

**3rd INTERNATIONAL CONFERENCE ON HYDROGEN DEUTERIUM EXCHANGE  
MASS SPECTROMETRY (HDXMS 2022)  
APRIL 24-26, 2022  
THE FRANCIS CRICK INSTITUTE  
LONDON, ENGLAND**



**PROGRAMME**

Sunday, 24 April 2022	
13:00-16:00	Registration
16:00-16:15	Opening Remarks
16:15-17:00	Open Plenary: <b>Perdita Barran</b> , The University of Manchester, <i>Structural Insights to Photoactive Dynamic Proteins with Hybrid MS methods</i>
17:00-18:45	<b>Technical Session 1: HDX-MS Methods</b> Chair: Miklos Guttman, University of Washington  <b>John Burke</b> , University of Victoria, <i>Combining HDX-MS with Cryo EM to study PI3K signalling complexes</i>  <b>Dario Segura-Pena</b> , University of Oslo, <i>HDX and MD simulation as tools to elucidate Aurora B kinase activation mechanisms</i>  <b>Charles Mundorff</b> , The University of Washington, <i>Monitoring structural changes on antigenic surfaces; Can HDX be performed on immobilized surfaces?</i>  <b>Malvina Papanastasiou</b> , The Broad Institute, <i>HDX in the –omics era: An unbiased, peptide-level analysis putting theory to the test,</i> <b>(Trajan Gold Speaker)</b>
18:45-19:00	Poster Flashes
19:00-20:30	Opening Catered Reception and Posters
Monday, 25 April 2022	
08:45-10:30	<b>Technical Session 2: Studies of Disease Processes</b> Chair: Chloe Martens, Université Libre de Bruxelles  <b>Elizabeth Topp</b> , Purdue University, <i>HDX-MS of fibrillating peptides</i>  <b>Benjamin Russell Lewis</b> , King's College London, <i>A switch in focus: targeting AcrA dynamics to inhibit the AcrAB-TolC multidrug efflux pump</i>  <b>Nikhil Tulsian</b> , National University of Singapore, <i>Antibody-induced allostery across Spike reveals multiple modes of SARS-CoV-2 neutralization</i>  <b>Jürgen J. Claesen</b> , Amsterdam UMC - Vrije Universiteit Amsterdam <i>Moderated test statistics for differential HDXMS</i>
10:30-11:00	Catered Morning Break

<p>11:00-12:45</p>	<p><b>Technical Session 3: Membrane Proteins</b>            Chair: Cherine Bechara, Institut de Génomique Fonctionnelle</p> <p><b>Joana Toporowska</b>, King's College London,  <i>Hydrogen Deuterium Exchange Mass Spectrometry reveals ligand-dependent conformational changes on B1-Adrenergic Receptor</i></p> <p><b>Wagas Javed</b>, King's College London,  <i>BmrA, A Bacterial ABC Multidrug Efflux Pump On The Move</i></p> <p><b>Chloe Martens</b>, Université Libre de Bruxelles,  <i>Linking function to global and local dynamics in an elevator-type transporter</i></p> <p><b>Ruyu Jia</b>, King's College London,  <i>Investigating the molecular mechanism of transport proteins using HDX-MS and MD simulations</i></p>
<p>12:45-14:00</p>	<p>Lunch Break (free time)</p>
<p>14:00-15:45</p>	<p><b>Technical Session 4: Protein Complexes 1</b>            Chair: Derek Wilson, York University</p> <p><b>Kasper Rand</b>, University of Copenhagen,  <i>Probing the conformational dynamics of the interleukin-4 and interleukin-13 receptor complexes by HDX-MS</i>  <b>(NovaBioassays Gold Speaker)</b></p> <p><b>David Balchin</b>, The Francis Crick Institute,  <i>Resolving nascent protein folding on the ribosome at peptide level</i></p> <p><b>George Chiduzo</b>, The Francis Crick Institute,  <i>Integrative structural modelling of the autophagy essential, ATG2A-9A lipid transfer-lipid scramblase complex</i></p> <p><b>Paula Booth</b>, King's College London,  <i>Capturing membrane protein folding intermediates on the ribosome</i></p>
<p>15:45-16:15</p>	<p>Catered Afternoon Break</p>
<p>16:15-18:00</p>	<p><b>Technical Session 5: Modelling</b>            Chair: Patrick Wintrode, University of Maryland, Baltimore County</p> <p><b>Lars Konermann</b>, Western University,  <i>Does HDX-MS Provide a Complete View of Protein Dynamics?</i></p> <p><b>Antoni Borysik</b>, King's College London,            HDXmodeller: An Online Webserver for High-Resolution HDX-MS</p> <p><b>Oliver Crook</b>, University of Oxford,  <i>Bayesian modelling of HDX-MS data</i></p> <p><b>Jochem Smit</b>, Katholieke Universiteit Leuven,  <i>PyHDX: Probing Universal Protein Dynamics Using Hydrogen–Deuterium Exchange Mass Spectrometry-Derived Residue-Level Gibbs Free Energy</i></p>
<p>18:00-18:15</p>	<p>Poster Flashes</p>
<p>18:15-20:30</p>	<p>Catered Reception and Posters</p>

