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Jointly organized by:

Dipartimento di Chimica
Dipartimento di Biologia e Biotecnologie “L. Spallanzani”

Integrative Structural Determination of Macromolecular Complexes

Integrative structural determination combines diverse biochemical and biophysical data to construct three-dimensional models of macromolecular complexes. By exploiting the complementarity and consistency of multiple datasets, this approach yields models that are more informative and accurate than those obtained from any single methodology.

A particularly useful framework combines chemical cross-linking coupled with mass spectrometry (XL-MS) and electron microscopy (EM), further enhanced by X-ray crystallography of individual domains or Artificial Intelligence-based structural predictions. These methods provide complementary insights: XL-MS defines proximities between residues, peptides, or domains within a complex, whereas EM reveals the overall shape and spatial organization of entire particles—from cellular components to large assemblies—captured as 2D images or 3D density maps.

This integrative strategy is especially effective for characterizing transient and dynamic macromolecular assemblies and for exploring interactions in situ. In this presentation, I will illustrate several biological applications of the method, highlighting its ability to provide structural insights that are otherwise inaccessible.

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October 9th, 3.00 pm

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