Elettra 2.0: New Structural Biology Opportunities

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Combining visual and X-ray sample characterization information in design of macromolecular crystallography experiments

Monday, July 3, 2023 10:00 AM (30 minutes)

The best thing one can do to determine the structure of a biological macromolecule at atomic resolution is to grow a large homogeneous crystal of it, then probe it with flat X-ray beam of the matching size, while rotating it using a perfect goniometer while measuring the complete reciprocal image of its electronic density with a perfect detector.

Though this ideal is not feasible in practice, it should stay the northern star of our struggle for quality. In this contribution we will address three points that have a promise of bringing us closer to the ideal.

First we will unravel the problem of achieving perfect sample alignement at arbitrary goniometer datum with mechanically imperfect goniometers.

Second we will address the problem of merging optical and x-ray sample characterization information into a coherent whole.

Third we will attempt to establish a way of optimal sampling of available diffracting volume for a more perfect measurement with beams of arbitrary size and intensity.

The talk will conclude with a discussion of the most desirable properties of a new MX beamline, with a view to the problems we will have attempted to unravel.

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Session Classification: Session 1 Macromolecular Crystallography Chair: Michele Cianci (Università Politecnica delle Marche)