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RESEARCH ARTICLE

EVALUATION OF PHENYLALANINE AMMONIA LYASE BETWEEN *PETROSELINUM CRISPUM* AND *RHODOSPORIDIUM TORULOIDES* BASED ON COMPUTATIONAL ALGORITHMS

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ABSTRACT

In this study, Phenylalanine ammonia lyase (PAL) was evaluated as one of the important enzymes in the pathway of phenylpropanoids synthesis in order to understand the structural fold and sequence homology; so that it was extracted from Protein Data Bank (PBD): X-ray crystallographic structures of *Rhodosporidiumtoruloides* (1T6J) as a genus of fungi category and (1W27) *Petroselinumcrispum* as a genus of plants category. In order to structural analysis of PAL has been used some software include Protein Structure Comparison Tool V 1.4, on-web PDBe version based on secondary structure matching (SSM) and Combinatorial Extension(CE) for Structure Alignment, calculation of statistical indicators such as Z-score, p-value, Q-score and etc. Finally PAL showed a significant relationship between structural sequences of 1T6J & 1W27 in terms of structural folds similarity and partialhomology with calculated indices between the two enzymes.

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INTRODUCTION

Structural biology is an important tool to understand the structural-functional details of bio-macromolecules at the atomic level. It is using for fund a mental studies of life from the evolutionary perspective and process engineering of metabolic pathways. Phenylalanine ammonia lyase (PAL) is playing an important role in dynamic control of primary and secondary metabolites converting process; also it catalyzes the converting reaction about non-oxidative elimination of phenylalanine (L-phe) amino group to trans-cinnamate. (Joseph *et al*., 2005) Trans-cinnamate, plays role as prefabricate for wide range of phenylpropanoids compounds such as phytoalexins, antioxidants, UV-absorbing compounds and pigments like anthocyanins. Also elimination of metabolic disorders is one of the pharmaceutical applications of PAL in patients with Phenylketonuria. (Holger Ritter and Georg E. Schulz, 2004) There are several computational methods have been reported such as dynamic programming, vector alignment and etc. Algorithms of proteins structure comparison are used in order to remote homologues evaluation. The importance of this is appeared well when it is not easy to check the evolutionary distance between them because of low similarity sequence in the structures. Studies show that three-dimensional structures of proteins are more conserved than sequences; also it is possible that two proteins with sequence similarity would have a very similar three-dimensional structure. It has provided development background of computational methods to predict the third structure of proteins such as Homology modeling. On the other hand, some proteins could have been a same evolutionary origin but different structure and function. This phenomenon could be occurred due to divergent evolution (Divergent evolution). (Zhang and Skolnick, 2005) In this work structure aligment analysis were done on PAL enzyme of *Rhodosporidiumtoruloides* (1T6J) and *Petroselinumcrispum* (1W27) (Figure 1)

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MATERIALS AND METHODS

In order to the structural alignment of two PAL enzymes, it was used two algorithms secondary structure matching (SSM) and Combinatorial Extension (CE) available at PDBe server. In this study, these tow enzymes have hadthe plant and fungi origin with PDB codes (1T6J) and 1W27. CE algorithm (Pair wise structural alignment) is able to perform quantitative assessment of how structural folding in tow proteins through

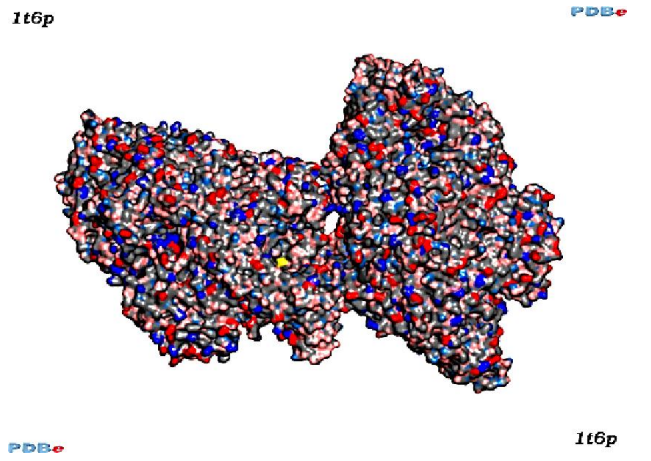
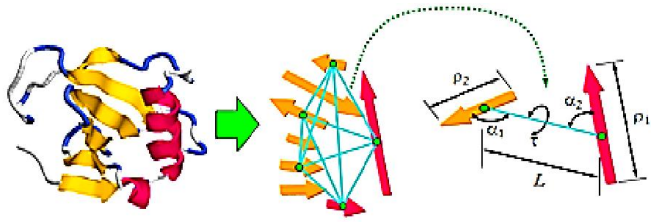


Figure 1. 3D Structure of *Rhodosporidiumtoruloides* (1T6J) PAL Enzyme



A)Graphical representation of SSEs algorithms (4)
B) Q-score equation represents the quality function of C-alignment, maximized by the SSM alignment algorithm.

