

2026-27 HIVE Summer Internship Project

Seeing the Pink Shift: Immersive Visualisation of AstaP-pink1

Primary Academic Supervisor

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Project Background

Carotenoids such as astaxanthin (AXT) are deep-red, powerful antioxidants widely used in aquaculture, nutraceuticals and cosmetics, but they are lipophilic and essentially insoluble in water. A small number of organisms produce water-soluble carotenoid-binding proteins that solubilise these pigments and, in some cases, shift their colour. AstaPs are a family of such proteins found only in Scenedesmaceae microalgae, where they protect the cells from photooxidative stress. Mitsui et al. (2026) focused on AstaP-pink1, a remarkable member of this family that converts orange AXT into a pink-coloured, UVA-absorbing complex, upon binding. This red shift is the same phenomenon that turns a raw, blue lobster bright red upon cooking (Cianci et al., 2002).

Mitsui et al. produced recombinant AstaP-pink1 in engineered *E. coli* and solved its X-ray crystal structure (PDB 9WM8) bound to AXT. The structure shows a FAS1-domain β -sandwich fold that clamps the pigment so one of its terminal rings is forced into an unusual 6-s-trans conformation, rather than the 6-s-cis/6'-s-cis form in the related protein AstaP-orange1. DFT calculations show this forced conformation, together with contacts from Gln46, Trp67 and Arg165, produces the larger red shift and distinctive UVA absorption that give AstaP-pink1 its colour.

This structure-function theory is arguably difficult to convey through static crystallography figures, yet it thrives in an immersive 3D environment. A handful of specific atomic contacts contort the ligand into a specific conformation, driving a directly visible optical change, analogous to the red shifts previously reported. We are seeking a HIVE intern to transform this molecular story into an interactive 3D visualization. This asset will serve dual purpose: a) enhancing high-impact research dissemination (graphical abstract, conference presentations, supplementary video) and b) driving

public engagement around structural biology and high-value pigment biotechnology.

Project Description, Expected Outputs, Possible Stretch Goals

Aim:

Build an interactive, structurally accurate visualisation of AXT-bound AstaP-pink1 (PDB 9WM8) that lets a viewer see, and physically explore, why binding to this protein turns astaxanthin from orange to pink.

Expected outputs:

- A high-fidelity 3D molecular model imported from PDB 9WM8 (and the related AstaP-orange1 structure), optimised and rendered for HIVE large-format displays (Dome/Wedge) and for VR headsets.
- An interactive VR experience enabling users to step inside the binding pocket, manipulate and rotate the astaxanthin chromophore, and toggle key interacting residues (Gln46, Trp67, Arg165) to inspect local steric and electrostatic contacts.
- A narrated explainer animation showing the ligand's conformational change (6/6'-s-cis to 6-s-trans/6'-s-cis) morphing in real time, synchronised with the measured UV-Vis spectrum, to visually connect the molecular shape to the orange-to-pink transition.
- A side-by-side comparison view of AstaP-pink1 and AstaP-orange1 binding pockets highlighting the structural differences (loop deletion, Tyr/Phe substitution) responsible for the difference in colour.

Possible stretch goals:

- Overlay of the DFT-calculated molecular orbitals (HOMO/LUMO) involved in the electronic transitions.
- An interactive comparison across all four known AstaP homologues (orange1, orange2, pink1, pink2).
- A lightweight web/mobile AR version for public outreach on astaxanthin's role in aquaculture and human health.
- Applying what we learned to PDB 1GKA, looking at the blue crustacyanin of lobster turning red upon cooking (Cianci paper). The two main structural features: 1) enforced planarity of the b-ionone rings with the polyene chain, and 2) the hydrogen bonding pattern around the end-ring keto-oxygens will be examined.

The outputs are intended to become supplementary/graphical-abstract material for a follow-up publication, a reusable outreach asset, and a template pipeline we can reapply to future protein structures from the lab.

Links to background reading and any relevant recent work in the field

- Mitsui et al. 2026, J. Structural Biology 218:108288 - <https://doi.org/10.1016/j.jsb.2026.108288>
- PDB entry 9WM8 (AXT-bound AstaP-pink1 crystal structure) - <https://www.rcsb.org/structure/9WM8>
- M. Cianci, P.J. Rizkallah, A. Olczak, J. Raftery, N.E. Chayen, P.F. Zagalsky, & J.R. Helliwell, The molecular basis of the coloration mechanism in lobster shell: β -Crustacyanin at 3.2-Å resolution, Proc. Natl. Acad. Sci. U.S.A. 99 (15) 9795-9800, <https://doi.org/10.1073/pnas.152088999> (2002).
- Gamiz-Hernandez, A.P., Angelova, I.N., Send, R., Sundholm, D. and Kaila, V.R.I. (2015), Protein-Induced Color Shift of Carotenoids in β -Crustacyanin†. Angew. Chem. Int. Ed., 54: 11564-11566. <https://doi.org/10.1002/anie.201501609>
- Kawasaki et al. 2020, Commun. Biol. 3:490 (discovery of AstaP-pink1/pink2) - <https://doi.org/10.1038/s42003-020-01206-7>
- Kawasaki et al. 2023, Algal Research 70:102982 (AstaP as a broad carotenoid solubiliser) - <https://doi.org/10.1016/j.algal.2023.102982>

What type of visualisation will the student develop or produce?

