The sequences of seven phosphoribosyl transferases were aligned using amino-acid homologies and secondary structure predictions. An average "folding pattern" \[1\] was computed for the transferase family and compared with the "folding patterns" of nucleotide binding proteins of known X-ray structures:

- the NAD dehydrogenases (ie Lactate dehydrogenase)
- the adenylate kinase.
- the GTP binding proteins (ie elongation factor Tu).

The folding pattern of the transferase family appeared related to the corresponding pattern of adenylate kinase and subsequent amino acid homologies were found with this protein. From this homology, we were able to build a 3D-model of phosphoribosyl transferase.

The analysis of conservative residues on this model allows to define the locations of both associated substrates and to propose a possible mechanism of the enzymatic reaction.


02. STRUCTURAL MOLECULAR BIOLOGY

02.2-2  
A 3D MODEL OF PHOSPHORIBOSYL TRANSFERASE by B. Busetta and M. Hospital, Laboratoire de Cristallographie UA 146, CNRS - Université de Bordeaux I - 33405 Talence Cedex, France.

02.2-3  
The crystal structure of the MBILF-BTRY complex was determined by molecular replacement and its 3-D molecular model was thereby derived. Mung bean trypsin inhibitor belongs to the Bowman-Birk inhibitor group, which is by far the most complicated among the ten fundamental groups of urinary protease inhibitors (Laskovski and Kato, 1980). The crystallographic data for the MBILF-BTRY complex are a=62.9, b=63.5, c=69.7 Å, space group P2_12_12_1, with Z=4. Its molecular weight is about 27500. On a Rigaku AFC-5 Four-circle diffractometer attached to a RU-300 rotating anode generator, 5142 independent reflections of up to 3 Á resolution were collected. Relative orientation angles between the model BTRY and BTRY in our crystal, α=235°, β=46°, and γ=75° (expressed in terms of Crouther angles), were obtained by using Crouther’s fast rotation function with diffraction data of 3Á resolution. Translational functions were calculated by applying Lattman’s program. From the three Harker sections, the relative translational components between the model BTRY and that in our crystal were found to be ΔX=10.1, ΔY=3.0 and ΔZ=13.3 Å. Group refinement (Huber and Schnaiter, 1985) improved the above rotational and translational parameters to a=236.4°, β=45.7°, γ=74.9° and ΔX=9.8 Å, ΔY=3.0 Å, ΔZ=13.1 Å. After the model BTRY molecule was oriented and located in the unit cell at the correct position using the refined parameters, the R-factor dropped to 0.39. Four cycles of EREF refinement (Jack and Levitt, 1978) of the tryptic inhibitor complex are now in progress. The 3-dimensional structure of MBILF-BTRY complex is now in progress. The 3-dimensional structure of MBILF-BTRY complex reveals the first Bowman-Birk type inhibitor complex which may lead to structure-function correlation studies.