

CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond

Argonne National Laboratory

June 19 - 26, 2017

All Lectures will be held in the Conference Center of Advanced Protein Characterization Facility, Building 446. All meals and refreshments will be arranged in the next room from the Conference Center, except for dinner on Monday the 19th, and all meals and refreshments on Tuesday, June 20. These will be served in the conference room C010 of Building 436.

Color code:

Meal or Coffee break

Lecture session

Practical session

Tutorial session

Other

Monday, 19th June

Introduction; Data collection and processing lectures; Beamline training; data collection planning; Registration.

08:00 – 08:30	Welcome and Introduction	B. Fischetti and N. Sanishvili, <i>Building 446</i>
08:30 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:45	All about data	Z. Dauter, <i>Building 446</i>
09:45 – 10:15	Applications of microdiffraction	N. Sanishvili, <i>Building 446</i>
10:15 – 11:00	Optimizing data quality with Hybrid Photon Counting detectors	A. Förster, <i>Building 446</i>
11:00 – 12:00	Data processing with MOSFLM	A. Leslie, <i>Building 446</i>
12:00 – 12:45	Lunch	<i>Building 446</i>
12:45 – 13:45	Data processing with HKL	D. Borek, <i>Building 446</i>
13:45 – 14:45	DIALS and BLEND	R. Gildea, <i>Building 446</i>
14:45 – 15:15	Data processing with XDS	T. Gruene, <i>Building 446</i>
15:15 – 15:30	Break. Walk to the sector 23	All students with crystals. The rest are optional
15:30 – 16:00	Sector Orientation	S. Corcoran, <i>Bld. 436, Sector 23</i>
16:00 – 16:30	Beamline tour	V. Nagarajan <i>Bld. 436, Sector 23</i>
16:30 – 18:00	Hands on training on Beamline Controls and Data Collection Software	GMCA staff, <i>Beamlines 23ID-B and 23ID-D</i>
18:00 – 19:00	Data collection planning	All participants <i>Building 436, C010</i>
19:00 – 20:00	Dinner Q&A session.	All participants. <i>Building 436, C010</i>
20:00 – 21:00	Prepare Samples	GM/CA staff <i>GMCA Lab</i>

Tuesday, 20th June

Data collection and processing

Beamlines 23ID-B and 23ID-D

08:00 – 09:00	Beamline setup	GM/CA staff <i>Beamlines 23ID-D and 23ID-B</i>
08:30 - 09:00	Breakfast	<i>Building 436, conference room C010</i>
09:00 – 12:00	Data collection and real-time processing	GM/CA staff, D. Borek, R. Gildea, T. Gruene, A. Leslie
12:00 – 12:45	Working Lunch with continued data collection and processing (Q&A session)	All participants <i>Building 436, conference room C010</i>
12:45 – 16:00	Data collection and real-time processing	GM/CA staff, D. Borek, R. Gildea, T. Gruene, A. Leslie
16:00 – 16:30	Break	
16:30 – 19:00	Data collection and real-time processing	GM/CA staff, D. Borek, R. Gildea, T. Gruene, A. Leslie
19:00 – 20:00	Dinner	<i>Building 436, conference room C010</i>
20:00 – 24:00	Data collection and real-time processing	GM/CA staff, D. Borek, R. Gildea, T. Gruene, A. Leslie

Wednesday, 21st June

***Overview of student's crystallographic problems;
Twinning; Data processing and tutorials***
Building 446 Auditorium

08:30 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 10:00	Overview of crystallographic problems	All participants
10:00 – 11:00	Twinning	Z. Dauter
11:00 – 12:00	Twinning and other pathologies, practical aspects	A. Lebedev
12:00 – 12:45	Lunch	
12:45 - 13:15	Overview of crystallographic problems, continued	All participants
13:15 – 14:45	Processing with MOSFLM. Student data	A. Leslie
14:45 – 16:15	Processing with HKL. Student data	D. Borek
16:15 – 16:30	Break	
16:30 – 18:00	Processing with DIALS. Student data	R. Gildea
18:30 – 19:30	Processing with XDS. Student data	T. Guene
19:30 – 20:30	Dinner	
20:30 – 22:00	Data processing	All participants

Thursday, 22nd June

Overview of CCP4; Experimental phasing; Finish data processing

Building 446 Auditorium

08:30 - 09:00	Breakfast	<i>Building 446</i>
9:00 – 09:30	Overview of CCP4	E. Krissinel
9:30 – 10:10	Crank/Crank2	R. Pannu
10:10 – 10:50	SHELXC/D/E	T. Gruene
10:50 – 11:30	Phasing and automation in Phenix	T. Terwilliger
11:30 – 12:10	Phaser – EP	A. Lebedev
12:10 – 13:00	Lunch	
13:00 – 13:40	Parrot/Buccaneer	B. Lohkamp
13:40 – 13:55	Tutorial Crank/Crank 2	R. Pannu
13:55 – 14:10	Tutorial Pirate Buccaneer	B. Lohkamp
14:10 – 14:25	Tutorial SHELXC/D/E	T. Gruene
14:25 – 14:40	Tutorial Phenix	T. Terwilliger
14:40 – 15:05	Tutorial Phaser EP	A. Lebedev
15:05 – 15:20	Break	
15:20 – 19:00	Hands-on problem solving	All participants
19:00 – 20:00	Dinner	
20:00 – 22:00	Hands-on problem solving	All participants

