Scientific program

Sunday

14:00–17:00	**Registration**	
17:00–17:15	**Conference opening**	
17:20–18:05	P. Hobza	Noncovalent Interactions: Theory and Applications
19:00–21:30	**Welcome party**	

Monday

chairman	*W. A. Sokalski*	
9:00–9:30	L. Gorb	DNA bases in Dickerson dodecamer: results of recent quantum-chemical calculations
9:30–10:00	P. Jurečka	Using QM Data in Force Field Development for RNA and DNA Simulations
10:00–10:30	J. Šponer	Computational studies of nucleic acids – the current trends.
	Coffee break	
chairman	*X. Assfeld*	
11:00–11:30	C. Lim	Principles Governing Biological Processes: Applications to drug design and drug target identification
11:30–12:00	T. Dudev	Determinants of Fe^{2+} over M^{2+} (M = Mg, Mn, Zn) Selectivity in Non-Heme Iron Proteins
12:00–12:30	N. Gresh	Polarizable molecular mechanics/dynamics potentials. Validations by QC computations on two sensitive issues: stacked guanine quartets and dizinc metalloenzyme binding sites.
	Lunch	
chairman	*P. Hobza*	
14:20–14:50	G. Mazzone	Computational Contribution to the Design of Effective Drugs in Photodynamic Therapy
14:50–15:10	S. Mutter	Metallobiology of Amyloid Beta Peptides by Ligand Field Molecular Mechanics
15:10–15:30	D. Bonhenry	Investigation of Ca^{2+} permeation in the Orail channel.
15:30–15:50	K. Mazmanian	Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions
	Coffee break	
chairlady	*C. Lim*	
16:20–16:50	W. A. Sokalski	Use of catalytic fields in biocatalyst design
16:50–17:20	J. Poater	How non-terran bio-solvents affect the structure and stability of B-DNA
17:20–17:40	R. Matute	Revisiting the Mechanism of DNA Polymerases with an Empirical Valence Bond Model
17:40–18:00	M. Růžička	Study of Structural and Elastic Properties of DNA Mutation Motifs Using Computational Methods
19:00–21:00	**Poster session**	

Tuesday

chairman	*R. Ettrich*	
9:00–9:30	T. Clark	Metadynamics Simulations of G-Protein Coupled Receptors
9:30–10:00	M. Hall	Modelling Hydrogenase Biomimetics
10:00–10:30	N. Russo	Enzyme promiscuity: A Computational Approach
	Coffee break	
chairman	*L. Gorb*	
11:00–11:30	P. Paneth	Binding isotope effects in design of HIV-1 reverse transcryptase inhibitors
11:30–12:00	S. Zaric	Modeling and elucidating role of aromatic and aliphatic side chain interactions in stability of amyloids
12:00–12:30	V. Moliner	Revealing the Origin of Enzyme Catalysis from Computational Studies
	Lunch	
chairman	*T. Clark*	
14:20–14:50	J. Kozelka	Anion-π interactions in flavoproteins involve a substantial charge-transfer component
14:50–15:20	P. Cysewski	Water solubility advantage of drugs cocrystalized with pharmaceutically acceptable coformers.
15:20–15:50	D. Řeha	Application of Charge Transfer Calculations on Computational Study of Proteins
	Coffee break	
chairman	*P. Paneth*	
16:20–16:50	R. Ettrich	Computational Modeling of 3'-Phosphoadenosine 5'- Phosphosulfate Synthase PAPSS
16:50–17:20	T. Wesolowski	
17:20–17:50	J. Urban	MP1- membrane interactions, MD study

19:30 **Concert in the Cathedral of St. Bartholomew**

Performed by **Pavel Šmolík**.

Compositions:

- Georg Muffat: Toccata prima (5´)
- Johann Pachelbel: Ciacona in f (9´)
- Johann Sebastian Bach: Toccata d moll (9´)
- Johann Sebastian Bach: O mensch, bewein (5´)
- Felix Mendelssohn-Bartholdy: Sonata c moll (Grave, Andante, Allegro Moderato, Fuga) (11´)
- Pavel Šmolík: Improvizace (8´)

Wednesday

chairman	*T. Wesolowski*	
9:00–9:30	K. Ruud	Modeling one- and multiphoton absorption in biomolecular systems
9:30–10:00	P. Bouř	Computations of Magnetic Circular Dichroism in Molecules
10:00–10:30	M. J. Ramos	Advances and Pitfalls in Computational Enzymatic Catalysis
	Coffee break	
chairman	*S. Roszak*	
11:00–11:30	A. Michalak	ETS-NOCV decomposition of the reaction force
11:30–12:00	X. Assfeld	Modeling Excited States Interactions in Biomolecules.
12:00–12:30	H. Dong	Exploring the Gating Mechanism of the Calcium Release-Activated Calcium Channel with Molecular Dynamics Simulations
	Lunch	
14:30–16:00	**Sightseeing tour in Pilsen**	
16:00–18:00	**Excursion to the Pilsner brewery**	
18:00	**Dinner in the brewery restaurant**	

