

## *5 Utilization of circular dichroism*

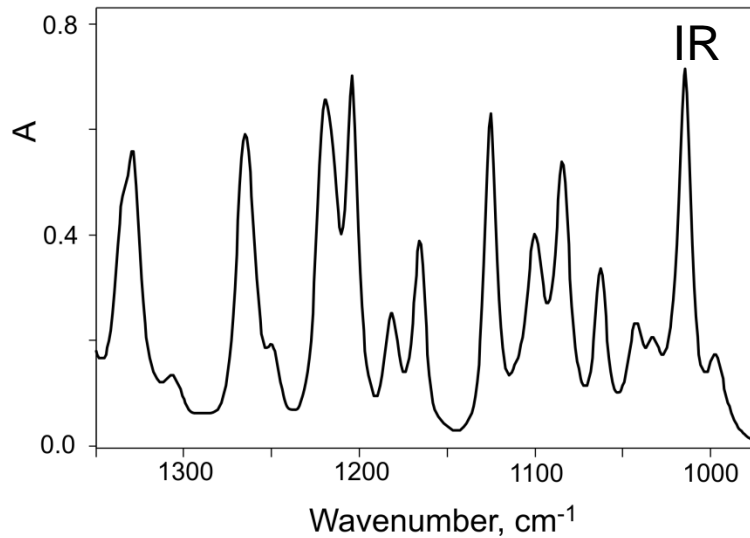
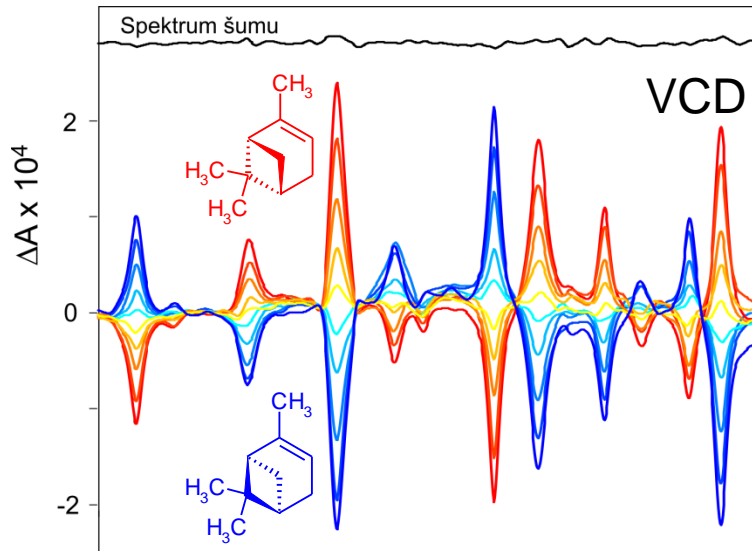
### Circular dichroism

- enantiomeric purity
- absolute configuration of small- and middle-sized molecules
- structure of peptides, proteins, oligonucleotides and DNA
- biologically interesting interactions
- structural studies of supramolecular interactions
- transcription of chiral information
- molecular recognition

# enantiomeric purity

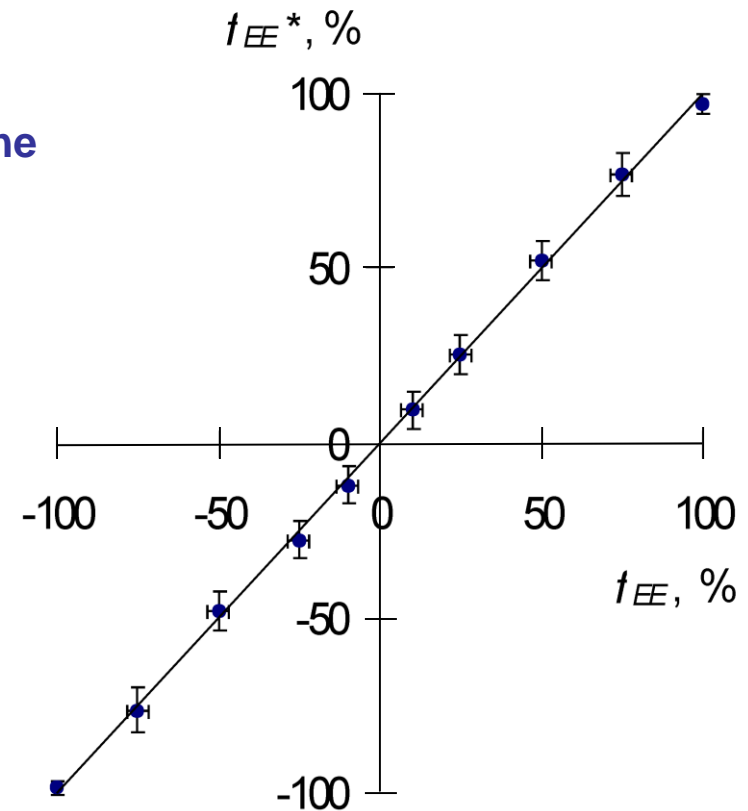
Enantiomeric excess:

