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In Silico Analysis of Dimethylsulfoxide Reductases from Phototrophic Rhodobacter Species

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Abstract

In the present study in silico modeling of Dimethylsulfoxide reductases were done and the results are presented. The composition of cysteine and lysine were lowest when compared to the aminoacids alanine and glycine. The instability index of all the enzymes varied but was less than 40 showing that all of them are stable. The negative aminoacids were more compared to the positively charged aminoacids. SOSUI server analysis has shown that all the enzymes were soluble in nature.

Keywords: DMSO Reductases; Rhodobacter sps; Silico Analysis; Instability Index

Introduction

Dimethylsulfoxide (DMSO) is a dipolar aprotic solvent, colorless liquid readily miscible in a wide range of organic solvents as well as water. DMSO is used as a solvent in NMR as a cryoprotectant for storage of embryonic stem cells and hematopoietic stem cell in the electronics industry. Dimethyl Sulfoxide may have anti-inflammatory, antioxidant and analgesic activities. Dimethylsulfoxide (DMSO) reductase family of molybdenum enzymes are found in bacteria and archaea. These enzymes are involved in reduction of certain toxic oxoanions. The molybdenum of the oxidized dimethyl sulfoxide (DMSO) reductase enzyme contains one terminal oxygen ligand (Mo=O), four thiolate ligands and one oxygen. The enzyme reduced by dimethylsulfide contains a desoxo active site with four Mo-S and two different Mo-O ligands. Recombinant wild-type *Rhodobacter sphaeroides* DMSO reductase expressed in *Escherichia coli*. [1]. High degree of similarity in tertiary structure DMSO reductase family. Reduced dimethylsulfoxide reductase (DMSOR) enzymes have an active-site which (a) lacks a terminal oxo ligand and has two pyranopterin-ene-1,2-dithiolate ligands [2]. Tungsten is also found in enzymes of the DMSO reductase and xanthine dehydrogenase family in thermophilic bacteria and archaea that grow under anaerobic reducing conditions [3] There exist very small differences in the active site of Mo indicating diversity of the enzyme catalyzed reaction mechanism [4]. Disruption of dmsA gene encoding Dimethyl sulfoxide/trimethylamine N-oxide reductase results in the inability to use DMSO or TMAO as the terminal electron acceptor [5].

Rhodobacter sphaeroides enzyme suggested hexacoordinated active site geometry, whereas for the R. capsulatus enzyme extended X absorption fine structure

indicated seven ligands [6]. The DMSOR from R. sphaeroides reveals plasticity at the active site where Mo is exists in a hexa coordinated and a pentacoordinated ligation sphere [7] the observed differences in the Mo co-ordination environment is due to structural flexibility at the active site [8]. The *Rhodobacter* enzyme catalyses the reduction of DMSO using the pentaheme c-type cytochrome DorC as the physiological source of reducing equivalents. Various spectroscopic studies on molybdenum center of DMSO reductases have been reported and were found to have unique absorption features [9-11]. X-ray crystallography studies on the group of these enzymes were also reported [12,13]. Li, et al. have determined the crystal structure of DMSO reductase at 1.3 Å resolutions and found the heterogenous nature of the oxidized enzyme with two conformations [6]. Dimethylsulfoxide (DMSO) is enzymatically reduced to dimethylsulfide (DMS) by bacteria, which helps in measurement of respiratory activity of bacteria. Hence in the present study, an insilico analysis was done to investigate the physico chemical characteristics and nature of the dimethyl sulfoxide enzymes from different Rhodobacter species.

Material and Methods

Retrieval of nitrogenase sequences was done from UniProtKB/Swiss-Prot [14]. These sequences were used for further analysis. ExPASy's ProtParam tool was used for the computation of various physical and chemical parameters [15]. SOPMA tool (Self-Optimized Prediction Method with Alignment) server was used to characterize the secondary structural features [16]. The transmembrane regions classified as membrane bound and soluble proteins were predicted by SOSUI server [17].

Results and Discussion

In continuation of earlier studies on phototrophic bacteria [18-23], a study has been done on the DMSO reductases which are known to play a crucial role in DMSO reduction by the bacteria. DMSO reductase is a membrane-bound terminal respiratory oxidase consisting of separate molybdenum- and ironsulfur-containing subunits in *Escherichia coli* while in phototrophic bacteria it is a soluble periplasmic protein with only a molybdenum center. This was found to over express when grown on Malate medium. The active site consists of pyranopterin cofactor via an enedithiolate linkage [24]. Reductases of different Rhodobacter species obtained from database are presented in (Table 1). Table 2 shows that the amino acid composition of six different DMSO reductases from Rhodobacter species. The composition of cysteine and lysine were lowest when compared to the aminoacids alanine and glycine. The number of negative charged residues was found to be more when compared to positively charged residues (Table 3). Molecular weight of DMSO5 was the highest while molecular weight of DMSO1 was the lowest. pI value of DMSO1 was the highest while the lowest pI was seen in DMSO4 .The instability index of all the enzymes varied but was less than 40 showing that all of them are stable. Aliphatic index which shows the relative volume of protein occupied by aliphatic side chains was found to be within a range of 75 to 77. From Table 4, Secondary structural analysis of the enzymes showed the dominance of α-helices and random coils almost equally for all the DMSO reductases. Beta turns were less in number for all the enzymes. SOSUI server analysis (Table 5) has shown that all the DMSO reductases so far characterized from Rhodobacter genus are soluble proteins.

