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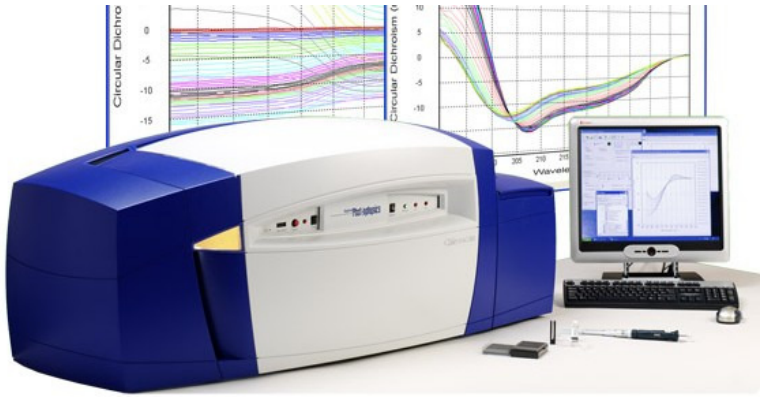
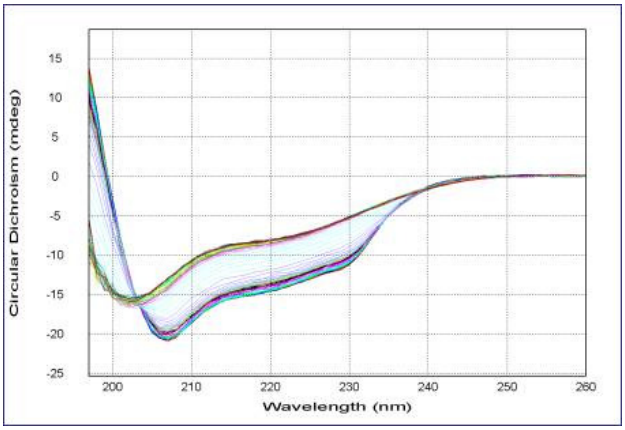
Protein Structure and Conformational Studies



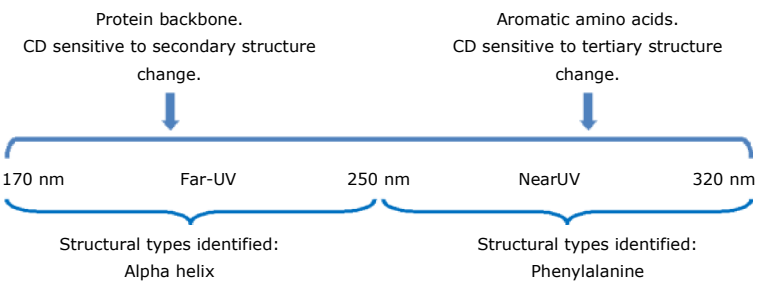
The Far UV region of a protein circular dichroism (CD) spectrum shows spectral features related to the structure of the backbone of the protein, and is directly relevant to the secondary structural elements that make up the protein structure. The spectral signatures can be used to predict the secondary structure makeup of a particular proteins structure. This is probably the most well known known application of CD spectroscopy, and there has been a number of analytical packages produced to aid in predicting secondary structure using circular dichroism data.



Far-UV CD spectrum thermal denaturation of lysozyme

The above figure illustrates clearly the change in CD signature as a function of temperature. Comparison of known CD signatures with the data in this experiment suggests that the initial CD signature is a combination of α-helical and β-sheet structure which, on heating, loses much of it's α-helical content to an unfolded state, whilst retaining some β-sheet character.

Secondary structure prediction is only part of the power of circular dichroism spectroscopy. CD spectra in the near UV regions of the CD spectrum are caused by side chain residues of the phenylalanine, tryptophan and tyrosine residues. When these residues are in highly structured environments (buried in a structured protein) they show distinct structured CD spectra, conversely when in unstructured environments (in bulk solution after unfolding of a protein for instance) they have very little structured CD spectral features. Changes in the CD spectra of the near UV show changes in the structure around these residues because of changes in the structure of the protein.



Beta turn	Tryptophan
Polyproline	Disulphide bonds
Irregular	

Relationship between regions of the CD spectrum and protein structural types.

Changes in the circular dichroism spectra of bio-molecules represent changes in their secondary and tertiary structures. When this is coupled with the facts that (i) spectra can be recorded in minutes and (ii) single wavelength kinetics can be recorded from milliseconds onwards, it can be seen that CD is a particularly powerful tool to follow dynamic changes in protein structure. For instance, changes induced by changing temperature, pH, ligands, or denaturants are all commonly studied.

Another powerful application of circular dichroism is to simply compare two proteins, and determine if they have a similar structure. This can be used simply to ascertain if a newly purified protein is correctly folded, determine if a mutant protein has folded correctly in comparison to the wild-type, or for the analysis of biopharmaceutical products to determine that the biopharmaceutical is still in a correctly folded active conformation.

Relevant Circular Dichroism References

Listed below are 5 selected recent references of studies of various protein structural using APL circular dichroism systems. A complete searchable database with all references can be accessed by logging into the APL members area.

Authors	Title	Year	Keywords	Journal/Proceedings
Sylvie Campagna, Nathalie Saint, G□rard Molle, and Andr□ Aumelas	Structure and Mechanism of Action of the Antimicrobial Peptide Piscidin [**Abstract**] [**URL**]	2007	Antibacterial Peptide, Structure and Mechanism, circular dichroism, NMR, secondary structure	BIOCHEMISTRY-USA, 2007, Vol 46, Iss 7, pp 1771-1778
Castelletto, V., Krysmann, M., Kelarakis, A. & Jauregi, P.	Complex Formation of Bovine Serum Albumin with a Poly(ethylene glycol) Lipid Conjugate [**Abstract**] [**URL**]	2007	Self-assembly, bovine serum albumin, formulation, circular dichroism, small-angle x-ray scattering	BIOMACROMOLECULES, 2007, Vol 8, Iss 7, pp 2244-2249
Sachin Kale, Palaniappa Arjunan, William Furey, and Frank Jordan	A Dynamic Loop at the Active Center of the Escherichia coli Pyruvate Dehydrogenase Complex E1 Component Modulates Substrate Utilization and Chemical Communication with the E2 Component [**Abstract**] [**URL**]	2007	crystallographic studies, Escherichia coli, kinetic, spectroscopic, and crystallographic studies.	J. Biol. Chem., Vol. 282, Issue 38, 28106-28116, September 21, 2007
Anna L. Mallam and Sophie E. Jackson	The Dimerization of an α/β-Knotted Protein Is Essential for Structure and Function [**Abstract**] [**URL**]	2007	Structure and function, α/β-Knotted proteins, biological self-assembly, polypeptide .	Structure, Volume 15, Issue 1, January 2007, Pages 111-122.
Denis B. D. O'SULLIVAN, Christopher E. JONES, Salama R. ABDELRAHEIM, Andrew R. THOMPSETT, Marcus W. BRAZIER, Harold TOMS, David R. BROWN and John H. VILES	NMR characterization of the pH 4 β-intermediate of the prion protein: the N-terminal half of the protein remains unstructured and retains a high degree of flexibility [**Abstract**] [**URL**]	2007	Prion diseases, misfolding, prion protein, α-helical isoform , β-sheet-rich oligomer.	Biochem. J. (2007) 401 (533□540)

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