

Chirascan: Fluorescence Detected Circular Dichroism (FDCD) data

The data below was collected on Chirascan in June 2010 as part of a customer evaluation.

FDCD data – R-CSA and S-CSA

Cell:	10 mm pathlength
Wavelength range:	182 to 350 nm in 1 nm steps
Optical filter:	375nm cut-off filter
Bandwidth:	4 nm
Step:	1 nm
Repeats:	2
Time per single scan:	~5 minutes
Sample properties:	(1R)-(-)-Camphorsulfonic acid: aqueous solution (0,06% tj. 0,6 g/L) – R-CSA (1S)-(+)-Camphorsulfonic acid : aqueous solution (0,06% tj. 0,6 g/L) – S-CSA

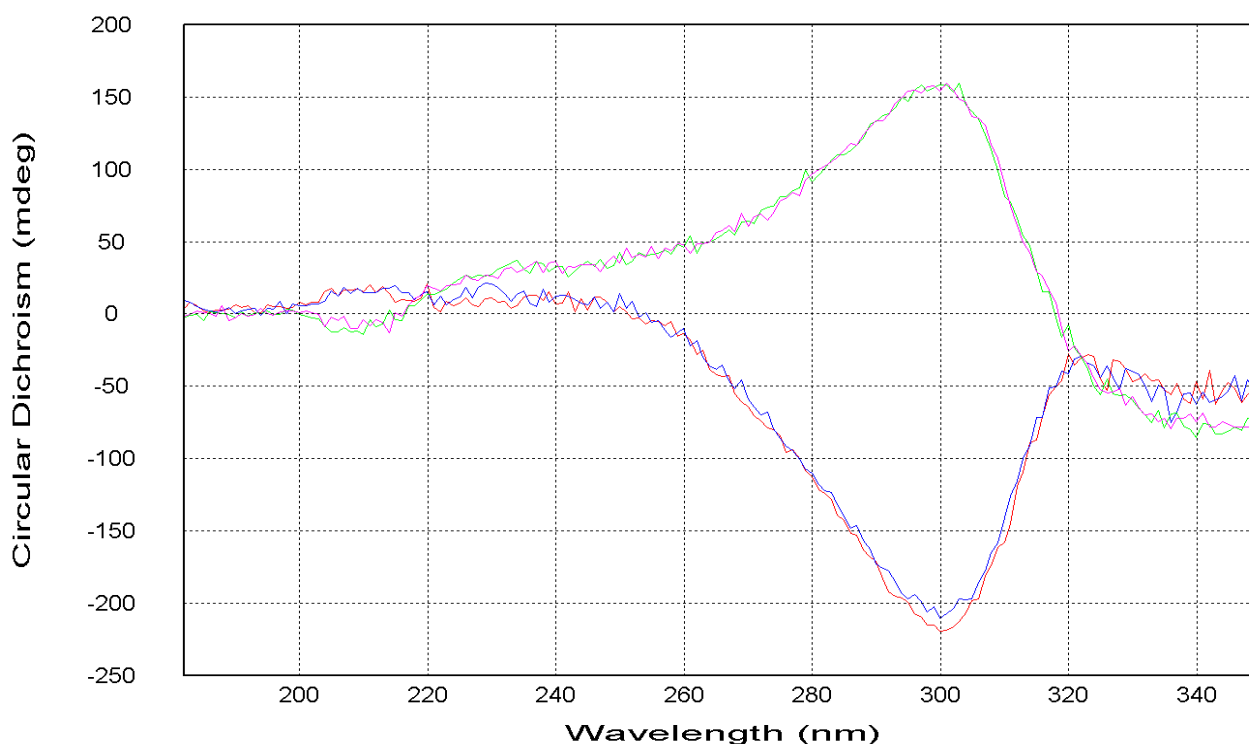


Figure 1 Raw, unsmoothed FDCD spectra. Over lay of two 5 minute scans of S-CSA (blue and red) and two 5 minute scans of R-CSA (light pink and green)

Background Substraction.