$$f_{EE} = \frac{c_R - c_S}{c_R + c_S} \cdot 100 \quad [\%]$$



EE ~ 2-3%

Urbanová M., Setnička V., Volka K.: *Chirality* **2000**, 12, 199.

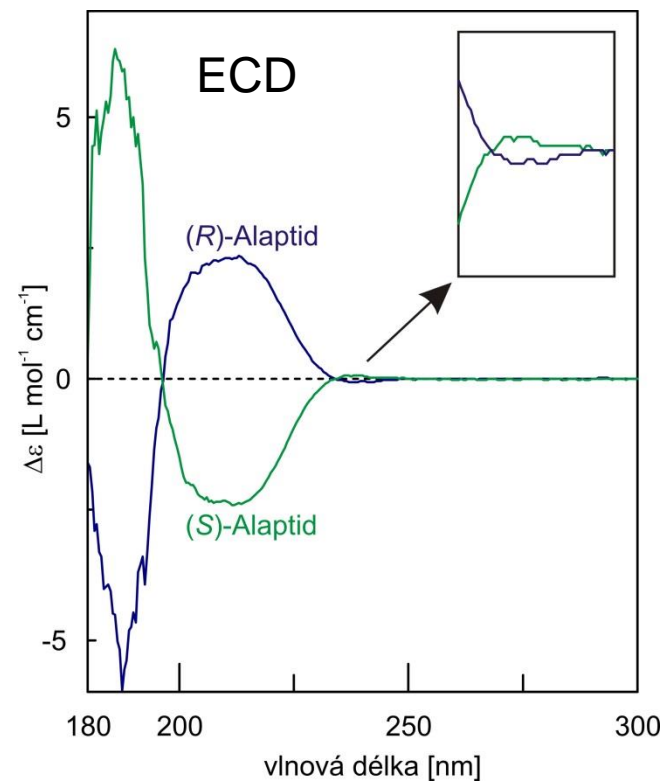
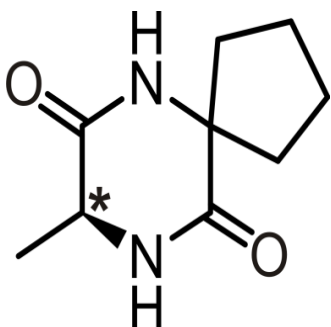


# absolute configuration of small- and middle-sized molecules

1. Conformation analysis
2. Optimization of structures/geometries
3. Calculation of the oscillator strength and rotational strength for all conformers (DFT methods)
4. Calculation of the spectra for all optimized structures
5. Boltzmann averaging from the particular spectra
5. Comparison with experiment

