

## Application News

# No. A609

### Spectrophotometric Analysis

## High Efficiency in Multi-Sample Analysis by Automatic Analysis System of LabSolutions™ UV-Vis

Ultraviolet and visible light (UV-Vis) spectrophotometers are used routinely in raw material receiving inspections and quality confirmation in various industries. In quantitative analyses of solutions, the technician measures the actual sample after first measuring a standard sample, then calculates the sample concentration and makes a pass/fail judgment by comparing the result with the standard value. This huge amount of manual work becomes a burden when several dozen samples are measured each day.

LabSolutions UV-Vis software includes an automatic analysis function that realizes high efficiency in this tedious, time-consuming work. All processes from measurement of the standard and quantitation samples to pass/fail judgments can be carried out automatically by using LabSolutions UV-Vis in combination with an autosampler (Teledyne CETAC Technologies).

This article introduces an example of automatic analysis of a food coloring.

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### Automatic Analysis

The options available with Shimadzu LabSolutions UV-Vis software include an automatic analysis function which can be used to control an autosampler in conjunction with spectra and photometric measurements. The autosamplers that can be controlled by this program are the ASX-280 and ASX-560 manufactured by Teledyne CETAC Technologies. Fig. 1 shows the appearance of the ASX-560. The maximum number of samples that can be set with the respective models is 120 vials with the ASX-280 and 240 vials with the ASX-560.

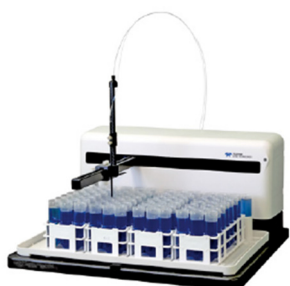


Fig. 1 Appearance of Teledyne CETAC ASX-560 Autosampler

As shown in Fig. 2, use of the spectra evaluation function of LabSolutions UV-Vis in combination with automatic analysis utilizing an autosampler makes it possible to automate all of the processes that had been required in manual quantitative analysis, including measurement of the standard sample and quantitation sample and analysis work using the obtained spectra. Automation of these processes is explained in the following section.

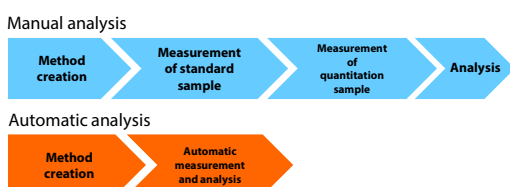


Fig. 2 Workflow of Quantitative Analysis

### From Preparation of Calibration Curve to Pass/Fail Judgment

All the processes from preparation of a calibration curve by measurement of the standard sample to measurement of the quantitation sample and the pass/fail judgment are possible by using a combination of this software and an autosampler. In this experiment, 5 standard samples and 20 quantitation samples were prepared using a red food coloring. For the pass/fail judgment, 17 samples with the same concentration and 3 samples with different concentrations were prepared. Fig. 3 shows the appearance of the samples set in the ASX-560.

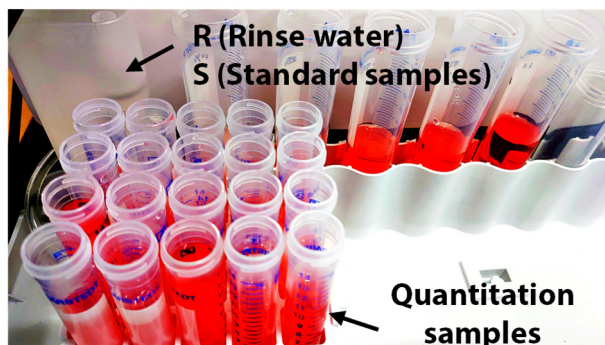


Fig. 3 Condition of Samples Set in ASX-560

A Shimadzu UV-1900i UV-Vis spectrophotometer was used in the spectrum measurements. Fig. 4 shows the appearance of the UV-1900i, and Table 1 shows the measurement conditions. When using the ASX autosampler, either a sipper unit or a syringe sipper is necessary.



Fig. 4 Appearance of UV-1900i UV-Vis Spectrophotometer

Table 1 Measurement Conditions

Measurement wavelength	: 505 nm
Slit width	: 1 nm
Suction speed	: High speed
Suction time	: 6 s
Discharge time	: 4 s
Stabilization time	: 2 s
No. of rinses	: 1
Accessory	: 160 L sipper unit

First, the measurement conditions are set in the quantitative measurement mode of the LabSolutions UV-Vis software. The measurement wavelength, concentration of the standard sample, suction speed, and other parameters are decided. Next, the measurement conditions of the autosampler are set from the automatic analysis screen. As shown in Fig. 5, the measurement locations and the measurement sequence of the standard sample (S), rinse (R), and quantitation sample (1A, 1B, ...) can be decided visually. It is also possible to determine the detailed conditions for each of these measurements, including whether to use the baseline correction and prewash functions or not. Existing measurement conditions can also be accessed, saving time and trouble in condition setting.

