May 31			hall
Saturday			
8.45-9.00	**Welcome**	**School directors & organizers**	SD
Session 01M	**Complex systems and Drug Design**		SD
9.00-9.45	Engineering GPCRs for use in Drug Design	M. Congreve	
9.45-10.30	Structural insights into activation and allosteric modulation of G protein coupled receptors	A. Kruse	SD
10.30-11.00	**coffee break**		SD & SR
11.00-11.45	*Membrane Protein Structures*	R. Stroud	SD
11.45-12.30	Epigenetics – the promise, the challenges, the use of target-based approaches	C.-w. Chung	SD
12.30-14.30	**Lunch**		
Session 01A			SD
14.30-15.15	Crystallography and Biopharmaceuticals	R. Pauptit	SD
15.15-16.00	**Workshop introduction**	C. Groom / I. Giangreco / Irwin / Tramontano / Lamzin / Prlic / Smart	SD
16.00-16.30	**coffee break**		SD&SR
Session 01C	**Workshops**		
16.30-18.00	Using the Cambridge Structural Database System in Drug Discovery	C. Groom / I. Giangreco	TBD
16.30-18.00	Computational Ligand Discovery	J.Irwin	TBD
16.30-18.00	How do we know how good a protein structural model is	A. Tramontano	TBD
18.00-18.30	An introduction to Erice	M. Schmidt	SD
20.00-	**Welcome buffet**		SF

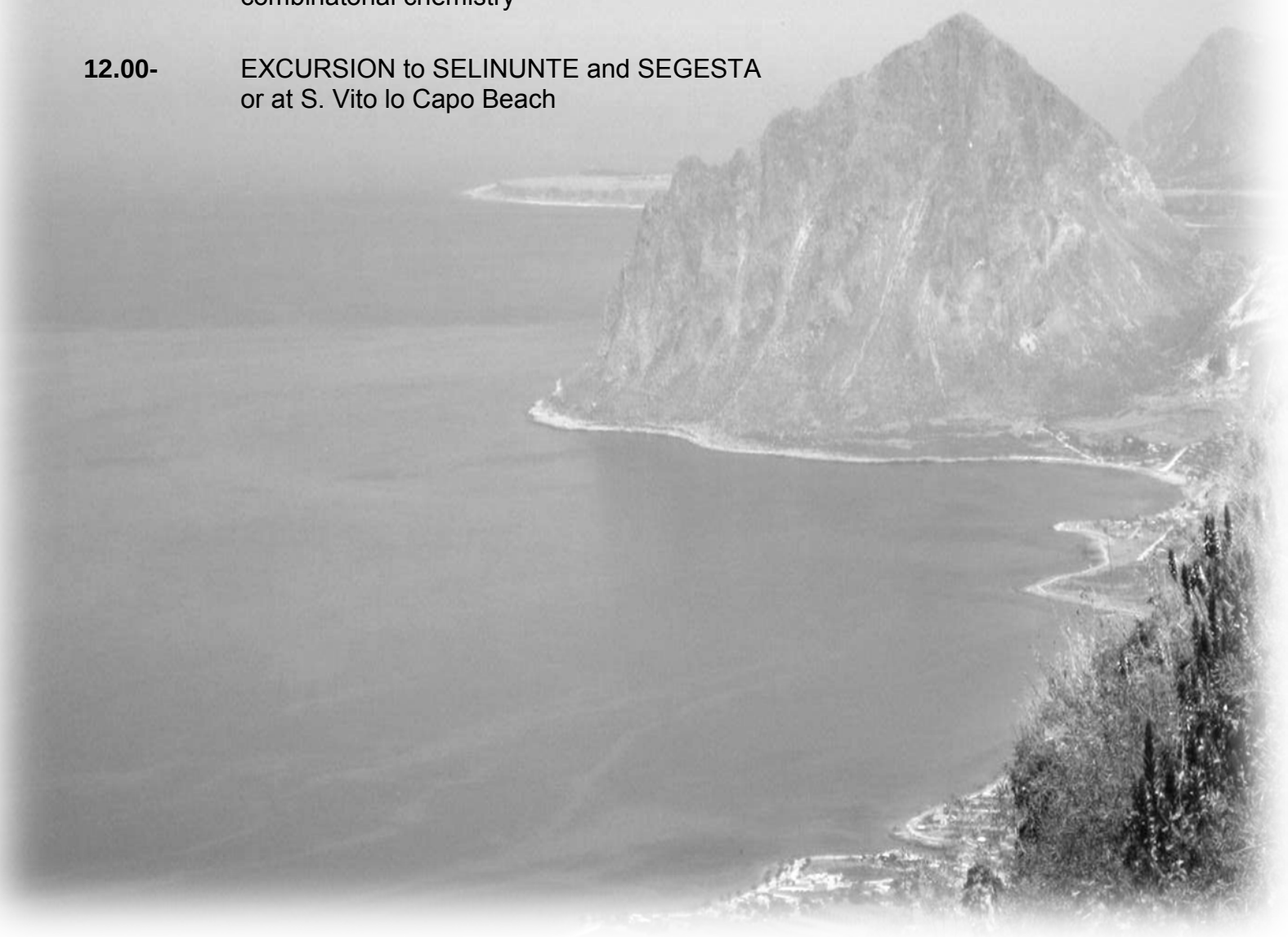
June 01			hall
Sunday			
Session 02M	**From hits to Drugs**		SD
9.00-9.45	Applying Molecular Modeling to Structure-Based Drug Design (SBDD)	J. Blaney	SD
9.45-10.30	*Structural bioinformatics*	A.Tramontano	SD
10.30-11.00	**coffee break**		SD&SR
11.00-11.45	Molecular docking for ligand discovery	J. Irwin	SD
11.45-12.30	Drug discovery: from lab bench to life cycle management.	G. Scapin	SD
12.30-14.30	**poster preview lunch**		SF
Session 02A	**Poster Preview**		**SD**
14.30-15.15	Short (2-3 minutes) poster presentations (odd numbers)		SD
15.15-16.00	Designing compounds against lipid kinases:NVP-BKM120 – a pan class 1 PI3K inhibitor	D. Bussiere	SD
16.00-16.30	**coffee break**		
Session 02C	**Workshops**		
16.30-18.00	Using the Cambridge Structural Database System in Drug Discovery	C. Groom / I. Giangreco	TBD
16.30-18.00	Computational Ligand Discovery	J.Irwin	TBD
16.30-18.00	How do we know how good a protein structural model is	A. Tramontano	**TBD**
18.00-20.00	Poster Session – Odd numbers		SF
20.00-	**Pasta Party**		**SF**

