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

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ABSTRACT

Abstract of paper – leave until everything is written.

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
* Existing QTY studies
* Intro to AlphaFold
* 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

The supplementary material can be found at...

DATA AVAILABILITY STATEMENT

The data for ... can be found at...

AUTHOR CONTRIBUTIONS

Detailed author contributions

FINANCIAL SUPPORT

No funding was received for this project.

ACKNOWLEDGMENTS

Thanks to ... for ...

COMPETING INTERESTS

The authors declare no conflict of interest.

ETHICS STATEMENT

There are no ethics issues related to the research in this paper. No animal or human data...

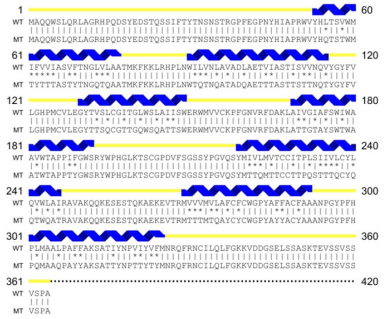
REFERENCES

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
ChR2	—	6.13	34.90	—	—
ChR2^{QTY}	0.235	6.13	35.30	35.53	22.22

Table 1. Protein characteristics

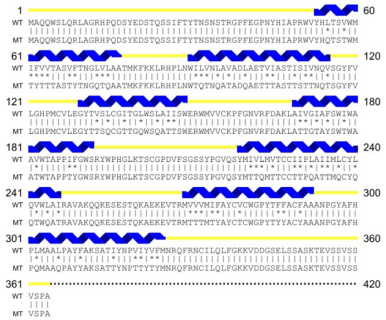
a) OPSG

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPSG	8.90	40.58	—	—
OPSG^{QTY}	8.82	40.85	41.86	19.78



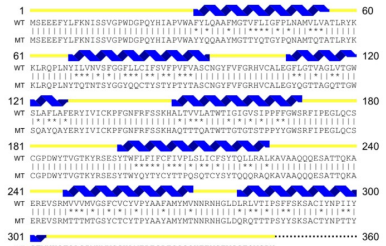
b) OPSR

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPSR	8.89	40.57	—	—
OPSR^{QTY}	8.83	40.76	40.12	18.96



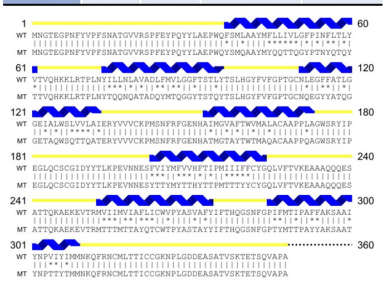
c) OPSB

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPSB	8.75	38.72	—	—
OPSB^{QTY}	8.66	39.30	46.51	23.19



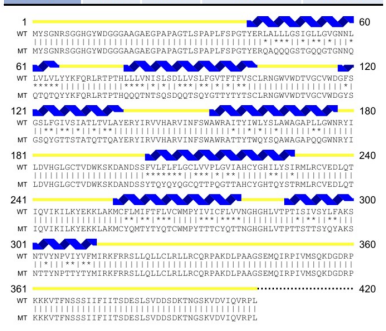
d) OPSD

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPSD	6.20	38.89	—	—
OPSD^{QTY}	6.20	39.29	46.58	21.55



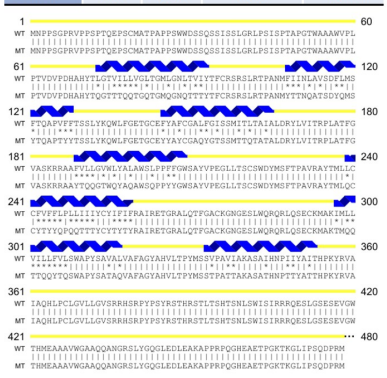
e) OPN3

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPN3	9.29	44.87	—	—
OPN3^{QTY}	9.18	45.47	49.12	20.90



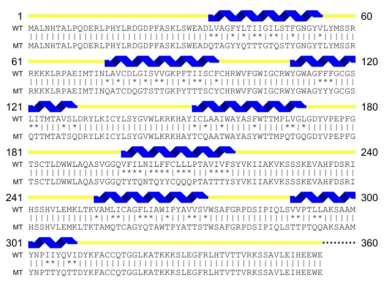
f) OPN4

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPN4	9.35	52.64	—	—
OPN4^{QTY}	9.19	53.08	50.34	15.48



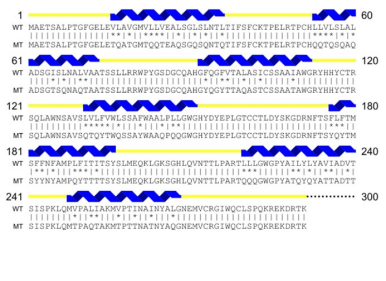
g) OPN5

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPN5	9.11	39.73	—	—
OPN5^{QTY}	9.02	40.04	45.58	18.93



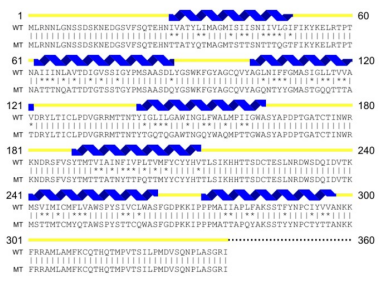
h) RGR

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
RGR	8.34	31.87	—	—
RGR^{QTY}	8.29	32.39	42.86	21.65



