

ISSN 2710-1185 (Online)  
ISSN 1813-1107 (Print)

ЕҢБЕК ҚЫЗЫЛ ТУ ОРДЕНДІ  
«Ә. Б. БЕКТҰРОВ АТЫНДАҒЫ  
ХИМИЯ ҒЫЛЫМДАРЫ ИНСТИТУТЫ»  
АКЦИОНЕРЛІК ҚОҒАМЫ

# ҚАЗАҚСТАННЫҢ ХИМИЯ ЖУРНАЛЫ

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## ХИМИЧЕСКИЙ ЖУРНАЛ КАЗАХСТАНА

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### CHEMICAL JOURNAL of KAZAKHSTAN

АКЦИОНЕРНОЕ ОБЩЕСТВО  
ОРДЕНА ТРУДОВОГО КРАСНОГО ЗНАМЕНИ  
«ИНСТИТУТ ХИМИЧЕСКИХ НАУК  
им. А.Б. БЕКТУРОВА»

1(93)

ЯНВАРЬ – МАРТ 2026 г.

ИЗДАЕТСЯ С ОКТЯБРЯ 2003 ГОДА

ВЫХОДИТ 4 РАЗА В ГОД

АЛМАТЫ  
2026

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«Қазақстанның химия журналы»

ISSN 2710-1185 (Online); ISSN 1813-1107 (Print)

Құрылтайшы: Еңбек Қызыл Ту орденді Ө.Б. Бектұров атындағы  
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келісім министрлігінде № 3995-Ж 2003 жылғы 25-маусымдағы

2003 жылы құрылған. Жылына 4 рет шығады.

Редакцияның мекен-жайы: 050010 (А26F3Y1), Қазақстан Республикасы, Алматы қ.,  
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«Химический журнал Казахстана».

ISSN 2710-1185 (Online); ISSN 1813-1107 (Print)

Учредитель: Ордена Трудового Красного Знамени Институт химических наук им. А.Б. Бектурова.

Регистрация: Министерство культуры, информации и общественного согласия Республики Казахстан № 3995-Ж от 25 июня 2003 г.

Основан в 2003 г. Выходит 4 раза в год.

Адрес редакции 050010 (A26F3Y1), Республика Казахстан, г. Алматы, ул. Ш. Уалиханова, 106, тел. 8 (727) 291-24-64, 8 (727) 291-59-31; ics\_rk@mail.ru

Отпечатано в типографии: ИП «Тойходжаев Н.О.», г.Алматы, Алмалинский район, ул. Нурмакова, 26/195 кв. 49; iparuna@yandex.ru

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### «Chemical Journal of Kazakhstan»

ISSN 2710-1185 (Online); ISSN 1813-1107 (Print)

Founder: A.B. Bekturov Institute of chemical sciences awarded by the Order of Red Banner of Labor.

Registration: Ministry of Culture, Information and Public Accord of the Republic of Kazakhstan No. 3995-Ж dated June 25, 2003 year.

«Chemical Journal of Kazakhstan» was founded in 2003 year, publishes four issues in a year.

Address of the Editorial board: 050010 (A26F3Y1), Republic of Kazakhstan, Almaty, Sh. Ualikhanov str., 106, A.B. Bekturov Institute of chemical sciences awarded by the Order of Red Banner of Labor, Fax: 8(727)291-24-64, ics\_rk@mail.ru

Printed in the printing house: IP " Toykhodzhaev N.O.", Almaty, Almainsky district, st. Nurmakova, 26/195 sq. 49, iparuna@yandex.ru

## REGULATION OF THE COMPOSITION AND PROPERTIES OF HUMIC SUBSTANCES DURING ACID TREATMENT

*U.Zh. Dzhusipbekov, G.O. Nurgalieva\*, Z.K. Bayakhmetova, D. Duissenbai, U.B. Aksakalova*

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**Abstract.** *Introduction.* Humic substances (HS) are promising natural sorbents that contain carboxyl, phenolic, hydroxyl and other functional groups, which ensures their high reactivity and tendency to complex with heavy and transition metals, influencing their migration, bioavailability and toxicity. *The aim of the work* is to investigate the influence of various factors on the production of humic acids from the domestic natural raw materials. *Methods:* standardized methods, elemental and functional analysis, IR spectroscopy, and thermogravimetry. *Results and discussion.* Research has been conducted on the production of humic acids (HA) by reacting sodium humate with hydrochloric acid. It has been shown that the regulation of the HCl concentration, liquid phase ratio, reaction time and temperature allows one to control the yield of HA<sup>daf</sup> (up to 78.31%), the content of COOH and OH<sub>phen.</sub> groups (up to 1.20 and 1.62 mmol/g), the total pore volume (up to 0.58 cm<sup>3</sup>/g) and static exchange capacity (up to 21.10 mg-eq/g). The determined optimal synthesis parameters (sodium humate concentration of 3.0%, liquid phase ratio 1:1, treatment for 15 min at 20°C) ensure reproducible properties of the HA and their high efficiency in the sorption of metal ions. The elemental analysis and the calculation of the H/C and O/C atomic ratios have shown that the structure of the synthesized HA is heterogeneous, including aromatic and aliphatic fragments. It has been found that an increase in the HCl concentration initiates an oxidative-hydrolytic destruction of the peripheral structures with a simultaneous increase in the oxygen-containing functional groups, which determine the sorption activity of the HAs. The data of the thermal analysis and IR spectroscopy confirm the preservation of the functional groups up to 350°C and are consistent with the degradation processes at higher temperatures. *Conclusion.* A process flow diagram for producing humic acids under the “mild” conditions has been developed. It is characterized by flexibility, low waste generation, and the ability to produce humic sorbents with a specified composition. The synthesized HA have sorption, ion exchange and other properties and are promising for practical application.

**Key words:** humic acids, hydrochloric acid, oxygen-containing functional groups, heavy metal ions, sorbent, process flow diagram

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**Citation:** Dzhusipbekov U.Zh., Nurgaliyeva G.O., Bayakhmetova Z.K., Duissenbai D., Aksakalova U.B. Regulation of the composition and properties of humic substances during acid treatment. *Chem. J. Kaz.*, 2026, 1(93), 5-14. DOI: <https://doi.org/10.51580/2026-1.2710-1185.01>

## 1. Introduction

Contamination of the liquid media with heavy metal ions (HMI) poses a serious threat to human health and the biosphere due to their high toxicity, stability, and tendency to bioaccumulate [1-3]. Various methods have been developed for the removal of the HMI from the aquatic systems [2-5], among which sorption is considered one of the most effective and versatile approaches [6-8]. Among synthetic and natural sorbents, HS, natural organic compounds with the oxygen-containing functional groups that provide high complexation and sorption capacity, are of particular interest for the HMI removal. The role of the HS as selective sorbents for  $Pb^{2+}$  in the multi-element systems with pH regulation and the introduction of activating groups into the sorbent structure has been demonstrated in [9]. It has been established that a combination of alkaline extraction of brown coal with membrane ultrafiltration makes it possible to obtain the HS with a low impurity content [10]. Biosolubilization of a lignite, using a cell-free fungal enzyme filtrate has demonstrated significantly higher humic acid yields [11]. The authors [12] have found that the alkaline extraction of a lignite, combined with the fermentation and subsequent organic decomposition, have improved the functional properties of humic acids.

Despite these results, the impact of the humic acid production methods on their properties, reproducibility, and industrial applicability remains poorly understood, which justifies the objective of this study - to investigate the influence of various factors on the process of obtaining humic acids from the domestic natural raw materials.

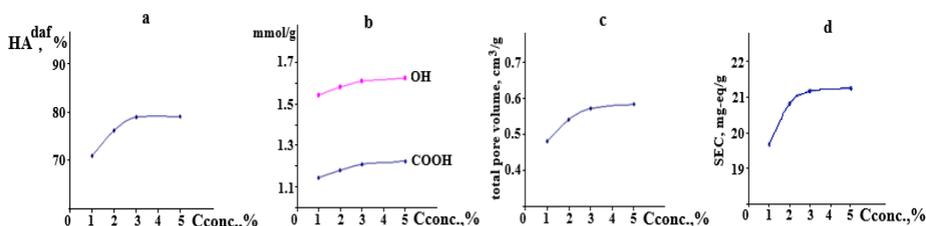
## 2. Experimental part

Humic acids were synthesized using sodium humate, extracted from brown coal from the Oikaragai deposit (the Almaty region). The yield of free humic acids ( $HA^{daf}$ ) was 47.0%, with the ash content ( $A^a$ ) of 24.80% and the moisture content ( $W^a$ ) of 12.80%.

Humic acids were synthesized, using 1.0-5.0% HCl at 20°C for 5-35 min with a liquid phase ratio (sodium humate:hydrochloric acid) of 1:0.4÷2 and a drying temperature of 20-150°C. The elemental composition of the HA (C, H, N, O) was analyzed on a FlashSmart elemental analyzer (Thermo Fisher Scientific Inc., USA), the yield of  $HA^{daf}$ , the content of COOH and  $OH_{phen.}$ -groups, the static exchange capacity (SEC), and the total pore volume were determined according to standard methods [13-16]. The IR spectra were recorded on a Nicolet 5700 Fourier-transform IR spectrometer (Thermo Electron, USA) in the range of 4000-400  $cm^{-1}$  in the KBr tablets; the absorption bands were interpreted according to the literature [14, 17]. A thermogravimetric analysis was performed on an SKZ1053 device (SKZ Industrial Co., Limited, China) in the air atmosphere up to 600°C at a heating rate of 1-80°C/min [18, 19].

### 3. Results and discussion

It follows from the results shown in Figure 1 that an increase in the HCl concentration is accompanied by a change in  $HA^{daf}$ , the content of the COOH- and  $OH_{phen}$ -groups, the total pore volume and the SEC of the obtained HA samples, reaching 79.10%, 1.23 and 1.63 mmol/g, 0.59  $cm^3/g$  and 21.23 mg-eq/g, respectively, at L:L=1:1, the reaction time of 35 min and the temperature of 20°C. An acid treatment of sodium humate probably initiates the oxidative-hydrolytic destruction of the organic macromolecule, accompanied by a structural rearrangement of the HA and the formation of the additional functionally active centers. An increase in the content of the COOH- and  $OH_{phen}$ -groups, characteristic of the HS [9, 10, 14], causes an increase in the number of active sites and, as a consequence, an increase in the sorption properties of the synthesized HA.

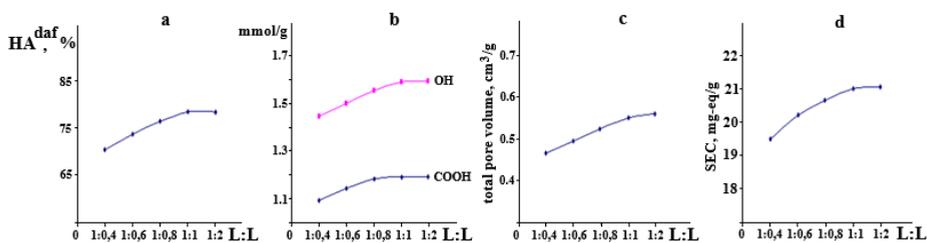


**Figure 1** – An isotherm of the dependence of the  $HA^{daf}$  (a), acidic groups (b), total pore volume (c) and SEC (d) on the concentration of hydrochloric acid.

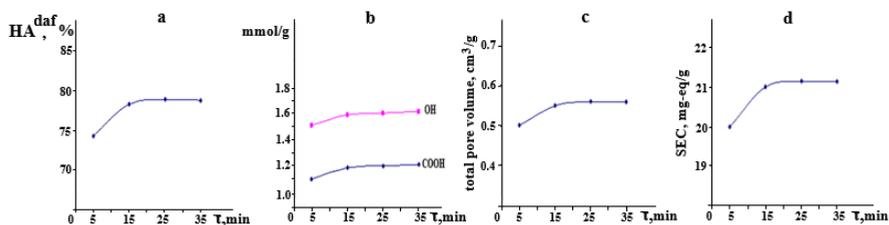
An analysis of the data presented in Figures 2 and 3 indicates that an increase in the L:L ratio from 1:0.4 up to 1:2, as well as an increase in time from 5 to 35 min, leads to an increase in  $HA^{daf}$  from 70.50 up to 78.75%, the content of the COOH groups from 1.09 up to 1.21 mmol/g and the  $OH_{phen}$  groups from 1.44 up to 1.61 mmol/g, the total pore volume from 0.46 up to 0.57  $cm^3/g$  and SEC from 19.50 up to 21.14 mg-eq/g, which is due to the dilution of the reaction suspension and intensification of the mass transfer, contributing to a more complete transition of the HA into the solution, acceleration of the decomposition of organic fragments of the humic sorbent and deepening of the oxidation of aliphatic structures, resulting in the formation of a more developed and porous structure of the material.

The obtained experimental data (Figure 4) indicate the presence of a pronounced temperature pattern in the formation of the structural and functional characteristics of the HA: an increase in the drying temperature from 20 up to 80°C promotes the removal of the physically bound moisture and stabilization of the porous structure, which leads to an increase in the yield of  $HA^{daf}$  up to 78.27%, the content of the COOH and  $OH_{phen}$ -groups – up to 1.19 and 1.59 mmol/g, respectively, the total pore volume – up to 0.55  $cm^3/g$  and SEC – up to 21.0 mg-eq/g. At the same time, a further increase in the drying temperature up to 150°C changes the direction of the process and causes a decrease in the above

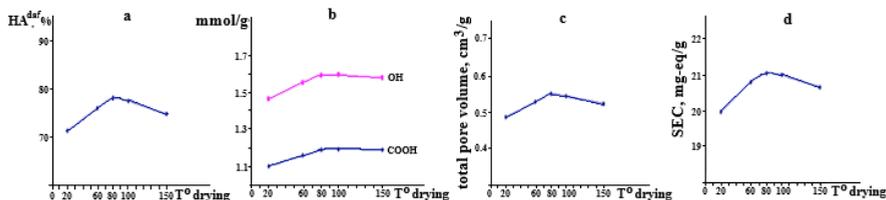
indicators, due to the intensification of the decarboxylation processes, partial oxidation and destruction of the aliphatic fragments of the HA macromolecules, leading to a decrease in the number of the oxygen-containing functional groups and degradation of the porous structure of the material. An elemental analysis of the HA characterizes their composition, transformation, aromaticity, and functional activity [14, 20]. The elemental analysis (Table 1) and calculated H/C and O/C atomic ratios demonstrate structural changes in the synthesized HA, affecting the ratio of the central and peripheral fragments of the molecules. A decrease in the content of C, H, N, and O with an increase in the concentration of HCl indicates the oxidative-hydrolytic destruction of the peripheral organic part. The H/C (0.92-1.08) and O/C (0.39-0.46) ranges reflect the presence of the aromatic and aliphatic fragments and enrichment of the HA with the oxygen-containing functional groups.



**Figure 2** – Changes in the HA<sup>daf</sup> (a), acidic groups (b), total pore volume (c) and SEC (d) depending on the L:L ratios.



**Figure 3** – Effect of time on the HA<sup>daf</sup> (a), acidic groups (b), total pore volume (c) and SEC (d).

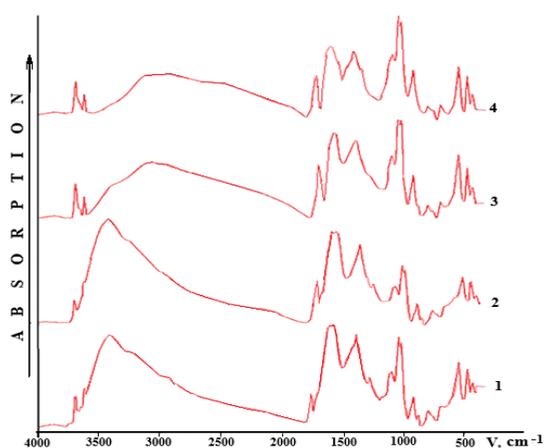


**Figure 4** – Dependence of the HA<sup>daf</sup> (a), acidic groups (b), total pore volume (c) and SEC (d) on the drying temperature.

An analysis of the IR spectra of the synthesized HA (Figure 5) has revealed the characteristic absorption bands of  $\nu$ -vibrations of the unbound OH groups at 3695–3690 and 3620–3615  $\text{cm}^{-1}$ , as well as the hydrogen-bonded OH groups in the region of 3415–3410 and 3235–3230  $\text{cm}^{-1}$  [14, 17]. The shoulder in the range of 3065–3000  $\text{cm}^{-1}$  is due to the vibrations of the aromatic =C–H bonds. The bands at 2965–2960, 2930–2925, and 2855–2850  $\text{cm}^{-1}$  correspond to the  $\nu_s$ -vibrations of the aliphatic -CH<sub>2</sub> and -CH<sub>3</sub> groups, and at 1710–1700  $\text{cm}^{-1}$  to the  $\nu$ -vibrations of the carbonyl groups of carboxylic acids and their derivatives, while the absorption in the region of 1580–1555  $\text{cm}^{-1}$  indicates the presence of secondary amides. The bands at 1390–1385  $\text{cm}^{-1}$  are associated with  $\nu$ - and  $\delta$ -vibrations of the C–O and O–H groups of carboxylic acids, esters, and phenols, and the range of 1095–1010  $\text{cm}^{-1}$  is associated with the  $\nu$ -vibrations of the C–O bonds in alcohols and esters. The bands in the region of 915–425  $\text{cm}^{-1}$  are due to the out-of-plane  $\delta$ -vibrations of the aromatic rings. An increasing in the HCl concentration is accompanied by an increase in the intensity of the carboxyl group bands in the region of 1710–1700  $\text{cm}^{-1}$ .

**Table 1** – An elemental analysis of the humic acid samples

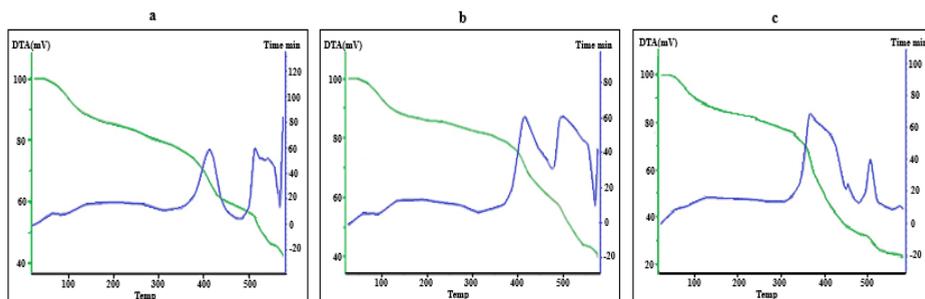
The concentration of hydrochloric acid, %	By weight %				Atomic %				Atomic relations	
	C	H	N	O	C	H	N	O	H/C	O/C
1	60.15	4.63	2.21	31.53	42.60	39.37	1.27	16.75	0.92	0.39
2	59.91	4.35	2.13	30.11	35.75	43.81	1.51	18.93	1.22	0.53
3	58.53	4.16	2.09	27.82	44.59	38.09	1.37	15.93	0.85	0.36
5	58.10	4.01	1.96	27.71	38.68	41.81	1.46	18.04	1.08	0.46



humic acids synthesized at different concentrations of hydrochloric acid,  
%: 1 – 1.0; 2 – 2.0; 3 – 3.0; 4 – 5.0

**Figure 5** – The IR spectra of the HA samples.

The thermal analysis data (Figure 6) are in good agreement with the IR spectroscopy results: the thermal stability of humic acids up to 350°C correlates with the presence of the intense bands of the carboxyl, hydroxyl, and aromatic groups in the IR spectra. The onset of degradation at 350-360°C corresponds to the degradation of the aliphatic fragments and carboxyl groups, indicated by the bands at 1710-1700 and 2960-2850  $\text{cm}^{-1}$ , while the exothermic effect at 510-550°C is consistent with the destruction of the aromatic ring, confirmed by the bands in the range of 1600-1500 and 915-425  $\text{cm}^{-1}$ .



humic sorbents obtained at different concentrations of hydrochloric acid, %: a – 1,0; b – 2,0; c - 3,0

**Figure 6** – The thermograms of the synthesized samples of humic sorbents.

Based on the experimental data, a process flow diagram for producing humic acids (Figure 7), implemented under the “mild” conditions, has been proposed. The process does not require high temperatures or pressures or the use of expensive or hazardous reagents, and the low reaction temperature (20°C) eliminates the need for additional energy. The technology is highly flexible due to the ability to vary parameters and use various mineral acids, enabling the production of humic sorbents with a specified composition and controlled physicochemical properties. An additional advantage is the low level of waste generation due to the ability to reuse the liquid phase in the process cycle.

Optimization of the humic acid synthesis parameters has been conducted under the laboratory conditions, resulting in the establishment of the optimal process conditions: the sodium humate concentration of 3.0%, phase ratio of 1:1, duration of 15 min, temperature of 20°C, and drying temperature of 80°C. A chemical analysis of the obtained test samples has been used to determine the contents of  $\text{HA}^{\text{daf}}$ ,  $\text{COOH}$  and  $\text{OH}_{\text{phen}}$  group, the total pore volume, and COE (Table 2). The results confirm the high efficiency of this technology, which ensures the production of humic sorbents with the reproducible physicochemical characteristics, suitable for the sorption of metal ions.

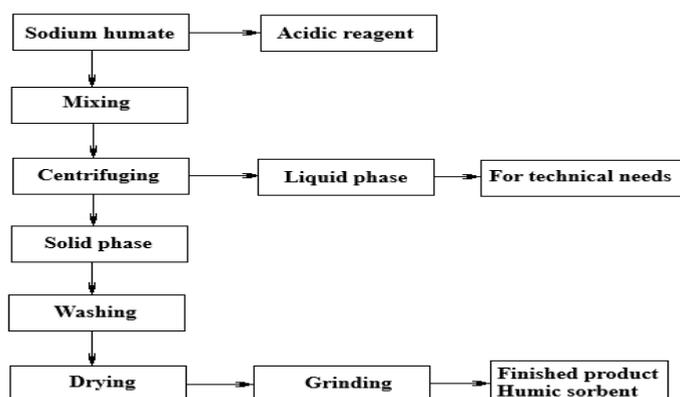


Figure 7 – The basic technological scheme for obtaining humic acids.

Table 2 – The characteristics of the prepared humic acid samples.

HA <sup>daf</sup> , mass. %	The content of the acidic groups, mmol/g		The total pore volume, cm <sup>3</sup> /g	COE, mg-equ./g
	COOH	OH <sub>phen.</sub>		
78.31	1.20	1.62	0.58	21.10

#### 4. Conclusion

The experimental results have demonstrated the feasibility of producing humic acids by reacting sodium humate with a low-concentration HCl solution. The composition and properties of the synthesized humic acids have been determined to depend on hydrochloric acid concentrations, drying time, temperature, and the ratios of the starting components. The elemental and functional analysis, IR spectroscopy, and differential thermal analysis (DTA) data indicate that the humic acids are characterized by the thermal stability, a high yield of the active ingredient, and a high content of the carboxyl groups and phenolic hydroxyls. They can participate in ion exchange and complexation reactions. The proposed humic acid production technology utilizes various types of acid reagents, variable process parameters, and the composition and properties of the humic acids, making it more flexible and enhancing their sorption capacity. The resulting humic acids can be used as effective natural sorbents for purifying the liquid and solid media from various contaminants.