June 02			hall
Monday			
Session 03M	**Antivirals**		SD
9.00-9.45	Towards novel anti-influenza drugs targeting the viral RNA-dependent RNA polymerase.	S. Cusack	SD
9.45-10.30	Drug design targeting HIV-1 reverse transcriptase: overcoming resistance via inhibitor strategic flexibility	E. Arnold	SD
10.30-11.00	**coffee break**		SD&SR
Session 03M-1	**Talks from poster abstracts**		
11.00-11.30	Biophysical and structural characterization of the p300/HIF-1α and eIF4e/eIF4g protein-protein interactions to enable drug design	H. Kyle	SD
11:30-12:00	Fragment screening against Bacteroides thetaiotaomicron glycoside hydrolase 84 reveals novel activators of O-GlcNAcase enzyme activity	J. Darby	SD
12:00-12:30	The HIV-1 pre-integration complexes: structure, function and dynamics	N. Levy	SD
12.30-	*Excursion 1*		

June 03			hall
Tuesday			
Session 04M	**Protein-protein and protein-ligand interactions 1**		SD
9.00-9.45	Protein-ligand interactions as the basis for drug action	G. Klebe	SD
9.45-10.30	The use of small molecule crystal structures in drug discovery and development	C. Groom	SD
10.30-11.00	**Coffee break**		
11.00-11.45	Prediction of aggregation in protein sequences and structures	S. Ventura	SD
11.45-12.30	Determination of protonation states in protein complexes using neutron and high resolution X-ray diffraction.	A. Podjarny	SD
12.30-14.30	**Lunch**		
Session 04A	**Protein-protein and protein-ligand interactions 1-cntd.**		SD
14.30-15.15	Protein-protein interactions: general aspect of druggability	T. Blundell	SD
15.15-16.00	DEMO: Using the Cambridge Structural Database System in Drug Development	C. Groom / I. Giangreco	SD
16.00-16.30	**Coffee break**		
Session 04C	**International Year of Crystallography Celebration**		SD
16.30-18.00	*Talks*	T. Blundell, H. Berman, J. Howard, E. Arnold	SD
18.00-20.00	*Game*	All	TBD
20.00-	**Dinner party**		TBD

