



Myoglobin Modeling to Study Species-Specific Differences in the Distance Between Heme Iron and Proximal and Distal Histidines

S. Mazunder¹, M. Denzer^{2*}, S. Suman³, S. Mohanty¹, G. Mafi², D. VanOverbeke², and R. Ramanathan²

¹Chemistry, Oklahoma State University, Stillwater, OK, USA

²Animal & Food Sciences, Oklahoma State University, Stillwater, OK, USA

³Animal & Food Sciences, University of Kentucky, Lexington, KY, USA

*Corresponding author. Email: mdenzer@ostateemail.okstate.edu (M. Denzer)

Keywords: histidine, meat color, myoglobin
Meat and Muscle Biology 3(2):157

Objectives

Species-specific differences in amino acid sequence influence myoglobin redox properties. Previous studies reported that the number and location of histidine residues can influence myoglobin redox stability. However, limited knowledge is currently available on the species-specific differences in the distances between the proximal (His 93) and distal (His 64) histidines and the heme iron in myoglobin. The objective of the current research was to utilize homology-based modeling to determine the distances between the proximal and distal histidines and the heme iron in the myoglobins from beef, pork, goat, bison, sheep, water-buffalo, venison, and emu.

Materials and Methods

The homology-based modeling was conducted using the Iterative Threading Assembly Refinement server (I-TASSER), which identifies the homologous structure models of myoglobins (beef, pork, goat, bison, sheep, water-buffalo, venison, and emu) from Protein Data Bank (PDB) using an algorithm named Local Meta-Threading-Server. The secondary structure of the target protein was predicted based on sequence information from the Protein Secondary Structure PREDiction algorithm. The lowest free energy conformations of the proteins were determined by SPICKER (a clustering ap-

proach to identify near-native protein folds). Refinement of the low free energy conformations were done by using Fragment Guided Molecular Dynamics simulations and ModRefiner. Prediction of the ligand-binding site of the target proteins were made by COACH algorithm. The distances between histidines (His 64 and His 93) and the iron in the heme group in the predicted structure of eight different species were determined using PyMOL, a computer software used for molecular visualization.

Results

The homology-based modeling has shown that despite having 80% sequence similarity and conserved histidine residues (His 64 and His 93), the distance between the distal histidine (His 64) and heme iron varied between 4.3–5.5 Angstrom. Pork myoglobin has the shortest distance, and beef myoglobin has the longest distance. The distance between the proximal histidine (His 93) to the heme varied between 1.9 to 3 Angstrom; sheep myoglobin had the shortest and bison had the longest.

Conclusion

The results suggest that in addition to the inherent differences in muscle biochemistry, variations in myoglobin structure also contributes to species-specific differences in meat color.