

# Circular Dichroism

J-1000 Series Spectrometers



**Jasco**

Performance  
Innovation  
Reliability



JASCO has produced the highest quality circular dichroism instrumentation for over 50 years. The J-1000 series is the result of many advances in technology combined with a great deal of customer input. These three new models adapt to meet any requirements and can be expanded as applications or budgets evolve.

Chiroptical spectroscopy has become one of the most important techniques for the characterization of biomolecules, determination of absolute configuration and stereochemical analysis. Since launching our first spectropolarimeter in 1961, JASCO has designed and built the finest in chiroptical instrumentation.

More than a half-century later, JASCO proudly presents the J-1000 series, our latest circular dichroism spectrometers. Unparalleled optical performance and available measurement modes are combined to make the J-1000 CD spectrometers true state-of-the-art chiroptical spectroscopy workbenches.

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# Features of the J-1000 Series

The three models of the J-1000 series offer the most robust feature set available, for applications ranging from education and routine analysis to complex research with strict requirements.

## Advanced Features of the J-1000 series

- High optical throughput
- Low stray light
- Advanced electronics: digital signal processing (DSP) using FGPA
- Simultaneous Multi-Probe (SMP): CD, LD, fluorescence, UV-visible, absorbance
- Wide dynamic range
- Highly efficient nitrogen purge system: low-volume monochromator designed using a flow simulator
- Integrated Hg lamp for wavelength calibration
- NIST traceable scale calibration standard
- Single USB connection for simplicity and easy PC changes in the future
- Measurement of micro-volume samples
- Three scanning modes: auto, step and continuous

## Unique Optical Features and Benefits

- Compact benchtop design
- Air-cooled 150W Xenon lamp
- Highest signal-to-noise ratio
- Collimated sample beam for artifact-free solid sampling and use of external accessories
- Precise temperature control accessories
- Automated titration and stopped-flow
- Spectra Manager™ software for control and data analysis
- Spectra Manager™ CFR option for 21 CFR Part 11 compliance
- Secondary Structure Analysis and Advanced Curve Fitting Analysis capabilities (standard)
- Flexible design allows for field upgrades for different measurement capabilities
- Ability to upgrade accessories as applications and budgets evolve

## Versatility for a Wide Range of Applications

- Protein conformational studies
- Protein folding studies
- DNA / RNA interactions
- Enzyme kinetics
- Formulation studies
- Purity testing of optically active substances
- Quantitative analysis of pharmaceuticals
- Natural products chemistry
- Material science
- Rapid kinetics (stopped-flow) CD
- Absorbance and fluorescence studies

## Validation and Data Confidence

Count on the accuracy and repeatability of your data. An integrated validation mode provides users with a list of up to nine instrument performance and calibration tests. Each J-1000 system includes a built-in Hg lamp wavelength calibration source. JASCO also offers the first traceable scale calibration substance (d-10-ammonium camphorsulfonate) for photometric accuracy and repeatability tests.



# Which model is right for you?



## J-1100

The basic model, perfectly suited for QA/QC and teaching applications.

## J-1500

Highest performance with a wide range of accessories to meet complex research demands.

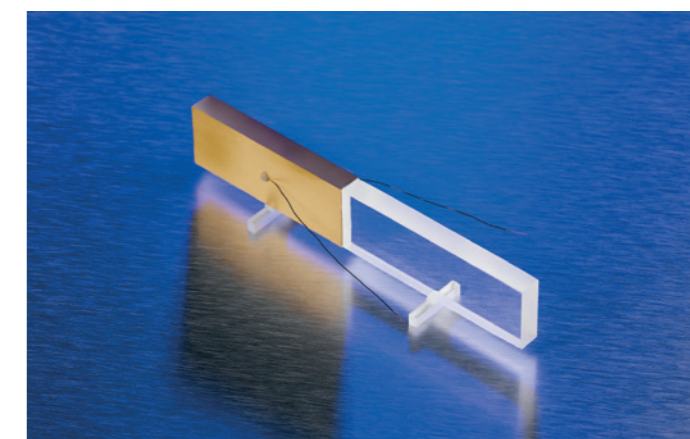


## J-1700

UV/Visible/NIR up to 2500 nm for MCD and specialized applications.

## Designed and Manufactured by JASCO

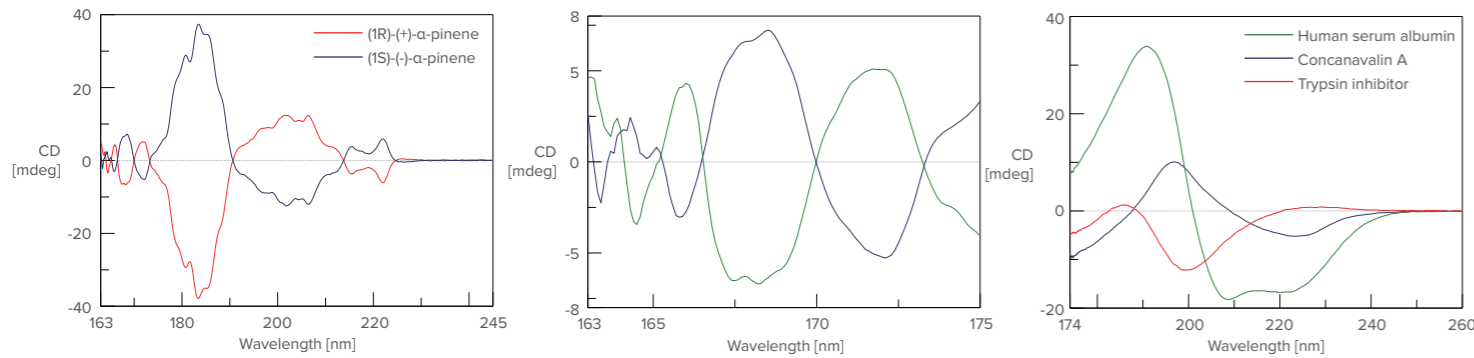
Since 1961, JASCO has designed and built the finest in chiroptical instrumentation. Instead of using instrument components from other manufacturers, the entire instrument is designed and manufactured by JASCO, including the PEM crystal, shown to the right. The result is the best performance and reliability in the industry.



# Instrument Performance

## Enhanced Vacuum-UV Measurement

The innovative optical system of the J-1500 permits the measurement of a CD spectrum in the vacuum-UV region down to 163 nm. The vacuum-UV region below 200 nm is of critical importance for biomolecules, particularly in protein secondary structure estimation.



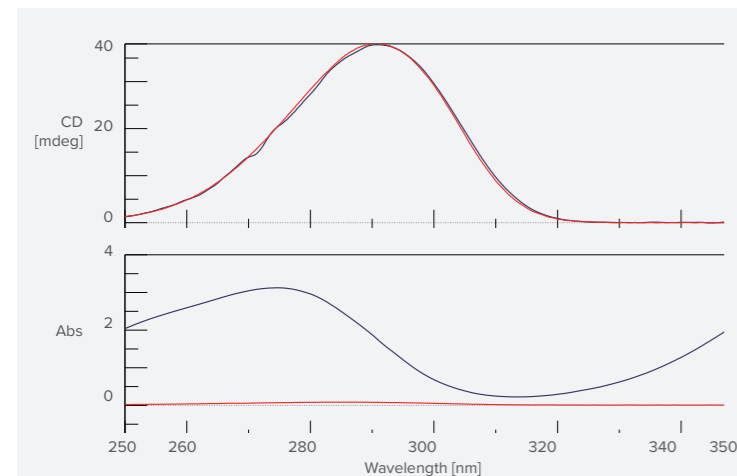
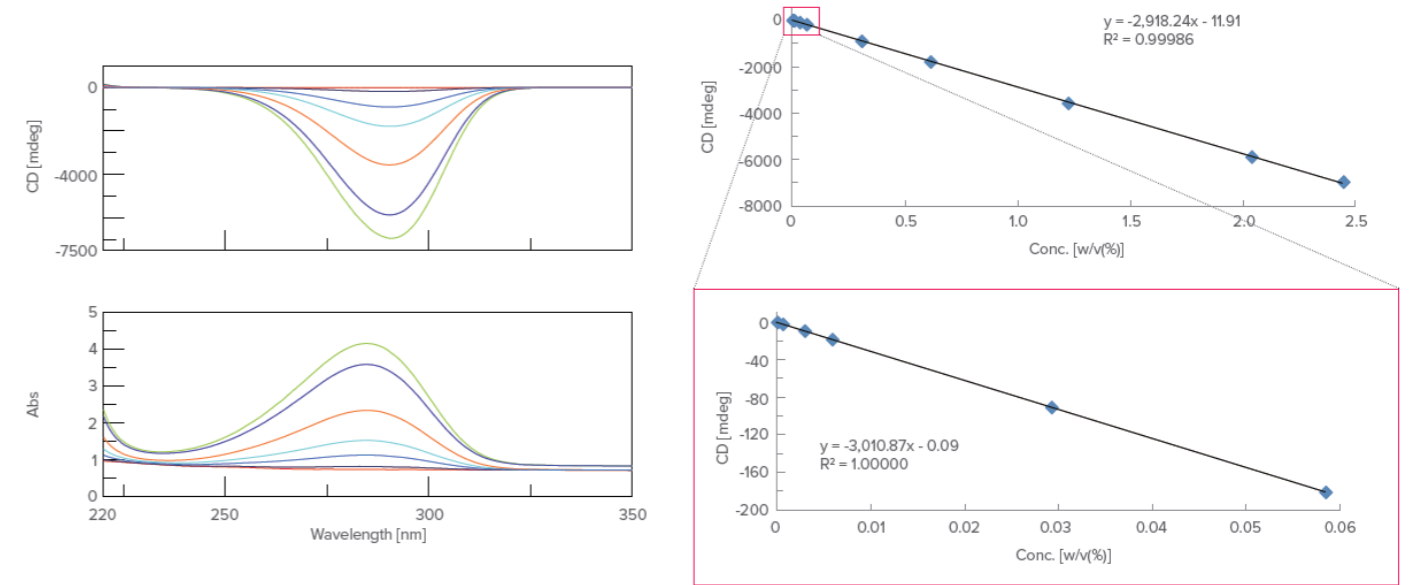
$\alpha$ -pinene enantiomers (gas phase) showing excellent performance in the far-UV region.

