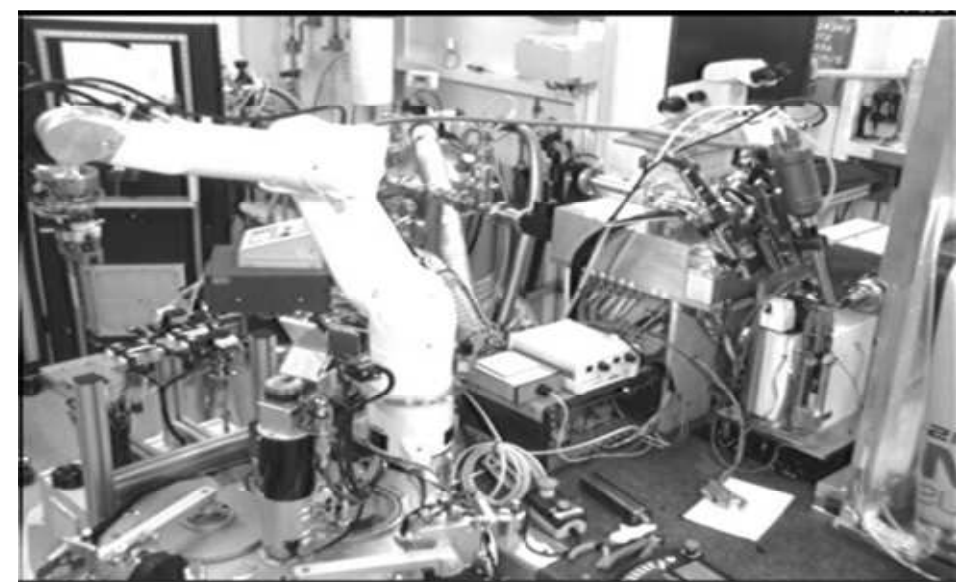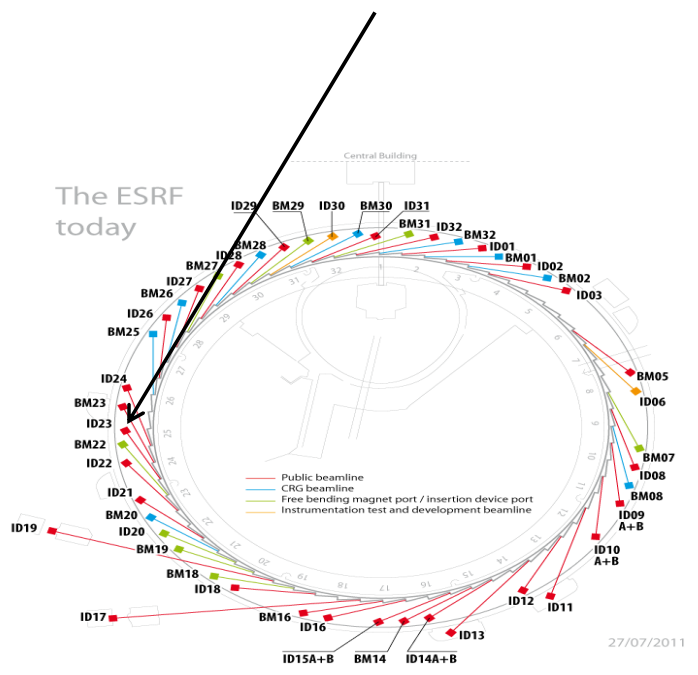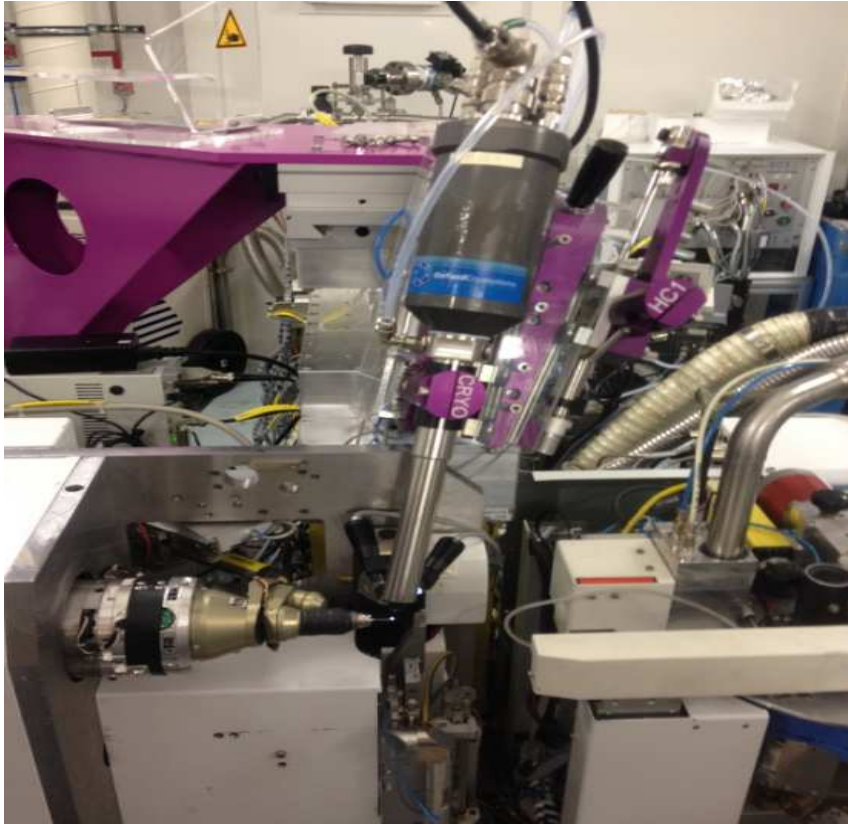# ID23-1 MX beamline news

Alexander Popov

ESRF, MX group

ID23-1 is a tunable MAD-capable station with a mini-focus X-ray beam which opened to users in 2004 (Nurizzo *et al.*, 2006).
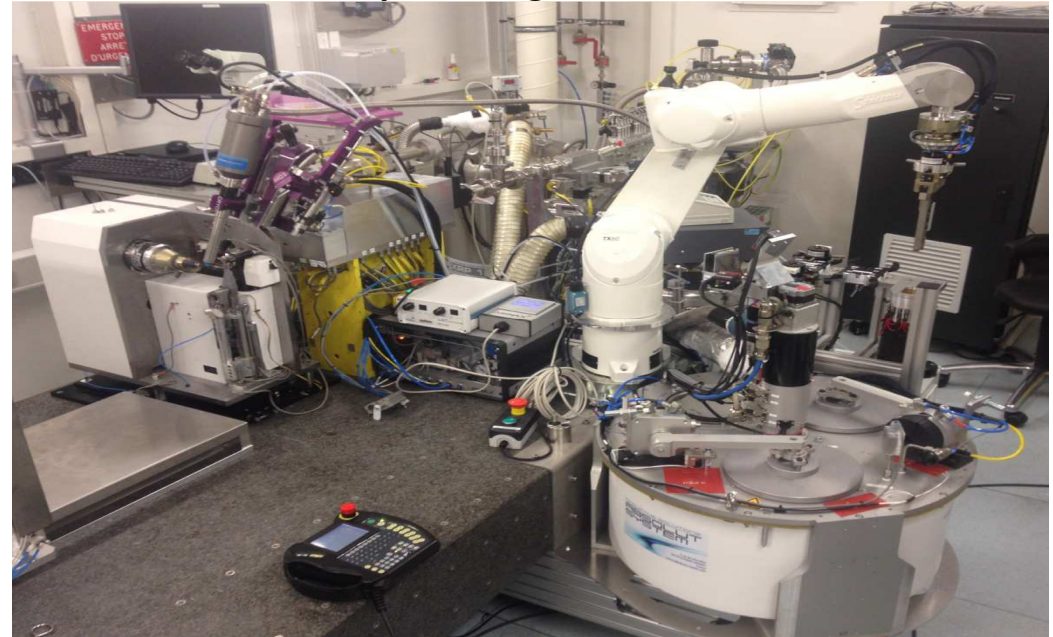
The experimental setup on ID23-1

