Conference and workshop program

September 10, 2006 (Sunday)

16.00-20.00	Registration - Entrance to B-4 building (corner of Smoluchowskiego & Łukasiewicza Streets)
16.00-20.00	Welcome reception

September 11, 2006 (Monday)

8.00-9.00	Registration - Entrance to B-4 building
9.00-9.10	Workshop opening - Room 409 B-4 building
	SESSION I - **Room 409 B-4 building** (Chair - J. Leszczyński)
9.10-10.00	**L1**: W. Minor - *Structural Genomics Changes the Molecular Modeling Approach*
10.00-10.45	**L2**: T. Brinck - *Computational Design of New Enzyme Catalysts*
10.45-11.00	Coffee break
	SESSION II - **Room 409 B-4 building** (Chair - G. Náray-Szabó)
11.00-11.40	**L3**: A. Koliński - *Modeling Protein Structure and Interactions in Reduced Conformational Space*
11.40-12.20	**L4**: L. Piela - *Theoretical Model of Conformational Autocatalysis*
12.20-13.00	**L5**: B. Lesyng - *Causality Analysis - A Strategy for the Analysis of Molecular Dynamics Data*
13.00-15.00	Lunch break
	SESSION III - **Room 409 B-4 building** (Chair - T. Brinck)
15.00-15.45	**L6**: G. Náray-Szabó - *On the Mechanism of Action of Enzymatic Phosphate Hydrolysis*
15.45-16.30	**L7**: P. Paneth - *Application of Different QM/MM Schemes to Studies of Enzyme-Catalyzed Reactions*
16.30-17.00	*FQS POLAND software presentation*
17.00-17.15	Coffee break
	SESSION IV - Rooms 448 & 446 B-4 building Optional session for participants registered earlier
17.15-18.45	L. Firlej, B. Kuchta - *Monte Carlo and Statistics*
	SESSION V - 4th floor B-4 building
19.30-21.00	Poster session A (P2-P6, P8-P11, P13-P14, P16-P28, P30-P38, P56)

September 12, 2006 (Tuesday)

SESSION VI - **Room 409 B-4 building** (Chair - L. Piela)

9.00-9.45 **L8**: H. Cheng - *Design and Development of Efficient Hydrogen Storage Materials to Enable the Hydrogen Economy*

9.45-10.30 **L9**: W. Grochala - *Towards the "Hydrogen economy" Dream – Catalysis of the Homo- and Heterolytic Splitting of the H2 Molecule*

10.30-11.00 **L10**: B. Kuchta - *Adsorption and Phase Transitions in Nanopores*

11.00-11.15 Coffee break

SESSION VII - **Room 409 B-4 building** (Chair - P. Paneth)

11.15-11.50 **L11**: P. Politzer - *Halogen Bonding as a Basis for the Design of New Materials*

11.50-12.25 **L12**: C. Ramseyer - *Modelling of Ionic Channels at the Molecular Level: Achievements and Perspectives*

12.25-13.00 **L13**: A. Miniewicz - *Design of Photochromic Polymers and Liquid Crystals for Dynamic Holography*

13.00-15.00 Lunch break

SESSION VIII - **Room 409 B-4 building** (Chair - C. Ghio)

15.00-15.40 **L14**: J. Leszczyński - *Nerve Agents - How To Uncover Their Characteristics and Not Get Killed?*

15.40-16.20 **L15**: I. Majerz - *Isotope Effects in Strong Hydrogen Bonds*

16.20-17.00 **L16**: J. Burda - *Computational Approach to Anticancer Metallodrugs*

17.00-17.15 Coffee break

SESSION IX - Rooms 448 & 446 B-4 building
Optional session for participants registered earlier

17.15-19.00 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*

September 13, 2006 (Wednesday)

9.30-10.00 Panorama Racławicka Gallery tour (Purkyniego Street)
optional upon request

10.00-13.00 Wrocław sightseeing (starting from Panorama Racławicka Gallery)
optional upon request, free