The same  $\alpha$ -pinene sample showing similar superior performance in the vacuum-UV region down to 163 nm.

CD spectra of Human Serum Albumin (helix rich), concanavalin A ( $\beta$ -sheet rich) and trypsin inhibitor (random rich) in water with excellent signal to noise to 174 nm.

## CD Dynamic Range and Linearity

The PMT detectors used in the JASCO system are specially selected for the highest sensitivity and lowest birefringence. The result is superior linearity compared to other types of detectors.



## Exceptional Stray-Light Rejection

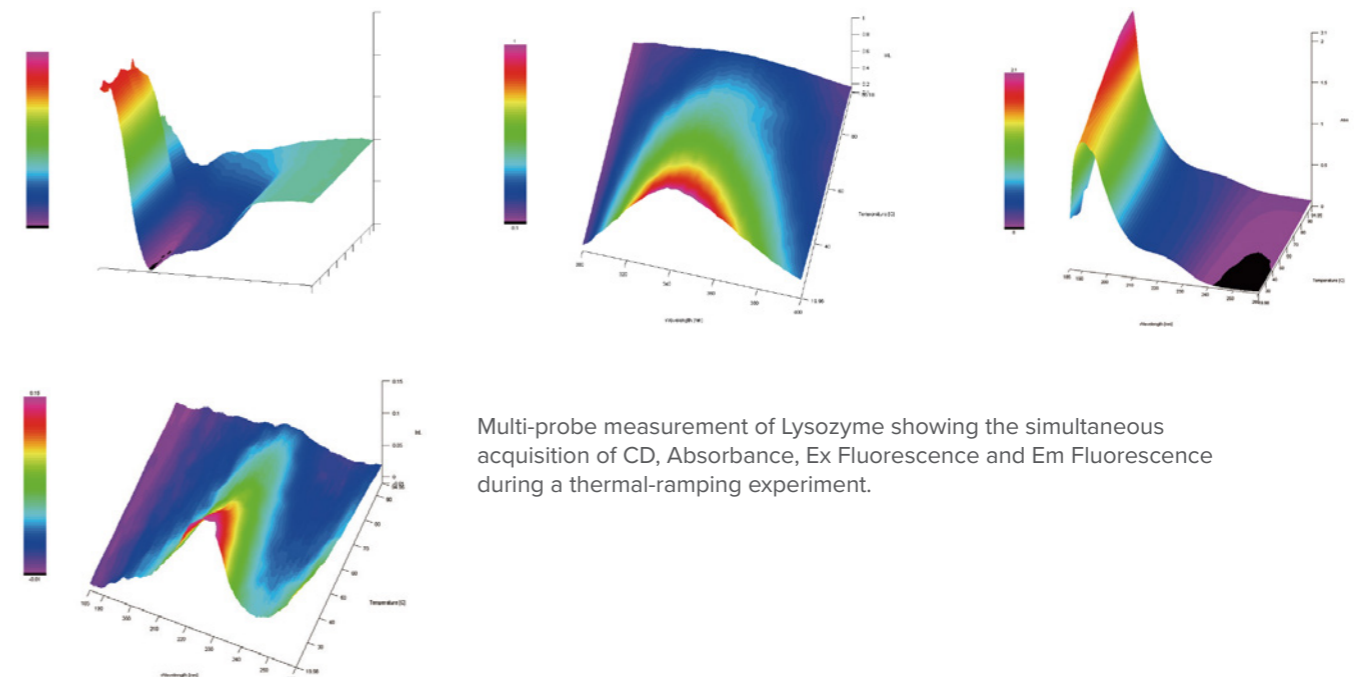
Stray light will result in distortion of the CD spectrum, particularly in the far-UV region where the sample absorbance is high. The dual polarizing prism optical design of the J-1000 series results in stray light lower than 0.0003%, enabling the instruments to obtain high-quality CD data even

## Rapid Scanning

High sensitivity combined with a 10,000 nm-per-minute maximum scan speed allows the J-1500 to measure samples quickly, increasing productivity in your lab. An additional benefit is the minimal time exposure of biological samples to the high-energy UV light, minimizing the risk of sample degradation.

## Simultaneous Multi-Probe Measurement

The latest quad-channel lock-in amplifier provides the simultaneous acquisition of up to four data channels including CD, absorbance, linear dichroism (LD), fluorescence, fluorescence-detected CD (FD CD), fluorescence-detected LD (FDLD) and fluorescence anisotropy.



Multi-probe measurement of Lysozyme showing the simultaneous acquisition of CD, Absorbance, Ex Fluorescence and Em Fluorescence during a thermal-ramping experiment.



# Temperature Control

## Single-Position Peltier Cell Holders

**PTC-510, 514, 517**

Three single-position Peltier thermostatted cell holders are available with a maximum light path length of 10 mm, to enable temperature control using the temperature control program. All feature a temperature setting range of -30 to 130°C with a measurement probe that can be placed inside or adjacent to the cell and a magnetic stirrer to eliminate thermal gradients.

**PTC-517** Single-position Peltier for J-1500 and J-1700 for use with rectangular cells up to 10 mm.

**PTC-514** Single-position Peltier for J-1100 for use with rectangular cells up to 10 mm.

**PTC-510** Single-position Peltier for J-1500 and J-1700 for use with rectangular and cylindrical cells up to 10 mm.

## Multiple-Position Peltier Cell Changers

**MPTC-511, 513**

The MPTC accessories are designed to enable high sample throughput and productivity. The six-position holder for rectangular cells allows automated spectral scans and parallel thermal ramps on up to six samples at a time. Applicable measurement modes include spectral scans, thermal ramping at single or multiple wavelengths, and thermal ramping with spectral scans at preset temperatures.

- Temperature setting range of -30 to 130°C
- Temperature sensors for each cell
- Magnetic stirrers for each cell to eliminate thermal gradient

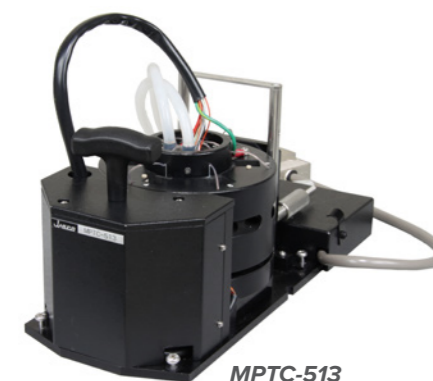
The MPTC-513 system is compatible with optional fluorescence modes including total fluorescence, scanning excitation/emission fluorescence (FMO-522) accessory and fluorescence polarization/anisotropy. (See the section on fluorescence on page 14.)



PTC-517



MPTC-511

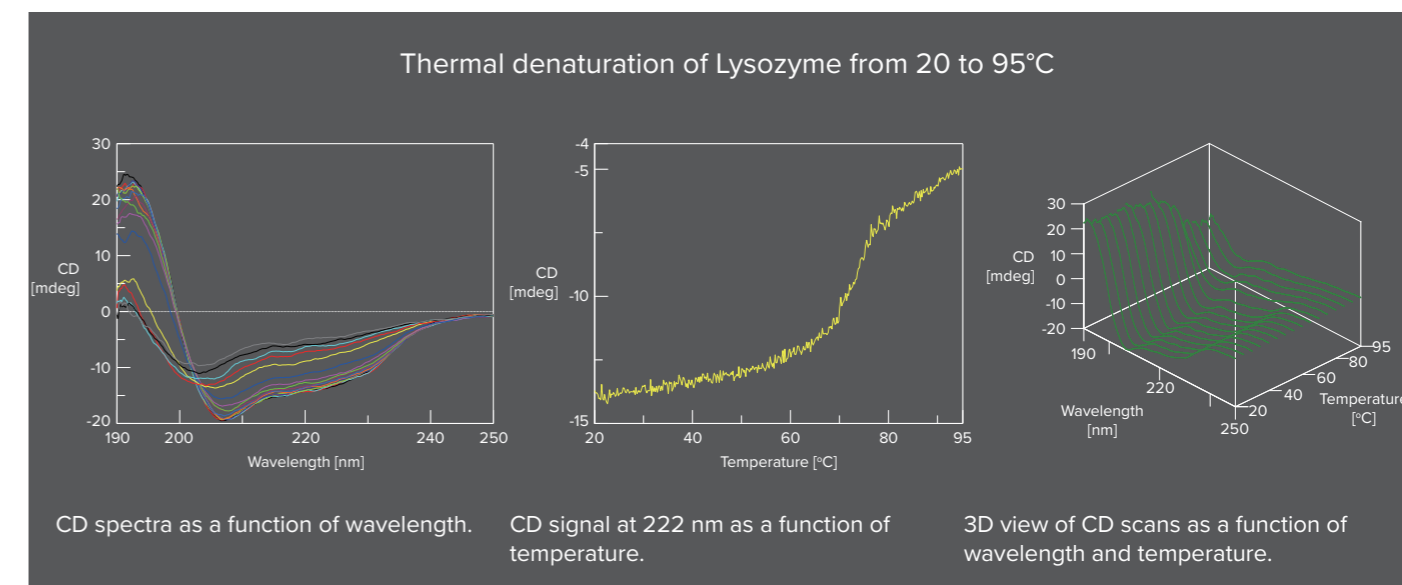


MPTC-513

## Temperature-Wavelength Scan

### Application

Measuring CD spectra while controlling the temperature of a sample provides important information about conformational changes associated with temperature perturbations and is used in the study of biopolymers. The Temperature Control Program measures the thermal denaturation curve (temperature scan) and CD spectra as a function of temperature, according to user-selected parameters. An optional thermal denaturation analysis program determines transition temperatures and thermodynamic parameters, such as  $\Delta H$  and  $\Delta S$ , from temperature scans.



## Other Temperature Control Accessories

### HTC-572 | Pressure-induced High-Temperature Measurement Cell

Thermal denaturation measurements at temperatures over 100°C are made difficult by the boiling point of water. Using the same principle as a pressure cooker, this accessory applies pressure to the sample to increase the boiling point, allowing for higher temperatures. Samples can be heated up to 170°C by applying up to 1 MPa pressure to the cell chamber.

### CAP-500 | Capillary Cell Jacket

For thermal ramping of microsamples, this new accessory allows only 10  $\mu\text{L}$  to be drawn into the capillary cell, which is inserted in a block that is placed in the Peltier cell holder. Accurate  $T_m$  measurement of such small sample volumes was not possible in the past.

