Third Annual Meeting
CA15135

BOOK OF THE ABSTRACTS

COST ACTION CA15135

MuTaLig & Companies: the multi-targeting drug discovery with implications at industrial level

University of Malta - Campus Historical building
Saint Paul street, Valletta (Malta)

www.mutalig.eu

INTRODUCTION

The MuTaLig COST Action aims to link interactions among highly-qualified research teams working in the emergent Medicinal Chemistry branch, known as multi-target or poly-pharmacology. Started in 2016, our COST Action has passed over the "turning point". Therefore, to start properly the second part of our four year activities, the third annual meeting has been designed to treat a special issue related to the involvement of industrial partners in the MuTaLig COST Action. Experts from known EU companies will present their activities in plenary talks, depict the impact of the multi-target drug discovery issue and contribute in the development of this field. All MuTaLig community will be involved to push the scientific activities toward the application, possibly at industrial level. Taking into account the special issue "Multi-Target Drug Discovery: an opportunity for novel and repurposed bioactive compounds" currently running on the prestigious European Journal of Medicinal Chemistry, the meeting will host also a plenary lecture of the associate editor Prof. Paola Barraja. Moreover, 20 short oral and 48 poster communications from experts within the European countries adhering the MuTaLig COST Action will enrich the intensive program, that will be closed with round table about the central topic of the meeting. Thanks to the availability of Dr. Claire Shoemake and Prof. David Magri, our two MC Malta Members, to organize it, the conference is fixed in two days: October 18th - 19th 2018. The location is the historical University building, within the beautiful center of Valletta, recently nominated 2018 European Capital of Culture. The meeting participation is free (no fee), limited to 125 participants registered on the e-cost platform and properly invited from it. All additional updates will be posted at www.mutalig.ue.

As Chair of this COST Action, I want to express my gratitude especially to the local organizers and LOS, to their local team, to the Grant Holder from University of Porto (Prof. Fernanda Borges and Dr. Joana Maria Neves Moreira Abrantes) and to the COST Association (Dr. Lucia Forzi, Science Officer and Dr. Svetlana Voinova, Administrative Officer) for their efforts in the meeting organization. A special thank is also due to Dr. Antonio Lupia (Università "Magna Græcia" di Catanzaro, Italy) for the support in the organization of this abstract book.

I wish a fruitful and stimulating annual meeting to all participants!

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Local Organizing Committee

Claire Shoemake

David Magri

Acknowledgments

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Poster communication 14

Pd(II) complexes with N-heteroaromatic hydrazones as dual targeting DNA/Topoisomerase 1 agents: experimental and *in silico* study

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Anticancer activity of five Pd(II) pyridine-based hydrazone complexes (**1**–**5**, Figure 1) was investigated against a human monocytic leukemia THP-1 (2D) cell line and a breast cancer MCF-7 (2D and 3D) cell line. For complexes with apoptosis as a mechanism of anticancer activity, further investigation revealed that they arrest the cell cycle in G0/G1 phase, induce ROS and *in vitro* inhibit topoisomerase I in a low micromolar range. *In silico* studies corroborate experimental findings and indicate binding to DNA's minor groove. The most active compounds are suitable to be transported *via* blood stream by human serum albumin, as results of CD and fluorescence spectroscopy showed.

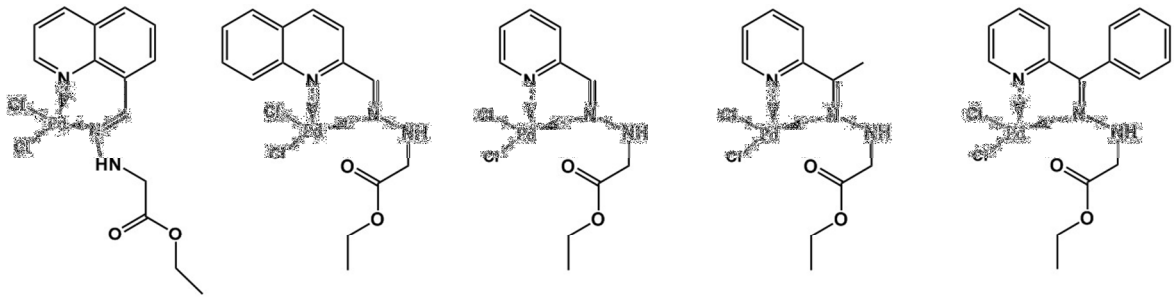

Figure 1: Structures of Pd(II) complexes with N-heteroaromatic hydrazone ligands, derivatives of ethyl hydrazinoacetate and *N*- heteroaromatic carbonyl compounds