



Chiral analysis of Ibuprofen using a Circular Dichroism Detector

Introduction

Ibuprofen is a well known non-steroidal anti-inflammatory drug and widely used for pain relief and fever reduction. Only the S enantiomer of ibuprofen has active antipyretic properties, but within the human body an enzymatic reaction can readily convert the R enantiomer into the S enantiomer.

The Circular Dichroism detector is well known for its high accuracy and selectivity for chiral analysis of compounds that have chromophores close to the chiral center. Both CD and UV signal are measured simultaneously and spectral scanning can be used to optimize the wavelength of interest, which is important in the measurement of chiral compounds. Not only can the CD detector help differentiate between two enantiomers, but it can also distinguish between achiral impurities and enantiomers of interest.

Keyword: Ibuprofen, enantiomer, CD detector, CHIRALPAK AD-RH

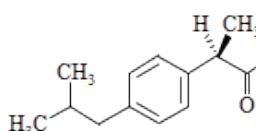
Experimental

[Equipment]

Pump: PU-4185
Pump option: Degasser unit
Autosampler: AS-4050
Column oven: CO-4060
Detector: RI-4095

[Conditions]

Column: CHIRALPAK AD-RH (4.6 mm I.D. x 150 mm L, 5 μ m)
Eluent A: 0.1% phosphoric acid aqueous solution
Eluent B: Acetonitrile
Composition: Eluent A/B (60/40)
Flow rate: 0.5 mL/min
Column temp.: 25°C
Wave length: 230 nm
Response: 1.5 sec
Scan speed: 10 nm/sec
Injection volume: 10 μ L
Standard sample: Mixture of 50 μ g/mL Caffeine and 200 μ g/mL racemic ibuprofen in eluent A/B (60/40)



Ibuprofen

Results

Fig. 1 Chromatograms of caffeine and racemic ibuprofen standards. The UV chromatogram shows that both compounds are detected, but in the CD chromatogram only ibuprofen can be detected, as the caffeine is achiral. Fig. 2 CD and UV spectra (measured using stopped-flow).

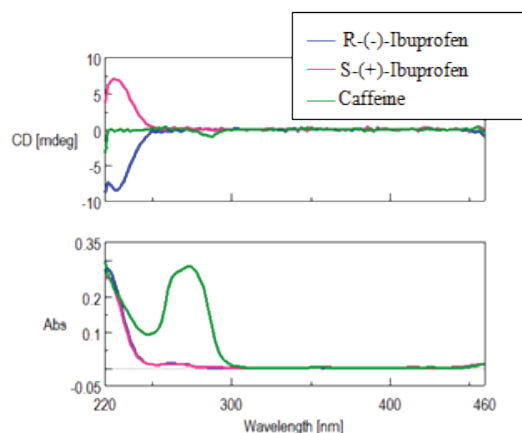
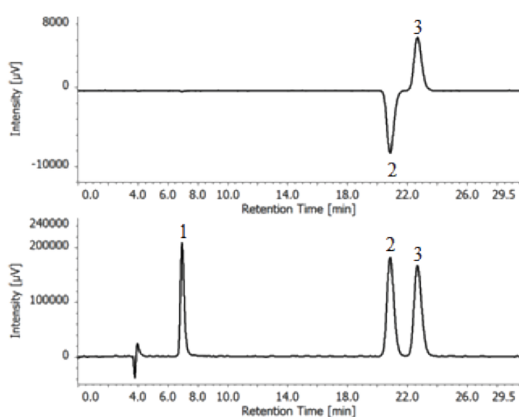


Figure 1. Chromatogram of Caffeine and Racemic Ibuprofen standards. Top: CD detection, Bottom: UV detection. 1: Caffeine, 2: R-(-)-Ibuprofen, 3: S-(+)-Ibuprofen

Figure 2. Spectral Measurement. Top: CD, Bottom: UV

P/N	Description
7003-J014A	PU-4185 RHPLC Semi-micro Pump (Base Unit)
7006-H003A	DG-4000-04 4-channel Degasser Unit, for Analytical
7017-J002A	AS-4050 HPLC Autosampler
7021-J002A	CO-4060 Column Oven
7029-J002A	CD-4095 Circular Dichroism Chiral Detector
7058-J011A	BS-4000-1 Bottle stand
7059-J012A	ChromNAV Ver.2 Chromatography Data System
6688-H564A	3x LC-Net CG cable
7001-H401A	HPLC Start Up Kit for LC-4000
7001-H405A	Maintenance tool kit
	19724 CHIRALPAK AD-RH manufactured by Daicel