s8a.m10.p9 **Crystallographic Determination of the Free Radical Intermediate of Pyruvate: Ferredoxin Oxidoreductase.** E. Chabriere, X. Vernede, M.H. Charon, B. Guigliarelli, E.C. Hatchikian, J.C. Fontecilla-Camps, *Laboratoire de Cristallographie et Cristallogenèse des Protéines, Institut de Biologie Structurale J.P. Ebel , CEA-CNRS, 41 rue Jules Horowitz, 38027 Grenoble cedex 1.*
Keywords: PFOR, radical, TPP.

The 1.87 Å resolution structure of the free radical form of pyruvate:ferredoxin oxidoreductase (PFOR) has been obtained using pyruvate-soaked crystals grown at pH 9.0. Surprisingly, the thiazole ring of the thiamine diphosphate cofactor is not planar indicating the loss of its aromaticity. Stereochemical considerations rule out models where the unpaired electron spin is located at either the methyl or the carbonyl components of the acetyl group of the intermediate. The CO_2 molecule resulting from the decarboxylation of pyruvate is still bound to the enzyme with its C atom close to the C2 of the ThDP-bound acetyl group. From the results reported here, it seems that in the crystal structure of the pyruvate/PFOR complex previously determined at pH 6.0, the substrate was bound in a non-productive manner.

[1] Chabriere E., Charon M.H., Vobeda A., Pieulle L., Hatchikian E.C., Fontecilla-Camps J.C., "Crystal Structure of pyruvate:ferredoxin oxidoreductase, a central enzyme in anaerobic metabolism, and of its complex with pyruvate", Nature Structural Biology, (1999), 6 : 182-190

s8a.m10.p10 **Crystal structure of an anti-interleukin-2 monoclonal antibody Fab fragment complexed with an antigenic nonapeptide**. P.V. Afonin, A.V. Fokin, I.N. Tsygannik, I.Yu. Mikhailova, V.Z. Pletnev, *Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry Russian Academy of Sciences, Ul. Miklukho-Maklaya, 16/10, 117871 Moscow, Russia.*
Keywords: Fab fragment complex, human interleukin, synthetic antigenic nonapeptide.

The three-dimensional organization of Fab fragment of monoclonal antibody LNKB-2 against human interleikin-2 (IL-2) complexed with synthetic antigenic nonapeptide

Ac-Lys-Pro-Leu-Glu-Glu-Val-Leu-Asn-Leu-OMe

has been determined at 2.6 Å resolution. In the structure found four out of six hypervariable loops L1, H1, H2, H3 of the Fab are involved in peptide binding by four hydrogen bonds, two salt bridges and a number of hydrophobic interactions. The Tyr residues in the Fab antigen binding site play the major role in this process. The CDR-L1 loop shows the largest structural changes upon binding. The peptide adopts α-helical conformation similar to that in the epitope fragment 64-72 of IL-2 antigen. The structural data show that the side chains of Leu66, Val69 and Leu70 residues of the epitope, internally buried in the IL-2 antigen structure, are involved in interaction with the Fab in the complex studied. This observation unequivocally indicates that antibody-antigen complexation causes the rotation of the antigen epitope helix around its axis.