Automated setup for *in crystallo* optical spectroscopy applied to Structural Biology at the ESRF

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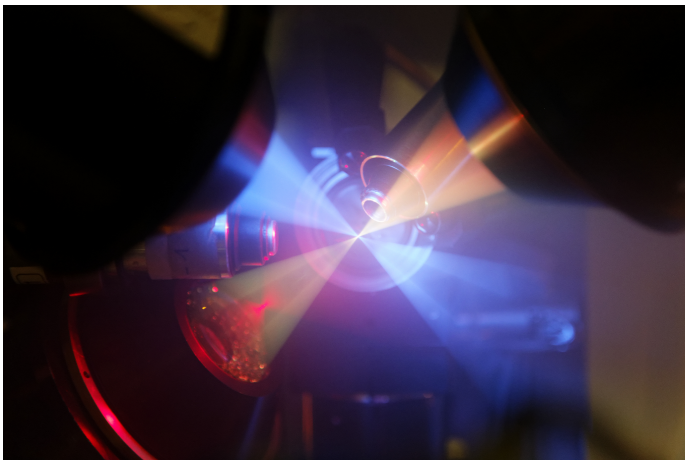
The analysis of structural data obtained by X-ray crystallography on biological macromolecules may benefit from information directly obtained on the crystalline sample by complementary techniques. In particular, various optical spectroscopies (UV-visible light absorption, fluorescence emission, Raman) have been crucial in establishing the nature of the physiological state adopted by certain macromolecules in the crystalline state, or controlling the extent of specific radiation damage to protein active sites. The biological systems of interest are generally coloured via light-absorbing chemical groups (cofactor, metal centre, chromophore), but not always. At the ESRF in Grenoble, the Cryobench laboratory has been developed since 2000 within the Structural Biology group to provide such complementary techniques either directly on the beamline (for online experiments), or next to the beamline (for offline, preparative experiments) [1]. This talk will introduce the latest developments of the ID29S-Cryobench laboratory, which include an improved setup for online Raman on beamline ID29 [2] and a fully motorized setup (Figure), which greatly facilitates the recording of spectra in the offline configuration of the laboratory.



The new offline microspectrophotometer of the ID29S-Cryobench laboratory at the ESRF. Three blue, green and red LEDs highlight the intersection of the focal volumes of the three optical objectives.

References

[1] von Stetten D. *et al.* (2015) '*In crystallo* optical spectroscopy (*ic*OS) as a complementary tool on the macromolecular crystallography beamlines of the ESRF' *Acta Crystallogr.* D**71**, 15-26.

[2] von Stetten D. *et al.* (2017) 'Online Raman spectroscopy for structural biology on beamline ID29 of the ESRF' *J Struct. Biol.* **200**, 124-127.