Figure 2.

So that in this way, the best likely alignment is made through combinational developing of a set of aligned fragment pairs (AFPs) and calculation of matrix similarity (Shindyalov and Bourne, 1998). Eventually it was presented distribution of existing structures in the PDB database via Z-score calculation so that Z›3.5 is demonstrated equality in structural folding (Adam Godzik and Philip E. Bourne, 2010). Q-score parameter is been made balance between RMSD and Nalign in SSM algorithm. It has shown moreaccuracy in structural similarity than other algorithms such as CE, VASD, DALI and geometric quantities (Krissinel and Henrick, 2004).

$$Q = N_{\text{align}}^2 / \left\{ \left[1 + (\text{RMSD}/R_0)^2 \right] N_1 N_2 \right\}$$

RESULTS AND DISCUSSION

Finding this study has demonstrated a significant relationship between structural similarity and partial homology in sequences of tow PAL enzymes (1T6J and1W27); note that was the calculative parameters such as RMSD and Z-score in CEalgorithm (Table 1) and P-score and Q-score in SSM algorithm (Table 2). Also the calculative parameters have shown advantage of SSM algorithm than CE algorithm about quantitative evaluation of structural similarity. It is matched with K. Henrick and E. Krissinel study (2004). In another study that was done by Longkuonxiang and *et al.* two PAL toruloides origins have been taken in one cluster for severance of PAL clusters with prokaryotic and eukaryotic origins based on Clustal x algorithm by Neighbor-joing method (Longkuan Xiang and Bradley S. Moore, 2005) also.

Results of Multiple structure alignment based on SSM algorithmwere shown in Figure 4. And Table 3. Rotation-Tralnslation Matrices of Best Superposition were calculated and represented in Table 4.

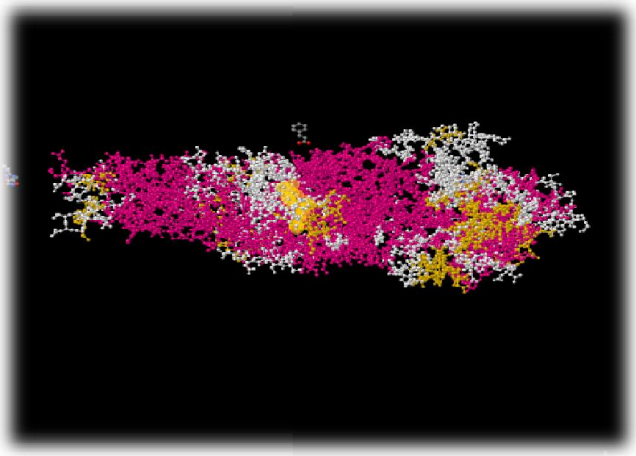


Figure 3. Graphical Output of pair wise Structural Alignment of 1W27 A vs1T6J B By Protein Structure Comparison Tool V 1.4 Software in RCSB PDB

Table 1. Resutlsof Pairwisestructural Alignments of PAL enzyme based on CE Algorithm between A and B chains

PDB ID	1W27 chain A vs 1T6J chain A	1w27 chain A vs 1T6J chain B	1w27 chain B vs 1T6J chain B	1w27 chainB vs 1T6J chain A
Z-score	7.74	7.84	7.84	7.84
Cα RMSD	2.14	2.16	2.22	2.21
(%)Id	36.36	35.53	36.16	36.22
(%)Similarity	54.55	54.55	54.4	54.32
Align- len	707	707	698	699
score	1201.98	1217.07	1870.18	1565.6
Gaps	102	102	84	86
eq	605	605	614	613

