	Experiment title:	Experiment number:
ESRF	Structural studies on the respiratory membrane proteins	LS-1609
Beamline: ID14/EH2,4	**Date of experiment:** 4-6 March (EH4), 4-6 May (EH2), 6-7 July, (EH4)	**Date of report:** 8/30/00
Shifts: 15 shifts	**Local contact(s):** Wim Burmeister, Vivian Stojanoff	*Received at ESRF:*

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Report:

The first beam time for this proposal was in March 2000 and we have not analyzed all the data yet. Here we summarize the data collection performed in March, May and July 2000.

Cytochrome bc_1 complex from bovine heart.
We have crystal structures from three different space groups of the bc_1 complex: $P6_522$ (a=b=212Å, c=342Å), $P6_5$ (a=b=130Å, c=720Å) and $I4_122$ (a=b=153 Å, c=599 Å). Native structures have been solved at 3.0Å for three crystal forms. We have collected data up to 2.5 Å from the $P6_5$ crystal form at ID14/EH4. The refinement of the structure is almost finished with R=24% and Rfree=26%. Ubiquinone binding sites structure of the bc_1 complex is very important for industry and medicine. We are studying the sites using specific inhibitors. Data from the crystals of 5 inhibitor complexes have been collected.

	Res (Å)	Unique data	Comp.	R-merge	R/FreeR
Native	2,5	204,063	0.911	0.126	0.24/0.26
NOA310018	3.0	120,855	0.902	0.114	
NOA283680	3.0	113,316	0.847	0.176	
NOA335326	3.0	118,153	0.876	0.121	
NOA362122	3.0	118,113	0.882	0.138	
NOA359689	3.0	118,023	0.882	0.155	

Succinate-ubiquinone oxidoreductase (SQR) from *Bacillus Subtilis*

We have recently obtained the crystals of *Bacillus subtilis* SQR. The crystals belong to the space group *R*32 with the cell dimensions of *a*=*b*=115 Å and *c*=667Å. The crystals diffract up to 3.5 Å.

	Res (Å)	Unique data	Comp.	R-merge
Native	3.7	13,358	0.713	0.111

Ubiquinol oxidase from *E.coli*

The crystal belongs to an orthorhombic space group $C222_1$ with the cell dimensions of *a*=92 Å, *b*=373 Å and *c*=233 Å. The structure has been solved at 3.5 Å and the paper has been accepted at Nature Structure Biology (Abramson, J. in press). We recently made fusion proteins of this complex with various soluble and membrane proteins and some of these fusion proteins were crystallizes. The data from these crystals have been collected. The resolution was not good enough but we could solved the structures by molecular replacement and show the crystal packing (Byrne, B, BBA in press). Further crystal improvement will be performed.

	Res (Å)	Total observation	Unique data	Comp.	R-merge
bo3+protein Z	6.0	25,814	15,317	0.776	0.047
bo3+Apo A-I	5.0	60,122	16,638	0.997	0,058

$F_{420}H_2$: NADP oxidoreductase from *Methanobacterium thermoautotrophicum*

This is a soluble enzyme, which catalyzes the reversible hydride transfer from $F_{420}H_2$, an analog of FMN, to $NADP^+$. We are studying the structure of the enzyme in relation to the catalytic reaction of the complex I of the oxygen respiratory chain. We performed the Se-Met MAD study at ID14/EH4. The data statistics are as follows.

	Res (Å)	Total observation	Unique data	Comp.	R-merge
Peak (0.9789)	2.5	48,187	12,878	0.921	0.044
Inflection (0.979)	2.5	48,178	12,882	0.922	0.047
Remote 1 (0.9395)	2,5	50,972	13,458	0.962	0.046
Remote 2 (0.9795)	2.0	67,135	27,244	0.973	0.051

The phases were calculated using the CCP4 program suit up to 3.0 Å. The initial overall figure of merit was 0.25. The problem of this low phasing power seems to be related a slight twining of the crystals. However, even in this map, we could recognize the clear solvent-protein boundary. After the density modification and phase extension (up to 2.0Å) using the program DM, the overall figure of merit has been improved to 0.78. It was very easy to trace the map and we have completed the model. The current R and R_{free} are 29 and 34%. Recently, we found another crystal form without twining. We are currently refining the structure using the data from this crystal form.