We show below the background subtracted FDCD data. As the two enantiomers will have equal and opposite FDCD signal, the background signal (B) can be obtained by averaging the recorded spectra for the S and R forms.

$$\text{i.e. } [(B + \text{FDCD}) + (B - \text{FDCD})]/2 = B$$

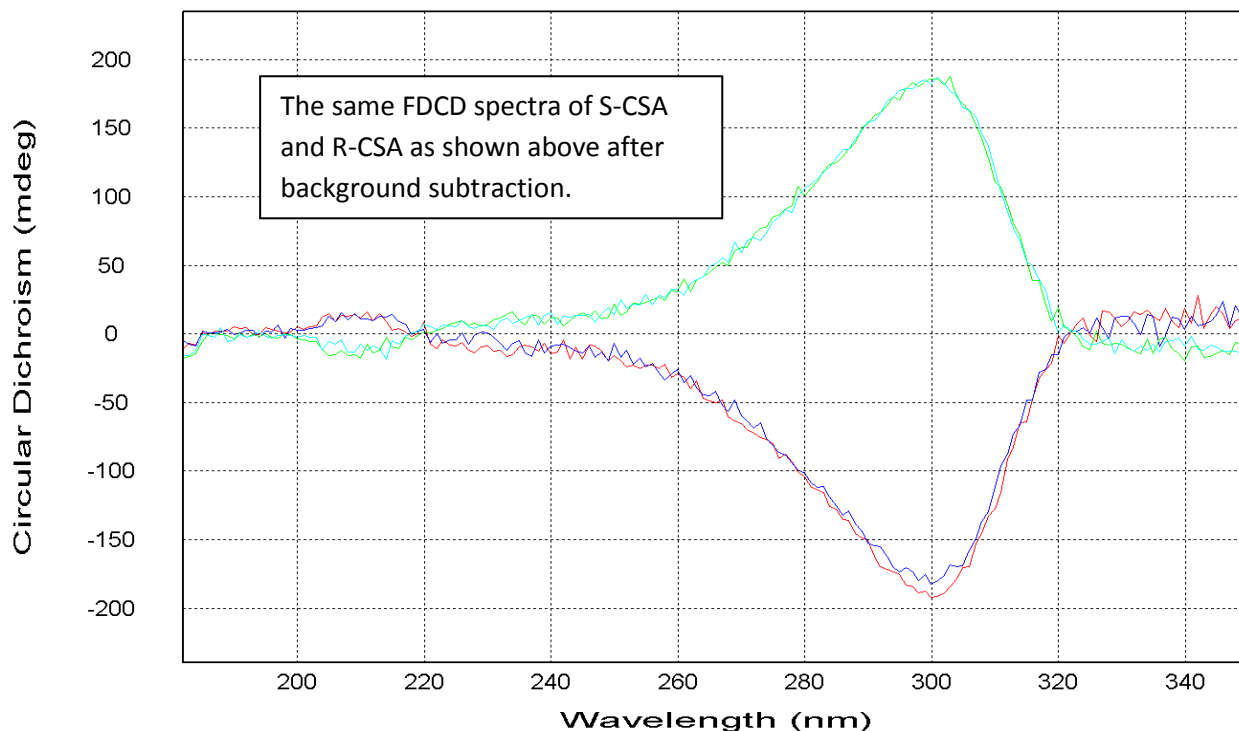


Figure 2 Unsmoothed FDCD spectra. **Background subtracted.** Over lay of two 5 minute scans of S-CSA (blue and red) and two 5 minute scans of R-CSA (light blue and green)

