ESRF	**Experiment title:** Test on truncated hemoglobins complexed with heme ligands	**Experiment number:** **LS1803**
Beamline: ID14-1	**Date of experiment:** from 23-11-2000 to 25-11-2000	**Date of report:** 14-06-01
Shifts to BAG: 9	**Local contact(s):** Hassan BELRHALI	*Received at ESRF:*

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CD81 complexes

Tetraspanins are a new protein family, composed of about 200 proteins which are invariably associated to the cell membrane, through four helices. They display two extracellular domains (a small- and a large-extracellular domain), which are responsible for their biological activity (cell-to-cell recognition, activation, differentitation …). CD81 from human hepatocyte is the tetraspanin acting as heptitis C virus receptor, being the receptor protein for the HCV E2 envelope protein. In the previous BAG activity we solved the structure of CD81, proposing a specific protein region as the likely target for HCV E2 binding. A series of peptidomimetic compounds, expected to bind at such surface patch, have been synthetized and co-crystallized with CD81. As a result, a new crystal form for CD81 was isolated. Data for three different liganded complexes have been collected at ID14-EH1, and the structure solved by molecular replacement. The crystalographic analysis, however, indicates that binding of the ligands is occurring with a low level of specificity, yielding very confuse images for the bound compounds, which may occupy the protein surface region with different levels of conformation/flexibility. Such a trend is supported by the low quality of the crystals grown, as opposed to those of native CD81, which diffract to 1.5 Å resolution.

Kitadokoro, K., Bordo, D., Galli G., Petracca, R., Falugi, F., Abrignani, S., Grandi, G., Bolognesi, M.
THE 3-D STRUCTURE OF HUMAN CD81 EXTRACELLULAR DOMAIN, A RECEPTOR FOR HEPATITIS C VIRUS, REVEALS THE TETRASPNIN SUPERFAMILY BASIC STRUCTURAL MOTIFS.*EMBO J.*, (2001), **20**, 12-18.

CD81 complexes with peptidomimetic ligands on ID-14-EH1

Data collection statistics

compound	resoln.	cell			mosaic	Rsym
inhibitor_1	2.6	102.862	102.862	34.157	0.592	0.087
inhibitor_2	2.6	102.491	102.491	32.394	0.495	0.029
inhibitor_3	2.0	101.926	101.926	35.725	0.337	0.034

Diffraction data

		In1	in2	in3
Wavelength (Å)			0.934	0.934 0.934
Resolution (Å)	2.6	2.6	2.0	
Unique reflections			11260	9279 14033
*R*merge (%)*	8.7	2.9	3.4	
Completeness (%)$^{+}$			90.0(97.6)79.1(84.9)96.6(99.7)	
Redundancy	2.2	1.5	4.0	

We lost about 6 hours due to beam dump.

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