Seminar științific

CHIMIA ECOLOGICĂ ASIGURĂ UN MEDIU SĂNĂTOS

Consacrat aniversării a 50 ani de la fondarea Laboratorului Resurse Minerale și Chimie a Apei,
30 de ani de la organizarea Laboratorului Chimie Ecologică și
comemorării talentatului chimist și ecolog dr. Valeriu ROPOT

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Chișinău, 16 septembrie 2022

INFLUENȚA GLUTATIONULUI ASUPRA CAPACITĂȚII DE AUTOPURIFICARE A SISTEMELOR ACVATICE

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Scopul lucrării constă în estimarea influenței glutationului (GSH) asupra procesului de autopurificare chimică și în formarea calității sistemelor acvatice.

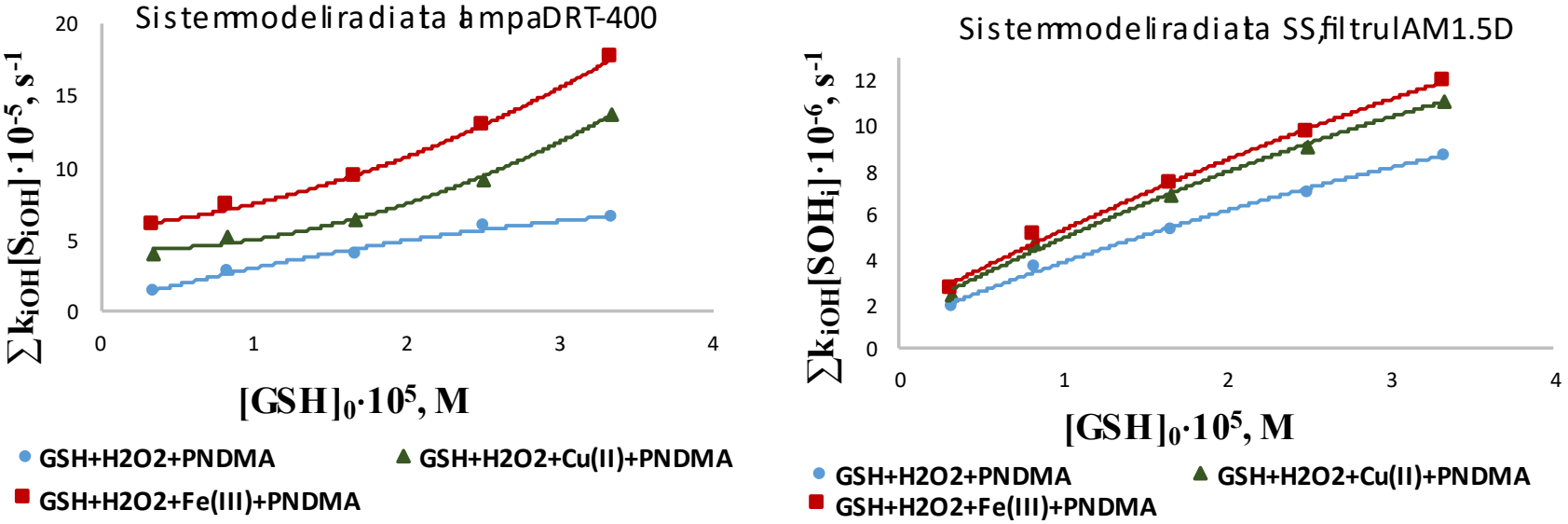

Fig. 1. Variația capacității de inhibiție în prezența GSH, $[PNDMA]_0 = 1{,}1\cdot10^{-5}$ M, $[H_2O_2]_0=1\cdot10^{-2}$ M, $[Cu(II)]_0=5\cdot10^{-6}$ M, $[Fe(III)]_0=5\cdot10^{-6}$ M, pH=6,8, t=20 °C

Concluzii. Ca urmare a cercetării date, s-a demonstrat că GSH, având un caracter puternic reducător, pe de o parte conduce la consumul echivalenților oxidativi în sistemele acvatice, iar pe de altă parte exclude ionii de Cu(II) și Fe(III), diminuând astfel intensitatea proceselor de autopurificare a sistemelor acvatice.

