

CCP4 Crystallographic School in South Africa

Data Collection to Structure Refinement and Beyond

University of Cape Town, South Africa
31 March 2020 – 08 April 2020

Detailed Program

Color code:

Lecture session

Questions and answers and one-on-one problem-solving

Tutorials

Meals and Coffee breaks

Other

March 31

Introductions; Basic concepts of Diffraction Crystallization and Data collection

All lectures and breaks will be in Electro Mechanical Building (EM Building), room 1.08 (lower level), Upper Campus, University of Cape Town

08:15 – 08:40	Check-in. Continued throughout the day	<i>Science Connect</i>
08:40 – 08:50	Welcome by UCT leadership?	Trevor? Management?
08:50 – 09:10	Opening notes and introduction	Organizers
09:10 – 09:30	Speaker self-introductions	All speakers
09:30 – 11:00	Overview of Projects and Problems	All participants
11:00 – 12:00	Roadmap for crystal structure determination, CCP4 cloud	E. Krissinel
12:00 – 13:30	Lunch	
13:30 – 15:00	Basic Theory of Diffraction, Crystals, symmetry	A. Leslie
15:00 – 16:30	Reciprocal space, Ewald sphere, Concepts and definitions in data collection	TBD
16:30 – 16:45	Q/A and Discussion	All participants
16:45 – 17:00	Break	
17:00 – 17:30	Students put up posters	All students
18:00 – 21:00	Opening reception and poster session	All participants

April 1

Data Collection and Processing theory; Radiation damage; MX capabilities at Diamond Light Source; Molecular Graphics

All lectures and breaks will be in Electro Mechanical Building (EM Building), room 1.08 (lower level), Upper Campus, University of Cape Town

09:00 – 11:00	A Synchrotron beamline for MX. New generation detectors	TBD
11:00 – 11:15	Q/A and discussion	All participants
11:15 – 11:30	Break	
11:30 – 12:00	Some practical tips for data collection	TBD
12:00 – 13:30	Lunch	
13:30 – 14:15	MX capabilities at Diamond Light Source	G. Evans
14:15 – 15:15	Radiation damage, Cryoprotection	E. Garman
15:15 – 15:30	Q/A and discussion	All participants
15:30 – 15:45	Break	
15:45 – 16:45	Coot	B. Lohkamp
16:45 – 18:15	General theory of data processing	A. Leslie
18:15 - 19:00	Plan data collection for April 3	<i>All with crystals and volunteer speakers</i>
19:00 – 20:00	Dinner	

April 2
Data processing

***All lectures and breaks will be in Electro Mechanical Building (EM Building),
room 1.08 (lower level), Upper Campus, University of Cape Town***

09:00 – 10:00	Data processing with iMOSFLM, Tutorial	A. Leslie
10:00 – 11:00	Data processing with DIALS, Tutorial	J. Parkhurst
11:00 – 11:15	Break	
11:15 – 12:00	Multi-crystal data collection at DLS, BLEND	J. Parkhurst
12:00 – 13:30	Lunch	
13:30 – 14:30	Data processing with XDS, tutorial	K. Diederichs
14:30 – 14:45	Q/A and Discussion	All Participants
14:45 – 15:00	Problem-solving. Process student data	All participants
15:45 – 16:00	Break	
16:00 – 19:00	Problem-solving. Process student data	All participants
19:00 – 20:00	Dinner	

April 3

Data Quality; Remote Data Collection

***All lectures and breaks will be in Electro Mechanical Building (EM Building),
room 1.08 (lower level), Upper Campus, University of Cape Town***

09:00 – 9:45	Data collection for experimental phasing	TBD
09:45 – 10:45	Data quality	K. Diederichs
10:45 – 11:00	Break	
Rest of the day	Data collection	All with crystals
12:00 – 13:30	Lunch	
16:00 – 16:15	Coffee	
19:00 – 20:00	Dinner	
20:00 –	Data collection	All with crystals

April 4

Free day

April 5

Experimental Phasing, Model Building

***All lectures and breaks will be in Electro Mechanical Building (EM Building),
room 1.08 (lower level), Upper Campus, University of Cape Town***

09:00 – 10:00	General theory of experimental phasing	P. Skubak
10:00 – 10:50	SHELX tutorial	T. Grune
10:50 – 11:00	Q/A and Discussion	All participants
11:00 – 11:15	Break	
11:15 – 12:15	Crank2 tutorial	P. Skubak
12:15 – 13:45	Lunch	
13:45 – 14:45	Model Building with ARP/wARP	TBD
14:45 – 15:00	Q/A and Discussion	All participants
15:00 – 16:00	Problem-solving	Student data
16:00 – 16:15	Break	
16:15 – 19:00	Problem-solving	Student data
19:00 – 20:00	Dinner	
20:00 – 22:00	Problem-solving	Student data

April 6

Molecular Replacement; Refinement; Model building at Lower Resolutions

All lectures and breaks will be in Electro Mechanical Building (EM Building), room 1.08 (lower level), Upper Campus, University of Cape Town

09:00 – 10:00	Molecular Replacement	R. Keegan
10:00 – 10:45	Molecular Replacement Tutorial	R. Keegan
10:45 – 11:00	Q/A and Discussion	All participants
11:00 – 11:15	Break	
11:15 – 12:00	Model Building at Lower Resolutions: ISOLDE	T. Croll
12:00 – 13:30	Lunch	
13:30 – 14:30	Refinement Theory	G. Murshudov
14:30 – 15:30	Refinement with CCP4 (REFMAC) and Tutorial	G. Murshudov
15:30 – 15:45	Q/A and Discussion	
15:45 – 16:00	Break	
16:00 – 19:00	Problem-solving	Student data
19:00 – 20:00	Dinner	
20:00 – 22:00	Problem-solving	Student data

April 7

Ligands; Model Completion and Quality

***All lectures and breaks will be in Electro Mechanical Building (EM Building),
room 1.08 (lower level), Upper Campus, University of Cape Town***

09:00 – 09:40	Ligands and ligand dictionary	G. Murshudov
09:40 – 10:20	Model Completion	R. Joosten
10:20 – 11:00	Validation, Deposition, Publication	R. Joosten
11:00 – 11:15	Break	
11:15 – 12:15	Model Quality	K. Diederichs
12:15 – 13:45	Lunch	
13:45 – 14:00	Q/A and Discussion	All participants
14:00 – 16:00	Problem-solving	Student data
16:00 – 16:15	Break	
16:15 – 19:00	Problem-solving	Student data
19:00 – 20:00	Dinner	
20:00 – 22:00	Problem-solving	Student data

April 8

Beyond X-ray Crystal structures; Feedback

All lectures and breaks will be in Electro Mechanical Building (EM Building), room 1.08 (lower level), Upper Campus, University of Cape Town

09:00 – 09:45	Analysis of macromolecular complexes (PISA)	E. Krissinel
09:45 – 10:45	Introduction to CryoEM	G. Murshudov
10:45 – 11:00	Break	
11:00 – 12:00	Introduction to Electron Diffraction	T. Gruene
12:00 – 12:15	Q/A and Discussions	As needed
12:15 – 13:45	Lunch	
13:45 – 14:00	Start Backups	All participants
14:00 – 15:00	Student feedback	All participants
15:00 – 15:15	Concluding remarks from the organizers and Speakers	Organizers and Speakers
15:45 – 16:00	Break	
16:00 – 19:00	Unaddressed questions and last minute problem-solving	As needed
19:00 – 20:00	Dinner	

Adjourned