PREDICTING SECONDARY STRUCTURE, PHYSICAL AND CHEMICAL PROPERTIES OF THE OVALBUMIN PROTEIN OF QUAIL EGG USING SOPMA AND PEPSTATS

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ABSTRACT
This research focused on the application of computational algorithms to predict secondary structure, physical and chemical properties of ovalbumin protein of quail eggs using SOPMA and PEPSTATS. Twenty (20) amino acid sequence data of Ovalbumin gene of quail was retrieved from the website of the National Centre for Biotechnology Information (NCBI). The amino acid sequence alignment of the species was carried out using Multalin software to obtain non-synonymous amino acid substitutions. The aligned sequence was reduced to eighteen (18). PEPSTATS was used for the computation of various physical and chemical properties of the Ovalbumin gene using amino acid sequences. SOPMA server was used to predict the secondary structure of the Ovalbumin protein. These changes affected the physical and chemical properties of the ovalbumin protein of quail as well as the protein-protein interaction.
Keywords: Ovalbumin gene, Amino acid, Quail

INTRODUCTION

The common quail (*Coturnix coturnix*), is mainly a migratory small ground-nesting game bird in the pheasant family *Phasianidae* with body weight between 70 to 140 g, body length of 16–18 cm in length with a wingspan of 32–35 cm (Takahashi *et al*., 2018). Ovalbumin belongs to the Ovalbumin gene family in poultry composed of three homologous genes located on chromosome 2. Ovalbumin is mainly expressed in the oviduct (Sugimoto *et al*., 2001), and more specifically by tubular gland cells of the magnum (Rehault-Godbert *et al*., 2013). The biological roles of Ovalbumin protein have not been fully understood especially in quails. However, increasing data in the literature have shown that its abundance is affected during incubation, suggesting a potential involvement of Ovalbumin in some aspects of fertilization or embryonic development (Yakubu *et al*., 2017).

MATERIALS AND METHODS

Twenty (20) amino acid sequence data on Ovalbumin gene of quail was retrieved from the website of the National Centre for Biotechnology Information (NCBI). The amino acid sequence alignment of quail species was carried out using Multalin software (http://multalin.toulouse.inra.fr/multalin/) to obtain nonsynonymous amino acid substitutions. The physical and chemical properties of the Ovalbumin protein of quail were determined using PEPSTATS as described by Madeira *et al*. (2019). Self- Optimized Prediction Method with Alignment (SOPMA) was used to predict the secondary structure of the Ovalbumin protein as described by Combet *et al*. (2000).

RESULTS AND DISCUSSION

The physico-chemical properties of the native protein and mutants of protein are presented in Table 1. The results revealed slight variation in the molecular weights (42107.18 – 42654.94) and average residue weight (109.940 – 111.081) of the native and mutants of proteins. The molecular weight showed the size and mass of the protein molecules. Protein with larger molecular weight tends to have more complex structure, solubility, stability and folding behaviour. The range of charges (-3.5 to -8.0) obtained for proteins varied widely. Moderate negative charge (-2 to -7) proteins have good solubility especially in neutral or slightly pH conditions, weaker binding affinity compared to highly negative charged proteins. Protein with high charge (> -7) has increased solubility due to electrostatic repulsion, enhanced binding affinity for positive charged surface and involvement in protein–protein interactions. Proteins with negative charges will be accompanied with high isoelectric point. A280 molar extinction coefficient and A280 extinction coefficient characterize native and mutants proteins. Values obtained showed that the protein absorbs lights at a wave length of A280 which is the concentration of a protein in a solution while A280 extinction coefficient obtained showed that the protein solution absorbs light at wavelength of 280.

Table 1: Physio-Chemical properties of the native and mutant protein

Variants	MW	ARW	IP	Charge	A280 MEC	A280 EC /mg/ml
Native	42209.32	110.207	5.1267	-7.0	29910	0.709
E151F	42285.41	110.406	5.1267	-7.0	29910	0.707
L233P	42249.38	110.312	5.1267	-7.0	29910	0.708
S241R	42365.50	110.327	5.2691	-6.0	29910	0.706
Q255K	42250.41	110.314	5.2691	-6.0	29910	0.708
K264E	42241.31	110.291	5.0216	-8.0	29910	0.708
L265I	42207.39	110.202	5.2626	-6.0	29910	0.709
E267V	42235.35	110.275	5.1267	-7.0	29910	0.708
S272Q	42208.33	110.205	5.2589	-6.0	29910	0.709
V279M	42253.43	110.322	5.1267	-7.0	29910	0.708
L283D	42223.30	110.244	5.0177	-8.0	29910	0.708
E289H	42189.24	110.155	5.4168	-6.0	29910	0.709
T304M	42209.32	110.27	5.1267	-7.0	29910	0.709
D305S	42260.36	110.340	5.1267	-7.0	31400	0.743
S308R	42236.39	110.278	5.4377	-5.0	29910	0.708
A333S	42107.18	109.940	5.2590	-6.0	28420	0.675
E355S	42225.32	110.249	5.1267	-7.0	29910	0.708
H368Y	42259.33	110.338	5.1267	-7.0	31400	0.743
V381Y	42225.36	110.249	5.1267	-7.0	29910	0.708
Cmutant	42654.94	111.081	5.8469	-3.5	31400	0.736

