Секция «Биоинформатика»

# ADMET properties of new copper(II) complexes derived from cyclohexylamine Schiff bases

**Научный руководитель – Сафин Дамир Амирович**

***Панова Елизавета Валерьевна***

*Postgraduate*

Тюменский государственный университет, Институт биологии, Тюмень, Россия

*E-mail: lizap-1999@mail.ru*

Nowadays, metal complexes of Schiff bases, including copper-based complexes, are in the limelight of studies to treat COVID-19. With this in mind we have directed our attention to copper(II) complexes $[Cu(L^{I})_2]$ (**1**) and $[Cu(L^{II})_2]$ (**2**) ($HL^{I}$ = *N*-cyclohexyl-3-methoxysalicylideneimin $HL^{II}$ = *N*-cyclohexyl-3-ethoxysalicylideneimine) [1]. According to ProTox-II, both complexes belong to a fourth class of toxicity with the predicted $LD_{50}$ of 1200 mg/kg (Fig. 1). The SwissADME bioavailability radar revealed that both complexes are preferred in three parameters, namely polarity, unsaturation and flexibility, and less preferred in lipophilicity, size and insolubility (Fig. 1). As it was evidenced from the BOILED-Egg method, both **1** and **2** exhibit a negative blood-brain barrier penetration and can potentially be absorbed by gastrointestinal tract and can be effluated from the central nervous system by the P-glycoprotein (Fig. 1).

## References

1) Panova, E.V., Voronina, J.K., Safin, D.A. Copper(II) Chelates of Schiff Bases Enriched with Aliphatic Fragments: Synthesis, Crystal Structure, in Silico Studies of ADMET Properties and a Potency against a Series of SARS-CoV-2 Proteins // Pharmaceuticals. 2023. Vol. 16(2). No. 286.

## Illustrations

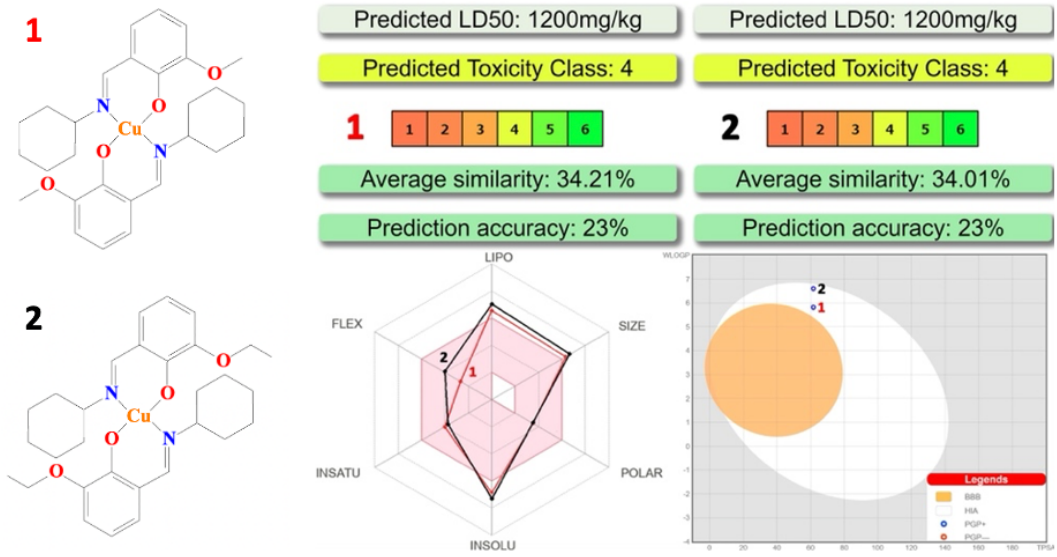


Рис. : Toxicity results of 1 and 2 calculated by ProTox-II. Bioavailability radar for 1 and 2 within the domain borders of ADME properties, calculated by SwissADME. The colored zone of the radar is the suitable physicochemical space for oral bioavailability. BOILED-Egg model of 1 and 2 calculated by SwissADME.