



BAG Beam time Progress Report

LSJ508

This represents a summary of the BAG progress in the reporting period, and is in addition to the standard ESRF report sheet for each project which will be used for the Review of the BAG.

BAG Title PROTEIN CRYSTALLOGRAPHY AT AFMB-CNRS, MARSEILLE

Allocation Period 01.02.99 – 31.07.99

List of publications resulting from ESRF beam time

- Florence VINCENT, Silvia SPINELLI, Roberto RAMONI, Stefano GROLLI, Paolo PELOSI, Christian CABBILLAU and Mariella TEGONI. Complexes of Porcine Odorant Binding Protein with Odorant Molecules Belonging to Different Chemical Classes., *J.Mol.Biol.*, submitted
- Silvia Spinelli, G.J. Leon Frenken, Pim Hermans, Theo Verrips, Kieron Brown, Mariella Tegoni and Christian Cambillau: Camelids heavy chain variable domains provide efficient combining sites to haptens, *Biochemistry*. **39**, 1217-1222 (2000).
- Valérie Campanacci, Sonia Longhi, Patricia Nagnan-Le Meillour, Christian Cambillau & Mariella Tegoni. Recombinant Pheromone Binding Protein 1 from *Mamestra brassicae* (Mbra1): functional and structural characterisation. *Eur. J. Bioch.* **264**,707-716 (1999).
- Kieron Brown, Jose J. Moura, Isabel Moura, Mariella Tegoni, Christian Cambillau, A new type of copper cluster at the active site of Nitrous oxide reductase *Nature Structural Biology*, **7**,191-195 (2000).
- Bourne, Y., Taylor, P. & Marchot, P. Mouse acetylcholinesterase part I, in preparation.
- Bourne, Y., Taylor, P. & Marchot, P. Mouse acetylcholinesterase part II, in preparation.
- Brown, K., Cambillau, C. & Bourne, Y., The catalytic machinery of GImU, in preparation.
- Florence Vincent, Kieron Brown, Dietrich Loebel, Silvia Spinelli, Suzanne Dixon, Heinz Breer, Christian Cambillau and Mariella Tegoni, Crystal Structure of Hamster Aphrodisin, a Copulatory Behaviour Eliciting Pheromone, in preparation
- C. Peneff, D. Mengin-Lecreux, Y. Bourne, Crystal structure of *Saccharomyces cerevisiae* glucosamine-6-phosphate N-acetyltransferase 1: a new member of the Gcn5-related N-Acetyltransferase superfamily, in preparation
- Sulzenbacher, G., Gal, L. & Bourne, I., Crystal structure of full length GImU from *Streptococcus pneumoniae*. Evidence for acetyl-CoA binding, in preparation.
- Gastinel, L.N., et al. Crystal structure of the bovine α 1,3GalT catalytic domain, a galactosyltransferase related with ABO blood group transferases (2000) (manuscript in preparation).
- M. Czjzek, B. Henrissat, V. Zamboni, W. Burmeister and A. Esen Crystal structure of Monnocot (Maize) beta-glucosidase and the mechanism of its aglycone substrate specificity, in preparation

Global Summary

The Architecture et Fonction des Macromolécules Biologiques lab, in Marseille, comprises 45 people among which 19 are dealing directly with Protein Crystallography. The lab is structured in 4 teams, which are working in different areas.

- 6 MAD structures have been solved.
- ca 40 data set of complexes and variants collected.

Visits made to the ESRF

Date(s) of visits	Beamline	No. of Shifts	Short Summary of each Visit
1. 16.09 99	ID14-4	6	4 projects (3 proteins), all solved within 24 hours , + high resolution data sets
2. 30.09.99	ID14-2	3	5 projects, 14 datasets
3. 29.10.99	BM14	6	2 MAD projects, solved..
4. 16.11.99	ID14-2	3	10 projects, 16 data sets.
5. 5.02.00	ID14-2	3	4 projects, 9 datasets.

LS-1508
22/9/99 – 5/2/00

BM14

Shifts used/allocated

1/6	2/6	3/6	4/6	5/6	6/6
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Date	User	Project	Status	Remarks
29/10/99	Herman van Tilbeurgh Marie-Pierre Egloff Gerlind Sulzenbacher	MP GlmU Full-length	solved by MAD solved by MAD	3.2Å resolution

ID14-4

Shifts used/allocated

1/6	2/6	3/6	4/6	5/6	6/6
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Date	User	Project	Status	Remarks
16-18/9/99	Yves Bourne Caroline Peneff Louis Gastinel Kieron Brown	GNA1 α 1,3 Aphrodisin	solved by MAD solved by MAD solved by MAD	

ID14-2

Shifts used/allocated

1/9	2/9	3/9	4/9	5/9	6/9
7/9	8/9	9/9			

Date	User	Project	Status	Remarks
30/9/99	Mirjam Czjzek	R Glu E191D+dimboa R Glu E191D+dhurrin R Glu E191D mutant		2.1Å 2.0Å 2.2Å
	Virginie Nahoum	α -amylase		1.38Å complex
	Marie-Pierre Egloff	MP	processed	first data collection
	Herman van Tilbeurgh	LICT		tests, no data
	Natalie Declerck			

Shifts used/allocated

1/9	2/9	3/9	4/9	5/9	6/9
7/9	8/9	9/9			

Date	User	Project	Status	Remarks
16/11/99	Mariella Tegoni	H369A	processed/refined	3.1Å, c-heme domain disordered
	Kieron Brown	N2OR	processed/refined	2.65Å oxidised structure 2.9Å SCN- complex 2.9Å N3- complex
	Florence Vincent	Aphrodisin	processed/refined	1.6Å high resln. dataset
	Mirjam Czjzek	Rglu E191D +dimboa-glucoside CelE	processed/refined	2.5Å dataset 2.1Å dataset 1.9Å data. Mol. Rep. Failed. SeMet in prep.
	Louis Gastinel	α 1,3+soaking 2 complexes		
	Virginie Nahoum	α amylase+BH4		1.38Å dataset. Ref. in progress
	Caroline Peneff	GNA1	refinement in	1.9Å CoA+GINAcGP complex 1.7Å CoA complex 1.3Å high resln. AcCoA cmplx.

Shifts used/allocated

1/9	2/9	3/9	4/9	5/9	6/9
7/9	8/9	9/9			

Date	User	Project	Status	Remarks
5/2/00	Mariella Tegoni	H369A	processed/refined	c-heme not visible
	Kieron Brown	N2OR-ox	processed/refined	2.8Å oxidised structure
	Caroline Peneff	AGX1	processed	data for native and substrate Complexed enzyme SeMet in prep.