

# Center for Eukaryotic Structural Genomics

## Protein Structure Data Summary

<b>Target ID</b>	GO.9161	
<b>Source Organism</b>	<i>Arabidopsis thaliana</i>	
<b>Target Name</b>	At2g43510.1	
<b>PDB Entry</b>	1JXC	Deposition: 06-Sep-2001
<b>BMRB Entry</b>	5056	Deposition: 13-Jun-2001
<b>Function</b>	ATT -- a trypsin/chymotrypsin inhibitor	
<b>Produced From</b>	<i>E. coli</i> BL21(DE3)/pLysS	
<b>Structure by NMR</b>	Restraints/Residue: 14	Subunits/Molecule: 1
	No. of Residues: 68	Molecular Weight: 7.5 kDa
	Backbone RMSD(10–64): 0.91 Å	All Heavy Atoms RMSD(10–64): 1.54 Å
<b>Data Collected At</b>	Nuclear Magnetic Resonance Facility at Madison (NMRFAM)	
<b>Authors</b>	Q. Zhao, Y.-K. Chae, J.L. Markley	



### Structural Features

The most similar structures in the PDB were brazzein (2BRZ) with 28% identical and 38% homologous residues. This represents the first structure of a new class of proteinase inhibitor (“rapeseed type proteinase inhibitor”) and thus a new fold-function relationship. The protein consists of a cysteine-stabilized  $\alpha\beta$  fold ( $CS\alpha\beta$ ), which has been associated with several other functions, including antifungal agent, sweet protein, and channel blocker.

Biochemical assays have confirmed that this protein is a trypsin inhibitor, and NMR spectroscopy was used to identify contact residues with the proteinase. This target aligns to domains within Pfam trusted matches for Toxin\_3 over residues 28–88. This family contains both neurotoxins and plant defensins. The mustard trypsin inhibitor, MTI-2, is a plant defensin. It is a potent inhibitor of trypsin with lower activity toward chymotrypsin. MTI-2 is toxic for Lepidopteran insects, but has low activity against aphids.

*References:* (1) Zhao, Q., Chae, Y.K., Markley, J.L. (2002) NMR solution structure of ATTp, an *Arabidopsis thaliana* trypsin inhibitor. *Biochemistry* 41(41):12284-96.

<b>Percent Identity with Nearest PDB Structure at Time Solved</b>	28% over 56 aa (2BRZ)
<b>Pfam Cluster</b>	Toxin_3
<b>Protonet Cluster Size : Structures in PDB</b>	16 : 2

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