CCP4/BGU Course on Advanced Methods for Macromolecular Structure Determination

Ben Gurion University of the Negev, Israel, 23.2-4.3.2020

PROGRAM

List of Speakers

Edward Lowe	Oxford University, Oxford, UK
Neil Paterson	Diamond Light Source, UK
Andrey Lebedev	CCP4, Harwell, UK
Kay Diederichs	University of Konstanz, Germany
David Waterman	CCP4, Harwell, UK
Mikhail Isupov	University of Exeter & Biomex Solutions, UK
Ronan Keegan	CCP4, Harwell, UK
Randy Read	University of Cambridge, UK
Kevin Cowtan	University of York, UK
Garib Murshudov	MRC-LMB, Cambridge, UK
Paul Emsley	MRC-LMB, Cambridge, UK
Eugene Krissinel	CCP4, Harwell, UK
Maya Topf	Birkbeck College, London, UK
Orly Dym	Weizmann Institute, Israel
Gabriel Frank	Ben-Gurion University, Beer Sheba, Israel
Yoel Shkolnitsky	Tel-Aviv University, Tel-Avib, Israel
Ran Zalk	Ben-Gurion University, Beer Sheba, Israel
Tom Burnley	CCP-EM, Harwell, UK
Colin Palmer	CCP-EM, Harwell, UK
David Aragao	Diamond Light Source, UK
Pavol Skubak	University of Leiden, The Netherlands

Color code

Breaks and meals	Hall
Lectures	Lecture room
Tutorials	Computer room

Sunday, 23rd February 2020

09:00 – 10:00	***Arrivals, registration and coffee***	
10:00 – 10:15	**Welcome**	Anat Shahar
10:15 – 11:30	**X-ray diffraction experiment**	Edward Lowe
11:30 – 12:30	**Remote data collection at DLS**	Neil Paterson/ David Aragao
12:30 – 13:30	***Lunch***	
13:30 – 14:15	**Data processing with XDS**	Kay Diederichs
14:15 – 15:00	**Data processing with DIALS (Groups 2-8)**	David Waterman
15:00 – 15:30	***Coffee break (times may vary)***	
Data collection sessions will run continuously, with breaks for coffee and dinner at convenient times, therefore, start/end times may change		
14:30 – 17:00	**Remote data collection at DLS (Group 1)**	Neil Paterson/ David Aragao
17:00 – 19:30	**Remote data collection at DLS (Group 2)**	Neil Paterson/ David Aragao
15:30 – 19:00	**Data processing with XDS (all available groups)**	Kay Diederichs
15:30 – 19:00	**Data processing with DIALS (all available groups)**	David Waterman
15:30 – 19:00	**Structure Solution with CCP4**	Eugene Krissinel / Andrey Lebedev / Ronan Keegan
19:00 – 20:00	***Dinner (times may vary)***	
19:30 – 22:00	**Remote data collection at DLS (Group 3)**	Neil Paterson/ David Aragao
20:00 – 22:00	**Working on data processing tutorials and own data (all available groups)**	All available tutors

Monday, 24th February 2020

Data collection sessions will run continuously, with breaks for coffee and dinner at convenient times, therefore, start/end times may change

09:00 – 11:30	**Remote data collection at DLS (Group 4)**	Neil Paterson/ David Aragao
11:30 – 14:30	**Remote data collection at DLS (Group 5)**	Neil Paterson/ David Aragao
09:00 – 10:00	**Data processing with DIALS (repeat)**	David Waterman
10:30 – 11:00	***Coffee break (times may vary)***	
10:00 – 12:30	**Data processing with XDS (all available groups)**	Kay Diederichs
10:00 – 12:30	**Data processing with DIALS (all available groups)**	David Waterman
10:00 – 12:30	**Structure Solution with CCP4**	Eugene Krissinel / Andrey Lebedev / Ronan Keegan
12:30 – 13:30	***Lunch (times may vary)***	
13:30 – 15:30	**Data processing with XDS (all available groups)**	Kay Diederichs
13:30 – 15:30	**Data processing with DIALS (all available groups)**	David Waterman
13:30 – 15:30	**Structure Solution with CCP4**	Eugene Krissinel / Andrey Lebedev / Ronan Keegan
14:30 – 17:00	**Remote data collection at DLS (Group 6)**	Neil Paterson/ David Aragao
15:00 – 15:30	***Coffee break (times may vary)***	
15:30 – 19:00	**Data processing with XDS (all available groups)**	Kay Diederichs
15:30 – 19:00	**Data processing with DIALS (all available groups)**	David Waterman
15:30 – 19:00	**Structure Solution with CCP4**	Eugene Krissinel / Andrey Lebedev / Ronan Keegan
17:00 – 19:30	**Remote data collection at DLS (Group 7)**	Neil Paterson/ David Aragao
19:00 – 20:00	***Dinner (times may vary)***	
19:30 – 22:00	**Remote data collection at DLS (Group 8)**	Neil Paterson/ David Aragao
20:00 – 22:00	**Working on data processing tutorials and own data (all available groups)**	All available tutors

Tuesday, 25th February 2020

09:00 – 09:45	**The impact of crystallization conditions, space groups and constructs on structure-based drug design**	Orly Dym
09:45 – 10:30	**Introduction to Space Groups**	Andrey Lebedev
10:30 – 11:00	***Coffee break***	
11:00 – 11:45	**Scaling and Merging**	Edward Lowe
11:45 – 12:30	**Assessing data quality**	Kay Diederichs
12:30 – 13:30	***Lunch***	
13:30 – 14:30	**Scaling and Merging**	Edward Lowe
14:30 – 16:30	**Data processing concluding (tutorial and own data)**	All students and tutors
16:30 – 17:00	***Coffee break***	
17:00 – 19:00	**Data collection and processing summary and analysis** *(students to report on their experience, difficulties and cases to highlight)*	All students and tutors
19:00 – 20:00	***Dinner***	
20:00 – 22:00	**Student projects presentation**	All students

