Application Note

CD-0008

Secondary structure estimation (SSE) program of multiple samples

Introduction

The multivariate SSE program can be used to analyze sets of CD data. A large number of samples can be automatically measured and efficiently analyzed using the high-throughput circular dichroism (HDX) system and multivariate SSE program.

Keywords: Secondary structure estimation, Multiple samples, HTCD, HDX

Sequence

Optical constants are automatically calculated in the multivariate SSE program after imputing parameters as the path length and mean residue molar concentration.

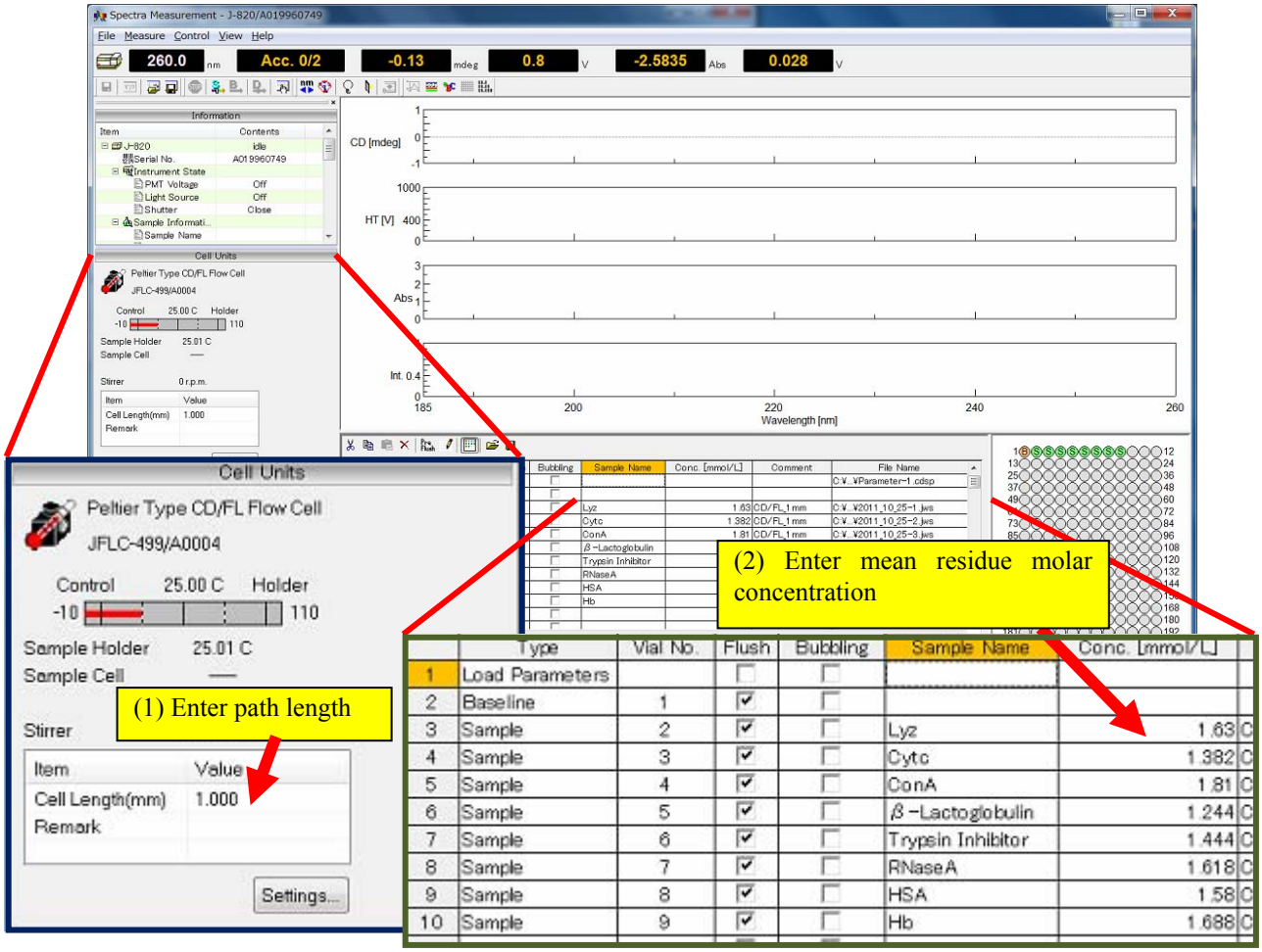

Fig. 1 Specifying path length and mean residue molar concentration

