ChemAICat 2026

Location: University of Liverpool
Date: 1st – 3rd September 2026

Tuesday 1st September 2026

09:00 – 09:30 | Arrival & Registration

09:30 – 09:45 | Welcome, Introductions and Information on the ChemAICat Workshop

09:45 – 11:15 | Introduction to Python – *Dr Jamie Cadge*

11:15 – 11:30 | Break

11:30 – 13:00 | Introductions to Cheminformatics – *Dr Ruben Laplaza*
Suggested Literature 1
Suggested Literature 2

13:00 – 14:00 | Lunch & Networking

14:00 – 15:30 | Practical session: Python & cheminformatics – *Dr Ruben Laplaza*

15:30 – 16:00 | Break

16:00 – 17:00 | Q&A and Custom Challenges

Wednesday 2nd September 2026

09:00 – 09:30 | Arrival & Refreshments

09:30 – 11:00 | Generation of molecular descriptors – *Dr Juan V. Alegre-Requena*
Suggested Literature 1

11:00 – 11:30 | Break

11:30 – 13:00 | Introduction to chemical AI & ML modelling – *Dr Juan V. Alegre-Requena*
Suggested Literature 1
Suggested Literature 2
Suggested Literature 3

13:00 – 14:00 | Lunch & Networking

14:00 – 15:30 | Practical session: descriptor generation & ML modelling – *Dr Jamie Cadge*

15:30 – 16:00 | Break

16:00 – 17:00 | Q&A and Custom Challenges

17:00 – Late | Social Evening at Fredericks, Hope Street

Thursday 3rd September 2026

09:00 – 09:30 | Arrival & Refreshments

09:30 – 11:00 | Chemical space exploration & catalyst sampling – *Dr Thijs Stuyver*
Suggested Literature 1
Suggested Literature 2

11:00 – 11:15 | Break

11:15 – 12:45 | AI-driven optimization of reaction conditions – *Dr Thijs Stuyver*
Suggested Literature 1
Suggested Literature 2

12:45 – 13:45 | Lunch & Networking

13:45 – 14:45 | Q&A and Custom Challenges

14:45 – 15:00 | Workshop Close