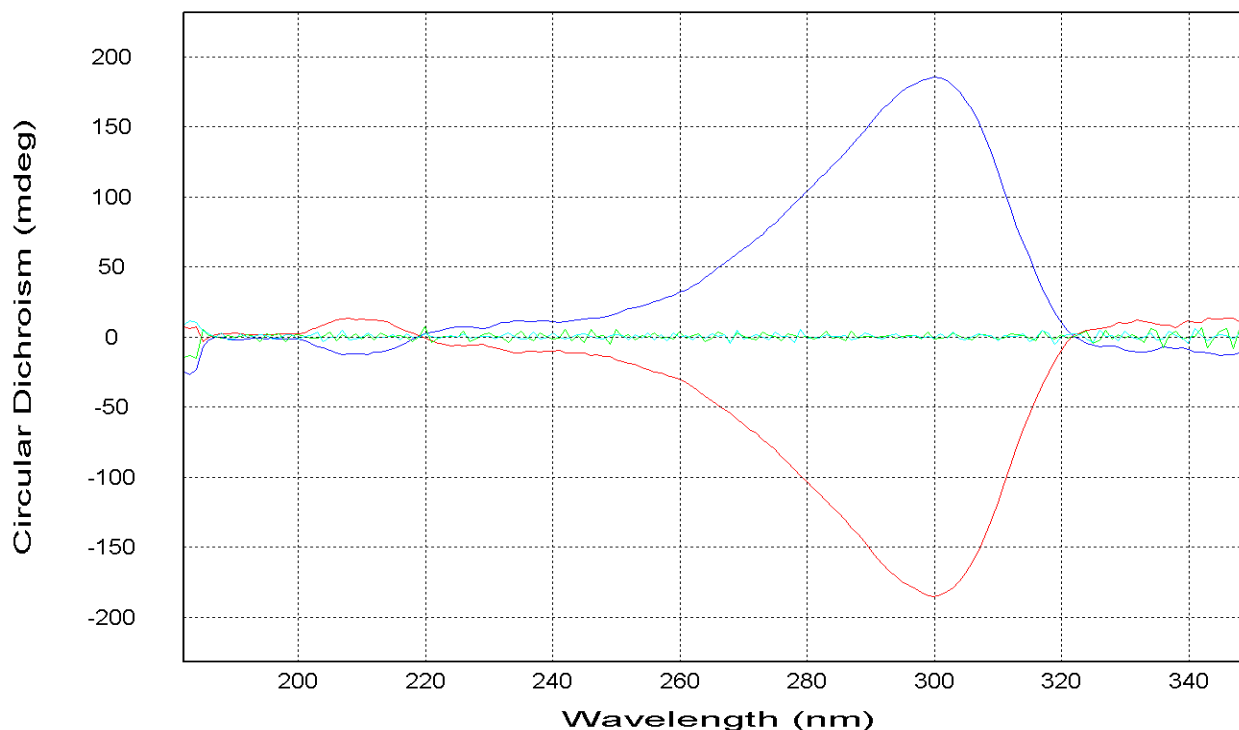


Figure 3. ... the same FDCD spectra following averaging of the two scans for each sample and post-acquisition smoothing (4-point Savitzky-Golay smooth). The residual curves (green and light blue) are also shown here to indicate that this smoothing operation did not produce any distortion of the CD spectrum.

CD data – R-BND and S-BND

Cell:	10 mm pathlength
Wavelength range:	200 to 350 nm in 1 nm steps
Bandwidth:	4 nm
Step:	1 nm
Repeats:	2
Time per single scan:	5 minutes
Sample properties:	(S)-(-)-1,1'-binaphtyl-2,2'-diol methanol soln (0,011g/L) – S-BND (R)-(+)-1,1'-binaphtyl-2,2'-diol: methanol soln (0,011g/L) – R-BND

