

KEMM15: Structural Biology and Bioinformatics HT2018

	Date	Time	Place	What	Activity	Teachers	Exam
week 1							
Structural bioinformatics							
Mon	5 November	9.30-10.15	B, (CR)	L	Upprop, short overview of course content;	DL	
		10.15-12.00	F	L	Integrated structural biology: an introduction	SA	
Tue	6 November	10.15-12.00	M	L	Overview of protein structure, sequence-structure relationships	SA	
		13.15-16.00	CR	E	Graphics, structural databases (PDB, PDBsum, etc.)	SA+CA	
Wed	7 November	10.00-12.00	F	L	Fold classification, domains and databases (CATH, SCOP)	SA	
		13.15-15.00	F	L	The thermodynamic driving forces for protein folding	IA	x
Thu	8 November	10.15-12.00	F	L	Molecular modelling of proteins	IA	x
		13.15-15.00	A	L	Crystallography I: Protein crystallisation	STH	x
Fri	9 November	10.15-12.00	CR	E	Interactive protein folding using FoldIt	IA / CA	
week 2							
Structural bioinformatics							
Mon	12 November	10.15-12.00					
		13.15-16.00	Bio-lab 2	E	Exercise I: Crystallisation	CA	
Tue	13 November	10.15-12.00	B	L	Crystallogr. Ib: Membrane proteins: structure and crystallisation	STH	x
		13.15-15.00	CR	E	Fold classification, domains, describing a structure	SA+CA	
Wed	14 November	10.15-12.00	F	L	Sequence analysis and database scanning	SA	
		13.15-16.00	CR	E	Sequence alignment and analysis tools (1 & 2, PS)	SA+CA	
Thu	15 November	10.15-12.00	CR	E	Chimera: getting started + surface properties/B-factor coloring	SA+CA	
		13.15-16.00	CR	E	Chimera: Analysis/comparison; attributes	CA	
Fri	16 November	10.15-12.00	F	L	Structure prediction, homology modelling and model quality	SA	
		13.15-16.00	CR	E	Homology modelling with SwissModel server	SA+CA	
week 3							
Structural bioinformatics							
Mon	19 November	10.15-12.00	CR	E	Chimera: Sequence/structure; similar sites	CA	
Tue	20 November	13.15-16.00	CR	E	Introduction to PyMOL	CA	
Wed	21 November	9.15-12.00	CR	E	HM: Modelling with Chimera and Modeller Independent project (HMP) and training paper continuation (if necessary)	SA+CA	
Thu	22 November	all day		E	Working independently on HMP		
Fri	23 November	10.00-16.00	CR	E	Projects discussion, continue HMP	SA	
week 4							
Structural bioinformatics / drug design							
Mon	26 November	10.15-12.00	CR	E	HMP - prepare presentations	SA	
Tue	27 November	10.15-12.00	B	E	Presentations	SA+CA	
		13.15-16.00	Biochem	E	Inspection of crystals from crystallisation practical	CA	
Wed	28 November	10.15-16.00			Pre-test: training paper	SA	
Thu	29 November	9.15-15.00	CR		Practical test	CA	
Fri	30 November	10.15-12.00	B	L	Basics of structure-based drug design	SA	x
		13.15-15.00	CR	E	COX1 - COX2 ligand specificity	SA/CA	
week 5							
Drug design & macromolecular crystallography							
Mon	3 December	10.15-12.00	M	L	Docking & scoring	SA	x
		13.15-15.00	CR	E	Introduction to AutoDock Vina	SA	
Tue	4 December	10.15-16.00	CR	E	Using AutoDock Vina & library screening	SA	x
Wed	5 December	10.15-12.00	F	L	Crystallography II: Crystals and symmetry	DL	x
Thu	6 December	10.15-12.00	F	L	Crystallography III: Waves, Fourier transforms and diffraction	DL	x
Fri	7 December	10.15-12.00	F	L	Crystallography IV: X-ray data collection	MT	x
		13.15-16.00	CR	E	Exercise II: Crystal packing analysis using PyMOL	CA	

week 6				Macromolecular crystallography			
Mon	10 December	10.15-12.00	L	L	Crystallography V: The phase problem: experimental phasing	DL	x
		13.15-16.00	CR	E	Exercise III: Bragg's law and Fourier transform	DL+CA	
Tue	11 December	9.15-12.00	LP3	E	Robotic crystallisation demo (G1)	MG	
		13.15-16.00	LP3	E	Robotic crystallisation demo (G2)	MG	
Wed	12 December	10.15-12.00	B	L	Crystallography VI: The phase problem: molecular replacement	DL	x
		14.00-15.30	MAX IV	L	Tour of MAX IV	AL	x
Thu	13 December	10.15-11.30	CR		KEMM15 lecturers present their research (~15 min each)		
		13.15-16.00	CR	E	Exercise IV: Diffraction data processing	DL+CA	x
Fri	14 December	10.15-12.00	CR	E	Exercise IIIb: Coot and the Electron Density Server (EDS)	CA	
		13.15-16.00	CR	E	Exercise V: Phase problem	DL+CA	
week 7				Macromolecular crystallography			
Mon	17 December	9.00-12.00	MAX IV		Data collection tutorial at BioMAX beamline	DL	
		13.00-16.00	MAX IV		Data collection tutorial at BioMAX beamline	DL	
Tue	18 December	9.15-12.00	CR	E	Exercise VI: Molecular replacement	DL+CA	
		13.15-16.00	CR	E	Exercise VI: Molecular replacement	DL+CA	
Wed	19 December	10.15-12.00	L	L	Crystallography VII: Electron density and model building	DL	x
Thu	20 December	8.15-10.00	F	L	Crystallography VIII: Refinement and validation	DL	x
Fri	21 December						
week 8				Macromolecular crystallography; other methods			
Mon	7 January						
Tue	8 January	10.15-12.00	CR	E	Exercise VII: Model building	CA	
		13.15-16.00	CR	E	Exercise VII: Model building	CA	
Wed	9 January	10.15-12.00	F	L	Small-angle X-ray scattering	DL	x
Thu	10 January	10.15-12.00	B	L	Applications of NMR in structural biology	KM	
Fri	11 January	10.15-12.00	F	L	Neutron scattering and neutron diffraction	EO	x
week 9				Final discussions, study and exam			
Mon	14 January	10.15-12.00	CR		Questions and discussion, course evaluation Hand in final lab report		
Tue	15 January						
Wed	16 January						
Thu	17 January						
Fri	18 January	8.00-13.00	Sparta A-C		Final written examination on weeks 1, 5-8 and crystallisation		

L = lecture; E = exercise

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

Teachers

IA – Ingemar André

SA – Salam Al-Karadaghi

AL – Ana Labrador (MAX IV Laboratory)

DL – Derek Logan

KM – Kristofer Modig (Biophysical Chemistry)

EO – Esko Oksanen (European Spallation Source)

MT – Marjolein Thunnissen (MAX IV Laboratory)

STH – Susanna Törnroth Horsefield

MG – Maria Gourdon (Lund Protein Production Facility)

CA - Course assistants (Rohit Kumar & Ipsita Banerjee)

from Biochemistry and Structural Biology unless otherwise noted

CR = Bioinformatics computer room, floor -1

Biochem = crystallisation room at Biochemistry