

POSTER - PROTEINS AND PROTEOMICS

**COMPUTATIONAL ASSESSMENT OF EIF4E ISOFORMS IN COWPEA
(VIGNA UNGUICULATA (L.) WALP): FROM GENOME MINING TO
STRUCTURAL PROFILING**

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Cowpea (*Vigna unguiculata* (L.) Walp) is an important crop in tropical and subtropical regions, due to its nutritional properties and adaptability. The eukaryotic translation initiation factor 4E (eIF4E) is a key protein involved in cap-dependent translation. Its interaction with viral proteins has been associated with host susceptibility/resistance to viruses of the Potyviridae family, such as the Cowpea aphid-borne mosaic virus (CABMV). This study provides a detailed *in silico* structural analysis of eIF4E isoforms in *V. unguiculata*, aiming to identify structural determinants that may influence viral resistance or susceptibility. Gene mining was performed using annotated genomes of common bean (*Phaseolus vulgaris*) and *V. unguiculata*, along with pre-release genomic assemblies from five Cowpea cultivars (BR14 Mulato,

IT85F-2687, Santo Inácio and Pingo de Ouro). Conserved sequence domains were identified using NCBI's CD-Search, and sequence alignments were subsequently performed with Clustal Omega and visualized in Jalview. Theoretical tridimensional models of the isoforms were generated using AlphaFold3, with model accuracy evaluated through pLDDT and PAE scores and validated using ProSa-web, PROCHECK and QMEANDisCo metrics. Molecular Dynamics (MD) simulations were performed using GROMACS 2022.4 with the GROMOS 53A6 force field in a solvated system under physiological conditions (0.15 M NaCl) for 100 ns. Structural stability and conformational flexibility were assessed via RMSD, RMSF, radius of gyration and hydrogen bond analysis. Electrostatic surface potential maps were generated using the APBS server to analyze the charge distribution across the molecular surfaces. Genomic mining of Cowpea cultivars revealed the presence of three genes encoding eIF4E isoforms, located on chromosomes 4, 6 and 7. The protein sequences corresponding to the isoforms from chromosomes 4 and 7 exhibited high sequence conservation, whereas the isoform encoded on chromosome 6 showed lower conservation, suggesting potential functional divergence, altered affinity for the 5' cap region, or distinct involvement in translation hijacking mechanisms during phytopathogen infections, such as those caused by CABMV. The tri-dimensional modeling revealed that eIF4E isoforms in *V. unguiculata* maintain a conserved "cupped hand" fold, typical of cap-binding proteins. Notably, isoforms encoded by chromosomes 4 and 7 showed significant structural similarity, particularly due to the presence of positively charged regions and flexible loops in the region involved in interacting with the mRNA 5' cap and eIF4G. In contrast, chromosome 6 isoforms displayed a distinct electrostatic potential and enhanced rigidity relative to the others, potentially impairing their interaction with the translation machinery. These findings suggest that the structural diversity among eIF4E isoforms may underlie differential responses to translation regulation and virus susceptibility in Cowpea cultivars. Altogether, these insights support future efforts in breeding and biotechnological approaches aimed at enhancing viral resistance in *V. unguiculata*.

Palavras-chave: translation initiation factor; potyvirus; pathogen resistance; structural characterization; molecular modeling; molecular dynamics.