PSL-Qlife Quantitative Biology Winter School 2026, February 9 to 13
AI-accelerated Design and Optimisation of Compounds for Biological Applications

Monday

8:20 - 8:40 am Welcome Coffee
ENS BIO - Cafeteria

8:40 - 9:00 am
G. Gasser/I. Ciofini & P. Charnay
Introduction to the shool
ENS BIO – Room 306

9:00 - 10:30 am
Thijs Stuyver
Introduction to machine learning for molecular property prediction
ENS BIO – Room 306

10:30 – 10:45 am Coffee break – 3F Hallway

10:45 – 12:00 am
Angelo Frei
Machine-Learning Guided Exploration of the Metalloantibiotic Space
ENS BIO – Room 306

12:00 – 1:30 pm Lunch
ENS BIO - Room 305

1:30 – 2:15 pm
Student presentations (Flash talks)
ENS BIO – Room 306

2:30 - 6:00 pm
Digital workshop
Hands-on workshop: machine learning for molecular property prediction
Thijs Stuyver
Basile Parmelli
Maxime Ferrer
Room Info 3

Tuesday

8:45 - 9:00 am Morning Coffee
ENS BIO – Room 305

9:00 - 10:15 am
Sylvestre Bonnet
Computational approaches towards the design and optimization of photoactivated chemotherapy metal-based compounds
ENS BIO – Room 306

10:15 - 10:35 am Coffee break – Room 305

10:35 – 11:50 am
Sophie Bombard
Cell proliferation and cytotoxicity assays
ENS BIO – Room 306

12:00 - 1:30 pm Lunch
Chimie ParisTech - Galerie

1:30 - 5:00 pm
Digital workshop
Predicting the cytotoxicity of organometallic complexes with machine learning
Thijs Stuyver
Basile Parmelli
Maxime Ferrer
Room Info 1 MMD

5:00 – 5:30 pm Coffee break - Chimie ParisTech

5:30 – 8:00 pm
Poster session I
Wine & Cheese
Chimie ParisTech - Library

Wednesday

8:45 - 9:00 am Morning Coffee
ENS BIO – Room 305

9:00 – 10:15 am
Ilaria Ciofini
Density functional Theory for photophysical property calculation
ENS BIO – Room 306

10:15 - 10:35 am Coffee break – Room 305

10:35 – 11:50 am
Davide Avagliano
Introduction to theoretical notions about computing photophysical properties
ENS BIO – Room 306

12:00 - 1:30 pm Lunch
Chimie ParisTech - Galerie

1:30 - 5:00 pm
Digital workshop
Computational modelling of photophysical properties of organometallic complexes
Davide Avagliano
Maxime Ferrer
Room Info 1 MMD

5:00 – 5:30 pm Coffee break - Chimie ParisTech

5:30 – 6:30 pm
Marta Vallejo
Layer-CAM for Localising Protein Aggregation in Multi-Cell Biomedical Images
Chimie ParisTech - Amphi Moissan

7:30 pm
Faculty dinner
for speakers & TAs

Thursday

8:45 - 9:00 am Morning Coffee
ENS BIO – 3rd Fl. Hallway

9:00 - 10:15 am
Victor Batista
Quantum Machine Learning Methods for Molecular Design and Optimization
ENS BIO – Room 306

10:15 - 10:35 am Coffee break – 3F Hallway

10:35 – 11:50 am
Davide Avagliano
Overview of the theories used to model environmental effects…
ENS BIO – Room 306

12:00 - 1:30 pm Lunch
Chimie ParisTech - Galerie

1:30 - 5:00 pm
Digital workshop
Computational modelling of environment effect on chemical properties
Davide Avagliano
Maxime Ferrer
Room Info 1 MMD

5:00 – 5:30 pm Coffee break - Chimie ParisTech

5:30 – 8:00 pm
Poster session II & Cocktail
Chimie ParisTech - Library

Friday

8:45 - 9:00 am Morning Coffee
ENS BIO – 3rd Fl. Hallway

9:00 - 10:15 am
Sherri McFarland
Light, Metal, and Medicine: Translating a Phototherapeutic Concept
ENS BIO – Room 306

10:15 - 10:35 am Coffee break – 3F Hallway

10:35 – 11:50 am
Fernanda Duarte
Modelling chemical reactions in solution with machine learning potentials
ENS BIO – Room 306

12:00 - 1:30 pm Lunch
Chimie ParisTech - Galerie

1:30 - 5:00 pm
Digital workshop
Development of a machine learning workflow to predict photophysical properties
Davide Avagliano
Thijs Stuyver
Room Info 1 MMD

5:00 – 5:30 pm Coffee break - Chimie ParisTech

5:30 – 6:00 pm
Closing remarks
Chimie ParisTech - Amphi Moissan