ASSESSMENT OF THE IMPACT OF BIOCHEMICAL PROCESSES AT THE SEDIMENT -WATER INTERFACE IN AQUATIC ECOSYSTEMS IN THE BIOSPHERE RESERVE „PRUTUL DE JOS" ON BIODIVERSITY IN THE CONTEXT OF CLIMATE CHANGE

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Conservation of biological diversity in ecosystems, species, populations and genes is one of the main concerns of mankind in the third millennium. The problem is that with the advancement of technological progress and the intensive use of natural resources, the anthropogenic impact on biological diversity has considerably increased, significantly reducing the number of species and varieties of living organisms that populate the Earth. Assessing the impact of biochemical processes at the sediment-water interface in aquatic ecosystems in the Biosphere Reserve „Prutul de Jos" on biodiversity in the context of climate change is important in that it includes biochemical research at the sediment-water interface, including the establishment of properties surface area and influence of the organic-mineral complex, amorphous phase, interstratular material of clay minerals, determination of mineralogical features, changes in the cation exchange complex, spatial dynamics of heavy metals in sediments, their chemical partition in particle constituents and their mobility in aquatic ecosystems, such as and evaluation of the complex influence of abiotic factors on water quality, establishing the kinetic characteristics of biochemical transformations of nitrogen in aquatic ecosystems, consumption of dissolved oxygen in water, self-purification capacity of the aquatic ecosystem, use of the model for ru biochemical simulations and for practical purposes, for modeling and forecasting ecological crisis situations in the water basins of the Biosphere Reserve „Prutul de Jos" and assessing the impact of these processes on the biodiversity of the aquatic ecosystem as a whole.

Climate change, changes in water circulation, intensification of water evaporation processes, eutrophication of water basins are becoming a concern for the environment and human health. That is why it is important to detect, monitor and evaluate the impact of different metabolites eliminated in the aquatic environment following the processes at the sediment-water interface and the impact on aquatic flora and fauna.

The object of study is the „Prutul de Jos" Biosphere Reserve (Republic of Moldova) located in the southwest part of the country. This biosphere reserve includes the Prut River and several floodplains Two thirds of the area is occupied by Lake Beleu. The aquatic ecosystems from the „Prutul de Jos" Biosphere Reserve have an impact on the Danube - Black Sea river basin.

This study addresses and integrates existing recommendations in a series of European Directives on water and biodiversity, and obtained results contribute to the scientific substantiation of the development of recommendations for the harmonization of the methods used and the improvement of water management exploited on the national territories of the Republic of Moldova and Romania.

Scientific seminar ECOLOGICAL CHEMISTRY ENSURES A HEALTHY ENVIRONMENT

ADSORPTION OF WATER SOLUBLE VITAMINS ON AUTOCHTHONOUS ACTIVATED CARBONS

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Introduction. The continuous and increasing pollution of water is one of the most pressing environmental problems in the world. A special type of contaminants are pharmaceutical products, that are ever more discovered in the environment, significantly affecting the quality of life. The increasing use of human and veterinary pharmaceutical products, accompanied by their infiltration into the aquatic and terrestrial environment, requires urgent solutions for the immobilization and removal of this category of pollutants. Adsorption is one of the most effective and practical techniques for removing pollutants from water. The use of carbonic adsorbents in water treatment technologies is justified by the fact that activated carbons are able to remove almost entirely a very wide spectrum of pollutants.

Materials and methods. In the Ecological Chemistry laboratory of the Institute of Chemistry, using different methods and conditions of activation, a set of activated carbons was obtained in order to identify samples with potential of use for the immobilization and removal of pollutant substances from aquatic systems. In this research were studied the adsorption parameters of vitamins B3 (Nicotinic acid, $C_6H_5NO_2$, MM 123,11) and B6 (Pyridoxine, $C_8H_{11}NO_3$, MM 169,18) on four samples of autochthonous activated carbon (CAS-23, obtained from peach kernels; CAN-8, obtained from walnut shells; AC-MR, obtained from apple wood, AC-C, obtained from apricot kernels). The influence of initial concentrations of adsorbates, contact time, temperature, granulometric compozition of carbons and their surface parameters on the adsorption process were investigated ..

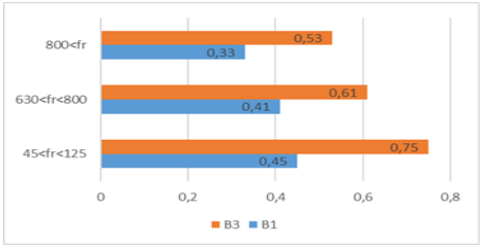

Fig.1. The vitamins B3, B6 adsorption capacity depending on the granulometric composition of AC-MC

Results and discussion. The influence of the granulometric composition of carbon adsorbents on the adsorption capacity of vitamins (fig.1) showed a considerable increase (about 30%) of the adsorption power value with the decrease of the carbon particle size (from 800-2000 μm to 90-125 μm).