**Funding:** This work has been completed under the Targeted Financing Program for 2025-2026 “Fundamental Principles for the Production of Innovative, Environmentally Safe, Multifunctional Chemical Products and Materials” (IRN BR27101179) of the Science Committee of the Ministry of Health, Education and Science of the Republic of Kazakhstan.

**Conflict of Interest:** The authors declare no conflicts of interest requiring the disclosure in this paper.

## ҚЫШҚЫЛМЕН ӨНДЕУ КЕЗІНДЕГІ ГУМИНДІ ЗАТТАРДЫҢ ҚҰРАМЫ МЕН ҚАСИЕТТЕРІН РЕТТЕУ

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**Түйіндеме.** *Кіріспе.* Гуминді заттар (ГЗ) – карбоксил, фенолды, гидроксил және басқа да функционалдық топтарды қамтитын перспективалы табиғи сорбенттер, бұл олардың жоғары реакциялық және ауыр және өтпелі металдармен кешен түзуге бейімділігін қамтамасыз етеді, олардың миграциясына, биожетімділігіне және уыттылығына әсер етеді. *Жұмыстың мақсаты* – отандық табиғи шикізаттан гумин қышқылдарын алу үдерісіне әртүрлі факторлардың әсерін зерттеу. *Әдістер:* стандартталған әдістер, элементтік және функционалдық талдау, ИҚ-спектроскопия және термогравиметрия. *Нәтижелер және талқылау.* Натрий гуматын тұз қышқылымен әрекеттесу арқылы гумин қышқылдарын (ГҚ) алу бойынша зерттеулер жүргізілді. HCl концентрациясын, сұйық фаза катынасын, реакция уақытын және температурасын реттеу  $\text{Na}^{\text{dat}}$  шығымын (78.31%-ға дейін),  $\text{COOH}$  және  $\text{OH}_{\text{фен.}}$  топтарының мөлшерін (1.20 және 1.62 ммоль/г дейін), жалпы кеуек көлемін (0.58  $\text{cm}^3/\text{g}$  дейін) және статикалық алмасу сыйымдылығын (21.10 мг-экв/г дейін) бақылауға мүмкіндік беретіні көрсетілді. Анықталған оңтайлы синтез параметрлері (натрий гуматының концентрациясы 3.0%, сұйық фаза катынасы 1:1, 20°C, 15 мин) ГҚ-ның қайталанатын қасиеттерін және металл иондарын сорбциялаудағы жоғары тиімділігін қамтамасыз етеді. Элементтік талдау және H/C және O/C атомдық катынастарын есептеу синтезделген ГҚ құрылымының гетерогенді екенін көрсетті, оның ішінде ароматты және алифатты фрагменттер бар. HCl концентрациясының жоғарылауы перифериялық құрылымдардың тотығу-гидролитикалық ыдырауына, ГҚ сорбциялық белсенділігін анықтайтын оттегі бар функционалдық топтардың артуына әкелетіндігі анықталды. Термиялық талдау және ИҚ-спектроскопия деректері функционалдық топтардың 350°C дейін сақталуын растайды және жоғары температурадағы ыдырау үдерістеріне сәйкес келеді. *Қорытынды.* «Жұмсақ» жағдайларда ГҚ алудың технологиялық сызбасы әзірленді, бұл икемділігімен, қалдықтардың аз түзілуімен және құрамы белгіленген гумин сорбенттерін алу мүмкіндігімен сипатталады. Синтезделген ГҚ сорбциялық, ион алмасу және басқа да қасиеттерге ие және практикада қолдану үшін перспективалы.

**Түйінді сөздер:** гумин қышқылдары, тұз қышқылы, оттегі бар функционалдық топтар, ауыр металл иондары, сорбент, технологиялық сызба

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## РЕГУЛИРОВАНИЕ СОСТАВА И СВОЙСТВ ГУМИНОВЫХ ВЕЩЕСТВ ПРИ КИСЛОТНОЙ ОБРАБОТКЕ

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**Резюме.** *Введение.* Гуминовые вещества (ГВ) – перспективные природные сорбенты, обладающие карбоксильными, фенольными, гидроксильными и другими функциональными группами, что обеспечивает их высокую реакционную способность и склонность к комплексообразованию с тяжелыми и переходными металлами, влияя на их миграцию, биодоступность и токсичность. *Цель работы* – исследование закономерностей влияния различных факторов на процесс получения гуминовых кислот из отечественного природного сырья. *Методы:* стандартизованные методы,

элементный и функциональный анализ, ИК-спектроскопия и термогравиметрия. *Результаты и обсуждение.* Проведены исследования по получению гуминовых кислот (ГК) путем взаимодействия гумата натрия с соляной кислотой. Показано, что регулирование концентрации HCl, соотношения жидкой фазы, времени реакции и температуры позволяет управлять выходом  $\text{HA}^{\text{daf}}$  (до 78.31%), содержанием COOH- и OH<sub>фен.</sub>-групп (до 1.20 и 1.62 ммоль/г), суммарным объемом пор (до 0.58 см<sup>3</sup>/г) и статической обменной емкостью (до 21.10 мг-экв/г). Определенные оптимальные параметры синтеза (концентрация гумата натрия 3.0%, соотношение жидких фаз 1:1, обработка 15 мин при 20°C) обеспечивают воспроизводимые свойства ГК и их высокую эффективность в сорбции ионов металлов. Элементный анализ и расчет атомных соотношений N/C и O/C показали, что структура синтезированных ГК является гетерогенной, включающей ароматические и алифатические фрагменты. Установлено, что повышение концентрации HCl инициирует окислительно-гидролитическое разрушение периферийных структур с одновременным ростом кислородсодержащих функциональных групп, определяющих сорбционную активность ГК. Данные термического анализа и ИК-спектроскопии подтверждают сохранность функциональных групп до 350 °C и согласуются с деградационными процессами при более высоких температурах. *Заключение.* Разработана технологическая схема получения ГК в «мягких» условиях, характеризующаяся гибкостью, низким уровнем отходаобразования и возможностью получения гуминовых сорбентов с заданным составом. Синтезированные ГК обладают сорбционными, ионообменными и др. свойствами и перспективны для практического применения.

**Ключевые слова:** гуминовые кислоты, соляная кислота, кислородсодержащие функциональные группы, ионы тяжелых металлов, сорбент, технологическая схема

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## LEAD-LIKE PROPERTIES OF A NOVEL PYRIDINE AMINOPHOSPHONATE: SYNTHESIS, PREDICTIVE EVALUATION AND BIOLOGICAL TESTING

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**Abstract.** *Introduction.* Aminophosphonate derivatives attract considerable interest as a class of low-molecular-weight compounds capable of exerting regulatory effects in biological systems of different origin. Early-stage characterization of biological potential can be achieved by combining predictive approaches with experimental investigation. *The aim* of this study is to synthesize a new aminophosphonate, obtain its water-soluble form and evaluate its biological activity in a “prediction-experiment” format. Dimethyl((3-phenoxyphenyl)((pyridin-2-ylmethyl)amino)methyl)phosphonate (**PMAAPh**) has been synthesized by the Kabachnik-Fields reaction, and then its succinate salt (**PMAAPh-Suc**) has been obtained to improve the solubility in water. The structure of the compound has been confirmed by the methods of a physicochemical analysis (NMR and IR spectroscopy). The predicted biological activity, pharmacokinetic properties, and toxicity have been assessed, using *in silico* tools. *Experimental studies* have been performed, using plant models *in vitro*, and a model of experimental pancytopenia *in vivo*. The computer screening has shown that aminophosphonate **PMAAPh** meets the main criteria for pharmacological similarity and belongs to toxicity class III. The experiment has demonstrated that **PMAAPh-Suc** stimulates the germination and vigor of wheat seeds, and also stimulates hematopoiesis. Taken together, these findings provide a basis for the further investigation of the biological activity of this aminophosphonate.

**Key words:** pyridin-2-ylmethanamine, aminophosphonate, *in silico* analysis, myelostimulating activity, plant growth-stimulating activity

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**Citation:** Ten A.Yu., Serdaly D.T., Seilkhanov T.M., Yu V.K. Lead-like properties of a novel pyridine aminophosphonate: synthesis, predictive evaluation and biological testing. *Chem. J. Kaz.*, **2026**, 1(93), 15-25. DOI: <https://doi.org/10.51580/2026-1.2710-1185.02>

## 1. Introduction

In recent years, a clear trend has emerged towards the use of integrated approaches that combine the computational prediction methods with the experimental studies [1,2]. The application of *in silico* tools makes it possible to assess drug-likeness, potential biological activity, and toxicological risks of new molecules at the early stages of the research, whereas subsequent *in vitro* and *in vivo* investigations allow for the characterization of their effects on the growth-related and regenerative processes in biological systems of different origins.

Such an integrative strategy is regarded as an effective means of identifying promising low-molecular-weight compounds with a regulatory activity and a balanced safety profile, thereby underscoring the relevance of the further research in this field.

## 2. Experimental part

The IR spectra were recorded on a Nicolet 5700 FT-IR spectrometer, using thin-films. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were obtained on a JEOL JNM-ECA 400 spectrometer in  $\text{CDCl}_3$ .

*Dimethyl* *((3-phenoxyphenyl)((pyridin-2-ylmethyl)amino)methyl)phosphonate (PMAAPh)*. A round-bottom flask equipped with a mechanical stirrer, a Dean–Stark apparatus, and a reflux condenser was charged with pyridin-2-ylmethanamine (0.02 mol), 3-phenoxybenzaldehyde (0.02 mol), and dimethyl phosphite (0.03 mol) in 150 mL of absolute benzene. The reaction mixture was refluxed for 48 h. After the completion of the reaction, the solvent was removed under reduced pressure, and the crude product was purified by column chromatography on  $\text{Al}_2\text{O}_3$  using chloroform/acetone (20:1, v/v) as the eluent. The second fraction was collected to afford **PMAAPh** as a yellow oil.  $R_f=0.43$  (chloroform/acetone (20:1, v/v))

Molecular formula:  $\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}_4\text{P}$ . Yield: 6.23 g (80%).  $n_D^{20}=1,382$ . IR (film),  $\nu$ ,  $\text{cm}^{-1}$ : 3459 (N–H); 1252 (P=O); 1056 (P–O–C); 1040 (C–O–C); 3020, 1585, 1491, 756, 683 (Ph).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.48 (d,  $J = 5.3$  Hz, 1H, pyridine–H), 7.55 (m,  $J = 7.0$  Hz, 1H, pyridine–H), 7.27 (q,  $J = 7.3$  Hz, 3H, Ar–H), 7.16 (d,  $J = 7.0$  Hz, 2H, Ar–H), 7.09 (d,  $J = 5.4$  Hz, 2H, Ar–H), 7.04 (q,  $J = 6.8$  Hz, 1H, pyridine–H), 6.93 (dt,  $J = 24.3, 6.8$  Hz, 3H, Ar–H, pyridine–H), 3.85 (dd,  $J = 14.3, 5.6$  Hz, 1H, CH–P), 3.73–3.62 (m, 4H,  $\text{CH}_3$ , N–H), 3.58 (dd,  $J = 10.6, 5.7$  Hz, 3H,  $\text{CH}_3$ ), 3.14 (s, 2H,  $\text{CH}_2$ ).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$ : 158.83 (Cq, pyridine), 157.54 (Cq, Ar–O), 157.11 (Cq, Ar–O), 149.39 (CH–N, pyridine), 137.48 (CH, pyridine), 136.54 (Cq, Ar), 129.97 (CH, pyridine), 129.83 (2CH, Ar), 123.62 (CH, Ar), 123.56 (CH, Ar), 123.42 (CH, Ar), 123.21 (CH, Ar), 122.44 (CH, Ar), 119.09 (2CH, Ar), 118.52 (CH, Ar), 60.57 (CH–P), 53.70 ( $\text{CH}_3$ ), 53.62 ( $\text{CH}_3$ ), 52.72 ( $\text{CH}_2$ ).

**PMAAPh Succinate (PMAAPh-Suc)**. **PMAAPh** (0.01 mol) and succinic acid (0.01 mol) were thoroughly ground in a mortar with a small amount of ethanol until a homogeneous mixture was obtained. The ethanol was evaporated at 50–

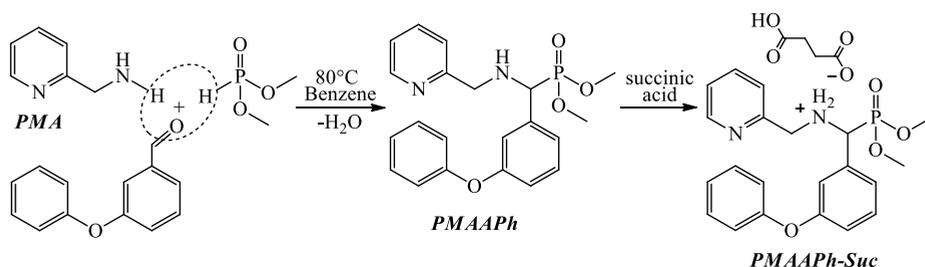
55°C in a drying oven. **PMAA $Ph$ -Suc** was obtained as a yellow powder. M.p.=176–177°C.

**Biological Assays.** The procedures for determining the seed germination energy, laboratory germination, and germination intensity of wheat seeds, as well as the methodology for evaluating myelostimulating activity, were carried out according to the previously described protocols [3].

*In silico* tools [4-6].

### 3. Results and Discussion

At the initial stage of the study, the target aminophosphonate derivative dimethyl ((3-phenoxyphenyl)((pyridin-2-ylmethyl)amino)methyl)phosphonate (**PMAA $Ph$** ) has been synthesized, using the three-component Kabachnik–Fields reaction, which is one of the most common and efficient approaches for the preparation of  $\alpha$ -aminophosphonates. The obtained compound has been isolated in an individual form. To improve the aqueous solubility of **PMAA $Ph$** , its succinate salt (**PMAA $Ph$ -Suc**) has been subsequently prepared by treating the free base with a succinic acid.



The IR spectrum of **PMAA $Ph$**  exhibits an absorption band corresponding to the N–H stretching vibrations at  $3459\text{ cm}^{-1}$ , as well as the characteristic bands of the dimethoxyphosphoryl fragment, namely the P=O and P–O–CH<sub>3</sub> stretching vibrations at  $1252$  and  $1056\text{ cm}^{-1}$ , respectively. The presence of the phenoxyphenyl substituent is confirmed by the aromatic ring bands at  $3020$ ,  $1585$ ,  $1491$ , and  $756\text{ cm}^{-1}$ , along with the C–O–C stretching band of the ether linkage at  $1040\text{ cm}^{-1}$ .

A key diagnostic feature of **PMAA $Ph$**  formation in the NMR spectra is the signal of the methine group at the phosphorus-containing center (CH–P). In the <sup>13</sup>C NMR spectrum, this signal is observed at  $\delta\ 60.57$ , while in the <sup>1</sup>H NMR spectrum the corresponding CH–P proton resonates at  $\delta\ 3.85$ . Its chemical shift and splitting pattern (dd,  $J = 14.3, 5.6\text{ Hz}$ , 1H) reflect the influence of the adjacent heteroatoms (P and N), which is typical for  $\alpha$ -aminophosphonates. The N–H proton falls within the signal region of the OCH<sub>3</sub> groups of the phosphonate moiety ( $\delta\ 3.73\text{--}3.62$ , m, 4H), so it is not considered as a separate resonance.

The *in silico* methods are an effective modern tool for the early-stage biologically active substance evaluation. They enable simultaneous assessment of

the drug-like properties, predicted biological activity, pharmacokinetic profile, and potential toxicity of the new compounds, enabling a rational selection of the most promising structures even before the experimental work.

In our initial study, an *in silico* analysis has been used for a comprehensive evaluation of the aminophosphonate (**PMAAPh**). The first step has been to evaluate the biological potential (predict the spectrum of the biological activity) of **PMAAPh**, using the PASS program (Table 1). The analysis indicates a notable cardiometabolic and regulatory potential of the compound. The types of activity with the highest probability of manifestation ( $P_a > 0.5$ ) are: cholesterol antagonism ( $P_a = 0.605$ ), treatment of restenosis ( $P_a = 0.539$ ), antianginal activity ( $P_a = 0.504$ ), and potential effectiveness in the treatment of Alzheimer's disease ( $P_a = 0.505$ ). The predicted inhibitory activity against glutamate-5-semialdehyde dehydrogenase also reaches high values ( $P_a = 0.531$ ), which demonstrates the possible effect of the compound on amino acid metabolism and energy metabolism. The moderate  $P_a$  values for the regulation of calcium metabolism ( $P_a = 0.479$ ), hypolipidemic effect ( $P_a = 0.356$ ) and treatment of atherosclerosis ( $P_a = 0.410$ ) also demonstrate the potential of the studied aminophosphonate in terms of cardiovascular and metabolic disorders.

**Table 1** – PASS-predictive analysis of the biological activity of **PMAAPh**

<b>Pa</b>	<b>Pi</b>	<b>Activity</b>	<b>Pa</b>	<b>Pi</b>	<b>Activity</b>
0.605	0.019	Cholesterol antagonist	0.410	0.035	Atherosclerosis treatment
0.539	0.005	Restenosis treatment	0.351	0.030	Stroke treatment
0.505	0.012	Alzheimer's disease treatment	0.346	0.025	HIV attachment inhibitor
0.531	0.054	Glutamate-5-semialdehyde dehydrogenase inhibitor	0.340	0.106	Neurodegenerative diseases treatment
0.473	0.004	Antischistosomal	0.332	0.015	Bone formation stimulant
0.504	0.041	Antianginal	0.299	0.003	Factor VIIa inhibitor
0.479	0.018	Calcium regulator	0.356	0.071	Hypolipemic

The activities predicted at lower  $P_a$  values, such as inhibition of HIV attachment, stimulation of bone formation, and inhibition of factor VIIa (Table 1), have not been a priority in this study. These areas require the further experimental verification. Based on the PASS profile, **PMAAPh** can be classified as a promising structure, primarily in the context of cardiometabolic regulation and enzyme inhibition. This justifies the further *in vitro* and *in vivo* studies.

Since the PASS algorithms are primarily focused on predicting the biological activity without considering the pharmacokinetic characteristics of the compound, an additional computational evaluation has been performed in the next step, using the SwissADME platform (Table 2). The data in Table 2 indicate that **PMAAPh** has a balanced physicochemical profile that meets the generally accepted requirements for orally active compounds. The compound is characterized by moderate lipophilicity (Consensus LogP = 3.03) and a high predicted gastrointestinal absorption rate. Furthermore, the bioavailability index has an

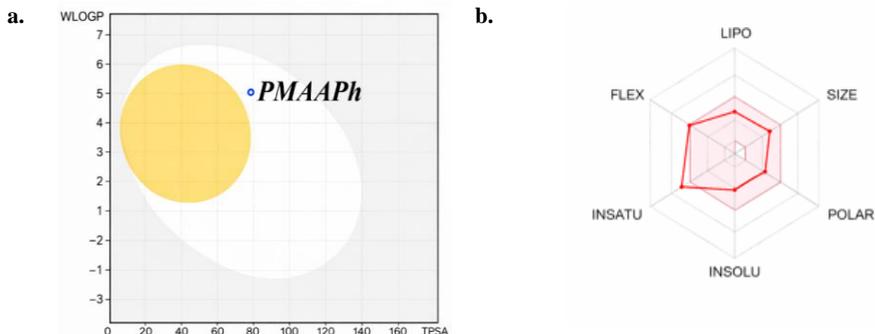
acceptable value (0.55). The topological polar surface area (TPSA = 79.49 Å<sup>2</sup>) indicates a predominantly peripheral pharmacological action. This is consistent with the lack of penetration across the blood-brain barrier predicted by the BOILED-EGG model (Figure 1a). Within this model, the white-colored region corresponds to a high probability of an intestinal absorption. The yellow zone indicates a potential permeability across the blood-brain barrier. Thus, the localization of *PMAAph* within the white region and outside the yellow zone indicates a favorable absorption profile. This also indicates a predominantly peripheral pharmacological action.

**Table 2** – The key calculated ADME and drug-likeness parameters of *PMAAph*

Parameter	Value	Extended comment
Molecular weight (MW)	<b>398.39 g/mol</b>	MW complies with Lipinski's rule (below 500 g/mol). MW places the compound within the classical lead-like range (300–450 g/mol).
Consensus LogP (Po/w)	<b>3.03</b>	This value falls within the range of moderate lipophilicity, indicating a good balance between membrane permeability and water compatibility. This means absorption in the gastrointestinal tract without an excessive hydrophobicity, which could lead to nonspecific binding or increased toxicity.
TPSA	<b>79.49 Å<sup>2</sup></b>	The TPSA assay shows that the standard threshold for blood-brain barrier penetration is exceeded. This indicates a primarily peripheral pharmacological profile and also explains the lack of a predictable CNS penetration.
Rotatable bonds	<b>9</b>	A relatively high number of rotatable bonds reflects an increased conformational flexibility, which may reduce an oral exposure consistency and contributes to the lead-likeness violations, but can enhance an adaptability to diverse biological targets.
Water solubility	<b>Low–moderate</b>	The differences between the ESOL/AlI and SILICOS-IT models indicate the marginal solubility of <i>PMAAph</i> in water, which significantly limits the ADME profile. Therefore, the formation of <i>PMAAph-Suc</i> is necessary.
GI absorption	<b>High</b>	Despite the limited intrinsic solubility, a high predicted gastrointestinal absorption suggests that <i>PMAAph</i> retains sufficient permeability, consistent with its moderate lipophilicity and BOILED-Egg analysis.
BBB permeation	<b>No</b>	The lack of the BBB permeation reduces the risk of the side effects upon the central nervous system, and supports the development of <i>PMAAph</i> for peripheral therapeutic applications.
P-gp substrate	<b>Yes</b>	The predicted interaction with P-glycoprotein suggests that efflux mechanisms may partially limit a systemic exposure, potentially contributing to the interindividual variability in pharmacokinetics.
Lipinski / Egan / Muegge	<b>Passed</b>	The compliance with multiple drug-likeness filters confirms a generally well-balanced physicochemical profile suitable for the further pharmacological development.
Bioavailability score	<b>0.55</b>	A moderate bioavailability score indicates a reasonable oral exposure potential, while leaving room for the improvement through the chemical or formulation optimization.

The radar diagram (Figure 1b) shows how the compound meets the key drug-likeness criteria, such as lipophilicity (LIPO), molecular size (SIZE), polarity (POLAR), solubility (INSOLU), saturation (INSATU), and molecular flexibility

(FLEX). As the diagram shows, most parameters are within the optimal ranges, with only flexibility and solubility showing slight deviations. Based thereupon, it seems justified to obtain succinate salt (PMAA $\text{Ph}$ -Suc) to improve solubility.



**Figure 1** – An illustration of the predicted ADME properties and pharmacokinetic profile of PMAA $\text{Ph}$  (**a** – BOILED-EGG diagram, **b** – radar plot).

To obtain a more comprehensive safety profile, the ADMET analysis has been supplemented with the computational toxicity prediction, using the ProTox-3.0 platform (Table 3). Overall, the compound exhibits a generally favorable predicted toxicology profile.

Specifically, hepatotoxic effects are not predicted (DILI: inactive, probability 0.74), and cardiotoxicity is also not expected (inactive, 0.71). The model also does not predict neurotoxicity or nephrotoxicity, with the corresponding inactive probabilities of 0.53 and 0.59. These results support the rationale for considering this compound early in the evaluation of the drug candidates. ProTox-3.0 does not predict the carcinogenic, mutagenic, immunotoxic, or general cytotoxic effects (inactive, probability range 0.57–0.86). Taken together, these results suggest the absence of the structural features typically associated with a significant toxicity.

