SCIENTIFIC PROGRAMME

Sunday, 1 September 2013

14:00 – 18:00	Registration
18:30 – 20:30	Get-together party

Monday, 2 September 2013

8:30 – 8:50	Opening Ceremony
	Computational chemistry of non-covalent interactions I. Session Chair: **Antonio Lagana**
8:50 – 9:30	**Ibon Alkorta, José Elguero, Janet E. Del Bene** Characterizing a new weak interaction: pnicogen bond
9:30 – 10:00	**Tore Brinck, Joakim Halldin Stenlid** Charge-Transfer Interactions in Halogen Bonds
10:00 – 10:20	**Manuel Yánez, Otilia Mó, Ibon Alkorta, José Elgueo, Al Mokhtar Lamsabhi, M. Merced Montero-Campillo** The Role of Closed-Shell Interaction in Modulating Intrinsic Molecular Properties
10:20 – 10:50	Coffee Break
	Computational chemistry of non-covalent interactions II. Session Chair: **Paul Mezey**
10:50 –11:20	**Stefan Grimme** Supramolecular interactions by dispersion corrected density functional theory
11:20 – 11:40	**Maxim Tafipolski, Bernd Engels** Intermolecular Force Field Parameterization from First Principles
11:40 – 12:00	**Anne-Marie Kelterer, W.M.F. Fabian, F.J. Iftikhar, G. Grampp, G. Uray** The excited state of lactams weakly interacting with the solvent
12:00 – 12:20	**Christian Mück-Lichtenfeld** Visualizing cooperativity: non-additive contributions to the deformation density
12:20 – 12:40	**Johannes Hoja, Alexander F. Sax, Krzysztof Szalewicz** Dispersion Interaction in Systems with Moderate Hydrogen Bonds

12:40 – 14:30	Lunch
	Cutting edge quantum chemistry I. Session Chair: **Géza Fogarasi**
14:30 – 15:10	**Mihály Kállay, Zoltán Rolik, Lóránt Szegedy, István Ladjánszki, Bence Ladóczki** Accurate calculations for large molecules: an efficient local CCSD(T) approach
15:10 – 15:30	**O. Demel, S. Kedzuch, Jozef Noga, J. Pittner** State specific explicitly correlated multi-reference coupled cluster method including perturbative triple-excitations correction
15:30 – 15:50	**Elisa Rebolini, Julien Toulouse, Andreas Savin** Influence of long-range correlation on molecular excitation energies calculated with range-separated TDDFT
15:50 – 16:20	Coffee Break
	Cutting edge quantum chemistry II. Session Chair: **Attila Bende**
16:20 –16:50	**Leticia Gonzalez** Disentangling molecular pathways after light irradiation
16:50 – 17:10	**Freija De Vleeschouwer, A. Chankisjijev, W. Yang, P. Geerlings, F. De Proft** Inverse Molecular Design: Pushing the Boundaries of Intrinsically Stable Radicals
17:10 – 17:30	**Alessandro Genoni** Extremely Localized Molecular Orbitals from X-ray Diffraction Data
17:30 – 17:50	**Itamar Borges** The Electronic and Ionization Specrta of the Energetic Molecule 1,1-Diamino-2,2-Dinitroethylene (Fox-7)
17:50 – 18:10	**Andrei L. Tchougréeff, Richard Dronskowski** RVB Electronic States in Solid State Quantum Chemistry: CuNCN
18:30 – 20:00	Dinner
20:00 – 21:00	Poster Session

Tuesday, 3 September 2013

Computational chemistry of solid states and surfaces I.
Session Chair: **Manuel Yanez**