SESSION X - Rooms 448 & 446 B-4 building
Optional session for participants registered earlier

15.15-19.00 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*

19.30-21.00 Conference reception - Museum of Architecture (Bernardyńska Street)

September 14, 2006 (Thursday)

SESSION XI - **Aula B-4 building** (Chair - P. Kafarski)

9.00-9.40 **L17**: L. Hua - *What controls enantioselectivity of carbonyl reductase?*

9.40-10.20 **L18**: C. Ghio - *Computational Prediction of Regio- and Stereoselectivities in the Hydroformylation of Chiral Olefins*

10.20-10.45 **L19**: N. Mishra - *A Theoretical Study of the Comparative Binding Affinities of PAIIL towards Monosaccharides*

10.45-11.00 Coffee break

SESSION XII - **Aula B-4 building** (Chair - L. Komorowski)

11.00-11.40 **L20**: T. Wesołowski - *First-principles Treatment of the Interface Between the Orbital and Orbital-free Levels of Description in Multi-scale Modelling*

11.40-12.25 **L21**: A. Tachibana - *A New Energy Density Visualization Scheme for External Field Effects on Molecular Systems*

12.25-13.00 **L22**: A. Daini - *The Effect of Interaction Range and Anisotropy on Surface Tension*

13.00-15.00 Lunch break

SESSION XIII - **Aula B-4 building** (Chair - Z. Latajka)

15.00-15.40 **L23**: J. Sauer - *Treating Dispersion Effects in Extended Systems by Hybrid MP2:DFT calculations: Hydrocarbons on Catalyst Surfaces*

15.40-16.20 **L24**: J. Wojdeł - *Computational Modelling of Double Metal Cyanide Catalyst for Propoxylation Reaction*

16.20-17.00 **L25**: E. Brocławik - *CYP 3A4: Modelling Substrate Binding and Electronic State of Oxyferryl Active Site Helps to Understand Reactivity*

17.00-17.15 Coffee break

SESSION XIV - Rooms 448 & 446 B-4 building
Optional session for participants registered earlier

17.15-19.00 L. Firlej, B. Kuchta - *Monte Carlo and Statistics*

SESSION XV - 4th floor B-4 building

19.30-21.00 Poster session B (P1, P3, P7, P12, P15, P17, P29, P31, P39-P55, P57-P58, P59)

September 15, 2006 (Friday)

	SESSION XVI - **Aula B-4 building** (Chair - J. Sauer)
9.00- 9.35	**L26**: M. Cieplak - *Stretching to Understand Proteins*
9.35-10.10	**L27**: S. Grabowski - *Characteristics of a Wide Spectrum of Dihydrogen Bonded Materials*
10.10-10.45	**L28**: H. Dodziuk - *Why Are Strained Hydrocarbons Worth Studying?*
10.45-11.00	Coffee break
	SESSION XVII - **Aula B-4 building** (Chair - J. Burda)
11.00-11.35	**L29**: P. Cysewski - *Accuracy of Gas Phase Acidities of Carboxylic Acids Predicted by Direct Scaling of Harmonic Vibrational Frequencies rom ab initio Calculations - A Perspective for Precise pKa Estimation*
11.35-12.00	**L30**: Z. Vokáčová - *NMR Parameters in RNA Molecules and Their Correlation with Molecular Structure*
12.00-12.20	**L31**: M. Pavelka - *Quantum Chemical Study of Cu(I)/Cu(II) Cations in a Peptide Environment*
12.30	Farewell - main campus building (A-1) photograph of workshop participants on the stairs