June 04			hall
Wednesday			
Session 05M	**Enzymes**		SD
9.00-9.45	Drug Discovery at Challenging Interfaces: “the high hanging fruit”	J. Wells	SD
9.45-10.30	Molecular interaction analysis for discovery of drugs targeting enzymes	H. Danielson	SD
10.30-11.00	**Coffee break**		SD&SR
	Methods		SD
11.00-11.45	Achieving high quality protein-ligand X-ray structures for drug design	O. Smart	SD
11.45-12.15	New tools for precise genome editing (from poster abstracts)	S. Stella	SD
12.15-12.45	Ligand discovery from GPCR crystal structures and homology models (from poster abstracts)	J. Carlsson	SD
12.45-14.30	**Poster preview lunch**		SF
Session 05°	**Poster Preview**		SD
14.30-15.15	Short (2-3 minutes) poster presentations (even numbers)		SD
15.15-16.00	Co-Evolution of Structural Biology and the Protein Data Bank	H. Berman	SD
16.00-16.30	**Coffee break**		SD&SR
Session 05C	**Workshops**		
16.30-18.00	Getting the most out of the RCSB PDB	A. Prlic	TBD
16.30-18.00	Achieving high quality ligand chemistry in protein X-ray structures	O. Smart	TBD
18.00-20.00	Poster Session – Odd numbers		SF
20.00-	**Pizza Dinner (Sponsored by EmeraldBio)**		SF

June 05			hall
Thursday			
Session 06M			SD
9.00-9.45	Structural insights for targeted drug design: from proteins to ribosomes	R. Zarivach	SD
9.45-10.30	Molecular Obesity, Potency and other addictions in Medicinal Chemistry	M. Hann	SD
10.30-11.00	**Coffee break**		SD&SR
Session 06M-1	**Talks from poster abstracts**		
11.00-11.30	Structure of Saffold virus at 2.5 Å resolution	P. Plevka	SD
11:30-12:00	Design of novel aspartic protease inhibitors from fragments exploiting dynamic combinatorial chemistry	N. Radeva	SD
12.00-	EXCURSION to SELINUNTE and SEGESTA or at S. Vito lo Capo Beach		



June 06			hall
Friday			
Session 07M	**SBDD: Applications**		SD
9.00-9.45	New Protein Engineered Tools for Signaling	J. Wells	SD
9.45-10.30	Enabling the Best Structure-Based Design Engine: a Human Expert	J. Blaney	SD
10.30-11.00	**Coffee break**		SD&SR
11.00-11.45	Bromodomains – from phenotypic hits to FT1H	C.-w. Chung	SD
11.45-12.30	Joys of X-ray Crystallographic Fragment Screening	J. Bauman	SD
12.30-14.30	**Lunch**		
Session 07A	**Hot topics – From Poster Abstracts**		SD
14.30-15:00	A new generation of more potent virus inhibitors resulting from structure based analysis of human Enterovirus71 (HEV71) capsid-binding molecule	L. De Colibus	SD
15:00-15:30	The mycobacterial F1Fo-ATP synthase as the target of a novel TB drug against tuberculosis	L. Preiss	SD
15:30-16:00	Structural basis for the inhibition of the eukaryotic ribosome	I. Prokhorova	SD
16.00-16.30	**Coffee break**		SD&SR
Session 07C	**Workshops**		
16.30-18.00	*The PDB*	A. Prlic	TBD
16.30-18.00	Achieving high quality ligand chemistry in protein X-ray structures	O. Smart	TBD
18.00-20.00	Free		
20.00-	**Dinner**		

June 07			hall
Saturday			
Session 08M	**Protein-protein and protein-ligand interactions 2**		SD
9.00-9.45	Targeting PPI: examples	T. Blundell	SD
9.45-10.30	Importance of protonation states for the binding of ligands to pharmaceutical targets	A. Podjarny	SD
10.30-11.00	**Coffee break**		SD&SR
11.00-11.45	Molecular interaction analysis for resolving biological function	H. Danielson	SD
11.45-12.30	Structural Chemistry and Molecular Modeling in the design of DPP4 inhibitors	G. Scapin	SD
12.30-14.30	**Lunch**		
Session 08A	**Protein-protein and protein-ligand interactions 2-cntd.**		
14.30-15.15	Structure-based drug design to perturb function of a tRNA-modifying enzyme by active site and protein-protein interface inhibition	G. Klebe	SD
15.15-16.00	Benzoxaborole compounds targeting leucyl-tRNA synthetase as novel anti-infectives	S. Cusack	SD
16.00-16.30	**Coffee break**		SD&SR
Session 08C			
16.30-17.15	Round Table		SD
17.15-18.00	Closing remarks and Awards	Directors	SD
18.00-20.00	Free		
20.00-	**Good Bye Buffet Dinner**		SF

HALLS:

SD: San Domenico Lecture Hall
SR: San Rocco
SF: San Francesco
TBD: to be determined