8:30 – 9:10	**Richard Dronskowski** Thermochemistry of Solid-State Materials from First Principles
9:10 – 9:40	**Steven Parker, M. Molinari, J. Grant, T. V. Shapley, Runliang Zhu** Atomistic simulation of structure, stability and adsorption at oxide and mineral surfaces
9:40 – 10:00	**Balázs Hajgató, S. Güryel, Y. Dauphin, J-M. Blairon, G. Van Lier, H. E. Miltner, F. De Proft, P. Geerlings** Intrinsic Mechanical Properties of Two-dimensional Graphitic Systems: A Computational Study
10:00 – 10:20	**Dario Alfe, Roberto Verucchi, Simone Taioli** Non-adiabatic ab-initio molecular dynamics of Supersonic Beam epitaxy of Silicon Carbide at room temperature
10:20 – 10:50	Coffee Break

Computational chemistry of solid states and surfaces II.
Session Chair: **György Lendvay**

10:50 –11:20	**Marcus A. Neumann, B. Doser** Algorithms for automated crystal structure prediction
11:20 – 11:40	**P. Gamallo, H. Prats, Ramon Sayos** ReaxFF Molecular Dynamics Study of CO Collisions on an O-preadsorbed SiO_2 Surface
11:40 – 12:00	**Nicholas Williams, M. Molinari, S.C. Parker, M. Storr** Atomistic Simulation of Structure and Transport Properties in Polycrystalline UO_2
12:00 – 12:20	**Anuar Aldongarov, I.S. Irgibayeva, H. Agren, K. Hermansson** Optical Properties of Small CdS Nanoclusters
12:20 – 12:40	**M. El Khatib, Stefano Evangelisti, T. Leininger, G.L. Bendazzoli** Finite-Size Effects in Graphene Nanostructures
12:40 – 14:30	Lunch
15:00 –	Excursion (including dinner)

Wednesday, 4 September 2013

Bridging grid- and super-computing for chemical calculations I.
Session Chair: Stefano Evangelisti

8:40 – 9:20	**Elda Rossi** Computational Chemistry and HPC: new technologies for data and computing
9:20 – 9:50	**Thomas Müller** High-End Supercomputers in Quantum Chemistry: Success Story or Failure?
9:50 – 10:10	**Emanuele Coccia, D. Varsano, L. Guidoni** Accurate quantum chemistry calculations for chromophores in photoactive proteins
10:10 – 10:30	**Neil S. Ostlund, Miroslaw Sopek** Applying the Semantic Web to Computational Chemistry
10:30 – 11:00	Coffee Break

Bridging grid- and super-computing for chemical calculations II.
Session Chair: **Ivan Cernusak**

11:00 –11:30	**Gergely Sipos** Bridging grid, cloud, supercomputing and storage resources at a global scale
11:30 – 11:50	**Andrea Lombardi, N. Faginas Lago, M. Bartolomei, A. Lagana** State-to-State Cross Sections and Rate Constants of Energy Transfer and Dissociation of Carbon Oxides in Gas Flows, Earth and Planetary Atmospheres
11:50 – 12:10	**Victor P. Vysotskiy, Valera Veryazov** Adaptation of the Molcas Quantum Chemistry Package to Modern Hardware
12:10 – 12:30	**Daniel Roca-Sanjuán, M. Merchán, R. Lindh** Towards the Understanding of the Chemiluminescence of Luminol
12:30 – 14:30	Lunch

