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OBTAINING BIOLOGICALLY ACTIVE COMPOUNDS BY EXTRACTION OF VALERIAN ROOTS

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Abstract. An effective method of obtaining biologically active substances from plant raw materials without changing their optical isomerism is extraction. The investigation results of achieving equilibrium conditions for isovaleric acid extraction from valerian roots and rhizomes are presented. The effect of the isovaleric acid chemical structure and extractant nature on achieving equilibrium conditions is shown. Extraction of valerian roots and rhizomes with 70% ethyl alcohol allows a traditional extraction process, i.e., an equilibrium straight line of $C_p=C_{1p}$ type. If desalinated water is used as an extractant, an unconventional case of $C_p \neq C_{1p}$ will arise, complicated by the solvation of isovaleric acid molecules and, consequently, the corresponding equilibrium conditions. The possibility of using ion exchange to isolate isovaleric acid from the polyextract of biologically active compounds was investigated. A technological scheme for obtaining isovaleric acid using ion technologies was proposed. Isovaleric acid was identified by gas chromatography.

Keywords: isovaleric acid, extraction, cellular volume, intercellular volume, ion exchange, equilibrium.

Introduction

Plants are an irreplaceable source for producing various types of biologically active compounds (BAS). BAS isolated from plant raw materials do not lose their relevance due to their high efficiency and low toxicity. The reason for this is the belonging of most of them to a certain type of optical isomerism, as well as the affinity of biochemical processes that occur in plant and human cells. An effective way to obtain BAS without changing the optical isomerism is extraction. This encourages the development of effective technologies for their production by the method of extracting plant raw materials. In addition, the production of BAS, where the extractant is water or aqueous-alcoholic solutions, does not harm the environment, and the technologies for their production can be considered environmentally safe. All this is of particular importance in times of environmental disasters.[1,2] Active substances, namely synthetic analogues of originally plant biologically active compounds, comprise approximately 40%, and in some cases up to 80% of the medicine list.[3-5] In medical practice, preparations are used both based on individual plants, such as valerian, and in combination with other medicinal plants, in particular, Persen, Novo-Passit, Sedavit, *etc*.

One of the methods to obtain them is extraction. That's why the obtaining of biologically active compounds via extraction continues to be actual, no matter how far the chemistry of organic synthesis has gone.[6-9.]

The extraction of biologically active compounds from plant raw materials is a process which efficiency affects the technical and economic indicators of production in various branches of the chemical industry. Improvement of the process itself allows to increase the number of target compounds after the extraction as well as to improve their quality. The raw plant extraction process efficiency depends first on the target compounds' solubility and the transition rates from one phase into another. The poor solubility of the target product can be overcome by selecting an extractant or mixture in a certain proportion. Such an approach should supply favourable conditions for the transition of required compounds into the extractant, and related impurities will remain in a solid phase.[2,4,6]

Analysis of the latest studies and publications showed that there is very little information on selecting an extractant for removing isovaleric acid from plant raw materials of different anatomical and morphological organs (leaves, fruits, roots with rhizomes, *etc*.).[1,2]

According to the different literature sources, isovaleric acid is contained in valerian roots and rhizomes, hop cones, viburnum fruits, *etc*. However, the highest concentration of isovaleric acid is found in the roots and rhizomes of Valeriana officinalis L. This gives reason to

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claim that Valeriana officinalis L. is the main source of this aliphatic acid. In the chemical industry, Valeriana officinalis L. is produced via stripping with water vapor from plant raw materials – valerian L., tea leaves, some citrus fruits, etc. Isovaleric acid is synthesized via isoamyl alcohol oxidation by an electrolytic method in the presence of sulfate acid (H_2SO_4) with adding manganese sulphate ($MnSO_4$) on an anode made of lead oxide (PbO_2) at 20°C; or heating in air with sodium hydroxide and potassium hydroxide (NaOH+KOH) in 2:1 ratio and a small quantity of H_2O at 285–295°C or with NaOH in the presence of copper carbonate $CuCO_3 \cdot Cu(OH)_2 \cdot 0{,}5H_2O$ at 140°C. The complexity of obtaining this acid motivates the development of simpler and cheaper methods.[3,4]

Isovaleric acid is mostly used in the chemical, pharmaceutical and food industries. In the pharmaceutical industry, isovaleric acid is used to produce sedative medicines - Validol, Bromisoval, Corvalol, Valocordin, and other drugs. Esters of isovaleric acid have fruit fragrance, so they are used as natural flavors in the food industry, perfumery and cosmetic industries. Concentrated ethyl ether of isovaleric acid has a fruit-wine fragrance, and diluted ether has an apple flavor.[1,3,4]

Humulus and viburnum fruits have some lower concentrations of isovaleric acid.[5] That is why valerian roots and rhizomes were chosen for further studies.

