

Wednesday, 21th March, 2018

12.00 – 15.00	Registration
15.00 – 15.10	Welcome: Nadica Maltar Strmecki (Local host) and Fraser MacMillan (Action Chair)
Session 1	Session Chairs: Fraser MacMillan (<i>University of East Anglia, UK</i>), Gabriela Guedez (<i>Åbo Akademi University, Finland</i>)
15.10 – 15.55	Plenary Lecture: Generic physics and molecular specificity in viruses - which is which? <i>Antonio Šiber (Institute of Physics, Croatia)</i>
15.55 – 16.25	Coffee Break
16.25 – 16.50	Biological physics of enterovirus coarsening – tiling, blobs, and all that <i>Ali Rana Atilgan (Sabanci University, Turkey)</i>
16.50 – 17.15	Exploring bacterial respiratory chains <i>Manuela Pereira (University of Lisbon, Portugal)</i>
17.15 – 17.40	Yeast <i>Saccharomyces cerevisiae</i> : a model system to study mitochondrial cytochrome c oxidases <i>Amandine Marechal (University College Lonon, UK)</i>
17.40 – 18.30	Poster presentations : 60 second bullet talks
18.30 – 20.30	Welcome Reception

Thursday, 22th March, 2018

Session 2	Session Chairs: Arwen Pearson (Action Vice Chair, <i>Universität Hamburg, Germany</i>), Gaby A. Frank (<i>Ben-Gurion University of the Negev, Israel</i>)
09.00 – 09.25	Computational tools for molecular simulation and visualization using Molecular Dynamics, Augmented Reality and Virtual Reality <i>Martin Calvelo Souto (University of Santiago de Compostela, Spain)</i>
09.25 – 09.50	Exploration of the chemical space with the multi-objective optimization software GaudiMM <i>José Emilio Sánchez (Aparicio Universitat Autònoma de Barcelona, Spain)</i>
09.50 – 10.15	Computational assessment of allosteric mutations on the dynamics of PDZ domains <i>Nazli Kocatug (Sabanci University, Istanbul, Turkey)</i>
10.15 – 10.40	Computational modeling of histamine metabolism in humans <i>Aleksandra Maršavelski (University of Zagreb, Croatia)</i>
10.40 – 11.10	Coffee Break
Session 3	Session Chairs: Manuela Pereira (<i>Universidade de Lisboa, Portugal</i>), Stephan Niebling (<i>University of Hamburg, Germany</i>)
11.10 – 11.35	Dissecting structure, function and dynamics of DNA gyrase: The mechanism of ATP-driven negative DNA supercoiling <i>Dagmar Klostermeier (University of Münster, Germany)</i>
11.35 – 12.00	A new evaluation method of Raman and infrared microscopic images <i>Csaba Bagyinka (Institute of Biophysics, Hungary)</i>
12.00 – 12.25	The role of the cation diffusion facilitator proteins cytoplasmic domain <i>Shiran Barber-Zucker (Ben-Gurion University of the Negev, Israel)</i>
12.25 – 12.50	Studying the movement of substrate-sequestering units of membrane transporters using advanced EPR techniques <i>Anna Mullen (University of East Anglia, UK)</i>
12.50 – 14.30	Lunch
Session 4	Session Chairs: Eurico Cabrita (<i>Faculdade de Ciências e Tecnologia, Portugal</i>), Tamara Šmidlehner (<i>Ruđer Bošković Institute, Croatia</i>)
14.30 – 15.00	Summary of STSM Presentations: 6 x 4 mins summary talks
15.00 – 15.25	The success of STSMs: Magnetic Resonance Spectroscopy of Molecular Transport Machines <i>Jenny Hall (University of East Anglia, UK)</i>
15.25 – 15.50	Mechanism of elevator-like membrane transport <i>Dirk Slotboom (University of Groningen, The Netherlands)</i>
15.50 – 16.15	ABC transporters with a degenerate NBS stay active by avoiding occlusion <i>Thomas Stockner (Medical University Vienna, Austria)</i>
16.15 – 16.45	Coffee Break
Session 5	Session Chairs: Serena Faggiano (<i>University of Parma, Italy</i>), Andrew Hartley (<i>University College London, UK</i>)

