



18th HELLENIC SYMPOSIUM

on Medicinal Chemistry

25-27 FEBRUARY 2021

Online Symposium

ORGANIZER:



HELLENIC SOCIETY
OF MEDICINAL
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POSTER 031

URINARY NMR METABOLOMIC ANALYSIS OF LATE PRETERM INFANTS ADMITTED IN NEONATAL INTENSIVE CARE UNIT (NICU) AND HEALTHY AGE-MATCHED LATE PRETERMS

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POSTER 032

SYNTHESIS OF NEW FLUOROQUINOLONE DERIVATIVES AND THEIR RHENIUM AND TECHNETIUM-99M COMPLEXES AND INITIAL BIOLOGICAL STUDIES

Tzovas Georgios, **Angelakou Eirini**, **Bompola Georgia**, **Sitsanli Anna**, **Papagiannopoulou Dionysia**

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POSTER 033

FUNCTIONALIZATION OF GOLD NANOPARTICLES WITH THIOL LIGANDS AND RADIOLABELING WITH ^{99m}Tc

Apostolopoulou Adamantia*, **Makrypidi Konstantina***, **Salvanou Eva-Alexandra***, **Chiotellis Aris***, **Pirmettis Ioannis***, **Papadopoulos Minas***, **Tsoukalas Charalampos***, **Koźmiński Przemysław****, **Bouziotis Penelope***

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POSTER 034

ANTIPROLIFERATIVE AND ANTIOXIDANT ACTIVITIES OF SYNTHETIC, TRYPTAMINE-DERIVED GRANULATAMIDE B AND ITS STRUCTURAL ANALOGUES

Matulja Dario^a, **Grbčić Petra^a**, **Kraljević Pavelić Sandra^{b,*}**, **Marković Dean^{a,*}**

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POSTER 035

DEVELOPMENT OF ANTHRAPYRAZOLE DERIVATIVES AND THEIR TRICARBONYL RHENIUM AND TECHNETIUM-99M COMPLEXES FOR POTENTIAL THERAPEUTIC OR DIAGNOSTIC APPLICATIONS

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POSTER 036

INFLUENCE OF XANTHINE DERIVATIVE CAFFEINE ON THE BINDING OF TIGECYCLINE TO HUMAN SERUM ALBUMIN

Emina Mrkalić*, **Miroslav Sovrlić****, **Ratomir Jelić****, **Stefan Stojanović****, **Nevena Prodanović****, **Jovica Tomović****

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POSTER 037

URINE NMR METABOLOMICS OF SPECIAL FORCES VOLUNTEERS UNDER PROLONGED INTENSE PHYSICAL EXERCISE

Sarbanı Ioanna¹, **Iliou Aikaterini¹**, **Mourtakos Stamatis^{2,4}**, **Benaki Dimitra¹**, **Gikas Evangelos³**, **Philippou Anastasios⁴**, **Koutsilieris Michael⁴**, **Papageorgiou Charalampos⁵**, **Sidossis Labros^{2,6}**, **Mikros Emmanuel¹**

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POSTER 038

SYNTHESIS AND ANTITUMOR ACTIVITY OF NOVEL STEROIDAL LACTAMS OF POPAM-OH

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POSTER 039

¹H NMR METABOLOMIC PROFILING OF MURINE LUPUS NEPHRITIS IN NZW/B-F1 KIDNEYS

Tsiara Ioanna*, **Manolaku Theodora****, **Nikolopoulos Dionysis****, **Benaki Dimitra***, **Garantziotis Panayiotis****, **Frangou Eleni*****, **Gikas Evangelos******, **Boumpas Dimitrios****, **Mikros Emmanuel***

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Certificate of Attendance

This is to certify that

TOMOVIC JOVICA

attended the **18th Hellenic Symposium on Medicinal Chemistry**,
organised on **February 25th - 27th, 2021** in **Athens**



**The President of the Hellenic Society
of Medicinal Chemistry
Prof. Emmanuel Mikros
National and Kapodistrian University of Athens
Symposium Chair**



**The Secretary of the Hellenic Society
of Medicinal Chemistry
Assoc. Professor Manolis Fousteris
University of Patras**

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POSTER036

INFLUENCE OF XANTHINE DERIVATIVE CAFFEINE ON THE BINDING OF TIGECYCLINE TO HUMAN SERUM ALBUMIN

Emina Mrkalić*, Miroslav Sovrlić**, Ratomir Jelić**, Stefan Stojanović**, Nevena Prodanović**, **Jovica Tomović****

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Simultaneous administration of the two drugs may lead to competition at the level of binding to human serum albumin (HSA), which may significantly affect the disposition of both drugs, with possible serious physiological consequences. Due to its characteristics, HSA is a unique protein model for the quantitative and qualitative study of protein-drug interactions [1]. The aim of this study is to evaluate the effect of caffeine (CAF) on the binding of tigecycline (TGC) to HSA. CAF shares the same binding site as tigecycline TGC. The interaction of TGC with HSA in the presence of competitive compounds may be realized through independent binding, competitive interference, or non-competitive interference [2]. For the research on the effects of the CAF on the HSA-TGC system, all fluorescence measurements were recorded at 298 K in the range of 300 to 450 nm, at an excitation wavelength of 295 nm. Various concentrations of TGC ($0.00\text{--}9.99 \times 10^{-6}$ M) were added to fixed equimolar concentration (2×10^{-6} M) of CAF and HSA. The fluorescence intensity of HSA decreased in the presence of CAF, indicating that TGC quenched the intrinsic fluorescence of HSA and form the HSA-TGC-CAF complex. The Stern–Volmer constant (K_{sv}) and binding constant (K_b) values were calculated. The K_{sv} value for the binary system was lower than K_{sv} value for the ternary system. Accordingly, the presence of CAF altered the ability of TGC to quench the intrinsic fluorescence of HSA. Calculated values of K_b of binary system HSA-TGC is lower than values of K_b of the ternary system (HSA-TGC-CAF) which indicate that the binding affinity of the binary system is enhanced in the presence of CAF. This can be explained by conformational changes in HSA caused by the presence of CAF (non-competitive interference). The increasing values of K_b implies a stronger binding of TGC to HSA and leads to the decreasing concentration of free TGC in plasma and reduce its maximum effectiveness. his research illustrates that the simultaneous uptake of coffee, tea, ...etc and drugs may cause interactions and thus an interesting field of future research.

References

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