The transition rate of the target substance from the solid phase to the extractant will be determined mainly by the penetration rate of the extractant into the internal volume of the solid cells, the diffusion rate of the target substance into the volume of the solid particles to the interface, overcoming the resistance of the cell membrane and the intercellular medium, and finally the transition rate of the target substance from the surface of the solid to the main volume of the extractant. This complex mass exchange mechanism (transportation of the target substance from its location in the plant raw material to the main volume of the extractant) is conducted until reaching the state of conditional equilibrium between the phases, which is considered to be the final stage of the extraction. The transition rate of the target substance from the solid phase into the liquid and vice versa at the equilibrium level is equal, and any concentration of this substance in one phase meets the equilibrium concentration in the other phase. The equilibrium conditions between phases are characterized by the equality of chemical potentials at constant temperature and pressure. Calculation of the chemical potential for the solid phase is quite complex and debatable, so the diffusion equilibrium state has been experimentally determined.[9,10]

The purpose of the work is to select an extractant for the selective extraction of isovaleric acid from valerian roots and rhizomes and to develop a mathematical description of the extraction process for the studied conditions and a technological scheme for its production using ion exchange.

2. Experimental

The content of free isovaleric acid in valerian roots and rhizomes is 5%, as well as borneol, bicyclic monoterpenes (camphene, a-pinene, d-terpineol, l-limonene), alkaloids - actinidine, which provides its stimulating effect, besides valerine, chatinine, tannins, saponins, sugars, organic acids (formic, acetic, malic, stearic, palmitic, *etc*.), glycosides (valeride, valerosides A, B, and Z), free monoterpene alcohol mertinol, and in the form of isovaleric acid ester. Raw material contains about 1% of valepotriates, polysaccharides, and organic acids.[3,4]

2.1. Materials

Roots and rhizomes of Valeriana officinalis L., Isovaleric acid (Wako Pure Chemical Industries, Ltd., WPCI), Kalii hydroxidum (PhEur), Hydrochloric acid (HCl, PhEur), Natrii hydrogenocarbonas ($NaHCO_3$, PhEur), Ethanol (WPCI), Strongly basic anionite AB-17-8, desalinated water.

2.2. Methods

2.2.1. Kinetic studies

Kinetic studies aim to simulate the extraction process of ground roots and rhizomes of Valeriana officinalis L. in a device with a stirrer (extractor).[10,11]

To obtain isovaleric acid, the roots and rhizomes of Valeriana officinalis L., crushed to a size of 3 mm, were used. Kinetic studies were conducted in a 2 dm^3 glass reactor with a stirrer. The temperature of the extraction process was maintained by a thermostat within 20 ± 1 °C. The scheme of the experimental unit for studying the extraction kinetics of plant raw materials is presented in Fig. 1.

The extraction technique was as follows: 50 g of chopped plant material was placed in a glass reactor with a stirrer (2) and filled with 1 dm^3 of water-alcohol solution. Later, the glass reactor was closed by a cover with a rubber gasket (4), and the stirrer (5) was turned on.

After that, for a certain time, which did not exceed 5 hours, in steps from 100 to 3600 s, samples of the obtained extract with a volume of 5-10 mL were taken, so the number of samples did not affect the extractant volume. Samples were analyzed for the isovaleric acid amount using the conductometric method of equivalence point determination corresponding to a certain acid number value of the studied sample.

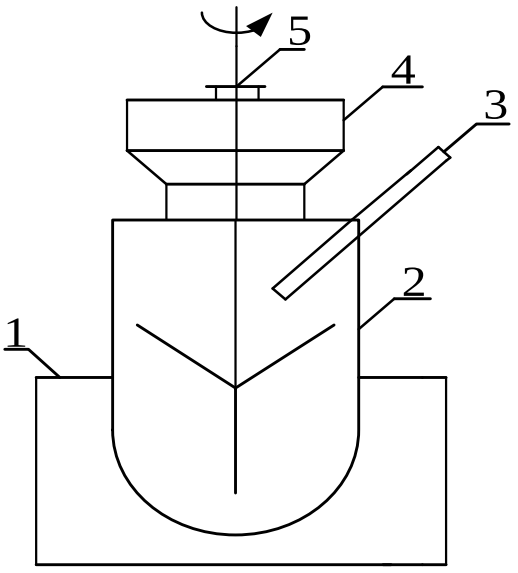


Fig. 1. Scheme of the experimental unit for studying the extraction kinetics of plant raw materials 1 – thermostat; 2 – glass reactor; 3 – sampling burette; 4 – cover with a rubber gasket; 5 – stirrer

2.2.1. Conductometric titration

To determine the content of isovaleric acid, an instrumental, indicator-free method of analysis was used - conductometry. Conductometry is an accurate and reliable method of analysis, economical in terms of time spent on establishing a constant conductivity value after adding the next portion of the titrant. Determination of the equivalence point by the conductometric method in the titration of solutions of organic acids of low concentration consists in establishing the dependence of the electrical conductivity of electrolyte solutions on their composition. This method is sensitive at concentrations of organic acids of medium strength at the level of 10-4 mol/L. The linearity and range of application of the method according to the results of the studies are within the limits of concentrations of organic acids from 1.10-4 to 8.10-4 mol/L.[10]