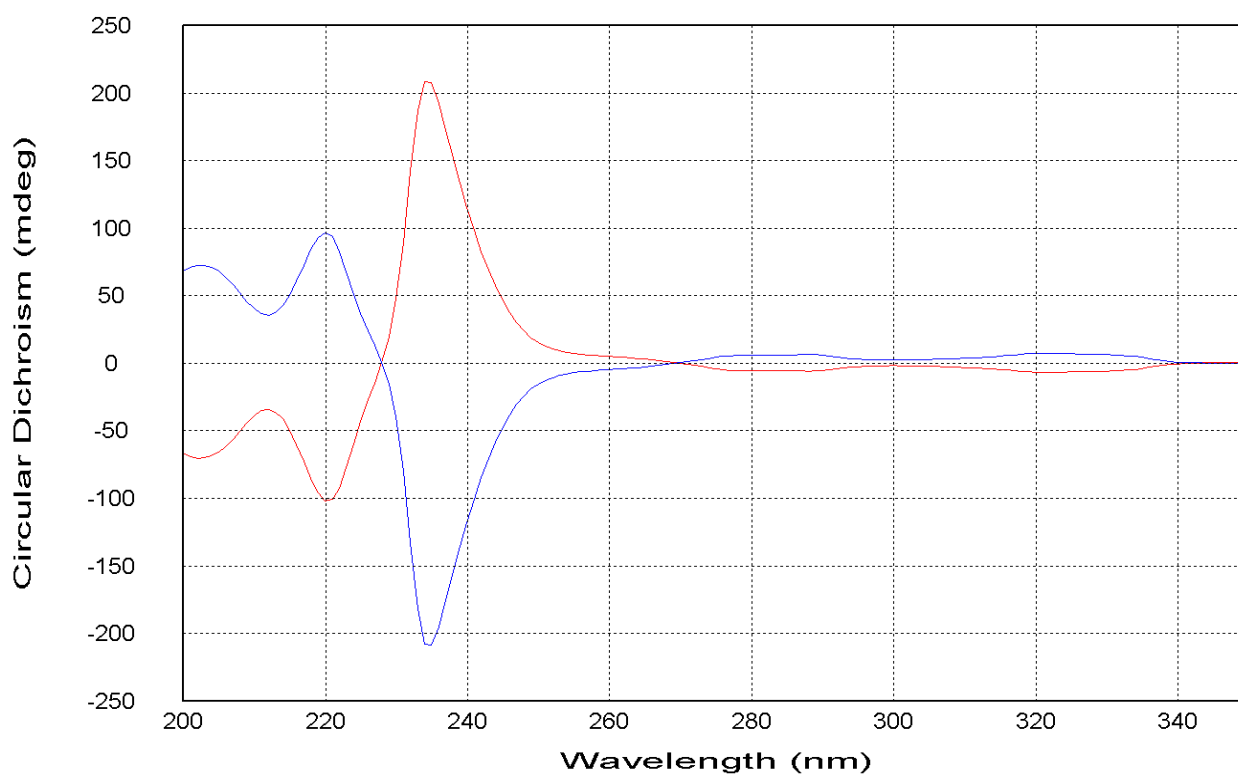


Figure 4 CD spectra of S-BND (red) and R-BND (blue) collected under the conditions tabulated. I.e. Both are 5 minute scans and are **unsmoothed** (e.g. no time constant filtering).

FDCD data – R-BND and S-BND

Cell: **10 mm** pathlength
Wavelength range: 200 to 350 nm in 1 nm steps
Optical filter: 375nm cut-off filter
Bandwidth: 4 nm
Step: 1 nm
Repeats: 2
Time per single scan: **~5 minutes**
Sample properties: (S)-(-)-1,1'-binaphthyl-2,2'-diol methanol soln (0,011g/L) – **S-BND**
(R)-(+)-1,1'-binaphthyl-2,2'-diol: methanol soln (0,011g/L)– **R-BND**