# absolute configuration of small- and middle-sized molecules I

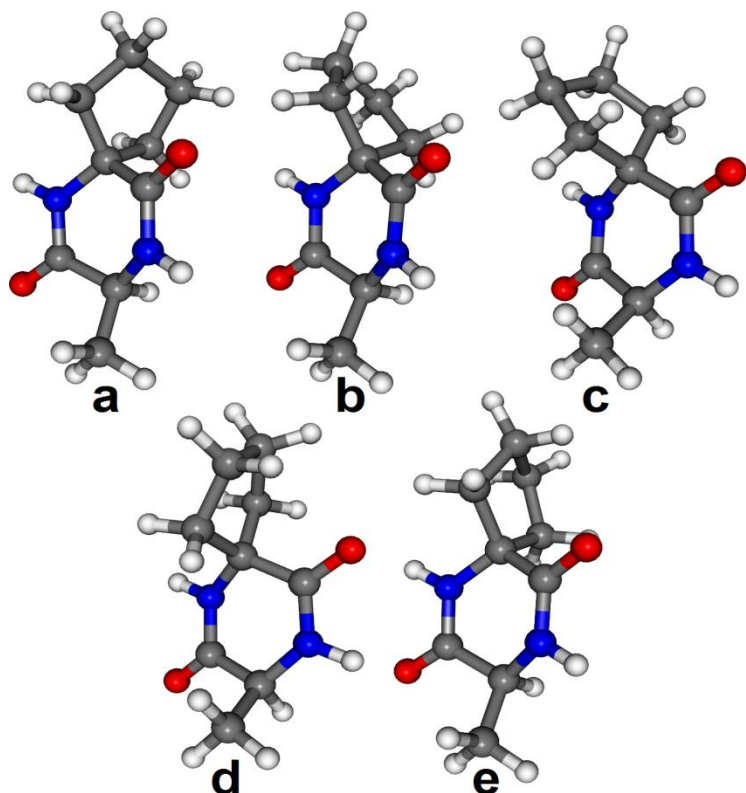
## Pharmaceutical industry (S)-alaptide



*J. Pharm. Biomed. Anal.* **2010**, *53*, 958.

# absolute configuration of small- and middle-sized molecules I

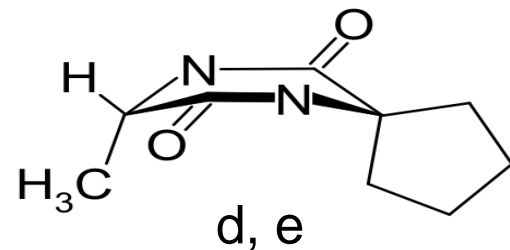
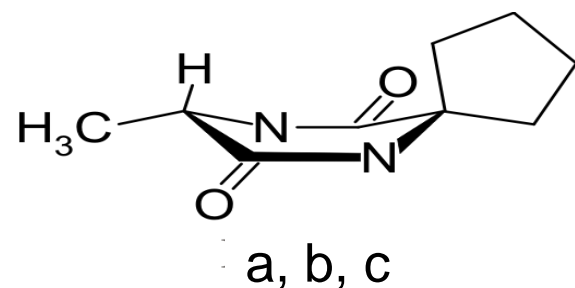
## Pharmaceutical industry (S)-alaptide



Gaussian 03, DFT

relative energies  $\Delta G$  [kJ mol<sup>-1</sup>]:  
 $T = 293.15$  K

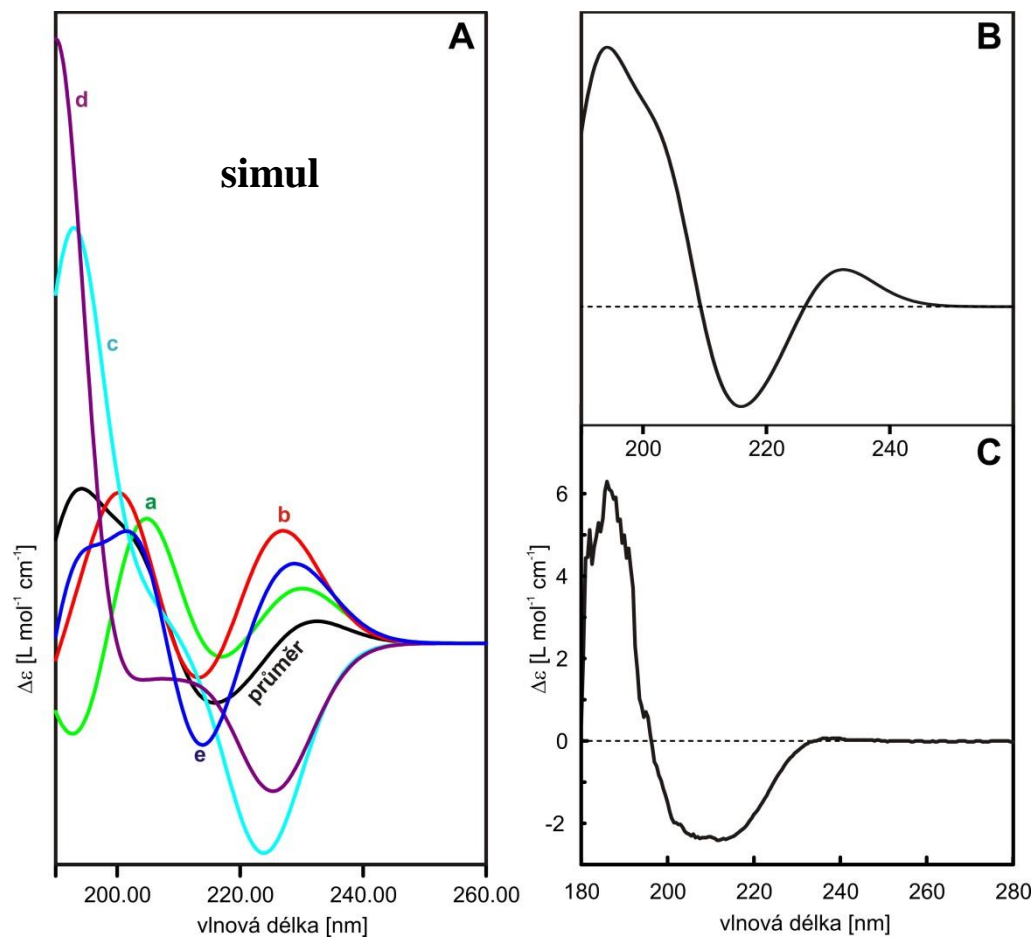
<b>a</b>	13 %
<b>b</b>	25 %
<b>c</b>	26 %
<b>d</b>	4 %
<b>e</b>	32 %