	Computational chemistry of biomolecules I. Session Chair: **Ramón Sayós**
15:00 – 15:30	**Josica Dolenc** Refinement of peptide and nucleic acid structures from solution NMR data using molecular dynamics simulations
15:30 – 16:00	**Roberto Improta** The excited state decay in strongly coupled multichromophore systems: the DNA as a test case
16:00 – 16:20	**Chandan Patel, Celine Dupont, Julian Garrec, Elise Dumont** QM/MM-MD Modelling of Some Complex DNA Lesions: Which Tools? Which Answers? Which Challenges question?
16:20 – 16:40	**Adam Liwo, M. Baranowski, C. Czaplewski, E. Gołaś, Y. He, D. Jagieła, P. Krupa, M. Maciejczyk, M. Makowski, M. Mozolewska, A. Niadzvedtski, S. Ołdziej, H.A. Scheraga, A.K. Sieradzan, A. Śleszyńska, R. Ślusarz, T. Wirecki, B. Zaborowski** A Unified Coarse-Grained Model of Biological Macromolecules Based on Mean-Field Multipole-Multipole Interactions
16:40 – 17:00	Coffee Break
	Computational chemistry of biomolecules II. dedicated to Gábor Náray-Szabó Session Chair: **György Ferenczy**
17:00 – 17:40	**Pavel Hobza** Structure and function of biomacromolecules and their complexes is determined by noncovalent interactions
17:40 – 18:00	**Tamas Beke-Somfai** Hyperfine Tuning in Complex Biomolecular Machines
18:00 – 18:20	**Paul Mezey** The Holographic Electron Density Theorem in Macromolecular Quantum Chemistry
18:20 – 18:40	**Ilona Hudaky, Gábor Náray-Szabó, György Juhász, Rosa M. Ortuno, András Perczel** Structure and stability of beta-peptide foldamers; toward a rational design
19:30 –	Dinner / Celebration of Prof. Náray-Szabó

Thursday, 5 September 2013

Bioinformatics and molecular modelling in drug discovery I.
Session Chair: Andrzej Sokalski

9:00 – 9:40	**Sándor Pongor, Roberto Vera, Zsolt Gelencsér, Dóra Bihary, Balázs Ligeti** Bioinformatics of microbial communication and cooperation: from data-integration to drug design
9:40 – 10:10	**Chris de Graaf** In crystallo, in silico, veritas: Computational prediction of protein-ligand interactions
10:10 – 10:30	**Emma Eriksson, J.P.M. Jämbeck, A.P. Lyubartsev, A. Laaksonen, L.A. Eriksson** Molecular dynamics studies of liposomes as carriers for photosensitizing drugs
10:30 – 11:00	Coffee Break

Bioinformatics and molecular modelling in drug discovery II.
Session Chair: **Gábor Náray-Szabó**

11:00 –11:30	**Slawomir Filipek** Binding of agonists and antagonists to GPCRS
11:30 – 11:50	**Adela Bobovska, J. Kóňa, I. Tvaroška** Building of 3D QSAR Model with DFT interaction energy descriptors for the design of inhibitors of a sugar processing enzyme with a zinc ion co-factor
11:50 – 12:10	**T. Mizushima, T. Kasumi, K. Araki, H. Kobayashi, Noriyuki Kurita** Ab initio molecular simulations for proposing novel peptide inhibitors blocking the ligand-binding pocket of urokinase receptor
12:10 – 12:30	**Andrzej Sokalski, W. Beker, E. Dyguda-Kazimierowicz, P. Kędzierski** Analysis of Theozyme Design Methodology
12:30 – 14:30	Lunch

2nd Workshop on Theoretical Chemistry and Computational Modelling

Thursday, 5 September 2013

First session
Chairman: **Stefano Evangelisti**

15:00 – 15:40 **Antonio Lagana**
Molecular collisions: from understanding to accurate predictions

15:40 – 16:00 **Leon Freitag, Leticia González**
Ab-initio multiconfigurational calculations on $[Ru(bipy)_3]^{2+}$

16:00 – 16:20 **Vijay Gopal Chilkuri, Georges Trinquier, Nadia Benamor, Jean-Paul Malrieu, Nathalie Guihéry**
A strategy to design organic compounds presenting a double exchange phenomenon

16:20 – 16:40 **Ana Martín Sómer, A. Cimas, M.-P. Gaigeot, R. Spezia, M. Yánez**
Reactivity of doubly charged cations in the gas phase: Insights from chemical dynamics and statistical approaches