- An interactive VR molecular experience (Quest 3) built from PDB entry 9WM8, letting users explore the AstaP-pink1 fold and manipulate the bound astaxanthin ligand;
- A narrated 3D explainer animation of the ligand's conformational change and the resulting colour shift; and
- A large-format HIVE Dome/Wedge render for talks, demos and Showcase Day.

How will the visualisation contribute to your research outcomes?

It lets us test structural hypotheses that are hard to grasp from static figures - the double ligand occupancy, the forced ring conformation, the electrostatic/pi-stacking network - and turn them into a clear visual story. This supports a follow-up publication's graphical abstract, strengthens conference and grant communication of the red-shift mechanism, and gives the lab a reusable public-engagement asset linking structural biology to astaxanthin's real-world biotechnology applications.

If the project is successful, where would you consider publishing the results?

We would aim to feature the visualisation as a graphical abstract or supplementary video for a follow-up article in Journal of Structural Biology, Communications Biology or Algal Research (our usual outlets for this work), and present it at structural biology and phycology conferences (e.g. the Asia-Pacific Phycological Forum, ACA/IUCr meetings).

Draft Project Timeline:

Week 1

Nov 16 - Full day HIVE induction

Nov 17 - Area and Project Induction with Primary supervisor

Develop project plan with HIVE and academic team

Literature and relevant project review

Project Familiarisation

Week 2

Deep dive into the structural biology background; download and process PDB 9WM8 (AXT-bound AstaP-pink1) and the related AstaP-orange1 model; learn PyMOL/ChimeraX for structural analysis; identify the key structural features (FAS1 fold, AXT-binding pocket, key residues) to visualise.

Week 3

Produce first high-quality static 3D renders of AXT-bound AstaP-pink1 (overall fold, binding pocket, key residues) in ChimeraX/Blender; set up the Blender (Molecular Nodes) or Unity pipeline for importing PDB coordinates; storyboard the VR experience and the explainer animation

Week 4

Build the first interactive VR prototype (Unity/Unreal or Blender VR) allowing free exploration of the protein structure; test on the Quest 3 headset in the HIVE Dome/Wedge; review with academic and HIVE supervisors and refine based on feedback.

Week 5

Build the side-by-side comparison of AstaP-pink1 and AstaP-orange1 binding sites, highlighting the structural determinants of the colour difference; refine VR interactions (grab/rotate the ligand, toggle residues and surfaces on/off).

Week 6

Animate the ligand's conformational change (6/6'-s-cis to 6-s-trans/6'-s-cis) and link it to the measured UV-Vis spectrum; integrate a dynamic orange-to-pink colour transition into the explainer animation.

Week 7

Polish visuals (lighting, materials, colour-accurate carotenoid rendering), add narration/captions to the explainer animation, and optimise the VR

build for smooth performance on HIVE hardware; run informal usability testing with lab members.

Week 8

Finalise all deliverables (VR build, explainer animation, HIVE Cylinder/Dome/Wedge render); prepare figures/video suitable for a journal graphical abstract; begin drafting the Showcase Day presentation and final report

Week 9

Focus on report writing and presentation (including demo) preparation

Week 10

*Focus on report writing and presentation (including demo) preparation
5th Feb Final Showcase Day and final report due*

Student Experience and Supervision:

How often will you meet with the student over the 10-week period?

At least once per week for a formal progress check-in, with ad-hoc support available by email throughout the project.

Your work desk location and the location of student desk

305.009 – there is a spare desk inside my office

Student Attributes:**Please indicate any preference for student's academic discipline or field of study**

Preference for Bioinformatics, Molecular Biosciences or a related life-science discipline, ideally with some exposure to structural biology or molecular visualisation tools (e.g. PyMOL, ChimeraX) or basic programming (Python). Students from Computer Science or Design with a strong interest in scientific visualisation will also be considered.

What competencies are required to start this project

Beginner - 2D art/editing

Beginner - Virtual Reality Development (rendering pipelines, scene content design, interaction)

Beginner - Data structures, analytics, statistical modelling

Beginner - PyMOL, ChimeraX

Intermediate - Video production/editing

Intermediate - 3D modelling software (Blender, 3ds Max)

Intermediate - Game engine development (Unity, Unreal. Godot, etc.)

Do you have any other student attributes you think are important to the project?

Enthusiasm for science communication and structural biology; comfortable working independently after initial guidance; a good eye for visual clarity and aesthetics; willingness to learn new 3D/VR software quickly in a research setting.