Chemical Crosslinking and Structural MS — Hands-on

Build a strong conceptual understanding of chemical crosslinking and structural mass spectrometry (XL-MS). This module focuses on crosslinker chemistry, experimental design, XL-MS data patterns and identification concepts, and how crosslink distance restraints are interpreted in the context of protein complex architecture and integrative structural models.

Chemical Crosslinking and Structural MS

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Crosslinking & Structural Restraints Foundations

What is chemical crosslinking and why use XL-MS

capturing proximity information **probing complexes and conformations** **complementing structural methods**

Distance restraints and structural interpretation ideas

linker length concepts **Cα–Cα distance thinking** **satisfied vs violated crosslinks (overview)**

Overview of XL-MS workflows at conceptual level

crosslinking reaction idea | digestion and LC–MS/MS readout | data interpretation and mapping

Session 2

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Crosslinker Types & Experiment Design (Concepts)

Crosslinker families and reactive group concepts

amine reactive crosslinkers (overview) | cleavable vs non cleavable ideas | homo vs heterobifunctional concepts

Spacer length, flexibility and solvent accessibility thinking

approximate upper distance limits | impact of protein dynamics | surface exposure concepts

Conceptual experiment planning for XL-MS projects

choice of complex and conditions | controls and replicate thinking | high level LC–MS/MS considerations

Session 3

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XL-MS Data Patterns & Identification Concepts

Types of crosslinked species in XL-MS data (concepts)

monolinks and loop links | inter and intra protein crosslinks | uncrosslinked background peptides

MS/MS patterns and interpretation at conceptual level

precursor mass shifts ideas | cleavable linker fragment concepts | complex fragmentation patterns awareness

Identification thinking and FDR concepts for crosslinks

search space considerations (overview) | target decoy style thinking for crosslinks | confidence and site assignment ideas

Session 4

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Mini Capstone: From Crosslinks to Structure

Mapping crosslinks onto structures or models (conceptual)

Theory + Practical (planning style)

Interpreting satisfied and violated restraints at high level

possible causes of conflicts | conformational heterogeneity ideas | model refinement thinking (overview)

Mini capstone deliverables (concept and planning focused)

crosslink table layout and annotation plan | distance summary and simple plots (idea level) | short narrative linking crosslinks to architecture