

## Integrated Modelling and Scattering for Biomolecules (IMSB)

Dates: Mon 18 - Wed 20 May 2026

Venue: Sheffield - [The Edge](#), 34 Endcliffe Cres, Sheffield S10 3ED,

Website: <https://www.ccpbiosim.ac.uk/scattering2026>

### Programme

#### Day 1: Monday, 18 May 2026

Time Slots	Duration	Session	Speaker	Room
11.30 - 12.00	30 min	Registrations		The Edge Bar (Ground floor)
12.00 - 13.00	60 min	<i>Lunch</i>		<i>The Edge Bar (Ground floor)</i>
13.00 - 13.10	10 min	Welcome		High Tor 2 (First floor)
13.10 - 15.10	120 min	Session 1: Introduction to Methods	Chair: Lorna Dougan	High Tor 2 (First floor)
13.10 - 13.50	40 min	Invited talk: T1.1: Dynamics of Biomolecular Systems Beyond Brownian Motion	Frank Schreiber	
13.50 - 14.30	40 min	Invited talk: T1.2:	Jonathan Essex	
14.30 - 15.00	30 min	Invited talk: T1.3:	Rob Rambo	
15.00 - 15.10	10 min	Poster flash talks (1 min/poster)	Presenters are listed in the order found at the end of this document.	
15.10 - 15.50	40 min	<i>Refreshments Break</i>		<i>The Edge Bar (Ground floor)</i>
15.50 - 17.10	80 min	Session 2: Codes, Software Platforms and Tools	Chair: Sarah Harris	High Tor 2 (First floor)
15.50 - 16.20	30 min	Invited talk: T2.1: SAXS-guided sampling of	Matteo Degiacomi	

		protein conformational ensembles		
16.20 - 16.40	20 min	Contributed Talk: T.2.2: Shapspyer – a structure generation toolchain for SAS data analysis	James Douch	
16.40 - 17.10	30 min	Invited Talk: T.2.3: Combining SANS, total neutron scattering and simulation to understand multiscale structure (for biomolecules)	Tom Headen	
17.10 - 18.30	80 min	Poster Session ♦	Chair: Lorna Dougan	High Tor 2 (First floor)

♦ List of poster's selected is available on the last page of programme.

## **Day 2: Tuesday, 19 May 2026**

Time Slots	Duration	Session	People	Room
8.45 - 9.00	15 min	<i>Arrival Refreshments</i>		<i>The Edge Bar (Ground floor)</i>
9.00 - 10.20	80 min	Session 3: Science 1: Intrinsically Disordered Proteins	Chair: Matthew Hughes	High Tor 2 (First floor)
9.00 - 9.30	30 min	Invited talk: T3.1: SAXS-Driven Ensemble Models of Highly Flexible Proteins	Pau Bernado	
9.30 - 10.00	30 min	Invited Talk T3.2: Bridging Scattering and Modelling - High-Throughput BioSAXS and Integrative Structural Workflows at ESRF BM29	Hayden Fisher	
10.00 - 10.20	20 min	Contributed Talk: T3.3: Ensemble Reweighting of the Amyloid Precursor Protein Intracellular Domain Revealed by Integrated SAXS and Molecular Dynamics	Nabanita Mandal	
10.20 - 11.00	40 min	<i>Refreshments Break</i>		<i>The Edge Bar (Ground floor)</i>

11.00 - 12.20	80 min	Session 4: Science 2: Biological Assemblies	Chair: Najet Mahmoudi	High Tor 2 (First floor)
11.00 - 11.30	30 min	Invited Talk: T4.1: New sample environment for BioSANS on D22	Anne Martel	
11.30 - 11.50	20 min	Contributed Talk: T4.2: Atomistic Dynamics to Macroscopic Function: Emergence of Enhanced Catalysis from Multiscale Force Propagation in All-Enzyme Hydrogels	Harrison Laurent	
11.50 - 12.10	20 min	Contributed talk: T4.3: Elucidating structural changes in <i>Klebsiella pneumoniae</i> during mercury biosorption via small-angle neutron scattering	Patricio Montecinos Munoz	
12.10 - 13.20	70 min	<i>Lunch</i>		<i>The Edge Bar (Ground floor)</i>
13.20 - 14.50	90 min	Session 5: Science 3: Examples of integrative methods where scattering is used alongside other methods	Chair: Hima Bindu Kolli	High Tor 2 (First floor)
13.20 - 13.50	30 min	Invited Talk: T5.1: Greater than the sum of its parts: the need for orthogonal measurement and modelling	Olwyn Byron	
13.50 - 14.20	30 min	Invited Talk: T5.2: Sampling Tyrosine kinase domains with large scale distributed MD simulations	Antonia Mey	
14.20 - 14.50	30 min	Invited Talk: T5.3: Atomistic scattering modelling in CCP-SAS provides essential mechanistic insights into human antibody structures	Steve Perkins	
14.50 - 15.30	40 min	<i>Refreshments Break</i>		<i>The Edge Bar (Ground floor)</i>
15.30 - 16.40	70 min	Session 6: Science 4: Nanomedicines and	Chair: Lorna Dougan	High Tor 2 (First floor)