16:40 – 17.00 **Daryna Smyrnova, Kirill Zinovievs, Benjamien Moeyaert, Peter Dedecker, Arnout Ceulemans, Inaki Tunón, Servaas Michielssens**
Hybrid MD and QM/MM study of the chromophore isomerization in GFP-like proteins Dronpa and mAG

17:00 – 17:30 Coffee break

Second Session
Chairman: **Daniel Roca**

17:30 – 17:50 **Muammar El Khatib, O. Brea, C. Angeli, S. Evangelisti, T. Leininger, G. L. Bendazzoli**
On the total position spread tensor

17:50 – 18:10 **Elisa Rebolini**
Molecular electronic excitation energies with range separated TDDFT

18:10 – 18:30 **Rafael García-Meseguer, Sergio Martí, J. Javier Ruiz-Pernía, Vicente Moliner, Inaki Tunón**
The Role of Protein Structure, Flexibility and Dynamics in Enzymatic Catalysis of a S_N2 Reaction

18:30 – 18:50 **Ana Cunha, N. Melo, A. Vries, S-J. Marrink**
Development of combined multiscaling methods

18:50 – 19:10 **Dumitru-Claudiu Sergentu, Daniel Roca-Sanjuán, Remco W.A. Havenith, Manuela Merchán, Ria Broer**
Revisiting the Intersystem Crossing in Benzophenone

19:10 – 19:30 **Lucy Cusinato, R.W.A. Havenit, R. Broer**
Magnetic interactions in organic-inorganic hybrid copper materials

Friday, 6 September 2013

Third Session

Chairperson: **Ria Broer**

9:00 – 9:20 **Oriana Brea, Manuel Yánez, Otilia Mó, Al Mokhtar Lamsabhi**
Gas phase $[(uracil)_2\text{-}Cu]^{2+}$ complexes stability. Reaction mechanisms for the formation of $[(uracil)_2\text{-}Cu]^{2+}$ and $[(uracil\text{-}H)(uracil)\text{-}Cu]^{+}$ enolic complexes

9:20 – 9:40 **Athanasios Arvanitidis**
Study of the molecular orbitals contribution to the induced magnetic field. The aromaticity concept

9:40 – 10:00 **Angelo Guissani, D. Roca-Sanjuán, M. Merchán**
On the photoinduced formation mechanism of cyclobutane pyrimidine dimers

10:00 – 10:20 **Dariusz Piekarski, S. Díaz-Tendero, F. Martín, M. Alcamí**
Stability and fragmentation dynamics of excited amino acids in gas phase: glycine and beta-alanine

10:20 – 10.40 **Andrii Rudavskyi, C. Sousa, C. Marian, C. de Graaf, R. Broer**
Intersystem crossings in $[Fe(phen)_3]^{2+}$ spin crossover complex

10:40 – 11:00 **Joaquin Calbo, J. Aragó, E. Ortí R. García, M. Roca, I. Tunón**
Hybrid QM/MM protocol to estimate binding free energies for π–π donor–acceptor supramolecular assemblies

Poster presentations

P-01 **Gerard Alcover, Maria-Angels Carvajal, Rosa Caballol, Coen de Graaf**
Spin-Crossover in Ni-porphyrin compounds

P-02 **A.P. Bhati, Dirk Andrae**
Quantum chemistry for complete classes of compounds

P-03 **Juan Aranda, K. Zinovjev, K. Swiderek, M. Roca, I. Tunón**
Reaction mechanism and molecular dynamics analysis of M. Hhai C5-Cytosine-methyltransferase

P-04 **Katharina Boguslawski, Pawel Tecmer, Gergely Barcza, Örs Legeza, Markus Reiher**
Quantum information analysis of bond-formation processes

P-05 **Johan Johansson, Nina Kann, Bengt Nordén, Tamás Beke-Somfai**
CLICKOMER: A combined theoretical and experimental study of δ-amino acid based peptidomimetic foldamers built from 1,5 triazole amino acids

