A Structural and Functional Bioinformatics Study of QTY-designed Retinylidene Proteins

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10 ABSTRACT

This is the abstract!

Keywords: Keyword1; Keyword2; Keyword3

INTRODUCTION

- 12 Intro
- * Families of opsins vertebrate vs. bacterial
- * General features of vertebrate opsin; structure and function
- * Activation mechanism of rhodopsin
- * Expression, function of each opsin
- * General features of bacterial opsin; structure, function, applications
- * Why solubilize
- * History of solubilizing studies of rhodopsin and bacteriorhodopsin
- * Intro to AlphaFold
- * Existing QTY studies
- * Intro to GROMACS
- * Existing rhodopsin bioinformatics studies

RESULTS AND DISCUSSION

25 Results

28

- * discuss the QTY code
- * describe and explain Table1
 - * describe and explain Fig1
- * describe and explain Fig2 ; I need more discussion here
- * describe and explain Fig3
- * discuss AlphaFold3 predictions
- * describe, explain, discuss MD results (Fig3 and Fig4) ; I need more discussion here
- * future scopes and potential applications
- * conclusion

METHODS

36 Methods

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- * protein sequences UniProt
- * AlphaFold3 server
 - * superimposition (PDB, AlphaFold, PyMOL)
- * Structure visualization (PyMOL, ChimeraX)
- * MD simulation (GROMACS, etc.; detailed params; analysis techniques)

42 SUPPLEMENTARY MATERIAL

Can be found at...

DATA AVAILABILITY STATEMENT

45 Can be found at...

46 AUTHOR CONTRIBUTIONS

- 47 A.O., A.T. and A.F. conceived the presented idea; A.O. wrote the main manuscript; All authors have read and agreed to
- the published version of the manuscript.

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54 COMPETING INTERESTS

55 The authors declare no conflict of interest.

56 ETHICS STATEMENT

No ethics issues...

58 REFERENCES