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Making routine native SAD a reality

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Experimental phasing by SAD (single-wavelength anomalous diffraction) is nowadays the dominant method for de novo structure determination owing to its experimental and operational simplicity. Most experiments still use selenomethionyl substitution or heavy-atom derivatization but native SAD, which exploits the weak anomalous scattering of light elements naturally present in the macromolecules (P, S, Cl, K and Ca), has made great progress in recent years and is gaining popularity [1]. With advances in both instrumentation and data collection strategies, as well as software, it is now possible to measure weak anomalous signals with very high accuracy.

A data collection strategy [2], which yields high quality anomalous data from a single crystal entity, was developed at beamline X06DA-PXIII at the Swiss Light Source (SLS). It benefits from very stable X-ray source and optics, a high-precision multi-axis PRIGo goniometer [3] and a readout noise-free PILATUS detector (Dectris, Ltd.) calibrated for low energies. I will present those instrumentation developments and data collection strategies, as well as ongoing work towards a very fast and fully automated native SAD data collection protocol using SmarGon (SmarAct GmbH), the commercial multi-axis goniometer based on PRIGo, in combination with a hybrid photon counting detector EIGER (Dectris, Ltd.).

I will show how native SAD is routinely performed at X06DA-PXIII for de novo structure determination of a wide range of targets solved in the past 3 years.

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