#### J-1000

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#### Circular Dichroism

#### J-1000 Series Circular Dichroism Spectropolarimeters

A circular dichroism spectrometer for exploring the structure and stability of small and biological chiral molecules.

The J-1000 Series Circular Dichroism spectrophotometers are specifically designed for high sensitivity measurements in the near- and far-UV regions, for scientists that need confidence in the data from characterization studies of biomolecule structure, function, and stability under a wide variety of experimental conditions.

Unlike some detectors which only provide good signal-to-noise for low absorbing materials, the J-1000 Series circular dichroism spectrophotometers use high dynamic range detectors to obtain high-quality spectra of samples with excellent signal-to-noise, especially for highly absorbing materials found in the far-UV.



**J-1500** Circular Dichroism Spectrophotometer

#### Features of the J-1000 Series

- High optical throughput
- · Double prism monochromator providing low stray light
- · Wide dynamic range PMT detector
- · Highly efficient nitrogen purge system
- · Digital signal processing
- Simultaneous Multi-Probe: CD, LD, HT, DC, absorbance, fluorescence

#### **Benefits and Accessories**

- Compact benchtop design
- · Range of precise temperature control accessories
- · High-throughput automated CD
- · Automated titration and stopped-flow
- Spectra Manager<sup>™</sup> software for control and extensive data analysis
- · Flexible design allows field upgrades for different measurement capabilities as applications and budgets evolve

#### Versatility for a Wide Range of Applications

- · Protein conformational studies
- · Quantitative analysis of pharmaceuticals
- · Formulation studies
- · Protein folding studies
- DNA/RNA interactions
- · Enzyme kinetics
- · Purity testing of optically active substances
- · Natural products chemistry

### J-1100 Circular Dichroism Spectrophotometer

The J-1100 Circular Dichroism spectrophotometer is a compact, general-purpose space-saving design. This simple yet powerful instrument is perfect for users looking to obtain more routine CD measurements in both industry and academia.

The J-1100 uses simple optimized parameters so that a wide range of users with different levels of CD knowledge can get right down to work and successfully obtain high quality data. The wavelength range from 180 to 600 nm is suitable for obtaining secondary and tertiary structure measurements in the



near- and far- UV. When fitted with a Peltier cell holder, the J-1100 be used for measurement of CD, LD and absorbance as a function of wavelength, temperature and time.

The intuitive Spectra Manager™ Suite of spectroscopy software provides the user with sample measurement, independent from the data processing and analysis. This allows users to obtain new measurements while simultaneously analyzing previously acquired data for increased productivity.

### J-1500 Circular Dichroism Spectrophotometer

The J-1500 allows for the maximum flexibility to upgrade your CD system with different measurement techniques. While the standard measurement modes are CD, LD, and absorbance, up to four simultaneous modes can be measured when combined with a wide range of sampling accessories.



These accessories can measure a variety of samples, from liquids to films to solid-states. Temperature control systems

can be coupled with multi-position cells to run thermal melts, providing researchers with CD and thermodynamic data sets for conformational and folding studies. Automated high-throughput CD can obtain measurements on up to 192 samples without user intervention, saving both time and money. Kinetic and protein dynamics studies can be performed with our dedicated stopped-flow systems that can measure both CD and fluorescence.

The wavelength range has also been significantly extended, allowing measurements to be obtained in both the vacuum-UV and NIR spectral regions using the standard PMT detector (163 – 950 nm) and an optional InGaAs detector (up to 1600 nm). Additional features now allow researchers to optimize their parameter specifications in order to obtain data with the highest resolution and S/N performance for a specific application set.

### J-1700 Circular Dichroism Spectrophotometer

The J-1700 was specifically designed for more demanding near-infrared CD applications. In addition to the enhanced far-UV capabilities, researchers probing the chiral activity of molecules in the NIR spectral region now have the ability to obtain data at wavelengths up to 2500 nm. The InGaAs detector has a wavelength range from 900-2500 nm, while the PMT ranges from 163-960 nm. The automatic detector interchange allows researchers to obtain both far-UV and



NIR measurements without having to manually switch detectors. The addition of a grating monochromator to the double-prism monochromator setup provides low stray light and high light intensity, generating CD signals with high S/N performance throughout a large spectral range.

NIR-CD applications vary from conformational and chirality studies of metal coordination complexes to tuning chiral properties of nanomaterials. Additionally, Magnetic Circular Dichroism (MCD) can be used in conjunction with NIR-CD to probe a chromophore's electronic structure as well as to induce chirality in compounds.