MD2M mini-diffractometer and
Rapid Exchanger (ReX) for automated exchange between HC1 humidifier
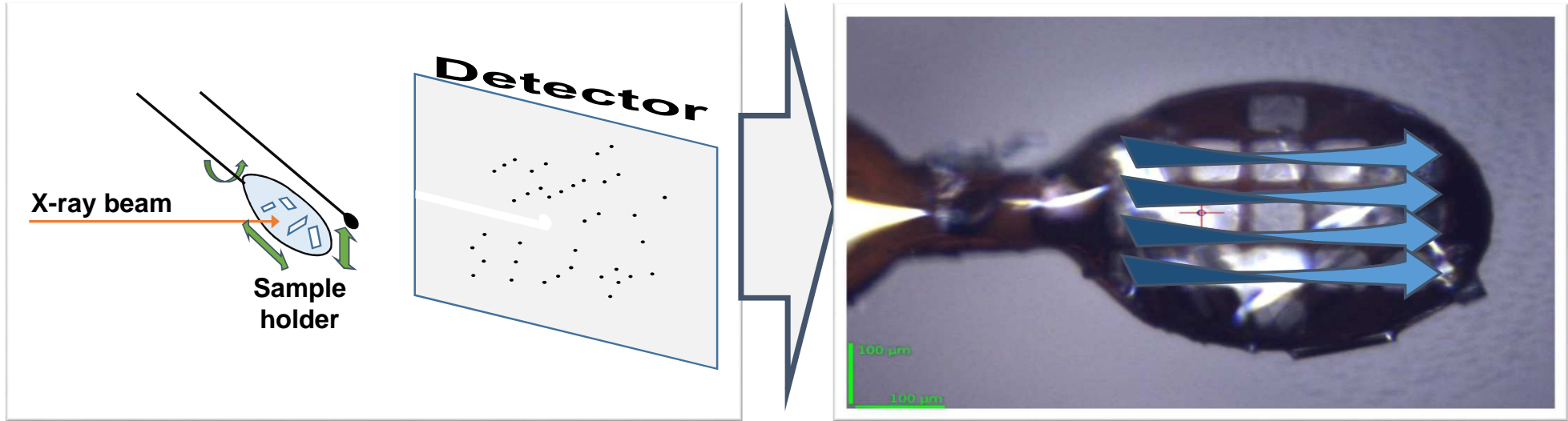**nozzle and cryo-stream nozzle. Including mechanical support system with**
alignment axes

FlexHCD sample changer

IcePAPS migration

✓**Fast crystal best position screening**
✓**X-ray centering**
✓**Crystal cartography**
✓**Helical Data Collection**
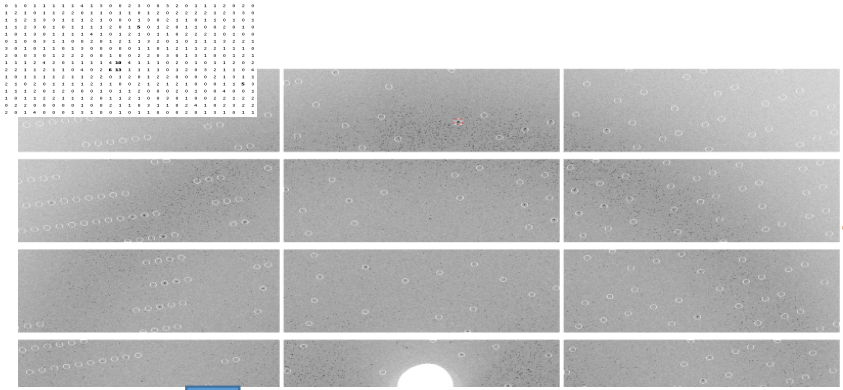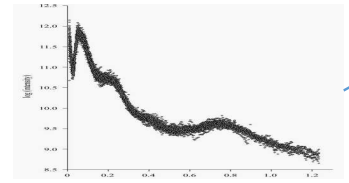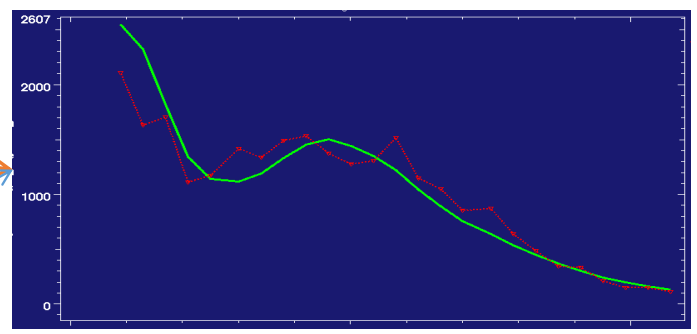✓**X-ray diffraction protein crystal detection**

Experimental setup for X-ray crystallography

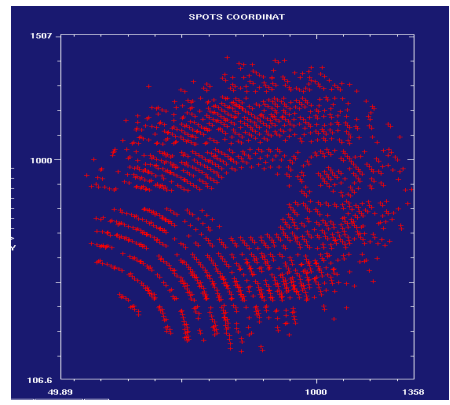The data are accumulated during translational movement

