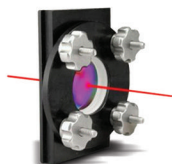


## VCD Accessories



**BioCell™**  
Cell for measurements  
of aqueous solutions



**TempCon™**  
Temperature controller  
for FT-IR cells

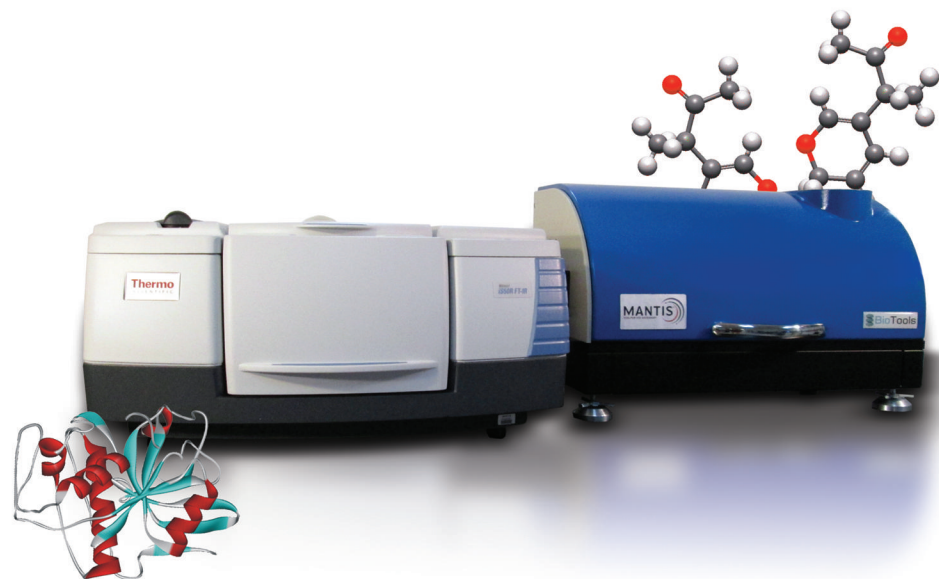


**SyncRoCell™**  
Rotating stage for  
elimination of cell artifacts  
and measurements of solids

# MANTIS™

DUALPEM VCD ACCESSORY

## VCD Accessory for Thermo FT-IR



LOOK AT MOLECULES WITH A *TWIST* OF LIGHT



Characterization Experts: Chirality & Biologics

17546 Bee Line Highway  
Jupiter, Florida 33478 USA  
ph. 561.625.0133 | fax. 561.625.0717  
email: [info@btools.com](mailto:info@btools.com)  
[www.btools.com](http://www.btools.com)

## Vibrational Circular Dichroism (VCD)

VCD is defined as the difference in the absorbance ( $A$ ) of left minus right circularly polarized infrared radiation,  $A = A_L - A_R$ . VCD extends the functionality of electronic Circular Dichroism (CD) into the infrared spectral region where vibrational transitions in molecules are observed.

VCD combines the structural specificity of FT-IR spectroscopy with the stereo-sensitivity of circular dichroism. This gives access to multiple, well-defined bands that provide molecular quantitative information. Measurements can be done in solids and solutions.

Thousands of molecules have been measured with VCD over the past few years; VCD data is accepted by regulatory agencies and all major journals.

## USP Chapters on VCD

### USP Chapters <782> & <1782>

Vibrational circular dichroism (VCD), an important analytical method for determining the absolute configuration (AC) and purity of chiral molecules, has been published as a new "standard method" in the U. S. Pharmacopeia (USP 39-NF34, Chapters 782 and 1782). The chapters became official on December 1st, 2016.

The chapters were written by a consortium of scientists from key pharmaceutical companies and the two co-founders of BioTools, VCD experts Dr. Rina K. Dukor and Prof. Laurence A. Nafie. Chapter <782> details aspects of VCD usages including qualification of VCD spectrometers, sample measurements, validation, and verification of measured spectra. Chapter <1782> provides specific examples of instrumentation, finer points of qualitative and quantitative analysis, comparisons between measured and calculated spectra, determination of enantiomeric excess (%EE), and concurrent use of AC and %EE.

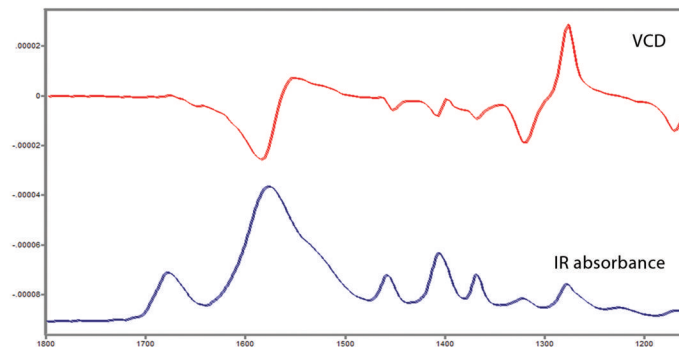
**THERMO FT-IR MODELS AVAILABLE FOR MANTIS™ UPGRADE:**

**Nicolet i550**

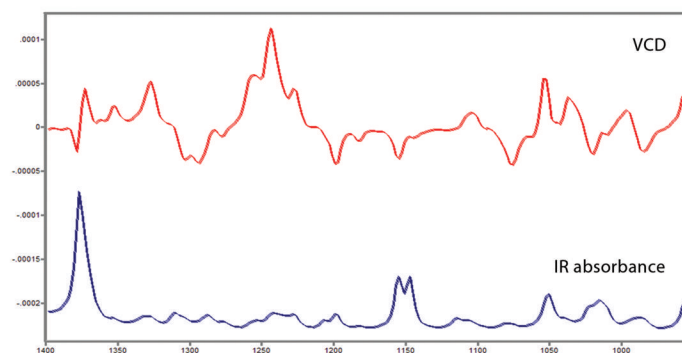
**Coming Soon iS10, 670, 870, 6700, 8700; Nexus 750, 550**

## Sample Spectra & Software

### L-Dialanine (H<sub>2</sub>O solution)



### R-Limonene (CCl<sub>4</sub> solution)



### ComputeVOA™ Software

An all inclusive package for calculation of VCD spectra. Combines: structure building, extensive conformational search, easy integration with Gaussian09 and plotting of calculated spectra.



### CompareVOA™ Software

Confidence level algorithm for comparing VCD (and ROA) experimental and theoretical spectra; the output generates two plots: IR and VCD comparisons of measured and calculated spectra, and statistical plot against a database of prior comparisons.