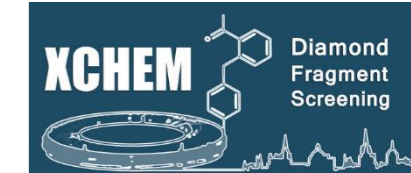


XChem Training Programme

Date: 9th -13th May



Diamond Ring Meeting Room: tbc by Stefania **RCaH:** Research Complex. Building outside zone 2 of Diamond **Lab XChem (lab34):** Diamond ring zone 5, downstairs, adjacent to I04-1

	09:00-10:00	10:00-11:00	11:00-12:00	12:00-13:00	13:00-14:00	14:00-15:00	15:00-16:00	16:00-17:00
Monday <ul style="list-style-type: none"> Introduction Imaging your plates Solvent tolerance test (DMSO): 1 hour and 3 hour soaks Unattended Data Collection <p>(50 drops with crystal minimum required)</p>	Room: Diamond House atrium <ul style="list-style-type: none"> DLS staff to start imaging 1 plate per group <p>9:30: head to Diamond Ring MR1.149 (Z10):</p> <ul style="list-style-type: none"> Welcome Housekeeping Plan for week 	Room: Diamond Ring MR1.149 (Z10) <p>XChem introduction:</p> <ul style="list-style-type: none"> XChem work flow TeXRank SoakDB Libraries <p><i>Own data:</i></p> <ul style="list-style-type: none"> Rank/assess crystal images Plan soak experiments in soakDB 	Room: Lab XChem <p>Lab induction:</p> <ul style="list-style-type: none"> Library (gate marks, spin) Echo (water level, plate carrier, source plates types - CP, GP, LDV) Shifter (troubleshooting, barcode, broken pins) Puck storage and tracking Pins cleaning Safety 	Room: Lab XChem <p>@12:00: groups 1 and 2 setup 3 hour soaks</p> <p>@12:30: groups 3 and 4 setup 3 hour soaks</p>	Room: Canteen <p>Lunch</p>	Room: Lab XChem <p>@14:00: groups 1 and 2 setup 1 hour soaks</p> <p>@14:30: groups 3 and 4 setup 1 hour soaks</p>	Room: Lab XChem <p>@15:00: groups 1 and 2 start fishing</p> <p>@15:30: groups 3 and 4 start fishing</p>	Room: i04-1 <ul style="list-style-type: none"> Load pucks and start data collection Questions/Close for day
Tuesday <ul style="list-style-type: none"> Image remaining plates Data collection review and re-collection Experiments: pre-screen with fragments (100-200 drops with crystals minimum required) <i>If necessary, repeat solvent tolerance</i> 	Room: RCaH atrium <ul style="list-style-type: none"> RCaH safety training and induction <p><i>Own data:</i></p> <ul style="list-style-type: none"> Image trays 	Room: Diamond Ring MR1.149 (Z10) <ul style="list-style-type: none"> ISPyB - data collection review Rank crystal images for remaining plates Plan pre-screen soak experiments in soakDB 	Room: Diamond Ring MR1.149 (Z10), Lab XChem and I04-1 <ul style="list-style-type: none"> Groups 1 and 2 setup soak experiments 	Room: Canteen <p>Lunch</p>	Room: Lab XChem <ul style="list-style-type: none"> Groups 3 and 4 setup soak experiments Groups 1 and 2 start mounting pre-screen 	Room: Diamond Ring MR1.149 (Z10), Lab XChem and I04-1 <ul style="list-style-type: none"> Mounting pre-screen Load pucks Questions/close for day 		
Wednesday <ul style="list-style-type: none"> Unattended data collection Intro to XCE and PanDDA Sample preparation 	Room: Diamond Ring MR1.149 (Z10) <ul style="list-style-type: none"> XChemExplorer and PanDDA intro Beamline setup and Unattended Data Collection 	Room: Diamond Ring MR1.149 (Z10) <ul style="list-style-type: none"> Unattended Data Collection Plan soak experiments in soakDB 	Room: Lab XChem <ul style="list-style-type: none"> Unattended Data Collection Groups 3 and 4 setup soak experiments 	Room: Canteen <p>Lunch</p>	Room: Lab XChem <ul style="list-style-type: none"> Groups 1 and 2 setup soak experiments Groups 3 and 4 start fishing samples 	Room: Diamond Ring MR1.149 (Z10), Lab XChem and I04-1 <ul style="list-style-type: none"> Mounting samples Prepare ground-state model 		
Thursday <ul style="list-style-type: none"> Data analysis Additional lab experiments 	Room: Diamond Ring MR1.149 (Z10) or Lab XChem and beamline I04-1 <ul style="list-style-type: none"> Finish lab experiments (if needed) Data processing in XCE Launch PanDDA jobs Data analysis (pandda.inspect, remodelling, pandda.export) 			Room: Canteen <p>Lunch</p>	Room: Diamond Ring MR1.149 (Z10) or Lab XChem and beamline I04-1 <ul style="list-style-type: none"> Finish lab experiments (if needed) Data processing in XCE Launch PanDDA jobs Data analysis (pandda.inspect, remodelling, pandda.export) 			
Friday <ul style="list-style-type: none"> Data review and annotation CompChem analysis Feedback & close 	Room: Diamond House MR G54 <ul style="list-style-type: none"> Multipins/new developments Intro to XChemReview and Fragalysis CompChem tools Automated Chemistry 	Room: Diamond House MR G54 <ul style="list-style-type: none"> Q&A Feedback 	Close					