However, there are several predicted endpoints: potential respiratory toxicity (activity, 0.69), ecotoxicity (activity, 0.66), food-related toxicity (activity, 0.60), and blood-brain barrier-related toxicity (activity, 0.70).

According to ProTox-3.0, the predicted  $\text{LD}_{50}$  value for PMAA $\text{Ph}$  is 200 mg/kg. This places the compound in toxicity class III (out of six), corresponding to a moderate acute toxicity.

Overall, the obtained data allow the compound to be considered an acceptable lead-like candidate in terms of its toxicological profile, with certain parameters requiring the further experimental validation and optimization. Thus, the results of the *in silico* evaluation provided a well-founded basis for the transition from the computational prediction to the experimental verification of the biological activity of the compound *in vitro* and *in vivo*.

**Table 3** – Toxicological profile of *PMAAPh* according to ProTox-3.0

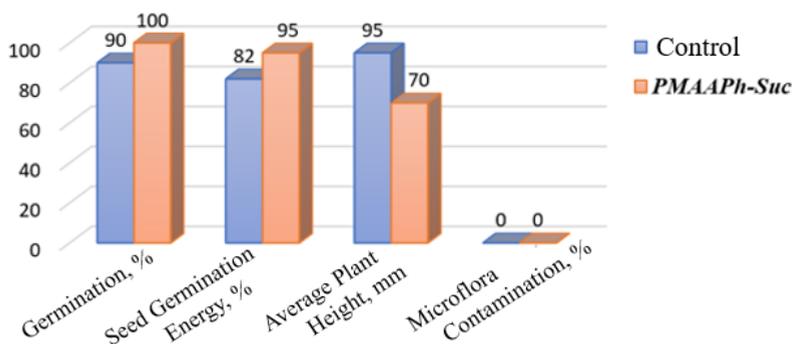
LD <sub>50</sub> (mg/kg)	Toxicity class		Toxicity endpoints		
200	III		Endpoint	Prediction	Probability
			Carcinogenicity	Inactive	0.57
<b>Organ toxicity</b>			Immunotoxicity	Inactive	0.86
Endpoint	Prediction	Probability	Mutagenicity	Inactive	0.66
Hepatotoxicity	Inactive	0.74	Cytotoxicity	Inactive	0.70
Neurotoxicity	Inactive	0.53	BBB-related toxicity	Active	0.70
Nephrotoxicity	Inactive	0.59	Ecotoxicity	Active	0.66
Cardiotoxicity	Inactive	0.71	Clinical toxicity	Inactive	0.52
Respiratory toxicity	Active	0.69	Nutritional toxicity	Active	0.60

Although PASS primarily predicted cardiometabolic and enzymatic activity, the study sought to expand the scope of the study and evaluate the compound's effects on plant growth and hematopoiesis as a manifestation of the broader metabolic potential of aminophosphonates. It should be noted that PASS algorithms are primarily focused on pharmacological and biomedical effects and are not intended to predict phytostimulating activity.

Given the previously reported ability of aminophosphonates to influence the growth-related processes in the biological systems of various origins [7], the next stage of this study has focused on investigating the plant growth–stimulating activity of *PMAAPh-Suc*. Under the laboratory conditions, the effect of the novel aminophosphonate, tested at a standard screening concentration of  $10^{-3}$  M, on the germination energy, laboratory germination, and germination intensity of wheat seeds (cultivar Kazakhstan 10) has been evaluated (Figure 2).

The seed treatment with *PMAAPh-Suc* has resulted in an increase in germination up to 100% and an enhancement of the germination energy up to 95.0% compared with the control group. At the same time, the average height of seedlings has slightly decreased, which may indicate a redistribution of the growth processes at the early stages of ontogenesis.

Previously, aminophosphonates of this structural series have been shown to exhibit myelostimulating activity, providing the rationale for further investigation of the obtained compound [8]. *PMAAPh-Suc* has been evaluated for the myelostimulatory activity (a stimulatory effect influencing the proliferative activity of erythro-, thrombocyto-, and leukopoiesis) (Table 4).



**Figure 2** – The diagram illustrating the effect of *PMAAPh-Suc* on the germination, growth, and development of wheat seedlings under the laboratory conditions.

**Table 4** – The key hematological parameters

Blood parameters	<i>PMAAPh-Suc</i>	Control group	Placebo group	Intact group
WBC, $\cdot 10^9/L$	$7.58 \pm 3.47$	$6.25 \pm 0.85$	$3.65 \pm 0.7$	$7.74 \pm 1.11$
RBC, $10^{12}/L$	$7.85 \pm 1.07$	$7.42 \pm 1.12$	$5.23 \pm 1.75$	$7.14 \pm 2.17$
HGB, g/L	$145 \pm 16.7$	$126.5 \pm 2.06$	$101 \pm 10.9$	$124.5 \pm 1.31$
PLT, $\cdot 10^9/L$	$797 \pm 29$	$698 \pm 17.2$	$617 \pm 14.6$	$745.0 \pm 15.71$
NEU, $\cdot 10^9/L$	$4.12 \pm 1.82$	$3.18 \pm 0.44$	$1.86 \pm 3.26$	$3.16 \pm 0.44$

Against the background of pancytopenia induced by the cytostatic agent cyclophosphamide, an administration of the studied *PMAAPh-Suc* has been accompanied by the pronounced leukopoiesis-stimulating activity, exceeding the effect of the reference drug methyluracil (control group (CG)). The compound moderately and in a balanced manner has stimulated proliferation in the erythrocytic, leukocytic, and thrombocytic lineages of hematopoiesis. The erythrocyte count (RBC) has recovered to  $(7.85 \pm 1.07) \cdot 10^{12}/L$ , exceeding the placebo group (PG) and corresponding to the control group (CG). Hemoglobin concentration (HGB) has been  $(145 \pm 16.7) \cdot g/L$ , exceeding the CG level  $(126.5 \pm 2.06) \cdot 10^9/L$ . The total leukocyte count (WBC) has reached  $(7.58 \pm 3.47) \cdot 10^9/L$ , which is slightly higher than in the CG  $(6.25 \pm 0.85) \cdot 10^9/L$  and 2.07 times higher than in the PG  $(3.65 \pm 0.7) \cdot 10^9/L$ . The Garkavi index has indicated a rapid recovery of hematopoiesis without disturbance of the lymphocyte-to-granulocyte ratio. The platelet count (PLT) has increased to  $(797 \pm 29) \cdot 10^9/L$ , exceeding the PG  $(617 \pm 14.6) \cdot 10^9/L$  and CG  $(698 \pm 17.2) \cdot 10^9/L$ . Effective restoration of the granulocyte–agranulocyte balance has been observed: the absolute neutrophil count (NEU) has been  $(4.12 \pm 1.82) \cdot 10^9/L$ , which is 1.29 times higher than in the CG, while the absolute lymphocyte count has reached  $(2.98 \pm 1.40) \cdot 10^9/L$ , exceeding the PG. Thus, *PMAAPh-Suc* has exhibited moderate leukopoiesis-, erythropoiesis-, and thrombocytopoiesis-stimulating activity, reaching the levels comparable to those of the intact animals. The

observed stimulation of hematopoiesis, a peripheral biological process, is also consistent with the proposed lack of BBB permeability (SwissADME). Further research is needed to clarify the underlying mechanisms.

#### 4. Conclusion

A new aminophosphonate, dimethyl ((3-phenoxyphenyl)((pyridin-2-ylmethyl)amino)methyl)phosphonate (**PMAAPH**), has been synthesized via the Kabachnik–Fields reaction, and its structure has been characterized by the IR and NMR spectroscopy. To improve an aqueous solubility, the succinate form of the compound (**PMAAPH-Suc**), has been obtained.

Based on the *in silico* analysis (PASS, SwissADME, ProTox-3.0), **PMAAPH** has been shown to possess a balanced physicochemical profile, meet the main criteria of drug-likeness, and exhibit the moderate predicted bioavailability with a predominantly peripheral activity. The toxicity prediction has indicated a moderate acute toxicity ( $LD_{50} = 200$  mg/kg, toxicity class III) in the absence of the pronounced organ-specific or genotoxic risks. The obtained *in silico* predictions, indicating the potential cardiometabolic activity of the compound, create a reasonable basis for further targeted research in this direction.

The results of the *in vitro* studies have demonstrated that **PMAAPH-Suc** affects the early plant growth processes, manifested by changes in the seed germination energy and laboratory germination of wheat seeds, indicating its potential as a regulator of growth processes.

Under the *in vivo* conditions in an experimental pancytopenia model, **PMAAPH-Suc** has exhibited a moderate and balanced effect on the main hematopoietic lineages, promoting restoration of the erythro-, leuko-, and thrombocytopoiesis parameters without a significant disturbance of their ratios.

Overall, the obtained data allow **PMAAPH** and its succinate form to be considered as promising lead-like compounds of interest for the further in-depth studies in the biomedical and agrobiological fields.

**Funding:** This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (BR27101179).

**Conflict of interests:** The authors declare that there are no conflicts of interests between the authors to disclose in this article.

#### LEAD-LIKE СВОЙСТВА НОВОГО ПИРИДИНАМИНОФOSFONATA: СИНТЕЗ, ПРЕДИКТИВНАЯ ОЦЕНКА И БИОЛОГИЧЕСКИЕ ИССЛЕДОВАНИЯ

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**Резюме.** Введение. Аминофосфонатные производные представляют интерес как класс низкомолекулярных соединений, способных оказывать регулирующее действие в биологических системах различной природы. Сочетание предиктивных и экспериментальных подходов позволяет

получить комплексную характеристику их биологического потенциала на ранних этапах исследования. Целью настоящей работы являлся синтез нового аминокислотного производного, получение его водорастворимой формы и проведение комплексной предиктивно-экспериментальной оценки биологической активности. Синтез dimethyl ((3-phenoxyphenyl)((pyridin-2-ylmethyl)amino)methyl)phosphonate (*PMAAPh*) осуществляли по реакции Кабачника–Филдса; для повышения растворимости получена его сукцинатная форма (*PMAAPh-Suc*). Структуру соединений подтверждали методами ЯМР- и ИК-спектроскопии. *In silico*-анализ включал оценку биологической активности, фармакокинетических и токсикологических параметров. *Экспериментальные исследования* проводили на растительных моделях и в условиях экспериментальной панцитопении *in vivo*. Установлено, что *PMAAPh* соответствует критериям лекарственноподобия и относится к III классу токсичности. *PMAAPh-Suc* проявляет регулирующее влияние на рост растений и показатели кровотока. Полученные данные позволяют рассматривать соединение как перспективный объект для дальнейших исследований биологически активных соединений.

**Ключевые слова:** 2-(аминометил)пиридин, аминокислота, *in silico* анализ, миелостимулирующая активность, стимулирующая рост растений активность.

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## ЖАҢА ПИРИДИНАМИНОФОСФОНАТТЫҢ LEAD-LIKE ҚАСИЕТТЕРІ: СИНТЕЗ, ПРЕДИКТИВТІК БАҒАЛАУ ЖӘНЕ БИОЛОГИЯЛЫҚ ЗЕРТТЕУЛЕР

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**Түйіндеме.** *Кіріспе.* Аминокислота туындылары әртүрлі табиғаттағы биологиялық жүйелерде реттеуші әсер көрсетуге қабілетті төмен молекулалы қосылыстар класы ретінде үлкен қызығушылық тудырады. Предиктивтік және эксперименттік тәсілдерді ұштастыра қолдану зерттеудің бастапқы кезеңдерінде олардың биологиялық әлеуетіне кешенді сипаттама беруге мүмкіндік береді. Осы жұмыстың мақсаты жаңа аминокислота туындысын синтездеу, оның суда жақсы еритін түрін алу және биологиялық белсенділігін кешенді предиктивтік-эксперименттік бағалау болды. Dimethyl ((3-phenoxyphenyl)((pyridin-2-ylmethyl)amino)methyl)phosphonate (*PMAAPh*) Кабачник–Филдс реакциясы бойынша синтезделді; ерігіштігін арттыру мақсатында оның сукцинаттық түрі (*PMAAPh-Suc*) алынды. Қосылыстардың құрылымы ЯМР және ИК-спектроскопия әдістерімен дәлелденді. *In silico* талдау биологиялық белсенділікті, фармакокинетикалық және токсикологиялық параметрлерді бағалауды қамтыды. *Эксперименттік зерттеулер* өсімдік модельдерінде және *in vivo* жағдайында эксперименттік панцитопения моделінде жүргізілді. Зерттеу нәтижесінде *PMAAPh* дәріге ұқсастық критерийлеріне сәйкес келетіні және уыттылықтың III класына жататыны анықталды. *PMAAPh-Suc* өсімдіктердің өсу процестеріне және қан түзу көрсеткіштеріне реттеуші әсер көрсететіні байқалды. Алынған деректер бұл қосылысты биологиялық белсенді заттарды әрі қарай зерттеу үшін перспективалы нысан ретінде қарастыруға мүмкіндік береді.

**Түйін сөздер:** 2-(аминометил)пиридин, аминокислота, *in silico* анализі, миелоциталандырығыш белсенділік, өсімдіктердің өсуін ынталандырушы белсенділік

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## HYDROMETALLURGICAL PROCESSING OF BRONZE PRODUCTION WASTE WITH SELECTIVE EXTRACTION OF COPPER AND ZINC

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**Abstract:** This article presents a study on the selective extraction of copper and zinc compounds from metallurgical bronze production slags using a hydrometallurgical approach. The relevance of the work is associated with the depletion of mineral resources and the increasing environmental burden of bronze production slags. The aim of the study was to evaluate efficient and environmentally friendly methods for recovering copper and zinc from these slags. Leaching experiments were conducted using nitric acid, ammonia solutions, and sulfuric acid, and their efficiencies were compared. The chemical and phase compositions of the slags were determined using inductively coupled plasma optical emission spectrometry, infrared spectroscopy, and X-ray phase analysis. The “hot leaching” method with 25% sulfuric acid at 80°C was applied for the selective separation of copper and zinc. The results demonstrated that sulfuric acid provides the most economical and environmentally effective separation. The process yielded tin precipitate, high-purity metallic copper via chemical and electrochemical methods, and zinc-rich solid residues. The proposed technological scheme reduces metal consumption, enhances the recyclability of bronze slags, and offers a practical, resource-saving approach to processing metallurgical waste.

**Key words:** bronze production slag, hydrometallurgical processing, sulfuric acid leaching, electrodeposition of metals, resource-saving technology.

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### 1. Introduction

The rapid development of technology has significantly expanded the applications of non-ferrous, rare, and precious metals, as well as their alloys. However, the extraction of these metals from ore raw materials presents several complex challenges. In particular, ore reserves of many metals are limited and

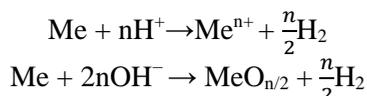
**Citation:** Yermukhanova S.T., Nazarova D.S., Akhmetova F.Zh. Hydrometallurgical separation of copper and zinc from bronze and brass slag. *Chem. J. Kaz.*, 2026, 1(93), 26-35. DOI: <https://doi.org/10.51580/2026-1.2710-1185.03>

irreplaceable, the metal content in mineral raw materials is decreasing, large capital investments are required for developing new deposits, and bronze production slag from industrial operations poses a negative environmental impact. These factors collectively hinder the expansion of metal production [1].

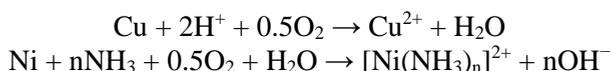
Non-ferrous and ferrous metals are present in large quantities in industrial bronze slag from the mining and metallurgical industries. Due to the lack of economical and environmentally friendly technologies for processing and recycling, these secondary raw materials are often stored and accumulated [2]. Comprehensive processing of bronze slag, aiming for maximal extraction of valuable components, is particularly important when it contains non-ferrous and rare metals, given the diverse composition of secondary raw materials [3,4]. A clear classification of secondary bronze slag is necessary to ensure efficient processing and utilization of metal-containing materials [5].

Bronze slag containing precious metals can be classified according to its origin: either as slag from the production of a specific product or as slag formed during a particular process. Non-ferrous metals in the original raw materials may be present in metallic form, as simple or complex oxides, or in various salts, among which sulfates, chlorides, chalcogenides, and arsenides are most common, with sulfides being particularly representative [6-9]. Typical raw materials with metals in elemental form include ores containing native metals (gold, silver, platinum group metals, and less commonly copper), secondary raw materials, and semi-finished products such as cementation precipitates and cinders after reducing roasting [10-13].

The chemical properties of electronegative metals (e.g., zinc, cadmium, aluminum) determine their high solubility in acidic and alkaline solutions:



Aeration is used to prevent the accumulation of explosive hydrogen concentrations. Electropositive metals dissolve only in the presence of both a solvent and an oxidizing agent. When the solvent has complexing or acidic properties and exhibits oxidizing activity (or when a mixture is used), the leaching process is significantly accelerated:



Certain metals (e.g., nickel, cobalt) are prone to passivation in air due to the formation of oxide films; therefore, leaching efficiency is higher for freshly reduced cinders [14,15]. The dissolution rates of alloys decrease in the presence of components that form insoluble films. The most rational method to prepare metallized raw materials for leaching is melting and spraying the melt, which

removes non-metallic inclusions and ensures homogeneity in chemical and phase composition, as well as a developed surface area [16].

In this study, the object of investigation was bronze slag obtained after smelting operations at a machine-building enterprise. The material represents a heterogeneous metallurgical residue consisting of oxidized phases and residual metallic inclusions. Throughout the manuscript, the term “slag” refers exclusively to this material.

Bronze slag was obtained from [Company/Plant]. Chemical reagents included sulfuric acid ( $H_2SO_4$ , 98%), hydrogen peroxide ( $H_2O_2$ , 30%), and deionized water. Copper cathodes (99.9%) and lead or chrome-plated steel anodes were used for electrolysis.

## 2. Experimental part

The main alloying element in bronze is tin, while in brass it is zinc; however, both alloys are copper-based. Depending on their composition, bronzes may be tin-containing or tin-free, whereas brasses may be binary or multicomponent alloys. Copper–tin bronzes can be produced by various methods, including smelting, co-smelting, and cementation.

Due to the depletion of high-grade mineral resources, complex and low-grade ores, as well as their processing products (slags, cakes, dusts, and sublimates), are increasingly involved in metallurgical production. In the present study, slag obtained from bronze smelting at a machine-building enterprise was used as the raw material.

To determine the chemical composition, the initial samples were crushed and divided into two fractions: crushed material (sample 1a) and uncrushed metallic phase (sample 1b). Photographs of the samples are shown in Figure 1.



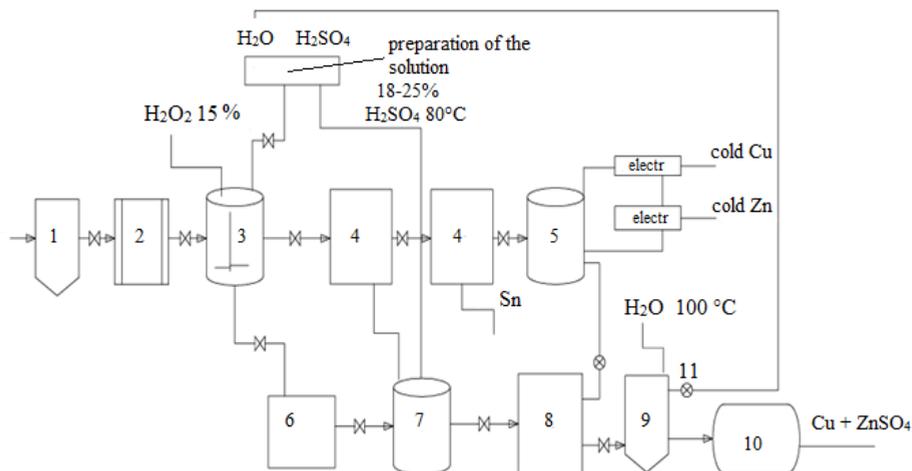
**Figure 1** – Bronze slag samples: 1a – abraded and 1b – non-abraded (metal phase).

The compositional differences between the crushed (1a) and uncrushed (1b) fractions confirm the heterogeneous distribution of metallic phases in the slag. Therefore, preliminary particle-size classification and controlled grinding are important steps in the processing scheme. Finer fractions enriched in copper are more suitable for oxidative sulfuric acid leaching, while coarser fractions

containing zinc-rich phases may require additional grinding or thermal treatment to improve metal accessibility.

The chemical and phase compositions of the slag were determined using inductively coupled plasma optical emission spectrometry (ICP-OES), infrared spectroscopy, and X-ray phase analysis (XRD).

Based on the analytical results, a technological scheme for the extraction of copper and zinc was developed (Figure 2).



**Figure 2** – Hot leaching flow chart for bronze production slag: 1 – classifier, 2 – calcination furnace, 3 – leaching reactor, 4 – filter, 5 – electrolyte collector, 6 – cake collector, 7 – leaching reactor, 8 – filter, 9 – rinse tank, 10 – dryer, 11 – circulation pump.

The process for extracting copper and zinc from bronze slag included the following stages:

Classification of slag to a particle size not exceeding 0.315 mm.

Calcination at 600°C for 8 hours to remove organic impurities.

Leaching in a reactor with 18–25% sulfuric acid at 80°C for 1 hour under constant stirring (400 rpm). After 20 minutes, 9–15% hydrogen peroxide was added as an oxidizing agent. Hydrogen peroxide oxidizes  $\text{Fe}^{2+}$  to  $\text{Fe}^{3+}$ :



Under strongly acidic conditions (25%  $\text{H}_2\text{SO}_4$ ),  $\text{Fe}^{3+}$  remains soluble; therefore, hydrogen peroxide primarily promotes oxidative dissolution of copper rather than iron precipitation.

After leaching, the suspension was allowed to settle for 20–30 minutes at 80°C. Metallic copper formed via cementation was separated by hot filtration.

The primary filter cake was retained, while the filtrate was allowed to cool for 30–40 minutes, resulting in tin precipitation. The tin precipitate was filtered, washed with water, and dried at 80°C.

The primary cake was returned to the reactor for secondary leaching with fresh 18–25% sulfuric acid. The deep blue coloration of the solution indicated further copper dissolution. After refiltration, the secondary filtrate was collected for electrolyte preparation.

The concentrations of free acid, copper sulfate, and zinc sulfate were monitored and adjusted prior to electrolysis. Wash waters were recycled back to the leaching stage.

The electrolyte was prepared from the filtrate containing copper and zinc sulfates in 18–25% H<sub>2</sub>SO<sub>4</sub> and adjusted to 80 g/L Cu<sup>2+</sup> and 20 g/L Zn<sup>2+</sup>.

Electrolysis was performed at a current density of 5 A/dm<sup>2</sup> using a copper cathode and a lead or chrome-plated steel anode for 1 hour at room temperature.

Selective copper deposition occurred due to the difference in standard reduction potentials:

$$E^{\circ}(\text{Cu}^{2+}/\text{Cu}) = +0.34 \text{ V}$$

$$E^{\circ}(\text{Zn}^{2+}/\text{Zn}) = -0.76 \text{ V}$$

Under these conditions, copper was deposited on the cathode, while zinc remained in solution. The cathode deposit contained 98.5% Cu with minor Zn and Sn impurities (<1%), confirming high copper purity. If higher copper purity is required, additional purification steps may be applied. These include electrolyte purification using solvent extraction or ion-exchange methods to remove trace metal ions, as well as secondary electrorefining under optimized electrochemical conditions. Such approaches are widely used in hydrometallurgical processing and can increase the purity of cathode copper to industrial standards.