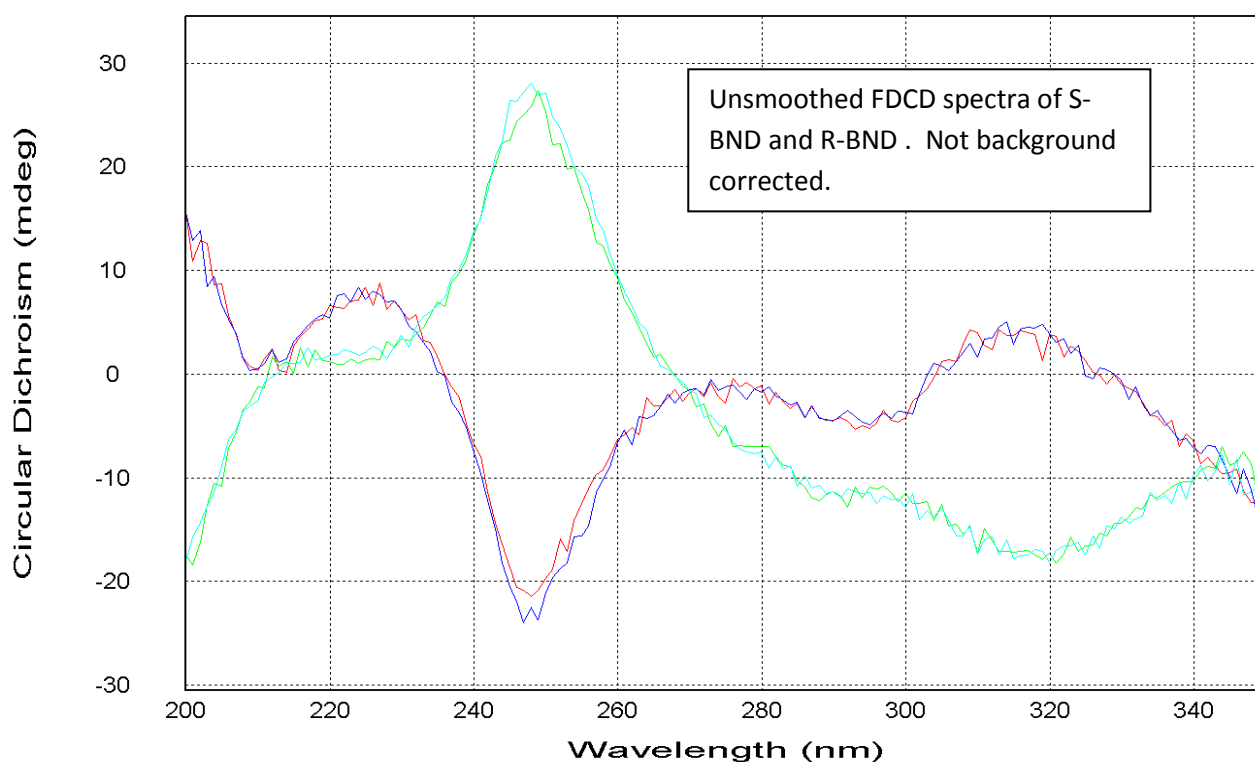


Figure 5 Unsmoothed FDCD spectra. Over lay of two 5 minute scans of S-BND (blue and red) and two 5 minute scans of R-BND (light blue and green). NOT background corrected