Conductometric determination of the equivalence point during the titration of isovaleric acid solutions present in the extract was carried out as follows: a selected extract sample of a certain volume, from 5 to 10 mL, was placed in a titration glass and diluted with distilled water to a volume of 100 mL. Then, the conductometer electrodes were immersed in the obtained 10-20 times diluted extract solution. After that, the extract solutions were titrated with an aqueous solution of 0.004–0.025M KOH in portions of 1 mL, and the specific electrical conductivity values were recorded for a conductometric titration curve. The titrant volume ($V_{TIT.}$) used for the isovaleric acid titration was calculated by the joint solution of linear equations to x, which describe the appropriate straight line areas of electric conductivity change of the extract solution before and after the equivalence point.[7]

The mass concentration of isovaleric acid in the extract was calculated according to the equation using the volume of standard solution ($V_{TIT.}$), which was spent for titration to the equivalence point:

$$C = \frac{C_{KOH} V_{KOH} 102}{V_{sample}}; [kg / m^3],$$

where C_t is the value of isovaleric acid mass concentration in the extract during sampling, kg/m^3; C_{KOH} is the concentration of KOH solution, mol/L; V_{sample} is the sample volume, mL; 102 is the isovaleric acid molecule weight, kg/kmol.

3. Results and Discussion

In the kinetics of this type of extraction, the most favorable situation is in the initial time, when the concentration difference in different phases reaches the maximum value. As a result of the extraction process, an equal distribution of solid phase on the whole machine volume is achieved. The concentration field on the surface of the solid phase always changes, and the extractant continuously increases its concentration. The increase of the extractant concentration lasts until equilibrium conditions are reached. Under the equilibrium conditions, the concentration of target substances $\boldsymbol{C_p}$ in the extract that fills the internal volume of the solid phase, corresponds to a certain equilibrium concentration of these substances $\boldsymbol{C_{1p}}$ in the main extract volume. The equilibrium concentration value $\boldsymbol{C_{1p}}$ will be determined by the initial content of target substances $\boldsymbol{C_o}$ in a raw plant material, and also by the internal anatomical structure of the solid particle of the raw plant material.

In the most general form, the internal structure of solid bodies of plant origin includes the presence of two media, cellular and intercellular. The notion of intercellular medium also comprises pores, capillaries, and receptacles. It is quite difficult to determine separately the volume of cellular and intercellular media; therefore, during the analysis of the equilibrium states, it is better to operate only on volume $\boldsymbol{V}$, the absolute value of which is equal to the conventionally named – the retained extractant volume.

Thus, the material balance equation was written in the most general form:

$$C_0 = VC_p + (W - V)C_{1p} \quad (1)$$

where M is a raw plant mass [kg]; C_o is an initial concentration of target substances in the raw plant material

[kg/kg]; W is an extractant volume [m^3]; C_{1p} is the equilibrium concentration of target substances in extract [kg/m^3]; V is the volume of extractant that is contained in cellular and intercellular medium [m^3]; C_p is the target substance concentration in extract, which is contained in cellular and intercellular medium [kg/m^3].

Under condition $C_p = C_{1p}$, or when gaining equilibrium concentration of target substances in the extract that is in cellular and intercellular mediums of raw plant solid phase C_p equals the concentration of these same substances in the main mass of the extract C_{1p}. The proof of this is a straight line on the dependence graph $\frac{C_{1p}}{\beta} = fC_{1p}$, and Eq. (1) turns into:

$$MC_0 = WC_{1p} \quad (2)$$

Eq. (2) can be rewritten:

$$C_0 = \frac{C_{1p}}{\beta} = const \quad (3)$$

where $\beta = \frac{M}{W}$.

Since the initial concentration of target substances in raw materials is constant, under phase ratio, the solid body is liquid, the extract concentration $\boldsymbol{C_{1p}}$ should constantly change under conditions of linear equilibrium dependence.

Analyzing experimental research data on achieving equilibrium conditions during the extraction of plant raw materials, it should be noted that the dependence $Cp=f(C_{1p})$ is linear since the ratio value $\frac{C_{1p}}{\beta}$ is constant.[1]

The analysis of the extraction results of isovaleric acid from the root and rhizome of valerian with 70% ethyl alcohol agrees well with the given theoretical basis. The dependence $Cp=f(C_{1p})$ has a truly linear character, and the ratio value $\frac{C_{1p}}{\beta}$ is constant (Table 1). However, using desalted water as an extractant, the obtained results show that $C_p \neq C_{1p}$, or in other words, when equilibrium is reached, the concentration of isovaleric acid in the extract, which is in the cellular and intercellular environment of the solid phase of plant raw materials C_p, is not equal to the concentration of these substances in the main mass extract $\boldsymbol{C_{1p}}$. This is confirmed by the curve line on $C_p=f(C_{1p})$ dependence graphic Fig.1, so Eq. (3) was refined according to the obtained experimental data:

$$C_p = C_{1p} + \frac{1}{\mathrm{h}}\left(C_0 - \left(\frac{C_{1p}}{\beta}\right)\right) \quad (4)$$

where $\mathrm{h} = \frac{V}{M}$.