P-06 **Zsuzsanna Benda, Péter G. Szalay**
Details of the excited state potential energy surfaces of adenine by coupled-cluster techniques

P-07 **Attila Bende**
Low-lying excited-states of benzyluracil isomers

P-08 **Agris Berzinš, A. Actinš**
Computational study of the dehydration process of mildronate dihydrate

P-09 **Agris Berzinš, A. Actinš**
Computational study of the intermolecular interaction energies in droperidol solvates

P-10 **Alba Campo-Cacharrón, Enrique M. Cabaleiro-Lago, Jesus Rodriguez-Otero**
Analysis of the interaction between ions and substituted buckybowls

P-11 **Jozef Federič, Ivan Černušák**
Microsolvation of halogen-ammonia ion-pairs

P-12 **Chi-Ruei Pan, Po-Tung Fang, Jeng-Da Chai**
Asymptotic Correction Schemes for Semilocal Exchange-Correlation Functionals

P-13 **J. Chandramohan, G. Ohanessian, C. Clavaguéra**
Structures, dynamics and ir spectra of hydrated tryptamine cluster ions

P-14 **Jennifer C. Crabtree, E.J. Mitchell, S.C. Parker, J.A. Purton**
Adsorption and transport of CO_2 at faujasite surfaces

P-15 **Zsófia Dubrovay**
Can a structural formula correctly represent the real molecular structure?

P-16 **Lisa A. Fredin**
Utilizing DFT to improve understanding of photochemical transition metal complexes

P-17 **Chunxia Gao, James A.L. Brown, Martin Scobie, Thomas Helleday, Leif A. Eriksson, Noel F. Lowndes**
Rational design of a histone acetyltransferase tip60 inhibitor

P-18 **Marcin Górecki, Wojciech Szczepek, Jadwiga Frelek**
Solid-state chiroptical study of linezolid and finasteride

P-19 **Arzu Hatipoglu, Hüseyin Dedeoglu, Zekiye Cinar**
Reactivity descriptors for the degradation reactions of organophosphorous compounds

P-20 **Svante Hedström, P. Persson**
Size-converged properties of light-harvesting polymers obtained by quantum chemistry

P-21 **LeoF. Holroyd, T. van Mourik**
Structure and energetics of the mutagenic dna base analog 5-bromouracil

P-22 **Ionel Humelnicu, Doina Humelnicu**
Non-covalent interactions of aromatic structures in nanotubes

P-23 **Imre Jákli, Attila Móricz, Dóra Papp, András Perczel**
Aromatic-anion interaction in the perspective of a new portable NBO visualization program

P-24 **Petra Kalinovčić, O. Jović, T. Hrenar**
Quantum chemical investigation of 2-(methylideneamino)acetonitrile

P-25 **Pharit Kamsri, A. Srisupan, P. Meewong, A. Punkvang, P. Saparpakorn, S. Hannongbua, P. Wolchann, U. Leartsakulpanich, P. Pungpo**
Elucidating the structural basis of diphenyl ether derivatives as highly potent enoyl-acp redutase inhibitors through molecular dynamics simulations

P-26 **A. Wernbacher, E. Rynkowska, L. Karpenko-Jereb, W. Kujawski, Anne-Marie Kelterer**
Interaction of cation exchange membrane with the solvent methanol and water

P-27 **Marta Knitter, Petter Persson**
Titanium dioxide nanoparticles modeled by quantum chemical methods

P-28 **Balázs Krámos, J. Oláh**
QM and QM/MM calculations reveal the mechanism of final step of the aromatization reaction catalyzed by human aromatase

P-29 **E. Shimizu, R. Hoshino, K. Nomura, V. I. Danilov, Noriyuki Kurita**
Reaction mechanism of DNA base pair with hydroxyl radical: DFT calculations in vacuum and in water

P-30 **Anikó Lábas, B. Krámos, G. N. Nagy, B. G. Vértessy, J. Oláh**
QM and QM/MM study of cation-π interactions

