	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
8:45		Introduction (Directors & IT)							
9	ARRIVALS *(Dinner provided)*	Historical Perspective **(T. Blundell)**	Measuring binding affinities **(F. von Delft)**	Machine learning in drug discovery **(C. Deane)**	General MedChem **(M. Congreve)**	Conformational landscaping of the SARS-COV-2 spike protein **(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**)	Data integration & pharmacology **(A. Bradley)**	Compound design **(A. Bradley)**	Accelerating drug discovery (**A. Kotecha**)	Rational design **(S.J. Fleishman)**	Case study 3 **(S. Jacob)**	
10:30		*Coffee*	*Coffee*	*Coffee*	*Coffee*		*Coffee*	*Coffee*	
11:00		CryoEM in drug discovery **(G. Scapin)**	Computing Drug Binding Kinetics **(R. Wade)**	Docking, Free energy calculation and Molecular Dynamics **(S. Riniker)**	In Silico SB optimization for accelerated drug discovery (**E. Davis**)	Talks from abstracts: G.A. Bezerra (4) J.C. Aschenbrenner (5) D. Vattovaz (58) C. Catalano (10) A. Chopra (12)	Biologics Developability **(R. Buick)**	Talks from abstracts: E. S. Cunha (13) M. Ruszkowski (45) S.S.R. Burman (44) Z. Kozicka (27) V. Yadrykhins'ky (62)	
11:45		High-throughput and automation **(F. von Delft)**	Targeted Allosteric Modulators **(G. Verkhivker)**	B. Vertessy (FEBS) Intro to FEBS	3D structures, interactions, and implications (**AY Sheikh**)		Atoms up protein engineering **(J. Williams)**		
12:30		*Lunch*	*Lunch with poster preview*	*Lunch*		Excursion	*Lunch with poster preview*	*Lunch*	
2:30		Project Moonshot **A. VonDelft**	WS	WS	WS		WS	Fragment-based design of MAT2 inhibitors **(M. Schimpl)**	
3:15		Machine learning and protein structure prediction: (**C. Outeiral Rubiera)**						Cu' havi 'na bona vigna, havi pani, vinu e ligna" – Startups **(J. Williams)**	
4:00		*Coffee*	*coffee*	*Coffee*	*coffee*		*coffee*	*coffee*	
4:30		WS Intro	WS	WS	WS		WS	Where will SB be in 10 years? (**S. Jacob**) + group discussion	
5:15		Ice Breaker						Ice breaker presentations	
6:00		Intro to Erice	Poster Session Odd Numbers				Poster Session Even Numbers	Closing remarks	
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 *C. Lesburg*	**Ligand crystallography /Hands on compound building** *C. Lesburg*	**General Machine Learning** *F. Boyles and C. O. Rubiera*	**General Machine Learning** *F. Boyles and C. O. Rubiera*	**Biologics design – Rosetta** *S. Fleishman*		**Hands-on single-particle cryoEM data analysis with cryoEDU** *M. Herzik*	
General Machine Learning *F. Boyles and C. O. Rubiera*	**General Machine Learning** *F. Boyles and C. O. Rubiera*	**Virtual Screening at Giga Scale** *S. Muchmore and M. Krier (OpenEye)*	**Virtual Screening at Giga Scale** *S. Muchmore and M. Krier (OpenEye)*	**In silico SB optimization for Accelerated Drug Discovery** *E. Abualrous and Z. Si Chaib (Schroedinger)*		**In silico SB optimization for Accelerated Drug Discovery** *E. Abualrous and Z. Si Chaib (Schroedinger)*	
Hands-on single-particle cryoEM data analysis with cryoEDU *M. Herzik*	**Hands-on single-particle cryoEM data analysis with cryoEDU** *M. Herzik*	**Drug Design using CSD-Discovery** *R. Chikhale and F. Montisci* (CCDC)	**Drug Design using CSD-Discovery** *R. Chikhale and F. Montisci Montisci* (CCDC)	**SmartEPU and G2** *A. Kotecha and A. Koh(TFS)*	**SmartEPU and G2** *A. Kotecha and A. Koh (TFS)*	**Biologics design – SabDab** *F. Boyles and C. O. Rubiera*	**Biologics design – SabDab** *F. Boyles and C. O. Rubiera*