



Indian Journal of Chemistry
Vol. 63, February 2024, pp. 145-158
DOI: 10.56042/ijc.v63i2.4273



Design, synthesis, *in vitro* and computational analyses of anticancer nicotinamide derivatives

Muhammed Gömeç^a, Vesim Nasif^b, Ayşe Hümeyra Taşkin Kafa^c, Koray Sayin^{b*}, Hayreddin Gezegen^d & Hilmi Ataseven^e

^aDepartment of General Surgery, Faculty of Medicine, Cumhuriyet University, Sivas, Türkiye

^bDepartment of Chemistry, Faculty of Science, Sivas Cumhuriyet University, Sivas, Türkiye

^cDepartment of Medical Microbiology, Faculty of Medicine, Cumhuriyet University, Sivas, Türkiye

^dDepartment of Nutrition and Dietetics, Faculty of Health Sciences, Cumhuriyet University, Sivas, Türkiye

^eDepartment of Gastroenterology, Faculty of Medicine, Sivas Cumhuriyet University, Sivas, Türkiye

E-mail: krysayin@gmail.com

Received 22 July 2023; accepted (revised) 19 January 2024

The search for ideal treatment continues for many health problems such as cancer and infection. In this context, new synthesis compounds have been promising and the nicotinamide derivative compounds, which is an important heterocyclic derivative, has attracted the attention of many researchers. Nowadays, anticancer, antifungal, antimicrobial, antibacterial and antibiofilm effects of some nicotinamide derivatives have been demonstrated. In this study, nine new nicotinamide derivative compounds have been designed and synthesized. The characterization of these synthesized compounds have been done by *in silico* methods. The anticancer effects of the compounds have been investigated in four different cancer types and compared with their effects on healthy fibroblast cells. N4 has been found to have a cytotoxic effect on MCF-7 human breast cancer, and the IC50 value has been calculated as 12.1 μ M. In addition, antibacterial, antifungal and antibiofilm activities were investigated by *in vitro* methods and they have been shown to be effective. As a result, it is observed that N4, one of the newly synthesized nicotinamide derivative compounds, has a serious cytotoxic effect in MCF-7 human breast cancer cells compared to healthy fibroblast cells. Pharmacophore map and ADME analyses of studied compound are performed in detail.

Keywords: Nicotinamide, Synthesis, DFT, *In silico*, Anticancer