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VABILO NA SERIJO PREDAVANJ LJUBLJANA - BENETKE (UL FKKT - Dipartimento di Scienze Molecolari e Nanosistemi, Università Ca' Foscari, Venezia)

"Pure and applied organic synthesis: a greener and more sustainable approach"

Predavanja bodo potekala 9. in 10. 4. 2015 v predavalnici P4 (3. nadstropje) na UL FKKT, Večna pot 113, po sledečem razporedu:

Četrtek, 9. 4. 2015:

14:00: Prof. Oreste Piccolo: *Innovation and sustainability in the synthesis of fine chemicals: issues, strategy and process evaluation.*

15:00: Marko Krivec and Marijan Kočevar: *Darco KB as a green catalyst for dehydrogenation.*

15:25: Aljoša Bolje and Janez Košmrlj: *Transition metal complexes with chelating triazolium N-hetorocyclic carbene ligands and their application in catalysis.*

15:50: *General discussion*

Petek, 10. 4. 2015:

10:00: Prof. Stefano Paganelli: *Hydrogenation and hydroformylation in water or in aqueous two-phase conditions: research contribution at Ca'Foscari Venice University.*

11:00: Jure Vajs and Janez Košmrlj: *Antibacterial activity of triazenes against Methicillin Resistant Staphylococcus Aureus and Mycobacterium Smegmatis.*

11:25: Luka Rejc and Andrej Petrič: *Cross-coupling reactions in the synthesis of molecular probes.*

11.50—14:00: *Informal discussion, lunch time.*

14:00: Prof. Oreste Piccolo: *More than thirty years of research and consulting activity for a sustainable synthesis of "Fine Chemicals": some examples of industrial realizations and new paths to explore.*

15:00: Gregor Strle and Janez Cerkovnik: *Simple and efficient catalytic generation of pure solution of hydrogen trioxide (HOOOH).*

15:25: Martin Gazvoda and Janez Košmrlj: *Recent advances in a selected carbon-carbon bond formation reaction.*

15:50: *General discussion; concluding remarks.*

W*orking group meeting and further plans for cooperation:*

16:15: Vikas D. Rathod, Oreste Piccolo and Stefano Paganelli: *Synthesis of fine chemicals, such as pharmaceuticals, agrochemicals, fragrances, by using catalytic reactions under homogeneous, heterogeneous and biphasic reaction conditions.*

Vikas D. Rathod and Marko Krivec: *Application of microwaves for the synthesis of pharmaceutical products: Preliminary results of cooperation Ljubljana – Venice.*

Vljudno vabljeni!

Prof. Marijan Kočevar (contact person) ***Prof. Matjaž Krajnc, Dean***

Ljubljana, 30. 3. 2015

Professor Stefano Paganelli
Università Ca' Foscari, Venezia, Italy

"Hydrogenation and hydroformylation in water or in aqueous two-phase conditions: research contribution at Ca'Foscari Venice University".

Abstract:

Homogeneous catalysis is an efficient tool to carry out hydroformylation and hydrogenation processes but the major drawback is represented by the separation of the expensive catalyst from the product mixture. Processes involving environmentally benign solvents, as water for instance, and easily recyclable water soluble catalysts are highly desirable for the realization of a more green sustainable chemistry [1-2]. Besides phosphines as TPPTS, many other new ligands and/or surfactants having different hydrophilic groups such as –COOH, NR_3, -OH, etc. have been designed to prepare new water-soluble catalytic precursors [3]. It is known that also natural compounds, such as aminoacids, peptides, proteins and sugars are able to bind metallic species and maintain them soluble and active in water [4, 5].
The presentation will discuss the results obtained in the hydroformylation and hydrogenation reactions catalyzed by new water soluble Rhodium- and Iridium-based complexes containing ligands as the protein Human Serum Albumin (HSA) [6, 7], thioaminoacids [8], the oligopeptitede [(S)-1-[(S)-3-mercapto-2-methylpropanoyl]pyrrolidine-2-carboxylic acid] (an ACE inhibitor named Captopril®) [9] and a very simple molecule as the dihydrothioctic acid (DHTA) [10].

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Professor Oreste Piccolo
Studio di Consulenza Scientifica, 23896 Sirtori (LC), Italy

"Innovation and sustainability in the synthesis of fine chemicals: issues, strategy and process evaluation".

Abstract:
A possible simplified strategy to adopt when you want to transform a project from the idea to the industrial realization is presented. It is based either on the state of art [1,2] or own direct experience of consulting activity with many fine chemicals companies. The analysis includes general considerations in the field of fine chemicals (in particular active pharmaceutical ingredients), process cost evaluation, relevance of IP issues and marketing requests, possibility of technological innovation and waste minimization,…. Some case studies of industrial preparations of enantiopure API or intermediates [3-6], such as for example Carnitine [7], Tolterodine [8], Pregabalin [9],… taken by the literature or by my work, with comparison of different stereotechnological approaches, are shown and discussed.

Some references:
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"More than thirty years of research and consulting activity for a sustainable synthesis of "Fine Chemicals": some examples of industrial realizations and new paths to explore".

Abstract:
Catalysis is an important tool to produce very often chemicals in a more sustainable way, in agreement with the principles of Green Chemistry [1-3]. My contribution and experience in some homogeneous and heterogeneous chemo- and bio-catalysis, working with many colleagues and co-workers, are here shown and exemplified [3-17]. Other examples are reported in the lecture of prof. Paganelli, during this meeting. In detail, very efficient enantioselective industrial applications are described, in particular some hydrogenations with [Ru](TMBTP), where TMBTP is a member of the family of atropisomeric bis-heterocyclic diphosphine [5]. Then, the comparison between commercial and home-made , easily prepared and with a low content of precious metal, heterogeneous catalysts is made; 0.18% Rh/alumina was prepared and used in the synthesis of an non-steroidal anti-inflammatory drug , Nabumetone, on multi-ton scale[6]; very recent, not yet published, results with this catalyst and similar metallic species are also presented. Later, some interesting applications of base [3,7] and acid [8-10,17] catalysts as well as advantages and issues working with some free [4] or immobilized [16] enzymes are described. Finally a new laboratory approach to use microorganisms to prepare and use biogenerated metallic species, embedded in a polysaccharidic structure, with catalytic [12,13] and biological properties, to implement in the next future for scaling-up is also presented. The main purpose of this lecture is to encourage, if possible, discussions and future collaborations in the field of applied catalysis.

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