The zinc-rich solution may be further processed for zinc recovery.

All leaching experiments were performed in triplicate. Extraction efficiencies are presented as mean values  $\pm$  standard deviation. The analytical error of the ICP-OES method was  $\pm 0.5\%$ , confirming reproducibility and reliability of the results.

### 3. Results and discussion

The chemical composition of the combined bronze slag sample showed the following contents (wt.%): TiO<sub>2</sub> – 0.07; MnO – 0.46; Na<sub>2</sub>O – 0.53; K<sub>2</sub>O – 0.14; SiO<sub>2</sub> – 2.66; MgO – 0.93; CaO – 4.40; Fe<sub>2</sub>O<sub>3</sub> – 1.94; Al<sub>2</sub>O<sub>3</sub> – 2.82; P<sub>2</sub>O<sub>5</sub> – <0.1; Zn – 28.49; Ni – 0.38; Cu – 55.69; Cr – 0.087; W – 0.006.

The results indicate the predominance of copper and zinc as the principal metallic components, while other oxides and alloying elements are present in minor quantities.

Solutions obtained after microwave digestion of crushed (1a) and uncrushed (1b) samples in a mixture of hydrochloric and nitric acids were analyzed by ICP-OES. Chemical analysis showed that in sample 1a, zinc (Zn) was 17.08%, nickel (Ni) 0.37%, copper (Cu) 72.97%, chromium (Cr) 0.036%, and tungsten (W) 0.007%. In sample 1b, zinc was 25.63%, nickel 0.26%, copper 41.57%, chromium 0.027%, and tungsten 0.005%. These results indicate that sample 1b

contains a higher zinc content and a lower copper content, reflecting the heterogeneity of the slag and uneven distribution of its phases.

Sample 1b contains significantly more zinc and less copper than sample 1a, indicating heterogeneity of the slag and uneven phase distribution.

X-ray diffraction suggested the possible presence of minor phases containing Ge, Se, and Co. However, chemical analysis showed that these elements were either below the detection limit or present only in trace amounts.

Therefore, identification of phases such as  $\text{Cu}_3\text{Ge}$  and Co- or Se-containing compounds should be considered tentative. Their appearance in the diffractogram may be explained by:

- trace micro-impurities,
- overlapping diffraction peaks,
- limitations of automatic database matching (PDF/ICDD).

Phase identification was refined by prioritizing phases consistent with the bulk Cu–Zn–Sn composition. Minor phases were interpreted cautiously.

Component composition of bronze samples:

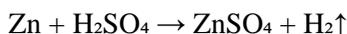
- Without calcination: Cu 54%, Zn 34%, Sn 5%, Pb 6%;
- Calcined 1 h: Cu 31%, Zn 56%, Sn 1.5%, Pb 4%;
- Calcined 8 h: Cu 26%, Zn 62%, Sn 1.3%, Pb 4%.

Prolonged calcination leads to redistribution of metallic components and relative zinc enrichment.

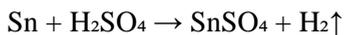
Sulfuric acid was selected as the leaching agent because it forms soluble sulfates of copper and zinc, while avoiding formation of poorly soluble by-products.

Since bronze is an alloy, dissolution must be considered as independent reactions of its components.

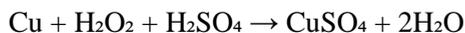
Zinc dissolves readily:



Tin may react as:

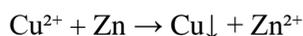


Copper does not dissolve in non-oxidizing sulfuric acid. In the presence of hydrogen peroxide:



Thus, zinc dissolves through a direct acid attack, reacting readily with sulfuric acid to form soluble zinc sulfate and release hydrogen gas. In contrast, copper dissolves via an oxidative mechanism, requiring the presence of an oxidizing agent such as hydrogen peroxide, which enables the formation of soluble copper sulfate.

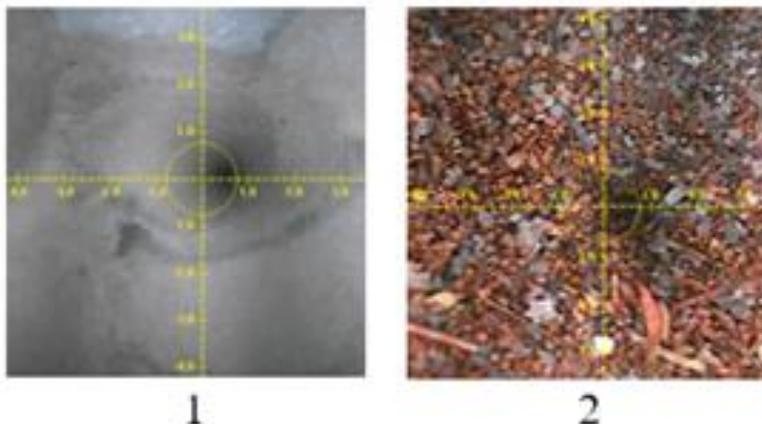
If  $\text{Cu}^{2+}$  forms, cementation may occur:



Therefore, metallic copper powder observed during leaching is attributed to cementation rather than direct acid dissolution.

Leaching was performed at 80°C in 25% H<sub>2</sub>SO<sub>4</sub> under constant stirring.

Figure 3 shows the solid products obtained.



**Figure 3** – Precipitates formed during leaching of bronze slag with sulfuric acid:

- 1 – tin powder formed after leaching bronze with sulfuric acid and hydrogen peroxide;
- 2 – metallic copper obtained after leaching bronze slag with sulfuric acid without hydrogen peroxide.

Metallic copper formed as a brown powder with minor zinc inclusions, as confirmed by XRD.

The study demonstrates that copper and zinc are the dominant components of bronze slag, while the particle size and thermal treatment of the material significantly influence the distribution of its phases. Oxidative leaching with sulfuric acid allows for the selective dissolution of copper, and the formation of metallic copper can be explained by the cementation process. Overall, the hot leaching method provides an effective and practical approach for obtaining high-purity copper, tin precipitates, and zinc-rich residues.

These findings establish a direct relationship between compositional analysis and the development of a resource-saving hydrometallurgical process for bronze slag recycling.

#### 4. Conclusion

The results of this study showed that bronze slag primarily consists of copper (Cu) and zinc (Zn), with other impurities present in minor amounts. The multicomponent structure of the slag significantly influences the leaching rate, as different metals respond differently to chemical treatment. When ammonium hydroxide and nitric acid were tested as leaching agents, several limitations were observed. In ammoniacal systems, copper dissolution occurs through the formation of ammine complexes, which requires strict control of pH and ammonia concentration. In addition, ammonia volatilization may lead to

atmospheric emissions and requires additional gas-capture systems. Nitric acid, although effective as an oxidizing agent, produces nitrogen oxide gases (NO<sub>x</sub>) during the leaching process, which require catalytic gas-treatment systems and increase operational costs. In contrast, sulfuric acid proved to be a much more efficient reagent, enabling selective extraction of copper and zinc while minimizing the formation of by-products.

To evaluate the efficiency of metal recovery, a material balance was established for copper, zinc, and tin. The results indicated that 81% of the total copper in the slag was recovered as a chemical precipitate, 70% of zinc remained in the solid residue after leaching, 59% of tin was obtained as a precipitate, and electrochemically deposited copper reached a purity of 98.5%. A total material balance accounting for all phases, including losses, chemical precipitates, electrochemical products, and residues, confirmed the transparency and effectiveness of the selective separation process. Furthermore, the washing solution from filtration can be reused to prepare fresh sulfuric acid, enhancing the sustainability of the process. Overall, these findings demonstrate that the proposed hot leaching method allows for the effective, resource-saving, and environmentally safe recovery of copper and zinc from metallurgical bronze production slag.

**Acknowledgements:** The authors express their deep gratitude to Professor Alexey Khatsrinov from Kazan National Research and Technological University for invaluable assistance in analyzing the samples.

**Conflict of Interest:** The authors declare no conflicts of interest that require disclosure in this paper.

## ҚОЛА ӨНДІРІСІНІҢ ҚАЛДЫҚТАРЫНАН МЫРЫШ ҚОСЫЛЫСТАРЫН БӨЛІП АЛУДЫ ЗЕРТТЕУ

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**Түйіндемe.** Бұл мақала қола мен жезді өндіру кезінде пайда болған металлургиялық қалдықтардан мырыш пен мыс қосылыстарын гидрoметаллургиялық әдіспен селективті бөлу технологиясын зерттеуге арналған. Зерттеудің өзектілігі минералды шикізаттың азаюымен және металлургиялық қалдықтардың қоршаған ортаға тигізетін экологиялық жүктемесінің артуымен байланысты. Жұмыстың мақсаты - қола мен жез шлактарын өңдеу кезінде мыс пен мырышты тиімді және экологиялық таза жолмен алу мүмкіндігін анықтау. Зерттеу барысында азот қышқылы, аммиак ерітінділері және күкірт қышқылы қолданылды, олардың шаймалау тиімділігі салыстырмалы түрде бағаланды. Шлактардың химиялық және фазалық құрамы индуктивті байланысқан плазмалық оптикалық эмиссиялық спектoметрия, инфрақызыл спектoскопия және рентгендік фазалық талдау арқылы анықталды. Жаңа әдістемелік тәсіл ретінде 80 °С температурада 25% күкірт қышқылын қолданатын «ыстық шаймалау» әдісі қолданылды. Зерттеу нәтижелері күкірт қышқылының мыс пен мырышты бөлуде экономикалық және экологиялық тұрғыдан тиімдірек екенін көрсетті. Бұл процесс қалайы тұнбасының, химиялық және электрохимиялық жолмен алынған жоғары таза металл мысының және мырышқа бай қатты қалдықтардың пайда болуына екедi. Ұсынылған технологиялық схема металл шығынын азайтады, қалдықтарды қайта өңдеу

мүмкіндігін арттырады және аз қалдықты, ресурстарды үнемдейтін металлургиялық технологияларды әзірлеу үшін практикалық маңызға ие.

**Түйінді сөздер:** металлургиялық қалдықтар, гидрометаллургиялық әдіс, күкірт қышқылымен шаймалау, металдарды электродтау, ресурс үнемдеуші технология.

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### ИССЛЕДОВАНИЕ ВЫДЕЛЕНИЯ СОЕДИНЕНИЙ ЦИНКА ИЗ ОТХОДОВ ПРОИЗВОДСТВА БРОНЗЫ

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**Резюме.** Данная статья посвящена изучению технологии селективного разделения соединений цинка и меди из металлургических отходов, образующихся при производстве бронзы и латуни гидрометаллургическим методом. Актуальность исследования связана с истощением минерального сырья и возрастающей экологической нагрузкой металлургических отходов. Цель работы – определить возможность эффективного и экологически безопасного получения меди и цинка при переработке бронзовых и латунных шлаков. В ходе исследования использовались азотная кислота, растворы аммиака и серная кислота, а также проводилась сравнительная оценка их эффективности выщелачивания. Химический и фазовый состав шлаков определялся методами оптической эмиссионной спектроскопии с индуктивно связанной плазмой, инфракрасной спектроскопии и рентгенофазового анализа. В качестве нового методического подхода использовался метод «горячего выщелачивания» с применением 25% серной кислоты при температуре 80 °С. Результаты исследования показали, что серная кислота является более экономически и экологически эффективной при разделении меди и цинка. В результате процесса образовался осадок олова, химически и электрохимически извлеченная высокочистая металлическая медь, а также твердые отходы, богатые цинком. Предложенная технологическая схема снижает расход металла, увеличивает возможности переработки отходов и имеет практическое значение для развития малоотходных, ресурсосберегающих металлургических технологий.

**Ключевые слова:** металлургические отходы, гидрометаллургический метод, выщелачивание серной кислотой, электроосаждение металлов, ресурсосберегающая технология.

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NEW *N*-BENZYLPIPERIDONE DERIVATIVES: SYNTHESIS AND PLANT GROWTH-STIMULATING ACTIVITYA.E. Malmakova<sup>1,2\*</sup>, K.B. Otegulova<sup>1</sup>, T.M. Seilkhanov<sup>3</sup><sup>1</sup> A.B. Bekturov Institute of Chemical Sciences, Almaty, Kazakhstan<sup>2</sup> Kazakh-British Technical University, Almaty, Kazakhstan<sup>3</sup> Sh. Ualikhanov Kokshetau University, Kokshetau, Kazakhstan

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**Abstract.** *Introduction.* Given their broad range of biological activities and potential for further structural modification, piperidine derivatives, particularly *N*-benzylpiperidones, have attracted considerable attention. Because of their easily accessible starting materials and relatively simple synthesis, these compounds are particularly attractive because they facilitate the effective design and development of novel molecules with specific physicochemical and biological characteristics. *The objective of this study* is to synthesize a new series of benzylpiperidone derivatives, generate more complex nitrogen-containing heterocycles through structural modification, and evaluate their plant growth-stimulating activity. *Results and discussion.* *N*-benzylpiperidin-4-one was reacted with 1-(3-methoxypropyl)amine and paraformaldehyde to yield 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one. The resulting ketone was converted to the corresponding oxime with a 76% yield under oximation conditions. Subsequent acylation of the oxime with benzoyl chloride produced *O*-benzoyloxime in 65% yield. At a concentration of 0.001%, the complex (KhZR-107) was evaluated for its impact on the germination, growth, and development of soybean (variety Zhansaya) and wheat (variety Kazakhstan-10) seedlings. *Conclusion.* Treatment with KhZR-107 improved wheat performance, raising germination from 90% to 100%, increasing germination energy from 82.5% to 95%, and promoting taller seedlings, all without compromising seed sanitary quality. In soybean, germination rates remained unchanged, but the seedlings appeared slightly more uniform, suggesting subtle benefits in early development.

**Keywords:** *N*-benzylpiperidone, diazabicyclononanone,  $\beta$ -cyclodextrin inclusion complex, plant growth stimulation.

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## 1. Introduction

Heterocyclic compounds, particularly nitrogen-containing systems, are widely distributed in natural products and pharmaceutical agents [1]. Owing to their pronounced physiological properties and key roles in biological processes,

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**Citation:** Malmakova A.E., Otegulova K.B., Seilkhanov T.M. New *n*-benzylpiperidone derivatives: synthesis and plant growth-stimulating activity. *Chem. J. Kaz.*, **2026**, 1(93), 36-47. DOI: <https://doi.org/10.51580/2026-1.2710-1185.04>

nitrogen heterocycles occupy a central position in medicinal and agrochemical research [2]. Among them, piperidine-containing compounds represent one of the most important structural motifs in modern drug design. The high prevalence of the piperidine ring in approved drugs is attributed to its synthetic accessibility, conformational adaptability, and favorable pharmacokinetic characteristics [3,4].

Sustained interest in piperidine derivatives is largely associated with the availability of diverse starting materials and well-developed synthetic methodologies, which enable systematic structural modification. In particular, the introduction of benzyl substituents allows fine tuning of lipophilicity, steric environment, and intermolecular interactions, parameters that directly influence biological activity and target affinity [5,6].

At the same time, analysis of the available literature indicates that most investigations of *N*-benzylpiperidone derivatives have been primarily focused on medicinal applications or on the development of synthetic approaches. Reports addressing their potential agrobiological activity remain limited and fragmented. In particular, systematic studies correlating structural modifications of the benzylpiperidone scaffold with growth-regulating effects in plants are scarce. Furthermore, the transformation of *N*-benzylpiperidones into more structurally complex nitrogen-containing heterocycles and the evaluation of their growth-stimulating properties have not been comprehensively explored [7-9].

Plant growth regulators are an essential component of modern crop production technologies [10]. Even when applied in small doses, they influence plant metabolism, significantly affecting growth, development, and yield, and are regarded as environmentally friendly and cost-effective tools for enhancing crop productivity and realizing the biological potential of plants. Therefore, studying the effects of next-generation growth regulators on the yield and grain quality of spring wheat under specific soil and climatic conditions remains highly relevant [11-13]. However, despite the established pharmacological relevance of this class of compounds, significant gaps persist in understanding their structure–activity relationships in the context of plant growth regulation.

Although *N*-(4-substituted benzyl, phenyl, and imidazolyl)piperidones have shown moderate plant growth-stimulating activity [14,15], the combination of a 3-methoxypropyl group with *N*-(4-substituted benzyl)piperidone has not been investigated. Here, we report a series of novel 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one derivatives, whose structures were confirmed by NMR, IR spectroscopy, and elemental analysis. Preliminary biological evaluation demonstrates that the *O*-benzoyloxime derivative significantly improves wheat performance, increasing germination from 90% to 100%, raising germination energy from 82.5% to 95%, and promoting taller seedlings.

## 2. Experimental part

### *Chemical Part*

Reaction progress was monitored by thin-layer chromatography employing aluminum oxide with second-degree activity. Infrared spectra were recorded on a

Nicolet 5700 FT-IR spectrometer.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a JEOL JNM-ECA 400 spectrometer at frequencies of 399.78 and 100.53 MHz, respectively, using  $\text{CDCl}_3$  as the solvent. Syntheses sensitive to oxygen or moisture were conducted under an inert gas atmosphere with dry solvents.

The synthesis of 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one and its derivatives followed procedures previously described [16].

*3-Benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one* (2). Yellow oil; 82%. Anal. calcd. for  $\text{C}_{18}\text{H}_{26}\text{N}_2\text{O}_2$ : C 71.49; H 8.67; N 9.26; Found: C 71.20; H 8.73. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1735 (C=O), 1118 (C-O-C).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 1.66, 2.33 (H-3,7); 1.65, 1.68, 1.71, 2.40 (H-2,4,6,8); 2.44 (H-10); 2.52 (H-11); 2.74 (H-12); 2.75 (H-13); 2.78 (H-15); 3.49 (H-16); 7.20-7.30 (H-18,19,20,21,22).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 57.23 (C-3,7); 54.34, 61.11 (C-2,4,6,8); 214.5 (C-9); 52.98 (C-11); 27.67 (C-12); 70.9 (C-13); 58.5 (C-15); 62.09 (C-16); 137.5 (C-17); 129.59 (C-18, 22); 128.48 (C-19,21); 127.03 (C-20).

*Oxime of 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one* (3). Yellow oil; 76%. Anal. calcd. for  $\text{C}_{18}\text{H}_{27}\text{N}_3\text{O}_2$ : C 68.11; H 8.57; N 13.24; Found: C 68.06; H 8.43. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 3222 (OH), 1671 (C=N).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 1.71, 1.71 (H-3,7); 2.26, 2.82, 2.186 (H-2,4,6,8); 6.93 (H-11); 2.75 (H-12); 1.73 (H-13); 3.42 (H-14); 3.32 (H-16); 7.12-7.49 (H-19, 20, 21, 22, 23).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 30.23 (C-3); 36.84 (C-7); 56.67, 57.16 (C-2,8); 58.06, 58.42 (C-4,6); 161.52 (C-9), 27.18 (C-13); 54.37 (C-12); 58.74 (C-16); 71.21 (C-14); 61.69 (C-17); 138.51 (C-18); 128.99 (C-19,23); 127.09 (C-21); 128.42 (C-20,22).

*O-Benzoyloxime of 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one* (4). Yellow oil; 65%. Anal. calcd. for  $\text{C}_{25}\text{H}_{31}\text{N}_3\text{O}_3$ : C 71.23; H 7.41; N 9.97; Found: C 71.42; H 7.21. IR (KBr) ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 1742 (C=O), 1637 (C=N).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 2.8 (H-3,7); 2.3 (H-2,4,6,8); 3.5 (H-14); 7.1-7.4 (H-16, 17, 18, 19, 20); 2.5 (H-21); 1.7 (H-22); 3.4 (H-23); 3.3 (H-25); 7.6-8.0 (H-27, 28, 29, 30, 31).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 38.09 (C-3); 41.09 (C-7); 60.57 (C-2,8); 59.43 (C-4,6); 168.99 (C-9); 158.91 (C-12); 62.04 (C-14); 138.86 (C-15); 127.03-132.12 (C-16,20,27,28,30,31); 27.67 (C-22); 70.49 (C-23); 58.5 (C-25); 133.35 (C-26).

*Inclusion complex of O-benzoyloxime with  $\beta$ -cyclodextrin (CD)* (5). Wight power decomposed in 200 °C. Anal. calcd. for  $\text{C}_{60}\text{H}_{96}\text{N}_2\text{O}_{37}$ : C 51.17; H 6.49; N 2.70; Found: C 51.05; H 6.24.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ),  $\delta$ , ppm (*J*, Hz): 0.98, 1.05 (H-3,7); 0.96, 1.00, 1.04, 1.83 (H-2,4,6,8); 3.26 (H-14); 3.30-3.44 (H-16,17,18,19,20); 3.45 (H-21); 3.46 (H-22); 3.6 (H-23); 4.84 (H-25); 7.2-7.27 (H-27,28,29,30,31); 7.29-7.89 (H-32,33,34,35,36,37,38).

#### Biological part

Model samples of wheat and soybean were used to evaluate the effects of stimulants, with the commercial preparation Baikal EM-1 serving as a reference. Water served as the medium for seed germination. For the germination test, four

replicates of 100 seeds each were selected from the main seed lot (combined sample). In this study, 10 seeds were sown in each of four replicates, corresponding to 100% seeding. Germination energy was assessed on day 3, and germination rate on day 7. For germination energy (after 3 days for wheat and soybean), normally germinated seeds were counted and removed, as were rotten seeds. Ungerminated and abnormally germinated seeds remained for further observation. For germination rate (after 7 days for wheat and soybean), all seeds were classified as normally germinated, abnormally germinated, swollen, hard (for legumes), or rotten, and the number of seeds in each group was recorded. The germination percentage was calculated for each sample, and the reliability of the results was verified. Both germination percentage and germination energy were determined. Spring wheat variety “Kazakhstan-10” and soybean variety “Zhansaya” from the collection of the Institute of Plant Biology and Biotechnology were treated during seed germination, seedling growth, and development for 24 hours according to standard protocols. Laboratory experiments were performed to assess the effects of stimulants on germination energy, germination rate, and germination intensity of wheat and soybean seeds.

The complex was evaluated at a concentration of 0.001% for its effects on germination, growth, and early development of wheat (variety “Kazakhstan-10”) and soybean (variety “Zhansaya”) seedlings under controlled laboratory conditions. A 0.001% solution of Baikal EM-1 served as a comparative reference. All experiments were conducted in triplicate, with at least 100 seeds per replicate.

#### *Methodology*

##### *Seed germination and growth measurements*

Seeds were sterilized in 1% sodium hypochlorite for 5 min, rinsed three times with distilled water, and placed on moistened filter paper in Petri dishes. Germination was monitored daily, and germination energy (percentage of seeds germinated within 3 days) and final germination (%) were calculated. Seedling height was measured at 7 days post-germination using a digital calliper, recording mean  $\pm$  SD for each replicate.

##### *Microbial contamination assessment*

Microflora presence was recorded qualitatively: “-” none, “+” low, “++” moderate, “+++” high contamination.