DMSO reductase	NCBI/Gen Bank Reference Sequence	Rhodobacter Species /strain
DMSO1	WP_012640770.1	Rhodobacter sphaeroides
DMSO2	AAB07230.1	Rhodobacter sphaeroides
DMSO3	AAB94874.1	Rhodobacter sphaeroides
DMSO4	ACM03079.1	Rhodobacter sphaeroides KD131
DMSO5	AAD13674.1	Rhodobacter capsulatus
DMSO6	CAA64689.1	Rhodobacter capsulatus

Table 1: Different DMSO Reductases From Rhodobacter Species

S.No	Dimethylsulfoxide reductase	No of Amino acids	MWt	PI	Negatively charged residues	Positively charged residues	Extinction coefficients	Instability index	Aliphatic index	GRAVY
DMSO1	Rhodobacter sphaeroides	763	83681.5	5.74	94	71	132850/132350	33.24	76.82	-0.29
DMSO2	Rhodobacter sphaeroides	822	89207.51	5.08	103	71	142835/142210	30.03	77.45	-0.214
DMSO3	Rhodobacter sphaeroides	822	89385.76	5.08	103	71	141345/140720	29.98	76.23	-0.243
DMSO4	Rhodobacter SphaeroidesKD131	819	89078.3	5.03	105	71	142835/142210	32.15	76.63	-0.247
DMSO5	Rhodobacter capsulatus	823	89561.39	5.39	101	76	143950/143700	27.91	76.35	-0.225

Table 2: Physico Chemical Characteristics Of Dimethylsulfoxide Reductase From Rhodobacter Species.

S.No	Ala	Arg	Asn	Asp	Cys	Gln	Glu	Gly	His	Ile	Leu	Lys	Met
DMSO1	11.9	7.6	2.6	5.5	1	3	6.8	9.8	4.7	3.4	8.7	1.7	3
DMSO2	11.2	4.9	3.3	6.1	1.2	2.8	6.4	10.5	2.4	3.9	8	3.8	2.8
DMSO3	10.2	4.6	3.4	6.1	1.2	3.2	6.4	10.7	2.4	3.9	7.8	4	2.9
DMSO4	10.3	4.6	3.3	6.2	1.2	3.1	6.6	10.7	2.4	4.2	7.7	4	2.8
DMSO5	10.1	4.4	2.7	6	0.5	2.3	6.3	10.7	2.7	4.1	7.2	4.9	3.2
DMSO6	10.1	4	2.6	6.2	0.5	2.4	6.3	10.7	2.8	4.2	6.9	5	3.1

Table 3: Amino Acid Composition of Dimethylsulfoxide Reductase From Rhodobacter Species.

S.No	Alfa Helix	310 Helix	Pi Helix	Beeta Bridge	Extended Strand	Beta turn	Bend region	Random Coil	Ambiguous State	Other state
DMSO1	36.17	0	0	0	15.99	10.75	0	37.09	0	0
DMSO2	36.01	0	0	0	16.67	11.68	0	35.64	0	0
DMSO3	33.82	0	0	0	18	12.53	0	35.64	0	0
DMSO4	33.58	0	0	0	18.56	12.33	0	35.53	0	0
DMSO5	33.9	0	0	0	18.96	12.15	0	34.99	0	0
DMSO6	33	0	0	0	19.14	12.09	0	35.77	0	0

Table 4: Secondary Structure Analysis of Dimethylsulfoxide Reductase from Rhodobacter Species.

Enzyme	Nature of the enzyme
DMSO1	This Amino acid sequence is of a SOLUBLE protein
DMSO2	This Amino acid sequence is of a SOLUBLE protein
DMSO3	This Amino acid sequence is of a SOLUBLE protein
DMSO4	This Amino acid sequence is of a SOLUBLE protein
DMSO5	This Amino acid sequence is of a SOLUBLE protein
DMSO6	This Amino acid sequence is of a SOLUBLE protein

Table 5: Sosui Analysis of Analysis of Dimethylsulfoxide Reductases from Rhodobacter Species.

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