# Extended Wavelength



EXPM-531

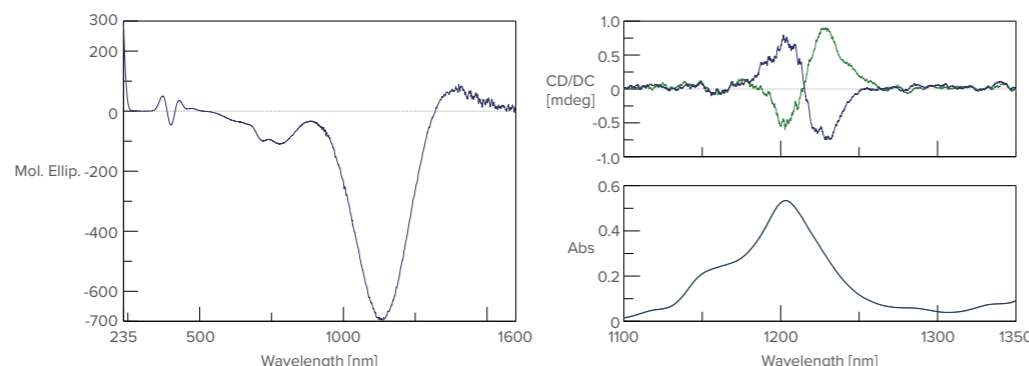


EXIG-532

## Extended Wavelength Options

### EXPM-531 (PMT), EXIG-532 (InGaAs)

Measurement in the near-infrared region is important for samples like colored proteins, including prosthetic groups, transition metal complexes and nanomaterials. The J-1500 with optional detector allows for the measurement of samples in the near-infrared region. The InGaAs detector kit includes a halogen lamp unit and allows for measurement up to 1,600 nm, covering a range where overtone VCD bands are present.



#### NIR-Region CD Spectra

Left: Sample: 0.24 M NiSO<sub>4</sub> + 0.36 M KNa-Tartrate  
 Measurement Condition: 235 - 940 nm Xe lamp + PMT  
 940 - 1,600 nm Wl lamp + InGaAs

Right: Sample: R-(+)-Limonene and S-(-)-Limonene  
 Measurement Condition: Wl lamp + InGaAs

## Extended Wavelength Accessories

### EXPM-531 | Extended wavelength option (PMT)

The EXPM-531 is a red-sensitive PMT detector covering the range from 700 to 1,250 nm. This has been the traditional method of extending the wavelength range of the CD system into the NIR range. Exchange is quick and easy, and data from the UV/Visible range can be linked with NIR data in the software.

### EXIG-532 | Extended wavelength option (InGaAs)

The EXIG-532 option includes an InGaAs detector combined with a halogen light source that expands the NIR measurement range to 1,600 nm.

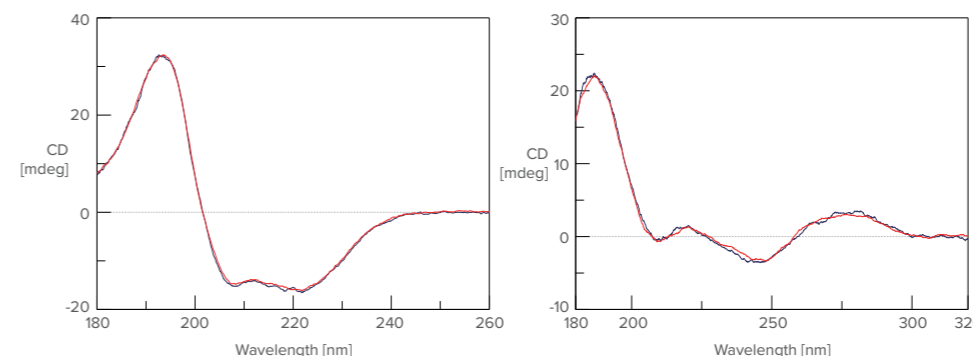
# Microsampling

Small quantities of very precious samples have always been a challenge for CD measurement. Conventional micro-cells typically have volumes as low as about 60  $\mu$ L, but a new breakthrough allows CD measurements for samples with volumes as low as 2  $\mu$ L.

## Microsampling Disk

### MSD-462

The microsampling disk is a new system designed for measurement of samples as small as 2  $\mu$ L. High-quality quartz windows with a special surface treatment utilize spacers of 1.0 and 0.2 mm for volumes of 10 and 2  $\mu$ L, respectively. The sample is applied using a micropipette, and cleaning is quick and easy.



		Helix (%)	$\beta$ -Sheet (%)	Turn (%)	Random (%)
Hemoglobin	X-ray	78.0	0.0	6.3	15.7
	Micro-sampling disk	73.8	0.0	10.9	15.3
	Cylindrical cell	72.2	0.0	12.0	15.8



MSD-462

**Comparative measurement and analysis**  
 Left: CD Spectra of DNA derived from bovine thymus

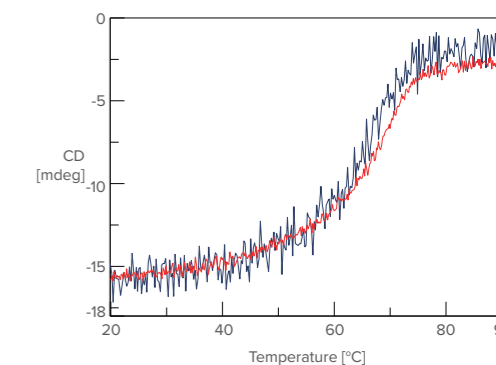
Right: CD Spectra of hemoglobin  
 Green: Cylindrical cell  
 Blue: Microsampling disk

Table: Comparison of secondary structural analysis

## Capillary Cell Jacket

### CAP-500

For thermal ramping studies of precious samples we also offer the CAP-500 system, which allows samples as small as 5  $\mu$ L to be placed in the Peltier cell holder. Melting curves are easily measured, including calculation of T<sub>m</sub>,  $\Delta$ S and  $\Delta$ H.



T<sub>m</sub> measurement of Hemoglobin  
 Wavelength: 222 nm  
 Temp.: 20°C - 90°C

— Capillary cell (10 $\mu$ L)  
 — Rectangular cell (250 $\mu$ L)

# Automated Titration

CD spectroscopists have often looked at changes in CD signal due to changes in solvent composition such as pH and buffer. In addition the studies of binding are also often of interest including protein-protein interactions as well as DNA and ligand binding. While these studies are often performed manually the use of automated titration systems has become more popular.

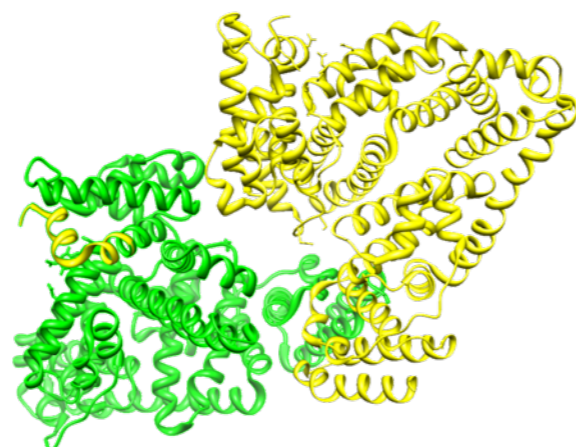


## Automated Titration Unit ATS-530

The ATS-530 is designed to automatically monitor changes in CD, absorbance and fluorescence as a function of solution pH, chemical denaturant or exogenous ligands in experiments such as protein denaturation or ligand binding. Dual syringes are employed, each equipped with a valve for automated refilling/flushing during extended runs and for maintaining a constant cell volume. Additionally, the titration measurement program automatically corrects for concentration.

The ATS-530 utilizes a 10 mm rectangular cell for mixing. It can be used with the PTC-517 or one position in either the MPTC-513 or the MPTC-511 Peltier cell holders.

- Automated titration measurement program included
- Macro command for complex/custom titrations
- Dual syringes (1 mL volume (standard), 1000 steps/syringe)
- Stirrer provided for mixing
- Temperature control
- Constant cell volume
- Concentration correction
- pH measurement (optional)



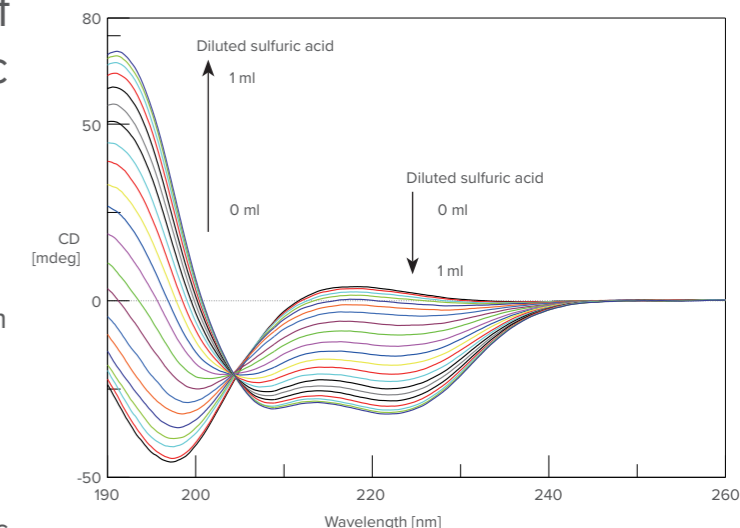
## Secondary Structure Changes of Poly-L-Glutamate During Sulfuric Acid Titration

### Application

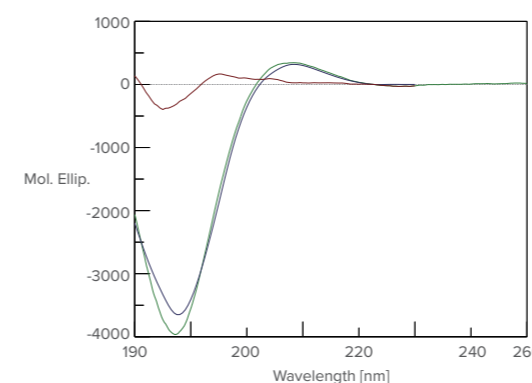
pH titration is an example of a typical experiment carried out with the ATS-530 system. Here we show the conformational changes of poly-L-glutamate from its native Alpha Helical state to random coil while lowering the pH with dilute sulfuric acid.

