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| | **Experiment title:**<br>Quaternary Structure of the Hexadecameric Carotenoprotein, α-crustacyanin | **Experiment number**:<br>SC873 |
| **Beamline**:<br>ID02 | **Date of experiment**:<br>from: 01/09/2001 to: 03/09/2001 | **Date of report**:<br>12/07/2002 |
| **Shifts:**<br>6 | **Local contact(s)**:<br>Stéphanie Finet | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

Véronique RECEVEUR*

Cosma DELLISANTI*

Silvia SPINELLI*

Christian CAMBILLAU

AFMB-CNRS - 31, chemin Joseph Aiguier – 13402 Marseille cedex 20

## Report:

Alpha-crustacyanin, the carotenoprotein responsible of the blue coloration of lobsters carapace, is a complex of 16 subunits assembled as an octamer made of heterodimers called beta-crustacyanins. Five different subunits have been identified and grouped into two different types. Subunits have an average mass of about 20kDa each and belong to the lipocalin family. In the hexadecameric native form each subunit binds a molecule of the chromophore astaxanthin. The way subunits bind the carotenoid is still partly unknown and it is of major interest because of the very typical bathochromic shift (150nm ca.) responsible of the blue coloration of the protein. The presence of the ligand is also essential for dimerisation and further octamerisation of dimers to occur. Some hypotheses were developed on the basis of cross-linking studies and preliminary electron microscopy investigations but never gave rise to any reliable model.

Therefore it has been so far virtually impossible to determine the quaternary structure of alpha-crustacyanin. Small angle X-ray scattering experiments have been performed on ID2 beamline to

determine the structural organisation of this protein. Data have been recorded at two camera length (3m and 1m) and this has enabled to reach a resolution of 10 angstrom with a very good statistics even at this resolution. The concentration dependence of the radius of gyration was determined and the measurement of I(0) showed that the protein was indeed hexadecameric in solution. The quality of the data enabled to calculate a beautiful distance distribution function P(r) (fig.1.). The shape of the protein has been calculated *ab initio* using the program GASBOR and has revealed an helicoidal structure (fig. 2.). We are now working on this strange new enveloppe of a protien and are trying to position the individual subunits of beta-crustacyanin within the envelope using their atomic coordinates. We hope then to propose a model of the hexadecameric assembly.

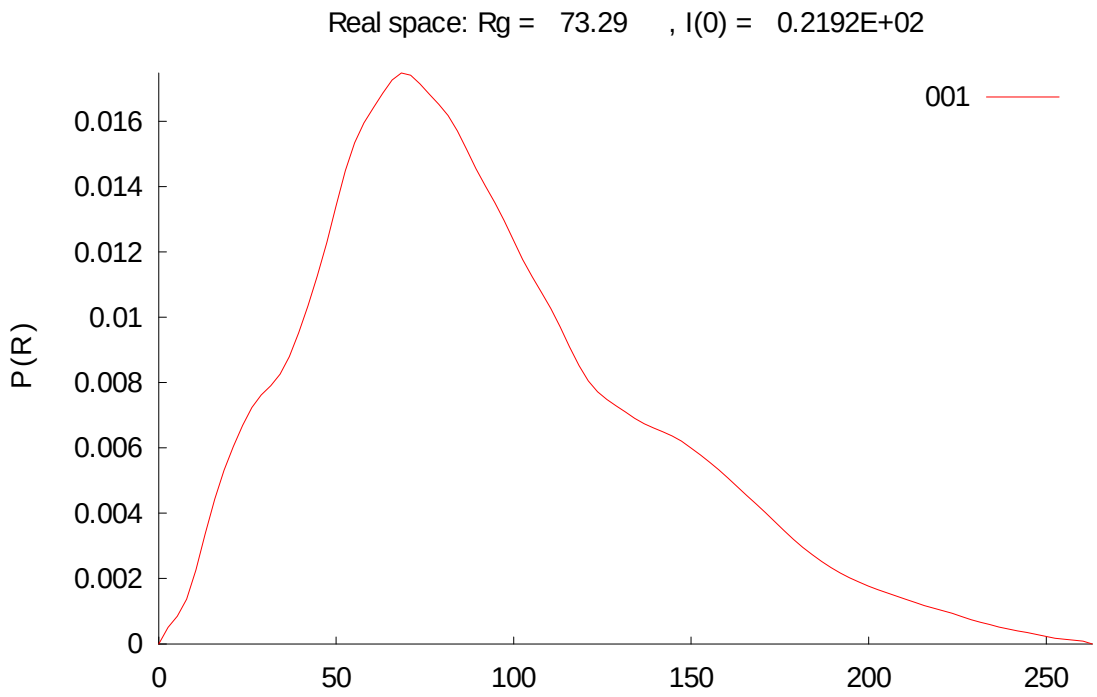


**Fig. 1. Distance distribution fuction of α-crustacyanin inferred from its scattering curve measured on ID2- beamline.**

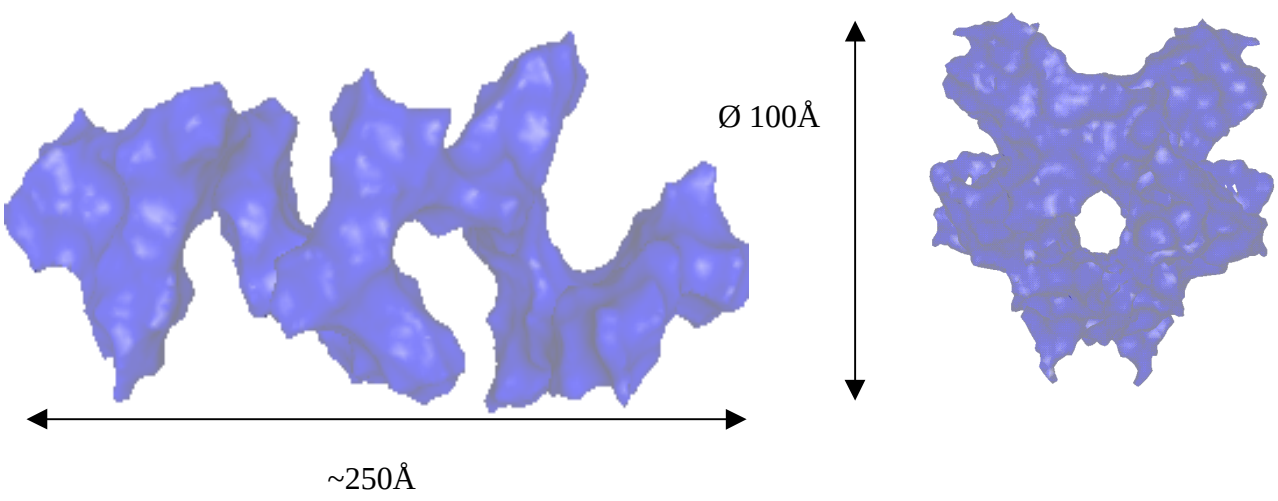

**Fig. 2. Envelope of α-crustacyanin calculated by GASBOR from its distance distribution function.**