Analysis of the biological anti-HIV activity of humic substances based on data on the molecular composition

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The problem of finding new sources and types of biologically active natural compounds is the most important task of modern medicinal chemistry. Humic substances are known to be a carrier of antiviral activity [1]. This study aimed to study the anti-HIV activity of the peloid hyalomelanic acid narrow fractions and to analyze its relationship with the molecular composition obtained by FTICR MS.

Solid-phase extraction was used to obtain narrow fractions followed by gradient elution on three Bond Elut cartridges: C8, C18 and CNE. The eluent was various mixtures of methanol and water. A total of 33 fractions were obtained, 11 from each of the 3 cartridges. Each fraction was characterized by FTICR mass spectrometry. Cytotoxicity and anti-HIV activity were measured.

The most active fractions for cartridges C8 and C18 were obtained by elution with mixtures of methanol:water from 60:40 to 80:20, and 70:30 to 90:10 for CNE.

Signals of impurities were removed from the obtained spectra. For each group of spectra, Tanimoto similarity matrices were calculated and Van Krevelen diagrams were plotted. Correlation diagrams were constructed for all 3 sets of fractions based on the 2d binning of Van Krevelen diagram. The correlation was calculated between the population densities of the squares on the van Krevelen diagram and the inverse decimal logarithm EC₅₀ (Fig. 1).

The correlation analysis suggests that tannins are associated with high anti-HIV activity.

Figure 1. The data of the correlation analysis that was carried out on the data of the descriptors of the population densities of the Van Krevelen diagram for the fractions of the HMA of peloids obtained from three different cartridges and the data of the anti-HIV activity. From left to right fractions got on cartridges C8, C18, CNE.

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References

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