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 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 transferases.

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.


02.2-2  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.

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 serine protease inhibitors (Laskovski and Kato, 1980). The crystallographic data for the MBILF-BTRY complex are \(a=62.9, b=63.5, c=62.7 \, \text{Å} \), 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\( \AA \) resolution were collected. Relative orientation angles between the model BTRY and BTRY in our crystal, \(q=23.5^\circ, b=46^\circ \), and \(Y=75^\circ \) (expressed in terms of Crowther angles), were obtained by using Crouther's fast rotation function with diffraction data of 3\( \AA \) resolution. Translational functions were calculated by applying Lattman's program. From the three Harker sections, the relative translational parameters \(a\theta=23.6^\circ, b\theta=45.7^\circ, Y\theta=74.8^\circ \) and \(a\theta=9.8 \, \text{Å}, b\theta=3.0 \, \text{Å}, Y\theta=3.1^\circ \). 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 intact complex molecule has reduced the R-factor to 0.353. A refined-weighted (Sin, 1958) electron density map both of 3\( \AA \) resolution were calculated. Dense contour levels apparently attributable to the MBILF could be seen clearly near the active center of BTRY molecule. The molecular size of MBILF was estimated at 15x15x25 \(\text{Å} \). It could be unambiguously seen that the electron density corresponding to the longer side chain of Lys 275 of MBILF molecule extends deeply into the specific pocket and terminates near ASP 189 OD1 of BTRY. The polypeptide folding could be traced in a Fourier map with reference to a difference Fourier. A preliminary stereochemical model of MBILF has been constructed. Five cycles of EREF refinement of the intact complex molecule has reduced the R-factor to 0.346. Further refinement of the 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.

02.4-2  CRYSTAL STRUCTURE DETERMINATION AND MOLECULAR MODEL OF MUNG BEAN TRYPsin INHIBITOR LYs ACTiVE FRAGMENT-BOwMAN TRYPsin (MBILF-BTRY) COMPLEX AT 3.0 Å RESOLUTION. By Chen Zhongguo, Li Genpei, Zeng Jia, Tang Youhui, Lu Guangying, Wei Zheheng, Institute of Physical Chemistry and Department of Biology, Peking University; Lin Guangda, Zhang Hongguang, Xuan Jianzhong, Chi Zhengwu, Tao Tiemchen, Institute of Biochemistry, Academia Sinica, Shanghai, China.

The crystallographic data for the MBILF-BTRY complex at 3.0 Å resolution were collected. Relative orientation angles between the model BTRY and BTRY in our crystal, \(q=23.5^\circ, b=46^\circ \), and \(Y=75^\circ \) (expressed in terms of Crowther angles), were obtained by using Crouther's fast rotation function with diffraction data of 3\( \AA \) resolution. Translational functions were calculated by applying Lattman's program. From the three Harker sections, the relative translational parameters \(a\theta=23.6^\circ, b\theta=45.7^\circ, Y\theta=74.8^\circ \) and \(a\theta=9.8 \, \text{Å}, b\theta=3.0 \, \text{Å}, Y\theta=3.1^\circ \). 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 intact complex molecule has reduced the R-factor to 0.353. A refined-weighted (Sin, 1958) electron density map both of 3\( \AA \) resolution were calculated. Dense contour levels apparently attributable to the MBILF could be seen clearly near the active center of BTRY molecule. The molecular size of MBILF was estimated at 15x15x25 \(\text{Å} \). It could be unambiguously seen that the electron density corresponding to the longer side chain of Lys 275 of MBILF molecule extends deeply into the specific pocket and terminates near ASP 189 OD1 of BTRY. The polypeptide folding could be traced in a Fourier map with reference to a difference Fourier. A preliminary stereochemical model of MBILF has been constructed. Five cycles of EREF refinement of the intact complex molecule has reduced the R-factor to 0.346. Further refinement of the 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.