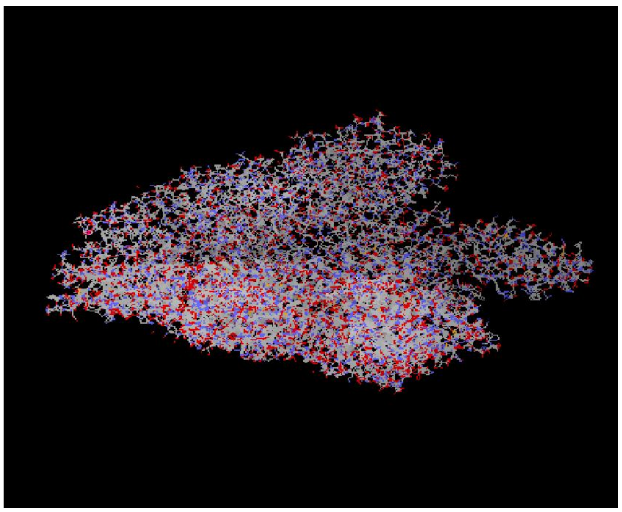


Figure 4. Graphical Output of Multiple Structure Alignment PAL Enzymes

Table 2. Results of Mutiple Structure Aligment of Rhodosporidiumtoruloides (1T6J) as a genus of fungi category and (1W27) Petroselinumcrispum

Q-score	P-score	Z-score	RMSD	N_{align}	N_g	$\%_{seq}$	%SSE	Match	%SSE	N_{res}	Title
1.00	113.6	32.2	0.00	647	0	100	100	1T6J:A	100	647	Crystal structure of phenylalanine ammonia lyase from rhodosporidium toruloides
1.00	61.7	23.7	0.15	647	0	100	96	1T6J:B	90	647	Crystal structure of phenylalanine ammonia lyase from rhodosporidium toruloides
0.54	19.5	14.1	1.77	569	21	37	81	1W27:B	73	690	Phenylalanine ammonia-lyase (pal) from petroselinum crispum
0.52	16.4	13.6	1.85	569	22	37	81	1W27:A	71	690	Phenylalanine ammonia-lyase (pal) from petroselinum crispum

Table 3. Results of Multiple Structure Alignment Based on SSM Algorithm

Structure	Nres	NSSE	Consensus Score	
			RMSD	Q-score
PDB 1W27:A	690	31	1.0074	0.7710
PDB 1W27:27:B	690	30	0.9393	0.7814
PDB 1T6J:B	647	29	0.9392	0.8333
PDB 1T6J:A	647	27	0.9489	0.8318
		Number of Aligned residues 592	Overall RMSD 1.566	
		Number of aligned SSEs 21	Overall Q-score 0.6169	

Table 4. Rotation-Tralnslation Matrices of Best Superposition

PDB 1w27:A	-0.311	-0.842	0.441	×	X	+	109.258
	0.217	-0.515	-0.830		Y		76.342
	0.925	-0.163	0.343		Z		62.425
PDB 1w27:B	0.048	0.843	-0.536	×	X	+	80.350
	-0.379	0.512	0.771		Y		-18.925
	0.924	0.166	0.344		Z		50.041
PDB 1t6j:B	0.466	0.845	0.262	×	X	+	8.339
	0.846	-0.513	0.148		Y		-46.978
	0.259	0.153	-0.954		Z		105.099
PDB 1t6j:A	1.000	0.001	0.001	×	X	+	-0.126
	-0.001	1.000	-0.000		Y		0.099
	-0.001	0.000	1.000		Z		0.060

Notes of table

Z-score represents the statistical significance of a match in terms of Gaussian de stributation. Sequence identity $\%_{seq}$ represents a quality characteristic of Cα-alignment RMSD (Root Mean Square Deviation) which calculated between Cα-atoms of matched residues at best 3D superposition of the query and target structures.

P-score shows minus logarithm of the P-value. Which represents *quality of match* at a chance, which has been calibrated on the non-redundant database containing all SCOP folds (about 700 structures).

Length of alignment N_{algn}, (number of matched residues) which is calculated at best 3D superposition Sequence identity $\%_{seq}$ is a quality characteristic of Cα-alignment.

Percent of matched SSEs: shows fraction of secondary structure of target chain has been identified in query protein Match is identified as a target structure name. The name may be one of the following PDB code, SCOP domain

Also Calabrese and *et al.* were demonstrated overall structural similarity in these structures via scrutiny of X ray crystallography structures of PAL At last; Finally it has been shown a significant relationship between structural sequences of 1T6J & 1W27 in PAL enzyme in terms of structural folds similarity and partial homology with calculated indices between the two proteins. In conclusion finding of present study confirm previous researches in this pathway.

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