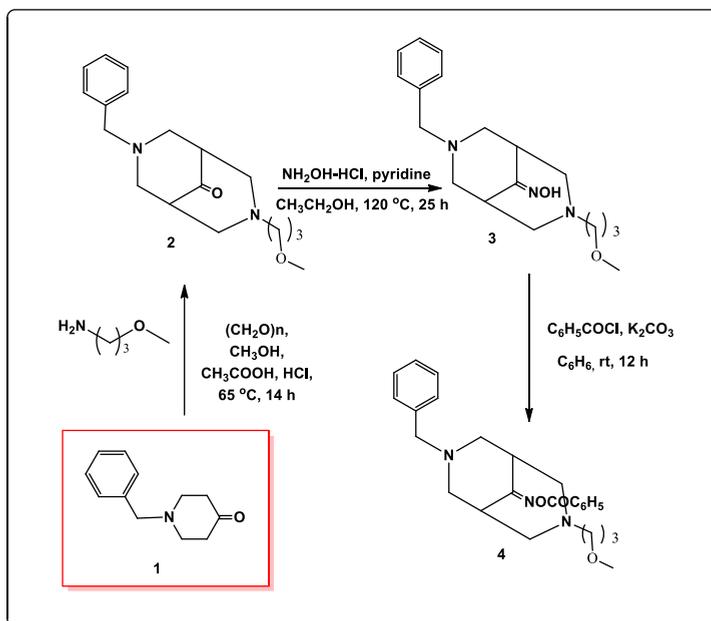
##### *Statistical analysis*

Data are expressed as mean  $\pm$  standard deviation (SD). Differences between control and treated groups were assessed using one-way ANOVA, followed by Tukey’s post hoc test. Differences were considered statistically significant at  $p < 0.05$ . Graphical representation includes error bars (SD) and asterisks for statistically significant differences.

### **3. Results and discussion**

Cyclization of 1-benzylpiperidin-4-one (**1**) with 1-(3-methoxypropyl)amine and paraformaldehyde via a Mannich condensation in an acetic acid-methanol mixture at 65 °C for 14 h afforded the bicyclic ketone (**2**) in 82% yield. The new

bicyclic ketone (**2**) was isolated by column chromatography ( $\text{Al}_2\text{O}_3$ , eluent: benzene/ *i*-propanol – 1:6), and the reaction product is a viscous oil.



The IR spectrum of 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one (**2**) displayed an intense absorption band at  $1735\text{ cm}^{-1}$ , characteristic of the stretching vibrations of the ketone carbonyl group at the C9 position. Additionally, the band at  $1118\text{ cm}^{-1}$  indicated the presence of a simple ether C–O–C linkage associated with the methoxypropyl substituent.

The  $^1\text{H}$  NMR spectrum showed signals for the protons of the bicyclic framework in the range 1.65–2.40 ppm (H3,7 and H2,4,6,8). The methoxypropyl fragment was identified by signals at 2.52 ppm (H11), 2.74 ppm (H12), 2.75 ppm (H13), and 2.78 ppm (H15). Aromatic protons of the benzyl substituent resonate in the region 7.12–7.35 ppm, confirming the presence of a phenyl ring. In the  $^{13}\text{C}$  NMR spectrum, the most downfield signal at 214.5 ppm corresponds to the carbonyl carbon C9. Signals for the bicyclic skeleton carbons C3 and C7 were observed at 57.23 ppm, while resonances for C2, C4, C6, and C8 appear in the range 54.3–61.1 ppm, which is characteristic of a 3,7-diazabicyclic system. Signals for the *N*-substituents (C10–C14) and the aromatic carbons of the benzyl fragment (127.03–137.5 ppm) were consistent with the proposed structure.

The structure of the compound (**2**) was additionally confirmed by two-dimensional NMR spectroscopy using COSY ( $^1\text{H}$ - $^1\text{H}$ ), HMQC ( $^1\text{H}$ - $^{13}\text{C}$ ), and HMBC ( $^1\text{H}$ - $^{13}\text{C}$ ) techniques, which enable the identification of homo- and heteronuclear spin-spin interactions. The observed  $^1\text{H}$ - $^1\text{H}$  COSY and  $^1\text{H}$ - $^{13}\text{C}$  HMQC correlations in the molecule are shown schematically.

In the  $^1\text{H}$ - $^1\text{H}$  COSY spectra of the compound, spin-spin correlations through three bonds were observed between protons of neighboring methylene-methylene, methyl-methine, and methane-methine groups: H12-H11 ( $\delta$  1.87, 2.61 and 2.61, 1.87), H16-H15 ( $\delta$  1.31, 3.59 and 3.59, 1.32), H12-H13 ( $\delta$  1.86, 3.60 and 3.60, 1.86), and H3,7-H4<sub>eq</sub>,6<sub>eq</sub> ( $\delta$  2.95, 3.16 and 3.16, 2.95 ppm).

Heteronuclear one-bond  $^1\text{H}$ - $^{13}\text{C}$  correlations were established by HMQC spectroscopy for the following proton-carbon pairs present in the compound: H16-C16 ( $\delta$  1.33, 15.53), H12-C12 ( $\delta$  1.83, 27.84), H11-C11 ( $\delta$  2.71, 47.05), H2<sub>ax</sub>,8<sub>ax</sub>, 2<sub>eq</sub>,6<sub>eq</sub>-C2,8 ( $\delta$  2.61, 53.81), H4<sub>ax</sub>,6<sub>ax</sub>-C4,6 ( $\delta$  2.94, 58.54), H4<sub>eq</sub>,6<sub>eq</sub>-C4,6 ( $\delta$  3.18, 58.58), H15-C15 ( $\delta$  3.61, 66.60), H13-C13 ( $\delta$  3.60, 68.68), H17-C17 ( $\delta$  3.70, 61.51), H21-C21 ( $\delta$  7.43, 126.88), and H19,23,20,22-C19,23,20,22 ( $\delta$  7.47, 128.60 ppm).

Long-range heteronuclear  $^1\text{H}$ - $^{13}\text{C}$  correlations through two or more bonds were identified by HMBC spectroscopy for the following pairs: H16-C15 ( $\delta$  1.31, 66.53), H12-C2,8 ( $\delta$  1.85, 53.81), H12-C13 ( $\delta$  1.85, 68.70), H17-C4,6 ( $\delta$  3.67, 58.49), H17-C19,23 ( $\delta$  3.67, 129.04), and H17-C18 ( $\delta$  3.67, 138.71 ppm).

Bicyclic ketone (**2**) was heated with a strong oximation agent in an alcoholic medium at 120 °C for 25 h, affording the corresponding oxime (**3**) in 76% yield. The oxime was purified by column chromatography on  $\text{Al}_2\text{O}_3$  (eluent: benzene/isopropanol, 1:20), and the product was obtained as a viscous oil.

In the IR spectrum of oxime (**3**), the characteristic C=O absorption band of the bispidinone fragment disappeared. A broad band at 3222  $\text{cm}^{-1}$ , corresponding to the stretching vibrations of the oxime hydroxyl group (C=NOH), and an intense band at 1671  $\text{cm}^{-1}$ , attributed to the C=N stretching vibration, were observed. These features confirmed the transformation of the carbonyl group of the initial ketone into an oxime.

In the  $^1\text{H}$  NMR spectrum of the compound, the methylene protons H-13,13 of the methoxypropyl fragment appeared as a two-proton multiplet at  $\delta$  1.71-1.76 ppm. The methylene protons H-12,12 of this fragment were observed as a two-proton broadened singlet at  $\delta$  1.89 ppm. The methylene protons H-13,12, H-14,14, and H-14,14 of the methoxypropyl fragment resonated as two-proton multiplets at  $\delta$  2.40-2.50, 3.41-3.45, and 3.49-3.76 ppm, respectively. The methyl protons H-16,16,16 of the methoxypropyl fragment appeared as a three-proton singlet at  $\delta$  3.32 ppm.

The diazabicyclohydroxyimino protons H-2<sub>ax</sub>,8<sub>ax</sub> were observed as a two-proton multiplet at  $\delta$  2.45-2.62 ppm. The diazabicyclohydroxyimino protons H-2<sub>eq</sub>,8<sub>eq</sub> and H-4<sub>ax</sub>,6<sub>ax</sub>,4<sub>eq</sub>,6<sub>eq</sub> appeared as a six-proton multiplet at  $\delta$  2.75-2.78 ppm. The diazabicyclohydroxyimino protons H-7 and H-3 were recorded as a one-proton multiplet and a singlet at  $\delta$  2.66-2.71 and 3.64 ppm, respectively. The hydroxyl proton H-11 resonated together with the aromatic protons H-19-23 as a six-proton multiplet at  $\delta$  7.22-7.34 ppm.

In the  $^{13}\text{C}$  NMR spectrum, signals of the carbon atoms of the methoxypropyl fragment were observed at  $\delta$  27.18 (C-13), 54.37 (C-12), 58.74 (C-16), and 71.21 ppm (C-14). Carbon atoms of the diazabicyclohydroxyimino fragment resonated

at  $\delta$  30.23 (C-3), 36.84 (C-7), 56.67 and 57.16 (C-2,8), 58.06 and 58.42 (C-4,6), and 161.52 ppm (C-9). The methylene carbon atom C-17 appeared at  $\delta$  61.69 ppm. Aromatic carbon atoms were detected at  $\delta$  127.09 (C-21), 128.42 (C-20,22), 128.99 (C-19,23), and 138.51 ppm (C-18).

The structure of the compound (**3**) was additionally confirmed by two-dimensional NMR spectroscopy using COSY ( $^1\text{H}$ - $^1\text{H}$ ), HMQC ( $^1\text{H}$ - $^{13}\text{C}$ ), and HMBC ( $^1\text{H}$ - $^{13}\text{C}$ ) techniques, which allow the identification of homo- and heteronuclear spin-spin interactions. The observed  $^1\text{H}$ - $^1\text{H}$  COSY and  $^1\text{H}$ - $^{13}\text{C}$  HMQC correlations in the molecule are shown schematically.

In the  $^1\text{H}$ - $^1\text{H}$  COSY spectra, three-bond spin-spin correlations were observed between protons of neighboring methylene-methylene, methyl-methine, and methine-methine groups: H13-H12 ( $\delta$  1.73, 2.42 and 2.42, 1.73), H13-H14 ( $\delta$  1.73, 3.40 and 3.40, 1.73), and H-2<sub>ax</sub>,8<sub>ax</sub>-H-7 ( $\delta$  2.52, 2.77 and 2.77, 2.52 ppm).

One-bond heteronuclear  $^1\text{H}$ - $^{13}\text{C}$  correlations were established by HMQC spectroscopy for the following proton-carbon pairs: H16-C16 ( $\delta$  3.30, 58.72), H12-C12 ( $\delta$  2.41, 54.29), H13-C13 ( $\delta$  1.74, 27.16), H-2<sub>ax</sub>,8<sub>ax</sub>,2<sub>eq</sub>,6<sub>eq</sub>-C2,8 ( $\delta$  2.77, 56.54), H-4<sub>ax</sub>,6<sub>ax</sub>,4<sub>eq</sub>,6<sub>eq</sub>-C4,6 ( $\delta$  2.76, 58.50), H-7-C7 ( $\delta$  2.61, 36.88), H-3-C3 ( $\delta$  3.63, 30.28), H-14-C14 ( $\delta$  3.40, 71.27), H-17-C17 ( $\delta$  3.49, 61.69), and H-19,23,20,22-C19,23,20,22 ( $\delta$  7.27, 128.60 ppm). Long-range heteronuclear  $^1\text{H}$ - $^{13}\text{C}$  correlations through two or more bonds were identified by HMBC spectroscopy for the following pairs: H13-C12 ( $\delta$  1.73, 54.76), H13-C14 ( $\delta$  1.73, 71.12); H12-C13 ( $\delta$  2.41, 27.09), H12-C2,8 ( $\delta$  2.41, 56.17), H12-C4,6 ( $\delta$  2.41, 58.42), H12-C14 ( $\delta$  2.41, 71.27); H14-C13 ( $\delta$  3.40, 27.15), H14-C12 ( $\delta$  3.40, 53.92); H16-C14 ( $\delta$  3.30, 71.45); H17-C2,8 ( $\delta$  3.49, 56.83), H17-C4,6 ( $\delta$  3.49, 58.86), H17-C20,22 ( $\delta$  3.49, 129.25), and H17, C18 ( $\delta$  3.49, 138.92 ppm).

Acylation of oxime (**3**) with benzoyl chloride in absolute benzene at room temperature for 12 h afforded the corresponding *O*-benzoyloxime (**4**) in 65% yield. The product was purified by column chromatography on  $\text{Al}_2\text{O}_3$  using benzene/isopropanol (7:1) as the eluent. The IR spectrum of compound (**4**) exhibits an intense absorption band at  $1742\text{ cm}^{-1}$ , corresponding to the ester carbonyl group of the benzoyl fragment, as well as a band at  $1637\text{ cm}^{-1}$  characteristic of the C=N bond of the oxime moiety, confirming the formation of the *O*-benzoylated derivative.

A crystalline inclusion complex (**5**) of compound (**4**) with  $\beta$ -CD was prepared in an equimolar ratio. The resulting complex (**5**), designated KhZR-107, exhibits high thermal stability, decomposing above  $240\text{ }^\circ\text{C}$ .

The inclusion complex of *O*-benzoylated derivative with  $\beta$ -CD (KhZR-107) was studied at a concentration of 0.001% for its effects on germination, growth, and development of wheat seedlings (variety Kazakhstan-10) and soybean seedlings (variety Zhansaya) under laboratory conditions. For comparison, a solution of Baikal EM-1 at 0.001% was used. The results of the study are presented in Tables 1 and 2 and Figures 1 and 2.

**Table 1** - Influence of KhZR-107 on germination and growth of wheat seeds under controlled laboratory conditions

Treatment	Germination, %	Germination energy, %	Mean height, cm	Contamination with microflora
Control	90 ± 2	82.5 ± 1.5	9.5 ± 0.4	-
KhZR-107	100 ± 0	95.0 ± 1.2*	11.0 ± 0.5*	-

\*Significant difference compared to control (p < 0.05)



**Figure 1** - Influence of KhZR-107 on germination, growth, and development of Kazakhstan-10 wheat seedlings under laboratory conditions.

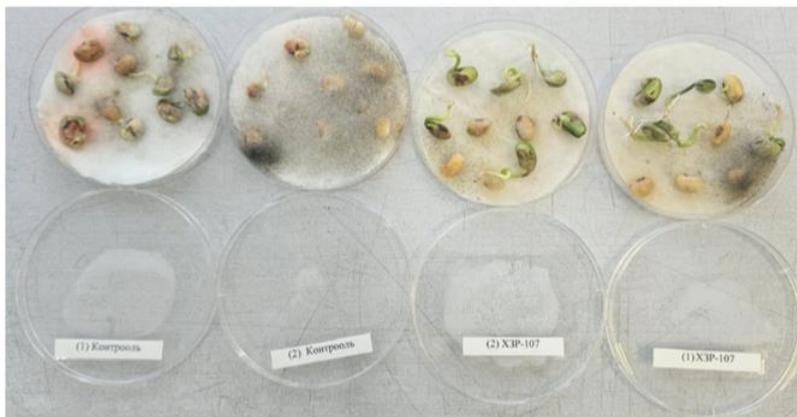
As shown in Table 1, treatment with KhZR-107 produced a pronounced stimulatory effect on wheat seeds. Laboratory germination increased from 90% in the control to 100%, while germination energy rose from 82.5% to 95.0%. In addition, treated seedlings exhibited more vigorous early growth, as indicated by a mean shoot height increase from 9.5 cm to 11.0 cm. The absence of visible microflora contamination in both control and treated variants indicates that the preparation did not negatively affect seed sanitary status. The simultaneous improvement of germination energy and seedling height suggests that the complex not only accelerated seed awakening but also supported subsequent metabolic activity during early ontogenesis.

**Table 2** - Effect of KhZR-107 on germination and seedling development of Zhansaya soybean under laboratory conditions

Treatment	Germination rate, %	Seed germination energy, %	Contamination with microflora
Control	50 ± 3	45.0 ± 2.0	+++
KhZR-107	50 ± 2	45.0 ± 1.8	+++

In contrast to wheat, soybean seeds showed no quantitative changes in germination rate or germination energy following treatment with KhZR-107 (Table 2). Both indicators remained at the control level (50% and 45.0%, respectively). Microflora contamination (+++) was observed in both experimental and control groups, indicating that the preparation did not exert a protective or inhibitory effect on associated microorganisms under the tested conditions.

Nevertheless, visual observations in the moist chamber indicated more uniform seedling development, suggesting that the preparation may influence post-germination physiological processes rather than the initial germination stage in soybean.



**Figure 2** - Effect of KhZR-107 on germination and early seedling development of Zhansaya soybean under laboratory conditions.

#### *Possible Mechanism of Growth-Stimulating Action of KhZR-107*

The growth-promoting effect of KhZR-107 in wheat may be attributed to enhanced bioavailability of the *O*-benzoylated oxime derivative resulting from its inclusion into  $\beta$ -cyclodextrin.

Such complexation [17,18] is known to improve solubility and facilitate penetration of the active compound into the seed during imbibition, thereby enabling more efficient interaction with metabolically active tissues. The observed increase in germination energy [19] suggests stimulation of early metabolic processes, particularly activation of enzymatic systems involved in reserve mobilization. Enhanced amyolytic activity and accelerated nutrient supply to the embryo may account for both faster germination and increased seedling height.

Furthermore, oxime-containing compounds may affect redox homeostasis. Controlled modulation of reactive oxygen species [20] during early ontogenesis could promote synchronized germination and stimulate cell division. The absence of significant quantitative effects in soybean indicates species-specific sensitivity, possibly related to differences in seed composition and metabolic pathways. Nevertheless, improved seedling uniformity suggests that KhZR-107 may influence post-germination physiological processes.

Overall, the findings indicate that KhZR-107 functions as a mild metabolic activator rather than a classical phytohormone analogue [21], enhancing early growth without exhibiting phytotoxic effects.

#### 4. Conclusion

A new series of 3-benzyl-7-(3-methoxypropyl)-3,7-diazabicyclo[3.3.1]nonan-9-one derivatives was synthesized from 1-benzylpiperidin-4-one and structurally confirmed by IR,  $^1\text{H}/^{13}\text{C}$  NMR, and 2D experiments. Incorporation of the *O*-benzoylated oxime into a  $\beta$ -CD inclusion complex (KhZR-107) enhanced biological activity. In wheat (Kazakhstan-10), KhZR-107 increased germination from 90% to 100%, germination energy from 82.5% to 95%, and shoot height from 9.5 to 11.0 cm, without affecting seed sanitary quality. In soybean (Zhansaya), germination remained unchanged, although seedling development was slightly more uniform. These results highlight KhZR-107 as a promising cereal growth stimulator, particularly for wheat, while further greenhouse and field studies are needed to optimize its application and confirm microbiological stability.

**Funding:** This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP22685628).

**Conflict of Interest:** The authors declare that there is no conflict of interest regarding the data presented in this article.

#### ЖАҢА N-БЕНЗИЛПИПЕРИДОН ТУЫНДЫЛАРЫ: СИНТЕЗІ ЖӘНЕ ӨСІМДІК ӨСУІН ҢНТАЛАНДЫРУШЫ ӘСЕРІ

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**Түйіндеме.** *Кіріспе.* Пиперидин туындылары, әсіресе *N*-бензилпиперидондар, кең фармакологиялық әлеуетке ие және әрі қарай химиялық түрлендіру үшін перспективалы болып табылады. Оларға деген қызығушылық бастапқы реагенттердің қолжетімділігімен және салыстырмалы түрде қарапайым синтез жолдарымен байланысты, бұл берілген физика-химиялық және биологиялық қасиеттері бар жаңа қосылыстарды жобалауға мүмкіндік береді. Осы жұмыстың мақсаты - бензилпиперидон туындыларының жаңа қатарын синтездеу, құрылымдық модификациялау арқылы күрделірек азотқұрамды гетероциклдерді алу және олардың өсімдік өсуін ынталандыру белсенділігін зерттеу. *Нәтижелер және талқылау.* 1-Бензилпиперидин-4-он 1-(3-метоксипропил)аминмен және параформальдегидпен әрекеттесіп, 3-бензил-7-(3-метоксипропил)-3,7-дизабизикло[3.3.1]-нонан-9-он түзді. Кетон оксимациялау жағдайында 76% шығыммен сәйкес оксимге айналдырылды. Оксимді бензойлхлоридпен ацилдеу нәтижесінде 65% шығыммен *O*-бензоилоксим алынды. ХЗР-107 кешені 0,001% концентрацияда бидайдың (Қазақстан-10 сорты) және сояның (Жансая сорты) тұқымдарының өнуіне, өсуі мен дамуына әсері тұрғысынан зерттелді. *Қорытынды.* ХЗР-107 препаратымен өңдеу бидай өсімін жақсартты: өсу көрсеткіші 90%-дан 100%-ға дейін өсті, өсу энергиясы 82,5%-дан 95%-ға дейін артты, ал бұл дәндер биіктігінің артуына әкелгенмен, бұл ұрықтың санитарлық сапасына әсер етпеді. Соя тұқымында өсу көрсеткіштері өзгермеді, бірақ көшеттер сәл біркелкі болып көрінді, бұл ерте даму кезеңіндегі оң әсерлерді көрсетеді.

**Түйінді сөздер:** *N*-бензилпиперидон, дизабициклононанон,  $\beta$ -циклодекстриннің инклюзиялық кешені, өсімдіктердің өсуін ынталандыру.

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## НОВЫЕ N-БЕНЗИЛПИПЕРИДОНОВЫЕ ПРОИЗВОДНЫЕ: СИНТЕЗ И РОСТСТИМУЛИРУЮЩАЯ АКТИВНОСТЬ РАСТЕНИЙ

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**Резюме.** *Введение.* Производные пиперидина, в частности N-бензилпиперидоны, проявляют широкий фармакологический потенциал и являются перспективными объектами для дальнейшей химической модификации. Интерес к ним обусловлен доступностью исходных веществ и относительной простотой синтеза, что позволяет конструировать новые соединения с заданными физико-химическими и биологическими свойствами. *Целью данной работы* является синтез новой серии производных бензилпиперидона, получение более сложных азотсодержащих гетероциклов путём структурной модификации и изучение их ростстимулирующей активности в отношении растений. *Результаты и обсуждение.* 1-Бензилпиперидин-4-он взаимодействовал с 1-(3-метоксипропил)амином и параформальдегидом с образованием 3-бензил-7-(3-метоксипропил)-3,7-дизабицикло[3.3.1]нонан-9-она. Кетон был превращён в соответствующий оксим с выходом 76% в условиях оксимации. Ацилирование оксима бензоилхлоридом привело к получению O-бензоилоксима с выходом 65%. Комплекс ХЗР-107 был исследован на влияние на прорастание, рост и развитие проростков пшеницы (сорт Казахстан-10) и сои (сорт Жансая) при концентрации 0,001%. *Заключение.* Обработка ХЗР-107 улучшила показатели пшеницы: всхожесть повысилась с 90% до 100%, энергия прорастания увеличилась с 82,5% до 95%, а рост семян стал выше, при этом санитарное качество семян не пострадало. У сои показатели всхожести остались без изменений, однако семена выглядели немного более равномерными, что указывает на умеренные положительные эффекты в раннем развитии.

**Ключевые слова:** N-бензилпиперидон, диазабициклононанон, комплекс включения β-циклодекстрина, стимулирование роста растений.

