

Day 0: Bioinformatics & Prep day (Monday, June 6, 2022)				
Chicago	London	Duration	Title	Presenter
8:00:00 AM	14:00:00	1:00:00	Introduction Software and Setup (Slack and Zoom)	All attendees
9:00:00 AM	15:00:00	1:00:00	Bioinformatics & AlphaFold	Daniel Rigden
10:00:00 AM	16:00:00	0:15:00	Break	
10:15:00 AM	16:15:00	0:30:00	Generating your models (AlphaFold and ADB)	Adam Simpkin
10:45:00 AM	16:45:00	1:00:00	Virtual computers & GMCA resources	
11:45:00 AM	17:45:00	1:00:00	Break	
12:45:00 PM	18:45:00	1:00:00	Problem solving in setup in Slack	
TODO: LIST of software to be installed on their own machines, slack help channel to troubleshoot beforehand?? linux cheatsheet				

Day 1: Introduction & Beamline (Monday, June 13, 2022)

Chicago	London	Duration	Title	Presenter
8:00:00 AM	2:00:00 PM	0:15:00	Welcome and Introduction	Robert Fischetti and Qingping Xu
8:15:00 AM	2:15:00 PM	1:00:00	Sample preparation	Elspeth Garman (BST)
9:15:00 AM	3:15:00 PM	1:00:00	Structural Biology Overview	Janet Smith (CST)
10:15:00 AM	4:15:00 PM	0:15:00	Break	
10:30:00 AM	4:30:00 PM	1:30:00	Student Presentation I	Students
12:00:00 PM	6:00:00 PM	1:00:00	Lunch break	
1:00:00 PM	7:00:00 PM	0:45:00	Student Presentation II	Students
1:45:00 PM	7:45:00 PM	0:30:00	GM/CA Overview & APS-U	Robert Fischetti
2:15:00 PM	8:15:00 PM	0:10:00	Break	
2:25:00 PM	8:25:00 PM	0:45:00	A Synchrotron Beamline & a Crystallographer's View	TBC
3:10:00 PM	9:10:00 PM	0:30:00	Data collection concept & parameters	TBC
3:40:00 PM	9:40:00 PM	0:10:00	Break	
3:50:00 PM	9:50:00 PM	0:45:00	Collecting Data with jBlulce	Nagarajan Venugopalan
4:35:00 PM	10:35:00 PM	0:40:00	Data Collection Demo, and Virtual Tour of GMCA Beamlines & QA	Nagarajan Venugopalan
5:15:00 PM	11:15:00 PM	1:00:00	Dinner break	
6:15:00 PM	12:15:00 AM	6:00:00	Students working on their own projects - unsupervised	Students (communication with tutors through SLACK channels)

Day 2: Data collection & processing (Tuesday, June 14, 2022)

Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	1:00:00	Radiation damage	Elspeth Garman (BST)
9:00:00 AM	3:00:00 PM	1:00:00	Data processing with XDS	Kay Diederichs (CET)
10:00:00 AM	4:00:00 PM	0:15:00	Break	
10:15:00 AM	4:15:00 PM	0:45:00	Good data with XDS, data quality indicators	Kay Diederichs
11:00:00 AM	5:00:00 PM	1:00:00	Data Processing with DIALS	DIALS team (BST)
12:00:00 PM	6:00:00 PM	1:00:00	Lunch break	
1:00:00 PM	7:00:00 PM	1:00:00	Data processing with HKL	Dominika Borek
2:00:00 PM	8:00:00 PM	0:15:00	Break	
2:15:00 PM	8:15:00 PM	2:45:00	Hand-on session: Working with data	Students & Kay, DIALS team, Dominika, CCP4 etc
5:00:00 PM	11:00:00 PM	1:00:00	Dinner break	
6:00:00 PM	12:00:00 AM	6:00:00	Students working on their own projects - Unsupervised	Students, communication with tutors through Slack channels
3:30:00 PM	9:30:00 PM	1:30:00	Data collection planning	Students with crystals & tutors
6:00:00 PM	12:00:00 AM	4:00:00	Prepare Samples	GM/CA staff

Day 3: Data collection & processing, overview of common GUI (Wednesday, June 15, 2022)