Conference posters

No.	Session	Main author	Title
P1	B	T. Borowski	*DFT Studies on the Reaction Mechanisms of Intra- and Extradiol Dioxygenases*
P2	A	G. Brancolini	*Mechanism for DNA Triple Helix Formation: a Computational Study*
P3	B	E. Broniatowska	*PLDB - Protein Ligands DataBase*
P4	A	H. Chojnacki	*Multiple Proton Transfer in Some Molecular Systems. Implications for Crystalline Phases*
P5	A	P. Czeleń	*Molecular Dynamic Simulation of the Effects of Oxidative Damage on the Structure of Telomeric DNA*
P6	A	M. Doskocz	*Studies of Hydrogen Bonds in C-H···O=P by NMR Chemical Shifts and 3hJ(13C-31P) Spin-Spin Coupling. Correlation of Experimental and ab inito Data*
P7	B	M. Doskocz	*The Theoretical Study of Five Heterocyclic Derivatives of Carbazole – Monomers Electroconducting Polymers*
P8	A	M. Feliks	*Reactivation mechanisms for sarin-inhibited acetylcholinesterase by oxime: a model DFT study*
P9	A	M. Fiet	*Theoretical Study of Concerted Proton Transfer in the Ground Electronic State of the Double Hydrogen Bonded Formic Acid Dimer*
P10	A	Z. Futera	*Activation of Ruthenium(II) Complexes and their Interactions with DNA bases*
P11	A	P. Gauden	*CO2 Sorption on N-, O-, and OH-substituted Carbonaceous Materials. A computational Chemistry Study*
P12	B	P. Gauden	*Argon Adsorption on Heterogeneous Carbon Surfaces: Accesible Pore volume and Width*
P13	A	A. Gorączko	*Modeling of Isotopomeric Molecular Clusters in Electron Ionisation Mass Spectra*
P14	A	H. Grebneva	*Causes of Rare Tautomer Forms Stabilization of DNA Bases Under Dimers Formation and DNA Synthesis*
P15	B	H. Grebneva	*Changes in Structure of DNA Bases as one of Reasons of the Untargeted UV-mutagenesis*
P16	A	D. Gront	*Optimizing the Parallel Tempering Monte Carlo method for biomolecular systems - insights from stat. thermodynamics*
P17	B	D. Gront	*BBQ - Backbone Building from Quadrilaterals: An Algorithm That Outperforms Existing Methods*
P18	A	R. Grzywa	*The Molecular Basis of Urokinase Inhibition: From the Analysis of Intermolecular Interactions to the Prediction of Binding Affinity*
P19	A	J. Handzlik	*DFT Study of Molybdena-silica System in Olefin Metathesis*
P20	A	K. Hernik	*cis-Diammine(orotato)platinum(II) - a Cisplatin Analogue. Density Functional Study*
P21	A	J. Hładyszowski	*DFT Study of Dihexanoyle Phosphatidylcholine Monolayer*
P22	A	T. Jaroń	*DFT Studies of Novel Hypothetical Hydrides of Late Lanthanide Metals: Route to high-TC Superconductivity?*
P23	A	A. Kaczmarek	*Experimental and Theoretical Investigations of Spectroscopic Properties of Azobenzene Derivatives in 1,1,2-trichloroetan*
P24	A	J. Kamiński	*Accuracy of Various Approximations to the Non-additive Kinetic Functional in Exactly Solvable Cases*