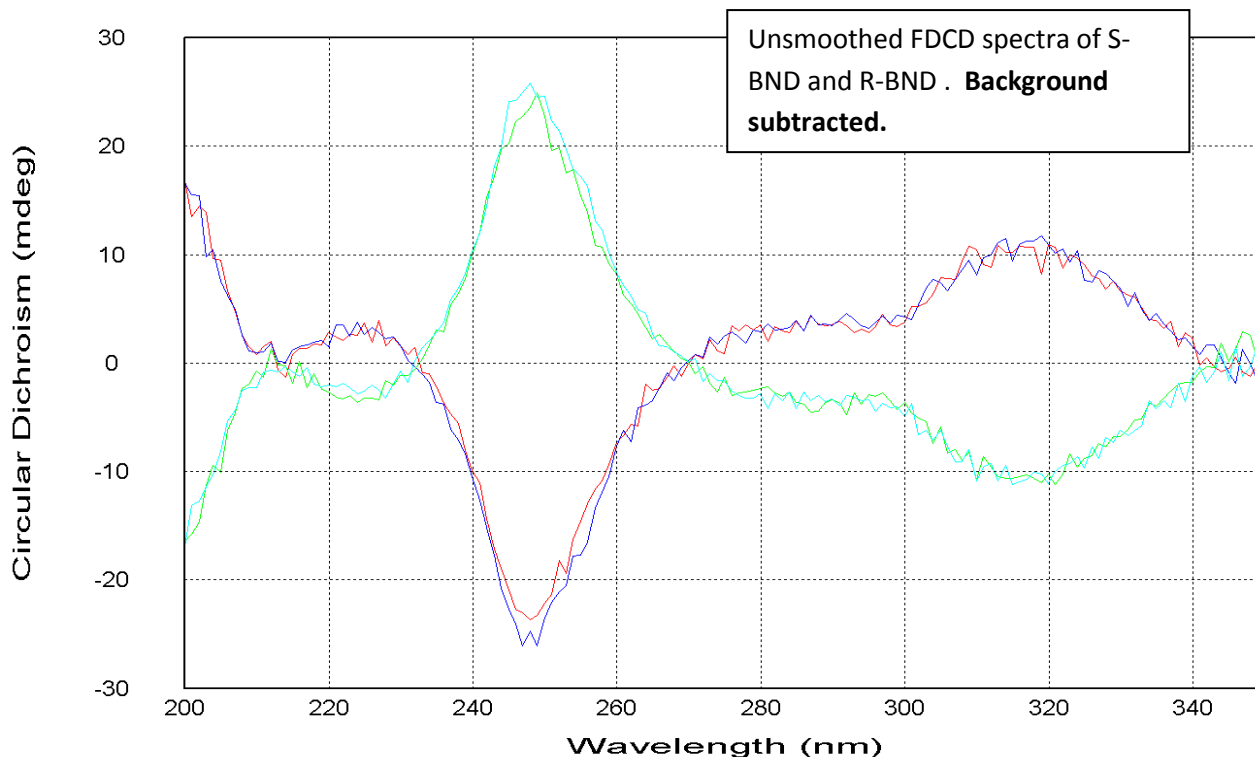


Figure 6 Unsmoothed FDCD spectra. **Background subtracted.** Over lay of two 5 minute scans of S-BND (blue and red) and two 5 minute scans of R-BND (light blue and green)

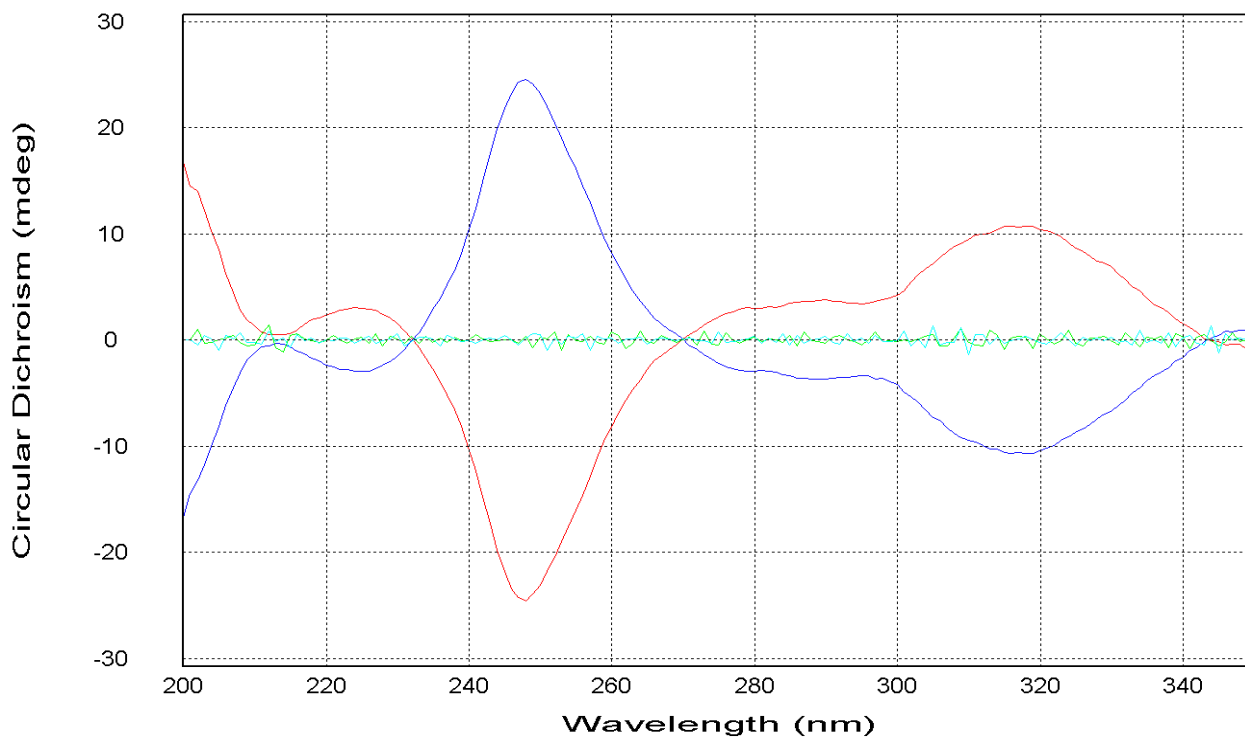


Figure 7. ... the same FDCD spectra following averaging of the two scans for each sample and post-acquisition smoothing (4-point Savitzky-Golay smooth). The residual curves (green and light blue) are also shown here to indicate that this smoothing operation did not produce any distortion of the CD spectrum.