Diffraction images analysis

- Use Wilson plot as a prior
- Use all pixels, not just the local maxima

score = total scattered intensity × radial shape similarity

Bragg spots search

SPOTS COORDINAT

Spots list

```
Program dozor /A.Popov & G.Bourenkov/
Version 1.3.6 //  02.02.2016
Copyright 2014 by Alexander Popov and Gleb Bourenkov
N  |     SPOTS     |        Powder Wilson          |   Main    Spot    Visible
image | num.of INTaver Res.| Scale B-fac. Res. Corr. R-factor|  Score   Score  Resolution
---------------------------------------------------------------------------------------
    1 |    44      4.  3.4| 154.25  26.5  2.9  72.0   26.7 |   1.426   1.74    2.73
    2 |    46     39.  3.6|  21.35  28.0  2.9  61.2   25.7 |   9.097  12.40    2.86
    3 |    40     76.  3.4|   5.88  44.6  2.8  69.1   28.2 |  22.485  29.69    2.73
    4 |    51     44.  3.4|  18.10  24.2  2.8  64.0   24.8 |  12.837  16.96    2.69
    5 |    46     32.  3.3|  22.98  30.4  2.9  71.6   24.9 |   9.561  13.63    2.62
    6 |    11      5.  6.4| 142.22  18.1  2.9  62.8   29.6 |   0.235   0.13    5.09
    7 |    43      4.  3.4| 232.69  16.7  2.8  62.9   31.0 |   1.258   1.97    2.69
    8 |    30     78.  3.4|  19.31  13.1  2.9  56.1   31.3 |  15.888  30.38    2.69
    9 |    33     83.  3.2|   9.34  28.5  2.9  52.3   25.0 |  20.799  40.67    2.59
   10 |    31     66.  3.4|   8.86  39.8  3.0  62.3   24.7 |  16.076  24.23    2.69
```
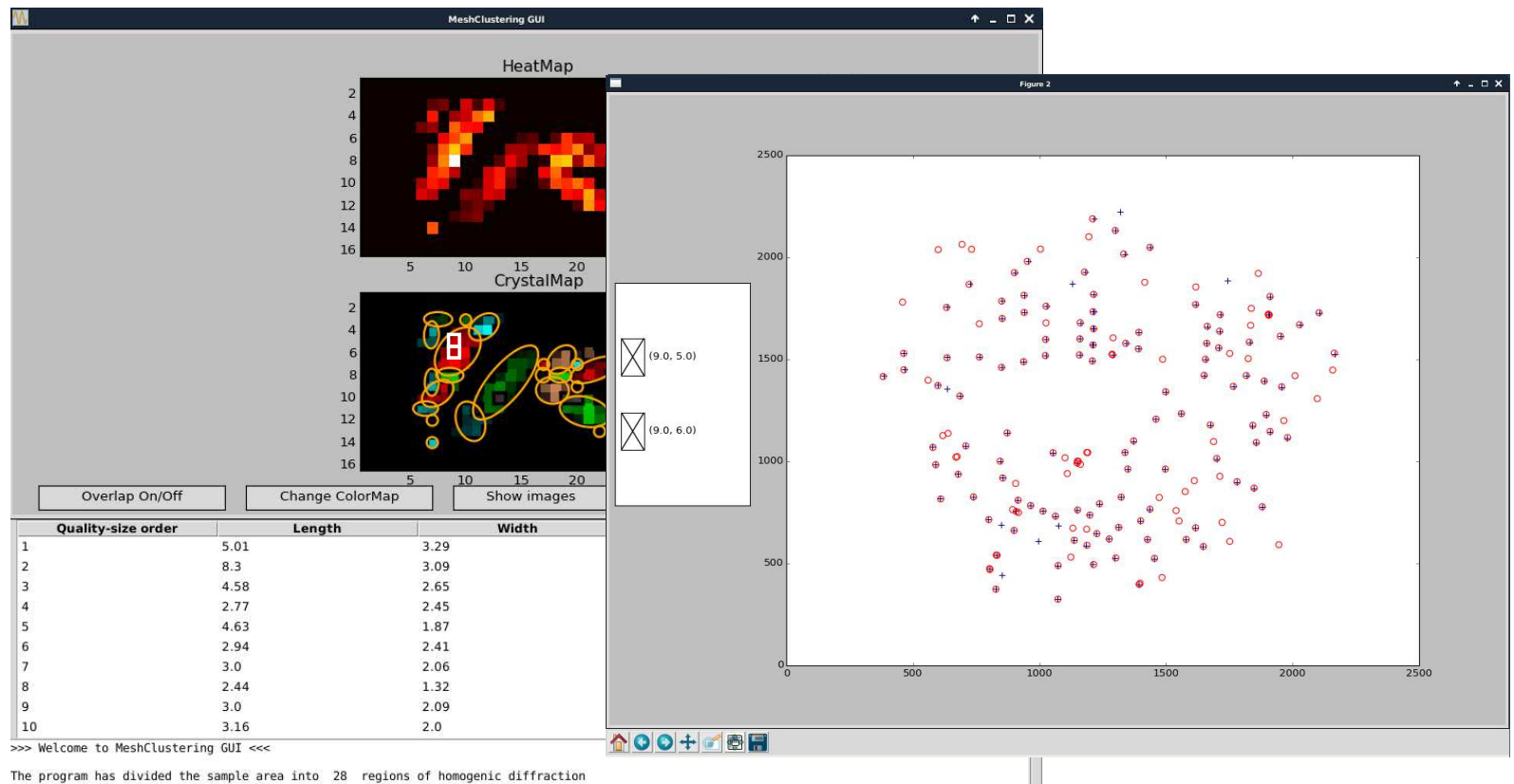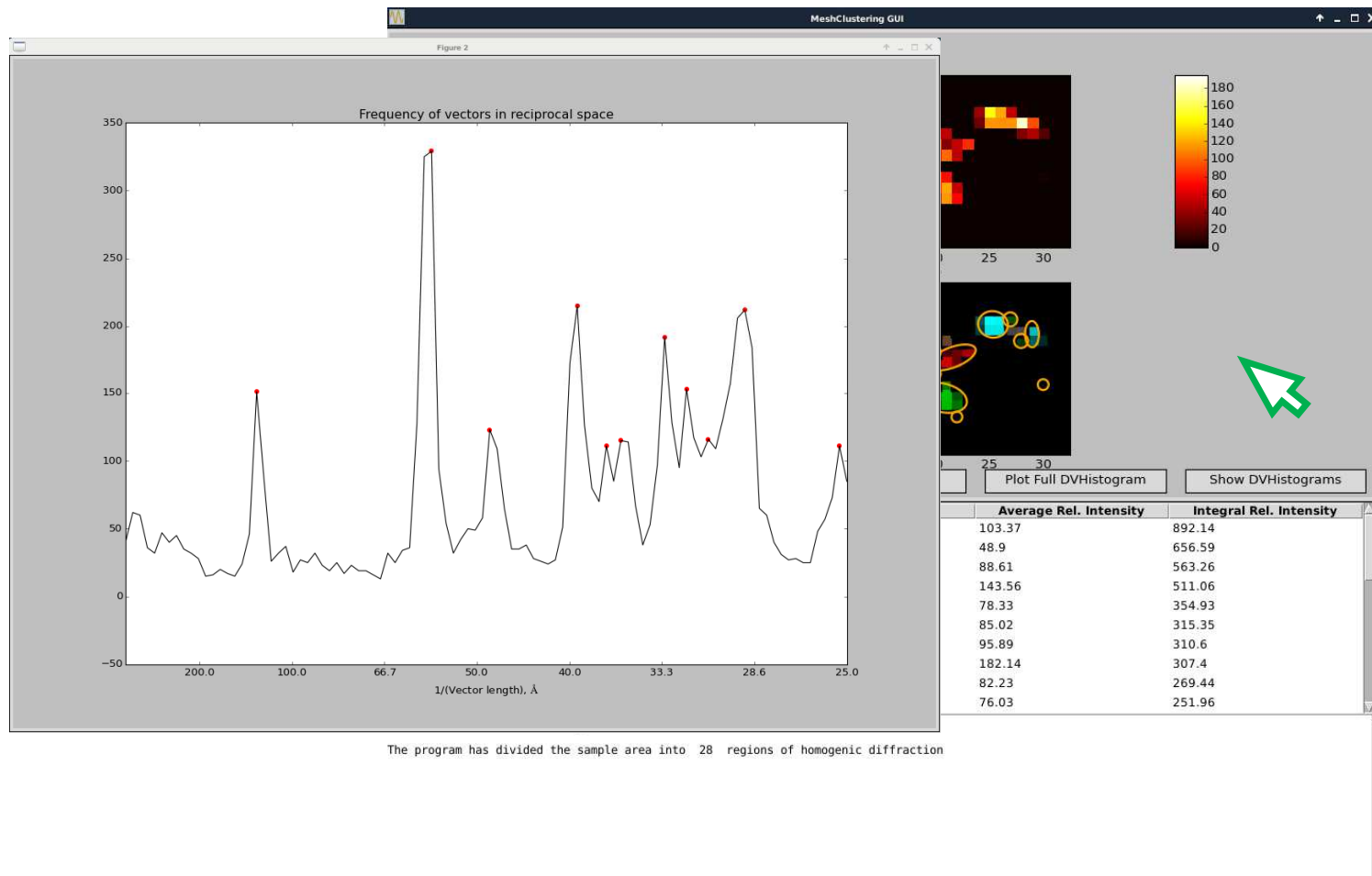
MeshBest GUI
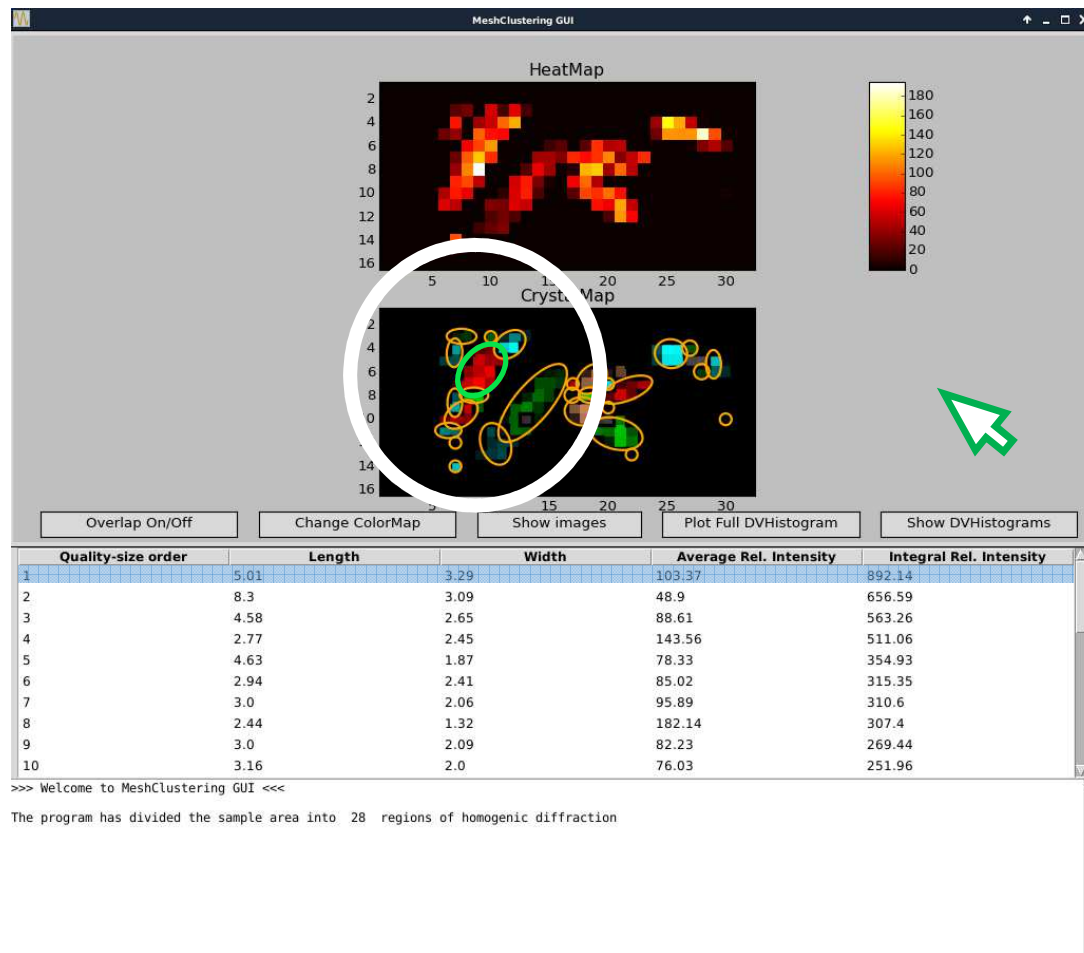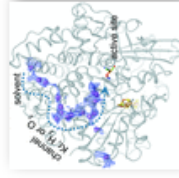
Igor Melnikov