No.	Session	Main author	Title
P25	A	M. Kluba	*Molecular Basis of Vampirism - Designing Anti-porphyria Drugs*
P26	A	S. Kmiecik	*De Novo Simulations of Protein-folding Pathways in a Reduced Conformational Space*
P27	A	M. Kurciński	*Model of Three-dimensional Structure of the Vitamin D Receptor Bound with Peptide Ligand Mimicking Co-activator Sequence*
P28	A	M. Kwiatkowski	*A Clustering Based Approach to Adsorption Modeling*
P29	B	M. Kwiatkowski	*Computer Analysis of Nitrogen Adsorption Isotherms on Active Carbons by an Employment of the New LBET Class Models*
P30	A	D. Latek	*Theoretically Predicted Contacts and Sparse NMR Data in De novo Protein Structure Prediction*
P31	B	J. Lundell	*Quantum Chemical Studies of Xenon Insertion Compounds of Formic Acid*
P32	A	J. Lundell	*Computational Study of Formic Acid Dimers Involving the Higher-energy Conformer, cis-HCOOH*
P33	A	Ł. Maj	*Design of Ti/Si/H Clusters and Surfaces of Cubic TiSi for Heterolytic Addition of H2*
P34	A	L. Michera	*Theoretical Study of Cisplatin Interactions with Glycine in Gas-phase and Implicit Water Solution – COSMO*
P35	A	P. Miszta	*Homology Modelling of G-protein Coupled Odorant Receptor AgOR1 from Malaria Mosquito Anopheles Gambiae*
P36	A	J. Mrázek	*Computational DFT Study of the Non-heme Iron Center of Photosystem II*
P37	A	J. Murray	*The Two Components of the Activation Energy*
P38	A	W. Niewodniczański	*Electronic Structure of Pyridinium N-phenolate Betaine Dye*
P39	B	S. Orłowski	*Locally Enhanced Sampling Molecular Dynamics Study of the Dioxygen Transport in Human Cytoglobin*
P40	B	A. Panczakiewicz	*Implementation of the QM/QM Method Based on the LocalSCF Algorithm*
P41	B	P. Paneth	*Continuum Solvent Models of Body Fluids on the Example of Serum*
P42	B	Ł. Pepłowski	*Insights Into the Catalytic Activity of Industrial Enzyme Co-Nitrile Hydratase. Docking Studies of Nitriles and Amides*
P43	B	J. Pietkiewicz	*Glycolytic enzyme enolase as a plasminogen receptor: in vitro interaction and theoretical modeling.*
P44	B	Y. Pivak	*Defect Transport Modelling in Monoclinic La(2-x)Pr(x)Ti(2-y)Nb(y)SiO(9+d)*
P45	B	M. Radoń	*Peculiarities of the Electronic Structure of Cytochrome P450 Active Site (Compound I) - DFT and CASPT2 Modeling*
P46	B	P. Rejmak	*Cu(I) Sites in Faujasite and their Interactions with the CO Molecule - Theoretical Studies*
P47	B	M. Rostkowski	*Charge Localization in Monothiophosphate Monoanions*
P48	B	D. Rutkowska-Zbik	*Preliminary Theoretical Studies on TiO2 Anatase System*
P49	B	J. Sebek	*Modeling of Circular Dichroism Spectra of Flexible Peptides in Water Solutions with Using Molecular Dynamics and Quantum Mechanics*
P50	B	W. Szczepanik	*Linear Response Kohn-Sham Equations with Constrained Electron Density Applied to a Nonheme Fe(IV)=O Complex*
P51	B	B. Szyja	*Modeling the Adsorption of Aromatic Compounds on a TiO2/SiO2 Catalyst*

No.	Session	Main author	Title
P52	B	K. Świderek	*Modeling Properties of Iridium Complexes*
P53	B	M. Ullrich	*Modelling of Transition States in Stereoselective Addition of Diethylzinc to Benzaldehyde Catalyzed by N,S-camphor Based Catalysts*
P54	B	Z. Velkov	*Predicted Antioxidant Activity of Amide and , Thioamide of o-Coumaric Acid*
P55	B	P. Wielgus	*Theoretical Description of Ge/Si Microclusters*
P56	A	M. Wiśniewski	*On the Reactivity of Curved Carbon Nanostructures to Amidogen*
P57	B	M. Wiśniewski	*Towards the Reactivity of Carbon to Izoelectronic (Cl- and K+) Adsorbates*
P58	B	T. Zimmermann	*The Interactions of Platinum Complexes with Sulfur-Containing Amino Acids; Theoretical Calculations*
P59	B	A. Zwiefka	*Study of Binding of Pseudomonas aeruginosa Alginate by Toll-Like 4 and CD18 Receptors*