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08:45-10:30	<p><b>Technical Session 6: Viruses and Antibodies</b> Chair: Eva Illes-Toth, LGC</p> <p><b>Edgar Hodge</b>, University of Washington, <i>Uncovering the Impact of HIV's Enormous Genetic Diversity on Fusion Protein Structural Dynamics</i></p> <p><b>Blaine Roberts</b>, Emory School of Medicine, <i>Determination of antibody epitopes against SARS-CoV2 N-protein with HDx and linear peptide footprint techniques</i> <b>(Agilent Gold Speaker)</b></p> <p><b>Clint Vorauer</b>, University of Washington, <i>Elucidating Mechanisms of Neutralization of Staph Enterotoxin B</i></p> <p><b>Haihong Zhou</b>, Merck, <i>HDX-MS of NLRP3 uncovers conformational heterogeneity and a novel mechanism of action for an inflammasome inhibitor</i></p>
10:30-11:00	Catered Morning Break
11:00-12:45	<p><b>Technical Session 7: Methods</b> Chair: Antoni Borysik, King's College London</p> <p><b>Sarah Cianferani</b>, University of Strasbourg, <i>Contributions of HDX-MS to integrative structural biology</i> <b>(Waters Gold Speaker)</b></p> <p><b>Owen Cornwell</b>, Waters, <i>Electron capture dissociation in a cyclic IMS Q-ToF provides high structural resolution in HDX-MS experiments</i></p> <p><b>Eric Largy</b>, Université de Bordeaux, <i>Biophysical characterization of G-quadruplex nucleic acids by Hydrogen-Deuterium exchange coupled to native mass spectrometry</i></p> <p><b>Elyssia Gallagher</b>, Baylor University, <i>Fundamentals and Applications of In-Electrospray HDX for Carbohydrate Analyses</i></p>
12:45-13:45	Lunch Break (free time)
13:45-14:15	<p><b>Workshop 1 - Auditorium 1</b> <i>Topic A: HDX-MS in the Alpha Fold 2 world</i> Moderated by: Benjamin Walters, Genentech &amp; Elyssia Gallagher, Baylor University</p> <p><b>Workshop 1 - Sherry Coutu Seminar Suite</b> <i>Topic B: HDX beyond the peptide unit</i> Moderated by: Antoni Borysik, King's College University &amp; Glenn Masson, University of Dundee</p> <p><b>Workshop 1 - Auditorium 2</b> <i>Topic C: HDX Data sharing</i> Moderated by: Kasper Rand, University of Copenhagen &amp; Miklos Guttman, University of Washington</p>

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14:20-14:50	<p><b><u>Workshop 2 - Auditorium 1</u></b></p> <p><i>Topic A: HDX-MS in the Alpha Fold 2 world</i> Moderated by: Benjamin Walters, Genentech &amp; Elyssia Gallagher, Baylor University</p> <p><b><u>Workshop 2 - Sherry Coutu Seminar Suite</u></b></p> <p><i>Topic B: HDX beyond the peptide unit</i> Moderated by: Antoni Borysik, King's College University &amp; Glenn Masson, University of Dundee</p> <p><b><u>Workshop 2 - Auditorium 2</u></b></p> <p><i>Topic C: HDX Data sharing</i> Moderated by: Kasper Rand, University of Copenhagen &amp; Miklos Guttman, University of Washington</p>
14:50-15:15	Catered Afternoon Break
15:15-15:45	Workshop Reports and Discussion
15:45-17:00	<p><b><u>Technical Session 8: Protein Complexes 2</u></b> Chair: John Burke, University of Victoria</p> <p><b>Julien Marcoux</b>, CNRS, Institute of Pharmacology and Structural Biology, <i>HDX-MS of mammalian proteasome subtypes reveals subtle structural rearrangements upon subunit substitution or regulator binding</i></p> <p><b>Esben Trabjerg</b>, University of Copenhagen, <i>Combining HDX-MS and XL-MS to study the binding of IgGs to the FcRn receptor</i></p> <p><b>Sheena D'Arcy</b>, The University of Texas at Dallas, <i>RNA-binding by RNA Helicase Mtr4</i></p>
17:00-17:30	International Society for HDX-MS Business Meeting and General Assembly
17:30-18:15	<p><b>Closing Plenary:</b> <b>Michael Gross</b>, Washington University, <i>HDX follows aggregation of Amyloid Beta and alpha Synuclein and Ca binding of Calprotectin</i></p>
18:15-18:20	Closing Remarks