Ligand and fragment screening: enabling technologies for pressing threats

Programme

Wednesday, 9th February 2022 - Microsymposium UDM2		
09:00 - 09:10	Introduction to the microsymposium UDM2 by **Gordon Leonard**	
Session I Chair: Max Nanao		
09:10 - 09:55	**XChem: A high throughput approach to screening**	**Ailsa Powell,** Diamond Light Source, UK
09:55 - 10:25	A fragment-based approach to develop trypanocidal drugs targeting trypanothione reductase	**Annarita Fiorillo** Sapienza University of Rome, Italy
Break		
Session II Chair: Adriana Miele		
11:00 - 11:45	**Utilisation of small-angle X-ray scattering for ligand screening and determination of affinities**	**Janosch Hennig** EMBL Heidelberg, Germany
11:45 - 12:15	Identification of fragments for the development of protein-protein-interaction inhibitors targeting the N-domain of p97	**Sebastian Bothe** University of Würzburg, Germany
Lunch Break		
Session III Chair: Didier Nurizzo		
14:00 - 14:45	**Generative AI drug discovery**	**Ho-Leung Ng** Kansas State University, USA
14:45 - 15:15	An integrative XRD/Cryo-EM approach for the identification of pre-clinical drug candidates against a parasite's drug target	**Matteo Ardini** University of L'Aquila, Italy
15:15 - 15:45	To design and generate specific protein inhibitors against Falcipain 2 from *Plasmodium falciparum*, a drug target for the malaria parasite	**Subhoja Chakraborty** Saha Institute of Nuclear Physics, India