# absolute configuration of small- and middle-sized molecules I

## Pharmaceutical industry (S)-alaptide

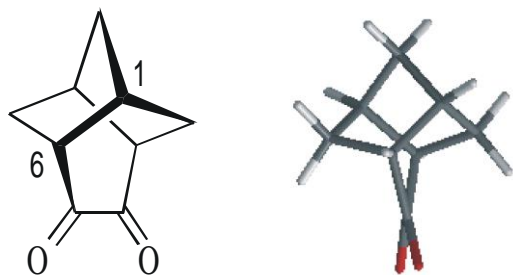
ECD



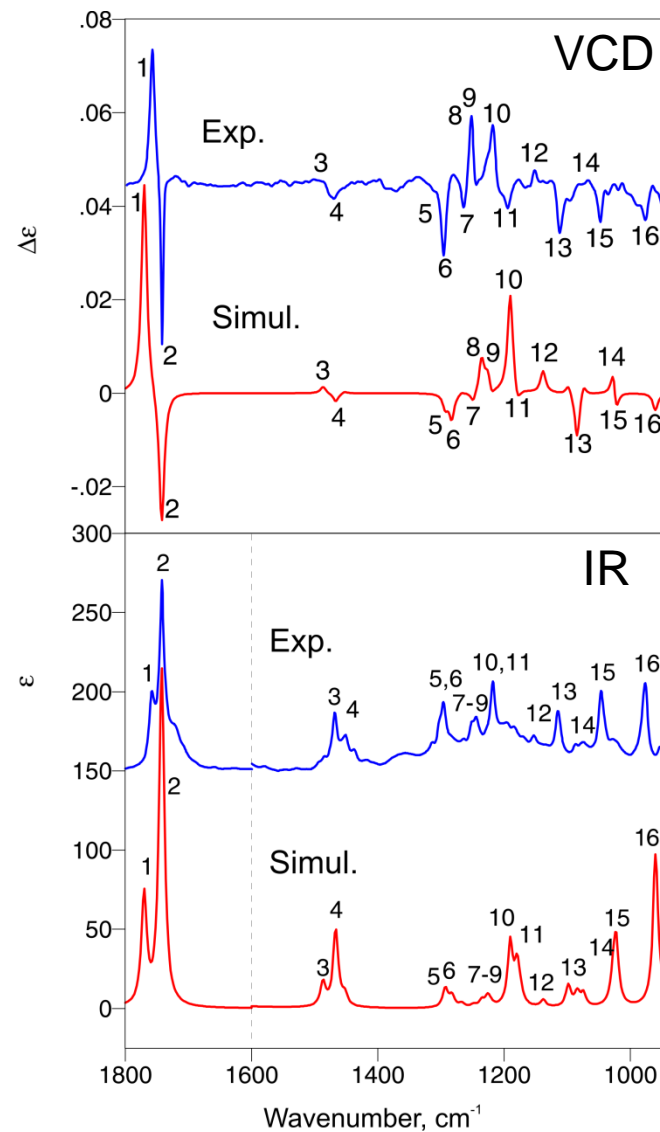
Gaussian 03, DFT

# absolute configuration of small- and middle-sized molecules II

## Tricyclo[4,3,0,0<sup>3,8</sup>]nonan-4,5-dione (twistbrendandione)

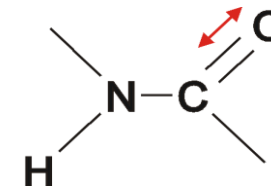
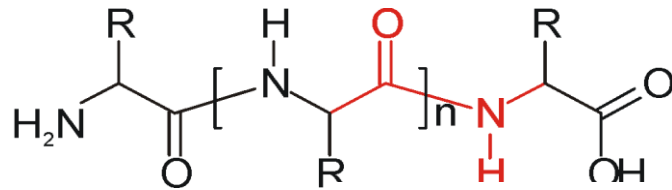