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CD Spectra Measurement

Path length:	1 mm	Concentration:	0.2 mg/ml	Temp.:	20ºC
Wavelength:	260-185 nm	Scan speed:	100 nm/min	Response:	2 sec
Data interval:	0.1 nm	Bandwidth:	1 nm	Accumulation:	2

Measurement time: 90 sec. per sample

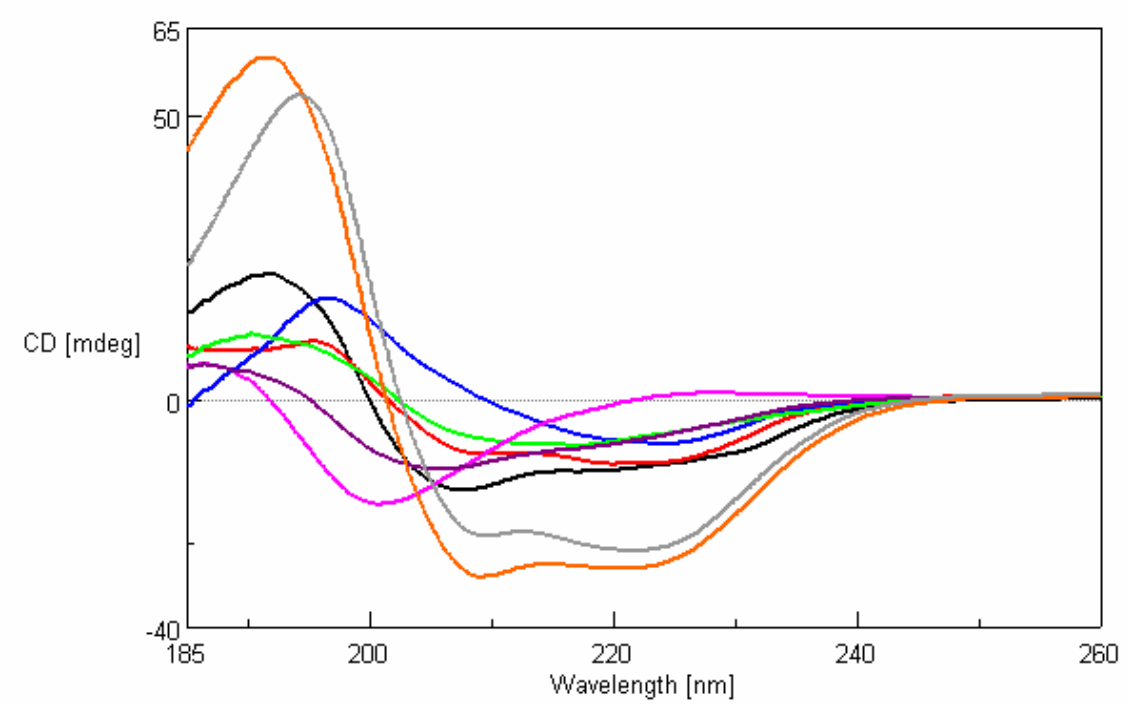

Fig. 2 CD spectra of eight proteins

Lysozyme: Cytochrome C: Concanavalin A:
b-Lactoglobulin: Trypsin Inhibitor: Ribonuclease A:
Human Serum Albumin: Hemoglobin:

Secondary Structure Estimation

In table 1, the results of secondary structure estimation of eight proteins conducted using the PLS method on CD spectra are compared with the results of X-ray crystallography.

