Unravelling the Mechanism of the Bathochromic Shift in the Lobster Carapace

Madeleine Helliwell[a], Giuditta Bartalucci[a], Jennifer Coppin[a], Gillian Hall[a], John R. Helliwell[a,b], Synnove Liaaen Jensen[c], *[a]Department of Chemistry, University of Manchester, UK. [b]CCLRC Daresbury Laboratory, Warrington WA4 4AD, UK. [c]Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway.* E-mail: Madeleine.Helliwell@manchester.ac.uk

The colouration mechanism in the lobster carapace was revealed at 3.2Å resolution by a protein crystal structure of β-crustacyanin [1]. The crystals are a vivid blue colour and this colour is provided by two bound molecules of the carotenoid astaxanthin. There are three candidate molecular parameters responsible for the bathochromic shift of astaxanthin, which is famously demonstrated via the colour change of lobsters on cooking, turning from blue/black to orange/red: 1. the coplanarisation of the end rings with the polyene chain, increasing the degree of conjugation; 2. an electronic polarisation effect stemming from H bonding of the keto oxygen atoms of the bound astaxanthins, to histidine and water molecules; 3. an exciton interaction due to the close proximity of the two bound astaxanthins.

In order to investigate these colour tuning parameters further, we have determined four new crystal structures of the carotenoids astaxanthin and canthaxanthin all of which are red. These have allowed us to investigate the atomic environment of the end rings and the crystal packing arrangements of the polyene chains. Further experiments are in progress and will also be reported.

[1] Cianci M., Rizkallah P.J., Olczak A., Raftery J., Chayen N.E., Zagalsky P.F., Helliwell J.R., *PNAS USA*, 2002, **99**, 9795-9800.

Keywords: lobster, colour, carotenoids