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## **OPTICAL SENSOR OF FLAVONOIDS BASED ON LIQUID CRYSTAL**

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Abstract. In order to solve the problems associated with the express registration of the presence of biologically active substances in callus biomass, we propose the use of cholesteric liquid crystal (CLC) with a spiral structure as a material of a sensitive element of optical sensor of flavonoids. Cholesteric liquid crystal BLO62 is proposed to use as a sensitive element. Spectral characteristics of alcohol solutions of flavonoids (20%, 40%, 70% and 90%) were obtained. The interaction of CLC with quercetin was analyzed. The scheme of the primary information signal converter is developed in which the current from the photodetector is transmitted to the developed signal converter. The device is implemented with the common use Atmega 328 microcontroller manufactured by Atmel. Speciality of this structural scheme is its flexibility and versatility, which makes it easy to reconfigure the parameters of the firmware for the registration of various types of investigated mediums.

Keywords: optical sensor, liquid crystal, flavonoids, quercetin

## OPTYCZNY CZUJNIK FLAWONOIDÓW BAZUJĄCY NA CIEKŁYCH KRYSZTAŁACH

Streszczenie. Aby rozwiązać problemy związane z szybką analizą obecności substancji biologicznie czynnych w biomasie kalusa, proponujemy zastosowanie materiałów ciekłokrystalicznych o spiralnej strukturze supramolekularnej jako wrażliwego elementu czujnika optycznego flawonoidów. Proponuje się stosowanie cholesterycznego ciekłego kryształu BLO62 jako wrażliwego elementu. Uzyskano charakterystykę spektralną roztworów alkoholowych flawonoidów (20%, 40%, 70% i 90%). Przeanalizowano interakcję cholesterycznego ciekłego kryształu z kwercetyną. Opracowano schemat pierwotnego przetwornika sygnału, w którym prąd z fotodetektora jest przesyłany do opracowanego przetwornika sygnałów. Urządzenie jest realizowane na bazie mikrokontrolera Atmega32 Atmega 328. Cechą tego schematu strukturalnego jest jego elastyczność i wszechstronność, co ułatwia rekonfigurację parametrów oprogramowania do rejestracji różnych typów badanych substancji.

Słowa kluczowe: czujnik optyczny, ciekły kryształ, flawonoidy, kwercetyna

### Introduction

Currently, the use of plant raw materials for the production of pharmaceutical and cosmetic products for the prevention and treatment of many diseases is extremely relevant. Availability, low toxicity, high efficiency, low number of side effects and the presence of secondary metabolites are advantages of plant biomass use [9]. Plants containing flavonoids have antiinflammatory, spasmolytic, antihistamines, antibacterial, antioxidant effects.

Many medicinal plants are rare or endangered species, therefore the arsenal of medicinal plant material is limited. Application of modern methods of biotechnology and cell biology solves problems of obtaining biomass of plants, namely in vitro.

Grass and seeds of Arnica montana were harvested in the phase of full flowering (July – August) from the wild population of Ivano-Frankivsk region [13]. Arnica montana belongs to plants that are under threat of destruction and are listed in the Red Book of Ukraine. This plant contains the various biologically active substances (terpenoids, alkaloids, organic acids, vitamins, glycosides, phenolic compounds and flavonoids) and used in combination therapy for hepatitis, cholangitis and cholecystitis [8]. It is known that in the grass of Arnica montana there are such flavonoids – quercetin, isoquercetin, routine, quercetin pentaoxiaacetate, eriodictiol, hesperidin, campsferol, luteolin, apigenin, which can be explained by the antiasthmatic effect of flavonoids [14].

However, it is necessary to control the availability and content of specific biologically active compounds in cultivated biomass in vitro and its extracts. In order to solve the problems associated with the rapid analysis of the presence of biologically active substances in callus biomass, we propose the use of liquid crystal (LC) materials [5, 6, 7, 11] as a sensitive element of optical sensors. In the sensitive element of the primary transducers of optical sensors an information signal is formed due to the selective reflection (transmission) of light.

