

ABSOLUTE CONFIGURATION BY VCD



Spring 2020 | AN-VCD04

UNAMBIGUOUS. FAST. IN SOLUTION.
NO CRYSTALLIZATION. NO DERIVATIZATION.

DISCOVER WHY VCD HAS BECOME THE
TECHNIQUE OF CHOICE FOR CHIRAL ANALYSIS

Determination of absolute configuration (AC) of chiral molecules is an important step in any field related to chirality but nowhere is it as critical as in the pharmaceutical industry. The phenomenon of “chiral recognition” – in which the enantiomers of a chiral drug may exhibit differences in biological activity or other processes such as distribution, uptake, and metabolism—makes it a necessity (or requirement) to know the AC not only of the final molecule but as early in the process of development as possible.

Within the past few years it has been conclusively demonstrated that vibrational circular dichroism (VCD) is a reliable method for AC determinations. VCD offers a novel alternative to X-ray crystallography, permitting AC determinations on neat liquid, oil, and solution samples. VCD requires no derivatization of the sample or growth of a pure single crystal. VCD is defined as the differential absorption of a molecules for left circularly polarized infrared (IR) light versus the right during a vibrational transition. VCD combines the structural specificity of vibrational IR absorption spectroscopy with the stereochemical sensitivity of a chiroptical spectroscopy such as CD. The absolute stereochemistry is established by comparing the solution-phase VCD spectrum to the results of an *ab initio* quantum chemistry calculation. The calculations are easily carried out in commercial packages such as Gaussian (Gaussian, Inc., Pittsburgh, Pennsylvania).

AWARD WINNING PATENTED TECHNOLOGY WHAT OUR CUSTOMERS ARE SAYING

“Over the last several years, the Vibrational Circular Dichroism (VCD) technique has dramatically revitalized the utility and visibility of vibrational spectroscopy within pharmaceutical drug discovery. The ability of VCD to deliver absolute chiral assignments without the need for standards or crystallizations, renders the technology a vital complement to traditional pharmaceutical analytical technologies.”

Dr. Don Pivonka, AstraZeneca

“As a long-standing analytical chemist in pharmaceutical research with a focus on vibrational spectroscopy, I recognized the potential impact VCD could have on many aspects of big pharma. With the ChiralIR I have successfully assigned the configurations of more than 600 exploratory drug molecules, providing an international service to research facilities in Europe and the United States. I consider this instrument to be world-class and a bargain for the price given its state-of-the art technology and incredible level of reliability.”

Dr. Douglas James Minick, Senior Research Investigator, GlaxoSmithKline



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WE PROUDLY SERVE HUNDREDS OF COMPANIES, UNIVERSITIES AND GOVERNMENT AGENCIES

Over **5,000** determinations have been carried out over the last few years and many results have been submitted and accepted by legal and regulatory agencies. Various research has been published in top scientific publications.

AbbVie
AIST
Amgen
AstraZeneca
Averca Discovery Services
BASF
Bayer Pharma AG
Beijing University
Biogen
Boehringer-Ingelheim
Bristol-Myers Squibb (BMS)
Caltech
Caymen Chemical
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Cell Therapeutics
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y de Estudios
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Dow AgroSciences LLC.
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Shanghai Institute of Organic
Chemistry (SIOC)
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University of the Air
University of Korea
University of California,
San Diego
U. of So. California
University of Illinois
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