



**UK Catalysis Hub & Physical Sciences Data-Science Infrastructure (PSDI)**  
**Joint Workshop 13<sup>st</sup> March 2026**

Meeting room 1&2, Research Complex at Harwell, Rutherford Appleton Laboratory, Harwell Campus

<b>9:30</b>	<b><u>Registration Opens &amp; Coffee</u></b>	
<b>Session 1</b>		<b>MR 1&amp;2, Research Complex at Harwell (Building R92)</b>
<b>Chair:</b>	Dr Ulrich Hintermair, Bath	Dr Ulrich Hintermair, Bath
10.00 -10.05	Welcome & Introduction	
10.05 -10.25	<b>Prof. Simon Coles</b> , UKRI STFC	Overview of PSDI
10.25 -10.45	<b>Dr. James Gebbie</b> , UKRI STFC	BioSimDR: Data tools and UK national infrastructure for biomolecular simulation.
10.45 -11:05	<b>Dr. Jas Kalayan</b> , UKRI STFC	A Case Study of Data provenance in Biomolecular Simulation
11:05-11:25	<b>Dr. Abraham Nieva de la Hidalga</b> , Cardiff	Connecting the Dots: Cataloguing, Linking, and Annotating UK Catalysis Hub Research Data: Promoting Reproducibility, Reuse, and FAIR Publishing of Data Outputs (2019–2026)
11:25-11:45	<b>Dr. Ulrich Hintermair</b> , Bath	Shifting the bottleneck - from integrated reaction monitoring to automated understanding of homogeneous catalysis
11:45-12:05	<b>Prof. Adrian Mulholland</b> , Bristol	Computational biocatalysis
<b>12:05 -12:50</b>	<b>LUNCH &amp; DISCUSSIONS FOYER (R92)</b>	
<b>Session 2</b>		<b>MR 1&amp;2, Research Complex at Harwell (Building R92)</b>
<b>Chair:</b>	Prof. Adrian Mulholland, Bristol	Why more is definitely more (at least when it comes to data): combining descriptors, HTE and mechanism in homogeneous catalysis
12:50-13:10	<b>Prof. Natalie Fey</b> , Bristol	Beyond the winners: building complete, metadata-rich enzyme kinetics datasets from high-throughput experiments
13:10-13:30	<b>Dr. Craig Markin</b> , Manchester	Data Challenges for AI-Augmented Electrocatalysis
13.30-13:50	<b>Dr. Vladislav Mints</b> , Imperial	Harwell facilities
13:50-14:10	<b>Prof. Andrew Beale</b> , UCL/Finden	Data Science/ML in Catalysis: Challenges and Opportunities
14:10-14:30	<b>Dr. Jamie Cadge</b> , Bath	Data Management for Automated Experimental Analysis: Progress and Challenges
14:30-14:50	<b>Dr. Dan Davies</b> , Imperial	
<b>14:50-15:10</b>	<b>TEA &amp; COFFEE</b>	
15.10- 16.30	Discussion	Challenges and opportunities - How to set up the service. Data standards and formats - how do we make sure this resource is used effectively (FAIR) and widely (easy) across the community? People need to think about what kind of data they have and how they can use it
		What training would be useful for community?
16:30	Close	