

	Friday Jun 2	Saturday Jun 3 General Techniques	Sunday Jun 4 Biophysics and binding	Monday Jun 5 Informatics	Tuesday Jun 6 Small molecule chemistry	Wednesday Jun 7	Thursday Jun 8 Biologics	Friday Jun 9 Case Studies	Saturday Jun 10		
9		Introduction (Directors & IT) (20') FEBS MIC (25')	Measuring binding affinities (F. von Delft)	Machine learning in drug discovery (C. Deane)	General MedChem (M. Congreve)	Case study 1 (G. McGaughey)	Intro to Biologics (C. Deane)	Viral evolution and drug resistance (E. Arnold)			
9:45		Historical Perspective (T. Blundell)	Protein Conformational Landscapes (M. Fischer)	Target selection drug discovery (A. von Delft)	Compound design (A. Bradley)	Accelerating drug discovery (A. Kotecha)	Rational design (S.J. Fleishman)	Case study 3 (S. Jacob)			
10:30		<i>Coffee</i>	<i>Coffee</i>	<i>Coffee</i>	<i>Coffee</i>		<i>Coffee</i>	<i>Coffee</i>			
11:00		Introduction to crystallography (C. Lesburg)	Rationalising biomolecular interactions (R. Wade)	Data integration & pharmacology (A. Bradley)	In Silico SB optimization for accelerated drug discovery (E. Davis)	Talks from abstracts	Biologics Developability (R. Buick)	Talks from abstracts			
11:45		CryoEM in drug discovery (G. Scapin)	Allostery & Dynamics (experimental) (J. Fraser)	Docking, Free energy calculation and Molecular Dynamics (S. Riniker)	CSP (AY Sheikh)		Small-molecule chimeras (J. Williams)				
12:30		Lunch	Lunch with poster preview	Lunch	Lunch & Power hour	Excursion	Lunch with poster preview	Lunch			
2:30		High-throughput and automation (F. von Delft)	WS	WS	WS		Excursion	WS	Case study 4 (J. Petersen)		
3:15		AlphaFold (C. Outeiral Rubiera)							Project Moonshot A. VonDelft		
4:00		<i>Coffee</i>	<i>coffee</i>	<i>Coffee</i>	<i>coffee</i>			<i>coffee</i>	<i>coffee</i>		
4:30		WS Intro	WS	WS	WS			Excursion	WS	Where will SB be in 10 years? (S. Jacob) + group discussion	
5:15		Ice Breaker								Closing Remarks	
6:00		Intro to Erice	Poster Session Odd Numbers						Poster Session Even Numbers		
8:00		Welcome buffet	Dinner at posters						Dinner at posters	Farewell dinner	

ARRIVALS
(Dinner provided)

DEPARTURES

Workshop schedule (proposed) based on three rooms

Sunday – 4 June		Monday – 5 June		Tuesday – 6 June		Thursday – 8 June	
2:30-4:00	4:30-6:00	2:30-4:00	4:30-6:00	2:30-4:00	4:30-6:00	2:30-4:00	4:30-6:00
Ligand crystallography /Hands on compound building <i>C. Lesburg</i>	Ligand crystallography /Hands on compound building <i>C. Lesburg</i>	General Machine Learning <i>Fergus Boyles</i>	General Machine Learning <i>Fergus Boyles</i>	Biologics design – Rosetta <i>Sarel Fleishman</i>		CryoEM <i>M. Herzik</i>	
General Machine Learning <i>Fergus Boyles</i>	General Machine Learning <i>Fergus Boyles</i>	Virtual Screening at Giga Scale <i>Steve Muchmore (OpenEye)</i>	Virtual Screening at Giga Scale <i>Steve Muchmore (OpenEye)</i>	In silico SB optimization for Accelerated Drug Discovery <i>Schroedinger</i>		In silico SB optimization for Accelerated Drug Discovery <i>Schroedinger</i>	
CryoEM <i>M. Herzik</i>	CryoEM <i>M. Herzik</i>	CCDC	CCDC	SmartEPU and G2 <i>A. Kotecha (TFS)</i>	SmartEPU and G2 <i>A. Kotecha (TFS)</i>	Biologics design – SabDab <i>Charlotte Deane</i>	Biologics design – SabDab <i>Charlotte Deane</i>