## Abstract

Anol synthase is multifunctional and NADPH dependent enzyme that can catalyze the conversion of coumaryl acetate into anol enzyme that transcript from AIS1 gene, also another enzyme in this pathway, t-anol/isoeugenol O-methyltransferase that catalyzed t-anethole synthesis reaction that transcript by AIMT1gene, t-anethole (1-methoxy-4-[(1E)-prop-1-en-1-yl]benzene), is one of The Phenylpropanoid Derivatives of secondary metabolism that find in Foeniculum vulgare (bitter fennel) and Pimpinella anisum. We have obtained amino acid sequences of isoeugenol O-methyltransferase and anol synthase from Uniprot database and we have used PYRE 2 software for predicting Tertiary and secondary structure and disorder based on Homology modeling algorithm of this enzymes with detecting sequence homologues with PSI-BLAST and scanning constructing Hidden Markove Model (HMM) this sequence with homologues detecting and constructing 3D model for sequence of this protein Based on the alignments between the HMM of query sequences and the HMMs of known structure with accuracy Based on core of the protein within 2-4 Å RMSD (Root Mean Square Deviation) from the native structure, secondary structure predicted at α-helix, β-strand, coil and disorder levels with their SS confidence line that indicates the confidence in the prediction, and with Average 78-80% accuracy (i.e. 78-80% of the residues are predicted to be in their correct state) and also domain analysis is done. In conclusion 3D structure is predicted and displayed.

### HMM, PYRE2, RMSD

**Presentation:** Poster