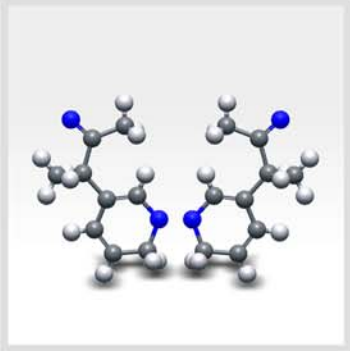
Absolute Configuration by VCD

Spring 2012
AN-VCD02

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).

Over 4,000 determinations have been carried out over the last few years and many results have been submitted and accepted by legal and regulatory agencies.

JOIN THE LEADERS IN VCD REVOLUTION (selected list)

- AIST
- Amgen
- AstraZeneca
- Biogen IDEC
- Boehinger-Ingelheim
- Bristol-Myers Squibb
- Cell Therapeutics
- Centro de Investigacion y de Estudios
- Creighton University
- Danish School of Pharmacy
- Drexel University
- Ehime University
- Eli Lilly
- ETH
- Food & Drug Administration (FDA)
- Galleon Pharmaceuticals
- Gilead
- GlaxoSmithKline
- Hokkaido University
- Inha University
- Intrexon Corp.
- Johnson & Johnson
- Medivation
- Merck
- Millennium Pharamaceuticals
- Naval Research Labs
- Neurocrine Biosciences
- Pfizer
- Roche
- Sanofi-Aventis
- Sunovion
- Syngenta Crop Protection
- Syracuse University
- Tokyo College of Pharmacy
- United Therapeutics
- University of the Air
- University of Korea
- U. of So. California
- University of Zurich
- Vanderbilt University
- Vertex Pharmaceuticals
- Viamet Pharmaceuticals
- York College

17546 Bee Line Highway • Jupiter, FL 33458 USA
Tel: (561) 625-0133 • Toll Free: (866) BTOOLS1
Fax: (561)625-0717 • Email: info@btools.com

BioTools
www.btools.com