### Measurement Parameters

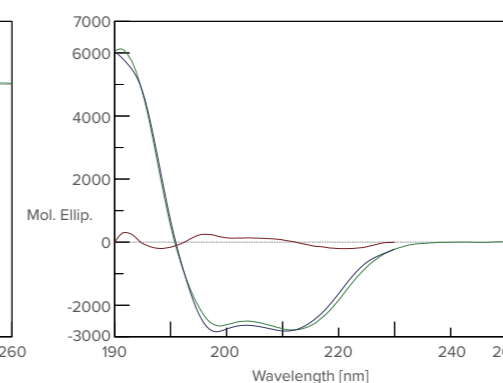
Starting solution: aqueous solution of sodium poly-L-glutamate (0.02 mg/mL, 2 mL); Titrant: diluted sulfuric acid ( $10^{-5}$  N); Titration step: 50  $\mu$ L, 20 times (total 1 mL)



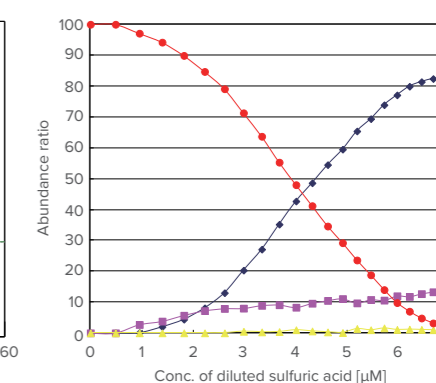
Above: 2D-CD Spectra of sodium poly-L-glutamate titrated with diluted sulfuric acid.



Comparison of experimental and calculated spectrum (before titration).  
Green: Experimental  
Blue: Calculated  
Red: Residual



Comparison of experimental and calculated spectrum (after titration).  
Green: Experimental  
Blue: Calculated  
Red: Residual



Change of SSE abundance ratio of sodium poly-L-glutamate.  
Blue: Helix  
Pink: Sheet  
Yellow: Turn  
Red: Random



# Fluorescence



FDT-538

## Total Fluorescence and Fluorescence Scanning

### FMO-522, FDT-538

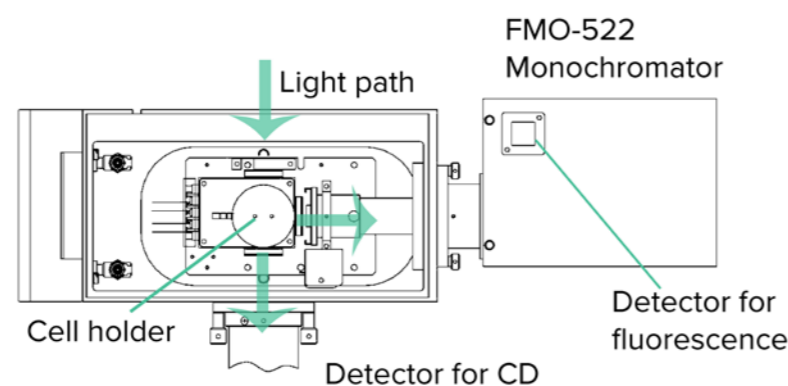
Intrinsic fluorescence can be measured on the J-1500 or J-1700 CD spectrometers, with either the single-position Peltier cell holders (PTC-510 and PTC-517) or turreted six-cell Peltier (MPTC-513). A simple low-cost system for detection of total fluorescence is available using a secondary detector and high-pass filters (FDT-538 and FST-470), allowing the user to select the excitation wavelength while detecting the emission at the wavelengths above the cut-off filter. This allows for simple, yet sensitive, detection of fluorescence changes during titration or thermal ramp experiments.

Alternatively, fluorescence data can be acquired by using the optional scanning emission monochromator (FMO-522) and emission detector (FDT-538). Excitation and fluorescence emission spectra can be scanned by fixing the emission or excitation wavelengths, respectively.

- Fluorescence scanning can be coupled with the titration and thermal ramping capabilities.
- With the MPTC-513, CD and fluorescence data can be collected, simultaneously or separately, on up to six samples.



FMO-522



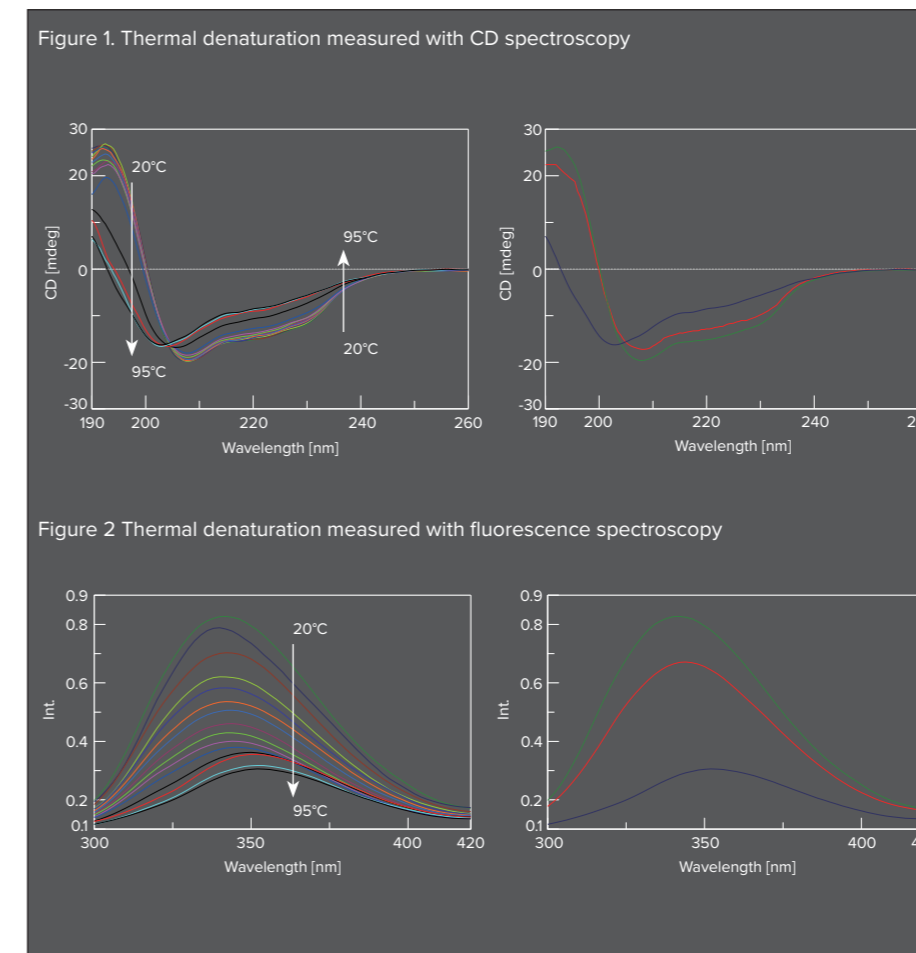
Above: Configuration for emission scanning with FMO-522

## Thermal Denaturation of Lysozyme Measured with CD and Fluorescence Spectroscopies

### Application

Lysozyme, a globular protein found in the white of a hen's egg, is a model protein used to investigate the denaturation of proteins at high temperatures. The secondary structure of lysozyme comprises about 38%  $\alpha$ -helix and 10%  $\beta$ -sheet.

Chicken egg-white lysozyme (1 mg) was dissolved in 15 mL of deionized water. The thermal denaturation of the protein was monitored using the JASCO J-1500 CD spectrophotometer equipped with an MPTC-513 Peltier temperature controller and an FMO-522 emission monochromator for detection of fluorescence. CD and fluorescence spectra were automatically measured at 5° intervals from 20 to 95°C. After the final measurement at 95°C, the sample temperature was returned to 20°C and a final spectrum was collected.



**Figure 1. Thermal denaturation measured with CD spectroscopy**

A. As the temperature increases, the intensity of the CD spectra decreases and the minimum at 208 nm blue-shifts to 203 nm.

B. Upon completion of the melt, the temperature is re-equilibrated at the initial 20°C. Comparison of the CD spectra measured at 20°C before and after the melt demonstrates that while the protein does refold, it does not recover its original structure. (Green: 20°C initial / Blue: 95°C / Red: 20°C final)

**Figure 2. Fluorescence data for the thermal denaturation of lysozyme from 20 to 95°C**

A. As the protein undergoes thermal denaturation, the fluorescence decreases in intensity and the emission maximum red-shifts from 338 to 347 nm. As with the CD data, the largest shift occurs between 75 and 80°C.

B. A comparison of the protein fluorescence spectra measured at 20°C before and after thermal denaturation supports the CD results, which indicate that the lysozyme structure does not return to its initial native state after denaturation. (Green: 20°C initial / Blue: 95°C / Red: 20°C final)



# Fluorescence (continued)

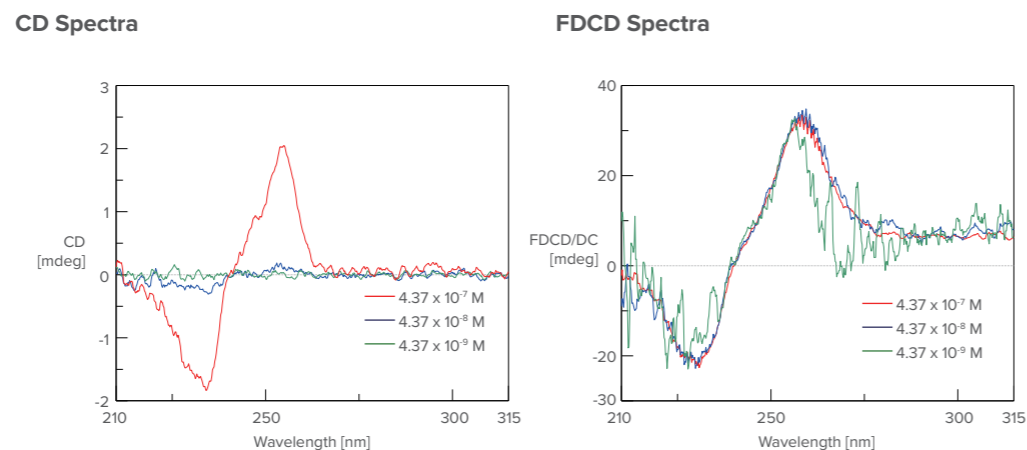
## Fluorescence-Detected Circular Dichroism

Fluorescence-detected circular dichroism (FDCD) is the measurement of the differential emission intensities from an optically active sample that is excited by left and right circularly polarized light. This method takes advantage of the chiral specificities and the structural sensitivities of CD, combined with the selectivity and sensitivity of enhanced fluorescence detection.