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## STRUCTURAL PARAMETERS OF SPATIALLY CROSS-LINKED COPOLYMERS OF POLYETHYLENE GLYCOL MALEATE AND ACRYLIC ACID

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**Abstract.** *Introduction.* The development of polymer binders for construction and composite materials requires purposeful control over the structure of spatially cross-linked polymer networks, since the internal structural parameters largely determine the mechanical, sorption, and performance characteristics of materials. In this context, the quantitative evaluation of crosslink density and the number of junctions in polymer networks as a function of system composition represents an important scientific task. *Methodology.* In this study, spatially cross-linked copolymers based on polyethylene glycol maleate modified with acrylic acid were synthesized by a “cold” radical curing method at various mass ratios of the components. The structure of the obtained materials was confirmed by Fourier transform infrared (FTIR) spectroscopy. Quantitative assessment of the structural parameters of the polymer network was performed using equilibrium swelling data of the copolymers in water. The crosslink density, number of network junctions, and average molecular weight between junctions were calculated using the Flory–Rehner equation. *Results of the study.* It was established that an increase in the polyester component content in the investigated systems leads to a decrease in the swelling degree and to the formation of a denser spatially cross-linked structure, characterized by an increase in crosslink density and a reduction in the molecular weight between network junctions. The obtained results demonstrate the possibility of purposeful control over the structural parameters and properties of polyester binders by varying the system composition, thereby opening prospects for their application in construction and composite materials.

**Keywords:** unsaturated polyester; “cold” curing; spatially cross-linked polymers; swelling; crosslink density; Flory–Rehner equation; molecular weight between crosslinks

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**Citation:** Burkeyeva G.K., Kovaleva A.K., Zhumabek N.M., Nukin N.A., Kenzhetayev R.R. Structural parameters of spatially cross-linked copolymers of polyethylene glycol maleate and acrylic acid. *Chem. J. Kaz.*, 2026, 1(93), 48-59. DOI: <https://doi.org/10.51580/2026-1.2710-1185.05>

## 1. Introduction

Currently, when creating polymer binders for construction and composite materials, special attention is paid to the study and targeted regulation of the structure of spatially cross-linked polymer networks, since the parameters of the structural organisation of the network largely determine the durability and performance characteristics of materials [1]. For thermosetting and network polymer systems, key characteristics of the internal structure include crosslink density and molecular weight between nodes, which affect mechanical strength, deformation behaviour, sorption properties, and resistance to moisture and temperature [2].

In polyester systems based on unsaturated polyesters and reactive monomers, the curing process is accompanied by the formation of a three-dimensional polymer network with nodes that unite macromolecular chains into a single spatial structure. The number of such nodes is one of the main quantitative characteristics of the degree of cross-linking and the level of structural organisation of the material [3]. An increase in node density usually leads to an increase in rigidity and a decrease in chain mobility, while less dense networks are characterised by increased elasticity and swelling capacity [4].

For systems based on polyethylene glycol maleate (p-EGM) modified with acrylic acid (AA), the formation of a polymer network occurs as a result of radical curing involving double bonds of the polyester component and acrylic monomer. The mass ratio of the components determines the concentration of reactive groups and, accordingly, the number of nodes in the spatially cross-linked structure [5], which makes the composition of the system an effective tool for controlling its structural parameters.

Quantitative assessment of the number of nodes is an important stage of structural analysis, allowing us to move from describing the composition and experimentally observed properties to characterising the internal structure of the material [6]. One of the most informative methods of such assessment is the study of the equilibrium swelling of network polymers, in which the degree of swelling reflects the balance between the elastic forces of the polymer network and the thermodynamic interaction of the polymer with the solvent [7]. For spatially cross-linked systems, an increase in the number of nodes is accompanied by a decrease in the material's swelling capacity [1].

Based on the swelling data, the calculation of crosslink density using the Flory–Rehner equation, which links the parameters of the polymer network with the thermodynamic characteristics of the system, is widely used [8]. Despite its known limitations, this approach remains one of the most common in the study of networked polyester and acrylate materials [3]. Its application is particularly relevant for polyester binders used in construction, where an optimal combination of strength, water resistance and dimensional stability is required [2]. Analysis of p-EGM–AA systems across a wide range of compositions allows establishing the relationship between the formulation, structural parameters and operational properties of materials [5].

Thus, calculating the number of nodes in the p-EGM-AA polymer network based on swelling data is a valid structural analysis tool that allows linking the characteristics of the composition and internal structure with the functional characteristics of materials and creates a basis for further optimisation of polyester binders [3].

## 2. Experimental part

The research was conducted in four stages. At the first stage, the starting unsaturated polyester, polyethylene glycol maleate, was synthesized, and its average molecular weight ( $M_w$ ) was determined by GPC and turbidimetry to be ~1232 Da.

In the second stage, using the ‘cold’ radical curing method of the initial p-EGM with acrylic acid at different mass ratios of the components, the following systems were obtained: p-EGM15 (p-EGM-AA 15:85 wt.%), p-EGM30 (p-EGM-AA 30:70 wt.%), p-EGM45 (p-EGM-AA 45:55 wt.%) and p-EGM60 (p-EGM-AA 60:40 wt.%). Benzoyl peroxide (BPO, initiator) and dimethylaniline (DMA, activator) were used as the initiating system in a mass ratio of 1.0:0.5 wt.%. Curing was carried out at a temperature of 293K without additional heat exposure [9,10]. The initial reaction mixtures were prepared by thoroughly mixing the components until a homogeneous system was obtained, after which the ‘cold’ curing initiation system was added and left at a set temperature until the formation of a spatially cross-linked structure was complete.

After curing, the cured samples were purified to remove unreacted monomers. Purification was carried out by sequential washing with dioxane and then distilled water. The composition of the cured polymers was determined by HPLC analysis of the resulting mother liquors in dioxane. After washing, the samples were dried at room temperature until a constant weight was achieved, which was monitored by repeated weighing.

The third stage of the study included determining the structure of the obtained systems based on p-EGM of various compositions by IR spectroscopy and determining their degree of swelling. The swelling study was carried out in distilled water. For each composition, weights of dry copolymer with a mass of ~3.0 g were used. The weights were placed in an excess of solvent and kept at a constant temperature until an equilibrium mass was established. The swelling equilibrium was considered to be reached when there was no change in the mass of the sample within the weighing error [11]. After reaching equilibrium, the samples were removed from the water, surface moisture was removed with filter paper, and they were weighed immediately.

The degree of swelling ( $S$ ) of the copolymers was calculated using formula (1):

$$S = \frac{m_{swel} - m_{dry}}{m_{dry}} \quad (1)$$

where  $m_{\text{swel}}$  is the mass of the sample in a state of equilibrium swelling (after blotting the surface), g;

$m_{\text{dry}}$  is the mass of the dry sample, g.

Each swelling measurement was performed in at least three parallel experiments. The deviation of mass values did not exceed  $\pm 2\%$ , indicating good reproducibility of the results. The tables present the average values of the measured parameters.

At the final stage, calculations were made of the number of nodes ( $N$ ) in the polymer network and the molecular mass ( $M_c$ ) between them. For this purpose, to calculate the structural parameters of the polymer network, the experimentally determined value of the degree of swelling  $S$ , calculated as the relative increase in sample mass, was converted into the mass swelling coefficient  $Q_m$  according to formula (2):

$$Q_m = 1 + S \quad (2)$$

The volume fraction of the polymer in the swollen state  $\varphi_2$  was determined taking into account the densities of the polymer and solvent according to equation (3):

$$\varphi_2 = \frac{1 / \rho_{\text{dry}}}{1 / \rho_{\text{dry}} + (Q_m - 1) / \rho_{\text{solv}}} \quad (3)$$

where  $\rho_{\text{dry}}$  is the density of the dry polymer,  $\text{g/cm}^3$ ;

$\rho_{\text{solv}}$  is the density of the solvent (for water,  $\rho_{\text{solv}} = 1 \text{ g/cm}^3$ ),  $\text{g/cm}^3$ .

The polymer density was assumed to be a constant value in accordance with generally accepted assumptions for calculations of spatially cross-linked polyester systems.

The assumption of a constant density of the dry polymer for all investigated compositions is based on the similarity of the chemical nature of the resulting cross-linked network structures and the absence of fundamentally different phase components in the system. Variation in the mass ratio of p-EGM and AA primarily leads to changes in crosslink density rather than to the formation of chemically heterogeneous materials.

The calculated density values for the different samples differ only slightly (Table 2), which confirms the validity of using an averaged approach. The potential error associated with this assumption does not exceed the experimental uncertainty in the determination of the swelling degree and does not affect the established qualitative trends in the variation of  $v_e$  and  $M_c$ .

The number of polymer network nodes (cross-link density) was calculated using the Flory–Rehner equation (4):

$$v_e = \frac{-\ln(1 - \varphi_2) - \varphi_2 - \chi\varphi_2^2}{V_1(\varphi_2^{1/3} - \frac{\varphi_2}{2})} \quad (4)$$

where  $v_e$  – concentration of network chains, mol/cm<sup>3</sup>;  
 $V_1$  – molar volume of solvent (for water  $V_1=18$  cm<sup>3</sup>/mol);  
 $\chi$  – was selected based on literature data for polyether-acrylate systems in an aqueous medium [8].

Next, the concentration of cross-linked chains was converted into the number of polymer chain nodes per unit volume using the expression (5):

$$N = v_e \cdot N_A \quad (5)$$

where  $N_A$  – Avogadro's number.

The obtained values were used for quantitative comparison of the structural characteristics of copolymers of different compositions and analysis of the effect of the degree of swelling on the parameters of the spatially cross-linked network.

The following reagents ('Sigma-Aldrich') were used for the study: acrylic acid, benzoyl peroxide, dimethylaniline, dioxane. All reagents were of analytical grade and used without additional purification. The starting unsaturated polyester, p-EGM, was previously obtained by the polycondensation reaction of ethylene glycol with maleic anhydride using a standard method [11].

### 3. Results and discussion

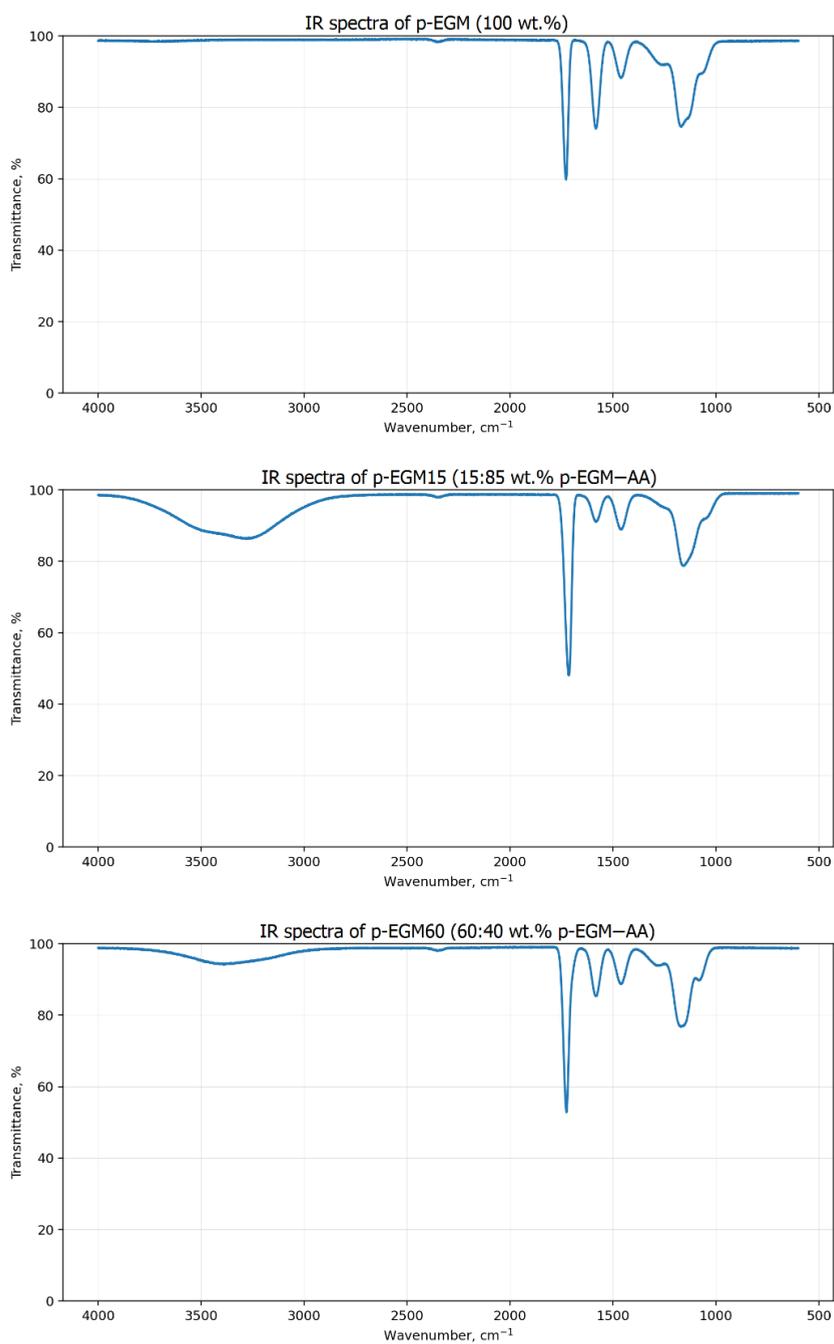
The curing of the initial unsaturated polyester – p-EGM – was carried out using a binary 'cold' curing initiation system consisting of BPO and DMA (1.0:0.5 wt.%) at a temperature of 293K.

The actual composition of the obtained cured systems p-EGM15, p-EGM30, p-EGM45 and p-EGM60 was determined by HPLC. The results are presented in Table 1:

**Table 1** – Dependence of the composition of copolymers and some of their parameters on the composition of the initial mixtures of p-EGM ( $M_1$ ) with AA ( $M_2$ )

Composition of the initial polymer-monomer mixture, wt.%		Composition of cured systems, wt.%		Yield, %	Degree of swelling, S
$M_1$	$M_2$	$m_1$	$m_2$		
15.04	84.96	13.98	86.02	92.8	38.29±1.91
30.21	69.79	28.87	71.13	91.2	11.51±0.58
45.06	54.94	43.54	56.46	89.7	2.17±0.11
60.12	39.88	58.12	43.88	89.1	1.44±0.07

\* The reported data represent average values; the relative error in the determination of the swelling degree does not exceed ±5%.



**Figure 1** – IR spectra of p-EGM and copolymers based on it.

The data obtained, presented in Table 1, indicate a direct dependence of the cured product yield on the AA content. It is also worth noting that varying the AA content allows products with different physicochemical properties to be obtained, which makes them promising materials in various industries, both as effective polymer gel sorbents and as hydrophobic compounds used as polymer binders for the manufacture of building materials.

The structure of the synthesized compounds was studied using IR spectroscopy. The spectra of the initial p-EGM and p-EGM-AA copolymers of various compositions are characterized by a set of absorption bands indicating the formation of the corresponding polymer structures (Fig.1). For the initial p-EGM, an intense band of valence vibrations of carbonyl groups of ester fragments in the range of 1725–1730  $\text{cm}^{-1}$  was recorded, as well as a band related to the vibrations of unsaturated  $\text{C}=\text{C}$  bonds of maleate units in the range 1575–1590  $\text{cm}^{-1}$ . Deformation vibrations of methylene  $\text{CH}_2$  groups appear in the range 1455–1465  $\text{cm}^{-1}$ . High-intensity bands in the range 1140–1160  $\text{cm}^{-1}$  correspond to vibrations of ether  $\text{C}-\text{O}-\text{C}$  bonds of the polyester chain.

When an increased content of AA (copolymer p-EGM15) is introduced, a broad absorption band appears in the IR spectrum in the range of 3100–3600  $\text{cm}^{-1}$ , caused by the contribution of valence vibrations of hydroxyl groups of carboxyl fragments involved in the formation of hydrogen bonds. A characteristic feature of the modification is an increase in the intensity of the carboxyl group  $\text{COOH}$  band in the range 1710–1715  $\text{cm}^{-1}$  compared to the initial p-EGM, which indicates an increase in the content of acrylic acid in the copolymer structure. At the same time, the band corresponding to the vibrations of unsaturated double bonds in the range 1575–1585  $\text{cm}^{-1}$  is preserved, but its intensity is noticeably reduced, which indicates a partial copolymerization reaction involving  $\text{C}=\text{C}$  bonds [12].

Next, the structural parameters of spatially cross-linked copolymers of the p-EGM-AA system were calculated, which made it possible to quantitatively characterize the features of polymer network formation and establish the relationship between the composition, internal structure, and properties of the materials. The use of equilibrium swelling data in water in combination with the Flory-Rehner equation made it possible to move from a qualitative description of the behaviour of copolymers to a quantitative assessment of the density of cross-links and the molecular organization of the polymer matrix.

It should be noted that in the calculation of the crosslink density  $\nu_e$  and the average molecular weight between network nodes  $M_c$ , the polymer-solvent interaction parameter  $\chi$  was taken from literature data for polyester-acrylate systems in an aqueous medium [8]. It is well known that the value of  $\chi$  can significantly influence the quantitative values of the calculated parameters, since it enters the Flory-Rehner equation in an exponential form.

Sensitivity analysis indicates that when  $\chi$  is varied within reasonable limits ( $\pm 0.02$ – $0.03$ ), the absolute values of  $\nu_e$  and  $M_c$  may change; however, the overall trend in the variation of structural parameters with changes in system composition

remains unchanged. Therefore, despite the possible uncertainty associated with the choice of  $\chi$ , the observed relationships are robust and reliably reflect the effect of the component mass ratio on the spatial organization of the polymer network.

It should be taken into account that the Flory–Rehner equation is based on several simplifying assumptions, including an ideal network structure, uniform distribution of crosslink junctions, and the absence of structural defects such as loops, dangling chains, and local inhomogeneities in crosslink density. In real polyester–acrylate systems, deviations from the idealized model are possible due to microstructural heterogeneity and the statistical nature of radical copolymerization. Therefore, the calculated values of crosslink density and molecular weight between network junctions should be regarded as effective (estimated) parameters reflecting the averaged characteristics of the polymer network.

The experimental swelling values were reduced to a dimensionless quantity  $S$  (degree of swelling), reflecting the relative increase in sample mass compared to the dry state. Based on the value of  $S$ , the mass swelling coefficient  $Q_m$  was calculated, and taking into account the densities of dry copolymers, the volume fraction of the polymer in the equilibrium swollen state  $\phi_2$  was determined. Subsequent calculation of the crosslink density  $\nu_e$  and the average molecular weight between the network nodes  $M_c$  allowed us to comprehensively characterize the structural parameters of the forming polymer network. The calculation results are presented in Table 2.

**Table 2** – Structural parameters of the polymer network of copolymers of the p-EGM–AA system

Composition (wt.%) p-EGM– AA**	$Q_m$	$\rho_{dry}, \text{g/cm}^3$	$\phi_2$	$\nu_e, \text{mol/cm}^3$	$M_c, \text{g/mol}$
p-EGM15	39.29	1.2697±0.0635	0.020	$(4.90±0.25) \cdot 10^{-6}$	$(2.59±0.13) \cdot 10^5$
p-EGM30	12.51	1.2842±0.0642	0.063	$(4.40±0.22) \cdot 10^{-5}$	$(2.92±0.15) \cdot 10^4$
p-EGM45	3.17	1.3041±0.0652	0.261	$(1.18±0.06) \cdot 10^{-3}$	$(1.11±0.06) \cdot 10^3$
p-EGM60	2.44	1.3195±0.0660	0.345	$(2.58±0.13) \cdot 10^{-3}$	$(5.11±0.26) \cdot 10^2$

\* The reported data represent average values; the relative uncertainty of the calculated structural parameters ( $\nu_e$  and  $M_c$ ) does not exceed ±5%.

\*\* Since the numerical compositions of the cured products are quite close to those of the initial mixtures, it is customary to designate the resulting polymers according to the values of the initial compositions for clarity

Analysis of the data obtained shows that a change in the mass ratio of components in p-EGM–AA systems is accompanied by pronounced changes in the structural characteristics of the polymer network. Copolymers with a high AA content are characterized by high  $Q_m$  values and low values of the polymer volume fraction  $\phi_2$ . This indicates the formation of a sparse spatially cross-linked structure in which macromolecular chains have high mobility and the number of polymer network nodes is small. Such systems are characterized by a significant

ability to sorb water, which is due to both the low density of cross-links and the presence of hydrophilic functional groups.

With an increase in the proportion of p-EGM in the composition of cured products, there is a regular increase in the volume fraction of the polymer in the equilibrium swollen state and a corresponding increase in the density of cross-links  $\nu_e$ . For compositions with a higher polyester content,  $\varphi_2$  values reach 0.26–0.35, and the crosslink density increases to about  $10^{-3}$  mol/cm<sup>3</sup>. This indicates the formation of a denser spatially cross-linked structure in which the mobility of macromolecular segments is significantly limited by the elastic forces of the polymer network. The decrease in the swelling ability of such systems is a direct consequence of an increase in the number of nodes and an increase in the elastic resistance of the network to solvent penetration.

Of particular interest is the analysis of the average molecular weight between nodes in the  $M_c$  network, which is an integral characteristic of the degree of structural organization of spatially cross-linked polymers. Calculation of  $M_c$  showed that as the density of cross-links increases, the value of this characteristic decreases by more than two orders of magnitude. For sparse networks with low node density,  $M_c$  values reach  $10^5$  g/mol, which corresponds to long and mobile macromolecular segments between cross-link nodes. At the same time, for denser networks,  $M_c$  decreases to values of the order of  $10^2$ – $10^3$  g/mol, which indicates a significant shortening of the chain segments and an increase in the rigidity of the polymer matrix.

The obtained trends are consistent with modern concepts of the behavior of spatially cross-linked polymers: an increase in crosslink density leads to higher network elasticity, restricted segmental mobility of macromolecules, and a reduced swelling capacity. The calculation of the parameters  $\nu_e$  and  $M_c$  makes it possible to quantitatively describe the internal organization of p-EGM–AA copolymers and to provide a well-founded interpretation of the changes in their sorption characteristics depending on composition.

Thus, the results of calculating structural parameters based on equilibrium swelling data demonstrate that varying the mass ratio of components in the p-EGM–AA system is an effective way to control the spatial organization of the polymer network. The data obtained provide a reliable basis for further analysis of the relationship between the operational characteristics of the copolymers obtained, and can also be used to justify their potential application as polyester binders for construction and composite materials.

In contrast to previously published studies on polyester network systems [3,5], the present work provides a comprehensive analysis of the effect of p-EGM–AA composition on the quantitative parameters of the network structure over a wide range of component ratios using an energy-efficient ‘cold’ curing method. This approach makes it possible to expand the understanding of the mechanisms of structural organization of polyester–acrylate networks and their regulation at the synthesis stage.

#### 4. Conclusions

Based on the data on equilibrium swelling in water, the structural parameters of spatially cross-linked p-EGM–AA copolymers were calculated. It was found that a change in the mass ratio of the components leads to variations in the volume fraction of the polymer in the swollen state, the density of cross-links, and the molecular weight between the network nodes. It was shown that an increase in the proportion of the polyester component is accompanied by an increase in the density of cross-links and a decrease in the inter-node molecular weight, which indicates a densification of the spatially cross-linked structure. A relationship has been identified between the structural parameters of the polymer network and the swelling ability of copolymers, which is due to the balance of elastic and thermodynamic factors. The calculation of the number of nodes confirmed the informative value of the equilibrium swelling method for the quantitative analysis of the structure of polyester network systems and substantiated the prospects for the use of p-EGM–AA copolymers as polyester binders for construction and composite materials.

