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Report:

We are elucidating the three-dimensional structure of the photosystem II (PSII) purified from the thermophilic cyanobacterium *Synechococcus elongatus*. Up to now we obtained electron density maps at relatively low resolutions, the most recent model determined at 3.8 Å (Zouni et al., 2001). Although the best heavy atom derivative diffract to 3.8 Å resolution, the reliable experimental phase information is available only to ~4.5 Å resolution. Therefore we wanted to collect additional derivatives and improve the phasing.
In former times the cadmium heavy atom derivatives had the best resolution. In these crystallisation trials, we tried to co-crystallise the protein with $CdCl_2$ instead of $CaCl_2$. We wanted to replace the calcium ion, placed close to the manganese cluster, by cadmium. According to HSAB principle the Ca^{2+} and Cd^{2+} ions are quit similar. Maybe these ions have a positive influence on the stabilisation of the protein.

From a Cd-PSII co-crystal (typical dimensions are 0.5 x 0.5 x 1.0 μm) we collected a data set with 97.2 % completeness. The data set was of reasonable quality to 3.7 Å resolution with R_{sym}=0.04 and $<I/\sigma(I)>$=10.9 (R_{sym}=0.108 and $<I/\sigma(I)>$=2.5, mosaicity 0.8°). Unfortunately the completeness in the higher resolution shells drops continuously to minimum of 52 %

between 3.8 to 3.7 Å because of the increasing number of overlapping reflection profiles due to the large unit cell constants an the high mosaicity of the crystal.
The good quality of the data is reflected by the anomalous Patterson function, which clearly shows the peaks corresponding to the difference vectors between the cadmium atom in the Harker section.

Reference

Zouni, A., Witt, H.-T., Kern, J., Fromme, P., Krauß, N., Saenger, W., Orth, P. (2001) Crystal structure of photosystem II from *Synechococcus elongatus* at 3.8 Å resolution. *Nature* **409**, 739-743.