Since $\frac{1}{\mathrm{h}}\left(C_0 - \left(\frac{C_{1p}}{\beta}\right)\right) > 0$, it is obvious that $C_p > C_{1p}$ (Tabl. 2). Therefore, Eq. (4) describes the peculiarities of the running extraction process well.

The dissolution conditions, and diphilic structure of the isovaleric acid molecule, a simultaneous combination of polar and nonpolar components in the molecule explain this phenomenon. In the presence of polar water molecules, hydrogen-bonded solvates are formed. Created solvates, as a result of big volume sizes, cannot penetrate through the membrane pores and hence cross the solid phase parts' borders. This is the reason for the slightly higher concentration of isovaleric acid under equilibrium conditions in the solution located in the internal volume of rhizome cells.

Table 1. Experimental data and calculated values obtained in the study of equilibrium conditions during the extraction of valerian roots and rhizomes with 70% ethanol

β; [kg/m^3]	C_{1p}; [kg/m^3] extraction substances isovaleric acid	$\frac{C_{1p}}{\beta}$ extraction substances isovaleric acid	C_o; [kg/kg] extraction substances isovaleric acid 5	C_p; [kg/kg] extraction substances isovaleric acid
500	131.85 5.50	0.264 0.011	0.264 0.011	0.211 $8.8 \cdot 10^{-3}$
250	65.93 2.75	0.264 0.011	0.264 0.011	0.11 $4.4 \cdot 10^{-3}$
166	43.95 1.83	0.265 0.011	0.264 0.011	0.070 $2.92 \cdot 10^{-3}$
125	32.96 1.38	0.264 0.011	0.264 0.011	0.053 $2.20 \cdot 10^{-3}$
100	26.37 1.10	0.264 0.011	0.264 0.011	0.042 $1.76 \cdot 10^{-3}$

In the presence of ethanol molecules, another dissolution mechanism takes place, the creation of a solvate with isovaleric acid molecules and ethanol molecules. In this case, the formation of solvates with alcohol molecules is predominant (Fig. 2). In this case, it is assumed that the concentration C_c of the intracellular substance (isovaleric acid) in the volume of the cell is greater than the concentration C of the same substance in the intercellular

medium and the greater concentration C_1 of the same substance in the main volume of the extractant is even under equilibrium conditions. That is the case of an unconventional course of the extraction process.[12-14]

The mathematical model of the extraction process given above should answer the following questions:

– how does the concentration of the isovaleric acid C_1 in the main volume of the extract increase over time?

– how to achieve the maximum extraction of isovaleric acid from a solid body of organic origin?

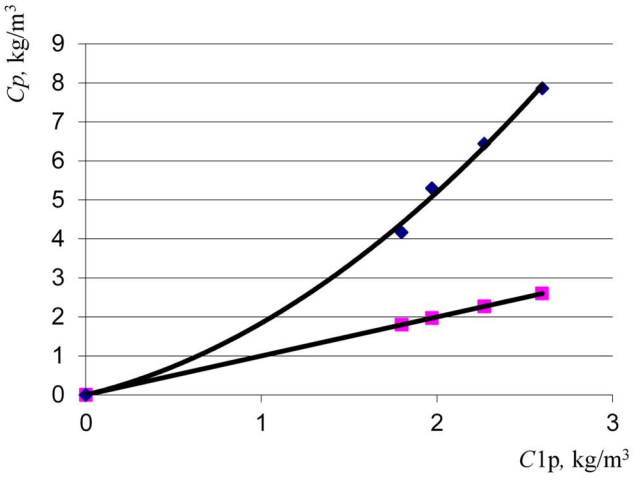


Fig. 2. Equilibrium line under extraction of isovaleric acid from roots and rhizomes of valerian with 70% ethanol - 1, and water - 2

Taking into account the different concentration values of the intracellular (target) substance in the cell volume C_c, in the intercellular space (C), and the main volume of the extract C_1, the differential equation of kinetics was written:

$$(W - V)\frac{dC_1}{dt} = KF(C_c - C_1); \qquad (5)$$

where K is the mass transfer coefficient, which includes the sum of the cell membrane diffusion resistance and the diffusion resistance of the intercellular medium.

