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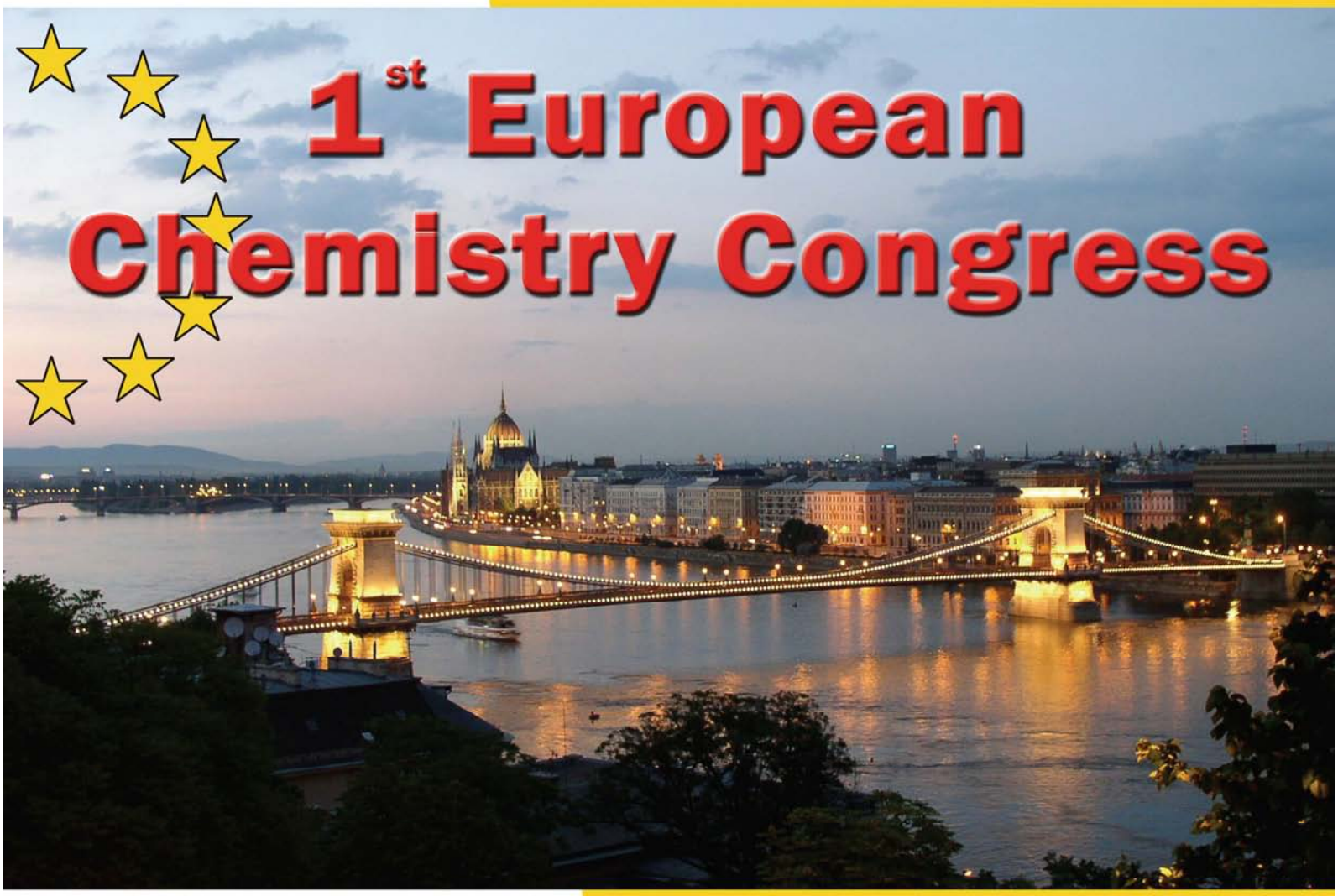

1st European Chemistry Congress

27-31 August 2006 Budapest, Hungary

ABSTRACT BOOK

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P-PO-45 **UNRAVELLING SUBSTRATE SPECIFICITY & FLEXIBILITY IN BINDING POCKETS OF THE TGT SYSTEM.** Naomi Tidten, Christoph Sotriffer, Hans-Dieter Gerber, Bernhard Stengl, Klaus Reuter, Gerhard Klebe, *Philipps-Universität Marburg, Institute of Pharmaceutical Chemistry, AG Klebe, Marbacher Weg 6, 35032 Marburg, Germany, tidten@staff.uni-marburg.de*