Because FDCD can selectively measure the CD of a specific fluorescent chromophore, it is particularly useful for the study of proteins, which have multiple chromophores. FDCD can be measured with the standard CD detector when paired with a PTC-510, PTC-517 or MPTC-513 cell holder. When samples are free from fluorescence anisotropy, this method is effective because the photoselection artifact is small. However, when the sample has a larger fluorescence anisotropy, the photoselection artifact will distort the FDCD spectrum. The FDCD-551 attachment is specially designed to reduce or eliminate this artifact while greatly enhancing sensitivity due to much more efficient light collection.

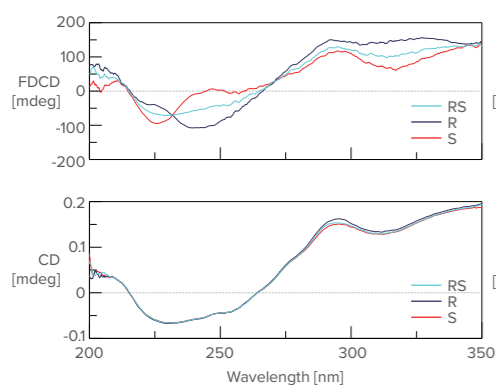
### Comparison with CD

FDCD offers a significant sensitivity advantage over absorption CD spectroscopy. The graphs illustrate CD and FDCD spectra of the same sample in concentrations varying by 10X. The sample is (1S,2S)-trans-cyclohexanediol bis(6-methoxy-2-naphthoate).

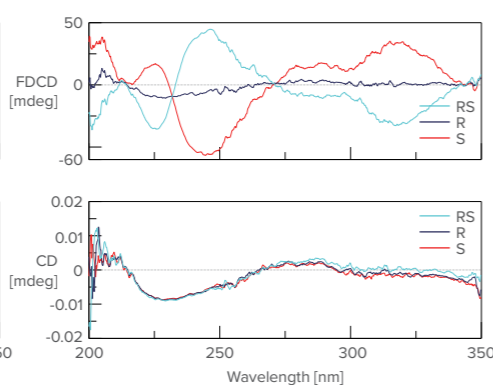


Data courtesy of Dr. Tatsuo Nehira, Faculty of Integrated Arts and Sciences, Hiroshima University, Japan, and Prof. Nina Berova, Department of Chemistry, Columbia University, USA.

### FDCD-550



### FDCD-551

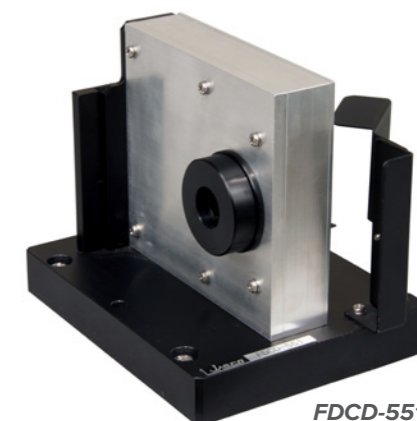
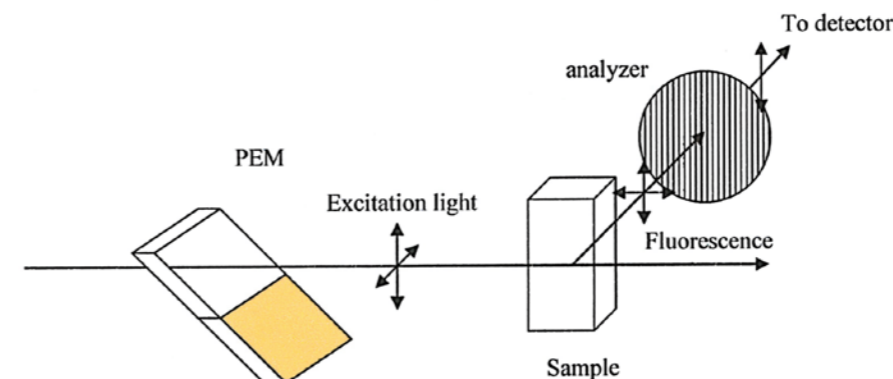


### Artifact Elimination

The graph on the left shows photoselection artifacts with conventional FDCD measurement using the FDCD-550. The graph on the right shows artifact-free FDCD spectra using the FDCD-551 system. The sample is RS-1,1'-Bi-2-Naphthol 0.4ppm / Glycerin.

## Fluorescence Polarization Anisotropy

The J-1500 and J-1700 CD instruments use circularly polarized light that is generated by phase modulation. By controlling the amplitude of the phase modulation, it is also possible to measure linear dichroism (LD), which is the differential absorption of light polarized parallel and perpendicular to an orientation direction. Using this same principle, when polarized light interacts with a fluorescent molecule, the resulting fluorescence emission has different intensities along different polarization axes. This fluorescence anisotropy can be measured as shown in the diagram below where the polarized light passes first through a polarizer (analyzer) and then a detector that is positioned 90° relative to the excitation beam. The polarizer is oriented so that only the vertical component of light passes to the detector.



FDCD-551



FDCD-550

## Additional Fluorescence Accessories

### FDCD-550 | FDCD Unit

Fluorescence-detected CD measurements are possible with this attachment, which comprises a sample holder for 90° detection, focusing lens, filter holder and a short wavelength cut-off filter. The sample can be temperature controlled with circulating water. For these measurements, the J-1500 CD detector is repositioned to the emission side.

### FDCD-551 | Artifact-Free FDCD Unit

The improvement in light collection efficiency and the ability to eliminate artifacts due to fluorescence anisotropy are two advantages of this FDCD accessory. Using a unique design that includes a sandwiched elliptical cylinder mirror with two plane mirrors, all fluorescence light emitted in a circumferential direction from the cell is collected. The end result is a highly sensitive, artifact-free FDCD spectrum.

### PTC-PLH | Polarizer for PTC-510/517

Adding this polarizer to the emission optics and utilizing the alternating horizontal and vertical polarization allows for the measurement of fluorescence polarization and anisotropy.

### FDCD-PLH | Polarizer for FDCD-550

This polarizer can be used with the FDCD-550 system to add fluorescence polarization and anisotropy capability in addition to fluorescence-detected CD.

# Stopped-Flow Series

Stopped-flow measurements involve the rapid mixing of two or more solutions to trigger a chemical reaction, the kinetics of which can be followed by CD, absorbance and fluorescence. All probe methods can be measured on the same instrument when the stopped-flow system is paired with a J-1500 CD spectrometer.

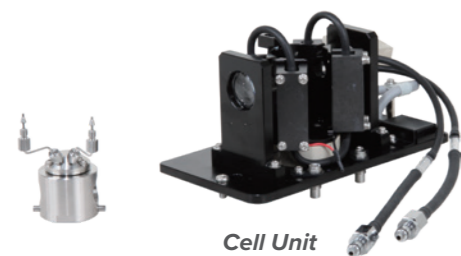


SFS-602

## Stopped-Flow Systems

### SFS-602

The SFS-600 series is an innovative stopped-flow measurement accessory with a modular design that allows the flow cell unit to be easily installed and removed from the sample compartment without alignment. Two-, three- and four-syringe models are available, offering flexible mixing as well as upgradeability for quench-flow. For temperature-dependent kinetic experiments, the options are Peltier temperature-controlled syringes. Stepper-motor-driven syringes allow infinitely variable mixing ratios and a mechanical mixer efficiently mixes solutions of different viscosities commonly used in protein folding experiments.



Cell Unit

- Applications to studies such as protein folding, substrate binding and enzyme kinetics
- Standard 2 mm cell (optional 0.5, 1 and 10 mm cells)
- Standard 10 mL syringe (optional 1, 2.5, and 5 mL syringes)
- 5 mL/sec flow rate with 10 mL syringe
- Exact control of flow rate
- Mixing ratio from 1:1 to 1:20
- Dead time: 0.57 msec with a 2 mm cell
- Peltier temperature control (SFS-602T/SFS-603T/SFS-604T) ranges from 5 to 80°C (with cell) and 5 to 60°C (with syringe)

**Note:** The SFS-500 series of stopped-flow accessories is still available for use with the J-1700 CD spectrometer.



## Unfolding of Concanavalin A by Trifluoroethanol

### Application

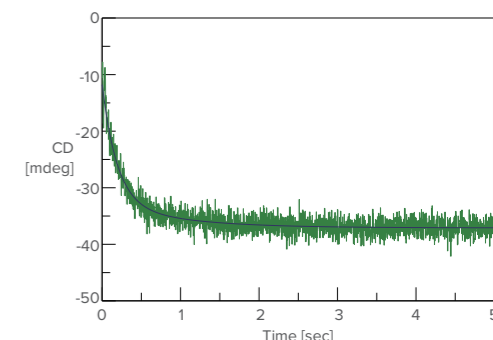
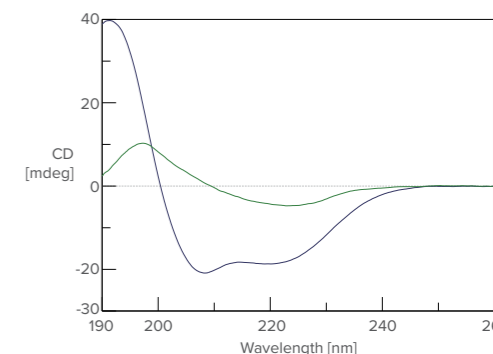
Concanavalin A is a lectin protein derived from the jack bean. In its native state, it is composed of abundant beta-sheet structures that change to alpha-helical form when exposed to trifluoroethanol (TFE).

The J-1500 and the SFS-602 high-speed stopped-flow system were used to measure the unfolding process of concanavalin A with TFE.