# High-Throughput Circular Dichroism System (HTCD)



J-1500-HTCD High-Throughput Circular Dichroism system

The high-throughput circular dichroism (HTCD) measurement system has been developed for use with either the J-1500 or J-1700 CD spectropolarimeter. This system can accommodate two 96-well plates (up to 192 samples) with protection at controlled temperature prior to measurement. Measurements using predetermined parameters for automated spectral scanning can be made with a Peltier thermostatted flow cell. In addition to CD, LD and absorbance data, fluorescence can be measured simultaneously (with optional accessory). Small sample amounts are required and can be recovered back to the micro-plate after measurement. The post-measurement analysis program allows batch processing of data and includes spectral correlation for quality control and secondary structure estimation.

- · Applications include peptides, proteins, nucleic acids, chiral organic components, monoclonal antibodies etc.
- Micro-plate temperature control
- Automated measurements with Spectra Manager-HTCD software; easily generated measurement sequences, including wavelength scan and temperature scan modes
- · Automated data processing

### Temperature Control

Three single-position Peltier thermostatted cell holders (PTC-510, 514, 517) are available for temperature control using the three Spectra Manager™ software programs. 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, as well as a magnetic stirrer to ensure thermal equilibrium. The cell holders can be used with cells of 10, 5, 2, 1 and sub-1 mm pathlengths.



The multi-position Peltier cell-changers are designed for high sample throughput and productivity. The six-position holder for rectangular cells is used for automated, simultaneous measurement of spectral scans and parallel thermal ramps for up to six samples. Thermal ramping at single or multiple wavelengths as well as thermal ramping with spectral scanning at preset temperatures are also possible.



The MPTC-513 cell holder can be used for fluorescence measurement, including total fluorescence (TFA-555), scanning excitation/emission fluorescence (FMO-522) and fluorescence anisotropy (FPA-580).

# Automated High-Throughput CD

Automated high-throughput CD can obtain measurements on up to 192 samples without user intervention, **removing the possibility of human error** and saving both time and money.

Recent trends in Combinatorial Chemistry and automated synthesis have lead to various new high-throughput measurement techniques. JASCO developed a high-throughput CD measurement system combining an autosampler, syringe pump and flow cell unit for use with the J-1500/1700.

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 measurements 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 Tm and secondary structure analysis.



J-1500-HTCD High-Throughput Circular Dichroism system

## Microsampling

In the case of samples where only very small volumes are available, two microsampling accessories are now available. The microsampling disk (MSD-462) is designed for sample measurements as small as 2  $\mu$ L with a 0.2 mm spacer and 10  $\mu$ L with a 1.0 mm spacer.



For thermal ramping studies of microvolume samples, JASCO also offers a capillary cell jacket (CAP-500), which allows for samples with volumes as small at 5  $\mu$ L to be placed in a Peltier cell holder. Melting curves are now easily measured, including Tm,  $\Delta$ S and  $\Delta$ H values.

### Stopped-Flow

Stopped-flow measurements involve the rapid mixing of two or more solutions to trigger a chemical reaction. The reaction kinetics can then be followed by CD, absorbance and fluorescence. All measurement techniques can be acquired on the same instrument when the stopped-flow system is paired with a J-1500 or J-1700 spectrophotometer.



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 and

T-jump experiments. For temperature-dependent kinetic measurements, the options include Peltier temperature-controlled syringes. Stepper-motor-driven syringes allow variable mixing ratios and a mechanical mixer efficiently mixes solutions commonly used in protein folding experiments.

- 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 of 2.1 ms with a 0.5 mm cell
- Peltier temperature control ranges from 5 to 80°C and 5 to 60°C for the cell and syringe, respectively



# Total Fluorescence & Fluorescence Detected Circular Dichroism

Intrinsic fluorescence spectra can be measured using the J-1500 or J-1700 Circular Dichroism spectrophotometers with the optional scanning emission monochromator (FMO-522) and emission detector (FDT-538). Alternatively, high-pass filters can be used to select specific excitation and emission wavelengths. The low-cost Total Fluorescence Accessory (TFA-555) is used to detect fluorescence changes during titration or thermal ramp experiments.



In addition, removing the filters allows the user to measure the sample's 90° light scattering,



FMO-522 fluorescence monochromator

FDT-538 fluorescence detector

simultaneously with CD and absorbance data collection.

