

Programme of the 4th MC meeting of the CM1306 COST ACTION

	Monday March 27
8.15-8.45	Registration
8.45-9.00	Welcome and Introduction
9.00-10.00	Collaboration Market Chair: <i>Arwen Pearson</i>
10.00-12.40	Scientific Session 1. Protein Systems Chair: <i>Eurico Cabrira</i>
10.00-10.20	Effects of translation initiation factors eIF4G and eIF4B on eIF4A activity and conformational dynamics <i>Alexandra Andreou</i>
10.20-10.40	Investigating structural/function relationship in type II NADH:quinone oxidoreductases <i>Manuela Pereira</i>
10.40-11.00	Coffee Break
11.00-11.20	AhR-Interacting Protein (AIP) interactions: Effect of mutations relevant to Pituitary Adenomas <i>Marita Vella</i>
11.20-11.40	Rate-limiting steps of the P-type ATPase transport mechanism revealed by single molecule FRET <i>Mateusz Dyla</i>
11.40-12.00	Metal selectivity studies of the cation diffusion facilitator protein family <i>Shiran Barber Zucker</i>
12.00-12.20	The magnesium transporter A ₁ is dependent on cardiolipin and selectively sensitive to free magnesium <i>Jens Preben Morth</i>
12.20-12.40	Stoichiometry and kinetics of mercury uptake by photosynthetic bacteria <i>Péter Maróti</i>
12.40-14.00	Lunch
14.00-16.00	Scientific Session 2. Spectroscopy Chair: <i>Diana Monteiro</i>
14.00-14.20	Observing conformational change in the substrate binding domain of a Mn ²⁺ -specific ABC transporter relevant to pathogen virulence <i>Anna Mullen</i>
14.20-14.40	New perspective on how photosynthetic and respiratory cytochrome bc complexes function safely in the presence of oxygen <i>Artur Osyczka</i>
14.40-15.00	Quantitative FRET studies and integrative modeling unravel the dynamic structure and the oligomerization of the large GTPase hGBP1 in vitro and in live cells <i>Claus Seidel</i>
15.00-15.20	Entrapment of <i>C. freundii</i> methionine γ -lyase in nanoporous silica gels <i>Serena Faggiano</i>
15.20-15.40	Towards dissecting the conformations and dynamics of GltPh using EPR spectroscopy and MD simulations <i>Jenny Hall</i>
15.40-16.00	Developing new labelling strategies to study fast protein dynamics for the example of T4 Lysozyme Stephen Niebling
16.00-16.20	Coffee Break
16.20-16.40	On the Rotary Mechanism of the Vacuolar Proton-ATPase, a true Biomolecular Engine <i>Tibor Páli</i>
16.40-17.40	Flash Presentations Chair: <i>Therese Hunter</i>
17.40-19.00	Poster Session (<i>pica pica</i>)

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	Tuesday March 28
8.15-9.00	Registration
9.00-11.20	Scientific Session 3: Computational Chair: <i>Matteo Levantino</i>
9.00-9.20	Stability and Dynamics of Dihydrofolate and Trimethoprim Binding to Wild Type and L28R Mutant of E.Coli Dihydrofolate Reductase <i>Canan Atilgan</i>
9.20-9.40	Advances in template-based modeling of protein complexes: interface based modeling towards structural interactome. <i>Attila Gursoy</i>
9.40-10.00	Protein-ligand docking for biometallic interaction: filling the gap between theory and experiments <i>Jean-Didier Maréchal</i>
10.00-10.20	GaudiMM: A Modular Multi-Objective Platform for Molecular Modeling <i>Jaime Rodríguez-Guerra Pedregal</i>
10.20-10.40	A multi-scale approach to ferret out behavior of iron-transport proteins <i>Ali Rani Atilgan</i>
10.40-11.00	Coffee Break
11.00-11.20	Membrane perturbation by nanopores and new tools for molecular visualization: outside matters <i>Rebeca Garcia-Fandino</i>
11.20-14.20	Scientific Session 4: Computational and Experimental Chair: <i>Gary Hunter</i>
11.20-11.40	Nucleotides control the conformation of the motor domains of ABC transporters <i>Thomas Stockner</i>
11.40-12.00	Combination of experimental restraints in structural modelling of large biomacromolecular complexes <i>Gunnar Jeschke</i>
12.00-12.20	Computer aided rational design of a novel enantioselective artificial metallohydratase <i>Lur Alonso-Cotchico</i>
12.20-12.40	Elucidation of interactions and chiral specificity of oxidovanadium drugs with lysozyme by an integrative EPR-docking strategy <i>Giuseppe Sciortino</i>
12.40-14.00	Lunch
14.00-14.20	Yeast Mitochondrial Cytochrome c Oxidase: Mechanism in Relation to Mammalian and Bacterial Homologues <i>Peter Rich</i>
14.20-16.00	MC Meeting <i>Fraser MacMillan</i>
16.00-16.20	Coffee Break
16.20-18.20	Scientific Session 5: Time resolved experimentation Chair: <i>Manuela Pereira</i>
16.20-16.40	Conformational states of substrate binding domains seen by smFRET and EPR <i>Florence Husada</i>
16.40-17.00	Protein flexibility observed in crystal structures <i>Lubica Urbanikova</i>
17.00-17.20	Cryo-EM – A Rapidly Evolving Tool: Insights from Heterogeneous RyR1 samples <i>Ran Zalk</i>
17.20-17.40	Hydrogenase enzyme catalysis <i>Miklos Haroth</i>
17.40-18.00	Links of Conformational sampling to biomolecular recognition: a single molecule perspective <i>Nikos Hatzakis</i>
18.00-19.00	Core Meeting
19.30-	Conference Dinner

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	Sunday 26th March 2017	Monday 27th	Tuesday 28th	Wednesday 29th
	ARRIVALS	REGISTRATION II	REGISTRATION III	DEPARTURES
08:00 - 08:45				
08:45 - 09:00		Introduction	Introduction	
09:00 - 09:20				
09:20 - 09:40		Collaboration Market		
09:40 - 10:00				
10:00 - 10:20		SCIENTIFIC SESSION 1 2X20 MIN	SCIENTIFIC SESSION 3 6 X 20 MIN	
10:20 - 10:40				
10:40 - 11:00		COFFEE	COFFEE	
11:00 - 11:20				
11:20 - 11:40				
11:40 - 12:00		SCIENTIFIC SESSION 1 5x 20 MIN	SCIENTIFIC SESSION 4 5 X20 MIN	
12:00 - 12:20				
12:20 - 12:40				
12:40 - 13:00		LUNCH	LUNCH	
13:00 - 13:20				
13:20 - 13:40				
13:40 - 14:00				
14:00 - 14:20		SCIENTIFIC SESSION 2 7x 20 MIN		
14:20 - 14:40			MC MEETING	
14:40 - 15:00				
15:00 - 15:20				
15:20 - 15:40				
15:40 - 16:00				
16:00 - 16:20		COFFEE	COFFEE	
16:20 - 16:40		Flash Presentations		
16:40 - 17:00				
17:00 - 17:20		60 min	SCIENTIFIC SESSION x5	
17:20 - 17:40		POSTER SESSION		
17:40 - 18:00				
18:00 - 18:20			CORE GROUP MEETING	
18:20 - 18:40				
18:40 - 19:00			conference dinner	

Protein systems
Spectroscopy
Computational
Computational and experimental
Time resolved experimentation