

## ChemAICat 2026

**Location:** University of Liverpool

**Date:** 1<sup>st</sup> – 3<sup>rd</sup> September 2026

---

### **Tuesday 1<sup>st</sup> 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 2<sup>nd</sup> 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

---

### Thursday 3<sup>rd</sup> 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

---