









Day 1 Monday, 6th September 2021

8:30 - 8:50	Registration	
8:50 - 9:00	Opening ceremony	
8:50	Javier De Las Rivas	Co-chair of Action, University of Salamanca, Spain
8:55	Ondrej Uhlik	Head of the Department of Biochemistry and Micro- biology, UCT Prague, patronage organization

9:00 – 12:3	5 Section I	Chair: Thomas Mohr
9:00	Virtual screening of large chemical databases with AI	Asan Agibetov (Austria)
10:00	Protein-drug networks based on pharmacogenomic data: un-	Alberto Berral-
	raveling the targets of anticancer drugs	González (Spain)
	Oxidative stress parameters can predict the response to eryth-	Ana Cristina
10:20	ropoiesis-stimulating agents in myelodysplastic syndrome pa-	Gonçalves (Portugal)
	tients	Goriçaives (i ortugai)
10:40	Coffee break	
11:20	Emerging targets and small molecule drug candidates to	Wolfgang Link
11:20	overcome cancer therapy resistance	(Spain)
	Carboplatin-induced TUBB3 expression differently impacts	A
11:40	mesenchymal-like ovarian cancer cells fate upon drug treat-	Anamaria Brozovic
	ment	(Croatia)
12:00	Characterization of DNA repair genes in ovarian cancer pa-	Karolina Šeborová
12:00	tients with regard to chemoresistance status	(Czech Republic)
12:20	New label-free approaches for analysis of cell structure and	Lenka Šídová
12:20	growth	(Sven Biolabs)

12:45 - 14:00	Lunch	

14:00 – 16:	Section II	Chair: Catherine Passirani
14:00	Biocompatible gold nanoparticles for therapeutic applications	Bertrand Philippe (France)
14:20	Dual Kinase & Topoisomerase I Inhibitors to Overcome Multidrug Resistant Cancers	Cooney Louise (Ireland)
14:40	In vitro evaluation of acute and chronic liver tox-icity of lipid nanocapsules: what formulation for a better biocompatibility?	Delaporte Flavien (France)
15:00	Drugs activation for the discovery and development of new targeted chemotherapeutic formulations	Hadjikakou Sotiris (Greece)
15:20	Coffee break	
16:00	Modulation of cancer-associated processes by multivalent gly- comimetic inhibitors of galectin-3	Vlachova Miluse (Czech Republic)
16:20	CytoFLEX SRT- Avalanche Photo Diode based cell sorting made easy	Andreas Wicovsky (Beckman Coulter)
17:00 – 18	00 CG meeting Chair: J	avier De Las Rivas









Day 2 Tuesday, 7th September 2021

9:00 – 12:55	Section III	Chair: Helena M. Vascondelos and Ana Bela Sarmento Ribeiro
	Repurposing an iron chelator:	
9:00	mitochondrially-targeted deferoxamine exhibits potent	Jaroslav Truksa
9.00	cytostatic, cytotoxic and migrastatic anti-cancer	(Czech Republic)
	properties and induces mitophagy	
10:00	Nischarin is expressed in pancreatic ductal adenocarci-	Jelena Grahovac
	noma and is a potential target for drug repurposing	(Serbia)
10.20	Unveiling the role of ATF4 in metastatic breast cancer	Christiana Neophytou
10:20	dormancy	(Cyprus)
10:40	Coffee break	
11:20	Unravelling resistance mechanisms to proteasome inhib-	Raquel Alves
11:20	itors in multiple myeloma	(Portugal)
11:40	Structure-activity relationship of triple-action plati- num(IV) prodrugs with albumin-binding properties and immunomodulating ligands	Isabella Poetsch (Austria)
12.00	Robotic platform for testing of multidrug resistance	Jitka Viktorova
12:00	modulators	(Czech Republic)
12.20	Cancer Organoids-on-a-Chip as a tool for drug screening	Enrico Cavarzerani
12:20	in platinum resistant ovarian cancer	(Italy)
12:40	Exploring Protein Dynamics within the RAS-RAF-MEK- ERK Pathway with NanoBRETTM –	Erik Bonke
	Applications for Drug Discovery	(Promega)