MW = Molecular weight; IP = Isoelectric Point; ARW = Average residue weight; 280 MEC = A280 Molar extinction coefficient; 280 EC = A280 extinction coefficient /mg/ml

Secondary structure using SOPMA (Self- Optimized Prediction Method with Alignment)

Secondary structure using SOPMA is presented in Table 2. SOMPA predicted secondary structure such as alpha helix, 3_{10} helix, Pi helix, Beta Bridge, Beta turn, extend strand, bend region, beta strands bends and turn and random coil. The prediction shows that Alpha helix at point 188 had confident score of 48.98% while 3_{10}helix, Pi helix, beta bridge, Bend region, Ambiguous states and others had confidence score of 0.00% (no prediction). The extend strand at point 60 had confident score of 15.62% while beta turn at point 20 had confident score of 5.21%. Random coil at point116 had confident score of 30.21%. In a related study, Abrusán and Marsh (2016) stated that the inclusion of predicted secondary structure changes shows significant utility for improving upon state-of-the-art pathogenicity predictions. With respect to the functional association analysis using SOPMA, the results obtained indicate that substitutions may alter cell cycle controls by disrupting genetic interactions involving Ovalbumin.

Table 2: Secondary structure prediction using SOPMA

Variants	Secondary Structure									
	Alpha helix	3_{10}helix	Pi helix	Beta bridge	Extend strand	Beta turn	Bend region	Random coil	Ambiguous states	Other states
Native	188(48.98)	0(0.00)	0(0.00)	0(0.00)	60(15.62)	20(5.21)	0(0.00)	116(30.21)	0(0.00)	0(0.00)
E151F	174(45.43)	0(0.00)	0(0.00)	0(0.00)	57(14.88)	20(5.22)	0(0.00)	0(0.00)	0(0.00)	0(0.00)
L233P	188(47.00)	0(0.00)	0(0.00)	0(0.00)	57(14.88)	19(4.96)	0(0.00)	127(33.16)	0(0.00)	0(0.00)
S241R	175(45.69)	0(0.00)	0(0.00)	0(0.00)	56(14.62)	23(6.01)	0(0.00)	129(33.68)	0(0.00)	0(0.00)
Q255K	178(46.48)	0(0.00)	0(0.00)	0(0.00)	59(15.40)	21(5.48)	0(0.00)	125(32.64)	0(0.00)	0(0.00)
K264E	176(45.95)	0(0.00)	0(0.00)	0(0.00)	60(15.67)	21(5.48)	0(0.00)	126(32.90)	0(0.00)	0(0.00)
L265I	182(47.52)	0(0.00)	0(0.00)	0(0.00)	56(14.62)	17(4.44)	0(0.00)	128(33.42)	0(0.00)	0(0.00)
E267V	177(46/21)	0(0.00)	0(0.00)	0(0.00)	60(15.67)	18(4.70)	0(0.00)	128(33.42)	0(0.00)	0(0.00)
S272Q	177(46.21)	0(0.00)	0(0.00)	0(0.00)	57(14.88)	20(5.22)	0(0.00)	129(33.68)	0(0.00)	0(0.00)
V279M	182(47.52)	0(0.00)	0(0.00)	0(0.00)	57(14.88)	18(4.70)	0(0.00)	126(32.90)	0(0.00)	0(0.00)
L283D	183(47.78)	0(0.00)	0(0.00)	0(0.00)	57(14.88)	17(4.44)	0(0.00)	126(32.90)	0(0.00)	0(0.00)
E289H	175(45.69)	0(0.00)	0(0.00)	0(0.00)	60(15.67)	20(5.22)	0(0.00)	128(33.42)	0(0.00)	0(0.00)
T304M	186(48.56)	0(0.00)	0(0.00)	0(0.00)	58(15.14)	16(4.18)	0(0.00)	123(32.11)	0(0.00)	0(0.00)
D305S	176(45.95)	0(0.00)	0(0.00)	0(0.00)	61(15.93)	26(6.79)	0(0.00)	120(31.33)	0(0.00)	0(0.00)
S308R					56(14.62)	22(5.74)	0(0.00)	125(32.64)	0(0.00)	0(0.00)
A333S	178(46.48)	0(0.00)	0(0.00)	0(0.00)	61(15.93)	23(6.01)	0(0.00)	121(31.59)	0(0.00)	0(0.00)
E355S	179(46.74)	0(0.00)	0(0.00)	0(0.00)	58(15.14)	22(5.74)	0(0.00)	124(32.38)	0(0.00)	0(0.00)
H368Y	180(47.00)	0(0.00)	0(0.00)	0(0.00)						
V381Y	176(45.95)	0(0.00)	0(0.00)	0(0.00)	65(16.97)	19(4.96)	0(0.00)	123(32.11)	0(0.00)	0(0.00)
Cmutant	178(46.35)	0(0.00)	0(0.00)	0(0.00)	63(16.41)	20(5.21)	0(0.00)	123(32.03)	0(0.00)	0(0.00)

CONCLUSION

It can be concluded from the study that the protein obtained have highly negative charges with increased solubility due to electrostatic repulsion and enhanced binding affinity for positive charged surface and involvement in protein–protein interactions. These changes affect the physical and chemical properties of the ovalbumin protein of quail as well as the protein-protein interaction.

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