

ELLIS Summer School 2026

Trustworthy & Responsible AI in Drug Discovery (TRAID26)

24–28 August 2026 · Saarland University Campus

pharma-science-hub.com/summerschools/traid26

Time	MONDAY 24 Aug Check-in: E2 1; Sessions: E2 2	TUESDAY 25 Aug E8 1 (HIPS)	WEDNESDAY 26 Aug E8 1 (HIPS)	THURSDAY 27 Aug E8 1 (HIPS)	FRIDAY 28 Aug E2 5
9:00					
9:30					
10:00		Robust and Faithful Explanations of AI Decision-Making <i>J. Fischer (MPI Saarbrücken)</i> 9:00–10:30 E8 1, 0.27	Trustworthy and Reliable Molecular Property Prediction: Requirements, Challenges and Best Practices <i>M. Mathea (BASF SE)</i> 9:00–10:30 E8 1, 0.27	Sim-to-Real: Generalizing from Synthetic to Real-World Data <i>P. Flotho (Saarland University)</i> 9:00–10:30 E8 1, 0.27	The Dual-use Nature Of General Purpose AI Increasingly Raises Biosecurity Concerns <i>G. Jaramillo-Gutierrez (EU AI Office, European Commission; Center for AI and Digital Policy, USA)</i> 9:00–10:30 E2 5, LH1
10:30		Coffee 10:30–11:00 E8 1, 0.27	Coffee 10:30–11:00 E8 1, 0.27	Coffee 10:30–11:00 E8 1, 0.27	Coffee & Snacks 10:30–11:00 E2 5, Foyer
11:00		A (Deep) Learning Journey from Point Clouds to Proteins <i>S. Imperatore (TU Eindhoven / Grisoni Group)</i> 11:00–12:30 E8 1, 0.27	Responsible AI: Explainability ... Trustworthiness ... Safety? <i>L. Kästner (University of Bayreuth)</i> 11:00–12:30 E8 1, 0.27	Startups in Drug Discovery <i>M. Lootus (Tehistark)</i> 11:00–12:30 E8 1, 0.27	Closing Session & Poster Awards 11:00–12:30 E2 5, LH1
11:30					
12:00					
12:30	Check-in & Snacks 12:30–13:00 E2 1, Foyer	Lunch 12:30–13:30 E8 1, 0.27	Grab Your Lunch Packet & Walk 5 Min Uphill to the Uni Mensa Bus Stop 12:30–13:15 E8 1, 0.27	Lunch 12:30–13:30 E8 1, 0.27	
13:00	Welcome <i>A. Volkamer, M. Fritz & K. Scherbaum</i> 13:00–13:30 E2 2		Social Event <i>Weltkulturerbe Völklinger Hütte</i> 13:15–17:00		
13:30	Trustworthy Machine Learning in Medical Research: Concepts, Tensions, and Practice <i>K. Lenhof (UMG Göttingen / CAIMed)</i> 13:30–15:00 E2 2	Earning Confidence In AI for Drug Discovery Through Rigorous Research <i>J. Schimunek (JKU Linz / ELLIS)</i> 13:30–15:00 E8 1, 0.27	Meeting point 13:15 @Bus stop Universität Mensa Bring your Student ID For connection details see backside	Can You Trust This Prediction? A Workshop on AI in Drug Discovery <i>D. Probst (Wageningen University)</i> 13:30–15:00 E8 1, 0.27	
14:00					
14:30					
15:00	Coffee 15:00–15:30 E2 2, Foyer	Coffee 15:00–15:30 E8 1, 0.27		Coffee 15:00–15:30 E8 1, 0.27	
15:30	Uncertainty in LLMs <i>G. Varoquaux (Inria / Probabl)</i> 15:30–17:00 E2 2	Right Answer, Wrong Reason <i>O. Crook (University of Oxford)</i> 15:30–17:00 E8 1, 0.27		Establishing Hands-On Talktorials on Trustworthy AI for Drug Design <i>Volkamer Lab</i> 15:30–17:00 E8 1, 0.27	
16:00					
16:30					
17:00	Elevator Pitches 17:00–17:30 E2 2	Poster Session B & Dinner 17:00–18:00 E8 1, 0.27		Closing Dinner (BBQ) 17:00–18:00 in Front of E8 1	
17:30	Poster Session A & Dinner 17:30–18:30 E2 2				
18:00					
18:30					

Speakers

Full speaker profiles
& event website



Oliver Crook University of Oxford. Statistician and group leader at the Kavli Institute; Bayesian machine learning for computational proteomics and structural biology.

