Advanced Techniques In Cheminformatics

8:45 AM - 10:15 AM: Session 1: Quantitative Structure-Activity Relationship (QSAR)

Introduction to QSAR modeling techniques.
Practical demonstration of building and validating QSAR models for predicting chemical activity.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Computational Chemistry Methods

Overview of computational chemistry methods in cheminformatics.
Hands-on workshop on molecular dynamics simulations and quantum chemistry calculations.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Machine Learning in Cheminformatics

Introduction to machine learning techniques in cheminformatics.
Practical session on applying machine learning algorithms to chemical data.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Cheminformatics in Drug Discovery

Discussion on the role of cheminformatics in drug discovery.
Case studies on using cheminformatics tools for virtual screening and lead optimization.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.
Dialogue on overcoming challenges in adopting new technologies in similar sectors.
Feedback session and closing remarks.
Certificate Issue

5:30 PM: Workshop Concludes