Herein were described results on the synthesis, spectroscopy analysis and biological activity evaluation of novel gramine derivatives.

Gramine is a natural indole alkaloid and it exhibits wide pharmaceutic activity. The significant role of derivatives of gramine in science, medicine and industry was declared in scientific literature. Up to now, gramine has been widely used as a pharmaceutical lead scaffold for constructing various biologically active indole-containing compounds. The chemical modifications of the lead gramine structure gave forty-nine new derivatives of gramine. The results were presented as five groups:

- Derivatives of N,O-diacetylindole-3-carbinol: series of ethers indole-3-carbinol and N-acetylindole-3-carbinol (I group)
- Compounds gramine with rings of phtalimide, imidazole and pyrrolidinedithiocarbamate (II group)
- The group of compounds gramine with uracil and its derivatives (III group)
- Compounds gramine with triazole ring (IV – Click group)
- Salts gramine and formyl- / acetoxy- cholic acids (V group)

All the obtained compounds were characterized on the basis of NMR, mass spectrometry, FT-IR spectra and elementary analysis. PM5 semiempirical calculations were performed. Heat of formation (HOF) of gramine derivatives were presented and the molecular structures of conjugates were shown. For predicting biological in silico activity spectra of obtained molecules were used PASS software and Molinspiration Property Calculator, v2016.10.

All synthesized compounds have been tested for their in vitro antibacterial, antiproliferate, antioxidant and haemolytic activities.