Identification and characterization of Nematode chemosensory GPCRs (*NemChRs*) in *Heterorhabditis bacteriophora*

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Introduction

- *H. bacteriophora* IJs locate insects by sensing universal host cue (CO_2) or insect/plant-derived odorants, which bind to various sensory receptors, including G-protein-coupled receptors (GPCRs)
- GPCRs: Largest family and most diverse group of membrane receptors in eukaryotes, including EPNs
- *NemChRs* bind to a diverse set of ligands, including odor molecules

Methods

H. bacteriophora proteome

↓ Length based filter

Sequences with >200 amino acid residues

↓ Check for 7-TM based on various algorithms

Consensus sequences with heptathetical transmembrane

↓ Search for GPCR domain using different tools

Final sequences predicted as GPCRs

↓ Pfam search

Chemosensory GPCRs

↓ AlphaFold, Galaxy Refine2 server and structural analysis with SAVES

Refined and validated 3-D models

↓ Molecular dynamics simulation @100ns in GROMACS in hydrated POPC bilayer

Stabilized models of *NemChRs*

- Pipeline validated by reciprocal BLAST, Interproscan, GPCR-CA, NCBI CDD search etc.
- Family-wide classification of GPCRs through reciprocal BLAST
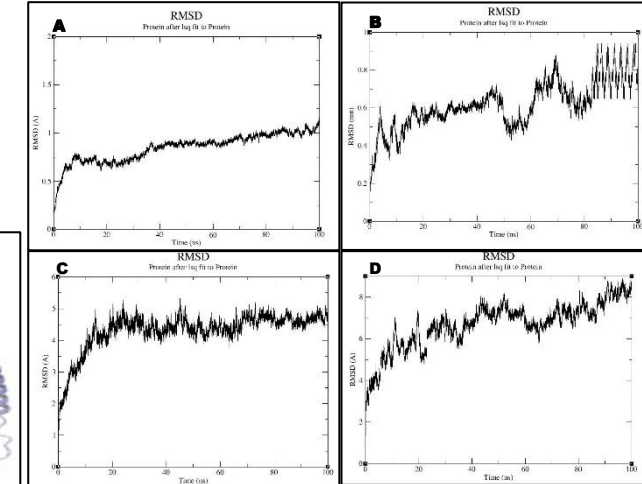
Results

- Fetched 21 GPCRs out of total 21,699 predicted proteins. Four are chemosensory out of those. a frizzled type, a secretin type and 19 rhodopsin types GPCRs.
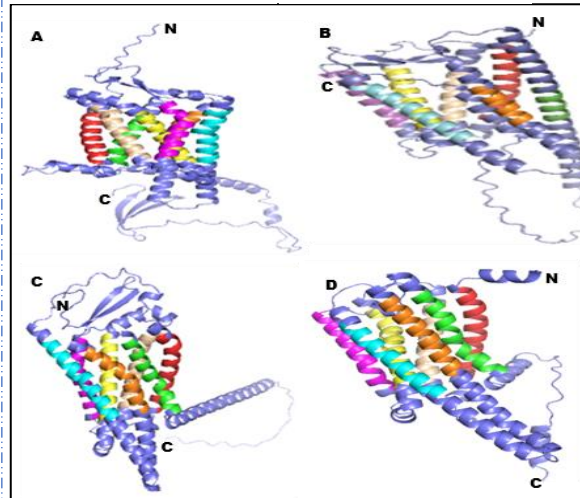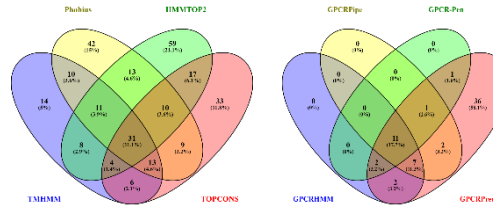
A. Hba_07805 B. Hba_17528 C. Hba_18427 D. Hba_18743

🟥 TM1 🟥 TM2 🟨 TM3 🟪 TM4 🟦 TM5 🟩 TM6 🟩 TM7

Predicted Local Distance Difference Test (plDDT) scores for all the models are >90

Root mean square deviation (RMSD) from crude models

- Ramachandran Plot showing >99% residues in highly preferred zone

Overall quality factor by SAVES

Hba_07805= 96.985, Hba_17528= 96.216

Hba_18427=92.879, Hba_18743= 98.792

Future Plan

- Molecular docking of these GPCRs with selected attractant and repellent molecules
- Expression analysis of *NemChRs* in response to these compounds