**(1*R*,3*R*,6*R*,8*R*)**

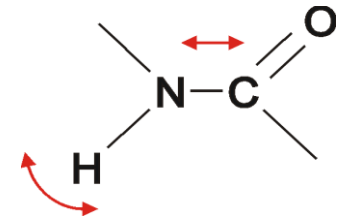


# structure of peptides, proteins, oligonucleotides and DNA

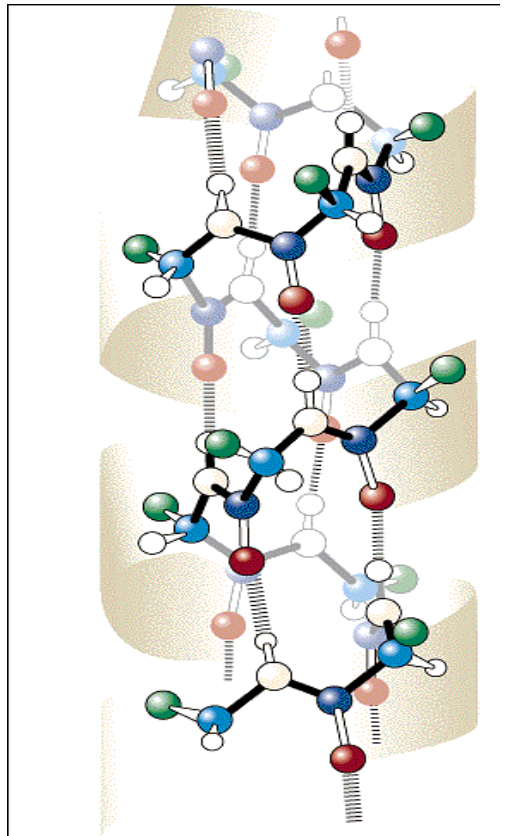
## Peptides, polypeptides, proteins



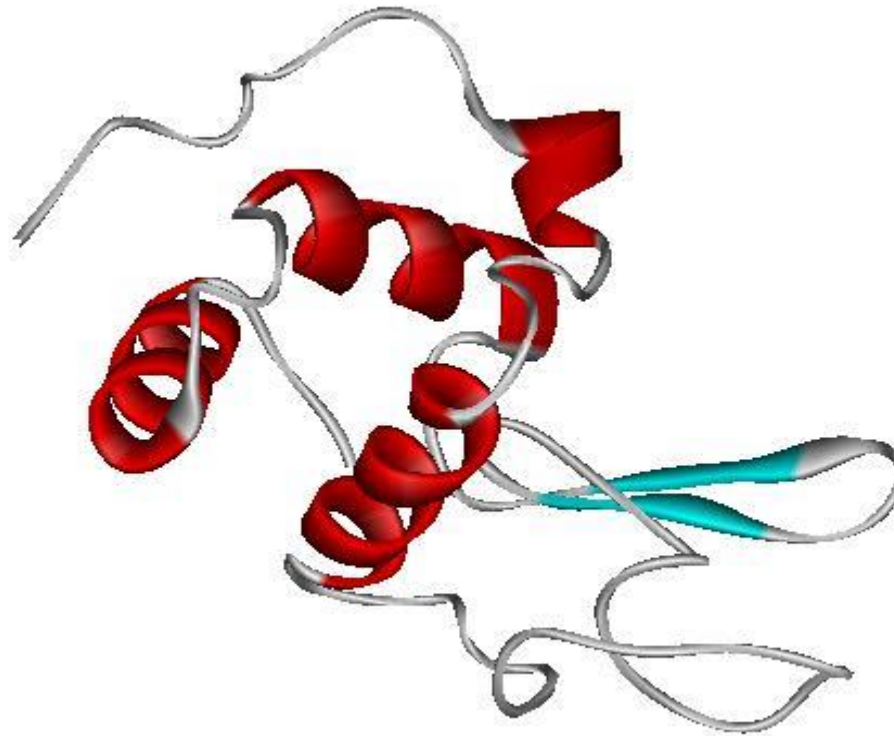
amide I



amide II



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Heme

Heme

<http://lysozyme.co.uk>

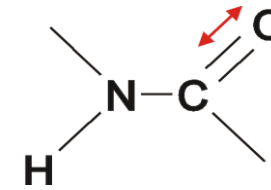
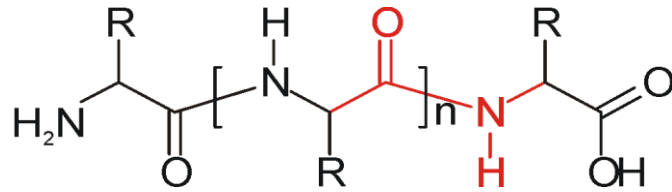
1e