### Unfolding of Concanavalin A by Trifluoroethanol

Top: CD Spectra of concanavalin A  
 Green: CD spectrum of concanavalin A in pH2 hydrochloric acid  
 Blue: CD spectrum of concanavalin A in solution with 50% TFE

Bottom: Unfolding process of concanavalin A in TFE and analysis result



## Refolding of Cytochrome C using GuHCl

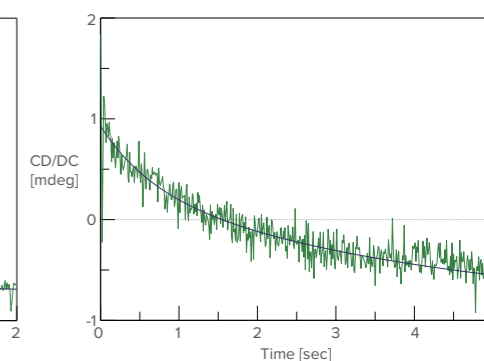
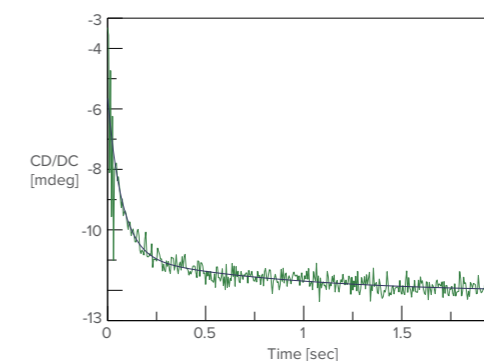
### Application

An aqueous solution of cytochrome C, which was denatured by guanidine hydrochloride (GuHCl), was prepared. CD stopped-flow measurement was performed using 0.1 M acetic acid buffer/water solution (1:9). The refolding process was observed at both 222 nm for the secondary structure and 289 nm for the environment of the aromatic side chain.

### Refolding of Cytochrome C

Left: Refolding measurement of cytochrome C (222 nm)

Right: Refolding measurement of cytochrome C (289 nm).



# High-Throughput CD

## Autosampling Systems

Recent trends in Combinatorial Chemistry and automated synthesis have lead to various new high-throughput measurement techniques. JASCO developed the high-throughput CD measurement system combining autosampler, syringe pump and flow cell unit for use with the J-1500 / J-1700. This system can accommodate two 96-well plates (up to 192 samples) and maintain a constant temperature prior to measurement. The system allows automated scanning measurements at predetermined parameters and/or temperature ramping measurement by using a Peltier thermostatted flow cell. In addition to CD, LD and absorbance data, fluorescence can be simultaneously measured as an option. Software control allows samples to be recovered after measurement for further analysis. The analysis program allows batch processing of data including determination of T<sub>m</sub> and secondary structure analysis.

- Applications include proteins, DNA, chiral organic components, monoclonal antibodies and more
- Sample cooling in autosampler
- Automated measurements with dedicated HTCD measurement software; easily generated measurement sequences, including wavelength scan and temperature scan modes
- Automated data handling



## HTCD-1500 Autosampling System

### J-1500 with ASU-800, ASP-849

The system comprises the ASU-800 microplate autosampler, ASP-849 syringe pump and a specialized flow cell and Peltier temperature controller, which is capable of automating CD measurement that includes sample pretreatment. The system is controlled via Spectra Manager™, JASCO's unique cross-platform program, which features a standard sequence measurement, as well as a sample measurement for prescreening samples; different load parameter options for running samples with different requirements in the same sequence; and advanced cleaning regimens.

# HPLC CD

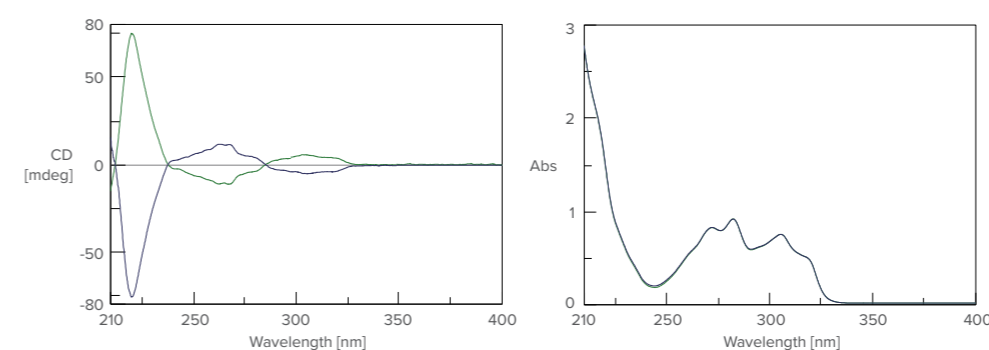
## Using the CD Spectrometer as a Chiral HPLC Detector of CD

HPLC is an effective method for quantitative detection of trace amounts of compounds and for mixture separation/purification. HPLC is also used for analysis of medicinal products and in food science. In these fields, samples often have optical activity allowing the analysis of enantiomeric excess and the separation/purification of the enantiomers. JASCO has been a pioneer in the development of chiral HPLC detection and offers an HPLC flow cell for J-1000 systems enabling acquisition of high-quality chromatographic data during chiral separations.

## HPLC-CD of Warfarin

### Application

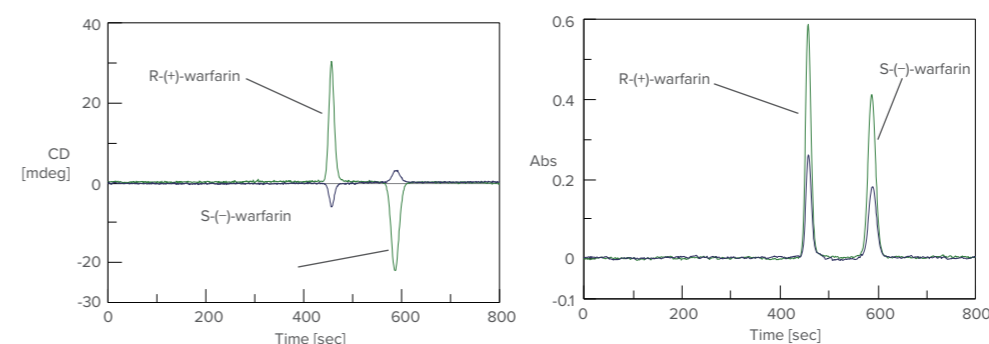
Warfarin was dissolved using a mixture of pH 2.0 aqueous phosphoric acid and acetonitrile. CD measurement was performed using a J-1500 outfitted with the LCCD-420 cell and connected to a conventional HPLC system.



**CD and Absorption Spectra of Warfarin**

Left: CD spectra of warfarin  
Right: Absorption spectra of warfarin

Green: R-(+)-warfarin  
Blue: S-(-)-warfarin



**CD and UV Absorption Chromatograms of Warfarin**

Left: CD chromatograms of warfarin  
Right: Absorption chromatograms of warfarin

Green: Chromatogram detected at 220 nm  
Blue: Chromatogram detected at 263 nm

### LCCD-420 | Flow Cell Attachment for LC-CD

The LCCD-420 enables the J-1000 to operate as an HPLC CD detector, and the chromatographic signal can be output

into any commercially available CDS (chromatography data system). Note: JWAOM-514 analog output function module program is required.



LCCD-420



# Magnetic CD

## Magnets and Cryostats

Placing the sample in a magnetic field allows measurement of magnetic circular dichroism (MCD) data. This method is a sensitive monitor of structural features that perturb the electronic states of an MCD-active chromophore. In protein molecules, MCD offers a probe of a chromophore's local environment because of its sensitivity to chromophoric electronic energy modulations induced by environmental perturbations. This technique has been generally used to study chromophores with large magnetic moments arising from rotational symmetries (aromatics, porphyrins), unpaired spins (metal complexes) or both (hemes). The MCD signal intensity is proportional to the magnetic field strength, which can be applied using either permanent magnets, electromagnets or super-conducting magnets:

JASCO offers a range of MCD options depending on the field strength and temperature desired, including:

- Permanent magnets with field up to 1.6 tesla at ambient temperature
- Electromagnets with field up to 1.5 tesla and low temperature cryostats
- Superconducting magnets with field of 8 tesla (and more)



MCD-581

## Magnetic CD Accessories

### MCD-581 | Electromagnet

Measure magnetic hysteresis and MCD spectra in a continuously variable field from -1.5 to 1.5 tesla. This magnet has a pole gap of 15 mm and a pole diameter of 21 mm. A regulated DC power supply unit is used to control the magnetic field strength. The magnet requires cooling water (minimum of 5 L/min) usually provided by a circulator system. Sample temperature can be maintained with an optional water-jacketed cell holder, which accommodates 10 mm cells. Spacers for 1, 2 and 5 mm cells are included. Low-temperature cryostats (CRYL-582 and CRYL-583) are also available.

accommodates 5 mm path length rectangular cells as standard. Optional holders are available for cells with 1 mm or 2 mm path lengths.

### CRYL-582 | Liquid Nitrogen Cryostat for Solid Samples

This cryostat is for solid samples up to 10 mm in diameter and has a temperature range from ambient down to -180 °C.

### CRYL-583 | Liquid Nitrogen Cryostat for Liquid Samples

For liquid samples, this cryostat has a temperature range from ambient down to -150 °C. Rectangular cells with path lengths up to 5 mm can be used.

### PM-491 | Permanent Magnet

Measure MCD spectra in a fixed magnetic field of + or -1.6 tesla, according to the orientation. With a weight of only 5.9 kg, this accessory can easily be placed in and out of the standard sample compartment. The magnetic field is easily reversed by turning the magnet 180°. This magnet

Note: For both cryostats, temperature control is achieved with the TC-22HK2 Temperature Controller. A vacuum pump is necessary for adequate insulation of the sample holder unit and the liquid nitrogen vessel (2 L capacity).



PM-491

# Linear Dichroism

## Couette Flow Cell Unit

### CFC-573

The most versatile approach to orienting macromolecules for LD measurements is the couette flow system. This system subjects the sample to a constant gradient over the annular gap between an inner quartz cylinder, which is rotating at high speed, and a fixed outer quartz cylinder (see Fig. 1). The CFC-573 Couette flow cell unit includes a built-in beam condenser, which focuses the beam onto the small LD flow cell to maximize light throughput. The cell unit is easy to install, remove and clean as needed.