Wednesday, 26th February 2020

08:30 – 18:00	**Trip to Masada**	
19:00 – 20:00	***Dinner***	
20:00 – 22:00	**Practical session: students projects**	All tutors

Thursday, 27th February 2020

09:00 – 09:45	**Twinning and Data Pathologies**	Andrey Lebedev
09:45 – 10:30	**Fundamentals of Molecular Replacement and Phaser-MR**	Randy Read
10:30 – 11:00	***Coffee break***	
10:30 – 11:15	**CCP4 Interface demo project**	Eugene Krissinel
11:15 – 12:30	**MR tutorial (Phaser)**	Randy Read
12:30 – 13:30	***Lunch***	
13:30 – 14:15	**MR model preparation and auto-MR**	Ronan Keegan
14:15 – 15:00	**Molecular Replacement Experiences**	Mikhail Isupov
15:00 – 15:45	**MR model preparation tutorial**	Ronan Keegan
15:45 – 16:30	**Practical session: students projects, MR approach**	All tutors
16:30 – 17:00	***Coffee break***	
17:00 – 19:00	**Practical session: students projects, MR approach**	All tutors
19:00 – 20:00	***Dinner***	
20:00 – 22:00	**Practical session: students projects continued**	All tutors

Friday, 28th February 2020

09:00 – 09:45	**Fundamentals of Experimental Phasing and Phaser-EP**	Randy Read
09:45 – 10:30	**Density Modification and Automatic Model Building**	Kevin Cowtan
10:30 – 11:00	***Coffee break***	
11:00 – 11:45	**Phaser Tutorial (EP)**	Randy Read
11:45 – 15:30	**Practical session: students projects**	All day's tutors
15:30	***Shabbath***	

Saturday, 29th February 2020

FREE DAY

Sunday, 1st March 2020

09:00 – 09:45	**Auto-EP in CCP4**	Pavol Skubak
09:45 – 10:30	**Refinement Theory and Practice**	Garib Murshudov
10:30 – 11:00	***Coffee break***	
11:00 – 11:45	**Auto-EP Tutorial**	Pavol Skubak
11:45 – 12:30	**Refmac Hands-on Tutorial**	Garib Murshudov
12:30 – 13:30	***Lunch***	
13:30 – 14:15	**AceDrg and Ligand Dictionary**	Garib Murshudov
14:15 – 15:00	**Model Building with Coot**	Paul Emsley
15:00 – 15:45	**Coot Ligand Building**	Paul Emsley
15:45 – 16:30	**AceDrg Hands-on Tutorial**	Garib Murshudov
16:30 – 17:00	***Coffee break***	
17:00 – 18:00	**Coot tutorial (Model Building)**	Paul Emsley
18:00 – 19:00	**Coot tutorial (Ligand Building)**	Paul Emsley
19:00 – 20:00	***Dinner***	
20:00 – 22:00	**Practical session: students projects & data backup**	Practical session: students projects & data backup

Monday, 2nd March 2020

08:30 – 22:00	**Election day (FREE DAY!!!)**	

Tuesday, 3rd March 2020

09:00 – 09:45	**Introduction to cryo-EM**	Tom Burnley
09:45 – 10:30	**Cryo-EM sample preparation for High Resolution**	Ran Zalk
10:30 – 11:00	***Coffee break***	
11:00 – 11:45	**Relion: EM Images to Maps**	Colin Palmer/ Tom Burnley
11:00 – 12:30	**Relion Hands-on Tutorial**	Colin Palmer / Tom Burnley
12:30 – 13:30	***Lunch***	
13:30 – 14:15	**EM vs MX maps and refinement**	Garib Murshudov
14:15 – 15:00	**Difficulties and solutions in solving Cryo-EM structures**	Yoel Shkolnitsky
15:00 – 16:30	**Relion Hands-on**	Colin Palmer / Tom Burnley
16:30 – 17:00	***Coffee break***	
17:00 – 18:15	**Relion Hands-on Tutorial**	Colin Palmer / Tom Burnley
18:15 – 19:00	**COOT: Tools for EM**	Paul Emsley
19:00 – 20:00	***Dinner***	
20:00 – 22:00	**Refmac/Coot EM Tutorial**	Garib Murshudov / Paul Emsley

Wednesday, 4th March 2020

09:00 – 09:30	**CCP-EM: Model building tools for EM**	Tom Burnley
09:30 – 10:15	**Flex-EM & TEMPy**	Maya Topf
10:15 – 10:45	***Coffee break***	
10:45 – 11:45	**Flex-EM & TEMPy**	Maya Topf
11:45 – 12:30	**Assesing the quality of EM data**	Gabriel Frank
12:30 – 13:30	***Lunch***	
13:30 – 14:15	**Efficient and cost effective image processing and data storage for cryo-EM labs**	Gabriel Frank
14:15 – 15:00	**Macromolecules, Complexes and Interactions**	Eugene Krissinel
15:00 – 16:00	**3D reconstructions of macromolecular complexes**	Ran Zalk
16:00 – 16:30	**Closing remarks**	Anat Shahar
16:30 – 17:00	***Coffee and departure***	