Thursday

chairman	*N. Gresh*	
9:00–9:30	B. Szefczyk	AIMD analysis of model protic ionic liquids
9:30–10:00	R. Friedman	Computer simulations to improve the understanding of drug resistance in cancers
10:00–10:30	S. Roszak	The breathing MOF's – chemistry of MIL-53 from first principles
	Coffee break	
chairman	*J. Kozelka*	
11:00–11:30	S. Záliš	Modelling of electron transfer in metal labelled proteins and systems containing multiple redox centers
11:30–12:00	H. Dos Santos	Predicting standard reduction potential for anticancer Au(III)-complexes: A DFT study
12:00–12:30	M. Srnec	Computational Electrochemistry of Mononuclear Non-Heme Iron Complexes: Redox Properties and their Contributions to Reactivity
	Lunch	
chairman	*P. Bouř*	
14:20–14:50	A. Wierzbicki	A modeling study of the binding of novel indenes to the catalytic site of mutant KRAS
14:50–15:10	T. Jeliński	Application of COSMO-RS methodology for screening of ionic liquids and deep eutectic solvents as effective media for enhancement of extraction and solubility
15:10–15:30	Z. Chval	Bonding and non-bonding interactions of Pt(II)-complexes
15:30–15:50	F. Šebesta	Reduction of Pt(IV) complexes by small biomolecules
	Coffee break	
chairman	*M. Hall*	
16:20–16:50	T. Ishida	Computational modeling of carbohydrate recognition in protein complex
16:50–17:20	W. Rocha	Release of NO from Ruthenium Nitrosyl Complexes in Aqueous Solution.
17:20–17:40	J. Novotný	Revealing structure of i-motif with purine stretches using NMR and molecular modelling
17:40–18:00	J. Jungwirth	Quantitative Determination of Ala-Ala Conformer Ratios by Decomposition of Raman Optical Activity Spectra

Friday

chairman	*S. Grabowski*	
9:00–9:30	M. Biczysko	Understanding structure and function of bio-molecular systems from spectroscopic 'fingerprints'
9:30–10:00	Z. Futera	Heterogeneous Electron Transfer Between Gold Surface and Adsorbed Deca-Heme Protein MtrF
10:00–10:30	R. Marek	Supramolecular Carriers for Anticancer Metallodrugs
	Coffee break	
chairman	*B. Szefczyk*	
11:00–11:30	T. Mančal	Ten years of coherent quantum biology: Paradigm change that almost happened
11:30–12:00	S. Grabowski	Dual character of boron as a Lewis acid center – ab initio calculations and QTAIM analysis
12:00–12:30	**Closing ceremony**	

Poster presentations

Poster no.	Author name	Poster title
1	E. Ahlstrand	Force Field Based Calculations of Zn Interaction Energies in Proteins
2	P. L. Bora	Supramolecular Covalence in Bifurcated Chalcogen Bonding
3	T. Bouchal	Influence of non-Watson-Crick base pairing on structure of DNA
4	R. Cajzl	Excited state dynamics of conjugated polyenes Ab-initio and semiempirical calculation of electronic absorption spectra
5	D. Cheshmedzhieva	Competition between Abiogenic Al^{3+} and Native Mg^{2+}, Fe^{2+} and Zn^{2+} Ions in Protein Binding Sites: Implications for Aluminium Toxicity
6	B. J. Cuyacot	Calculation of Pt-195 NMR Chemical Shifts for Pt(IV)-Based Metallodrugs
7	P. Czeleń	Docking and molecular dynamics study of CDK2 inhibition by new indoline derivatives
8	O. Dvořáčková	The effect of substituents on the kinetics of the hydration reactions of trans-Platinum complexes
9	H. Georg	Elucidating the structure of merocyanine dyes with the ASEC-FEG method
10	W. Jedwabny	Testing a simple non-empirical scoring model on inhibitors of EphA2-ephrinA1 protein-protein interaction
11	N. Kircheva	Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga^{3+} and Fe^{3+} Ions in Metalloproteins
12	P. Krawczyk	The reactive group effects on the photophysical and biological properties of the fluorescent probe based on chalcone derivatives
13	M. Krupová	Circularly Polarized Luminescence in Study of Protein Folding – Experimental and Theoretical Study
14	E. Kutálková	Molecular-dynamics simulations of hyaluronan-ions interactions
15	S. Malali	Paramagnetic NMR study of Ru(III) complex for calculating NMR chemical shift
16	M. Melichercík	The influence of site Mutations on Activity of XPB Protein
17	M. Misini Ignjatovic	Structure and thermodynamics of water at the binding site of galectin-3 with two diastereomers of different affinities
18	V. Nikolova	Determinants of the host–guest interactions Q1 between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study
19	I. Niksic-Franjic	Reactions of free radicals with haloorganics in buffered aqueous solutions: modeling proton-coupled electron transfer and competing mechanisms
20	J. Petrova	Assessment of the Effect of Oligomer-Water Interaction on Polyaniline Properties
21	M. Pizl	Vibrational spectroscopy of metal complexes derived from vitamin B6: Experimental and DFT study
22	L. Plačková	Theoretical study of PAPSS2 kinase domain
23	T. Smetanová	Estimation of Ir(III) empirical parameters for molecular mechanical force fields
24	Z. Sochorová Vokáčová	Theoretical study of a lipase-catalyzed reaction in organic solvent
25	B. Szefler	Theoretical Study on Cisplatin Binding to B-Vitamins: Could the therapeutic effect of cisplatin be decreased if a patient with lung cancer drinks carrot or beet juice?
26	M. Turner	Modelling Pt^{II}(Ligand) – Amyloid-β Interactions: Prediction of Ligand Effects
27	M. Zgarbová	Recent Force Fields for RNA Simulations – Performance, Comparison and Challenges