Keywords: tRNA-guanine transglycosylase (TGT); Molecular dynamics simulation

tRNA-guanine transglycosylases (TGT) - present in all three kingdoms of life - catalyze a base exchange reaction in tRNA anticodon loops. In eubacteria, the mechanistic pathway of the guanine exchange towards the modified base preQ1 is well characterized due to elaborate studies of Zymomonas mobilis TGT. As TGT plays a key role in pathogenicity of Shigella flexneri, the causative agent of bacterial dysentery, it has been established as a target for structure-based drug design.

However, eukaryotes also possess a TGT highly homologous to the eubacterial one. In an analogous reaction the base queuine is incorporated into tRNA. Hence, it is of utmost importance to study selectivity-determining features.

Since no crystal structure of an eukaryotic TGT is yet available, we genetically engineered a human TGT binding pocket based on Z. mobilis TGT. The crystal structure was determined at high resolution. As the mutated TGT showed enzymatic activity as well it seems to be appropriate to treat it as a model system for human TGT binding pockets.

To probe structural and dynamic effects of the mutations, MD simulations were performed, providing insights into flexibility within TGT binding pockets.

P-PO-46 **REBINDING MOLECULAR DYNAMICS SIMULATIONS OF NITRIC OXIDE TO THE V68F MIOGLOBIN MUTANT.** Stefka Tsintsarska, Markus Meuwly, *Department of Chemistry, University of Basel, Stefka.Tsintsarska@unibas.ch*

Keywords: molecular dynamics; myoglobin; ligand rebinding

The study of reactive processes in chemically and biologically relevant systems is a topic of much current interest. Here, an atomistically detailed picture of NO rebinding from myoglobin V68F is presented. Using reactive molecular dynamics (RMD) [1] the rebinding probability as a function of time after dissociation is calculated. RMD considers two intersecting potential energy manifolds which dissociate to different adiabatic states. During the simulations, crossings are detected by monitoring an energy criterion and the surfaces are mixed over a finite number of time steps. The unbound surface (Fe...NO) is a standard force field, whereas the bound surface (Fe-NO) is based on ab initio calculations.

The rebinding is nonexponential in time, in agreement with experimental studies,[2] and can be described using two time constants. Particular emphasis is paid to the asymptotic separation Delta between the two potential energy manifolds. An extension of the original RMD approach with a conformationally varying Delta is discussed.

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P-PO-47 **GLYCOSAMINGLYCAN BINDING AFFINITY AND AVIDITY RESOLVED FROM VACCINIA VIRAL ENVELOPE PROTEIN A27L/HEPARIN INTERACTIONS.** Der-Lii M. Tzou, Min-Hsiang Yang, Yu-Chang Peng, Feng-I Chu, Yu Ho, Jye-Chian Hsiao, Wen Chang, *Institute of Chemistry, Academia Sinica, tzou@ccvax.sinica.edu.tw*

Keywords: vaccinia virus; avidity; heparin

Vaccinia virus envelope protein A27L interacts with glycosaminoglycan (GAG), predominantly heparan sulfate (HS), on cell surface to facilitate the attachment of virions onto host cells. The wild-type A27L protein forms a stable trimer and the self-assembly is mediated by hydrophobic interaction of the coiled-coil domain at the C-terminus. A Lys/Arg enriched random coil segment at the N-terminus is the GAG-binding site (GBS) as responsible for the multivalent interaction with HS. In this study, we have employed site-directed mutagenesis to construct a series of A27L mutant covering a wide variety of degree of oligomerization. The HS binding ability of these mutants was determined by either sPR or ITC. We here report a strong linear correlation derived from a semi-logarithmic plot of heparin binding constant versus degree of oligomerization. As indicated by linear curve fitting, the intercept of the y-axis represents intrinsic GBS binding affinity, and the slope is a measure of the heparin binding avidity. Here, we sough to resolve the GAG binding affinity and avidity of the vaccinia viral envelope protein A27L upon interaction with heparin.