Overview
Spot diagram display

Interspot distance histogram

Picking the crystal

Gas-sensitive biological crystals processed in pressurized oxygen and krypton atmospheres: deciphering gas channels in proteins using a novel `soak-and-freeze' methodology
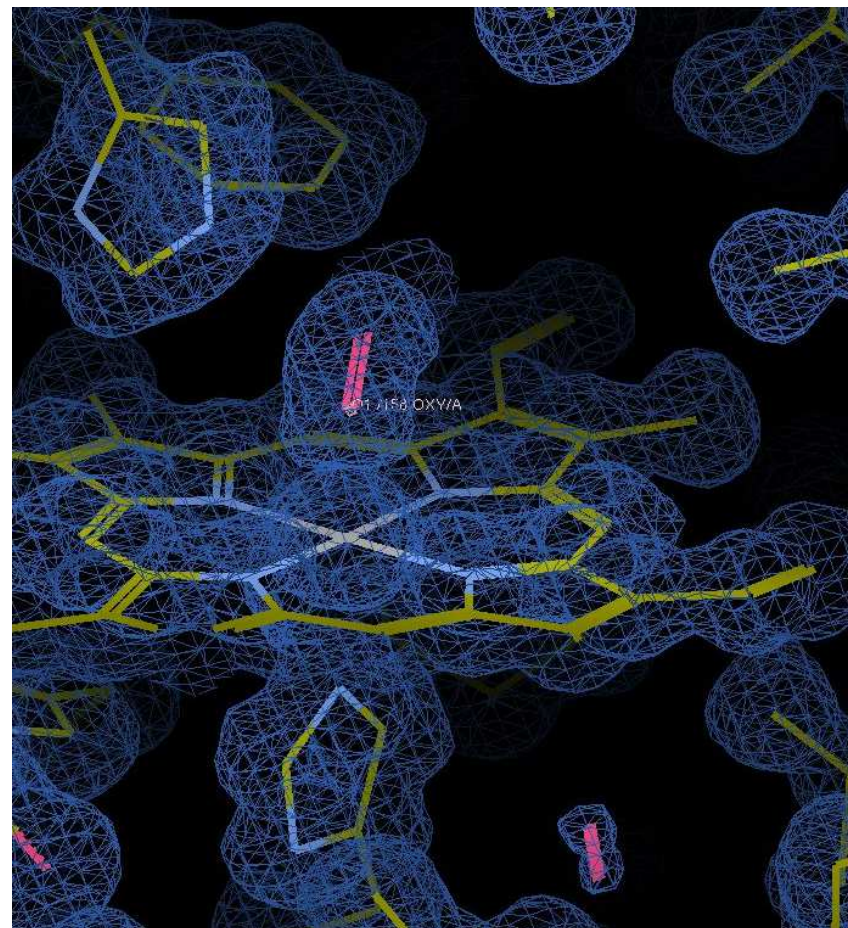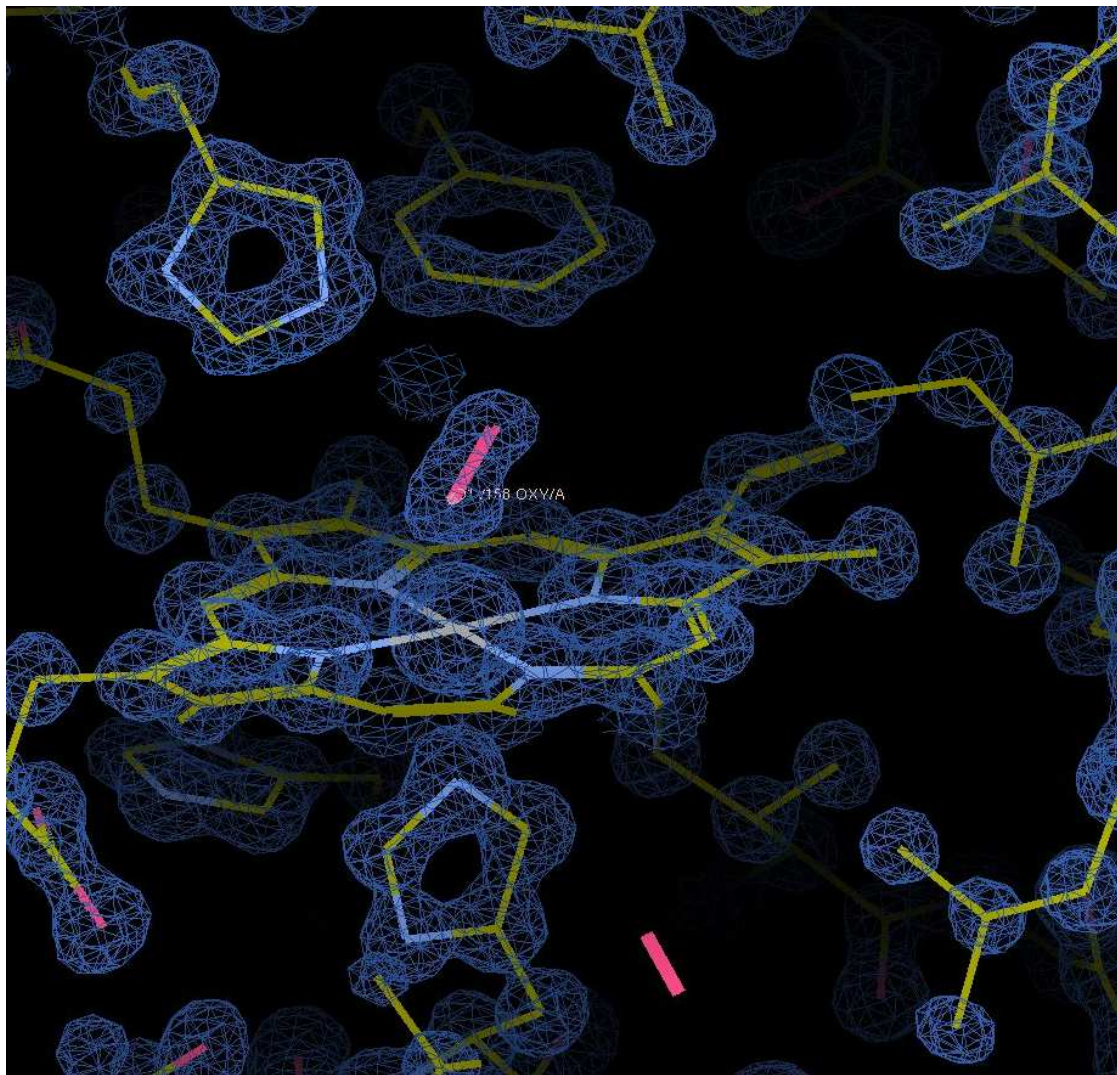
B. Lafumat, C. Mueller-Dieckmann, G. Leonard, N. Colloc'h, T. Prangé, T. Giraud, F. Dobias, A. Royant, P. van der Linden and P. Carpentier

A novel cryogenic gas pressure cell has been designed for structural studies of enzymes requiring gaseous substrates. The proof of principle is demonstrated for test crystals. The pressure cell has