P-31 **Al Mokhtar Lamsabhi, Otilia Mó, Manuel Yánez, Violette Haldys, Jean-Yves Salpin, Jeanine Tortajada, Jean-Claude Guillemin**
Cu^+ reactions with aminoacetonitrile, a potential pre-biological precursor of glycine

P-32 **Marco Lerario, Alexandre L. Magalhaes**
A study of interaction potentials for H_2 adsorption in SWNT: a possible way to more realistic predictions

P-33 **Yuan Liu, Annika Lenz, Lars Ojamäe**
IR Spectra of $(H_2O)_{100}$ and Contributions from Specific H-Bond Topologic Configurations Studied by DFT Calculationations

P-34 **Ayyaz Mahmod, Ricardo Luiz Longo**
Structure of 1-Benzyl-5-amino-1H-tetrazole studied by X-ray diffraction, DFT calculations, NMR, FTIR and UV-visible spectra

P-35 **S. Maintz, V. L. Deringer, A. L. Tchougréeff, R. Dronskowski**
Projecting local chemical information from delocalized plane-wave calculations

P-36 **Alpeshkumar K. Malde, Alan E. Mark**
Validation of ligands in X-ray crystal structures: Molecular Dynamics simulations and Free Energy calculations

P-37 **Gergely Matisz, A. Wernbacher, A-M. Kelterer, W. M. F. Fabian, S. Kunsági-Máté**
Liquid structure of methanol – water binary mixture – a theoretical study

P-38 **James L. McDonagh, David S. Palmer, Tanja van Mourik, John B. O. Mitchell, Maxim V. Fedorov**
A First Principles Prediction of Intrinsic Aqueous Solubility of Crystalline Drug-like Molecules

P-39 **Paul McKeown, J.C. Crabtree, V. P. Ting, T. J. Mays, S. C. Parker**
Molecular Modelling of Hydrogen Storage in Nanoporous Materials

P-40 **Satoshi Miyagi, Kyoshiro Murata, Mitsuko Ishihara-Sugano, Satoshi Itoh, Noriyuki Kurita**
Specific interactions and dimerization mechanism between aryl hydrocarbon receptor and co-factor protein: classical MD and *ab initio* FMO simulations

P-41 **Antonio Monari**
Photophysics of Chromophores Interacting with Biological Macromolecules: TD-DFT and QM/MM

P-42 **Salvador Moncho, E. N. Brothers, B. G. Janesko**
Density functional's performance in modeeling the decomposition of CH_3OH by Cu_4 clusters

P-43 **Marc Mulet-Gas, N. Cheng, A. Rodríguez-Fortea, L. Echegoyen, J. M. Poblet**
Electronic structure and stabilization of non-IPR sulfide cluster fullerenes

P-44 **Akisumi Okamoto, A. Yano, K. Nomura, S. Higai, N. Kurita**
Global search for stable conformation of amyloid-β peptide in explicit water by replica exchange MD simulations combined with *ab initio* MO method

P-45 **Marta K. Olszówka, M. Musiał**
Multireference coupled cluster study of molecular and atomic oxygen

P-46 **J. Noga, Gabriela Orešková, J. Šimunek**
Quantum-chemical calculation of geometry and spectral properties of glycolato peroxido complex of vanadium (V) with $[Zn(H_2O)_6]^{2+}$ cation

P-47 **Hiroki Otaki, K. Ando**
Dipole induction and isotope effect on dielectric phase transition in hydrogen-bonded molecular crystal

P-48 **K. Csankó, B. Tolnai, P. Sipos, O. Berkesi, István Pálinkó**
Structural features of heteroatom-containing cinnamic acid dimers and their extended, hydrogen-bonded aggregates

P-49 **Predrag V. Petrović, Jean-Pierre Djukic, Stefan Grimme, Snežana D. Zarić**
On the self-agregation of oxaliplatin in solution and in the gas phase: experimental and theoretical investigations on the origins of self-association.