16.45 – 17.10	Structural studies of magnetosome-associated proteins <i>Raz Zarivach (Ben-Gurion University of the Negev, Israel)</i>
17.10 – 17.35	New insights in the nucleotide-dependent conformational cycle of Roco proteins <i>Wim Versées (Vrije Universiteit Brussel, Belgium)</i>
17.35 – 18.00	Engineering Methionine γ -Lyase from <i>Citrobacter freundii</i> for improved catalytic activity <i>Andrea Mozzarelli (University of Parma, Italy)</i>
18.00 – 20.00	Poster Session and Dinner

Friday, 23th March, 2018

Session 6	Session Chair: Thomas Stockner (<i>Medical University of Vienna, Austria</i>), Marta Sans (<i>University of Hamburg, Germany</i>)
09.00 – 09.25	Design of molecular origami nanostructures and folding pathways <i>Roman Jerala (National institute of chemistry, Slovenia)</i>
09.25 – 09.50	Conformational sampling to biomolecular recognition by single molecule studies for <i>in silico</i> design of ligands and advanced protein regulation <i>Nikos Hatzakis (University of Copenhagen, Denmark)</i>
09.50 – 10.15	Fuzzy Sarcomeric Z-disk Complexes: α -Actinin Intercatome <i>Kristina Djinovic Carugo (University of Vienna, Austria)</i>
10.15 – 10.40	Exploring the role of Q89 in the allosteric modulation of human serine racemase by ATP <i>Serena Faggiano (University of Parma, Italy)</i>
10.40 – 11.10	Coffee Break
Session 7	Session Chairs: Dagmar Klostermeier (<i>University of Münster, Germany</i>), Martin Calvelo Souto (<i>University of Santiago de Compostela, Spain</i>)
11.10 – 11.35	Photoprotective mechanisms in photosynthesis studied by time-resolved FTIR difference spectroscopy <i>Alberto Mezzetti (Sorbonne Université, France)</i>
11.35 – 12.00	The link between anisotropic B-factors and function of trypsin <i>Gergely Katona (University of Gothenburg, Sweden)</i>
12.00 – 12.25	Towards direct correlation between structure and function <i>Gaby Frank A. (Ben-Gurion University of the Negev, Israel)</i>
12.30 – 14.00	Lunch
13.30 – 14.30	Core Group Meeting
15.00 – 19.00	City Tour
20.00	Conference Dinner

Saturday, 24th March, 2018

	Fraser MacMillan (<i>Action Chair</i>), Arwen Pearson (<i>Action Vice Chair</i>), Eurcio Cabrita (<i>Dissemination manager</i>)
09.00 – 09.30	Participant feedback on the past 4 years of the CM1306 Action
Session 8	Session Chair: Raz Zarivach (<i>Ben-Gurion University of the Negev, Israel</i>), Anna Mullen (<i>University of East Anglia, UK</i>)
09.30 – 09.55	N-terminal splicing extensions of the hMYO1C gene fine-tune the kinetics of the three full-length myosin IC isoforms <i>Arnon Henn (Technion- Israel Institute of Technology, Israel)</i>
09.55 – 10.20	Chemical Rescue of Proton Transfer to Q _B in Reaction Center of Photosynthetic Bacteria <i>Peter Maroti (Institute of Medical Physics, Hungary)</i>
10.20 – 10.45	Using light as a trigger to understand biological mechanisms <i>Marta Sans (University of Hamburg, Germany)</i>
10.45 – 11.00	What is all the fuss about COST Actions! <i>Fraser MacMillan (University of East Anglia, UK)</i>
11.00 – 11.20	Coffee Break
11.20 – 12.45	MC Meeting
12.45 – 13.00	Brief discussion about future COST Actions, expressions of interest
13.00	Closure of Meeting and Departure