P-PO-48 **STRUCTURAL FEATURES OF LIPOPOLY-SACCHARIDE FROM PISCIRICKETTSIA SALMONIS, THE CAUSATIVE AGENT OF SALMONID RICKETTSIAL SEPTICEMIA.** Pavol Vadovic, Marcela Fodorova, Marianne Bordevik, Ludovit Skultety, Rudolf Toman, *Institute of Virology, Slovak Academy of Sciences, 845 05 Bratislava, Slovakia, virutoma@savba.sk*

Keywords: Piscirickettsia salmonis; lipopolysaccharide; composition and structure

Piscirickettsia salmonis infects a wide range of salmonid species and causes a systematic infection that targets kidney, liver, spleen, heart, intestine, ovary, and gills of salmonids. Pleomorphic, predominantly coccoid bacteria that range in diameter from 0.5 to 1.5 micrometer are found within cytoplasmic vacuoles of cells from infected tissues. The major carbohydrate antigen of the bacterium is thought to be a lipopolysaccharide (LPS) but its composition and structure are unknown. Using a conventional hot phenol-water method, an LPS was isolated from P. salmonis. SDS-PAGE electrophoresis did not show a ladder-like banding pattern typical for enterobacterial LPSs but indicated the presence of a core region LPS. Compositional analyses revealed the presence of mannose (Man), glucose (Glc), galactose (Gal), L,D heptose (Hep), and glucosamine (GlcN) in a molar ratio 3.0:4.8:3.0:1.0:0.4, respectively. Methylation-linkage analysis indicated mainly the presence of terminal Man and Glc, 6-linked Glc and Gal, and 2,3- and 3,6-di-substituted hexoses that could not be specified in a more detail thus far. It appears that some of hexose residues are heavily phosphorylated. More detailed studies are in progress.

P-PO-49 **A LFER STUDY OF 4-PHENYL-2,4-DIOXOBUTANOIC ACID DERIVATIVES PROTOLYTIC EQUILIBRIA IN ACIDIC SOLUTIONS.** Tatjana Z. Verbic, Branko J Drakulic, Mire F Zloh, Jovana R Pecelj, Gordana V Popovic, Ivan O Juranic, *Faculty of Chemistry, University of Belgrade, P. O. Box 158, 11000 Belgrade, Serbia and Montenegro, tatjanad@chem.bg.ac.yu*

Keywords: acidity constants; 4-Phenyl-2,4-dioxobutanoic acid derivatives; LFER

P

4-Phenyl-2,4-dioxobutanoic acid derivatives exert widespread biological activities. Targeting the HIV-1 integrase is among the most important ones. By the appropriate structural modifications on the phenyl ring, a different type of biological activity was assessed. Part of the current studies of physico-chemical profiling of these compounds describes the protolytic equilibria of 11 4-phenyl substituted derivatives (limited set) in acidic aqueous solutions. These compounds simultaneously exist in two enolic forms (conformationally locked by the pseudo-ring) and one diketo form (two rotatable bonds responsible for the conformational flexibility). The carboxylic group ionization distorts it from the plane of the rest of the molecule in enolic forms. H NMR spectra (278 K, pH<5) proved the existence of all tautomeric forms. Using extended Hammet correlation, determined pKa values were correlated with literature sigma R and I values. Predicted pKa are in good accordance with those experimentally obtained. Inductive effect is the main term that influences transmission of substituent effects from phenyl ring to carboxylic group, as expected according to previously discussed conformations of existing molecular and anionic tautomeric forms.

P-PO-50 **STRUCTURAL CHANGES INDUCED BY NICKEL BINDING TO THE N-TAIL OF HISTONE H4: AN NMR STUDY.** Maria A. Zoroddu, Serenella Medici, Massimiliano Peana, *University of Sassari, zoroddu@uniss.it*

Keywords: histone H4; nickel ions; NMR study

Carcinogenicity of certain nickel compounds has been confirmed by the combination of epidemiological evidence in humans and carcinogenesis bioassays in animals. We have previously reported that nickel is a potent suppressor of histone H4 acetylation in both yeast and mammalian cells. We have recently carried out a study on the coordination ability of Ni(II) to the N-terminal tail of histone H4 by the use of multidimensional NMR techniques (1D, 2D TOCSY and NOESY spectra) [1]. The data thus collected allowed us to calculate a structural model for the square planar complex formed by the Ni(II) ion and our peptide, pointing out the important structural changes induced by nickel coordination on the peptide.

Reference

[1] CERM (University of Florence) and Prof. Bertini are gratefully acknowledged for the use of NMR facility.