According to the equation of the material balance, at any time of extraction, equality is fulfilled:

$$V(C_{co} - C_c) = (W - V)C_1; \qquad (6)$$

Eqs. (5) and (6) form a system that formulates a mathematical model of the studied non-traditional case of the extraction process.

$$\begin{cases} (W - V)\dfrac{dC_1}{dt} = KF(C_c - C_1) \\ V(C_{co} - C_c) = (W - V)C_1 \end{cases} \qquad (7)$$

The solution of this system consists in determining the concentration C_c, from the material balance Eq. (6) and substituting its value into the differential equation of kinetics (5). The solution of the mathematical model has the form:

$$\frac{C_1}{C_{co}} = [1 - \exp(-\frac{KFct}{(W - V)})]; \qquad (8)$$

given that $C_{co}c = \dfrac{C_o V}{W} = C_{1\max}$;

Provided that the entire amount of intracellular substance will pass into the extract, then:

$$\frac{C_1}{C_o c} = \frac{C_1}{C_{1\max}};$$

Eq. (8) will be rewritten in the form:

$$\left(1 - \frac{C_1}{C_{1\max}}\right) = \exp(-\frac{KFt}{W(\frac{1}{h} - 1)}); \qquad (9)$$

$$\text{or } C_1 = C_{1\max.}(1 - Ae^{-k^*t}); \qquad (9^*)$$

where

$$k^* = \frac{KF}{W(\frac{1}{h} - 1)}; \qquad (10)$$

Eq. (9*) in logarithmic coordinates describes a straight line whose tangent angle is k^*. Based on the known k^* value, the mass transfer coefficient K can be determined from formula (10), hence the diffusion resistance of the cell membrane is $\dfrac{D_c}{\delta_c}$ and the diffusion resistance of the intercellular medium is $\dfrac{D}{l}$. In addition, analyzing Eq. (9), it should be noted that with an increase in the volume of the extractant W, the mass transfer coefficient k^* will decrease, then the value of Ae^{-k^*t} will increase. As a final result, all this will cause a decrease in the concentration of the extractant - C_1, accordingly (9), which will have a positive effect on the driving force of the process: $\Delta C = C_c - C_1$. It will be maximal, contributing to the complete extraction of the target component from plant raw materials.[11-13]

Thus, for the maximum extraction of isovaleric acid, it is necessary to take as much extractant W as possible, or h should be as small as possible, but in this case, a large amount of extract with a low content of the target substance will be obtained. The priority should be balancing the cost of the obtained extraction product and the cost of energy resources spent on the extract concentration.

This feature occurs during extraction from fresh plant raw material. On the diffusion path of biologically active substances, there is a living cell wall, the physiological state of which depends on many factors. One of them is a state of protoplasm that leaves prints on the permanent membrane wall layer, making it semipermeable.

The extractant easily penetrates the internal volume of the cell (osmosis), and the reverse diffusion process (plasmolysis) is complicated.

A mixture with a range of biologically active substances is formed by extracting valerian roots and rhizomes. An ion exchange method is suggested for the removal of isovaleric acid. Isovaleric acid is a weak acid; for its extraction efficiency, a strong basic type of anionite should be used. One of such anionites is commonly known AB-17-8.

Table 2. Experimental data and calculated values obtained in the study of equilibrium conditions during the extraction of valerian roots and rhizomes with desalinated water

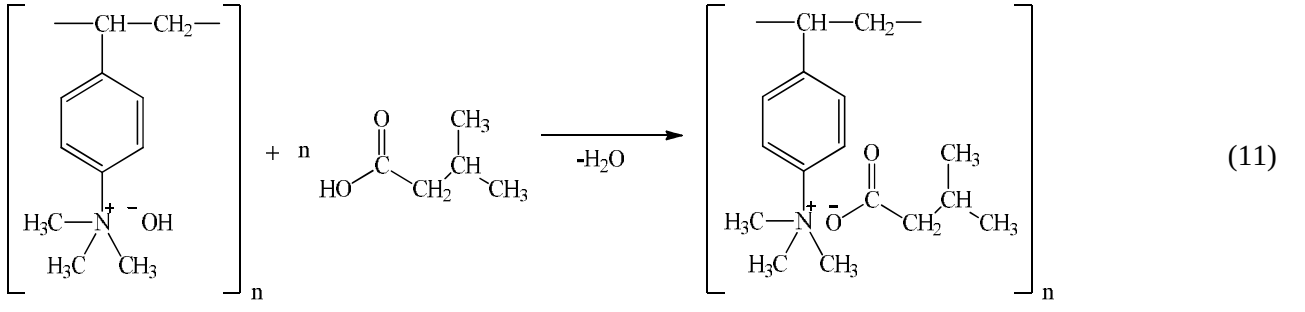
β; [kg/m^3]	C_{1p}; [kg/m^3] isovaleric acid	$\frac{C_{1p}}{\beta}$ isovaleric acid	C_o; [kg/kg] isovaleric acid	C_p; [kg/kg] isovaleric acid	C_p; [kg/m^3] isovaleric acid
500	-	-	0.024	0.024	9.60
250	2.90	0.012	0.024	0.020	7.86
166	2.27	0.014	0.024	0.016	6.44
125	1.97	0.015	0.024	0.013	5.30
100	1.80	0.018	0.024	0.011	4.17