been designed for the study of O_2-sensitive proteins to reveal pores, channels and reactive centres, and thus to decipher O_2 traffic in proteins.
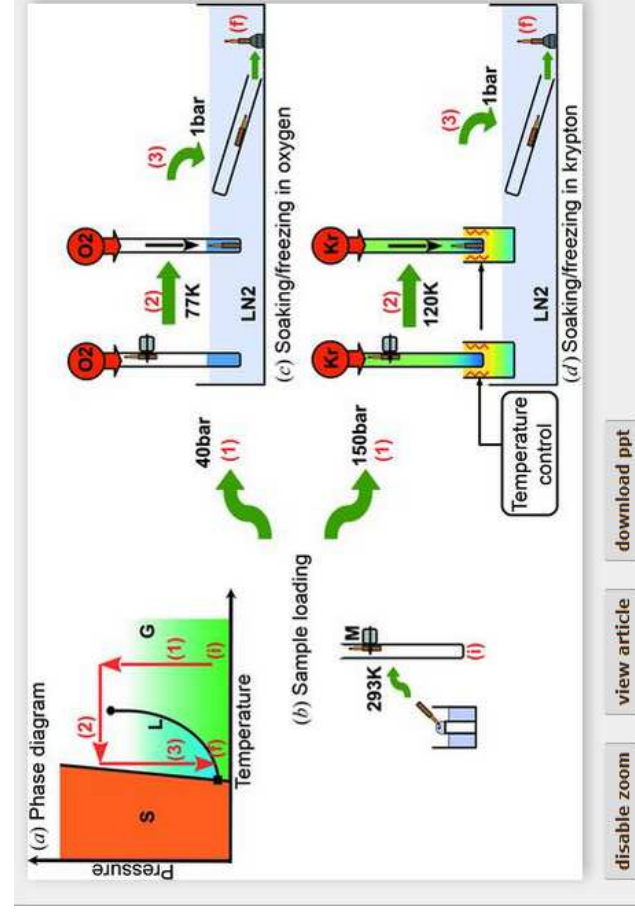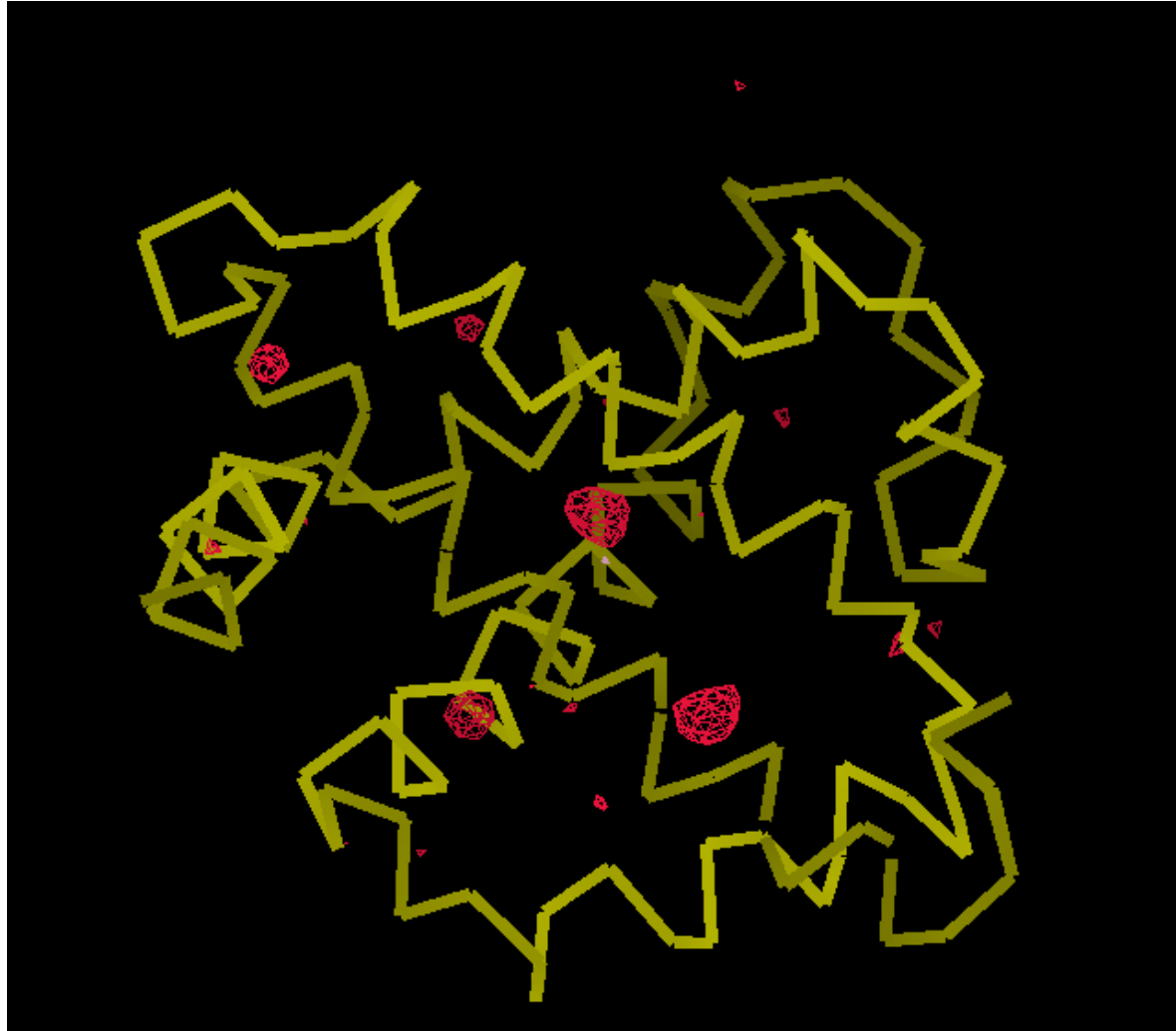
Figure 1
Soak-and-freeze thermodynamics. (*a*) A typical phase diagram (*P*, *T*), displaying the soak-and-freeze pathway subdivided into its three transformations. (*b*) Sample fishing from the crystallization tray and loading into the pressure cell. The sample is held at the top of the tube by an external magnet. (*c*) Soaking and freezing in oxygen. (*d*) The same process for krypton, with temperature regulation at the bottom of the tube.

