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UNIVERSITY OF BANJA LUKA
ТЕХНОЛОШКИ ФАКУЛТЕТ
FACULTY OF TECHNOLOGY

# BOOK OF ABSTRACTS

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## XIV CONFERENCE OF CHEMISTS, TECHNOLOGISTS AND ENVIRONMENTALISTS OF REPUBLIC OF SRPSKA

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# SYNTHESIS, CHARACTERIZATION AND CRYSTAL STRUCTURE OF THE 2-QUINOLONE DERIVATIVE

Lidija Radovanović[1], Jelena Lađarević[2], Bojan Božić[3], Marijana Kasalović[4], Nebojša Pantelić[5], Dušan Mijin[2], Jelena Rogan[2]

[1]Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia
[2]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
[3]University of Belgrade, Faculty of Biology, Institute of Physiology and Biochemisty „Ivan Đaja“, Belgrade, Serbia
[4]University of Kragujevac, Faculty of Science, Kragujevac, Serbia
[5]University of Belgrade, Serbia, Faculty of Agriculture, Belgrade, Serbia
Corresponding author e-mail: lradovanovic@tmf.bg.ac.rs

## Abstract

2-Quinolones represent important structural motifs in the numerous biologically active compounds and naturally occurring alkaloids. Their derivatives show remarkable diversity of pharmalogical properties such as antibacterial, antifungal, anticancer, antitubercular, anti-inflammatory, and antihypertensive and play a significant role in the development of the new pharmaceuticals. On the other hand, propanoic acid derivatives are known for their uniqe terapeutic activity. In an effort to merge these two structural motifs, two-step synthesis of 3-(4-methyl-2-oxoquinolinyl)propanoic acid, **1**, was performed. The obtained compound was characterized by melting point, FTIR and NMR spectra. The single crystals of molecule **1**, was prepared by slow evaporation from the ethyl acetate solution. The single crystal X-ray analysis revealed that molecule **1** crystallizes in monoclinic $P2_1/c$ space group with $Z = 4$. The main structural feature is pseudo wavy layer formed by O–H···O and C–H···O interactions between adjacent molecules, whereas among the layers $\pi\cdots\pi$ stacking and C–H···$\pi$ interactions were observed, resulting in the formation of supramolecular network. The main crystallographic data for **1**: $C_{13}H_{13}NO_3$, $a = 9.2414(4)$, $b = 9.0128(3)$, $c = 13.6567(6)$ Å, $\beta = 109.676(4)$ °, $V = 1071.06(8)$ Å$^3$. The refinement based on $F^2$ (156 parameters) yielded: $R_1 = 0.0456$, $wR_2 = 0.1287$, $S = 1.068$ for all data, and $R_1 = 0.0433$ for 1765 reflections with $I \geq 2\sigma(I)$.

**Keywords**: Crystal structure, wavy topology, 2-quinolone, propanoic acid derivative.

University of Banja Luka
Faculty of Technology

Vojvode Stepe Stepanovića br. 73
78 000 Banja Luka
Tel./Faks: +387 51 434 357
e-mail: savjetovanje@tf.unibl.org
web: www.tf.unibl.org