Automated crystal centering by use of UV LED

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The continuously increasing demand for synchrotron beam-time, both from academic and industrial users, is a direct outcome of the exponential growth of macromolecular crystallography. Fully automated procedures at every level of the experiments are being implemented at all synchrotron facilities, allowing the screening of a profusion of sample crystals for more and more projects. However, the sample recognition and centering in the X-ray beam represents one of the major obstacles to achieving such automation.
Several independent algorithms have been developed to achieve crystal recognition and centering. The most popular method relies on pattern recognition of the loop encircling the crystal (1). Ideal for high-throughput data collections, this frequently used routine has the advantage to allow the screening of plenty of samples in a timely and efficient manner. Nevertheless, when dealing with crystals of small sizes or shifted from the loop center, it suffers from a lack of precision. Other techniques include diffraction-based analysis crystal centering (2), increase of crystal-to-surrounding contrast by differential lights (3), X-ray fluorescence (4) and UV-fluorescence recognition (5).
UV-based crystal centering takes advantage of the capacity of UV-light to specifically react with aromatic residues present in proteins or with DNA base pairs. Although very efficient, a well-known side effect of illuminating biological samples with strong UV-sources resides in the damages induced on the irradiated samples (6). In the present study, the effectiveness of a softer UV-light for crystal centering, by taking advantage of low power LED sources was investigated. Detailed analysis will be done on the impact of such UV-light source on the irradiated sample. Finally, it will be shown how the use of UV LED can represent a low-cost solution for non-damaging crystal centering with high specificity.

References

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