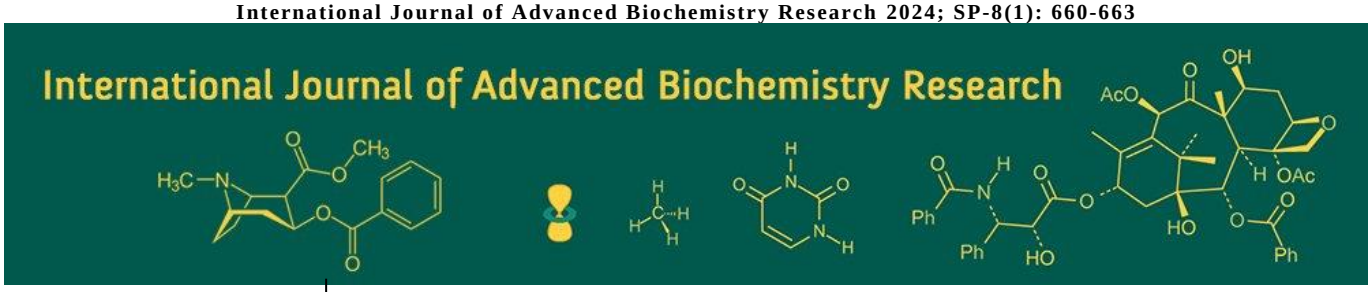

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In-silico analysis of phylogeny, physicochemical and structural properties of nucleocapsid proteins of Peste des Petits Ruminants virus across India and globally

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Abstract
Peste des Petites Ruminants (PPR) is an important livestock disease affect small ruminant productivity especially goats. PPR virus is known to be ssRNA virus and is continuously evolving and mutating which increases infectivity and spread of disease. Phylogenetic analysis, physicochemical and structural properties provide a better base for characterisation of PPR virus. The evolutionary trace back revealed that there are more than one lineage circulating around the world. Physicochemical properties i.e. pI, aliphatic index and GRAVY also differs greatly in all the samples. Homology and structural modelling also differ in its sequence resemble in all nucleocapsid proteins of the virus. Overall, this study provided a snapshot view of representative variants of nucleocapsid proteins around the world.

Keywords: PPR, phylogeny, MEGA, nucleocapsid

1. Introduction
Peste des petits ruminants (PPR) is an important disease of small ruminants with acute course of occurrence and it is also notifiable disease by OiE (world organization for animal health). It negatively impacts the economics of small ruminant production. PPR virus belongs to the family of morbilli virus and encoded by various structural and non-structural proteins. India harbours 65.06 and 135.17 million of sheep and goats, respectively (19th Livestock census, 2019; http://dahd.nic.in/dahd/WriteReadData/Livestock.pdf) which is 16.1 and 6.4% of the world's total goat and sheep population, respectively. PPR was first detected in West Africa (Gargadennec *et al*., 1942) [5]. In India, PPR was first recorded in 1987 from Tamil Nadu (Shaila *et al*., 1989) [7]. The prevalence rate of PPR disease is 45.66% in sheep and 38.54% in goats as studies performed by Balamurugan and co-workers in 2014. The disease also negatively impacts about 70% of livestock landless farmers in India. Due to its widespread effect on low-income group of society, international organizations i.e. FAO & OIE set a target of global eradication by 2030 (http://www.fao.org/ppr/en/).
The various structural proteins included are The PPRV genome encodes for 6 signature and its measurement provides useful information structural proteins like Nucleocapsid protein (N), Matrix protein (M), transmission Pattern phosphoprotein (p), matrix protein (M), fusion protein (F). PPR virus is enveloped negative single-stranded virus (Domingo, 2010) [3]. Like, other RNA virus, PPR virus shows error prone replication machinery and undergo several mutations, recombination under different pressures (Drake and Holland, 1999) [4]. It is also frequently evolutionary changes in protein structure, thereby conferring high infectivity to the virus. For efficient implementation and success of eradication of PPR by 2030. There is a need for elaborate characterisation of PPR isolates around the world. There are several methods for better characterisation including PCR, antigen binding characterisation. One of the important ways is through construction of phylogenetic tree of important clades of isolates to study diversity of a particular disease or condition either through its gene sequence (Singh *et al*., 2023) [1] or expressed peptide sequence. The evolutionary proximity of diverse proteins expressed in viral structure reveals better picture of the extent of transmission of the disease. Moreover, physicochemical parameters, homology and two-dimensional modelling

also increases in-depth study of viral structure. So, the current study was employed to understand the similarity and differences of diverse evolutionary, physicochemical and modelling parameters of nucleocapsid protein expressed in PPR virus within India and globally.