P-50 **Tadeusz S. Pluta, M. Kolaski, J. Kauczor**
Excitation energies and electric properties of the excited states of the PNA molecule

P-51 **Yulia G. Polynskaya, D.A. Pichugina, N.E. Kuz'menko**
Oxygen interaction with silver clusters and bimatallic gold-silver cluster

P-52 **Eszter S. Pós, György Tarczay, Péter G. Szalay**
Matrix-isolation uv and computational study of the excitation spectrum of adenine

P-53 **Maitreyi Robledo, Sergio Díaz-Tendero, Fernando Martín, Manuel Alcamí**
Charge transfer in molecules and ultrathin insulating films deposited on metal surfaces

P-54 **Fabiola E. Medina, Jesus Rodriguez-Otero, Enrique M. Cabaleiro-Lago**
Interaction between halogen anions and heterasumanenes

P-55 **Kai I. Ruusuvuori, P. Hietala, O. Kupiainen, T. Kurtén, H. Vehkamäki**
The charging of amine containing clusters using protonated acetone

P-56 **Sergi Saureu, Coen de Graaf**
The role of the solvent effects on the electronic transitions in Fe^{II} and Ru^{II} complexes

P-57 **Paweł Artur Siuda, J. Sadlej**
NMR shielding constants of methane and carbon dioxide clathrate hydrates

P-58 **Paweł Artur Siuda, J. Sadlej**
Nucleation and growth of methane clathrate hydrate crystal - molecular dynamics study

P-59 **Ján Skoviera, Ivan Cernusák, Florent Louis**
Structure and reactivity of Cs_xH_y clusters

P-60 **Sriraj Srinivasan, Robert G. Syvret**
Fluorination over Chromium Oxide Catalyst to Produce Hydrofluoroolefins: a Quantum Chemical Study

P-61 **Maria Sudolská, L. Cantrel, I. Černušák**
Complexes of Cs, CsOH, CsI and Cs_2I_2 with water

P-62 **Borys K. Szefczyk, R. Roszak**
First-principlesmolecular dynamics simulations of $NaYF_4$ hexagonal phase

P-63 **Tibor Szilvási, T. Veszprémi**
How to synthesize reactive species: the case of hexasilabenzene and hexagermabenzene

P-64 **Attila Tajti, György Lendvay, Péter G. Szalay**
Theoretical investigation of the singlet oxygen dimer using multi-reference Techniques

P-65 **Guido Todde, S. Hovmöller, A. Laaksonen, F. Mocci**
Glucose oxidase from Penicillium amagasakiense: a Molecular Dynamics study of its stability.

P-66 **C. Selçuki, Gülin Ürgenç**
Investigation of the reactions of hydroxyl radical with glycine and alanine by computational methods

P-67 **Romain Vandeputte, Florent Louis, Laurent Cantrel**
Thermochemistry of $Cs_xB_yO_z$ compounds and microsolvatation of $CsBO_2$

P-68 **Jonas Boström, Victor P. Vysotskiy, Valera Veryazov**
Constrained fragment optimization in internal coordinates

P-69 **Min Wu, Ake Strid, Leif Eriksson**
Prediction of the three-dimensional structure of the plant uvr8 photoreceptor dimer, and the key residues in UV-B regulated signalling pathway

P-70 **Z.N. Ling, S. Yue, I.K.S. Yap, Wai Keat Yam**
Molecular docking simulation of ganoderic acid compounds on anti-hypertensive targets

P-71 **Stephen R Yeandel, M. Molinari, S.C. Parker, D.C. Sayle, R. Freer**
Atomistic Simulation of Thermoelectric Oxides

P-72 **Yahya Yasin Yilmaz, C. Selcuki**
Effect of implicit and explicit solvent models on the zwitterionic form of anserine