

KEMM25: Structural Biology and Bioinformatics HT2020

Date	Time	Place	What Activity	Teachers	Exam
week 45			Structural bioinformatics		
Mon	2 November	9.30-10.15	L	Upprop, welcome & short overview of course content	DL
		13.15-15.00	L	Integrated structural biology: an introduction	DL x
Tue	3 November	10.15-12.00	L	The thermodynamic driving forces for protein folding	IA x
Wed	4 November	10.15-12.00	L	Overview of protein structure, sequence-structure relationships	SA
		13.15-15.00	E	Graphics, structural databases (PDB, PDBsum, etc.)	SA
Thu	5 November	10.15-12.00	L	Fold classification, domains and databases (CATH, SCOP)	SA
		13.15-16.00	E	Fold classification: CATH	SA
Fri	6 November	10.15-12.00	L	Sequence analysis and database scanning	SA
week 46			Structural bioinformatics		
Mon	9 November	10.15-12.00	E	Sequence alignment and analysis tools	SA
Tue	10 November	10.15-12.00	E	Chimera: getting started + surface properties/B-factor colouring	SA+CA
		13.15-16.00	E	Chimera: analysis/comparison; attributes	CA
Wed	11 November	10.15-12.00	L	Structure prediction, homology modelling and model quality	SA
Thu	12 November	10.15-12.00	E	Introduction to PyMOL	CA
		13.15-16.00		Chimera: Sequence/structure; similar sites	CA
Fri	13 November	10.15-12.00	E	SwissModel server; Independent project (HMP)	SA+CA
			E		
week 47			Structural bioinformatics		
Mon	16 November	10.15-12:00	E	HM: Modelling with Chimera and Modeller	SA+CA
Tue	17 November		E	Working independently on HMP	
Wed	18 November	10.15-11:00	E	Q&A Continue HMP	SA
Thu	19 November	10.15-12:00	E	Q&A, HMP - prepare presentations	SA
Fri	20 November	10.15-13:00		HMP - Presentations	SA,DL,CA
week 48			Macromolecular crystallography		
Mon	23 November	10.15-12.00	L	Crystallography Ia: Protein crystallisation	ZF x
		13.15-15.00	L	Crystallogr. Ib: Membrane proteins: structure and crystallisation	STH x
Tue	24 November	10.15-12.00	L	Crystallography II: Crystals and symmetry	DL x
Wed	25 November	10.15-12.00	L	Crystallography III: Waves, Fourier transforms and diffraction	DL x
Thu	26 November	10.15-12.00	E	Crystallography IV: X-ray data collection	DL x
		13.15-16.00	E	Exercise II: Crystal packing analysis	CA
Fri	27 November	9.15-12.00	E	Data collection tutorial at BioMAX beamline (Zoom)	AG+DL
week 49					
Mon	30 November	10.15-12.00	E	Crystallography V: The phase problem: experimental phasing	DL x
		13.15-15.00	E	Workshop: Help with installing crystallography software	DL x
Tue	1 December	10.15-12.00	L	Crystallography VI: The phase problem: molecular replacement	DL x
		13.15-16.00	E	Exercise III: Bragg's law and the Fourier transform	DL+CA
Wed	2 December	9.00-12.00	E	Exercise I: Crystallisation (groups 1 + 2)	CA
		13.00-16.00	E	Exercise I: Crystallisation (groups 3 + 4)	CA
Thu	3 December	9.00-12.00	E	Exercise I: Crystallisation (groups 5 + 6; if necessary)	CA
		13.00-15.00	E	Demo video of robotic crystallisation + Q&A	MG/CS
Fri	4 December	10.15-12.00	E	Exercise IIIb: Coot and the Electron Density Server (EDS)	CA
		13.15-16.00	E	Exercise IV: Diffraction data processing	DL+CA

week 50							
Mon	7 December	10.15-12.00	E	Exercise IIIb: Coot and the Electron Density Server (EDS)	CA		
		13.15-16.00	E	Exercise V: Phase problem	DL+CA		
Tue	8 December	10.30-12.00	E	Exercise VI: Molecular replacement	DL+CA		
		13.15-16.00	E	Exercise VI: Molecular replacement	DL+CA		
Wed	9 December	10.15-12.00	L	Crystallography VII: Electron density and model building	DL	x	
			E	Inspection of crystals from Exercise I (groups 1-3)	CA		
Thu	10 December	10.15-12.00	L	Crystallography VIII: Refinement and validation	DL	x	
		13.15-16.00	E	Inspection of crystals from Exercise I (groups 4-6)	CA		
Fri	11 December	10.15-12.00	E	Exercise VII: Model building	CA		
		13.15-16.00	E	Exercise VII: Model building	CA		
week 51		Structural biology in drug design / other methods 1					
Mon	14 December	10.15-12.00	L	Basics of structure-based drug design	SA	x	
		13.15-15.00	E	From hit to lead structure	ML		
Tue	15 December	9.15-12.00	L	E: COX1 - COX2 ligand specificity; L: docking & scoring	SA	x	
		13.15-16.00	E	Docking	SA		
Wed	16 December	10.15-12.00	L	Small-angle X-ray scattering (SAXS)	OB	x	
		13.15-16.00	E	SAXS data processing tutorial	OB	x	
Thu	17 December	10.15-12.00	L	Applications of NMR in structural biology	KM		
Fri	18 December	10.15-12.00	L	Neutron scattering and neutron diffraction	EO	x	
week 52							
Mon	21 December	10.15-12.00		RESERVE DAY			
week 2		Other methods 2					
Thu	7 January	10.15-12.00		Cryo-electron microscopy 1	DL	x	
Fri	8 January	10.15-12.00		Cryo-electron microscopy 2	DL	x	
week 3							
Mon	11 January	10.15-12.00	CR	Questions and discussion, course evaluation			
				Hand in final lab report			
Tue	12 January			FREE FOR STUDY			
Wed	13 January			FREE FOR STUDY			
Thu	14 January			FREE FOR STUDY			
Fri	15 January	8.00-13.00		Final written examination on weeks on material marked with "x"			

L = lecture; E = exercise

Elements marked with an "x" are included in the final written examination

Teachers

IA – Ingemar André

SA – Salam Al-Karadaghi

OB – Oskar Berntsson (MAX IV)

ZF – Zoë Fisher (ESS)

AG – Ana Gonzalez (MAX IV)

MG – Maria Gourdon (Lund Protein Production Facility)

DL – Derek Logan

KM – Kristofer Modig (Biophysical Chemistry)

EO – Esko Oksanen (ESS)

CS – Céleste Sele (Lund Protein Production Facility)

STH – Susanna Törnroth Horsefield

ML - Marco Lolli (University of Turin)

from Biochemistry and Structural Biology unless otherwise noted

CR = Bioinformatics computer room, floor -1

CA - Course assistants (Ipsita Banerjee, Niels Meijer)