

	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	
8:30		Introduction (Directors & IT) (15') FEBS MIC (15')								
9	ARRIVALS <i>(Dinner provided)</i>	Historical Perspective (T. Blundell)	Measuring binding affinities (F. von Delft)	Machine learning in drug discovery (C. Deane)	General MedChem (M. Congreve)	Case study 1 (G. Verkhivker)	Intro to Biologics (C. Deane)	Structure-based drug discovery targeting HIV reverse transcriptase (E. Arnold)	DEPARTURES	
9:45		Introduction to crystallography (C. Lesburg)	Protein Conformational Landscapes (M. Fischer)	Target selection drug discovery TBD	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		CryoEM in drug discovery (G. Scapin)	Computing Drug Binding Kinetics (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		High-throughput and automation (F. von Delft)	Allostery & Dynamics (experimental) (J. Fraser)	Docking, Free energy calculation and Molecular Dynamics (S. Riniker)	CSP (AY Sheikh)		Atoms up protein engineering (J. Williams)			
12:30		<i>Lunch</i>	<i>Lunch with poster preview</i>	<i>Lunch</i>	<i>J. William How to start a company</i>	Excursion	<i>Lunch with poster preview</i>	<i>Lunch</i>		
2:30		Project Moonshot A. VonDelft	WS	WS	WS		WS	WS		Case study 4 (J. Petersen)
3:15		Machine learning and protein structure prediction: present and future (C. Outeiral Rubiera)								Cu' havi 'na bona vigna, havi pani, vinu e ligna" – Startups (J. Williams)
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		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

Workshop schedule

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>		Hands-on single-particle cryoEM data analysis with cryoEDU <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>	
Hands-on single-particle cryoEM data analysis with cryoEDU <i>M. Herzik</i>	Hands-on single-particle cryoEM data analysis with cryoEDU <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>