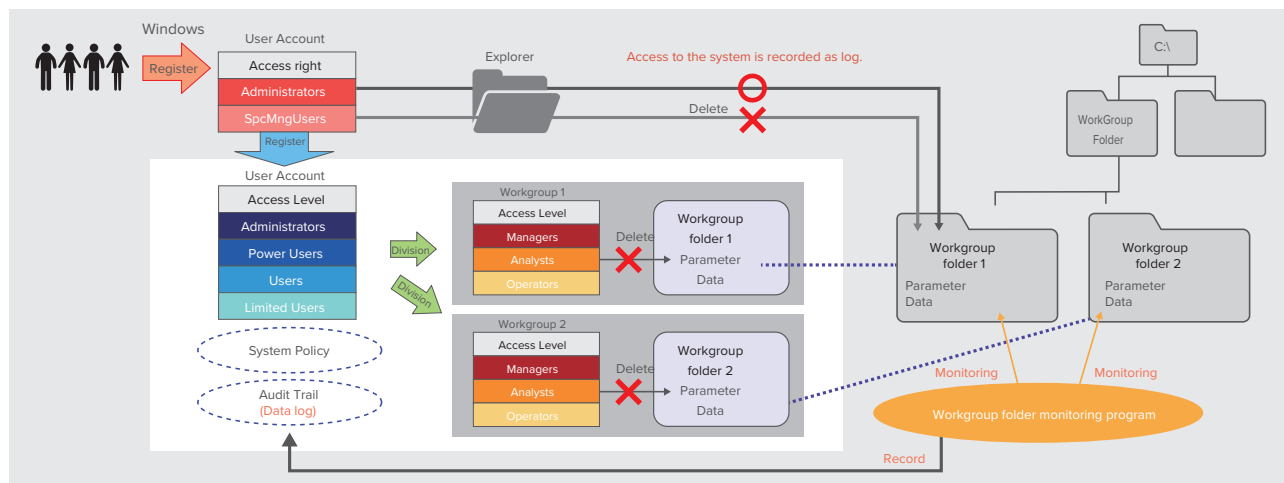
NRMSD = 0.02



This program utilizes 'BeStSel engine', which is an algorithm developed by Dr. József Kardos and Dr. András Micsonai, et. al. at ELTE (Eötvös Loránd University, Hungary).

# Regulatory Compliance with Spectra Manager™ 2.5 CFR

JASCO Spectra Manager™ 2.5 CFR is designed and developed under ALCOA+ and is a total solution platform to create accurate and complete data.



Overview

## Solution for data integrity



### User Management

Based on the dual security category ([Access Level] and [Work Group]), it is possible to manage different authorization processes in flexible and independent as total analysis systems, instrumentations and analytical applications.

### User Account Security

Based on functions to prevent account duplication or to protect password, and to prevent unauthorized access, administrative authorizations such as system access and electronic signature etc., can be managed strictly.

### Enduring Electronic Record

Based on prohibiting function to delete electronic record and to overwrite save, and also functions for backup and restore data, electronic records can be saved properly and can be searched accurately during the data lifecycle.

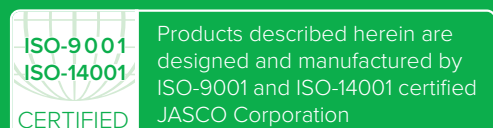
### Audit Trail

It is categorized as 4 different records (system log, application log and data log), and it is recorded. Each log can be filtered and displayed under recorded date, user name etc, and it can be exported for audit trail review.

### Computerized System Validation

Spectra Manager™ 2.5 CFR is developed and manufactured properly under quality control system adapted ISO 9001, and adapted CSV standard.

The contents of this material are for reference and illustrative purposes only. Information, descriptions, and specifications in this publication are subject to change without notice. JASCO assumes no responsibility and will not be liable for any errors or omissions contained herein or for incidental, consequential damages or losses in connection with the furnishing, performance or use of this material.



Products described herein are designed and manufactured by ISO-9001 and ISO-14001 certified JASCO Corporation



### JASCO CORPORATION

2967-5, Ishikawa-machi, Hachioji-shi, Tokyo 192-8537 Japan  
Tel: +81-42-649-5177 Fax: +81-42-646-4515  
Web: [www.jasco-global.com](http://www.jasco-global.com)