- Applications to studies of proteins, DNA and biological or synthetic polymers
- Small (100  $\mu$ L) sample volume requirements and 0.5 mm path-length cell
- Continuously variable spinning speeds up to 5,000 RPM
- Temperature control using an external circulator



CFC-573

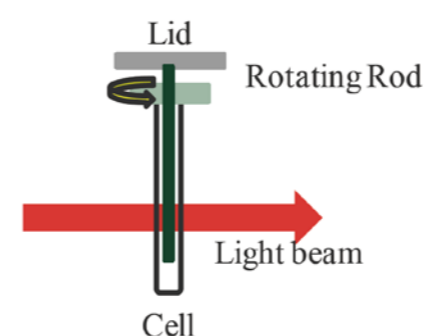
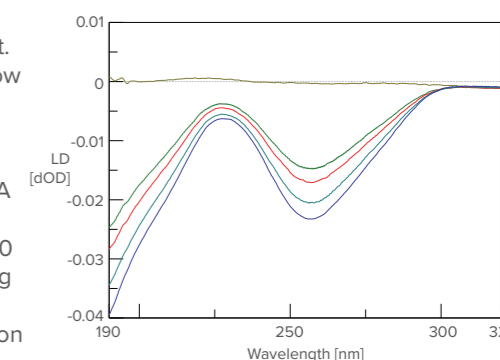


Figure 1. Schematic of the couette cell unit.

### Couette Flow Measurement

**Left:** Schematic of the couette cell unit. With the sample in the annular gap, flow orientation is achieved by rotating the inner cylinder.

**Right:** Linear dichroism spectra of DNA from calf thymus measured at rotation speeds of 500, 1,000, 2,000 and 3,000 rpm. The spectra were measured using data pitch of 0.2 nm with a scanning speed of 200 nm/min, a data integration time of 0.5 sec and a 1 nm bandwidth.



# Optical Rotatory Dispersion

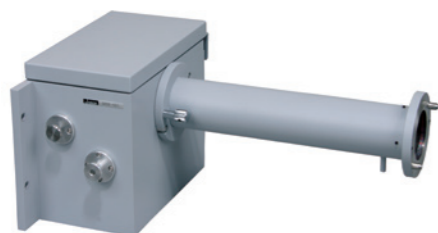


ORDM-520

## Optical Rotatory Dispersion

Complimentary and related to CD is the measurement of optical rotatory dispersion (ORD). This technique provides information on chiral molecules even without chromophores, such as saccharides. It can be used to measure the chirality of non-absorbing samples and the determination of absolute configuration.

JASCO offers two methods of ORD detection: optical null and intensity measurement systems. The intensity measurement method, using a fixed analyzer, is simpler and more economical, while the optical-null approach, with its rotating analyzer, is intrinsically more accurate because the measurement is absolute. Because ORD is very sensitive to the effect of strain in the sample cell window cylindrical cells are strongly recommended for use ORD measurement.



ORDE-521

## ORD Accessories

### ORDM-520 | ORD Attachment

This accessory allows detection of ORD over a wide angular range (90°) with very high accuracy using a rotating analyzer. No calibration is required, and switching back and forth from CD to ORD is handled automatically by the PC software. The system uses a separate optical path with a servo-driven analyzer and a dedicated PM tube.

### ORDE-521 | ORD Attachment

The electrical ORD accessory has an angular range up to 2°. Since the measurement principle is based on an electrical measurement method, the apparatus is simpler and is also able to respond faster to changes in ORD signals.

# Diffuse-Reflectance CD

## Diffuse-Reflectance CD

Samples that are insoluble or may change conformation when in solution have traditionally been difficult to characterize by CD. Diffuse reflectance, using an integrating sphere, is an effective way to analyze these samples, often dispersed into a finely ground scattering matrix such as KBr powder. In addition, diffuse transmission measurements of pellets or films is easily accomplished with the same integrating sphere, substantially increasing the collection efficiency for scattering samples and providing a suitable alternative to conventional transmission measurements.



DRCD-574



DRCD-575

## DRCD Accessories

### DRCD-574 | DRCD Attachment

The DRCD-574 unit utilizes a BaSO<sub>4</sub> interior for economical reflectance and transmittance measurements.

### DRCD-575 | DRCD Attachment

The DRCD-575 offers a Spectralon™ interior as well as N<sub>2</sub> purge port for improved performance at low wavelengths.



# Spectra Manager™ Software Suite

## Instrument Control

Drivers are available to control each JASCO spectroscopy system. Parameter dialogs allow easy editing of pre-saved parameter files. Data acquired from each instrument is automatically loaded into the analysis program (running in the background) in order to free up the PC and control software to acquire more data. Each instrument driver also has a module to allow for instrument hardware diagnostics and validation.

## Flexible Display Features

User-friendly features include overlay printing in colors and patterns, autoscale mode, full control of style and font, plus customized toolbars.

## Data Processing and Spectral Analysis

View and process several types of measurement data files (UV/Vis/NIR, FTIR, Fluorescence, etc.) in a single window, using a full range of data manipulation functions. Features include arithmetic operations, derivatives, peak detection and processing, smoothing (several methods) and baseline correction.

## Report Publishing

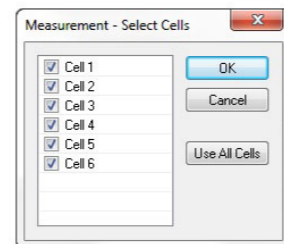
JASCO canvas allows the user to produce hard-copy layouts of data to meet individual reporting requirements.

## Macro Command Option

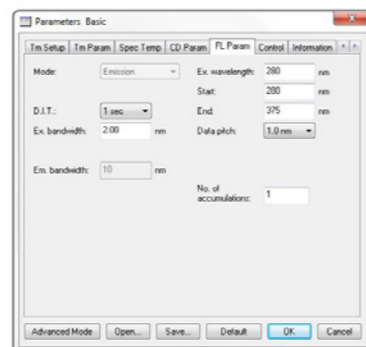
This software provides customized programs for a complete range of tasks, including data acquisition, post-run data manipulation and report printing.

## Secure Access with Spectra Manager™ CFR

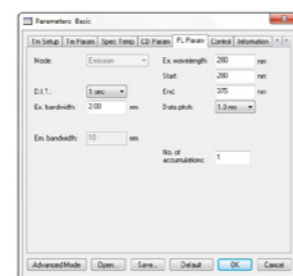
Spectra Manager™ CFR provides secure access and compliance features for 21 CFR Part 11. System access requires a username and password, which are assigned by the Workgroup Manager. Individual access levels determine the access to administrative tools, which includes instrument installation, analysis application installation, user setup, workgroup setup and security policies, as well as system and application history logs. Three levels of electronic signatures are required, including creation, review and approval stages. An audit trail is assigned to every data file, recording any manipulation on spectral data.



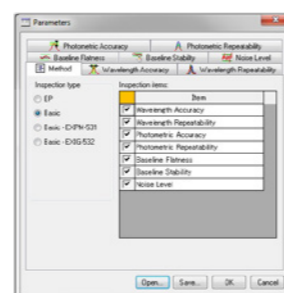
Sample selection of up to six cells with optional holder.



Parameter selection including three scanning modes.



Fluorescence parameter selection.



Easy-to-use software to validate instrument performance.

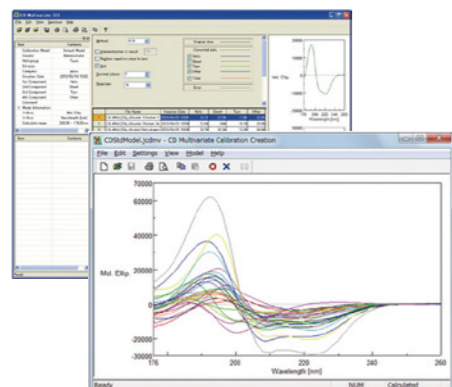


# A SINGLE PLATFORM FOR EVERY INSTRUMENT.

JASCO is the only manufacturer to develop a powerful, cross-platform 64-bit Windows software package for controlling a wide range of spectroscopic instrumentation. Spectra Manager™ is a comprehensive lab companion for capturing and processing data, eliminating the need to learn multiple software programs and allowing data from more than one instrument to be manipulated and displayed together on the same platform.

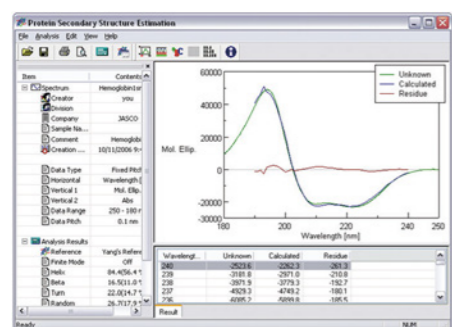


# Applications Software



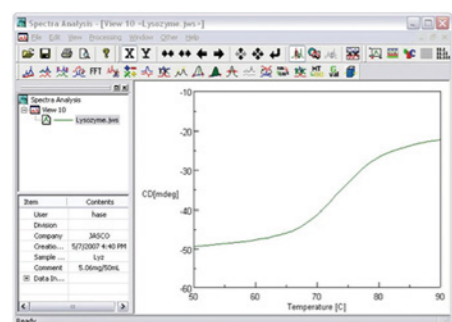
## Multivariate SSE Analysis Program

JWMVS-529 is a quantitative multivariate analysis (PCR/PLS) program for the estimation of protein secondary structures from CD spectra. The reference data set supplied includes 26 proteins and is flexible to allow the user to add additional proteins as desired or even create an entirely new reference data set. Quick and easy to use this program finally makes it easy to get the information often desired from CD spectroscopy.



## Interface for CDPro Secondary Structure Analysis

CDPro has been a popular program for many years combining several methods of secondary structure analysis in one package. The program uses methods developed by the Woody group at Colorado State University and also methods from the Johnson group at Oregon State University, Fasman group at Brandeis University and Provencher group at EMBL, Heidelberg. In the past, its use was difficult due to restricted OS and data file formats, but JASCO has developed an interface to run it quickly and easily, directly from the Spectra Manager™ program.

