



Experiment title: Nuclear Receptor Ligand Binding Domain human RXR α bound to 9- <i>cis</i> retinoic acid	Experiment number: LS 1364
Beamline: ID14 EH2	Date of report: 26/02/1999
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Report:

Retinoids (9-*cis* and all-*trans* retinoic acid) are powerful morphogens. These pleiotropic hormones are involved in the control of cellular differentiation, division and apoptosis. They are implicated in the embryogenesis and the general homeostasis in the Vertebrates.

They act through binding to their cognate receptors RXRs and RARs, these receptors belong to the superfamily of nuclear receptors. These receptors are ligand regulated transcription factors that regulate transcription by interacting with specific DNA target sequences (the so called Hormone Response Elements) located in the promoter regions of genes.

We crystallized the ligand binding domain of human RXR α bound to its natural ligand 9-*cis* retinoic acid. The crystals (50 μm x 50 μm x 400 μm) are obtained through several round of micro and macroseeding by the hanging and sitting drop vapour diffusion method at room temperature. They are cryoprotected in liquid ethane in the crystallization mother liquor.

A data set was collected on ID14-EH2 within a resolution range of 8 to 2.9 \AA (resolution limit 2.5 \AA). The crystals belong to space group $P2_12_12_1$ with cell parameters $a=66 \text{\AA}$ $b=86 \text{\AA}$ and $c=90 \text{\AA}$ and $\alpha=\beta=\gamma=90^\circ$. There are 2 monomers in the asymmetric unit. These data set is very incomplete but is being used for structure determination

global $R_{\text{sym}}=8\%$ from 8 to 2.7 \AA resolution

last resolution shell $R_{\text{sym}}=25\%$ from 2.8 to 2.7 \AA

We wish to collect a full and complete native data set of hRXR α bound to 9-*cis* RA and to a synthetic agonist compound of pharmaceutical interest at the highest resolution (2.5 \AA); crystals are being optimized for such purpose.

For this project we will need 3 shifts on a high brilliance and flux beamline such as ID14 EH4.