13:00 - 14:00	Lunch

14:00 – 17:20	Section IV	Chair: Simona Saponara and Ivanka Tsakovska
14:00	Cardio-oncology: cardiovascular effects of the anti-	Radek Pudil
14.00	tumor treatment, diagnosis and management	(Czech Republic)
15:00	PARP inhibition: from idea to registration -	Zdenek Hostomský
15:00	A personal perspective	(Czech Republic)
16:00	Coffee break	-
16:40	Predictive in silico off-target profiling for the	Miguel X. Fernandes
16:40	H2S-releasing doxorubicin derivative Sdox	(Spain)
	Recent progress in the synthesis of ciprofloxacin deriva-	- Ryszard Ostaszewski
17:00	tives as a new therapeutic agents against multidrug re-	,
	sistant tumors	(Poland)

19:00	Dinner	







Day 3 Wednesday, 8th September 2021

9:00 - 12:55	Section V		Chair: Jitka Viktorova
9:00	Horizontal transfer of mitochondria and mitocho	ondrial	Jiri Neuzil
9.00	respiration		(Czech Republic)
10:00	Natural products ingredients with metal ions for r	new ef-	Banti Christina
	ficient targeted chemotherapeutics		(Greece)
	Predicting progression and recurrence using	g	
10:20	Deep Learning in small cancer cohorts and applied	cation	Oscar González-
	of Explainable Machine Learning as a tool to eluc	cidate	Velasco (Spain)
	resistance to therapy		
10:40	Identifying Unique Molecular Targets to Use N	ovel	Preeta Ananthana-
	Gene Group Based Shotgun Treatments in Malig	gnant	
	Pleural Mesothelioma		rayanan (Italy)
11:00	Coffee break		
11:40 - 12:55	Poster section		
13:00 – 14:00	Lunch		
14:00 – 16:30	in parallel:	Chair: J	avier De Las Rivas
4= 00	MC meeting / Poster section		
	Coffee break		
15:00			







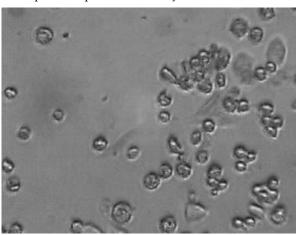
Natural products ingredients with metal ions for new efficient targeted chemotherapeutics

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Abstract: Carvacrol, the main constituent of the essential oil of oregano possesses antiproliferative activity. The organoantimony derivative of formula [Ph₂Sb(Carv)₂] (**TPAC**) (CarvH= carvacrol) was synthesized and characterized in solid state by melting point, X-ray Fluorescence (XRF), Attenuated Total Reflection Furrier Transform Infra Red (ATR-FT-IR) spectroscopies, Thermogravimetric Differential Thermal Analysis (TG-DTA), Differential Scanning Calorimetry (DTG/DSC), while UV-Vis spectroscopy was used for the characterization in solution. The crystal structure of **TPAC** has been determined by X-ray crystallography.

The *in vitro* anti-proliferative activity of **TPAC** was evaluated against human breast adenocarcinoma cancer cell lines: MCF-7 (positive to hormones receptor (HR+)), MDA-MB-231 (negative to hormones receptor (HR-)). Its *in vitro* toxicity was checked against normal human fetal lung fibroblast cells (MRC-5). The *in vitro* genotoxicity of **TPAC** was tested on normal human fetal lung fibroblast cells (MRC-5) with the micronucleus (MN) assay using fluorescence microscopy. Moreover, the *in vivo* toxicity and genotoxicity of **TPAC** was tested by *Artemia salina* assay and *Allium cepa* assays. The MCF-7 cells morphology suggests apoptotic pathway for their death, especially though the mitochondrion damage, which was confirmed by DNA fragmentation, Acridine Orange/Ethidium Bromide (AO/EB) Staining and permeabilization of the mitochondrial membrane tests. The binding affinity of **TPAC** toward the calf thymus CT-DNA was *ex vivo* investigated by Uv-Vis, Fluorescence spectroscopies and viscosity measurements.



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