The adsorption kinetic curves were determined in a time interval between 10-300 minutes at 25°C The obtained data shows that the amount of immobilized vitamins on investigated carbon adsorbents growths with increasing contact time between vitamins solution and carbon adsorbent surface. It was found that the equilibrium of the adsorption process was achieved after 3 hours of stirring/contacting .

The adsorption isotherms of vitamins on local carbon adsorbents were determined at three values of temperatures (25°C, 35°C and 45°C). According to the obtained data the increase of the temperature is accompanied by the decrease of the amount of immobilized adsorbates. The adsorption capacity of the autochthonous carbon adsorbents towards investigated vitamins (fig. 2) was determined from their adsorption isotherms. The obtained results are in accordance with the method of obtaining of researched carbons and their structural parameters, being obvious the advantage of samples AC-MR and AC-C, which showed the highest adsorption values: about 0,9 mmol/g. The adsorption values of CAN-8 and CAS 23 samples indicated near 0.65 mmol/g.

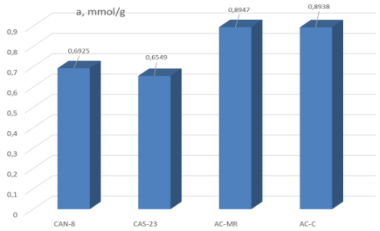

Fig.2. The adsorption capacity of CAN-8, CAS-23, AC-C and AC-MR towards vitamin B6

Conclusion: *The pharmaceuticals such as vitamins B3 and B6 can be effectively removed from aqueous solutions using autochthonous activated carbon, obtained from the local vegetable raw materials.*

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FINE ORGANIC SYNTHESIS APPROACHES FOR OBTAINING MONASTROL BY GREEN CHEMICAL METODOLOGIES

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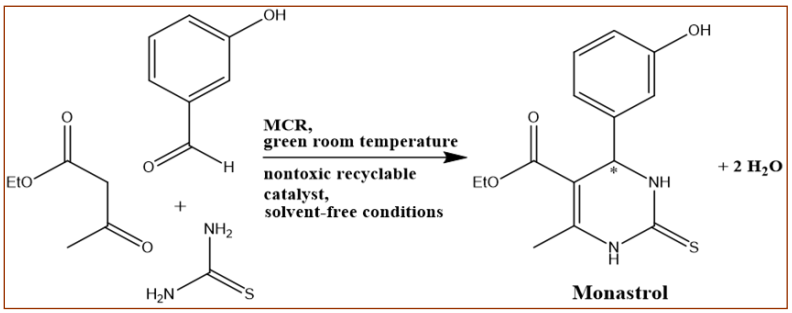
Introduction

Monastrol (M) is an important target molecule for organic chemists in virtue of its remarkable biological properties, e.g. antitumoral activity [1] and inhibition of the motility of the mitotic motor protein kinesin Eg5, thus serving as a particularly useful tool for study of mitotic mechanisms [2].

The most useful and smart method actually applied for M synthesis is the Biginelli multicomponent reaction (MCR), discovered in 1891 by Pietro Biginelli [3]. MCRs have the advantage of performing the reaction in a one-pot version, thus avoiding waste from multistep purifications and residue generation. Moreover, MCR adducts include in their structures almost all atoms (atom economy), the common by-product being water.

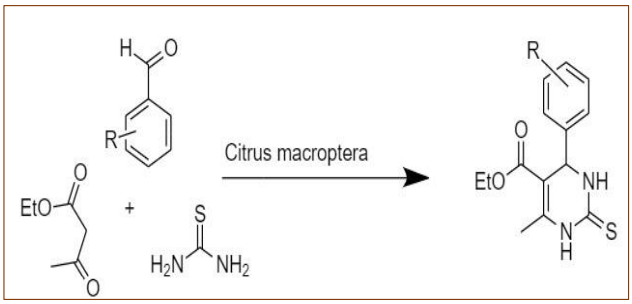


Schematic representation of Biginelli reaction applied for the preparation of (+/-)-Monastrol in eco-friendly conditions

The Biginelli reaction has been known for more than a century but it is ambiguous, that's why scientific researchers have changed catalysts of an inorganic nature to those of green chemistry or even the lack of them. An eloquent example of obtaining monastrol by means of harmless organic catalysts is the replacement of the Lewis acid (it is toxic) that is used as a catalyst in the classic reaction by lemon juice (*Citrus macroptera*) [4]. This reaction took place at room temperature for 12 h and without the presence of the solvent. The obtained product was filtered and purified by recrystallization with hot ethanol until the pure substance was obtained.

