Unexpected synthesis, characterization, biological evaluations, and computational details of novel nucleosides containing triazine-pyrrole hybrid

Ahmed I. Khodair
Department of Chemistry, Faculty of Science, Kafrelsheikh University, El-Geish Street, P.O. Box 33516, Kafrelsheikh, Egypt; E-mail: khodair2020@yahoo.com

Abstract: A series of novel nucleosides containing 1,2,4-triazine and pyrrole moieties were efficiently prepared and characterized via analytical, spectral, and computational methods. The synthesized compounds had no effect on human immunodeficiency virus type 1 (HIV-1) (HTLV IIIB). Moreover, the triazine derivatives **8a** and **8b** were screened for their anticancer activity against five human cancer types [breast adenocarcinoma (MCF-7), pancreatic carcinoma (Paca2), lung carcinoma (A-549), human bone cancer cell line (Hos), and a normal human (BJ-1)] cell lines using MTT assay. The obtained results revealed that the tested nucleosides **8a** and **8b** had significant inhibitory activity against Paca2, but no activity against A-549, Hos, and BJ-1 cell lines. The structure-activity relationship displayed an increase in anticancer potential of compound **8a** with the increase of number of hydrogen bond interactions with Lys 89 as the key interactive amino acid of CDK-2 kinase.

Keywords: 1,2,4-Triazines, pyrrole; nucleosides, anticancer evaluation, computational studies

Prof. Dr. Ahmed I. Khodair (1962) has been graduated at Faculty of Science; Tanta University, Egypt in 1984 and got has Ph. D. (Org. Chem.) at Faculty of Science, Tanta University, Egypt in 1993. He has been promoted to full Professor of Organic Chemistry at Faculty of Science, Kafrelsheikh University, 2005. He is specialized in the synthesis of heterocyclic organic compounds and their nucleosides. He is a Humboldt fellow since 2001. He served as a referee for many international organization and scientific journals. He is a member of the permanent scientific committee for promotion of Egyptian universities staff members (Organic Chemistry). He has supervised more than ten master and doctoral theses. He has published more than 50 publications in renowned scientific journals. He spent two years in Denmark at Odense University as a Ph. D. student. He spent seven months at Technical University of Copenhagen/Lyngby (Denmark). He spent two years at Poitiers University (France). He spent sixteen months at Konstanz University (Germany). He spent seven years at King Saud University (Saudi Arabia). He is the head of Chemistry Department of Faculty of Science at Kafrelsheikh University since 2010 for three years. He is the Vice Dean for Education and Student Affairs of Faculty of Science at Kafrelsheikh University since 2011 for three years. He is the Dean of Faculty of Science at Kafrelsheikh University since 2015 for three years. He is the head of Chemistry Department of Faculty of Science at Kafrelsheikh University since 2021 for one year.



Presenting author details
Full name: Ahmed I. Khodair
Contact number: +201011789920
Email id: khodair2020@yahoo.com
Category: Oral presentation
Session name:
Research interest: Drug design and drug development