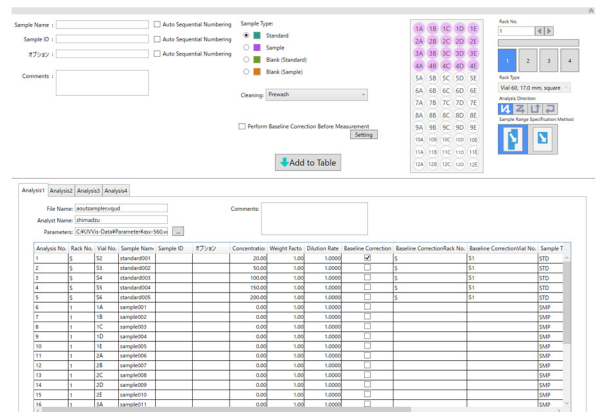


Fig. 5 Setting of Automatic Analysis Screen

During a measurement, it is possible to check the remaining time, measurement position, number, and results on both the automatic analysis and quantitative measurement software. Figs. 6 and 7 show the respective screens during a measurement.

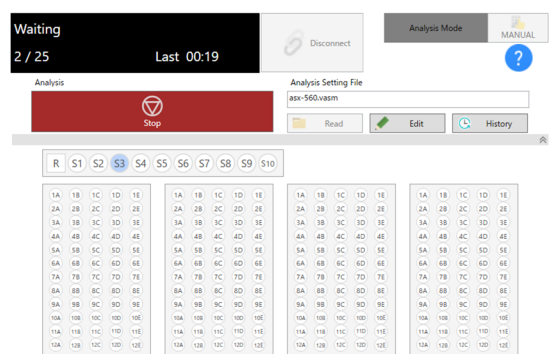


Fig. 6 Automatic Analysis Screen During Measurement

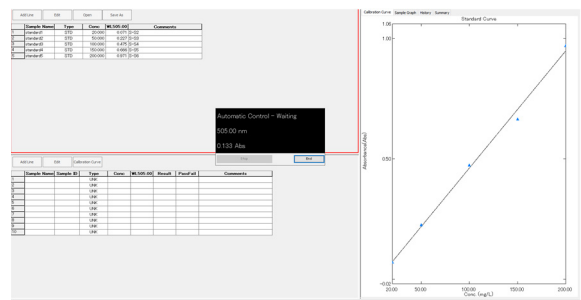


Fig. 7 Quantitative Measurement Mode Screen During Measurement

	Sample Name	Conc	WL505.00	Pass/Fail	Comments
1	Sample1	106.096	0.492	Passed	1-1A
2	Sample2	111.564	0.519	Passed	1-1B
3	Sample3	108.933	0.506	Passed	1-1C
4	Sample4	112.016	0.521	Passed	1-1D
5	Sample5	109.138	0.507	Passed	1-1E
6	Sample6	103.794	0.481	Failed	1-2A
7	Sample7	113.249	0.527	Passed	1-2B
8	Sample8	110.577	0.514	Passed	1-2C
9	Sample9	111.605	0.519	Passed	1-2D
10	Sample10	110.988	0.516	Passed	1-2E
11	Sample11	151.478	0.713	Failed	1-3A
12	Sample12	111.605	0.519	Passed	1-3B
13	Sample13	114.688	0.534	Passed	1-3C
14	Sample14	109.960	0.511	Passed	1-3D
15	Sample15	109.549	0.509	Passed	1-3E
16	Sample16	107.494	0.499	Passed	1-4A
17	Sample17	110.988	0.516	Passed	1-4B
18	Sample18	154.150	0.726	Failed	1-4C
19	Sample19	109.138	0.507	Passed	1-4D
20	Sample20	108.933	0.506	Passed	1-4E

Fig. 8 Measurement Results and Pass/Fail Judgment Results

Fig. 8 shows the measurement results and results of an automatic evaluation. The table shows the concentrations calculated from the calibration curve. Pass/fail judgments based on criteria set in advance can be made from these results. In this experiment, concentrations in the range of 105 ppm to 115 ppm are judged "pass." The 3 sample solutions that did not satisfy this criterion were judged "fail." The measurement location is shown in the comments column. The information in this table can also be pasted into other applications by using the csv output and the copy & paste function, supporting creation of reports in various formats.

A manual analysis of 20 samples from setting of the measurement conditions to the pass/fail judgment required approximately 1 hour. In contrast, the same analysis could be completed in about 30 minutes by using the automatic analysis function of LabSolutions UV-Vis. Thus, the analysis could be completed in half the time necessary in a manual analysis.

Conclusion

In this experiment, all process from preparation of the calibration curve to measurement of the quantitation sample and the pass/fail judgment were conducted automatically by using the automatic analysis function of the LabSolutions UV-Vis software. The time required in routine measurements can be reduced substantially by using this automatic analysis function and an autosampler.

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