(Rsym = 0.109) were collected on a Siemens multiwire X200-B area detector. The structure was solved by molecular replacement with Crowther's fast rotation and translation function, and the search molecule constructed from one subunit(L) of *C. atrox* venom PLA_2. The structure was refined using programs PROLSQ and X-PLOR and model building techniques. The current model gives a crystallographic R-factor of 0.19. The root-mean-square (rms) deviation from ideality for bond lengths is 0.012Å, for bond angles is 2.9°, and for planarity of the peptide bond is 23.8°. The structure of acidic PLA_2 shows that the main chain folding is similar to that of *C. atrox* venom PLA_2, with the exception of several flexible loops and the stretch 115-124 where the extra residue Ser121 is inserted. The enzymatic active center, the hydrophobic channel to accessing the catalytic center and the binding region of calcium ion resembles closely those of other PLA_2. The structure details will be described and the relationship between the structure and function including inhibiting platelet aggregation will be discussed.

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PS–03.07.29 THE CRYSTAL STRUCTURE OF THE TERNARY COMPLEX OF MUNG BEAN TRYPSIN INHIBITOR WITH TWO PORCINE TRYPSIN (PTRY-MBI-PTRY) AT 2.8 Å RESOLUTION. Jin Yi, Liu Shenping, Li Genpei, Tang Youchi, Institute of Physical Chemistry, Peking University, Beijing 100871, P.R. China; Chi Zhengwu, Shanghai Institute of Biochemistry Academia Sinica, Shanghai 200031, P.R. China

Mung bean trypsin inhibitor is a Bowman-Birk type serine proteinase inhibitor with a single peptide chain of 72 residues and possesses two active sites of antitrypsin. Both sites bind strongly to trypsin synchronously, but not to chymotrypsin. The crystallization of the complex was carried out by the combination of vapor diffusion and reseeding methods. The crystal was orthorhombic with space group I222 and unit cell dimensions of a=122.4, b=123.0, c=112.8Å. The 2.8Å resolution data set composed of 18409 unique reflections above significant level, corresponding to 88.7% expected unique reflections, was collected on a Simens X-200B area detector. The structure of the complex was determined by molecular replacement method and refined by stereochemically restrained least-squares and simulating annealing procedure to a current R value of 0.217 at 2.8Å resolution. The root-mean-square deviations from the ideal bond distances and angles for the model are 0.015Å and 3.4°, respectively. The model of MBI molecule is composed of two structural domains which are similar in conformation, but distinctly different in atomic details. The two domains relate to each other by an approximate dyad axis and their binding modes with trypsin are remarkably similar. A model of ternary PTRY-MBI-PTRY complex will be presented.

PS–03.07.30 THE CRYSTAL STRUCTURE OF THE COMPLEX OF PORCINE PANCREATIC ELASTASE WITH C/E-1 INHIBITOR, A MEMBER OF A NOVEL INHIBITOR FAMILY OF SERINE PROTEINASES. Kui Huang, Robert J. Peanasky and Michael N.G. James, Dept. of Biochemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2H7 and Dept. of Biological Chemistry, The University of South Dakota Medical School, Vermillion, South Dakota 57069, U.S.A.

A 63 amino acid protein isolated from the intestinal parasite *Ascaris suum* is a very strong inhibitor of chymotrypsin and elastase, with a Ka of 1.6×10^{10} M^{-1} for porcine pancreatic elastase. This inhibitor (C/E-1) shares little sequence homology with known protein inhibitors of proteolytic enzymes, thus representing a distinct family of protein inhibitors of serine proteinases, including several other small proteins isolated from *Ascaris suum*.

The C/E-1 inhibitor has been crystallized in complex with porcine pancreatic elastase. The crystals grow as thin plates from 12% PEG (6000), at pH 6.5, in 50 mM sodium citrate buffer. The space group was determined from precession photos, as $P2_12_12$, with $a = 74.51$ Å, $b = 114.33$ Å, $c = 70.45$ Å. There are two molecules of complex per asymmetric unit. X-ray diffraction data have been collected using synchrotron radiation to 2.5 Å resolution. The initial phases for the structure of the complex were determined by the molecular replacement method, using the refined crystal structure of porcine pancreatic elastase as a search model. The highest peak given by the Navaza fast rotation function was 9.2 sigma above the mean. The second highest peak was significantly lower (4.5 sigma), suggesting that the two complex molecules are in almost the same orientation. The Brute translation search carried out with two molecules in the same orientation gave two peaks, one for each of two molecules. The best orientation for each molecule was determined by a 6-dimensional fine search of one molecule, while the other one was fixed. The molecular replacement solution gave a reasonable crystal packing pattern, exhibiting abundant intermolecular interactions and no collision of main chain atoms in the interfaces of neighboring molecules. The relatively limited number of interactions along the b-axis explains the fact that the complex crystal is very thin in that direction (about 0.01 mm thickness).

The initial electron density map reveals parts of the polypeptide chain of the C/E-1 inhibitor in the vicinity of the reactive site. Progress on the detailed structure analysis of the C/E-1 inhibitor, the comparisons of the structure and inhibitory mechanism of C/E-1 inhibitor with those of inhibitors from other families, and prediction of common features of the novel *Ascaris suum* inhibitor family represented by C/E-1 will be reported.

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