Philipp Flotho Saarland University. Computer Vision and Deep Learning researcher solving cross-domain challenges in bioinformatics and neuroscience.

Sofia Imperatore TU Eindhoven / Grisoni Group. Works at the intersection of ML, computational chemistry, and drug discovery, developing AI methods for molecular design and prediction in biomedical applications.

Kerstin Lenhof UMG Göttingen / CAIMed. Research focuses on developing novel and trustworthy ML algorithms for oncological applications.

Meelis Lootus Tehistark (Founder & CEO). Former Director of AI Engineering at Sharecare Inc., leading teams deploying AI models in production; expert on clinical-trial innovation (PhD in ML).

Miriam Mathea BASF SE. Works in chemical informatics, developing digital tools for chemists using ML. Her work connects molecules with algorithms and supports research.

Daniel Probst Wageningen University. Research interest is efficient machine learning and data visualisation applied to natural sciences, focusing on the intersection of chemistry and biology.

Johannes Schimunek JKU Linz / ELLIS. Postdoctoral Researcher in Machine Learning for Drug Discovery; few-shot learning and molecular representations. Background in mathematics and physics.

Jonas Fischer MPI Saarbrücken. Research on interpretable and robust machine learning, with a focus on faithful explanations of model decisions.

Giovanna Jaramillo-Gutierrez EU AI Office, European Commission; Center for AI and Digital Policy, USA. Works on AI governance and the biosecurity implications of general purpose AI.

Lena Kästner University of Bayreuth. Philosopher of science and technology working on explainability, trustworthiness and safety of AI systems.

Gaël Varoquaux Inria / Probabl. Research director working on statistical learning and its applications; co-creator of scikit-learn.

Address / Venues

Main venue

Universität des Saarlandes

Campus Saarbrücken
66123 Saarbrücken
Germany



Google Maps

WLAN

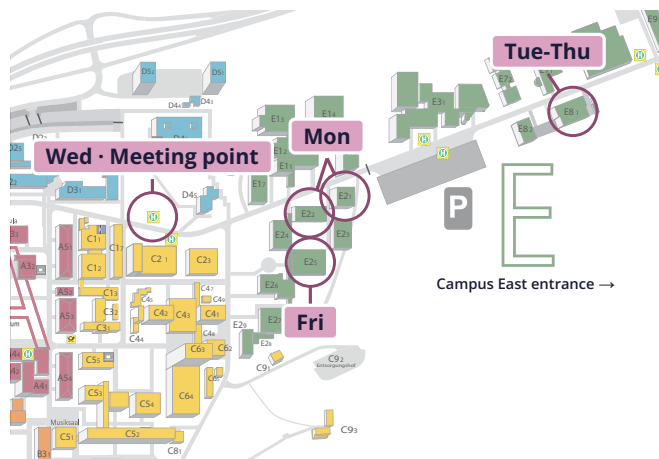
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Getting here by train & bus

<https://www.uni-saarland.de/en/sites/saarbruecken/train-bus.html>

Interactive campus map

https://www.uni-saarland.de/fileadmin/upload/footer/lageplan/saarbruecken_klickbar.pdf



Social Event · Wed 26 Aug

Meet @ bus stop Uni Mensa, 13:15 latest

Bring your student ID

Plan 5 min walk from E8 1

- @ 13:24 take bus 101 to the main train station
- @ 13:44 take train RB70 to Völklingen
- Arrival 14:13, then walk to the entrance of Völklinger Hütte

Backup connection

- @ 13:48 take bus 124 to the main train station
- @ 14:08 take train RE1 to Völklingen
- Arrival 14:26, then walk to the entrance of Völklinger Hütte

Weltkulturerbe Völklinger Hütte

Europäisches Zentrum für Kunst und Industriekultur
Rathausstraße 75–79
66333 Völklingen



Google Maps