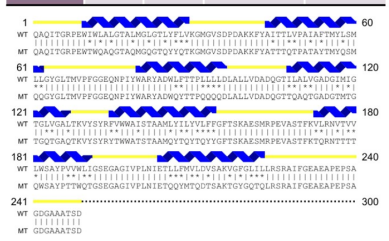
i) OPSX

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
OPSX	8.77	37.42	—	—
OPSX^{QTY}	8.72	37.46	40.96	20.18



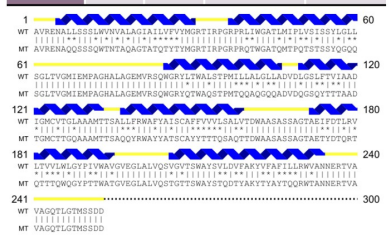
j) BACR

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
BACR	4.75	26.92	—	—
BACR^{QTY}	4.75	27.40	46.67	25.30



k) BACH

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
BACH	5.34	26.96	—	—
BACH^{QTY}	5.34	27.50	44.19	30.04



l) ChR2

Name	pI	MW (kDa)	Variation rate (TM, %)	Variation rate (%)
ChR2	6.13	34.90	—	—
ChR2^{QTY}	6.13	35.30	35.53	22.22

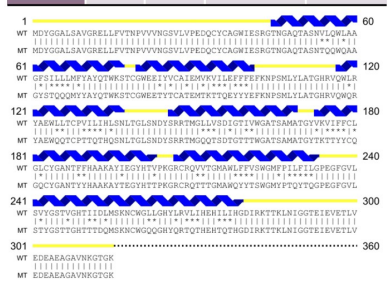


Figure 1. Protein sequence alignments

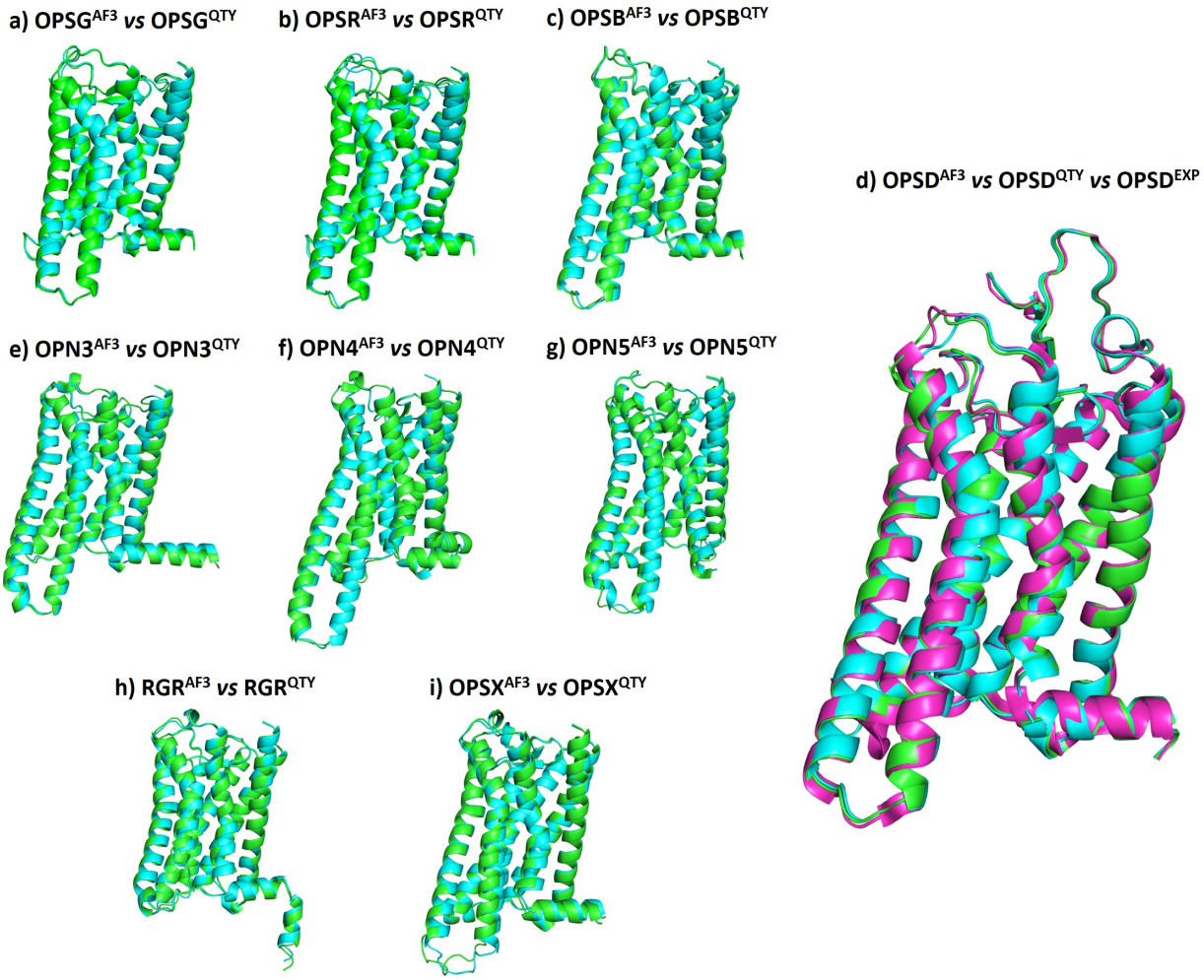


Figure 2. Superimposition of human retinylidene proteins