



# **Gdansk, 16-19 September 2019**

## **Novotel Gdansk Marina Hotel**

### **Monday, September 16<sup>th</sup>**

16.00 19.00 **Registration**

19.30 21.00 **Welcome Drink + Dinner**

### **Tuesday, September 17<sup>th</sup>**

#### **Breakfast**

9:00 9:10 **Opening remarks** R. Dutkiewicz M. Piccioli

**Session 1 Chair:** Rafal Dutkiewicz

9:10 9:45 **Keynote 1** Jaroslaw Marszalek

9:45 10:05 **Oral 1** Annalisa Pastore

10:05 10:25 **Oral 2** Carlos Acevedo-Rocha

10:25 10:45 **Oral 3** Wilfred Hagen

10:45 11:10 **Coffee break**

**Session 2 Chair:** Antonio J. Pierik

11:10 11:30 **Oral 4** Salvatore Adinolfi

11.30 11:50 **Oral 5** Smilja Todorovic

11:50 12:10 **Oral 6** Pawel Lipinski

12:10 12:30 **Oral 7** Simone Ciofi-Baffoni

13.00 14.30 **Lunch**

**Session 3 Chair:** Eva Horakova

14:30 14:50 **Oral 8** Marie-Pierre Golinelli

14:50 15:10 **Oral 9** Hubertus Haas

15:10 15:30 **Oral 10** Christine Cavazza

15:30 15:50 **Oral 11** Kerstin Gari

15:50 16:20 **Coffee break**

**Session 4 Chair:** Mario Piccioli

16:20 16:40 **Oral 12** Oliver Stehling

16:40 17:00 **Oral 13** Katarzyna Sikorska

17:00 17:20 **Oral 14** Georgios A.Spyroulias

17:20 17:55 **Keynote 2** Sandrine Ollagnier de Choudens

20.00 **Dinner**

## Wednesday, September 18<sup>th</sup>

### Breakfast

**Session 5 Chair:** Sandrine Ollagnier de Choudens

9:00 9:35 **Keynote 3** Silke Leimkuehler

9:35 9:55 **Oral 15** Antonio J. Pierik

9:55 10:15 **Oral 16** Kostas Tokatlidis

10:15 10:35 **Oral 17** Rachel Nechushtai

10:35 11:25 **Coffee break. Group Photo**

**Session 6 Chair:** Kostas Tokatlidis

11:25 11:45 **Oral 18** Eva Horakova

11:45 12:05 **Oral 19** Jelena Bogdanovic Pristov

12:05 12:25 **Oral 20** Jordi Tamarit Sumalla

12:25 12:45 **Oral 21** Kourosch Honarmand-Ebrahimi

12:45 13:05 **Oral 22** Daili J Aguilar Netz

13:05 14:30 **Lunch**

14:30 16.00 **Poster Session**

**Session 7 Chair:** Oliver Stehling

16:00 17:00 **Flash Talk Session**

Marila Alfano

Francesca Camponeschi

Maria Teresa Pellicer

Maria Politi

Ines Trindade

Milan Zizic

17:00 17:20 **Oral 23** Benoit D'Autréaux

17:20 17:40 **Oral 24** Ana Carolina Cordeiro

17:40 18:00 **Oral 25** Peter Leon Hagedoorn

18:00 18:35 **Keynote 4** Miroslaw Cygler

20:00 24:00 **Banquet**

## Thursday, September 19<sup>th</sup>

### Breakfast

7.00 12.00 **Departures**

8.30 11.30 **Management Committee Meeting**

### Closure

# Structure of biliverdin and its interaction with copper

ORAL presentation

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The structure of biliverdin (BV) and its complexation capacity with  $\text{Cu}^{2+}$  in dependence of solvent choice has been examined. We first examined coordinate/redox interactions of BV with  $\text{Cu}^{2+}$  in phosphate buffer at pH 7.4, using spectrophotometry, HESI-MS, Raman spectroscopy, <sup>1</sup>HNMR, EPR, fluorimetry, and electrochemical methods. BV formed a stable coordination complex with copper in 1 : 1 stoichiometry. The structure of BV was more planar and energetically stable in the complex. The complex showed strong paramagnetic effects that were attributed to an unpaired delocalized  $e^-$ . The delocalized electron may come from BV or  $\text{Cu}^{2+}$ , so the complex is formally composed either of BV radical cation and  $\text{Cu}^{1+}$  or of BV radical anion and  $\text{Cu}^{3+}$ . The complex underwent oxidation only in the presence of both  $\text{O}_2$  and an excess of  $\text{Cu}^{2+}$ , or a strong oxidizing agent, and it was resistant to reducing agents. The biological effects of the stable BV metallocomplex containing a delocalized unpaired electron should be further examined, and may provide an answer to the long-standing question of high energy investment in the catabolism of BV, which represents a relatively harmless molecule per se. The complex possibility was quite different after changing the solvent. BV structure in DMSO was analyzed by using NMR techniques and unrestricted density function theory simulations to explain the incapacity of BV to build coordination complex(es) with  $\text{Cu}^{2+}$  in dimethyl sulfoxide, which was confirmed by UV-Vis, EPR and NMR spectroscopy. NMR showed that N atoms of BV are protonated in all four pyrrole rings. The structure is stabilized by two hydrogen bonds between NH moieties and carbonyl oxygens from opposite terminal pyrrole rings, and by the bending of propionyl chain with carboxyl group out of the plane toward central position of BV. The simulations of deprotonated BV, which builds copper complexes in water and chloroform as described previously, showed a different conformation and organization of hydrogen bonds. Taking into account that deprotonation represents a critical step in coordinate bonds formation, the protonation of an additional N atom may represent a key difference between the interactions of BV with copper in different solvents.