Chicago	London	Duration	Title	Presenter
8:00:00	14:00:00	0:30:00	Get started with CCP4 cloud	Maria Fando or Eugene Krissinel (BST)
8:30:00	14:30:00	0:30:00	Coot basics	TBC (BST)
9:00:00	15:00:00	0:30:00	Get started with Phenix GUI	Dorothee Liebschner (Pacific)
9:30:00	15:30:00	2:30:00	Data collection and real-time processing	Naga, David/Qingping, D. Borek, DIALS team, K. Diederichs
12:00:00	18:00:00	1:00:00	Lunch break	
13:00:00	19:00:00	4:00:00	Data collection and real-time processing	Naga, David/Qingping, D. Borek, DIALS team, K. Diederichs
17:00:00	23:00:00	1:00:00	Dinner Break	
18:00:00	0:00:00	6:00:00	Data collection and real-time processing	Craig, Michael and Qingping, D. Borek, DIALS team, K. Diederichs

Day 4: Symmetry, Twinning; Data processing and tutorials (Thursday, June 16, 2022)

Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	0:30:00	RABDAM -- radiation damage detection	Kathryn Shelley (BST)
8:30:00 AM	2:30:00 PM	1:00:00	Space groups, symmetry and all that	Charles Ballard (BST)
9:30:00 AM	3:30:00 PM	0:15:00	Break	
9:45:00 AM	3:45:00 PM	1:15:00	Scaling and merging the data/multi crystal	DIALS team (BST)
11:00:00 AM	5:00:00 PM	1:00:00	Twinning and other pathologies, practical aspects	Andrey Lebedev (BST)
12:00:00 PM	6:00:00 PM	1:00:00	Lunch break	
1:00:00 PM	7:00:00 PM	4:00:00	Hands-on session: Data processing	All participants
5:00:00 PM	11:00:00 PM	1:00:00	Dinner break	
6:00:00 PM	12:00:00 AM	6:00:00	Hands-on session: Data processing	All participants

Day 5: Experimental phasing; Finish data processing Molecular replacement (Friday, June 17, 2022)

Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	1:00:00	The Phase Problem	Edward Lowe (BST)
9:00:00 AM	3:00:00 PM	1:00:00	Model Preparation for MR and assessing the solution	TBC (BST)
10:00:00 AM	4:00:00 PM	0:15:00	Break	
10:15:00 AM	4:15:00 PM	0:45:00	Phaser MR	TBC (BST)
11:00:00 AM	5:00:00 PM	0:30:00	ARCIMBOLDO	Isabel Uson (CET)
11:30:00 AM	5:30:00 PM	0:45:00	MR pipelines in CCP4	Andrey Lebedev (BST)
12:15:00 PM	6:15:00 PM	1:00:00	Lunch break	
1:15:00 PM	7:15:00 PM	0:45:00	MR in Phenix	Dorothee Liebschner (Pacific)
2:00:00 PM	8:00:00 PM	3:00:00	Hands-on problem solving	All participants via slack and zoom
5:00:00 PM	11:00:00 PM	1:00:00	Dinner break	
6:00:00 PM	12:00:00 AM	6:00:00	Hands-on session	All participants

Day 6: Phasing, Density modification, Model building (Monday, June 20, 2022)

Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	1:15:00	SHELXC/D/E lecture and demo	Isabel Uson (CET)
9:15:00 AM	3:15:00 PM	0:45:00	Theory of experimental phasing and density modification	Navaraj Pannu (Pacific ??)
10:00:00 AM	4:00:00 PM	0:15:00	Break	
10:15:00 AM	4:15:00 PM	0:45:00	Phaser EP and MR-SAD	Ed Lowe (BST)
11:00:00 AM	5:00:00 PM	1:15:00	CRANK2	Navaraj Pannu (Pacific)
12:15:00 PM	6:15:00 PM	1:00:00	Lunch break	
1:15:00 PM	7:15:00 PM	1:30:00	Phasing and automation in Phenix	Dorothee Liebschner (Pacific)
2:45:00 PM	8:45:00 PM	2:30:00	Hands-on problem solving	
5:15:00 PM	11:15:00 PM	1:00:00	Dinner break	
6:15:00 PM	12:15:00 AM	6:00:00	Hands-on problem solving	All participants via slack and zoom