This anionite easily exchanges a hydroxide ion for an anion from the solution; its exchange capacity also depends on pOH of the solution, as the exchange capacity of cations depends on pH. Anionites of this type contain quarter amines (≡N+OH–) that easily dissociate to ions hydroxide OH^- and $\equiv N^+$, which are included in an ionite framework. The extract of target substances formed during extraction was concentrated and sent to a filter and an ion exchange column. The mechanism of ion exchange is as follows: first, the isovaleric acid anion is transferred to the outer layer surface around the AB-17-8 anionite grain; then the anions move through the phase separation boundary into the anionite grain then the chemical exchange reaction between the anionite and isovaleric acid occurs. Then there is the anion diffusion into the ion grain to the phase distribution boundary and the diffusion of ions through the layer into the main volume of the solution.

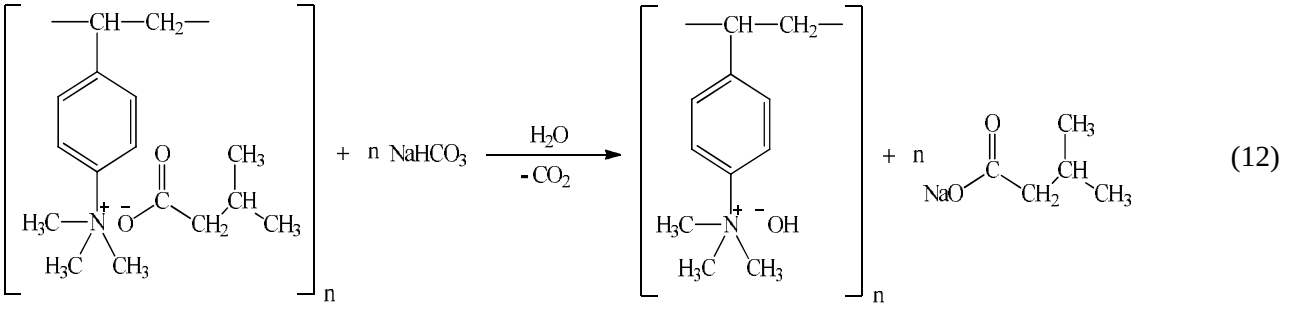
The stages of isovaleric acid extraction by the ion exchange method on the surface of anionite AB-17-8 are depicted by reactions (11-13).

As shown in reaction (11), anion exchange occurs between isovaleric acid and AB-17-8 anionite, as a result of which it remains on the anionite granules.

Soda ($NaHCO_3$) was used to displace the acid from the anionite and regenerate it.



(11)



(12)

The technological scheme for obtaining isovaleric acid is shown in Fig. 3.

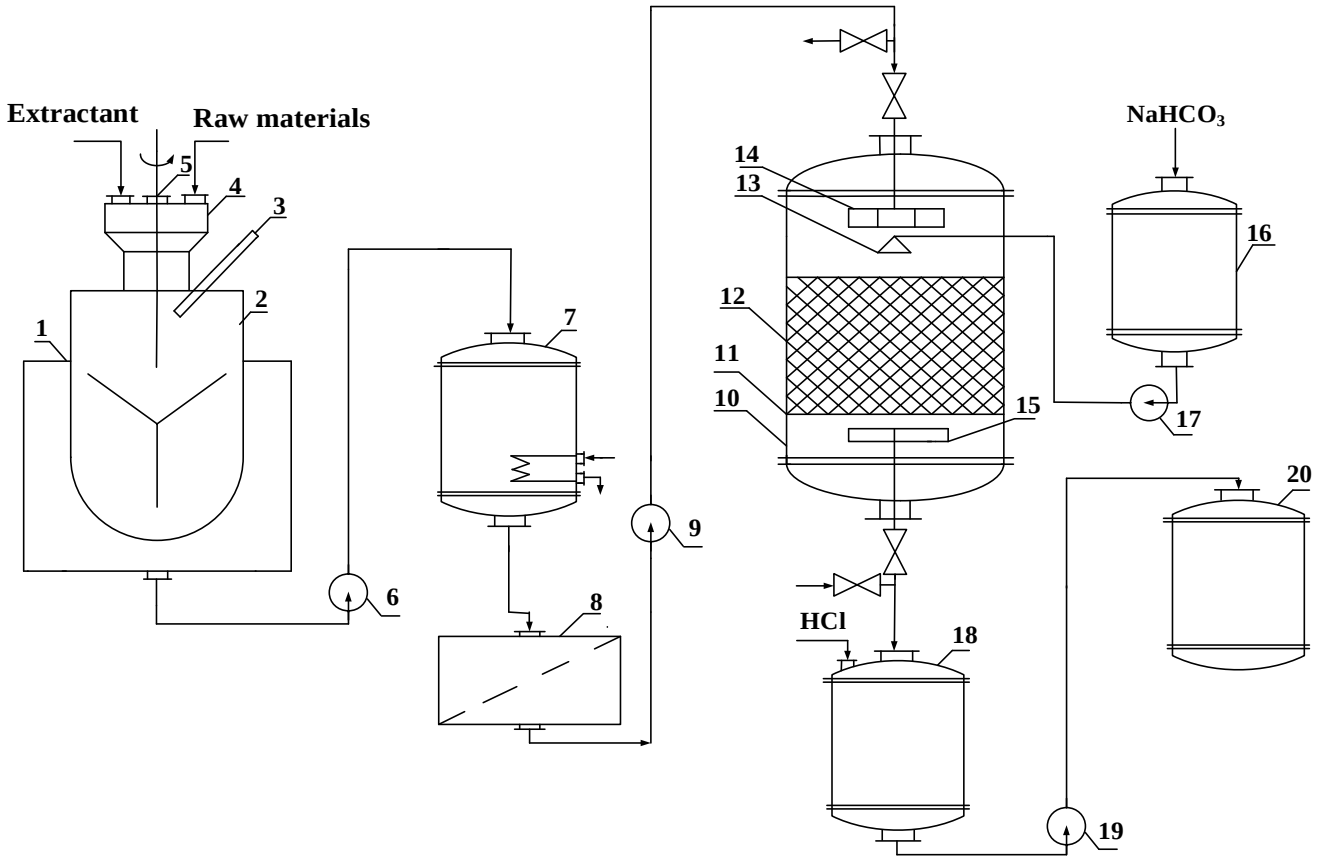
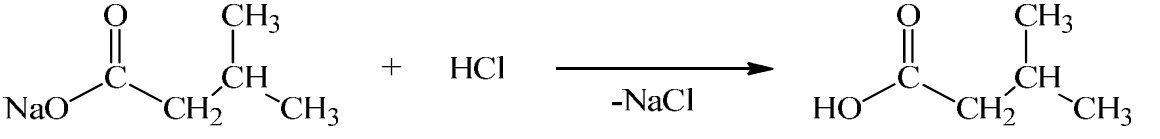