- When used with the MPTC-513 temperature control accessory, CD and fluorescence data can be acquired either simultaneously or separately for up to six samples.
- Fluorescence scanning can be coupled with the titration and temperature control accessories.

#### Fluorescence-Detected Circular Dichroism

Fluorescence-detected circular dichroism (FDCD) is used to measure the difference in fluorescence emission when an optically active sample has been excited with circularly polarized light. This method takes advantage of the chiral specificities and the structural sensitivities of CD and fluorescence and is more specific than standard CD measurements.

Since FDCD selectivity measures the circular dichroism of a specific fluorescent chromophore present in a group of non-fluorescent chiral molecules, it is particularly useful for the study of proteins that have multiple chromophores. FDCD can be measured using the standard CD detector when paired with the PTC-510, PTC-517 or MPTC-513 cell holder. When samples have no fluorescence anisotropy, this method is effective because the photo selection artifacts are small. However, when the sample has a larger fluorescence anisotropy, the photo selection artifact will distort the FDCD spectrum.



The FDCD-551 attachment is specifically designed to reduce or eliminate these artifacts while greatly enhancing sensitivity due to much more efficient light collection.

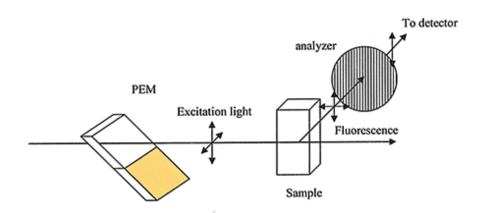


FDCD-550 Standard accessory for measurement

FDCD-551 enhanced sensitivity accessory for measurement

#### **Fluorescence Polarization Anisotropy**

Fluorescence anisotropy occurs when polarized light interacts with a fluorescent molecule and the resulting fluorescence emission has different intensities along different polarization axes. 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, fluorescence anisotropy can be measured. Adding the FPA-580 polarizer to the emission optics and utilizing the alternating horizontal and vertical polarization allows for the measurement of fluorescence polarization anisotropy.



### **Automated Titration**

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 for studies involving protein denaturation or ligand binding. Dual syringes are employed and are each equipped with a valve for automated refilling and flushing during extended runs and for maintaining a constant cell volume. Additionally, the titration measurement program automatically corrects for concentration.



### Magnetic CD

Placing a sample in a magnetic field allows for magnetic circular dichroism (MCD) measurements to be obtained. In protein molecules, MCD can be used as a probe to monitor a chromophore's local environment. Chromophores with large magnetic moments arising from either rotational symmetries (aromatics, porphyrins), unpaired spins (metal complexes), or both (hemes) are sensitive to electronic perturbations and therefore provide information regarding the molecule's electronic state. The MCD signal intensity is proportional to the magnetic field strength, which can be applied using either permanent magnets, electromagnets or super-conducting magnets.

- Permanent magnets with field strengths up to 1.6 tesla at ambient temperature
- Electromagnets with field strengths up to 1.5 tesla
- Superconducting magnets with field strengths of 8 tesla



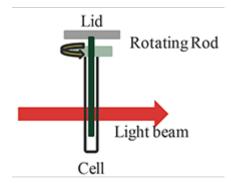


#### Linear Dichroism

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 r

otating at high speed, and a fixed outer quartz cylinder. The CFC-573 Couette flow cell unit includes a built-in beam condenser that 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.

- Small (100 µL) sample volume requirements and 0.5 mm pathlength cell
- Continuous variable spinning speeds up to 7,000 RPM
- Temperature control using an external circulator





CFC-573

### Optical Rotary Dispersion

Optical Rotatory Dispersion (ORD) 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. Since ORD is very sensitive to strain in the sample cell window, cylindrical cells are strongly recommended for use ORD measurement.





## CD of Solid Samples

Samples that are insoluble or may change conformation when in solution have traditionally been difficult to characterize by CD. Diffuse reflectance uses an integrating sphere to effectively analyze these samples. 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.





# Extended Wavelength

Near Infrared (NIR)-ECD spectra of metallo-protein and metal complexes are known to be sensitive to conformations of the metal's ligands as well as the configuration around the central metal atom, which is used for structural analysis of these molecules.

The J-1500 CD spectrometer can be used for spectral measurements into the NIR region using an extended wavelength range light source and detector. In this configuration, the InGaAs detector kit includes a halogen lamp unit and allows for measurement up to 1600 nm.





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