1S

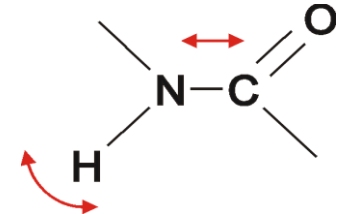


# structure of peptides, proteins, oligonucleotides and DNA

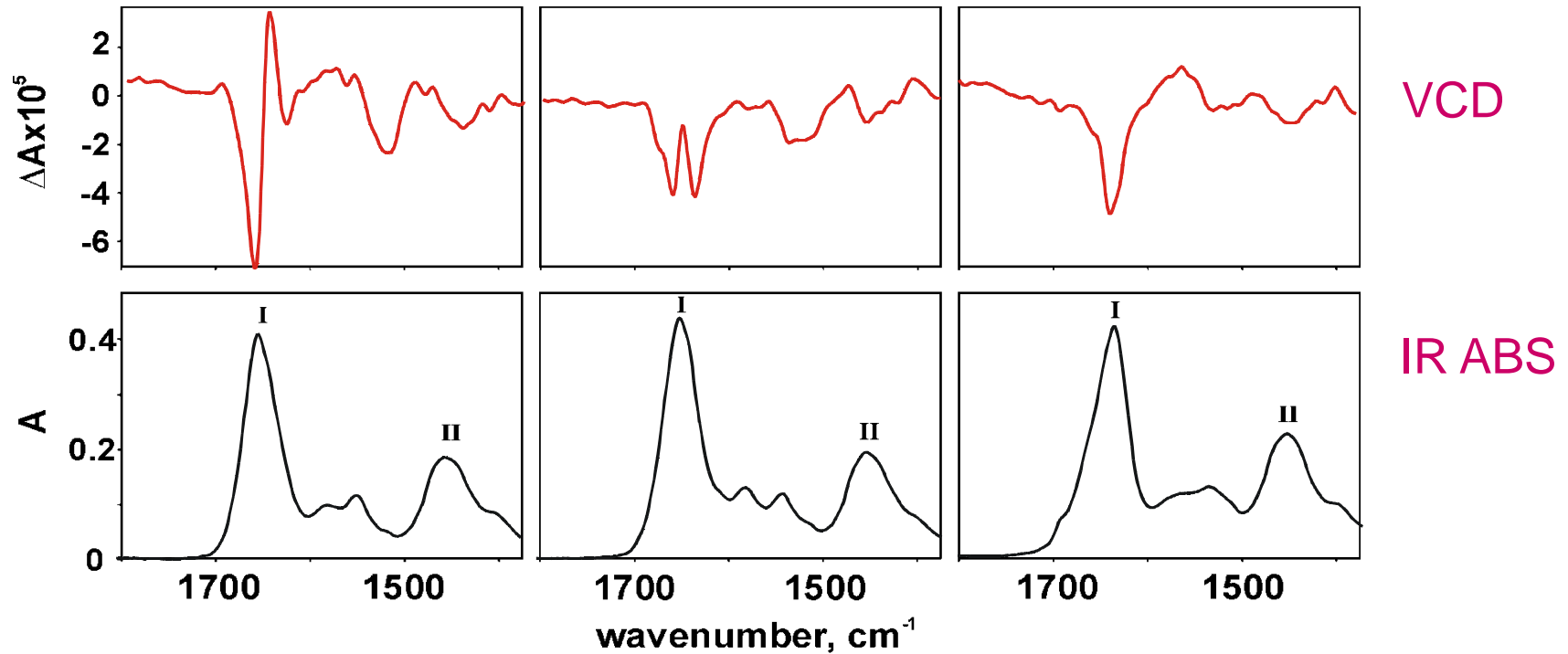
## Peptides, polypeptides, proteins



amide I



amide II