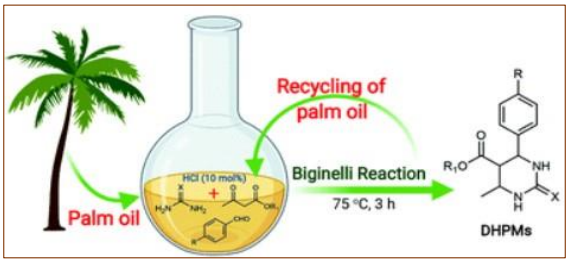
Discussion

Dihidropyrimidinones (DHPMs) obtained by the Biginelli rection play an essential role in human life, due to their biological activity, being widely used in the pharmaceutical field as anticancer, antihypertensive, antibacterial, anti-inflammatory and antiviral agents [1].



Green synthesis of DHPM derivaties

Some recent advances are described in the literature, regarding the convenient synthesis of M, based on the environmentally benign methods in sustainable conditions [5,6]. Virgin palm oil exhibited clear solvent effects, including enhanced solubility of substrates and promotion of keto-enol tautomerization, leading to increased reaction productivity compared to previously published bio-based solvents such as p- cymene and ethyl lactate. Multicomponent one-pot Biginelli reactions were successfully performed using vegetable oil as bio-based, non-toxic, and ecological solvents. Palm oil has been shown to be a highly efficient greener solvent compared to petroleum-based solvents such as cyclohexane, with comparable yields for the Biginelli reaction of urea, benzaldehyde and methyl 3-oxobutanoate of 74% and 74%, respectively 73% [7].



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SCIENTIFIC SEMINAR *'ECOLOGICAL CHEMISTRY ENSURES A HEALTHY ENVIRONMENT'*, 16.09.2022

STUDY OF THE ADSORPTION OF *BACILLUS SUBTILIS* AND *BACILLUS CEREUS* ON DIFFERENT FRACTIONS OF ACTIVATED CARBONS OBTAINED FROM APPLE WOOD

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The paper presents the results of scientific research related to the study of adsorption processes of *Bacillus subtilis* and *Bacillus cereus* bacteria on activated carbon obtained from apple wood. The activated carbons used have a specific BET area of about 2018 m^2/g and a total sorption volume of the pores equal to 1,573 cm^3/g. The study of the kinetics of the adsorption processes of the *Bacillus subtilis* and *Bacillus cereus* bacteria showed that the value of the maximum adsorption for the fraction 630-800 µm is established within 90 and 70 min, respectively.

The maximum adsorption capacity for the *B. subtilis* bacteria is 0,54-0,55 McF*10^8/g, higher than activated charcoal obtained from apricot stones that has the values of 0,375 -0,385 at 27°C. For the *B. cereus* bacteria the maximum adsorption was attested at the value of 0,45 McF*10^8/g, also higher than the adsorption capacity of the activated charcoal obtained from apricot stones, that has the value of 0,33 McF*10^8/g at 27°C. An example of a peak adsorption after 90 minutes of the contact for the *B.subtilis* bacteria is presented in the figure bellow:

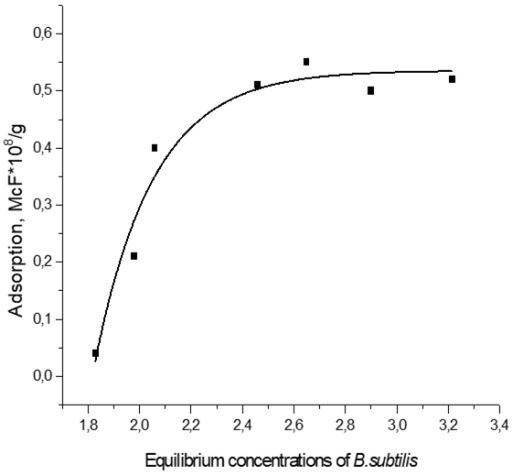

Fig. 1 Asorption isotherm of *B. subtilis* bacterium on AC-apple, fraction 630-800 µm , at 27°C

The kinetics of the adsorption processes of activated carbon obtained from apple wood (fraction 800 -2000 µm) for the same bacteria were evaluated at 27 °C. The main sorptive properties were attested after 90 to 120 minutes of contact. The adsorption values were in the range of 0,21 -0,25 McF*10^8/g for *B. subtilis* and 0,26-0,28 McF*10^8/g for *B. cereus* depending on the contact time, lower than in the case of the fraction 630 -800 µm.