Day 7: Refinement and Autobuilding (Tuesday, June 21, 2022)				
Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	1:00:00	Refmac and TLS	Rob Nicholls (BST)
9:00:00 AM	3:00:00 PM	0:45:00	ModelCraft	Paul Bond (BST)
9:45:00 AM	3:45:00 PM	0:15:00	Break	
10:00:00 AM	4:00:00 PM	1:00:00	Model building: ARP/wARP and other tools	Grzegorz Chojnowski (CET)
11:00:00 AM	5:00:00 PM	1:00:00	Coot: An Introduction (Part 1)	Paul Emsley (BST)
12:00:00 PM	6:00:00 PM	1:00:00	Lunch break	
1:00:00 PM	7:00:00 PM	1:00:00	Coot: An Introduction (Part 2)	Paul Emsley (BST)
2:00:00 PM	8:00:00 PM	2:00:00	Phenix refinement and ligand building	Pavel Afonine (Pacific)
4:00:00 PM	10:00:00 PM	2:00:00	Hands-on problem solving	All participants via slack and zoom
6:00:00 PM	12:00:00 AM	1:00:00	Dinner break	
7:00:00 PM	1:00:00 AM	6:00:00	Hands-on problem solving	All participants via slack and zoom
			Buidling nucleic acids ??	

Day 8: Ligands and validation (Wednesday, June 22, 2022)

Chicago	London	Duration	Title	Presenter
8:00:00 AM	2:00:00 PM	0:45:00	Ligands and ligand dictionary	Murshudov's group (BST)
8:45:00 AM	2:45:00 PM	0:45:00	Polysaccharride modeling	Jon Agirre (BST)
9:30:00 AM	3:30:00 PM	0:30:00	ARP/wARP ligands	Grzegorz Chojnowski (CET)
10:00:00 AM	4:00:00 PM	0:15:00	Break	
10:15:00 AM	4:15:00 PM	1:15:00	Coot ligand building	Paul Emsley (BST)
11:30:00 AM	5:30:00 PM	0:45:00	Hands on problem solving	
12:15:00 PM	6:15:00 PM	1:00:00	Lunch Break	
1:15:00 PM	7:15:00 PM	2:30:00	Hands on problem solving	
3:45:00 PM	9:45:00 PM	1:30:00	Model completion and validation in Phenix	Pavel Afonine (Pacific)
5:15:00 PM	11:15:00 PM	1:00:00	Dinner Break	
6:15:00 PM	12:15:00 AM	6:00:00	Hands on problem solving	All participants

Day 9: Structure Analysis, Molecular Graphics, PDB deposition (Thursday, June 23, 2022)				
Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	1:30:00	How good is my model and can it be improved?	Robbie Joosten (CET)
9:30:00 AM	3:30:00 PM	0:15:00	Break	
9:45:00 AM	3:45:00 PM	0:20:00	CCP4 beyond structure solution	Eugene Krissinel (BST)
10:05:00 AM	4:05:00 PM	0:40:00	Analysis of macromolecular Complexes (PISA)	Eugene Krissinel
10:45:00 AM	4:45:00 PM	0:15:00	Break	
11:00:00 AM	5:00:00 PM	1:00:00	CCP4mg – Advanced options Demo and tutorial	Stuart McNicholas (BST)
12:00:00 PM	6:00:00 PM	1:00:00	Lunch break	
1:00:00 PM	7:00:00 PM	1:00:00	wwPDB OneDep tools for deposition and validation	Brian Hudson (EST)
2:00:00 PM	8:00:00 PM	3:00:00	Hands on problem solving	All participants
5:00:00 PM	11:00:00 PM	1:00:00	Dinner break	
6:00:00 PM	12:00:00 AM	6:00:00	Hands on problem solving	All participants

Day 10: CryoEM and Feedbacks (Friday, June 24, 2022)				
Chicago	London	Duration	Title	Presenter (TZ)
8:00:00 AM	2:00:00 PM	1:00:00	CryoEM overview	TBC (CET)
9:00:00 AM	3:00:00 PM	1:00:00	CCPEM & Relion	CCPem (BST)
10:00:00 AM	4:00:00 PM	0:15:00	Break	
10:15:00 AM	4:15:00 PM	0:45:00	CryoEM and Model Fitting	Grzegorz Chojnowski (CET)
11:00:00 AM	5:00:00 PM	1:00:00	An introduction to single particle cryo-EM & low resolution refinement	Murshudov's group (BST)
12:00:00 PM	6:00:00 PM	1:00:00	Lunch break	
1:00:00 PM	7:00:00 PM	1:00:00	CryoEM and Phenix	Pavel Afonine (Pacific)
2:00:00 PM	8:00:00 PM	0:05:00	Concluding remarks	Organizers
2:05:00 PM	8:05:00 PM	4:00:00	Final hands-on session and Data Backup	All students