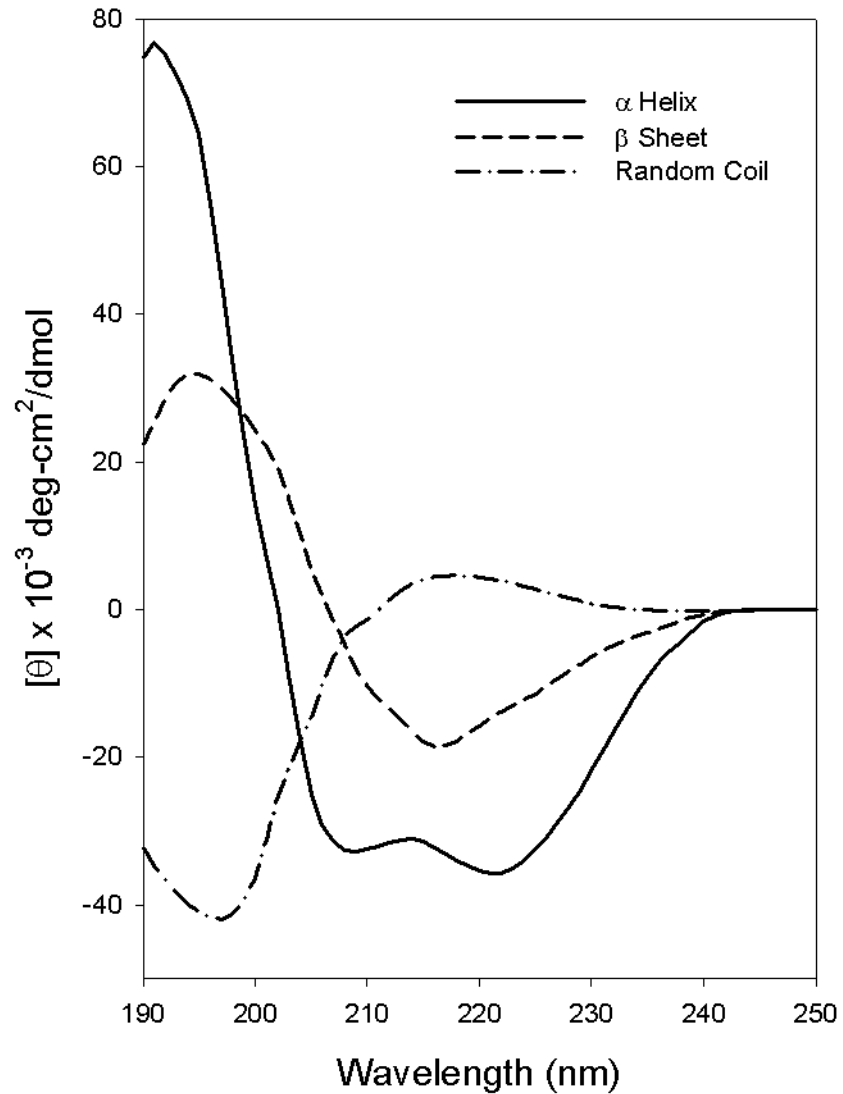
Hemoglobin  
 $\alpha$ -helix

Lysozyme  
 $\alpha + \beta$

Concanavalin A  
 $\beta$ -structure

# structure of peptides, proteins, oligonucleotides and DNA

## Polypeptides, proteins



ECD