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

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ABSTRACT

This is the abstract!

Keywords: Keyword1; Keyword2; Keyword3

INTRODUCTION

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

Results

* 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

Methods

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

SUPPLEMENTARY MATERIAL

Can be found at...

DATA AVAILABILITY STATEMENT

Can be found at...

AUTHOR CONTRIBUTIONS

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.

COMPETING INTERESTS

The authors declare no conflict of interest.

ETHICS STATEMENT

No ethics issues...

REFERENCES