It is also worth noting that people suffering from alcohol use disorder in most cases don't have higher educa-tion. So, among our patients only 4 people out of 49 (8,1%) had a higher education, and this percentage is much lower than the average in the Republic of Belarus.

It can be concluded that people's alcohol dependence imposes a burden on society, and the more people suffer from alcohol use disorder, the higher this load is.

CONIINE, PHYSICO-CHEMICAL PROPERTIES AND ITS APPLICATION IN THE ENVIRONMENTAL INDUSTRY

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For the first time the geometric parameters of the coniine molecule were calculated, the electronic and UV spectrum of coniine was calculated by an ab initio method (M062X). The intermolecular interaction between the molecules of the coniine and the molecules of CO of the air has been established. It has been found that coniine is a powerful absorber of CO air.

Keywords: coniine, adsorption, DFT, non-bonded interaction, NBO analysis.

For the first time in the present study, the non-bonded interaction of the Coniine (C8H17N) with carbon monoxide (CO) was investigated by density functional theory (DFT/M062X/6-311+G*) in the gas phase and solvent water. The adsorption of the CO over C8H17N was affected on the electronic properties such as EHOMO, ELUMO, the energy gap between LUMO and HOMO, global hardness. Furthermore, chemical shift tensors and natural charge of the C8H17N and complex C8H17N/CO were determined and discussed. According to the natural bond orbital (NBO) results, the molecule C8H17N and CO play as both electron donor and acceptor at the complex C8H17N/CO in the gas phase and solvent water. On the other hand, the charge transfer is occurred between the bonding, antibonding or nonbonding orbitals in two molecules C8H17N and CO. We have also investigated the charge distribution for the complex C8H17N/CO by molecular electrostatic potential (MEP) calculations using the M062X/6-311+G* level of theory. The electronic spectra of the C8H17N and complex C8H17N/CO were calculated by time dependent DFT (TD-DFT) for investigation of the maximum wavelength value of the C8H17N before and after the non-bonded interaction with the CO in the gas phase and solvent water [1].

1. The adsorption energy of CO over C8H17N in the gas phase (-2,67 eV) is greater than solvent water (-1,33 eV).
2. It is found that some geometrical parameters of C8H17N are changed after adsorption process due to the formation of intermolecular non-bonded interaction.
3. NBO analysis predicted a charge transfer from the molecule C8H17N to CO and from CO to C8H17N. It was found that the electronic properties of the molecule C8H17N are sensitive to the adsorption of the CO. The complex C8H17N /CO in the gas phase has a high chemical activity, low chemical stability and it is a soft system rather than complex in the solvent water.
4. The non-bonded interaction between the C8H17N and CO is changed the value of λmax. Therefore, C8H17N may be used for development of filters in order to adsorption of carbon monoxide as environmental pollution [1].

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ANTIOXIDANT ACTIVITY CHARACTERISTICS OF THE GANODERMA LU-CIDUM SPOROCARPS EXTRACT

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Currently, the search for new natural compounds capable of neutralizing the activity of certain substances is constantly being conducted. Basidiomycetes cause increased interest in many scientists as producers of a wide range of compounds with different biological activity, including antioxidant. Ganoderma lucidum contains various compounds that exhibit a variety of biological activities, including increased immunity, antitumor, antimicrobial, anti-inflammatory and antioxidant activity.

Keywords: Ganoderma lucidum, antioxidant activity, biologically active substances.

Introduction

Free radicals and reactive oxygen species, which are formed as by-products of certain metabolic processes, can cause serious damage to cells as a result of uncontrolled oxidation. Some studies show that Ganoderma lucid-um extracts increase the activity of superoxide dismutase and catalase, as well as other enzymes involved in the elimination of highly reactive oxygen species [1].

Material and research methods

An extract of Ganoderma lucidum fungus sporocarp was used as an object of study. In the work, spectrophotometric, chemical and statistical methods were used.

Ethanol extracts were obtained from the dry milled sporocarps of Ganoderma lucidum. Next, the extract was filtered and dried at a temperature of 100–105 °C until a constant mass was obtained. The content of dry extrac-tive substances in fungi extracts was determined by the gravimetric (weight) method.

Determination of the total content of phenolic compounds in the extract of the fungus by the method of Folin – Ciocalteu

To determine the total content of phenolic substances in the studied fingi extracts, a calibration curve was constructed for the standard substance with which gallic acid was chosen. Using the calibration curve, a direct equa-tion of the form y = kx+b was derived, according to which further calculations were performed.

Determination of the antiradical activity of the extract of the fungus by ABTS

The formation of $ABTS^{\cdot}+$ radical cations was started by adding crystals of ammonium persulfate to a final concentration of 2,45 mM. After adding ammonium persulfate, the mixture was thoroughly mixed and left for 12–16 hours in the dark at room temperature.

In the process of determining the antiradical activity, equal aliquots of the studied extracts were added to the radical solution, and the degree of quenching of the radical was assessed over time. The measurements were carried out in a cuvette with an optical path length of 1 cm, λ=734 nm.

Results

The content of dry extractive substances determined by the gravimetric method in all the studied extracts of the fruiting bodies of fungi was 0.0033±0.00001 g. According to the data obtained, it was shown that the content of total phenolic compounds in terms of gallic acid in 50 μl of the extract was 454,3±12,4 mg/l.

Phenolic acid has a pronounced antiradical activity. With increasing concentration, the antioxidant activity of phenolic acid increases and reaches a maximum at a concentration of 10-2 mol. This allows us to make the as-sumption that it is precisely this acid that is likely to make the maximum contribution to the manifestation of the antioxidant properties of the extracts of the fruiting bodies of the studied fungus. It was shown that the obtained fungi extract from fruiting bodies showed antiradical activity in this model. The percentage inhibition of 50 μl of the extract was 36,8±0,5, which suggests that this extract has a pronounced antioxidant activity.

Conclusion

The obtained extract of Ganoderma lucidum fungus sporocarp contains phenolic compounds and has a pronounced antioxidant activity, the manifestation of which can be explained by the high antioxidant activity of phenolic acid, which is one of the components of the extract.