Friday, 23rd June

Molecular replacement

Building 446 Auditorium

08:30 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:50	Molecular Replacement in CCP4	A. Lebedev
09:50 – 10:30	Model Preparation for MR and assessing the solution	R. Keegan
10:30 – 11:10	AMPLE, a pipeline for unconventional MR	R. Keegan
11:10 – 11:35	SHELXE for Molecular Replacement	T. Gruene
11:35 – 12:00	Structural Biology with Electron Diffraction	T. Gruene
12:00 – 12:45	Lunch	
12:45 – 13:00	Tutorial: Molecular Replacement	A. Lebedev
13:00 – 13:15	Tutorial: Phaser MR	A. Lebedev
13:15 – 13:30	Tutorial: MR in CCP4	R. Keegan
13:30 – 13:45	Tutorial: AMPLE	R. Keegan
13:45 – 14:00	Tutorial: SHELX	T. Gruene
14:00 –	Afternoon and evening: free time	

Saturday, 24th June

Refinement and Autobuilding

Building 446 Auditorium

08:30 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:45	Refmac	G. Murshudov
09:45 – 10:30	Phenix refinement and ligand building	P. Afonine
10:30 – 11:15	TLS and all that	E. Merritt
11:15 – 12:00	Automated Protein Model Building with ARP/wARP 7.4	G. Chojnowski
12:00 – 12:45	Lunch	
12:45 – 13:15	Coot: An Introduction	B. Lohkamp
13:15 – 13:45	CCP4MG: Introduction	S. McNicholas
13:45 – 14:00	Tutorial: Refmac	G. Murshudov
14:00 – 14:15	Tutorial: Phenix	P. Afonine
14:15 – 14:45	Tutorial: TLS	E. Merritt
14:45 – 15:00	Tutorial: Classic Model Building in ARP/wARP	G. Chojnowski
15:00 – 15:15	Tutorial: Coot	B. Lohkamp
15:15 – 16:15	Hands on problem solving	All participants
16:15 – 16:30	Break	
16:30 – 19:00	Hands on problem solving	All participants
19:00 – 20:00	Dinner	
20:00 – 22:00	Hands on problem solving	All participants

Sunday, 25th June

Ligands and validation

Building 446 Auditorium

08:30 - 09:00	Breakfast	<i>Building 446</i>
9:00 – 9:30	Ligands and ligand dictionary	G. Murshudov
9:30 – 10:00	Automatic Building of Ligands and Nucleotides in ARP/wARP 7.4	G. Chojnowski
10:00 – 10:40	Coot ligand building	B. Lohkamp
10:40 – 11:20	Validation in Phenix	P. Afonine
11:20 – 12:00	How good is my model and can it be improved?	R. Joosten
12:00 – 12:45	Lunch	
12:45 – 13:30	wwPDB OneDep tools for deposition and validation	B. Hudson
13:30 – 13:45	Tutorials: Ligands and ligand dictionary	G. Murshudov
13:45 – 14:00	Tutorials: Automatic Building of Ligands and Nucleotides in ARP/wARP	G. Chojnowski
14:00 – 14:15	Tutorial: Coot ligand building	B. Lohkamp
14:15 – 14:30	Tutorial: PDB-REDO and validation	R. Joosten
14:30 – 16:00	Hands on problem solving	All participants
16:00 – 16:30	Break	
16:30 – 19:00	Hands on problem solving	All participants
19:00 – 20:00	Dinner	
20:00 – 22:00	Hands on problem solving	All participants

Monday, 26th June

Structure Analysis, Molecular Graphics and Feedback

Building 446 Auditorium

08:30 - 09:00	Breakfast	<i>Building 446</i>
09:00 – 09:20	CCP4 beyond structure solution	E. Krissinel
09:20 – 10:00	Analysis of macromolecular Complexes (PISA)	E. Krissinel
10:00 – 10:45	CCP4mg – Advanced options Demo and tutorial	S. McNicholas
10:45 – 11:30	An introduction to single particle cryo-EM	G. Murshudov
11:30 – 12:00	Start backups	All participants
12:00 – 12:45	Lunch	
12:45 – 16:00	Hands on problem solving	All participants
16:00 – 16:15	Break	
16:15 – 17:30	Hands on problem solving	All participants
17:30 – 19:30	Overview of crystallographic problems and backups	All participants
19:30 – 19:40	Concluding remarks	Organizers
19:40 – 20:40	Dinner	

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