Here is a cumaltive report from several sessions at ID23-1, ID30

1. Crystal structures of nanobody 85-Vietnam 026 P domain complex

Dataset for a single crystal of nanobody 85 bound to Vietnam 026 P domain was processed at 2.1Å resolution with completeness 94.8%, space group P 1 21 1. Data proccesing was done with XDS. Molecular replacement was performed using apo structure of Vietnam 026 P domain and structure of nanobody with higest aminoacid homology (Protein Data Bank code 3P0G). Refinement led to the R_{work} and R_{free} values 0.21 and 0.26, respectively, and well-defined electron density for a vietnam P domain dimer with 2 bound nanobodies. The binding site is located at the bottom part of P domain. Further refinement to reduce R-factors is in progress.

2. Crystal structures of nanobody 27-Vietnam 026 P domain complex

Dataset for a single crystal of nanobody 27 bound to Vietnam 026 P domain was processed at 2.7Å resolution with completeness 99.7%, space group P 6 2 2. Data proccesing was done with XDS. Molecular replacement was performed using apo structure of Vietnam 026 P domain and structure of nanobody previously solved in our laboratory (nanobody 25). Refinement led to well-defined electron density for a Vietnam P domain dimer with 2 bound nanobodies. The binding site is located at the bottom part of P domain. Further refinement to reduce R-factors is in progress.

3. Crystal structures of nanobody 13-Vietnam 026 P domain complex

Dataset for a single crystal of nanobody13 in complex with Vietnam 026 P domain was processed at 2.7Å resolution with completeness 95.5%, space group P 6 2 2. Data proccesing was done with XDS. Molecular replacement is currently in progress, as models apo structure of Vietnam 026 P domain and structure nanobody 25 were taken.

4. 026 P domain – NIH clinical collection drugs

Dataset for a single crystal of 026 P domain cocrystallized with 10 drugs from NIH clinical collection mixed with compound 78 was processed at 1.52Å resolution by EDNA. The F_o-Fc map for some parts of compound78 was observed after molecular replacement. Datasets for 026 P domain cocrystallized with 21 more drug batches were collected with average resolution of 1.7 Å and currently are beeing processed.

5. Crystal structure of norovirus UNSW Polymerase

Dataset for a single crystal of norovirus polymerase from UNSW strain was processed at 1.6Å resolution and space group C 1 2 1. Data proccesing was done with XDS. Molecular replacement was performed using structure of Norwalk Virus polymerase (Protein Data Bank code 3BSO). Refinement led to the R_{work} and R_{free} values 0.23 and 0.27, respectively, and well-defined electron density for 2 Mg ions in active site. Further refinement to reduce R-factors is in progress. Several dataset for polymerse cocrystalized with RNA primer and DNTP were collected and processed, but no electron density for ligands was found.