Application Note

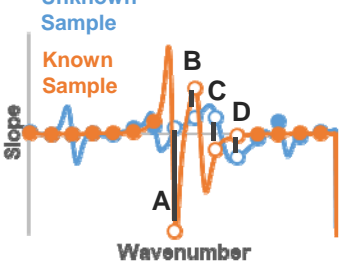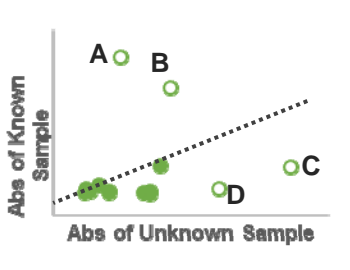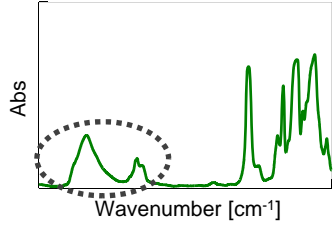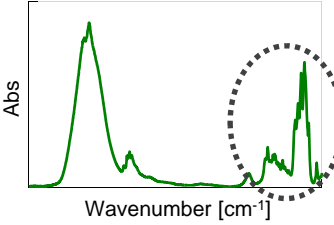## Q. Which algorithm should be selected when using [Data Comparison] of [Spectral Analysis] program?

A. There are eight comparison algorithms in [Data comparison], but in the analysis of IR spectra, three of the following are mainly used: (1) Euclidean distance, (2) Derivative euclidean distance, and (3) Correlation coefficient. In general, (1) is used for evaluating broad peaks, (2) is used when the baseline is distorted or user wants to evaluate sharp peaks, and (3) is used when the spectrum is noisy. The outlines, advantages, disadvantages and usage examples of the three algorithms are shown in following table.

	Euclidean Distance	Derivative Euclidean Distance	Correlation Coefficient
Outline of Algorithm	Evaluates the sum of differences in the absorbances at each point.	Evaluates the sum of the differences in the slopes of absorbance (derivative of spectrum) at each point	Evaluates the strength of correlation of absorbance
	A, B, C and D of the three graphs show the same points		
Advantage	Emphasizes the broad peak	Emphasizes the sharp peak The influence from baseline distortion is small.	The influence from noise is small.
Disadvantage	Does not emphasize the sharp peak	Susceptible to noise	Does not emphasize the fine differences in spectra
Usage Example	In case that user wants to evaluate broad peaks	In case that user wants to evaluate sharp peaks	In case that the spectrum is noisy

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