Fig. 3. Technological scheme for obtaining isovaleric acid by extracting valerian roots and rhizomes:
1 – thermostat; 2 – glass flask; 3 – sampling equipment; 4 – rubber gasket; 5 – mixer;
6, 9, 17, 19 – pumps; 7, 18 ,20 – collectors; 8 – filter; 10 – ion exchange column; 11 – grille; 12 – ionite layer;
13, 15 – dispensers; 14 – drip trap; 16 – regenerating solution capacity



(13)

As a result of the reaction (12) sodium salt is formed from isovaleric acid. Chloric acid was used to release isovaleric acid (13).

The identification of isovaleric acid obtained by this technology was confirmed by gas chromatography according to the conditions stipulated in State Pharmacopoeia of Ukraine, 1 edition. 2.2.28 on a gas chromatograph, Shimadzu GC-2010, with a flame ionization detector, under the following conditions:

- chromatograph 1 μL of the test solution of isovaleric acid and the reference solution, the standard of isovaleric acid;
- capillary column 60 m long and 0.53 mm internal diameter, coated with a layer of macrogol 20000 R 1 μm thick, or similar;
- carrier gas – helium for chromatography R;
- carrier gas speed - 5 mL/min;
- carrier gas flow split - 1:1;
- the column temperature is programmed: initial temperature 100 °C, hold at this temperature for 5 min, then the temperature is increased to 230 °C at a rate of 10 °/min and hold for 22 min;
- evaporator temperature - 200 °C;
- detector temperature - 300 °C.

On the chromatogram of the tested solution (Fig. 4), the retention time of the isovaleric acid coincides with the retention time of the isovaleric acid on the chromatogram of the standard solution (Fig. 5).