Fig. 2 Bacterial solution of *B.cereus* in contact with AC from apple wood and bacterial cultivation on peptone-agar

Conclusion: The sorption capacity of the activated carbon of the fraction 630-800 µm obtained from apple wood is approximately 2 times higher than in the case of the 800-2000 µm fraction of the same carbons for both bacterial species taken into study.

Acknowledgement : This research was carried out with the financial support of the institutional project "The reduction of the environmental and health impact of toxic chemicals through use of adsorbents and catalysts obtained from local raw material" DISTOX, No 20.80009.7007.21

SCIENTIFIC SEMINAR „ECOLOGICAL CHEMISTRY ENSURES A HEALTHY ENVIRONMENT"

ADSORBTION OF BENZENESULFONATE AND DODECYLBENZENESULFONATE BY ACTIVATED CARBON OBTAINING FROM WOOD CHARCOAL

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Introduction

Among the most common chemicals used in household and industrial applications are surfactants. Due to widespread use surfactants are often found in the domestic and industrial wastewater as these may not be completely utilized in the application. Obviously part of surfactant discharged could be degraded naturally. However biodegradation alone is not sufficient when the surfactant is present in large concentration. The surfactants have an impact of the humans if these enter into the food chain. Their presence can also affect the treatment efficacy of the wastewater treatment plants.

The surfactants are widely used in detergent, shampoos and cosmetics. Surfactants increase solubility of organic compounds in water and hence presence of surfactants can lead to enhancement in carcinogenic potential and dermatitis as reported in literature [1]. Considering environmental and health impacts, permissible limits for surfactants is 1 mg/L in water intended for domestic purposes and still low at 0.5 mg/L for potable water [2].

Materials and methods

Adsorptive separation of commercial sodium benzenesulfonate (SBS) and sodium dodecyl-benzenesulfonate (SDBS) was investigated in the present work using activated carbon obtaining from wood charcoal by different methods. In the case of activated carbons from wood charcoal obtained by the fluidized layer method (CAML-SF) more effective results were obtained than in case of charcoals obtained by the classical method (CAML-MC). The samples were stirred at the speed of rotation 150 rpm, amplitude 4 and the temperature of 298 K. Kinetic study yields important information about the rate of removal and time required to achieve equilibrium.

Results and discussion

Rapid adsorption rate of SDBS from solution on both CAML-SF and CAML-MC samples was observed in first 15 min which decreased and became negligible after 120 min. Around 91% SDBS removal was achieved in initial 15 min from solutions having an initial concentration as 0.5 mmol/L on CAML-SF samples which continued to 97 % at 240 min. In the case of CAML-MC samples approximately 51 % were removed in the first 15 minutes and respectively until 62 % at 240 min.

Langmuir isotherm is a broadly used model, assuming adsorption to occur on specific sites uniformly spread on the surface of the adsorbent. It is commonly used for description of processes, where adsorbed species form a monolayer, and is described by the following equation:

$$C_{eqv}/q_{eqv} = 1/K_L * q_{max} + 1/q_{max} * C_{eqv}$$

where C_{eqv} is the concentration of solute remaining in solution after equilibrium to be reached (mmol/L); q_{eqv} is the amount of solute adsorbed in the same condition (mmol/g); q_{max} is the maximum adsorption capacity in the monolayer and K_L is the equilibrium constant of the adsorption process.

For data description experimental Langmuir theoretical models were applied, which allowed the calculation of sorption parameters (Table 1):

Sample	q_{max}, mmol/g	Langmuir		
		q_{max}, mmol/g	K_L (L/mmol)	R^2
DDBS/Na--CA ML-SF	0,785	0,818	31,31	0,9994
DDBS/Na--CA ML-MC	0,551	0,560	78,95	0,9998

The effect of temperature conditions on extent of SBS removal has been studies. Adsorption isotherms of SBS at different temperatures namely: 298 K, 308 K and 318 K were measured. Initially stock solutions of SBS and SDBS having 5 mmol/L were prepared. The required solutions having different initial concentration for experiments were obtained after appropriate dilution. BET surface area of adsorbents and the pore size distribution have been analyzed based on the Brunauer-Emmett-Teller (BET) method using the Autosorb-1 instrument based on N_2 adsorption-desorption.

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