MICROCOMPUTER PREDICTION OF PROTEIN STRUCTURE FROM AMINO ACID SEQUENCE DATA

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A program package was developed for IBM compatible PCs with color graphics to make structural and functional predictions for different proteins. All calculations are performed on amino acid sequences. For most of the procedures these sequences are converted to numerical vectors on given amino acid properties. The prediction methods used are based on statistical, stereochemical and other physico-chemical observations. Different types of secondary structure calculations and one type of tertiary structure estimate can be made. To identify transmembrane and surface active segments in given sequences, hydrophobic moments and cooperative effects are also taken into account. Autocorrelation and Fourier analysis is used to study internal homology within a sequence. Crosscorrelation calculations are performed to compare features implied by different sequences. A new algorithm was introduced to compare two sequences and find the optimal alignment between them (insertions and deletions are automatically included) The system is flexible: the user can introduce new parameters and measure their predictive power. The programs were shown to be useful for transmembrane proteins, immunological site predictions and on unknown structures from DNA sequencing. Examples will be given.

CONFORMATIONS OF OXYTOCIN IN SOLUTIONS DETERMINED BY 2D NMR AND DISTANCE ALGORISM

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The neurohypophyseal hormone, oxytocin, is a nonapeptide with the sequence of Cys-Tyr-Ile-Gln-Asn-Cys-Pro-Leu-Gly-NH_2. Recent two reports, experimental(1) and theoretical(2), have pointed out again the importance of conformational flexibility in this molecule which has long been a main subject in the NMR studies(3). In the X-ray study(2), two chiral conformers about a disulfide bond were shown. Recent our finding with NMR(400Mhz) of two distinctive conformations in solution(DMSO) have corresponded to the result. The combination of 2D NOE and distance alogorism(4) in conjunction with the systematic assignment by 2D NMR were utilized to characterize the two conformers. Due to the inherent flexibility in structure, distance algorism did not work well. Two approaches were made to overcome this difficulty: (1) to find out a position fixed commonly in various structures and (2) to reduce the flexibility by embedding it into micelle.

1) S.P. Wood et al., Science, 232, 633-636 (1986).
2) A.T. Hagler et al., Science, 227 1309-1315(1985).
3) V.J. Hruby, in "Topics in Molecular Pharmacology" (North-Holland) p100(1981).
4) A.D. Kline et al., J. Mol. Biol. 189, 377-382(1986).

2D NMR AND CD STUDIES OF *ESCHERICHIA COLI* INITIATION FACTOR 3 TERTIARY STRUCTURE.

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Escherichia coli translational initiation factor 3 protein (IF3) is one of the simplest systems to study in order to obtain a detailed and fundamental understanding of protein–nucleic acid interactions in the regulation of translation. IF3 is an RNA helix destabilizing protein, with sequence specificity for the initiation codon AUG, and a conserved sequence near the 3' end of 16S ribosomal RNA. In order to obtain sufficient IF3 for physical studies, purification was optimized for speed (2–5 days), yield (300 mg/100 g cells), and purity (99% long form) from a heat–inducible IF3 gene in a high copy number plasmid. 360 MHz 2D NMR spectra implied that His 139 and Tyr 109 do not experience NOE interactions with other aromatic residues. Tyr 71 and Tyr 76, on the other hand, showed significant NOE interactions with Phe side chains. Peak broadening by aggregation made further interpretation difficult. In order to inhibit aggregation of IF3 at 1–5 mM, solvent perturbation was studied by CD. A broad sigmoidal reduction of the induced Tyr and Phe 282 nm trough was seen with both 0–1 M urea and 0–10% EtOH; no more than 0.1 M urea or 1% EtOH could be added without significant loss of signal, implying great sensitivity of tertiary structure to perturbants. In contrast, the peptide bond 222 nm trough was not reduced by urea until more than 1 M, implying moderate sensitivity of secondary structure. This work was supported by grants from the US NIH (E. W.) and the Max Planck Gesellschaft (C. O. G.).

A COMPARATIVE STUDY OF THE PHYSICO-CHEMICAL PROPERTIES OF TOMATO BUSHY STUNT VIRUS STRAINS

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Tomato Bushy Stunt Virus (TBSV) is a small, quasi-spherical virus responsible for a family of diseases in dicotyledons. Infective particles of one variant in particular ("Type Strain") have been well characterised. Other strains however are known to have different host plants and symptoms. In an attempt to correlate this behaviour with physico-chemical properties we have performed a comparative study on isolates of TBSV variants ("Type Strain" , Petunia Asteroid Mosaic, Pelargonium Leaf Curl and Carnation Italian Ringspot) with regard to sedimentation velocity behaviour (both sedimentation coefficient and concentration dependence behaviour), molecular weight (by low speed sedimentation equilibrium), viscosity (intrinsic viscosity and concentration dependence behaviour) and quasi-elastic light scattering (apparent diffusion coefficients). The usefulness of TBSV for testing out hydrodynamic concentration dependence theories for near-spherical particles (along the lines performed on Turnip Yellow Mosaic Virus (TYMV) by Harding, S.E. and P. Johnson; 1985, Biochem. J., 231, 549-555) is explored.