P-PO-51 **FLUORESCENT INOSITOL ANALOGS FOR PROBING CELLULAR SIGNAL TRANSDUCTION PATHWAYS.** Hervé Bazin, Olivier Hernout, Françoise Chrétien, Emmanuel Bourrier, Eric Trinquet, Yves Chapleur, Gérard Mathis, *CIS biointernational DRD/M/HTRF, BP 84 175, F-30204 Bagnols/Ceze Cedex, France., hbazin@cisbiointernational.fr*

Keywords: lanthanides; cyclitols; immunofluorescence

New D-myo-inositol-1-phosphate analogs bearing an aminolinker attached to the C-2 or C-3 position were synthesized. Camphor acetal was used for optical resolution and transient protection of the 2,3-diol. The introduction of the aminolinker was made by opening of a 2,3-cyclic carbonate ring thus generating two isomeric IP1 analogs which were separated on RP-HPLC. Both C-2 and C-3 analogs were conjugate to BSA and used to raise monoclonal antibodies which were shown to be specific for D-myo-inositol-1-phosphate. A Homogeneous Time Resolved Fluorescence (HTRF) assay was designed to probe the phospholipase C coupled receptors pharmacology through the monitoring of D-myo-inositol-1-phosphate accumulation into living cells. The method is particularly relevant in the domain of High Throughput Screening.

P-PO-52 **THE ELECTROCHEMICAL AND MOLECULAR DYNAMICS STUDY OF ALIPHATIC-ALIPHATIC INTERACTIONS IN COPPER(II) AMINO ACID COMPLEXES**. Gina Branica, Jasmina Sabolovic, *Institute for medical research and occupational health, Ksaverska cesta 2, Zagreb, Croatia, gbranica@imi.hr*

Keywords: steric hindrance; force field; cyclic voltammetry

Copper amino acidates are considered to be good models of active sites of copper containing redox enzymes. This paper deals with the cyclic voltammetry of bis-copper complexes with aliphatic L-amino acids and their N-dimethyl derivatives in aqueous solution. The influence of N-dimethyl substitutents and of aliphatic amino acid residues on the redox behaviour of the complexes were investigated under physiological conditions (0.15 mol/L). All studied complexes showed two-electron and quasi-reversible electrochemical reactions. Lower stabilities deduced from the redox potential were obtained for the dimethylated than for unsubstitued copper complexes, as we expected [1]. However, bis(L-leucinato)copper(II) showed the lowest stability and its N,N-dimethyl derivative the highest stability among the complexes with natural and dimethylated amino acids, respectively. To examine whether different electrochemical behaviour can be explained with sterical reasons and aliphatic-aliphatic interactions, the molecular dynamics calculations using the force field developed for copper(II) amino acidates [2] are attempted in aqueous medium.

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P-PO-53 **NEW CHIRAL PEPTIDE NUCLEIC ACIDS BEARING A DIPEPTIDE-MIMIC MONOMER WITH TWO LYSINE-DERIVED STEREOGENIC CENTERS.** Stefano Sforza, Tullia Tedeschi, Roberto Corradini, Arnaldo Dossena, Rosangela Marchelli, *Department of Organic and Industrial Chemistry, University of Parma, Parma, Italy., arnaldo.dossena@unipr.it*

Keywords: peptide nucleic acids; DNA recognition; chirality

Peptide Nucleic Acids (PNAs) are oligonucleotide analogues with a pseudopeptide backbone first indtroduced in 1991 by Nielsen and coworkers. A huge number of applications, both in diagnostic and in therapeutic fields, have been reported in the literature since PNA first appearance and many modifications of the original achiral backbone have been introduced.

In this communication we present the DNA binding abilities of PNA bearing in the middle of the strands monomeric units with two lysine-based stereogenic centers. Melting temperatures of these PNAs bound to their complementary DNA strands and CD spectra of the duplexes demonstrated that the configurations of the stereogenic centers determine the preferential helicity of the PNA strand and that the DNA binding affinities are strictly related to the extent of the preference for the right-handed helical conformation in the PNA strand, being the DNA helix right-handed.

Moreover, by inserting two stereogenic centers per PNA monomeric unit a PNA bearing a peptide sequence "embedded" in the pseudopeptide backbone can be obtained, thus achieving a "double-face" molecule behaving at the same time like a peptide and like an oligonucleotide.

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