



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



Providing eight types of secondary structure information



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

Secondary structure

Helix 1 – regular α -helix

The middle part of α -helices

Helix 2 – distorted α -helix

2-2 residues at the ends of α -helices

Anti 1 – left-twisted β -strand

Left-hand twisted antiparallel β -sheet

Anti 2 – relaxed β -strand

Relaxed (slightly right-hand twisted) antiparallel β -sheet

Anti 3 – right-twisted β -strand

Right-hand twisted antiparallel β -sheet

Parallel β -strand

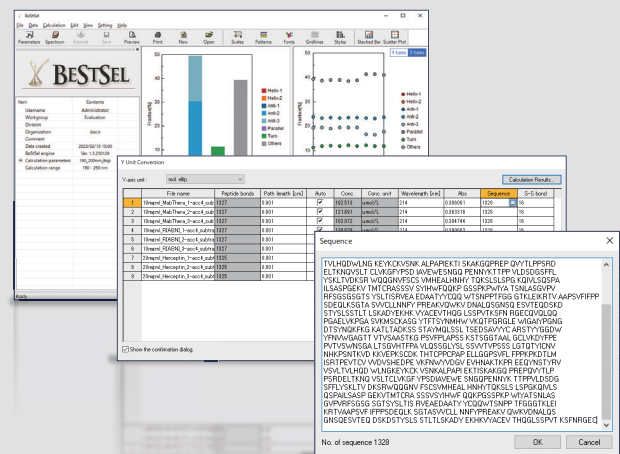
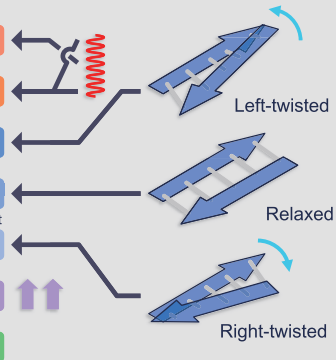
Parallel β -sheet

Turn

Turn, as defined by DSSP

Others

3,10-helix, π -helix, β -bridge, bend, loop/irregular and invisible regions of the structure



Secondary structure information obtained by BeStSel algorithm

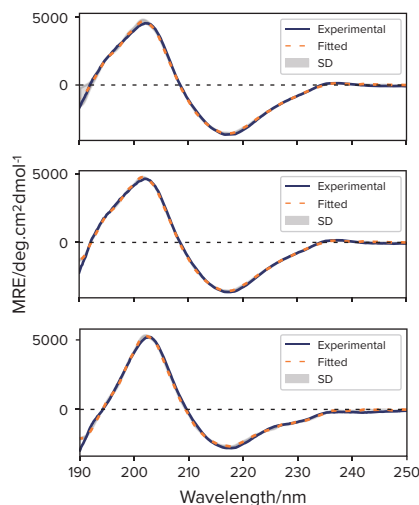
Automatic Y-axis conversion and concentration calculation by amino acid sequence and absorption

APPLICATION

Secondary structure prediction of therapeutic antibodies

CD spectra of antibodies

Secondary structure prediction



MabThera®

NRMSD = 0.02



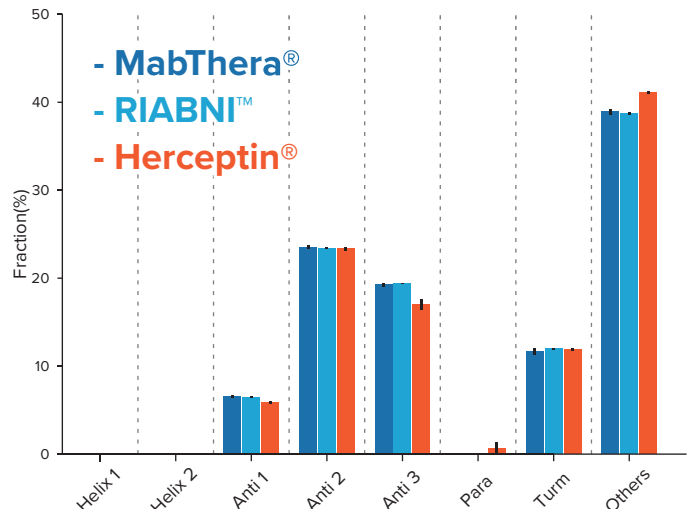
RIABNI™

NRMSD = 0.01



Herceptin®

NRMSD = 0.02

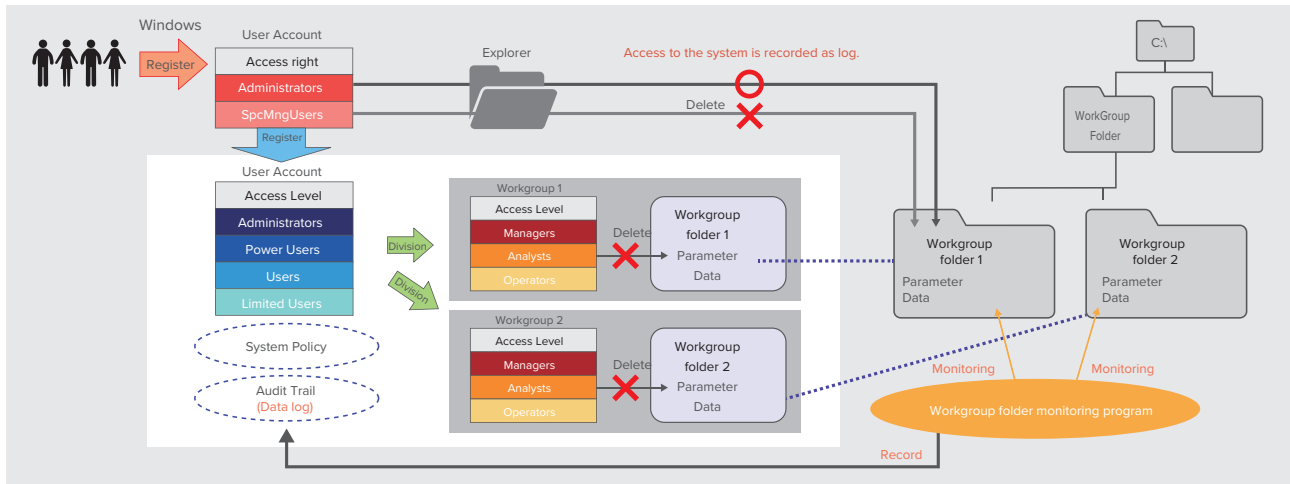


This program utilizes 'BeStSel engine', which is an algorithm developed by Dr. József Kardos and Dr. András Micsonai, et. al. at ELTE (Eötvös Loránd University, Hungary).



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



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.

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.

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