We propose to use as an active medium LC materials that are characterized by high sensitivity to external influences, namely temperature, pressure, humidity, action of gas molecules [12, 15]. Among the wide range of electro-optical effects in LC materials, the effect of selective scattering in CLC was chosen. These LC materials are characterized by the presence of a spiral supramolecular structure. Works [16, 17, 18] present the results of using a CLC active medium as an optical sensor of biological substances. Therefore, it is relevant to determine the concentration of flavonoids in alcohol solutions.

## **1.** Preparation of experimental samples and technique of investigation

The object of the study was biologically active substances extracted from callus biomass of Arnica montana.

The biotechnological method of obtaining biomass of plants by in vitro cultivation method is used [10]. The method has many advantages, since the production of biomass does not depend on weather, seasons, soil quality, and callus biomass contains the same biologically active substances as the biomass of an intact plant. Callus biomass at pH 5.5–5.8 with the addition of  $\beta$ -indolylactic acid (2.0 mg/l),  $\alpha$ -naphthylacetic acid (0.1 mg/l) and kinetin (0.5 mg/l) was used to obtain and maintain a tissue culture. The cultivation was carried out with illumination of 2000 lux, a 16-hour photoperiod and a temperature of 23°C. After 50 days, the callus biomass was obtained in light yellow color and loose consistency.

As an extractant, ethanol of different concentrations (20%, 40%, 70% and 90%) was used. To study the dependence of flavonoids and the completeness of extraction from raw materials, alcohol extracts were obtained at various concentrations of the extractant. The presence of flavonoids was detected and confirmed using color reactions and UV spectroscopy. In the grass, Arnica montana contains  $3.85 \pm 0.017\%$ , in callus biomass  $4.04 \pm 0.008\%$  of flavonoids.

A multicomponent cholesteric liquid cristal (CLC) mixture of BLO-62 produced by EM Industries, characterized by high temperature stability of optical characteristics, was chosen as an active LC medium. The nematic liquid crystal 5CB was added in to BLO-62. Concentration of nematic liquid crystal was chosen so that maximum selective reflection ranged within 400–850 nm. The choosing of CNM was characterized by minimum optical transmission at 529 nm of wavelength at room temperature. The CNM with alcohol solution of callus biomass with the following percentage ratios: 20%, 40%, 70% and 90% was studied. Spectral studies were using by means of a spectrophotometer USB-2000 in the range of wavelengths of 200–1000 nm.

In the work [8] the technique of experimental investigations and processing the obtained results is described. The method of obtaining experimental mixtures based on a CNM with the addition of solutions (aqueous, alcohol) of biological substances is considered in the paper [12].

## 2. Results and discussion

On the basis of the spectral studies carried out, spectral dependences were obtained. The typical dependence is shown in Fig. 1.

As can we was concluded from the all spectrals dependencies of the addition of alcoholic solution of flavonoids in the CNM, there is a shift of the minimum transmission in the long-wavelength region of the spectrum (for mixtures of 20%, 40% and 70%) and in the short-wave region with an increase in the percentage composition of the alcohol solution (for 90%).

We observed the linear changing of wavelength of minimum transmission versus of concentration of quercetin alcohol solutions.

As can be seen from Fig. 2 the course of the dependence of the minimum wavelength of the optical transmission from the concentration of 70% and 90% (curve 3 and 4) of the alcohol solution in CNM are observed the shift of minimum wavelength of the optical transmission into smaller wavelengths.

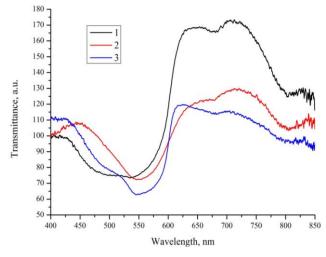


Fig. 1. The typical spectral dependencies of CNM with 20% alcohol solution of quercetin in callus biomass: 1 - 13.00 wt.% (alcohol solution); 2 - 26.09 wt.% (alcohol solution); 3 - 30.88 wt.% (alcohol solution)

Explaining the process of interaction of CNM with flavonoids, we can assume the following. Quercetin molecule is typical flavonoid (Fig. 3) and contains the  $\pi$ -electron aromatic structure, in solution it has a planar structure with a high degree of polarity. Due to the extended  $\pi$ -electron system in the quercetin molecule,

an effective dispersion interaction with the surrounding LC medium is provided. In addition, in the quercetine molecule, there are five phenolic groups, and in the LC molecule there are many carboxyl groups that can form a hydrogen bonds with each other. This hydrogen bond is not strong but sufficient for effective interaction. A complex is formed between the impurity molecules (quercetin) and the LC and its deformation takes place.

