steroid. The density for four rings and two methyl groups of the substrate is clear in the difference map. The steroid is surrounded by hydrophobic protein residues on all sides and makes no contact with external solvent. There is only one water molecule left in the active site. It bridges N5 of the FAD(3.04A), NE2 of His447(3.14A), OD1 of Asn485(2.88A), OE1 of Glu361(2.99–3.29A, because of flexibility) and O1 of the substrate(3.05A) with strong hydrogen bonding interactions to FAD, the protein and the substrate. A loop formed by residues from 72 to 86 constitutes of one wall of the active site, and is the only region to show a major protein conformational change during the substrate binding. It suggests that this is the entrance for the substrate to the enclosed binding site.
some hints have been received regarding the oxidation reaction, the reducability of the FAD, the activation and reoxidation of the enzyme from this substrate structure and related experiments, all of which lead to this protein crystallographic results. With other substrate binding structures and product complex structures which are in progress, combined with other information about related structures and biological research, would reveal that how does this enzyme work.

**PS–03.11.04** X-RAY STRUCTURE ANALYSIS OF ABRIN-A FROM THE SEEDS OF ABRUS PRECATORIUS. By Tahir H. Tahirov*, Tian-Huey Lu, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 300, China; Yen-Chywan Liaw, Institute of Molecular Biology, Academia Sinica, Nankand Taipei, Taiwan 11529, China and Jung-Yaw Lin, Institute of Biochemistry, College of Medicine, National Taiwan University, Taipei 10018, Taiwan, China.

Abrin-a is one of the four isoabrins isolated from the seeds of Abrus precatorius (Lin, Lee, Hu & Tung, Toxicon 1981, 19, 41-51). The antitumor activity of the four isoabrins were studied, and was found that abrin-a showed the highest inhibitory effects on the protein biosynthesis of Sarcoma 180 tumor cells and on the growth of Sarcoma 180 tumor cells in experimented animals (Lin, Lee & Tung, Cancer Res., 1982, 42, 276-279). The toxic protein consists of two subunits, the A and B chains containing 250 and 267 amino acids each, are linked by a disulfide bond. The crystals of abrin-a in the form of rhombic prisms were obtained by vapor diffusion method and belong to monoclinic system, space group $P2_1$, a=84.58, b=73.07, c=48.23 Å, $\beta$=96.20°. There is one molecule in an asymmetric unit. Unit cell dimensions and intensity data from native crystal and three heavy-atom derivatives [$(CH_3COO)_2Hg$, $HgCl_2$ and $DyCl_3 \cdot 6H_2O$] with appoximately equal dimensions 0.35x0.40 x0.25 mm were collected on the SDMS twin area detector system (Hamlin, Methods Enzymol., 1985, 114, 452). The X-rays were from a Rigaku RU-300 generator running at 50 kV and 80 mA. A total of 113,198 reflections were measured from native crystal at 2.2 Å, of which 27,470 were independent, giving the merging R factor 0.063. A three dimensional structure determination simultaneously by the MIR method and by the molecular replacement method using model of ricin (Monfort et al., J. Biol. Chem., 1987, 262, 5398-5403) (homology 42% for A-chain and 59% for B-chain) are in progress.

**PS–03.11.05** MOLECULAR BASIS OF CELL ADHESION: CRYSTAL STRUCTURES OF A FIBRONECTIN FRAGMENT AND A MOLECULAR MIMIC FOR FIBRINOGEN. By K. R. Ely*, C. Dickinson, B. Veerapandian, C.-Z. Ni, and R. Kodandapani, La Jolla Cancer Research Foundation, La Jolla, CA 92037 USA.

Cell surface receptors (integrins) mediate diverse cell-adhesion phenomena through recognition of an RGD sequence present in proteins such as fibronectin and fibrinogen. This recognition is important in cell attachment and metastasis (fibronectin) and platelet aggregation and thrombosis (fibrinogen). Efforts to date to use NMR analyses to examine the RGD structure have been unsuccessful due to marked flexibility of a loop containing the tripeptide. We have crystallized two proteins to study the conformation of the RGD site. Both of these structures have been solved by molecular replacement methods: 1) the 10th Type III module (RGD) of fibronectin (space group $P2_1$ with $a$ = 30.7, $b$ = 35.1, $c$ = 37.7 Å, $\beta$ = 107°; and 2) the OP-G2 Fab fragment that contains an RYD sequence and functions as a molecular mimic for fibrinogen (space group $P2_12_12$ with $a$ = 93.1, $b$ = 83.8 and $c$ = 53.7 Å. The high-resolution structures of these proteins will be presented and the atomic configuration of the RGD (RYD) sequences will be compared.

**PS–03.11.06** A NEW STRUCTURE TYPE OF INSULIN HEXAMER, $T_3R_3^t$ By Da-Cheng Wang*, Zong-Hao Zeng and Yong-Lin Hu, Institute of Biophysics, Academia Sinica, Beijing 100101, China.

Some recent finding from X-ray structural analysis revealed that the hexameric zinc insulin displays the properties of an allosteric protein. So for three conformational states designated as $T_6$, $T_3R_3$, and $R_6$ have been found in the crystal structures of 2 Zn insulin, 4 Zn insulin and phenol insulin respectively. Here we report a new structure type of insulin hexamer which was observed in the crystal structure of a protein-engineered mutant, A21-Ser human insulin, at 1.8 Å resolution and designated as $T_3R_3^t$. Compared with the $R_3$ conformational state discovered in $T_3R_3$ and $R_6$, the $R_3^t$ structure in the new structural species possesses the following characteristics: (1) the first cycle of B-chain helix appeared in $R_3^t$ is lost to a $\beta$-turn-like conformation; (2) the coordination pattern of zinc ion on the 3-fold axis adopts an octahedral array composed of six ligands (like a T type) including three Asn-B3 and three His- B10, other than the tetrahedral array composed of four ligands including one chloride ion or water molecule and three His-B10 in R structure; (3) the effector inducing the conformational changes to $R_3^t$ is a neutral organic molecule, 1,4-dioxane, which binds to a pocket on the hexamer surface to trigger the conformational transition, other than the phenol or chloride ion.

The $T_3R_3^t$ seems to represent a new particularly stable intermediate in the $T_6$ to $R_6$ conformational transition and may provide a new insight into the insulin property as an allosteric protein. The detail characteristics of $T_3R_3^t$ structure and its significance will be presented and discussed.

  