Scientific Program

Monday		
13:00 – 17:00	**Registration**	
17:00 –17:20	Conference opening	
Chairman	*N. Gresh*	
17:20 – 18:05	P. Politzer	The σ-Hole at Age Ten: Healthy but with Some Growing Pains
18:05 – 18:35	J. Urban	Interactions of DNA, RNA Aptamers – Computational Study
19:00 - 22:00	**Welcome party**	

Tuesday		
Chairman	*F. J. Luque*	
9:00 – 9:30	M. Kaupp	Insights from Computations of NMR/EPR Parameters of Paramagnetic Metalloenzyme Sites
9:30 – 10:00	N. Gresh	Addressing the Issues of Non-Isotropy and Non-Additivity in the Development of a Quantum-Chemistry-Grounded Polarizable Molecular Mechanics/Dynamics Potential
10:00 – 10:30	M. Sodupe	Fluorescence Markers for Amyloid-β Fibrils Detection. Insights From Computational Approaches
	Coffee break	
Chairman	*J. Šponer*	
10:50 – 11:20	A. Michalak	ETS-NOCV Description of Chemical Reactions
11:20 – 11:50	M. P. Mitoraj	From Polar to Non-Polar Dihydrogen Bonding - An Insight from Computational Perspective
11:50 – 12:10	I. Cukrowski	Destabilizing a Molecule Classical Intramolecular H-Bonding. An Insight from the FAMSEC Perspective
12:10 – 12:30	J. H. de Lange	Deformation Densities for Intramolecular Interactions without Unphysical, Radical Reference States
	Lunch	

Chairlady	*M. Sodupe*	
14:30 – 15:00	A. Klamt	COSMO Polarization Charge Densities as Valuable Descriptors for Hydrogen Bonding and Free Energies of Binding
15:00 – 15:30	J. S. Murray	Electrostatic Potentials of Interacting Atoms: Giving Atoms Back Their Identities
15:30 – 15:50	B. Herrera	The Role of Water in the Mechanism of Proton Transfer of Formamide and Thioformamide
15:50 – 16:00	**Conference photo**	
	Coffee break	
Chairman	*A. Michalak*	
16:20 – 16:50	S. J. Grabowski	Protonation of Hydrocarbons by Carborane Superacids and Their Aluminum Analogues – Towards the Topological Acidity Scale
16:50 – 17:10	J. Šebera	Catalytic Mechanism of the hOGG1 Base-excision Repair Enzyme; the Theoretical Modeling of Reaction Pathway
17:10 – 17:30	S. D. Zarić	Noncovalent Interactions of Water Molecule
	Dinner	
19:00 – 21:00	**Poster session**	

Wednesday

Chairman	*M. Kaupp*	
9:00 – 9:30	P. Paneth	Isotope Effects on Binding Inhibitors to HIV-1 Reverse Transkryptase
9:30 – 10:00	M. B. Hall	When Modeling Hydrogenase Mimics, Expect the Unexpected
10:00 – 10:30	F. J. Luque	On the Inhibition Mechanism of the Influenza A M2 Proton Channel by Amantadine-like Inhibitors
	Coffee break	

Chairman	*P. Paneth*	
10:50 – 11:20	R. Ettrich	Structure and Function of the Motor Subunit of the EcoR124I Restriction-Modification Complex
11:20 – 11:50	V. Moliner	Computer Aided Design of New Biocatalysts
11:50 – 12:10	D. Řeha	Theoretical Study of Crystal Structure of WrbA from *E. coli* in Complex with Benzoquinone using QM Calculations of Charge Transfer Rates and MD Simulations
	Lunch	
14:00 - 19:00	**Sightseeing tour**	starts from Václavské nám. "at the horse"
19:00- 20:15	**Concert**	in church St. Martin in the Wall

Thursday

Chairlady	*J. S. Murray*	
9:00 – 9:30	T. Brinck	Designing New Enzyme Activities
9:30 – 10:00	L. Rulíšek	Computational Electrochemistry: From Small Molecules to Metalloproteins
10:00 – 10:30	T. Borowski	Reaction Mechanisms of Mononuclear Metalloenzymes
	Coffee break	
Chairman	*J. Leszczynski*	
10:50 – 11:20	S. Roszak	Comparative Study of Hydrolytic and Electron-driven Processes in Carboplatin Biotransformation
11:20 – 11:50	P. Cysewski	Rules for Efficient Co-Formers Selection for Co-Crystals Screening of Active Pharmaceutical Ingredients
11:50 – 12:10	P. Adamczyk	Permanganate Oxidation of Carbon-Carbon π-Bond
12:10 – 12:30	O. Kroutil	Structure and Dynamics of Hydration Shell of Pt(II) Complexes
	Lunch	

Chairman	*L. Rulíšek*	
14:30 – 15:00	J. Kozelka	Physical Origin of Lone-Pair-π Interactions
15:00 – 15:30	J. Korchowiec	Inclusion Complexes of β-Cyclodextrin: DFT and Molecular Dynamics Simulations
15:30 – 15:50	R. Friedman	Forcefield and QM Calculations for Zn-Protein Interactions
15:50 – 16:10	C. Fonseca Guerra	Covalence, not Resonance-Assistance, behind Cooperative Hydrogen and Halogen Bonds
	Coffee break	
Chairman	*J. Korchowiec*	
16:30 – 17:00	W. A. Sokalski	Possible Improvements in Biocatalyst Design Methodology
17:00 – 17:30	M. Straka	Molecular Properties of Endohedral Fullerenes
17:30 – 17:50	J. Leszczynski	To Heal or to Kill: Comprehensive Evaluation of Large Pool of Fullerenes
17:50 – 18:10	A. Wierzbicki	Selective Inhibition of PP5 versus PP4 by Norcantharidin-Based Compounds
	Dinner	

Friday

Chairman	*S. J. Grabowski*	
9:00 – 9:30	J. Šponer	Multiscale Modelling of G-Quadruplex DNA
9:30 – 10:00	P. Jurečka	Deriving and Testing Force Field Torsion Parameters for RNA and DNA Simulations
10:00 – 10:30	R. Marek	Designing Nucleic Acid Bases for Quadruplexes
	Coffee break	

Chairman	*W. A. Sokalski*	
10:50 – 11:20	P. Bouř	Modeling of Chiroptical Spectra of Large Molecules
11:20 – 11:40	H. F. Dos Santos	Chemically Modified Tetracyclines as Inhibitors of MMP-2 Matrix Metalloproteinase: A Molecular and Structural Study
11:40 – 12:00	W. Rocha	Reaction Mechanism for Methane Oxidation Reaction Promoted by a Structural Model of the pMMO Enzyme
12:00 – 12:30	Concluding remarks	