

	Experiment title: Structural studies on the respiratory membrane proteins	Experiment number: LS-1609
Beamline: ID14/EH2,4	Date of experiment: (not yet used) from: to:	Date of report: 2/28/00
Shifts: -----	Local contact(s): Wim Burmeister	<i>Received at ESRF:</i>

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Report:

Since we have not used the beam time, we summarize our current progress here.

(1) Cytochrome bc1 complex from bovine heart.

Following data were collected at ID14/EH4 using beam time for our BAG application (LS-1027).

	Resolution (Å)	Unique data	Comp. (%)	R-merge (%)	R-factor/R-free (%)
P65 form ("lnl" form)					
Native	2.5	204,063	91.1	12.6	29.5/32.2 (480 water and 5 lipid molecules)
MOA-stilbene complex	3.0	117,243	87.3	16.4	30.9/33.2
Myxothiazol complex	3.5	77,411	92.5	20.2	33.1/36.6
P6522 form ("c1" form)					
Native	3.0	79,396	88.9	7.0	28.5/32.5
Antimycine complex	3.3	55,170	79.0	10.5	32.5/35.5
Ascochlorin complex	3.0	57,246	61.8	7.9	32.0/36.0
I4122 form ("b" form)					
Native	3.0	59,804	83.4	15.9	32.6/36.6

1. Complete structure of the *bc1* complex has been revealed at 2.5 Å resolution.
2. Molecular mechanism of "Q-cycle" was proposed based on the Rieske FeS protein motion.
3. Quinone binding site structures have been revealed.
 - (a) Cause of a genetic disease, exercise intolerance, has been revealed.
 - (b) Development of new fungicides based on the structure.
4. The *bc1* complex is bifunctional; the core subunits are involved in protein transport to mitochondria.

(2) Cytochrome c oxidase from *Rhodobacter sphaeroides*.

Following data were collected at ID14/EH4 and EH3 using beam time for our BAG application (LS-1027).

	Resolution (Å)	Unique data	Comp. (%)	R-merge (%)	R-factor/R-free (%)
Wild type	2.3	119,310	70	8.0	24.8/29.7
Mutant E286Q	3.0	71,181	89.9	12.4	-----

Major results of this study

High Resolution Structure of cytochrome c oxidase *Rhodobacter sphaeroides*

- (a) Two proton pathways were confirmed. Water molecules in the pathway were assigned.
- (b) Oxygen channel was determined.
- (c) First evidence of Glu286 motion which could be the key of proton gating.

(3) Ubiquinol oxidase from *E. coli*.

Following data were collected at ID14/EH3 using beam time for our BAG application (LS-1027).

	Resolution (Å)	Unique data	Comp. (%)	R-merge (%)	R-factor/R-free (%)
Native	3.5	48,154	94.5	17.4	30.2/34.5

Major results of this study

First structure of Ubiquinol Oxidase

- (a) Subunits and most of the helices are assigned.
- (b) Quinone binding site was revealed.