ESRF	**Experiment title:** **Serial snapshot microcrystal crystallography on small organic molecules**	**Experiment number**: CH-4317
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Report:

The first target of the experiments was to test the serial snapshot crystallography approach as a tool for structure solution from microcrystal too small to give enough information before radiation destruction. The second target was to evaluate the possibility to use intensive semi-monochromatic wavelength for structure solution from microcrystal. For the experiment we had used both model compound of a known structure as well as samples of unknown structures:

A) Model compounds with previously known crystal structure
I. co-crystal of agomelatine with citric acid (prepared by controlled crystallization targeted to get uniform sub 63 μm crystal size)
II. lisuride maleate

B) Compounds of unknown structure impossible to solve from standard monocrystal
III. agomelatine phosphate
IV. agomelatine chloride
V. epi-ergokryptinine (ergot alkaloid)
VI. ginkgetin (flavonoid)
VII. epi-taxol
VIII. tenofovir disoproxil fumarat

For each of the compound it was at first measured an 180 degree 1 degree step scan from microcrystals. The size of the microcrystal was sub 50 μm in maximal dimension. Semi-monochromatic wavelength with average λ=0.3542 Å was used. The images were processed in CrysAlisPro software and potentially solved in CRYSTALS software.

It was possible to solve structures I, II, III,V and VI. After structure solution of V it was found it is already a known one (incorrect chemical analysis of source material). It was possible to index structures VII and VIII, but to do a solution was not possible due to low angle diffraction. Data for structure IV was impossible to index at all. Structures III and VI were not solved due to luck of enough big crystals up to now so a solution from sub 50 μm microcrystal is a useful result itself. During data processing and crystal refinement it was impossible to achieve as good Rint and refinement R factors as for standard monocrystal measurement. It will be necessary to find optimal data processing for measurement based on semi-monochromatic wavelength and only partial data coverage.

Based on the mentioned single microcrystal measurement the compounds I,II,III and VI were chosen for experiments related to the potential serial-snapshot crystallography. The microcrystals were distributed on a non diffracting grid. The grid was positioned perpendicular to the beam. The grids were scanned with 50 μm step in x,y direction. For each position 3 snaps were made with -5, 0 and 5 degree rotation. Small grids were scanned in 10x10 steps mode, big in 25x25 so 300 or 1877 images per grid were recorded. We work on this data processing in cooperation with the Catherine Dejoie group.

Expected results and publications:

- fine tone the data processing obtained by semi-monochromatic wavelength and publication of structures III and VI measured from single microcrystal
- test the algorithm for serial snapshot crystallography on data measured on compound I,II,III,IV and publish the result in cooperation with C. Dejoie