		Interactions		
15.30 - 16.00	30 min	Invited Talk: T6.1: Insight into quality of pharmaceutical mRNA nanoparticles from advanced biophysical characterization	Henrich Haas	
16.00 - 16.20	20 min	Contributed Talk: T6.2: Combining molecular generation tool Shapespyer with SANS measurements of short-chained antimicrobial peptides interacting with model bacterial membranes	Anna Stephens	
16.20 - 16.40	20 min	Contributed Talk:T6.3:	Mona Sarter	
19.00 onwards		<i>Conference Dinner</i>		<i>The COSYCLUB, Sheffield</i>

### **Day 3: Wednesday, 20 May 2026**

Time Slots	Duration	Session	People	Room
9.00 - 9.30	30 min	<i>Arrival Refreshments</i>		<i>The Edge Bar (Ground floor)</i>
9.30 - 10.20	50 min	Session 7: Science 5: Liquid-liquid phase separation	Chair: Najet Mahmoudi	High Tor 2 (First floor)
9.30 - 10.00	30 min	Invited Talk: T7.1: Deciphering the molecular origin of liquid-liquid phase separation in monoclonal antibody solutions.	Vito Fodera	

10.00 - 10.20	20 min	Contributed Talk: T7.2: Reversible binding of patchy spheres: a bridge between experimental evidence and computational simulations of proteins under LLPS?	Luis Fernando de Camargo-Rodrigues	
10.20 - 10.30	10 min	Session 8: Introduction to General Discussions	Chair: Oliver Henrich	High Tor 2 (First floor)
10.30 - 11.30	60 min	Working Coffee Break		The Edge Bar (Ground floor)
11.30 - 12.15	45 min	Session 9: Future	Chair: Lorna Dougan and Oliver Henrich	High Tor 2 (First floor)
		Feedback, next steps, roadmap		
12.30 - 13.30	60 min	Packed Lunch		The Edge Bar (Ground floor)
13.30		Conference Ends		

Accepted Posters:

Presenting Author	Affiliation	Abstract title
Chin W Yong	STFC Daresbury Laboratory	D_ATA: Chemistry-based atom typing and analysis software for atomistics systems
Rayan ABO ARAB	Institut Max von Laue–Paul Langevin (ILL), France, Centre de Biologie Structurale (CBS), Université de Montpellier, INSERM and CNRS, France	Increasing Resolution in SANS Experiments by Amino Acid–Selective Protein Deuteration
Nga Man (Mandy) Cheng	University of Nottingham	Impact of formulation condition on mRNA structure and their interaction with lipids
Eli Hughes	School of Biochemistry	Full Protein Jacket - Analysing Encapsulation of Iron Oxide Nanoparticles in a Ferritin Nanocage via SAXS

	and Biomedical Sciences (BABS), University of Bristol	
Issy Sutton	University of Leeds and ISIS Neutron and Muon Source	Molecular resolution of biomolecular assembly by combining neutron scattering and coarse-grained simulation
Jeremy Cai	Durham University, Diamond Light Source	Resolving protein dynamics using SAXS and XFMS
Naoto Hori	University of Nottingham	Modelling long mRNA structures in solution
Josh Mckeown	Durham University	Carbonara: SAXS-Guided Conformational Seeding Accesses Solution-State Ensembles Inaccessible to Conventional Molecular Dynamics
Victoria Byelova	University of Leeds	Capturing dynamic conformational change in proteins during gel network formation
Dorothy Xiaoyu Wang	University of Copenhagen, Denmark and Institut Laue-Langevin, France	Combining Monte Carlo Simulations and Small Angle Scattering to Investigate Alpha-Synuclein Conformational Changes during Liquid-Liquid Phase Separation