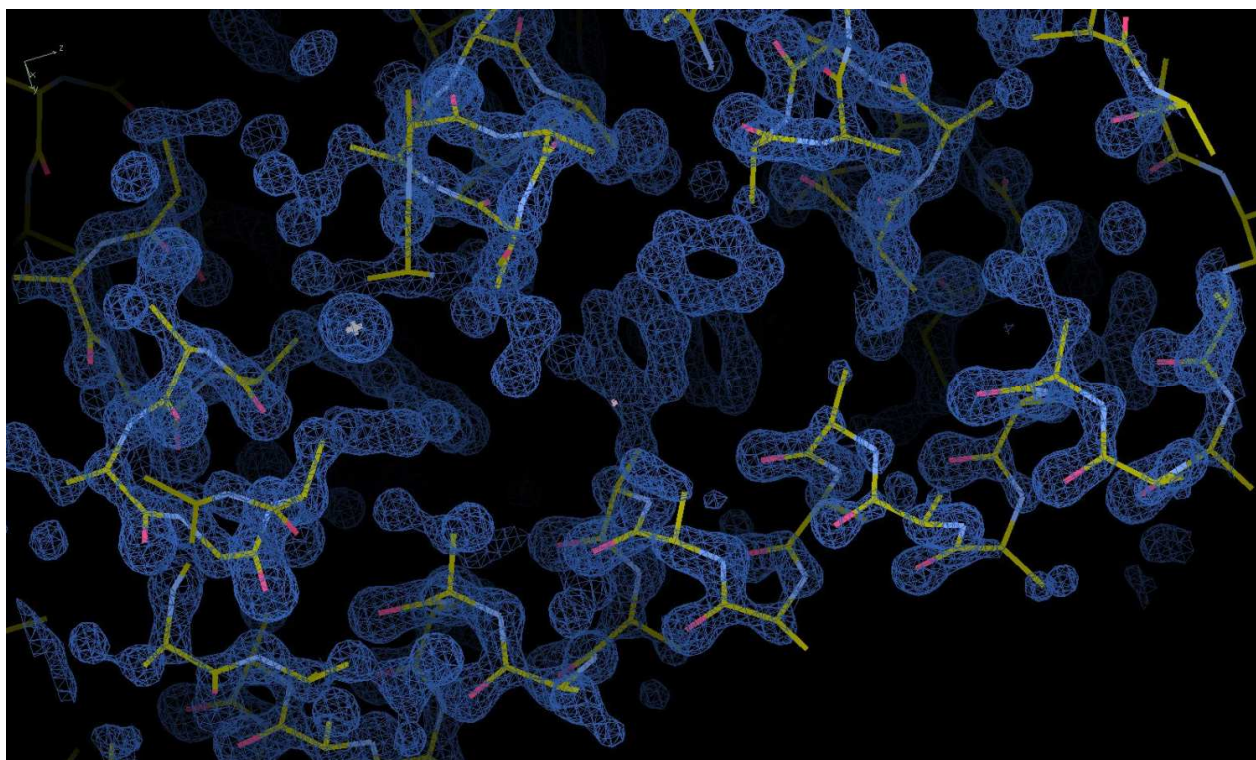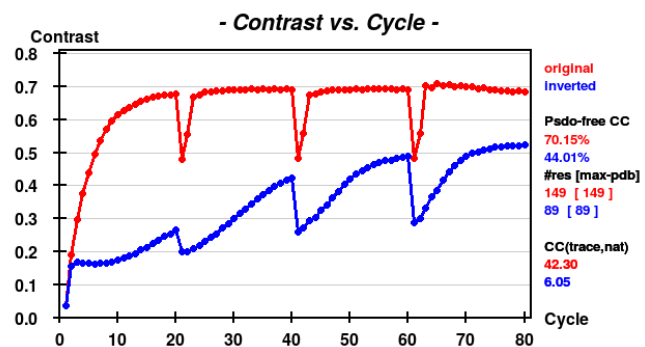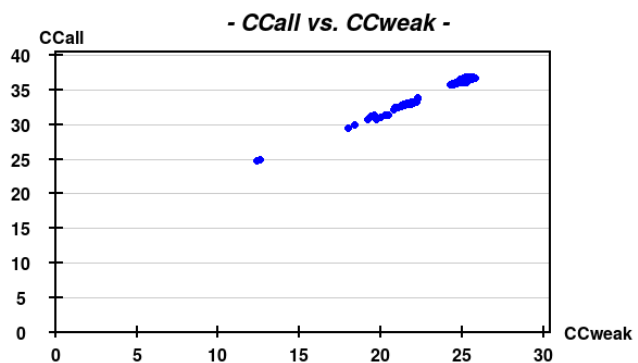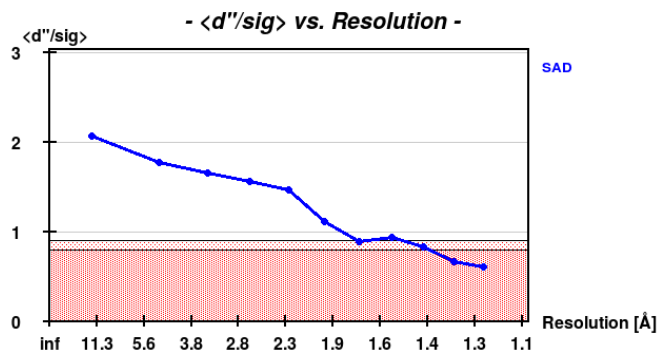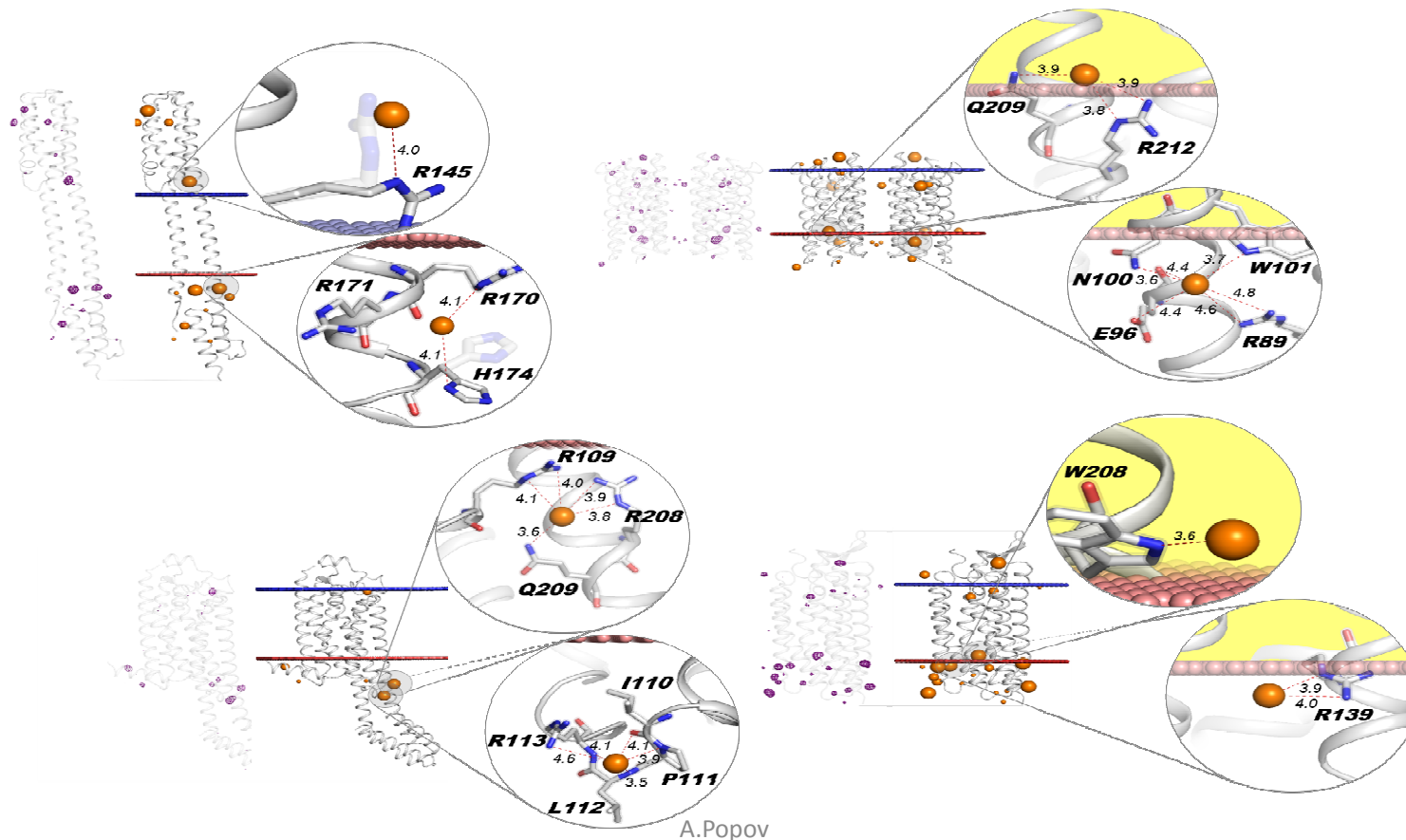[disable zoom] [view article] [download ppt]