**Funding:** This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23488036).

**Conflict of Interest:** There is no conflict of interest between the authors.

#### ПОЛИЭТИЛЕНГЛИКОЛЬМАЛЕИНАТ ПЕН АКРИЛ ҚЫШҚЫЛЫНЫҢ КЕҢІСТІКТІК ТІГІЛГЕН СОПОЛИМЕРЛЕРІНІҢ ҚҰРЫЛЫМДЫҚ ПАРАМЕТРЛЕРІ

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**Түйіндемe.** *Кіріспе.* Құрылыс және композициялық материалдарға арналған полимерлі байланыстырғыштарды әзірлеу кеңістіктік тігілген полимерлік торлардың құрылымын мақсатты түрде басқаруды талап етеді, өйткені ішкі құрылым параметрлері материалдардың механикалық, сорбциялық және пайдалану сипаттамаларын айқындайды. Осыған байланысты жүйе құрамына тәуелді тігілулер тығыздығы мен полимерлік тор түйіндерінің санын сандық тұрғыдан бағалау өзекті ғылыми міндет болып табылады. *Әдістеме.* Жұмыста акрил қышқылымен модификацияланған полиэтиленгликольмалеинат негізіндегі кеңістіктік тігілген сополимерлер әртүрлі компоненттердің массалық қатынастары кезінде «суық» радикалды қатайту әдісімен алынды. Алынған материалдардың құрылымы инфрақызыл спектроскопия әдісімен расталды. Полимерлік тордың құрылымдық параметрлерін сандық бағалау үшін сополимерлердің суда тепе-теңдік ісіну деректері пайдаланылды. Тігілулер тығыздығы, тор түйіндерінің саны және түйіндер арасындағы орташа молекулалық масса Флори–Ренер теңдеуі негізінде есептелді. *Зерттеу нәтижелері.* Зерттелетін жүйелерде полиэфирлік компоненттің үлесінің артуы ісіну дәрежесінің төмендеуіне және тігілулер тығыздығының артуы мен тор түйіндері арасындағы молекулалық массаның кемуімен сипатталатын неғұрлым тығыз кеңістіктік тігілген құрылымның қалыптасуына әкелетіні анықталды. Алынған нәтижелер жүйе құрамын өзгерту арқылы полиэфирлік байланыстырғыштардың құрылымдық параметрлері мен қасиеттерін мақсатты түрде реттеуге болатынын көрсетеді және олардың құрылыс пен композициялық материалдарда қолданылу болашақтарын ашады.

**Түйінді сөздер:** канықпаған полиэфир; «суық» катайту; кеністіктік тігілген полимерлер; ісіну; тігілулер тығыздығы; Флори–Ренер тендеуі; түйіндер арасындағы молекулалық масса

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## СТРУКТУРНЫЕ ПАРАМЕТРЫ ПРОСТРАНСТВЕННО-СШИТЫХ СОПОЛИМЕРОВ ПОЛИЭТИЛЕНГЛИКОЛЬМАЛЕИНАТА И АКРИЛОВОЙ КИСЛОТЫ

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**Резюме.** *Введение.* Разработка полимерных связующих для строительных и композиционных материалов требует целенаправленного управления структурой пространственно-сшитых полимерных сетей, поскольку параметры внутреннего строения в значительной степени определяют механические, сорбционные и эксплуатационные характеристики материалов. В этой связи актуальной задачей является количественная оценка плотности сшивок и количества узлов полимерной сети в зависимости от состава системы. *Методология.* В работе исследованы пространственно-сшитые сополимеры на основе полиэтиленгликольмалеината, модифицированного акриловой кислотой, полученные методом «холодного» радикального отверждения при различных массовых соотношениях компонентов. Структура полученных материалов была подтверждена методом ИК-спектроскопии. Для количественной оценки структурных параметров полимерной сети использованы данные равновесного набухания сополимеров в воде. Расчет плотности сшивок, количества узлов и средней молекулярной массы между узлами выполнен с применением уравнения Флори–Ренера. *Результаты исследования.* Установлено, что увеличение доли полиэфирного компонента в исследуемых системах приводит к снижению степени набухания и формированию более плотной пространственно-сшитой структуры, характеризующейся ростом плотности сшивок и уменьшением молекулярной массы между узлами сети. Полученные результаты демонстрируют возможность целенаправленного управления структурными параметрами и свойствами полиэфирных связующих путем варьирования состава, что открывает перспективы их применения в строительных и композиционных материалах.

**Ключевые слова:** ненасыщенный полиэфир, «холодное» отверждение, пространственно-сшитые полимеры; набухание; плотность сшивок; уравнение Флори–Ренера, межузловая молекулярная масса

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## FEATURES OF THE INTERACTION OF INTERGEL SYSTEMS BASED ON POLYACRYLIC ACID AND POLY-2-METHYL-5-VINYLPYRIDINE WITH GOLD IONS

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**Abstract.** *Introduction.* In the interpolymer system of polyacrylic acid and poly-2-methyl-5-vinylpyridine, the change in the mutual activation of polymer hydrogels with different degrees of crosslinking as a result of remote interaction of the two hydrogels was determined, and their effect on the process of gold ion sorption was studied [1,2]. The purpose aim of the work is to study the sorption capacity of intergel systems based on poly-2-methyl-5-vinylpyridine and polyacrylic acid in relation to gold ions [3,4]. *The obtained results* The maximum degree of sorption of the gPAA:gP2M5VP interpolymer systems increased to 0.645 mol/L at a polymer molar ratio of 5:1 within 48 hours of interaction, and then gradually decreased to 0.575 mol/L. The maximum pH values of the intergel system gPAA:gP2M5VP are observed at a ratio of 3:3, corresponding to a pH of 2.99. The minimum pH value is 2.96 at a ratio of 2:4. The overall swelling ratio (Ksw) increases from 0.8 to 3 during the conformational rotation of the interstitial unit. *Conclusion.* According to the results, the electrochemical properties of hydrogels of polyacrylic acid and poly-2-methyl-5-vinylpyridine in the interpolymer system were studied and the optimal molar ratios were determined. Thus, as a result of these studies: the obtained experimental data on specific electrical conductivity of the solution, pH of the medium and swelling coefficient of hydrogels showed that the presence of remote interaction between acrylic acid and 2-methyl-5-vinylpyridine hydrogels has a significant effect on the initial polymer network and physicochemical properties of the solution.

**Keywords:** interpolymer system, ion-exchangers, hydrogels, polyacrylic acid, poly-2-methyl-5-vinylpyridine, remote interaction, mutual activation, sorption.

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**Citation:** Jumadilov T.K., Dyussebaeva G.T., Mukataeva Zh.S., Khimersen Kh., Erzhet B., Gražulevičius J.V. Features of the interaction of intergel systems based on polyacrylic acid and poly-2-methyl-5-vinylpyridine with gold ions. *Chem. J. Kaz.*, 2026, 1(93), 60-68. DOI: <https://doi.org/10.51580/2026-1.2710-1185.06>

## 1. Introduction

In recent years, work that has attracted the attention of scientists and has been intensively studied is primarily focused on the separation of gold ions from solutions by creating interpolymer systems of cross-linked polymers with high sorption properties and selectivity, as well as on the determination and analysis of their sorption capacity [5,6]. A distinctive feature of the ionization process in interpolymer systems is the absence of a counterion in one part of the ionized chains. This is a consequence of interpolymer interactions, leading to mutual activation of polymers and the formation of unbalanced charges along the polymer chain. During the dissociation of acidic polymers, a proton is separated from the carboxyl group, and this ion combines with a heteroatom of the base polymer in an aqueous medium, resulting in the formation of a neutralized charge. In this case, the charge density of the base polymer is limited by the degree of dissociation of the acidic polymer. As a result, the polyacid undergoes ionization, followed by dissociation of the carboxyl group, and then the association of protons with the polybase heteroatom, resulting in both polymers having equally charged groups in the interstitial chain links without counterions. Therefore, interpolymer systems have a higher sorption capacity compared to individual polymers [7-9]. Based on the long-distance interaction, hydrogels of polyacrylic acid (PAA) and poly-2-methyl-5-vinylpyridine (P2M5VP) were selected for the formation of an intergel pair in intergel systems. Purpose of the study is to study the sorption capacity of intergel systems based on gold ions.

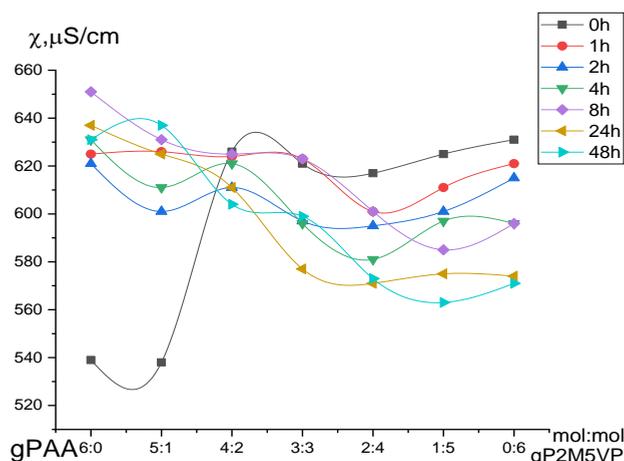
## 2. Materials and Methods

The study was conducted at room temperature over various time intervals. The interpolymer system was prepared as follows: each dry mass of hydrogel was weighed and placed separately into specially prepared individual polypropylene cells (filters) permeable to molecular ions and molecules, but not to hydrogel dispersions. Electrochemical changes (specific conductivity, pH) of the aqueous solution were measured at various time intervals. The mass of the empty cell (g) was subtracted from the mass of the cell filled with hydrogel. gPAA:gP2M5VP. The swelling degree of the hydrogels was calculated. We poured 200 ml of the prepared solution into seven glasses and added seven different ratios of gPAA:gP2M5VP. We conducted a study by placing a cell containing gels in an intergel system. A polyacrylic hydrogel was synthesized in the presence of the cross-linking agent N,N-methylene-bis-acrylamide and the  $K_2S_2O_8$ - $Na_2S_2O_3$  redox system. Poly(2-methyl-5-vinylpyridine) hydrogel (gP2M5VP) was synthesized from the linear polymer in a dimethylformamide medium in the presence of epichlorohydrin at 60°C. The degree of purification was monitored using a conductivity meter. During the study, the synthesized poly(2-methyl-5-vinylpyridine) hydrogel was washed with distilled water for two weeks, dried for one week, and used for experimental work. Conductometer MARK 603 for determining the electrical conductivity of aqueous solutions. The study was

conducted by Expert 002 (Econix-Expert, Moscow, Russian Federation). To measure pH values, use pH Lab 827 (Metrohm, Heritau, Objects (Switzerland) were used. The study of the electrochemical properties of polymers allows us to predict the formation of highly ionized regions of polymer structures during long-range interaction.

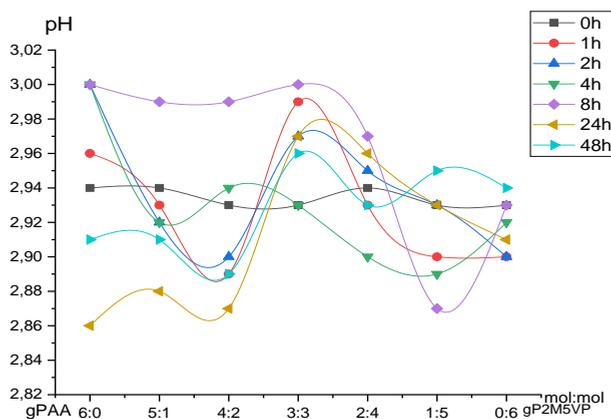
### 3. Results and discussion

Based on our systematic work, we first synthesized the required acidic hydrogels based on polyacrylic acid (gPAA) and poly-2-methyl-5-vinylpyridine (gP2M5VP) and analyzed their properties using various methods. Having created an intergel system, we studied the selective adsorption of the gold ion  $\text{HAuCl}_4$  in various gPAA:gP2M5VP ratios. Previous studies have shown that hydrogels interact with each other at a distance in various combinations, changing their electrochemical and volumetric-hydrodynamic properties [10]. To create an intergel system by mixing poly (2-methyl-5-vinylpyridine) gel with poly(acrylic acid) in different ratios, we first studied the changes in electrical conductivity, pH, and swelling coefficient of the synthesized poly (acrylic acid). Figure 1 shows the changes in the specific electrical conductivity of the medium over certain time intervals at different molar ratios of the gPAA:gP2M5VP intergel system. We observe that at ratios of 6:0 and 5:1 in the intergel system, the specific electrical conductivity of the medium reaches its maximum value, suggesting mutual activation of the hydrogels and their transition to a highly ionized state based on long-distance interactions. The maximum degree of sorption of the gPAA:gP2M5VP intergel system is observed at a molar ratio of polymers of 5:1 over 48 hours of interaction. We see that the concentration of gold ions increases to 0.645 mol/L and then gradually decreases to 0.575 mol/L. The figure also shows high conductivity values at a hydrogel ratio of 4:2, which is 0.625 mol/L. The maximum values observed at the top point indicate an increase in the concentration of electrical conductivity charge carriers, which is explained by the maximum formation of ionic bonds and the corresponding increase in electrical conductivity as a result of the optimal number of carboxyl and amino groups. High values of specific electrical conductivity of the intergel system gPAA:gP2M5VP in a ratio of 1:5. Indicates the presence of  $\text{H}^+$  ions in an aqueous medium. The concentration of  $\text{H}^+$  ions depends on the degree of dissociation of the carboxyl groups. The presence of a maximum on the curve indicates that the speed of ion movement in dilute solutions of strong electrolytes does not depend strongly on concentration. In a solution of  $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$ . Changes in pH of the environment are shown in Figure 2.



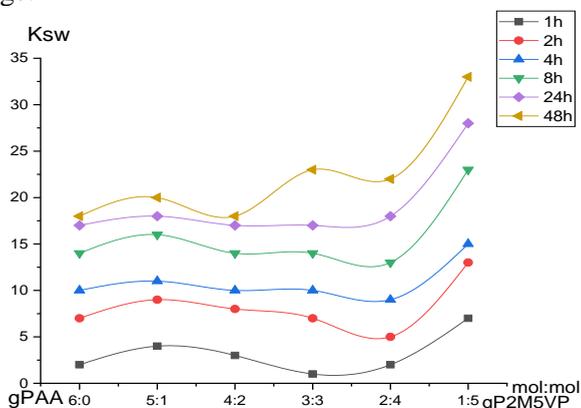
**Figure 1** – Dependence of parameters of intrinsic electroconductivity of gPAA:gP2M5VP hydrogels with different ratios on molar ratios.

The results of the study show that the minimum and maximum pH values are observed in the  $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$  solution. The maximum pH point of the medium is close to neutral at a ratio of 6:0,  $\text{pH}_{\text{max}} = 3.03$ . The minimum pH values of the gPAA:gP2M5VP intergel system medium are observed at ratios of 4:2 and 1:5, and the maximum values are at ratios of 5:1 and 3:3, respectively, at a ratio of 3:3,  $\text{pH}_{\text{max}} = 2.99$ . These values indicate that a low pH value indicates an increase in the concentration of hydrogen ions, and a high pH value indicates a low concentration of  $\text{H}^+$  ions. At a ratio of 4:2,  $\text{pH}_{\text{max}} = 2.98$ , and at a ratio of 2:4,  $\text{pH}_{\text{max}} = 2.96$ . These values indicate that the concentrations of  $\text{H}^+$  and  $\text{OH}^-$  ions in the solution are close. In a  $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$  solution, the pH of the medium slowly increased at a ratio of 2:4, and then the hydrogen concentration remained constant, indicating the formation of hydroxyl ions as a result of the interaction of the base with water molecules in the solution. In the intergel system, at an equimolar ratio of 3:3, complete neutralization of  $\text{H}^+$  and  $\text{OH}^-$  ions occurs. At this ratio, the electrical conductivity of the system is minimal. At a ratio of 1:5, the pH decreases, and the electrical conductivity reaches its maximum. As can be seen from the figure, the low pH and high electrical conductivity are due to the influence of  $\text{H}^+$  ions. gPAA:gP2M5VP The dependence of the swelling coefficients ( $K_{\text{sw}}$ ) of the intergel system on different time intervals is shown in Figure 3. The swelling ratio of the gPAA hydrogel remains constant at a ratio of 6:0 over different time intervals. This indicates that the hydrogel has a limited capacity to absorb water, as only one polymer, gPAA, is present in this system.



**Figure 2** - Dependence of pH of the intergel system of polyacrylic acid and poly-2-methyl-5-vinylpyridine on the molar ratios of hydrogels.

The swelling coefficients of the hydrogels were  $K_{sw}(\text{gPAA})=10.1$  and  $(\text{gP2M5VP}) = 0.46$ . These data indicate a high degree of ionization of both hydrogels at this stage. The concentration of  $\text{H}^+$  and  $\text{OH}^-$  ions is proportional to the concentration of the hydrogels and their degree of swelling. In the  $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$  solution, at a certain ratio of acidic to basic hydrogels, we observed the highest swelling coefficient ( $K_{sw}$ ) at a ratio of 1:5 after 48 hours compared to the initial hydrogels, indicating a high degree of ionization of the hydrogel at this stage.



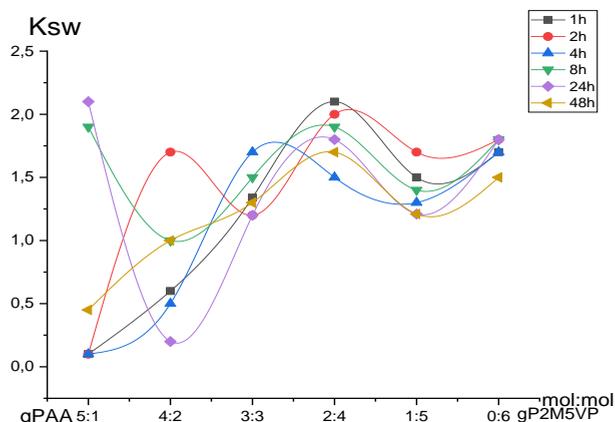
**Figure 3**– Dependence of the degree of swelling of gPAA in the presence of hydrogel P2M5VP on the molar ratio of hydrogels.

The high degree of  $\text{H}^+$  ionization is explained by the excess of polyacid in the solution and the high dissociation of  $\text{COOH}$  groups. The figure shows that the swelling coefficient ( $K_{sw}$ ) increases with time, and after a certain time, swelling

ceases. The swelling coefficient ( $K_{sw}$ ) of the polyacrylic acid hydrogel in the intergel system in the presence of poly(2-methyl-5-vinylpyridine) demonstrates that the volumetric and gravimetric properties of the hydrogels change during long-distance interaction. A sharp increase in the size of the poly(2-methyl-5-vinylpyridine) gel is observed in the ratios of 4:2 and 3:3. As a result of long-distance interaction in the  $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$  solution, a sharp decrease in the swelling coefficient is observed in the ratio of 3:3, which is due to an insufficient swelling rate and low concentrations of the main groups.

gPAA:gP2M5VP Figure 4 shows the dependence of the swelling degree ( $K_{sw}$ ) of poly-2-methyl-5-vinylpyridine gel on time at different time intervals in the intergel system. Unlike the cross-linked hydrogel gPAA, the hydrogel P2M5VP exhibits a stepwise change in the swelling degree ( $K_{sw}$ ) over time. The maximum swelling of the gel gP2M5VP is observed at ratios of 5:1 and 4:2, which is evident from the change in the swelling coefficient of poly-2-methyl-5-vinylpyridine gel with a certain time interval, which increases to a minimum value of 0.1 and a maximum value of 2.1, as evidenced by the change in the volumetric-gravimetric properties of poly-2-methyl-5-vinylpyridine hydrogel and polyacrylic acid hydrogel.

The maximum swelling values of the hydrogels are also maintained at a ratio of 2:4. This is explained by the neutralization of hydroxyl ions by protons and a very low degree of dissociation of carboxyl groups while maintaining a high concentration of positive ions in the solution. gPAA:gP2M5VP hydrogels in the intergel system showed a minimum value at a ratio of 4:2 in a  $\text{HAuCl}_4 \cdot 4\text{H}_2\text{O}$  solution, which is due to the insufficient swelling rate of the main groups and their low concentration.



**Figure 4** – Dependence of the degree of swelling of gP2M5VP in the presence of gPAA hydrogel on the molar ratio of hydrogels.

Thus, the poly(2-methyl-5-vinylpyridine) hydrogel changes its volumetric and gravimetric properties compared to the polyacrylic acid hydrogel. Overall,

( $K_{sw}$ ) increases from 0.8 to 3 during the conformational rotation of the internodal unit ( $K_{sw}$ ). That is, the swelling coefficient increases by 3.8 times. The minimal reduction in swelling in this region is associated with the formation of an intramolecular bond of the  $\geq NH^+ \dots N \leq$  type or the formation of an intramolecular association. As the gPAA concentration in the aqueous medium increases, the swelling process intensifies, and  $K_H$  increases significantly. In this case, the local conformational change and the inverse arrangement of interstitials are explained by an increase in chain charge density, which leads to the rupture of intramolecular bonds.

#### 4. Conclusion

The results of numerous studies and analyzes, depending on the amount and volume of cross-linked polymers used in the synthesis, show that mutual activation of interpolymer systems of polyacrylic acid and poly-2-methyl-5-vinylpyridine leads to a significant increase in their sorption capacity. Experimental data on the specific electrical conductivity of the solution, pH of the medium and the swelling coefficient of the hydrogels showed that the presence of long-range interactions between acrylic acid and 2-methyl-5-vinylpyridine hydrogels has a significant effect on the initial polymer network and the physicochemical properties of the solution; the presence of areas of abnormally high electrical conductivity at the lowest gPAA:gP2M5VP ratio indicates the presence of highly concentrated charged ions; in an equimolar gPAA:gP2M5VP ratio, association of  $H^+$  and  $OH^-$  ions with each other and intermolecular duplication of hydrogels occurs; As a result of long-distance interaction, additional activation of the hydrogels occurs, i.e., the interstitial chain acquires an additional charge without a negative ion; long-distance interaction leads to a conformational change in the interstitial chain in both hydrogels, which causes their additional swelling; at a certain ratio of gPAA:gP2M5VP, a zone of intramolecular association formation was identified in the gP2M5VP hydrogel, which leads to rotation of the polymer network.

