

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

Siqi Pan<sup>1</sup> and Shuguang Zhang<sup>2</sup>

<sup>1</sup>Shanghai World Foreign Language Academy, No. 400, Baihua Road, Shanghai 200233, China

<sup>2</sup>Lab of Molecular Architecture, Media Lab, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

Corresponding author:

Shuguang Zhang<sup>2</sup>

Email address: Shuguang@MIT.EDU

## 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)

42 **SUPPLEMENTARY MATERIAL**

43 Can be found at...

44 **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  
48 the published version of the manuscript.

49 **FINANCIAL SUPPORT**

50 This work was supported ... For the purpose of open access, the author has applied a CC BY public copyright licence to  
51 any Author Accepted Manuscript version arising from this submission.

52 **ACKNOWLEDGMENTS**

53 Thank...

54 **COMPETING INTERESTS**

55 The authors declare no conflict of interest.

56 **ETHICS STATEMENT**

57 No ethics issues...

58 **REFERENCES**