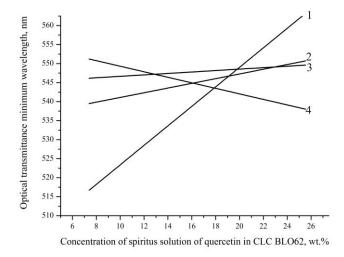


Fig. 2. Dependence of the minimum wavelength of optical transmission on the concentration of alcohol solution of quercetin in callus biomass in CNM: 1-20%, 2-40%, 3-70%, 4-90%

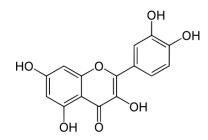


Fig. 3. Structural formula of quercetin molecule (2-(3,4-dihydroxyphenyl)-3,5,7trihydroxy-4H-chromen-4-one

## 3. The principal electrical realization of flavonoids optical sensor

The principle of operation of an optical sensor lies in the process of registering an information signal from the source of radiation that has passed through the active medium to the photodetector [10, 16, 17, 18]. In our case, the information signal is the wavelength [1, 2, 3].

The device (Fig. 4) is implemented with the use of the Atmega 328 microcontroller. The main structural elements are the light source, the active medium, the photodetector, the microcontroller, the interface and the elements of the signal transducer – the input amplifier, the clock detector, the integrator [2, 3, 4].

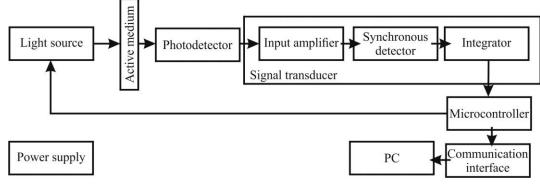
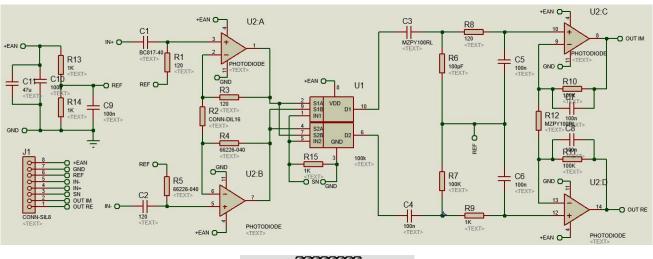


Fig. 4. The block diagram of an optical sensor of flavonoids



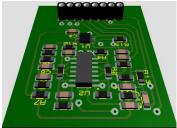


Fig. 5. Electric circuit diagram of the signal converter and its 3D realization

The light source forms an microcontroller modulated optical signal, which crosses the active medium by photodetector registration. The informative signal thus formed after the previous amplification is detected with the subsequent integration and enters the analog input of the microcontroller. Further processing of the received signal is carried out programmatically according to the algorithm of the created software, which is placed in the built-in memory of the microcontroller. Output measurements via the interface unit are transmitted to the PC for their digital and graphical representation.

The peculiarity of this structural scheme is its flexibility and versatility, which makes it easy to reconfigure the parameters of the firmware for the registration of various types of investigated environments.

Figure 5 depicts the electrical principle diagram of the signal converter, which is implemented using modern energy-efficient microelectronic components in particular amplifiers AD8544 and switch AG736.

The simulation was performed and the optimal operating mode of the sensor was selected in the Proteus software environment.

#### 4. Conclusion

- As can been concluded cholesteric-nematic mixture is useful to designed the sensitive element of flavonoids optical sensor for detection in callus biomass.
- 2) Take in to account the influence, we can to suggest the extended  $\pi$ -electron system in the flavonoids (quercetin) molecule, an effective dispersion interaction with the surrounding LC medium.
- 3) The proposed structural scheme is its flexibility and versatility, which makes it easy to reconfigure the parameters of the firmware for the registration of various types of biological investigated mediums.

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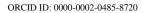
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