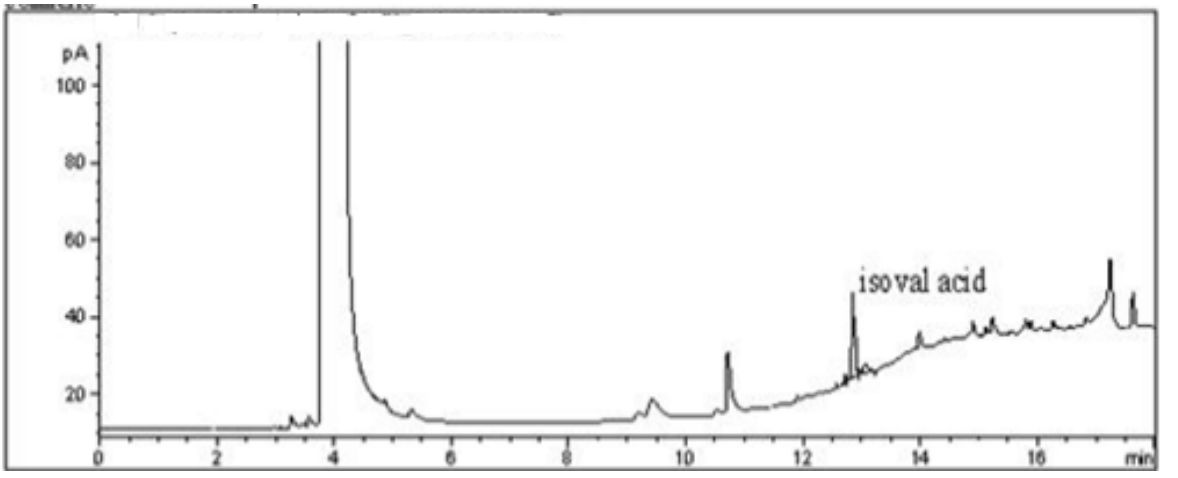


Fig. 4. Chromatogram tested solution

The first maximum corresponds to a solution of ethyl alcohol.

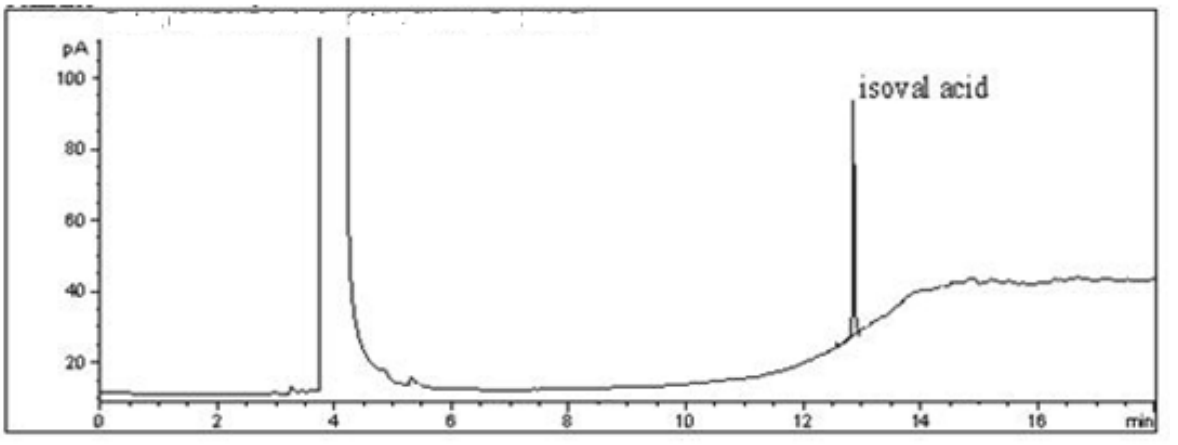


Fig. 5. Chromatogram of standard sample solution

4. Conclusions

It was established that the chemical structure of the extracted substances and the nature of the selected extractant significantly influence the state of equilibrium. Extraction of valerian roots and rhizomes with 70% ethyl alcohol yielded the traditionally straight equilibrium line $C_p=C_{1p}$. In the case of using desalinated water as an extractant, the results indicate an unconventional case, $C_p \neq C_{1p}$, complicated by the solubility characteristics of isovaleric acid, and therefore, the conditions for achieving equilibrium.

A mathematical description of the extracting process of the target substance is given in the case when the concentration of the intracellular substance in the cell volume - C_c is greater than the concentration of the same substance in the intercellular medium - C, and the greater concentration of the same substance in the main volume of the extractant - C_1 under equilibrium conditions.

Ion exchange is proposed to release isovaleric acid from the extract of biologically active substances. Also, the technological scheme for obtaining isovaleric acid was projected.

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ОТРИМАННЯ БІОЛОГІЧНО АКТИВНИХ СПОЛУК ЕКСТРАГУВАННЯМ КОРЕНІВ ВАЛЕРІАНИ

Анотація. *Дієвим способом одержання біологічно активних речовин з рослинної сировини, не змінюючи їхню оптичну ізомерію, є екстрагування. Представлено результати вивчення умов досягнення рівноваги під час екстрагування ізовалеріанової кислоти з коренів і кореневищ валеріани. Показано вплив хімічної структури ізовалеріанової кислоти та природи екстрагенту на умови досягнення рівноваги. Так, у ході екстрагування коренів і кореневищ валеріани 70% етиловим спиртом отримуємо традиційний випадок екстракційного процесу, а саме: рівноважну пряму типу $C_p=C_{1p}$. Якщо використовувати як екстрагент опріснену воду, то отримаємо нетрадиційний випадок, $C_p\neq C_{1p}$, який ускладнюється сольватацією молекул ізовалеріанової кислоти та відповідними умовами досягнення рівноваги. Виділення ізовалеріанової кислоти з екстракту біологічно активних речовин проводили методом іонного обміну. Запропоновано технологічну схему одержання ізовалеріанової кислоти. Отриману ізовалеріанову кислоту ідентифіковано методом газової хроматографії.*

Ключові слова: *ізовалеріанова кислота, екстракція, клітинний об'єм, міжклітинний об'єм, іонний обмін, рівновага.*