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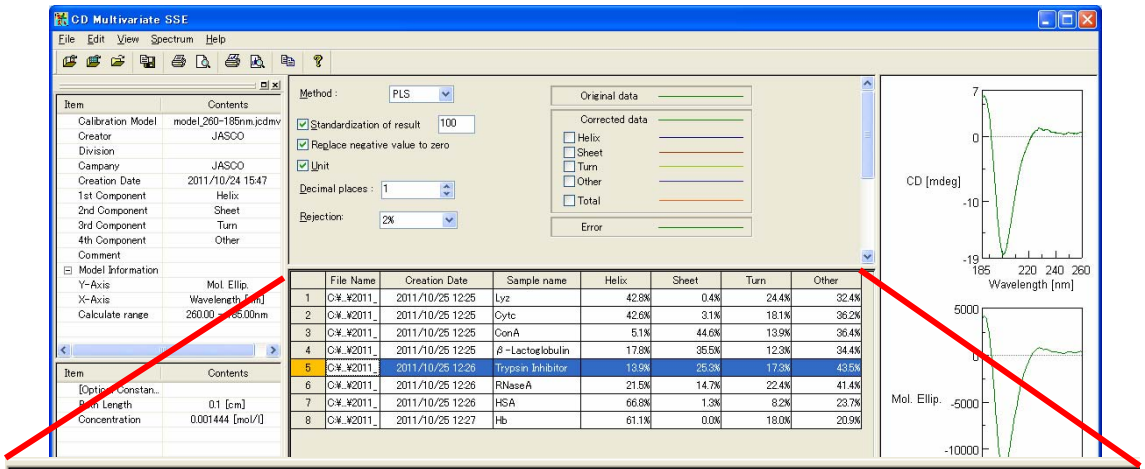

	File Name	Creation Date	Sample name	Helix	Sheet	Turn	Other
1	C:¥...¥2011_	2011/10/25 12:25	Lyz	42.8%	0.4%	24.4%	32.4%
2	C:¥...¥2011_	2011/10/25 12:25	Cytc	42.6%	3.1%	18.1%	36.2%
3	C:¥...¥2011_	2011/10/25 12:25	ConA	5.1%	44.6%	13.9%	36.4%
4	C:¥...¥2011_	2011/10/25 12:25	β-Lactoglobulin	17.8%	35.5%	12.3%	34.4%
5	C:¥...¥2011_	2011/10/25 12:26	Trypsin Inhibitor	13.9%	25.3%	17.3%	43.5%
6	C:¥...¥2011_	2011/10/25 12:26	RNaseA	21.5%	14.7%	22.4%	41.4%
7	C:¥...¥2011_	2011/10/25 12:26	HSA	66.8%	1.3%	8.2%	23.7%
8	C:¥...¥2011_	2011/10/25 12:27	Hb	61.1%	0.0%	18.0%	20.9%

Fig. 3 Results using multivariate SSE program

Table 1 Comparison with X-ray crystallography

Sample name		Helix (%)	Sheet (%)	Turn (%)	Other (%)	Reference
Lysozyme (Lyz)	PLS	42.8	0.4	24.4	32.4	
	X-ray	41	4	19	35	1
Cytochrome C (CytC)	PLS	42.6	3.1	18.1	36.2	
	X-ray	42	8	9	42	1
Concanavalin A (ConA)	PLS	5.1	44.6	13.9	36.4	
	X-ray	2	36	12	49	1
β-Lactoglobulin	PLS	17.8	35.5	12.3	34.4	
	X-ray	13	34	13	41	1
Trypsin Inhibitor	PLS	13.9	25.3	17.3	43.5	
	X-ray	2	33	10	55	2
Ribonuclease A (RNaseA)	PLS	21.5	14.7	22.4	41.4	
	X-ray	22	19	11	48	1
Human Serum Albumin (HSA)	PLS	66.8	1.3	8.2	23.7	
	X-ray	72	0	8	20	2
Hemoglobin (Hb)	PLS	61.1	0	18	20.9	
	X-ray	75	0	10	15	1

Helix: a-helix + 310-helix, Sheet: b-strand, Turn: turns, Other: rest

References

(1) W. Curtis Johnson, *PROTEINS: Structure, Function, and Genetics*, **35**, 307-312, (1999)
(2) PROTEIN DATA BANK: Trypsin inhibitor: 1ba7 (DSSP), HAS: 1bm0 (DSSP)

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