

Computational insights into Ani s 12– major allergen of *Anisakis simplex*

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Allergens of *Anisakis simplex* are one of the most common hidden allergens in food. Anis 12 is one of the major allergens of A. simplex, however, Ani s 12 is still poorly investigated. Therefore our goal was to characterize this allergen using a bioinformatics approach.

Ani s 12 protein sequence was retrieved from UniProt database (accession no. E9RFF6). Different software packages and servers were used to increase the accuracy of analysis and to validate the results. Physicochemical characterization of protein is shown in Table 1. Secondary structure and tertiary (3D) structure models were reconstructed. Crystal structure of the human SF3b core complex, yeast activated spliceosome, cryo-EM structure of the activated spliceosome (Bact complex), and crystal structure of the nuclear export complex CRM1-snurportin1-ranGTP were identified as the best structural analogs of Ani s 12. Gene Ontology (GO) and enzyme activity predictions are shown in Table 2. Molecular docking of Ani s 12 and human IgE antibody is displayed in Fig. 1.

In silico methods were used to predict physicochemical prosperities, function, structure of Ani s 12 and interaction between allergen and IgE antibody. These analyses of Ani s 12 were performed for the first time. Computational investigations are important prior to experimental studies on the immunological determination of IgE-binding epitopes of Ani s 12 which will be carried out in a further step.

Table 1. Physicochemical characterization of Ani s 12

Number of amino acids	295
Molecular weight	32942.86
Theoretical pI	5.36
Total number of negatively charged residues (Asp + Glu)	38
Total number of positively charged residues (Arg + Lys)	32
Atomic composition	C (1425), H (2259), N (387), 0 (444), S (32)
Instability index	49.07
Aliphatic index	69.12
Grand average of hydropathicity (GRAVY)	–0.310

Table 2. Gene ontology and enzyme activity prediction of Ani s 12

Gene ontology terms	
Molecular function	protein transporter activity, RNA binding, nuclear export signal receptor activity
Biological process	protein localization to organelle, regulation of catabolic process, regulation of centrosome cycle, regulation of nucleocytoplasmic transport, centrosome duplication, response to other organism, regulation of intracellular protein transport, regulation of protein metabolic process, protein catabolic process, mRNA transport
Cellular component	organelle envelope, kinetochore, nucleolus, ribonucleoprotein complex, Cajal body, annulate lamellae, cytoplasmic part
Enzyme activity	
Enzyme	protein farnesyltransferase, protein geranylgeranyltransferase type I, protein-serine/threonine phosphatase, protein geranylgeranyltransferase type II, protein farnesyltransferase

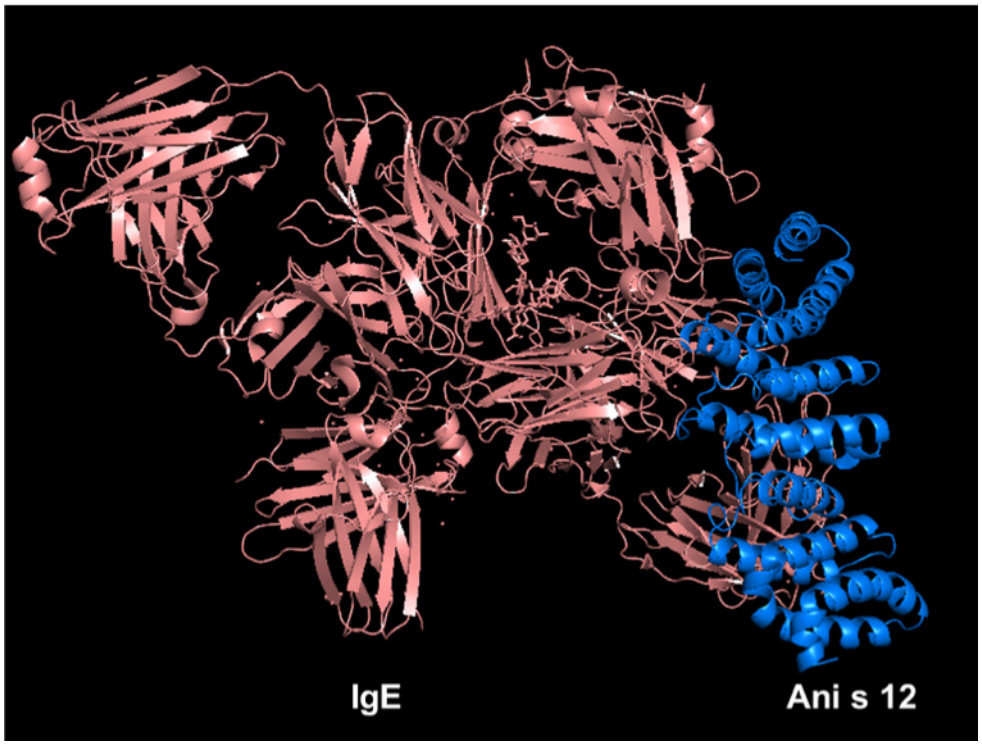

Fig. 1. Molecular docking analysis of the interaction between Ani s 12 and human IgE antibody