



## Toward automated and optimized operations of hard x-ray diffraction experiments

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### 1. 背景と研究目的

The aspects of sample preparation is of great interest and tremendous influence for automating sample handling and studies at synchrotron sources. The Nagoya University BL2S1 beamline at the Aichi Synchrotron proposes a unique setup that gives structural biologists access to experiments performed at higher pressures. This particular setup is unique in Japan, and rarely encountered at other synchrotron facilities worldwide. One of the main issue when experimenting with this setup remains in the sample handling procedures. In order to gain further insights in the use and manipulation of this fantastic tool, screening of protein crystal conditions of one particular protein (namely the human neuraminidase *hNeu2*) has been initiated.

### 2. 実験内容

During the current shift, a classical crystallization condition of *hNeu2* has been characterized at BL2S1, under HPPX diffraction experiments. In practice, several protein crystals were disposed inside a Diamond Anvil Cell (DAC). After applying various pressures ranging from 200 MPa to 700 MPa, the diffraction properties of the protein crystals were challenged and the quality of the diffraction patterns assested.

### 3. 結果および考察

Diffraction experiments were performed at pressures of 280 MPa, 460 MPa and 680 MPa, respectively. Experiments were perfored on two crystals originating from the same crystallization condition, for redundancy. An estimation of the cell parameters in these conditions gave an approximation of both the diffracting power of the crystals at these various pressures, and their resistance to higher pressures. Fig. 1 shows the diffraction pattern of small crystals at below 500 MPa.

Surprisingly, the crystals behaved well under higher pressures, with a tendancy to witness a reduction in the values of their cell parameters. Because of the size of the crystals, no full data could be recorded during this present shift, however, important information were obtained in regard to the sample preparation and quality, which will permit to optimize the crystallization conditions prior to future experiments on larger crystals.

### 4. 参考文献

None

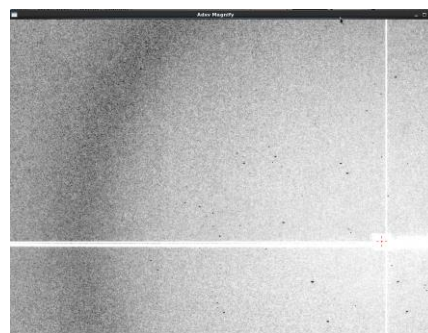


Fig. 1. Diffraction pattern of *hNeu2* under a pressure of 460 MPa.