2. Materials and Methods

2.1 Retrieval of sequences

The various peptide sequences of one of most important Protein, Nucleocapsid protein representing several geographical locations within India and across world were retrieved from https://www.ncbi.nlm.nih.gov/protein/ with accession number QCY50238, WGO49596, AEL30504, AGI51686, AHJ59531, ABG68020, AVH80635, AMY61458, QIH45827, AID69933, ACU78077, AYD75854.

2.2 Phylogenetic analysis of Nucleocapsid protein

Retrieved peptide sequences were aligned through multiple alignment through MUSCLE algorithm. The phylogenetic tree was constructed using MEGA (Molecular Evolutionary Genetic analysis) software. The evolutionary relationship between different clades and lineage was established through Maximum Likelihood of the Kimura two-parameter model (Kimura, 1980) with testing of phylogeny by 1000 bootstrap value in software.

2.3 Physicochemical Properties of infective protein across diverse sample

Physicochemical properties like pI, number of amino acid residues, aliphatic index and GRAVY (Grand average of hydropathicity) were determined using ProtParam tool of EXPASY. (https://web.expasy.org/protparam/) (Gasteiger *et al.*, 2005) [8].

2.4 Prediction of structure of infective protein

2D and 3D structure of protein helps in further assessing the functionality of infective nucleocapsid protein of PPR virus. Two -dimensional structure of protein was predicted through online PSIpred server. Secondary structure determines strandedness, helix and primary coiling of protein structure.

3. Results & Discussion

3.1 Evolutionary relatedness of isolated nucleocapsid proteins across diverse geographical areas

When defining phylogenetic analysis of different proteins, it has been well established that Nucleocapsid protein shows more variability as compared to other proteins (F, H) (Kumar *et al.* 2014) [6]. There are several biological evidence for existence of four distinct lineage for different genes of the PPR virus (Banyard *et al.* 2010) [2]. Phylogenetic analysis revealed close relatedness of various Indian samples with diverse association of different clades even among Indian partial nucleocapsid peptide sequences. The findings of this study are supported by previous studies including. As reported by Senthilkumar *et al.*, 2014 [6], the variable N gene which leads to nucleocapsid protein formation provides the best phylogenetic tree prediction for PPR virus. Nucleocapsid protein being infective protein and is chiefly associated with pathogenicity. The phylogenetic tree focused on close association of African nucleocapsid isolates. Moreover, other PPR virus isolates were scattered with showing clustering with different lineages.

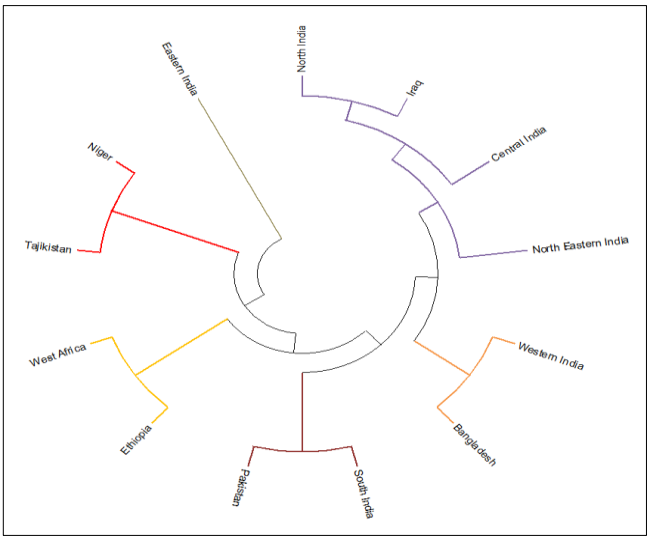


Fig 1: Phylogenetic tree of Nucleocapsid Protein of PPR virus within India and around the world