OXY - Myoglobin

Myoglobin and Kr

SHELX and Leghemoglobin+Kr

- ⟨d"/sig⟩ vs. Resolution -

⟨d"/sig⟩

SAD

Resolution [Å]

inf 11.3 5.6 3.8 2.8 2.3 1.9 1.6 1.4 1.3 1.1

- CCall vs. CCweak -

CCall

CCweak

- Contrast vs. Cycle -

Contrast

original
inverted

Psdo-free CC
70.15%
44.01%

#res [max-pdb]
149 [149]
89 [89]

CC(trace,nat)
42.30
6.05

Cycle

Fast iodide-SAD phasing for high throughput membrane protein structure determination

Igor Melnikov [a] *, Vitaly Polovinkin [bce] *, Kirill Kovalev[ce], Ivan Gushchin[ce], Mikhail Shevtsov[e], Vitaly Shevchenko[cde], Alexey Mishin[e], Alexey Alekseev[ce], Francisco Rodriguez-Valera[f], Valentin Borshchevskiy[e], Vadim Cherezov[eg], Gordon Leonard[a], Valentin Gordeliy[bce] **, Alexander Popov[a] **

We describe a fast, easy and potentially universal method for solving the crystal structures of membrane proteins via iodide-single-wavelength anomalous diffraction. The potential universality of the method is based on a common feature of membrane proteins – availability at hydrophilic-hydrophobic interface of positively charged residues with which iodide strongly interacts. We show that the method is efficient for different data collection strategies based on either standard or serial X-ray crystallography techniques.
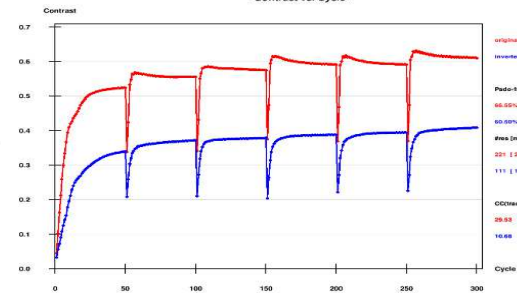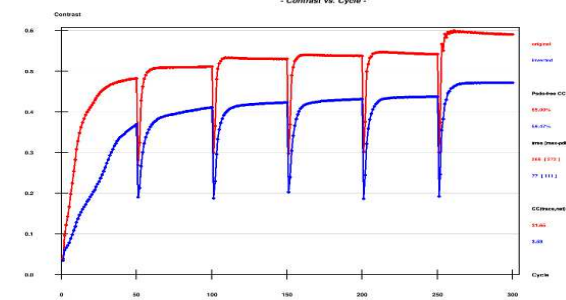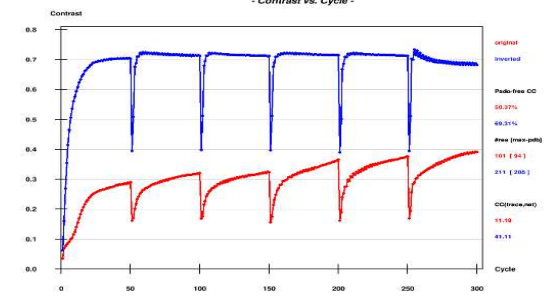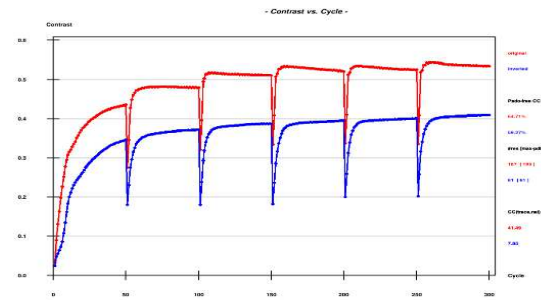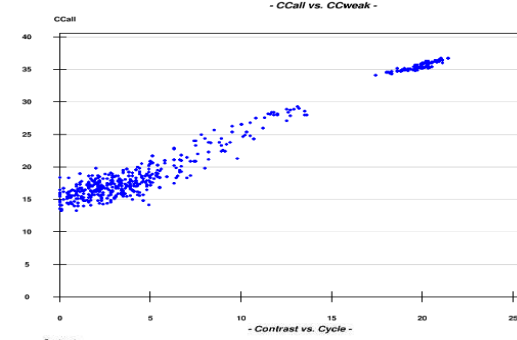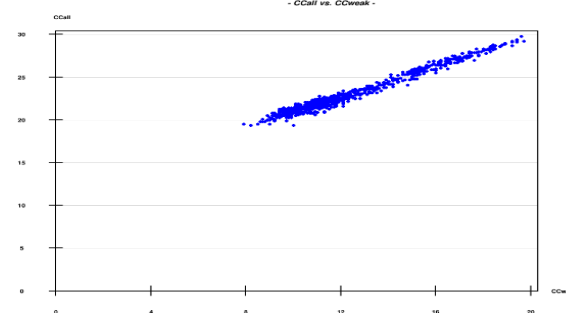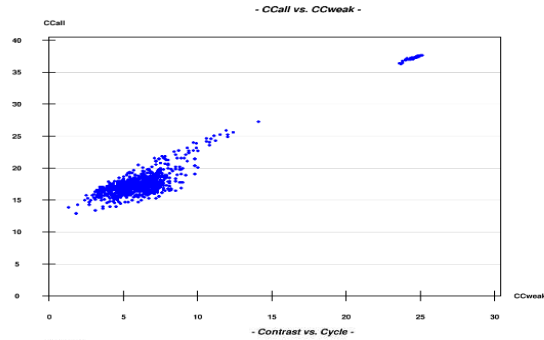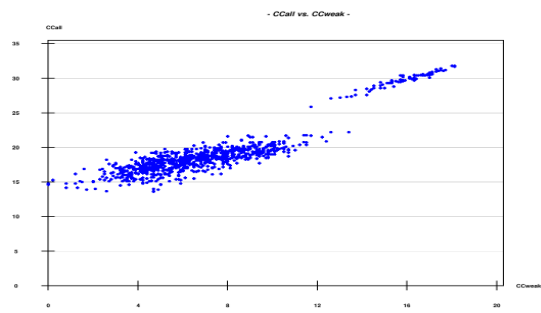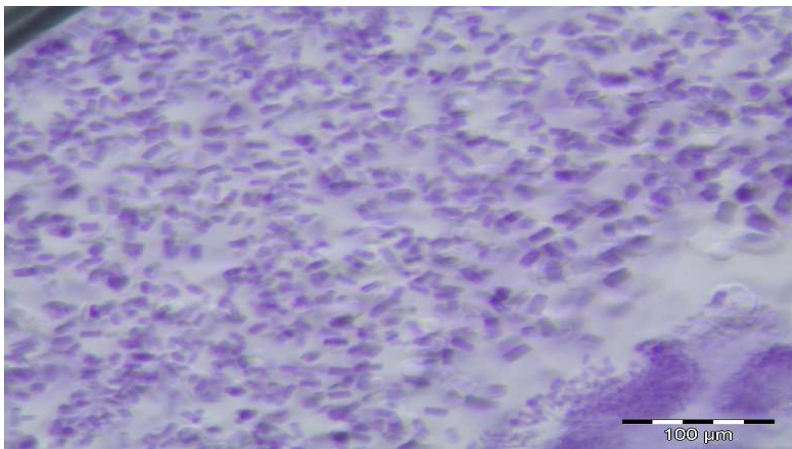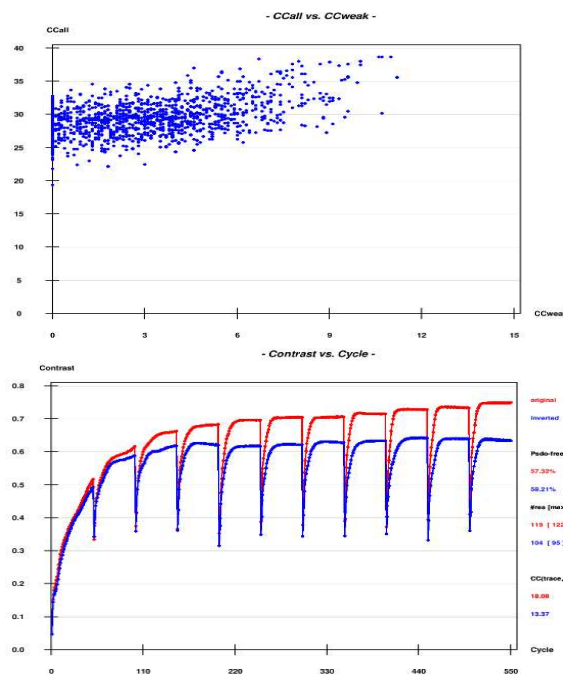
NarQ in F222

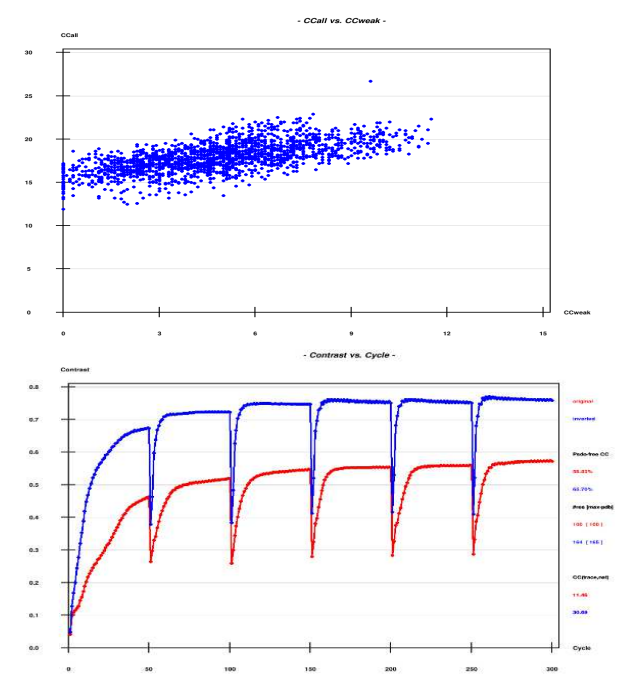KR2 in I222

MacR in P1

A2A in C2221

SAD within Mesh&collect pipeline

KR2 small crystals of an average size of 10-15μm

SAD, 136 serial datasets merged together

SIRAS, 39 serial datasets merged together + one native dataset from standard collection