CHEMISTRY ViA COMPUTATION
SYMPOSIUM PROGRAM
OCTOBER 30, 2017 ALBERT LONG HALL (SOUTH CAMPUS)

08:45-09:30	Registration
09:30-09.45	Opening Remarks: Şaron Çatak, Yüksel İnel
	Session I Chair: Tereza Varnalı
09:50-10:35	Gerald Monard, University of Lorraine, Nancy, France *Molecular modeling of the reaction of deamidation in peptides and proteins using combined approaches*
10:35-10:55	Bülent Balta, Istanbul Technical University, Turkey *GTP hydrolysis in the elongation factor EF-Tu*
10:55-11.15	İlke Uğur, Technische Universität München , Munich *1,3-Dipolar cycloaddition reactions of low-valent rhodium and iridium complexes with arylnitrile N-oxides*
11:15-11:30	Coffee Break
	Session II Applications on Molecular Nanoscience **Chairs: İlknur Doğan, Duygu Avcı**
11:30-12:15	Paul Geerlings, Vrije Universiteit Brussel, Belgium *From conceptual density functional theory to molecular electronics*
12:15-12:35	Sondan Durukanoğlu, Sabancı University, Istanbul, Turkey *Molecular motion on metal surfaces: Quantum and classical mechanical approaches*
12:35-12.55	Hande Toffoli, Middle East Technical University, AnkaraTurkey *A comparative study of the polymer-nanotube interface through a reactive force field and density functional theory*
12:55-14:15	Lunch Break-Lunch box (Group photo)
	Session III Chairs: Mine Yurtsever, Canan Ünaleroğlu
14:15-15:00	Michael Feig, Michigan State University, USA *Molecular dynamics simulations of biomolecules: Facing the challenges in connecting with biology*
15:00-15:20	Canan Atılgan, Sabancı University, Istanbul, Turkey *Deciphering equilibrium and kinetic properties of iron transport proteins by computational means*
15:20-16:05	Maria J. Ramos, University of Porto, Portugal *Predicting catalytic mechanisms of enzymatic reactions*
16:05-16:25	Nilsun İnce, Boğaziçi University, Istanbul, Turkey *A Bridge between Computational Chemistry and Environmental Science*
16:25-16:40	Coffee Break
	Session IV Chair: Safiye S. Erdem
16:40-17:25	Viktorya Aviyente, Boğaziçi University, Istanbul, Turkey *What have we learned with computational tools in chemistry?*
17:25-17:50	Video Presentation (Comments from collaborators)
17:50-18:00	Closing Remarks: Prof. Ersin Yurtsever
18:00-19:15	**Poster Session**
18:00-18:45	*Round table meeting on "Applications on Molecular Nanoscience"*