3.2 Physicochemical properties of nucleocapsid protein across samples

The theoretical physicochemical parameters of different peptide sequences were obtained by utilizing FASTA sequence of nucleocapsid protein. The parameters predicted are number of positive and negative amino acid residues, isoelectric point (pI), aliphatic index (AI), grand average of hydropathicity (GRAVY). Thirteen samples from within India and world were physiochemically characterised by ProtParam tool. Majpr physicochemical parameters are listed in Table 1.

Table 1: Physicochemical parameters of various PPRV variants

PPRV isolate	(Asp + Glu	Arg + Lys	pI	Aliphatic Index	GRAVY
North India	20	16	5.12	52.33	-1.117
South India	15	16	8.54	50.74	-1.086
Central India	25	18	4.86	54.09	-1.139
Western India	19	12	4.56	61.95	-1.280
Eastern India			5.2		
North-East India	20	14	4.84	54	-1.219
Ethiopia	14	13	5.87	55.95	-1.079
West Africa	16	17	8.18	50.28	-1.221
Bangladesh	13	12	5.84	58.21	-1.011
Pakistan	13	12	5.84	54.76	-1.057
Tajikistan	15	14	5.90	54.76	-1.121
Niger	15	14	5.90	53.57	-1.129
Iraq	27	17	4.65	61.50	-0.984

3.3 Homology and Structural modelling of nucleocapsid protein

Homology modelling by swiss model depicted that highest sequence identity with hetero-tetramer orthoretroviral capsid protein. GMQE score (Global Model Quality Estimation) is estimated to be 0.08 for sample isolated from North India. Similarly, GMQE score of viruses from Nigeria has score of about 0.11.

