CERTIFICATE OF ATTENDANCE

This is to certify that

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participated in

25TH IUBMB 46TH FEBS 15TH PABMB | 2022

9-14 JULY

LISBON PORTUGAL

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Abstracts submitted to the virtual The Biochemistry Global Summit (25th IUBMB Congress, 46th FEBS Congress and 15th PABMB Congress) from 9th to 14th July 2022 and accepted by the Congress Organizing Committee are published in this Supplement of *FEBS Open Bio*. Late-breaking abstracts are not included in this supplement. The abstracts are available as two PDF files: Talks (Plenary Lectures, Symposia and FEBS Special Sessions) and Posters.

About these abstracts

Abstracts submitted to the Congress are **not peer-reviewed**. In addition, abstracts are published as submitted and are **not copyedited** prior to publication.
We are unable to make **corrections of any kind** to the abstracts once they are published.

Indexing

Abstracts published in *FEBS Open Bio* Supplement for The Biochemistry Global Summit will be included individually in the Conference Proceedings Citation Index published by Web of Science.

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* Each poster has been given a unique number beginning with the letter P; the next part relates to the session in which the poster will be presented (see p.68 for key).

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polymerization of α/β-tubulin plays a key role in mitosis. Thus, in rapidly dividing cancer cells, it offers an enticing target for drug screening programmes. Notably, inhibitors of natural and synthetic origin act as destabilizing agents and exert their effect by interaction at the β-tubulin colchicine-binding domain. In order to search for new tubulin inhibitors, pharmacophore-based virtual screening was employed, an established *in silico* drug discovery approach. To cover a large part of the active space, several pharmacophore models for tubulin inhibitors were developed with two different types of modelling software, LigandScout and Discovery studio. Models were optimised against a dataset of active inhibitors from literature (n = 100) and a corresponding decoy set (n = 4,901). The best performing models were used to virtually screen vendor databases of natural products (n = 736) and synthetic compounds (n = 208,761). Among predicted hits, candidates were prioritised for *in vitro* screening based on consensus overlap, fit values, and drug-like properties. For hit validation, a set of 46 purchased compounds were tested in a cell-free fluorescence based tubulin polymerisation assay (Cytoskeleton, inc). Compounds were screened at 30 μM and inhibition was observed across varying scaffold types. Thiadiazole, sulfonate, and benzodioxole derivatives showed activity within range of the colchicine control (3 μM). As a next step, a dose-response study will be performed on the best candidates and IC50 values determined. Furthermore, potent inhibitors will be tested in cancer cell lines to assess activity. The combination of *in silico* screening and *in vitro* validation provides us with a powerful tool to identify novel tubulin inhibitors from synthetic and natural origin. Project funded by EUREGIO (IPN 119) 'HERBAL'.

P-01.1-068
Transcriptional factors and genes expression regulation in response to alternating oxygenation conditions, *in vitro*

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Hypoxia-inducible factor-1 (HIF-1) is a key regulator of tumor cell hypoxia of several genes related to oxygen homeostasis in response to hypoxic stress. Carbonic anhydrase 9 (CA9) has been found to be a stable marker of acute or chronic hypoxia. *N*-myc downstream-regulated gene 1 (NDRG1) is a tumor suppressor with the potential to suppress metastasis, invasion, and migration of cancer cells. It is regulated under stress conditions such as starvation or hypoxia. NDRG1 regulation is both induced and controlled by HIF-1α-dependent and -independent pathways under hypoxic conditions. We aimed to define the time-dependent pattern of CA9 and NDRG1 mRNA and protein expression in human glioblastoma cell lines in extreme hypoxia and after re-oxygenation as well as under normoxic conditions. Here, the regulation of the transcription factors HIF-1α, SP1, CEBPα, YB-1, and Smad7 was examined in a time-dependent manner. The human malignant glioma cell lines U87-MG, and GaMG were cultured for 1, 6, and 24 h under hypoxic (0.1% O_2) conditions with following re-oxygenation. The mRNA expression of NDRG1, CA9, HIF-1α SP1, CEBPα, YB-1, and Smad7 was measured via semi-quantitative RT-PCR analysis. Protein expression was analyzed using western blotting. Long-term (24 h), but not short-term hypoxia led to the induction of NDRG1 expression in human glioma cell lines while CA9 was induced upon short- and long-time hypoxic oxygenation conditions. CA9 and NDRG1 expression was found to correlate with the protein expression of HIF-1α, SP1, CEBPα, YB-1, and Smad7. These transcriptional factors, each separately or in combination, may possess the potential to become important regulative molecules that can be targetted during antitumor targetting.

P-01.1-069
Herbicides and structurally relevant Schiff bases as human protoporphyrinogen oxidase inhibitors

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Protoporphyrinogen oxidase (PPO, EC 1.3.3.4) catalyses the oxygen-dependent six-electron oxidation of protoporphyrinogen IX to protoporphyrin IX. Relevant work found that PPOs are overexpressed in some cancer types (e.g. colorectal cancer). In addition, targeting PPO could be a promising way to enhance photodynamic activity based on the application of 5-aminolevulinic acid. Possible human PPO inhibitors could be based on the structural motif of herbicides targeting plant PPO. However, prospective strategies for the preparation of anticancer agents could combine additional structural motifs, such as Schiff bases, for their molecular design. Schiff bases possess a wide range of biological activities, including the repression of oncological processes and signalling pathways. Schiff bases bearing 2-hydroxyaryl moieties can bind arginine groups and thereby possibly target Arg-98 or Arg-59, which are key amino acids that maintain PPO activity. Therefore, beside commercial herbicides, we study two novel series as potential inhibitors: 2-hydroxybenzaldehyde-based on anticancer pharmacophores Schiff bases and chromanone derivatives. Some tested inhibitors display potent activity against human PPO, but prepared compounds did not display any significant effect on enzyme activity. Nevertheless, obtained compounds could be used to better prediction PPO herbicidal toxicity and improve the design of synthetic inhibitors. The research was funded by the Ministry of Health of the Czech Republic (grant no. NU21-08-00407). The authors also thank Operational Programme Research, Development and Education, within the project Center for Tumor Ecology—Research of the Cancer Microenvironment Supporting Cancer Growth and Spread (reg. no.CZ.02.1.01/0.0/0.0/16_019/0000785).

P-01.1-070
Novel synthetic inhibitors of Il-6R based on structure motif of pentamethinium salts

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Interleukin-6 (IL-6) and its receptor play important roles in the tumor development (e.g. development of malignancies, promotes

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