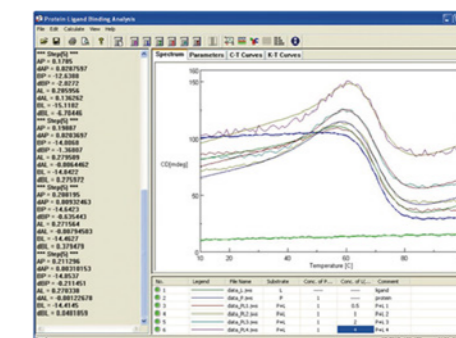


## Denatured Protein Analysis Program

JWTDA-519 enables calculation of the thermodynamic parameters ( $T_m$ ,  $\Delta H$ ,  $\Delta S$ ) of protein from the data with variable temperatures.

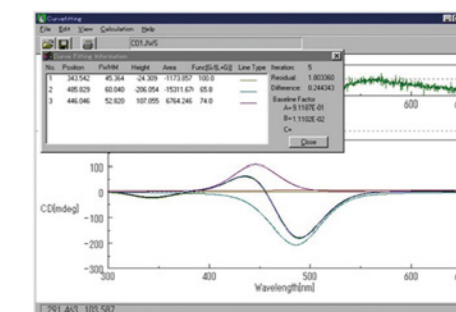
## Protein-Ligand Analysis Program

JWPLB-525 allows the dynamic analysis of proteins that are denatured in the presence of ligand, based on CD spectra with variable temperature of both the isolated ligand in solution and a set of spectra of protein and ligand mixtures.



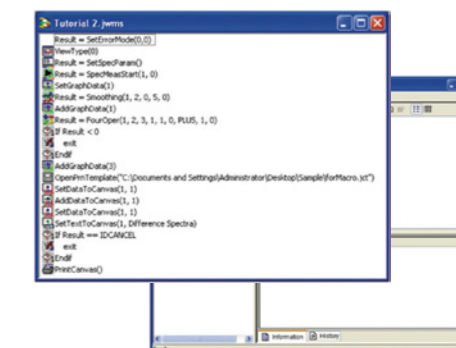
## Curve Fitting Program

Curve fitting is a function that can be applied to a variety of spectroscopic techniques, including FTIR and UV-visible. The JWCVF-518 program applies this analysis technique to CD spectra. Curve fitting is a method used to resolve multiple components by finding the heights, widths and positions of overlapping bands contained in a spectrum and using a variety of regression algorithms including variable bandwidths.



## Macro Command Program

JWMCRC-512 allows full automation from data measurement to complete analysis—and even presentation using preset templates in the JASCO Canvas program. Routine measurements become easy; it's a matter of inserting the sample, pressing go and finding the analyzed results on the printer or network. The simple GUI-driven interface allows even novices to compose macro scripts using editable tools for parameter setting.



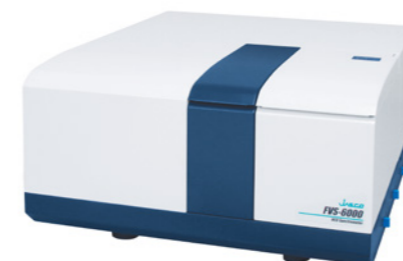
# Specifications

Model	J-1100	J-1500	J-1700
Light Source	150W air-cooled Xe lamp	150W air-cooled Xe lamp (J-1500-150) or 450W water-cooled Xe lamp (J-1500-450)	150W air-cooled Xe lamp (J-1700-150) or 450W water-cooled Xe lamp (J-1700-450) 150W halogen lamp
Optional Light Source	N/A	20W Halogen lamp, 150W air-cooled Hg-Xe lamp	N/A
Light Source for Validation	Integrated Mercury lamp		
Detector	PMT	PMT, ExPMT (option), InGaAs (option)	PMT, Dual InGaAs
Monochromator	Double-prism polarizing monochromator		Double-prism polarizing monochromator and grating monochromator
Wavelength Range	180 to 600 nm	163 to 950 nm (standard) 163 to 1600 nm (option)	163 to 2500 nm 163 to 950 nm (PMT), 900 to 2500 (InGaAs)
Wavelength Accuracy	±0.2 nm (180 to 250 nm) ±0.4 nm (250 to 500 nm) ±0.8 nm (500 to 600 nm)	±0.1 nm (163 to 250 nm) ±0.2 nm (250 to 500 nm) ±0.5 nm (500 to 800 nm) ±1.5 nm (800 to 950 nm)	±0.1 nm (163 to 250 nm) ±0.2 nm (250 to 500 nm) ±0.5 nm (500 to 800 nm) ±1.5 nm (800 to 950 nm) ±2.0 nm (1200 to 1600 nm) ±5.0 nm (1600 to 2500 nm)
Wavelength Reproducibility	±0.05 nm (163 to 500 nm) ±0.1 nm (500 to 600 nm)	±0.05 nm (163 to 500 nm) ±0.1 nm (500 to 800 nm) ±0.5 nm (800 to 950 nm)	±0.05 nm (163 to 500 nm) ±0.1 nm (500 to 800 nm) ±0.5 nm (800 to 1600 nm) ±1 nm (1600 to 2500 nm)
Wavelength Resolution	0.025 nm		
Spectral Bandwidth	1 nm	0.01 to 16 nm	0.01 to 16 nm (163 to 950 nm) 5, 10, 20, 30, 40, 50 nm (950 to 2500 nm)
Slit Width	1 to 4000 μm		
Digital Integration Time	8 msec to 8 sec	0.1 msec to 30 sec	
Measurement Mode	Continuous scan, step scan, auto-scan		
Scanning Speed	up to 5,000 nm/min	up to 10,000 nm/min	
CD Full Scale	±8000 mdeg		
CD Resolution	0.00001 mdeg		
CD Dynamic Range	No CD distortion even with an OD=3 sample in the optical path		
Stray Light	less than 0.0003% (at 200 nm)		
RMS Noise (185 to 500 nm: SBW 1 nm, DIT 8 sec.) (1500 nm: SBW 10 nm, DIT 8 sec.)	0.03 mdeg (200, 500 nm)	0.004 mdeg (185nm, 150W) 0.003 mdeg (185nm, 450W) 0.007 mdeg (200, 500 nm)	0.004 mdeg (185nm, 150W) 0.003 mdeg (185nm, 450W) 0.007 mdeg (200, 500 nm) 0.06 mdeg (1500 nm, W1 light source)
Baseline Stability	0.05 mdeg/hr	0.02 mdeg/hr	
LD Measurement	Provided as standard, Full scale ±1 ΔOD		
UV Measurement	Provided as standard, Full scale up to 5 Abs		
External Input Terminals	Two channels (input range: -1 to 1 V DC)		
Nitrogen Gas Purge	High efficiency N <sub>2</sub> purge with internal optimization for light source unit, monochromator unit and sample compartment		
Accessory Auto-Recognition	Standard		
Communication / Control	USB 2.0 / Spectra Manager™ or Spectra Manager™ CFR		
Sample Compartment Size	105 W x 150 D x 110 H mm	150 W x 310 D x 165 H mm	
Dimensions	740 W x 545 D x 325 H mm	1055 W x 545 D x 390 H mm (J-1500-150) 1135 W x 610 D x 420 H mm (J-1500-450)	1266 W x 545 D x 390 H mm (J-1700-150) 1346 W x 610 D x 420 H mm (J-1700-450)
Weight	70 kg	77 kg (J-1500-150), 82 kg (J-1500-450)	87 kg (J-1700-150), 92 kg (J-1700-450)
Power Input Voltage	100, 115, 200, 220, 230, 240 V, 50/60 Hz		
Power Consumption	315 VA	315 VA (J-1500-150), 685 VA (J-1500-450)	600 VA (J-1700-150), 1000 VA (J-1700-450)

# Additional Instruments

## Vibrational Circular Dichroism

### FVS-6000



The system is capable of measuring conventional IR absorption along with vibrational CD and is controlled by the Spectra Manager™ spectroscopy software suite.

- Digital signal processing (DSP) to enhance sensitivity
- Thermally stabilized modulator system to eliminate baseline drift
- Extra large dewar to allow up to 15 hours of operation without refill
- Auto-alignment system to eliminate linear anisotropy artifacts
- High-intensity ceramic light source for maximum energy and lifetime up to 10 years

## Circularly Polarized Luminescence

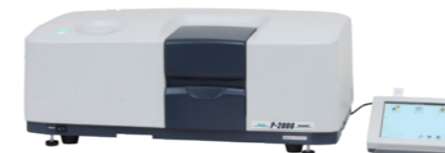
### CPL-300



Circularly polarized luminescence systems are designed to supplement other chiroptical techniques like circular dichroism, providing chiral information of the excited state properties. The CPL-300 uses the original 180° fluorescence collection approach proposed by Steinberg. The standard ozone-free 150W Xe lamp can be user-replaced with an Hg/Xe source. The instrument's double-prism excitation and emission monochromator delivers very low stray light and no spurious linear polarization effects caused by diffraction gratings.

## Digital Polarimeter

### P-2000



The P-2000 is designed as a customizable polarimeter with various options for an array of applications and budgetary requirements. The system can also be field-upgraded as application requirements change. Options for wavelength filters and source lamps provide a wide range of analytical wavelengths from UV-Vis to NIR.



**JASCO INTERNATIONAL CO., LTD.**

11-10, Myojin-cho 1-chome, Hachioji, Tokyo 192-0046, Japan

Tel: +81-42-649-3247 Fax: +81-42-649-3518 <http://www.jascointl.co.jp/english/>

Australia, China, Hong Kong, India, Indonesia, Japan, Korea, Malaysia, New Zealand, Pakistan, Philippines, Russia, Singapore, Taiwan, Thailand

**JASCO, INCORPORATED**

28600 Mary's Court, Easton, Maryland 21601, U.S.A.

Tel: +1-410-822-1220 Fax: +1-410-822-7526 Web: [www.jascoinc.com](http://www.jascoinc.com)

Argentina, Bolivia, Brazil, Canada, Chile, Colombia, Costa Rica, Guatemala, Mexico, Paraguay, Peru, Puerto Rico, United States of America, Uruguay, Venezuela

**JASCO EUROPE S.R.L.**

Via Luigi Cadorna 1, 23894 Cremella (LC), Italy

Tel: +39-039-9215811 Fax: +39-039-9215835 Web: [www.jasco-europe.com](http://www.jasco-europe.com)

**JASCO Deutschland** [www.jasco.de](http://www.jasco.de) | **JASCO UK** [www.jasco.co.uk](http://www.jasco.co.uk) | **JASCO France** [www.jasco.fr](http://www.jasco.fr)

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BFP-1808 Printed in Japan



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