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.

FINANCIAL SUPPORT

This work was supported ...

ACKNOWLEDGMENTS

Thank...

COMPETING INTERESTS

The authors declare no conflict of interest.

ETHICS STATEMENT

No ethics issues...

REFERENCES

Table 1. TWO

Name	RMSD (Å)	pI	Mw (kDa)	TM variation (%)	Overall variation (%)
OPSG		8.90	40.58		
OPSG QTY	0.468	8.82	40.85	41.86	19.78
OPSR		8.89	40.57		
OPSR QTY	0.611	8.83	40.76	40.12	18.96
OPSB		8.75	38.72		
OPSB QTY	0.486	8.66	39.30	46.51	23.19
OPSD		6.20	38.89		
OPSD QTY	0.559	6.20	39.29	46.58	21.55
OPN3		9.29	44.87		
OPN3 QTY	0.454	9.18	45.47	49.12	20.90
OPN4		9.35	52.64		
OPN4 QTY	0.307	9.19	53.08	50.34	15.48
OPN5		9.11	39.73		
OPN5 QTY	0.555	9.02	40.04	45.58	18.93
RGR		8.34	31.87		
RGR QTY	0.537	8.29	32.39	42.86	21.65
OPSX		8.77	37.42		
OPSX QTY	0.548	8.72	37.46	40.96	20.18
BACR		4.75	26.92		
BACR QTY	0.448	4.75	27.40	46.67	25.30
BACH		5.34	26.96		
BACH QTY	0.296	5.34	27.50	44.19	30.04