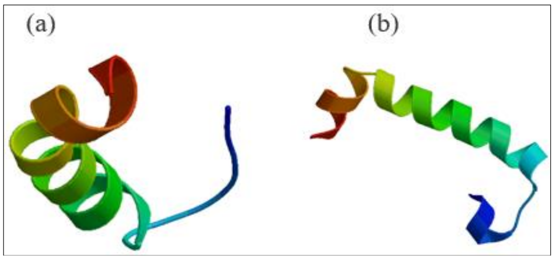
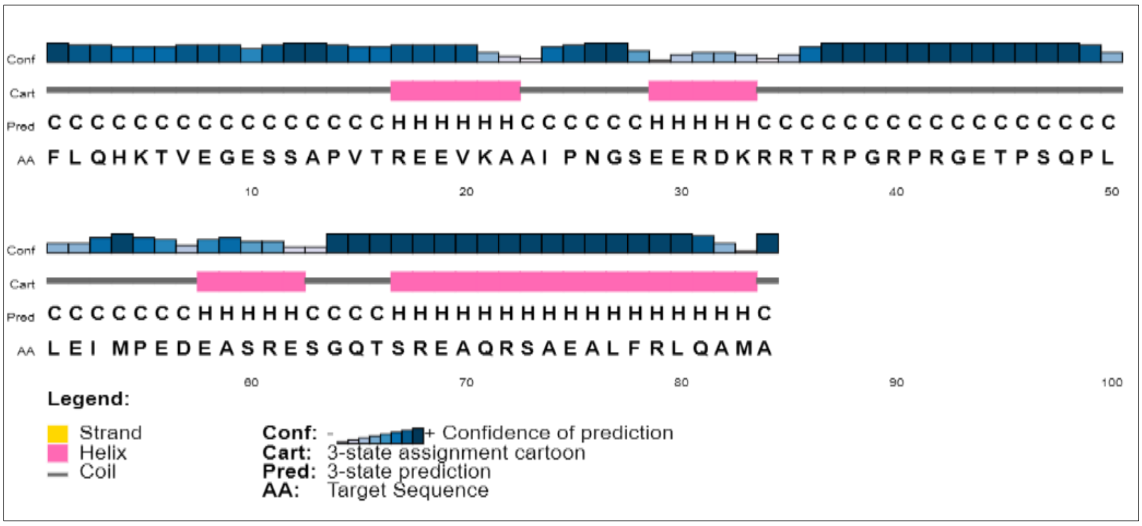
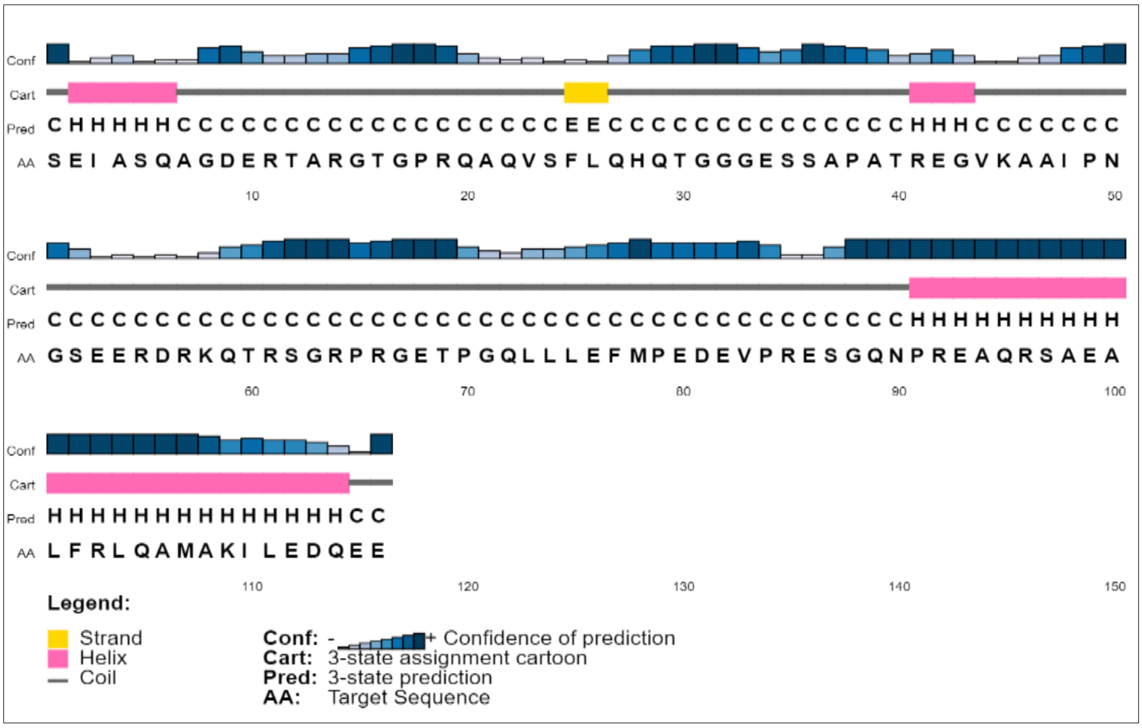


Fig 2: Homology modelling of nucleocapsid protein of PPR virus isolated from (a) North India; (b) Nigeria

Secondary structure of partial nucleocapsid proteins were predicted using PSIpred server. Secondary structure from few nucleoproteins is depicted in Figure 2.



(a)



(b)

Fig 3: Two-dimensional structure of partial nucleocapsid protein of PPR virus isolated from Niger (a) and North India (b)

4. Conclusion

In silico characterization of nucleocapsid protein of PPR virus revealed the different lineage present across the world. The virus isolated from India were closely related to each other as compared to samples isolated from African countries spanning Nigeria, West Africa. The physicochemical properties suggested that N protein has pI ranging from 4 to 8. Even the homology modelling and 2-D model provided better insights into the structure of nucleocapsid protein of virus from different geographical locations. Overall, this study focuses on the importance of phylogenetic analysis of nucleocapsid protein pan-world level to prevent the spread of PPR over the international transboundary and ultimately eradicate the disease in the near future.

5. Conflict of Interest

The authors declare that there is no competing conflict of interest.

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