**Funding:** This research was supported by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP26195783).

**Conflicts of Interest:** The authors declare no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

**ПОЛИАКРИЛ ҚЫШҚЫЛЫ ЖӘНЕ ПОЛИ-2-МЕТИЛ-5-ВИНИЛПИРИДИН ГИДРОГЕЛЬДЕРІ НЕГІЗІНДЕ ҚҰРЫЛҒАН ИНТЕРГЕЛЬДІ ЖҮЙЕЛЕРДІҢ АЛТЫН ИОНДАРЫНА ҚАТЫСТЫ ӘРЕКЕТТЕСУ ЕРЕКШЕЛІКТЕРІ**

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**Түйіндеме.** *Кіріспе.* Полиакрил қышқылы мен поли-2-метил-5-винилпиридин интерполимерлік жүйесінде екі гидрогелдің қашықтықтан әрекеттесуі нәтижесінде торлану дәрежесі әр түрлі полимерлік гидрогелдердің өзара активтенуінің өзгерісі анықталып, олардың алтын иондарының сорбциялау үдерісіне тигізетін әсері зерттелді [1,2]. *Жұмыстың мақсаты* поли-2-метил-5-винилпиридин және полиакрил қышқылы негізінде құрылған интергельді жүйелердің алтын иондарына қатысты сорбциялық қабілетін зерттеу [3,4]. *Алынған нәтижелер.* гПАК:гП2М5ВП интерполимерлі жүйелерінің максималды сорбция дәрежесі 48 сағат әрекеттесу кезінде полимерлердің 5:1 молярлық қатынастарында алтын иондарының концентрациясы 0.645 моль/л мөлшеріне дейін жоғарлап, ары қарай біртіндеп 0.575 моль/л азайған. ПАК:П2М5ВП интергельді жүйесінің рН ортасының максималды мәндері 3:3 қатынасында байқалады, сәйкесінше рН 2.99 тең. Ал минимум 2:4 қатынасында рН мәні 2.96 тең. Жалпы ісіну дәрежесінің ( $K_i$ ) түйінаралық буын конформациялық айналу үрдісінде ( $K_i$ ) 0.8 ден 3-ке дейін өседі. *Қорытынды.* Көптеген зерттеулер мен талдаулардың нәтижелері синтездеу барысындағы пайдаланған сызықтық полимерлермен ондағы қосымша реагенттердің мөлшеріне, көлеміне қарай алынған мәліметтер полиакрил қышқылы мен поли-2-метил-5-винилпиридин интерполимерлі жүйелерінің өзара активтенуі олардың сорбциялық қабілетінің айтарлықтай жоғарылауына әкелетінін көрсетеді.

**Түйін сөздер:** интерполимерлік жүйе, иониттер, полиакрил қышқылы, поли-2-метил-5-винилпиридин, қашықтықтан өзара әрекеттесу, гидрогельдер, өзара активтену, сорбция.

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## ОСОБЕННОСТИ ВЗАИМОДЕЙСТВИЯ ИНТЕРГЕЛЕВЫХ СИСТЕМ НА ОСНОВЕ ПОЛИАКРИЛОВОЙ КИСЛОТЫ И ПОЛИ-2-МЕТИЛ-5-ВИНИЛПИРИДИНА С ИОНАМИ ЗОЛОТА

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**Резюме.** *Введение.* В результате дистанционного взаимодействия двух гидрогелей в интерполимерной системе полиакриловой кислоты и поли-2-метил-5-винилпиридина было определено изменение взаимной активации полимерных гидрогелей с различной степенью сшивания, а также изучено их влияние на процесс сорбции ионов золота [1,2]. *Целью работы* было изучение сорбционной способности интергелевых систем на основе поли-2-метил-5-винилпиридина и полиакриловой кислоты по отношению к ионам золота [3,4]. *Полученные результаты.* Максимальная степень сорбции интерполимерных систем гПАК:гП2М5ВП увеличилась до 0.645 моль/л при молярном соотношении полимеров 5:1 в течение 48 часов взаимодействия, а затем постепенно снизилась до 0.575 моль/л. Максимальные значения рН среды интергелевой системы гПАК:гП2М5ВП наблюдались при соотношении 3:3, соответственно, рН 2,99. А при минимальном соотношении 2:4 значение рН составляет 2,96. Общая степень набухания ( $K_n$ ) увеличивается с 0.8 до 3 в процессе конформационного вращения междоузлового звена. *Вывод.* По результатам исследований изучены электрохимические свойства гидрогелей полиакриловой кислоты и поли-2-метил-5-винилпиридина в интерполимерной системе и определены оптимальные молярные соотношения. Таким образом, в результате проведенных исследований: полученные экспериментальные данные по удельной электропроводности раствора,

pH среды и коэффициенту набухания гидрогелей показали, что наличие дистанционного взаимодействия между акриловой кислотой и 2-метил-5-винилпиридином гидрогелей оказывает существенное влияние на исходную полимерную сетку и физико-химические свойства раствора.

**Ключевые слова:** интерполимерная система, иониты, гидрогели, полиакриловой кислота, поли-2-метил-5-винилпиридин, дистанционное взаимодействие, взаимная активация, сорбция.

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**STUDY OF THE SURFACE-BULK PROPERTIES OF AN ACRYLIC DISPERSION IN THE PRESENCE OF AN AMINE-CONTAINING ADDITIVE**

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**Abstract.** *Introduction.* Waterborne coating materials based on polymer dispersions are regarded as a priority direction in coating technology due to reduced environmental impact and increasingly stringent requirements for production and application safety. However, aqueous acrylic dispersions retain technological limitations associated with film formation, interfacial interactions, and resistance to moisture exposure. One promising approach to improving performance is the incorporation of amine-containing additives capable of regulating charge–associative processes and the structure of the interfacial layer. The aim of this study was to determine the effect of an amine-containing additive on the surface–bulk properties of an aqueous acrylic dispersion and to identify the factors governing changes in interfacial activity and structural organization within the bulk phase. The research objectives included a comparative analysis of the “water–additive” system and the “acrylic dispersion–water–additive” system, as well as an examination of the mechanisms responsible for the redistribution of protonated and less ionized forms of the additive between the bulk phase and the phase boundary. *Methods.* Interfacial characteristics were evaluated using an ACAM series instrument equipped with video recording of the droplet profile and calculation of interfacial parameters by drop shape analysis based on the Young–Laplace equation. Bulk properties were monitored by conductometry (specific electrical conductivity) and potentiometry with pH measurements while varying the content of the amine-containing additive polyethylene polyamine. *Results and discussion.* It was shown that in an aqueous medium the additive exhibits limited interfacial activity. In the presence of an acrylic dispersion, the interfacial effect is enhanced, indicating the involvement of the additive in specific interactions with functional groups of the film-forming polymer and a change in its distribution between the surface and the bulk phase.

*Conclusion.* The results obtained substantiate the use of polyethylene polyamine as a tool for controlling interfacial and bulk processes in aqueous acrylic dispersions and may be applied in the development of waterborne coating systems.

**Keywords:** waterborne coating materials; acrylic dispersion; amine-containing additive; interfacial interactions; surface–bulk properties.

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**Citation:** Dyuryagina A.N., Ostrovnaya D.Yu., Byzova Yu.S., Lutsenko A.A. Study of the surface–bulk properties of an acrylic dispersion in the presence of an amine-containing additive. *Chem. J. Kaz.*, **2026**, 1(93), 69-78. DOI: <https://doi.org/10.51580/2026-1.2710-1185.07>

## 1. Introduction

In recent years, a steady global trend toward replacing solvent-borne coatings with water-dispersible systems has been observed [1]. This transition is primarily driven by increasingly stringent environmental regulations on volatile organic compound (VOC) emissions, corresponding changes in technical standards, and advances in polymer synthesis technologies that enable the design of materials with tailored properties [2].

According to Coherent Market Insights, in 2025 waterborne coatings accounted for approximately 40.5% of the total global paint and coatings production volume, reflecting a systematic shift in market demand toward environmentally safer systems with reduced emissions of hazardous substances [3]. Furthermore, estimates by Precedence Research indicate that the global market volume of waterborne coatings reached USD 96.15 billion in 2025, with a compound annual growth rate (CAGR) of 5.5% [3,4].

However, replacing organic solvents with water presents several technological challenges, as water exhibits fundamentally different physicochemical properties compared with organic solvents [5]. In addition, most conventional film-forming agents are insoluble in water, and only a limited number of water-soluble film formers are capable of producing transparent (true or molecular) solutions in aqueous media [6]. For this reason, aqueous dispersions of polymers and oligomers have become the most widely used systems, among which acrylic dispersions occupy a leading position [7].

Coatings based on acrylic film-forming agents are characterized by high weather resistance, including light, thermal, and chemical stability, as well as resistance to contamination and to acidic and alkaline environments [8,9]. At the same time, such coatings typically do not allow the production of high-solids formulations and may exhibit insufficient mechanical strength, limited water resistance, and relatively low corrosion resistance [10-12].

One of the main approaches to the targeted modification of the properties of polymer composite materials and their coatings is the use of additives exhibiting surfactant activity [13]. The selection of polyethylene polyamine as an additive in the present study was determined by two factors. First, the amphiphilic nature of its macromolecules, resulting from the presence of polar amine groups within a mixture of high-molecular-weight amines (characterized by the amine number) and hydrocarbon fragments, provides pronounced interfacial activity and the ability to participate in specific interactions within aqueous dispersion systems. Second, the additive ( $M = 5000$ ) is water-soluble, which facilitates its incorporation into the aqueous phase [14-16].

From a physicochemical standpoint, modification induced by differences in the thermodynamic characteristics of the film-forming polymer and the additive is accompanied by concentration fluctuations of the introduced substance between the bulk phase of the aqueous polymer system and its interfacial surface energy at the air interface, primarily due to the development of adsorption processes. The variety of processes occurring in the bulk and interfacial phases differs only

slightly in terms of the energy required for their initiation [17]. The narrow energy range within which various states of the initial and modified forms are realized implies the necessity for precise and selective control of these processes in order to achieve the desired effects while preventing undesirable outcomes [18].

At the same time, understanding the physicochemical processes occurring in aqueous polymer dispersions is also important from a practical perspective. Changes in surface tension and electrokinetic characteristics of such systems can influence pigment wetting, dispersion stability, and film formation processes, which ultimately affect the performance properties of coatings, including adhesion, mechanical strength, and protective efficiency [19]. Therefore, the study of the influence of surface-active additives on the interfacial and bulk properties of aqueous polymer systems is relevant not only for fundamental research but also for the rational design of waterborne coating formulations.

In this context, it was considered appropriate to determine the effect of the additive concentration on the regularities of processes occurring both in the bulk of the aqueous acrylic dispersion (dissociation processes, hydrogen ion concentration, pH) and at its interface with air (surface tension).

## 2. Experimental Section

The objects of investigation were an aqueous acrylic dispersion based on the glossy acrylic varnish “Solax” and an amine-containing additive, polyethylene polyamine (PEPA), TU 2413-357-00203447-99. The studies were carried out using model compositions of the “water–PEPA” type and ternary systems of the “film former–water–PEPA” type, with the additive concentration varied within the range of 0–1.2 % in increments of 0.2 %. All solutions and compositions were prepared immediately prior to measurement and examined at a temperature of 295 K.

PEPA solutions of the required concentration were prepared individually: a weighed portion of the additive was measured on an analytical balance and dissolved in a specified volume of distilled water under stirring until complete homogenization. The ternary compositions were obtained by introducing PEPA into a calculated volume of the acrylic varnish “Solax” under stirring until a visually homogeneous state without observable aggregates was achieved. According to preliminary kinetic experiments, equilibrium in the investigated systems was established within 30 min; therefore, all subsequent measurements were performed after a standardized equilibration period of this duration.

The surface tension of the investigated systems was determined using an automated ACAM instrument by the pendant drop method (Figure 1). A droplet was formed at the tip of a dosing needle, its profile was recorded using a video system, and the surface tension was calculated by drop shape approximation in the instrument software based on the Young-Laplace equation. Measurements were carried out in parallel, and the results were averaged.



**Figure 1** – Image of a water droplet dispensed for surface tension determination.

The specific electrical conductivity was measured using a “Multitest” conductometer. Prior to measurements, the instrument was calibrated with a standard solution. The measuring cell was rinsed with distilled water and with the test sample, after which conductivity was recorded once the readings stabilized at 295 K. The final value was taken as the average of three measurements.

The hydrogen ion concentration (pH) was determined using a “Multitest” potentiometer equipped with a combined glass electrode. Before measurements, calibration was performed using buffer solutions. The electrode was rinsed with distilled water and the test sample, and the pH value was recorded after stabilization of the readings at 295 K.

### 3. Results and Discussion

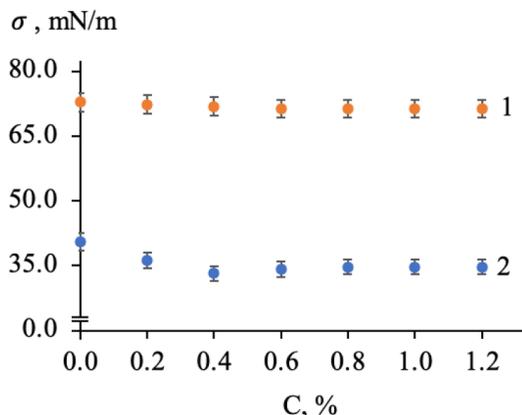
The results of the study are presented sequentially.

#### 3.1. Surface Properties of Binary “Water–PEPA” Systems at the Air Interface

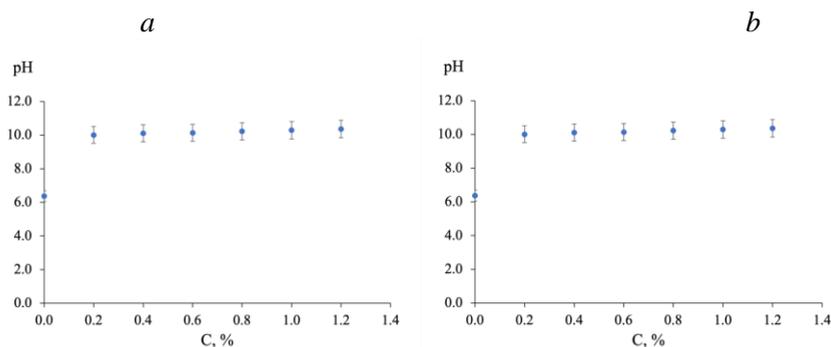
The surface tension isotherm ( $T = 295$  K) of aqueous polyethylene polyamine solutions at the air interface demonstrates only minor changes in the liquid-gas surface tension ( $\sigma_{l-g}$ ) (Figure 2). The maximum surface tension depression ( $\Delta\sigma = 1.49$  mN/m) was observed at a PEPA concentration of 0.6 %. Beyond this concentration range ( $C > 0.6$  %), the surface tension remains essentially constant ( $\sigma = 71.28$  mN/m).

The weak surface activity of polyethylene polyamine compared with classical additives is due to the peculiarities of its chemical composition and structure, characterized by a large number of amine groups of different types ( $-\text{NH}_2-$  and  $-\text{NH}-$ ) and short hydrophobic fragments ( $-\text{CH}_2-\text{CH}_2-$ ) [20,21]. The shift of the hydrophilic–lipophilic balance (HLB) toward polar groups reduces the tendency of PEPA to accumulate at the water–air interface. The quantitative dissociation characteristic of polyethylene polyamine, resulting from protonation of amine groups by water (accompanied by the formation of hydroxide ions), promotes hydrophilization and, consequently, the preferential localization of hydrated species within the bulk phase. The increase in the fraction of ionized

forms is clearly reflected in the observed changes in electrical conductivity (Figure 3a) and hydrogen ion concentration (Figure 3b) of aqueous polyethylene polyamine solutions.



**Figure 2** – Surface tension isotherms ( $T = 295\text{ K}$ ) for the “water-PEPA” (1) and “film former-water-PEPA” (2) systems.

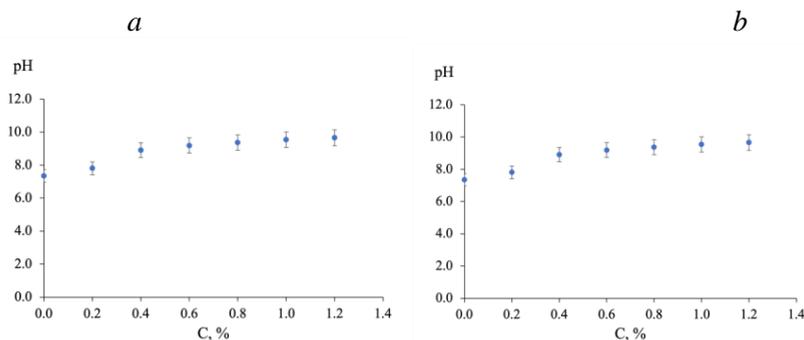


**Figure 3** – Effect of polyethylene polyamine concentration in the binary “water-PEPA” system on: (a) specific electrical conductivity; (b) hydrogen ion concentration (pH).

As the polyethylene polyamine content increases up to 1.00–1.20 %, a continuous rise in solution conductivity (from 4.90 to 368.00  $\mu\text{S}/\text{cm}$ ) and pH (from 6.38 to 10.36) is observed. The pH shifts from near-neutral conditions ( $\text{pH} = 6.38$ ) to an alkaline medium ( $\text{pH} \geq 10$ ) as hydroxide groups accumulate in the aqueous phase, indicating a substantial increase in the fraction of ionized species.

### 3.2. Surface Properties of Ternary “Film Former–Water–Additive” Systems at the Air Interface

Upon introduction of PEPA into the film-forming solution, a different behavior is observed (Figure 4a and b).



**Figure 4** – Effect of polyethylene polyamine concentration in the ternary “film former-water-PEPA” system on: (a) specific electrical conductivity; (b) hydrogen ion concentration (pH).

In contrast to the behavior observed in the “water-PEPA” system, the increase in hydrogen ion concentration (pH) in the “film former-water-PEPA” system was accompanied by the opposite effect – a decrease in electrical conductivity as the additive concentration increased (Fig. 4a and b).

Moreover, the absolute values of conductivity ( $\chi$ ) in the ternary system were tens of times lower than those recorded for the binary system. This is confirmed by the relative conductivity values  $\omega$  (1):

$$\omega = \chi_1 / \chi_2, \quad (1)$$

where  $\chi_1$  is the electrical conductivity of the binary “water-additive” system, and  $\chi_2$  is the electrical conductivity of the ternary “film former-water-additive” system.

**Table 1** – Effect of additive concentration on the ratio of conductivity values  $\omega$

$C_{PEPA}, \%$	0.2	0.4	0.6	0.8	1.0	1.2
$\omega$	30.54	43.63	56.76	64.52	74.05	81.06

The resulting effect of acrylic binder macromolecules in the “film former-water-PEPA” system, in which the water content is 69 %, on the surface activity of polyethylene polyamine is clearly illustrated by the surface tension isotherm (Fig. 1, curve 2). In the region of low additive concentrations ( $C_{PEPA} \leq 0.4 \%$ ), the polymer present in the composition induces the migration of non-ionized forms of the polyelectrolyte to the air interface. This is evidenced by the observed decrease in specific surface energy. The maximum reduction in surface tension ( $\Delta\sigma = 14.56 \text{ mN/m}$ ) was recorded at  $C_{PEPA} = 0.4 \%$ . This decrease in specific surface energy was observed in a weakly alkaline medium (pH = 8.91) at a specific electrical conductivity of 5.57 mS/cm (Fig. 3a and b).

Further addition of polyethylene polyamine (above 0.4 %) promoted its preferential localization in the bulk liquid phase rather than at the air interface:

instead of a continued decrease, the surface tension remained constant at  $34.03 \pm 0.07$  mN/m (plateau on curve 2, Fig. 1). The appearance of a plateau at higher PEPA concentrations indicates the development of association processes, accompanied by a decrease in conductivity values (Fig. 3a) and an increase in pH (Fig. 3b).

Spontaneous association of the acrylic film-forming macromolecules and the polyelectrolyte upon reaching a critical association concentration (onset of the plateau on curve 2, Fig. 1) is likely driven by electrostatic interactions between ionized species, hydrogen bonding, and van der Waals forces. As the additive concentration increases further, the degree of association rises and the mobility of larger associates decreases, which accounts not only for the absence of surface activity ( $\sigma_{l-g} = \text{const}$ ) but also for the observed reduction in specific electrical conductivity (Fig. 3a).

#### 4. Conclusion

In the binary “water–PEPA” system, polyethylene polyamine exhibits weak interfacial activity due to its quantitative dissociation resulting from protonation of amine groups by water, accompanied by hydroxide ion formation. As the PEPA concentration increases to 1.00–1.20 %, a steady rise in conductivity from 4.90 to 368.00  $\mu\text{S}/\text{cm}$  and a simultaneous increase in pH from 6.38 to 10.36 are observed.

In the ternary “film former–water–PEPA” system, the reduced extent of PEPA dissociation due to the lower solvent content (69 %) enhances its surface activity at the air interface. The maximum reduction in surface tension ( $\Delta\sigma = 14.56$  mN/m) was recorded at a PEPA concentration of 0.4 %. The highest surface activity effect was achieved in the weakly alkaline region (pH = 8.91) at a specific electrical conductivity of 5.57 mS/m.

**Conflict of interest:** The authors declare that there is no conflict of interest between the authors that requires disclosure in this article.

#### ҚҰРАМЫНДА АМИН БАР ҚОСПАНЫҢ ҚАТЫСУЫМЕН АКРИЛ ДИСПЕРСИЯСЫНЫҢ БЕТТІК-КӨЛЕМДІК ҚАСИЕТТЕРІН ЗЕРТТЕУ

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**Түйіндемe.** *Кіріспе.* Полимерлік дисперсиялар негізіндегі су арқылы сұйылтылатын лак-бояу материалдары экологиялық жүктемені төмендету және өндіру мен қолдану қауіпсіздігіне қойылатын талаптардың артуына байланысты жабындарды дамытудың басым бағыты ретінде қарастырылады. Сонымен қатар су негізіндегі акрил дисперсиялары плёнка түзілуі, фазалар аралық өзара әрекеттесулер және ылғалдың әсеріне төзімділікке байланысты технологиялық шектеулерін сақтайды. Қасиеттерді жақсартудың перспективалы бағыттарының бірі – зарядтық-ассоциациялық процестерді және фазалар аралық қабаттың құрылымын реттеуге қабілетті аминқұрамды беткі-белсенді заттарды енгізу. *Жұмыстың мақсаты* су негізіндегі акрил

дисперсиясының беткі және көлемдік қасиеттеріне аминқұрамды қоспаның әсерін анықтау және фазалар аралық белсенділік пен компоненттердің көлемде құрылымдануының өзгеруін айқындайтын факторларды белгілеу болды. Зерттеу міндеттеріне «су–қоспа» және «акрил дисперсиясы–су–қоспа» жүйелерінің мінез-құлқын салыстыру, сондай-ақ протондалған және аз нондалған қоспа формаларының көлем мен фазалар аралық шекара арасында қайта бөліну себептерін талдау кірді. *Әдістері.* Фазалар аралық сипаттамалар АСАМ сериялы аспаптарда тамшы профилін бейнетіркеу және Юнг-Лаплас теңдеуіне негізделген тамшы пішінін аппроксимациялау әдісі арқылы есептелді. Көлемдік қасиеттер кондуктометрия (меншікті электрөткізгіштік) және потенциометрия әдістерімен, аминқұрамды қоспа – полиэтиленполиаминнің мөлшерін өзгерте отырып, сутектік көрсеткішті (рН) өлшеу арқылы бақылауға алынды. *Нәтижелер мен талқылау.* Су ортасында қоспаның фазалар аралық белсенділігі шектеулі екені көрсетілді. Акрил дисперсиясының қатысуында фазалар аралық әсердің күшеюі байқалады, бұл қоспаның плёнка түзушінің функционалдық топтарымен спецификалық өзара әрекеттесулерге тартылуын және оның бет пен көлем арасында таралуының өзгеруін көрсетеді. *Қорытынды.* Алынған нәтижелер полиэтиленполиаминді су негізіндегі акрил дисперсияларындағы фазалар аралық және көлемдік процестерді басқарудың тиімді құралы ретінде қолдануды негіздейді және су арқылы сұйылтылатын жабындарды әзірлеуде пайдаланылуы мүмкін.

**Түйін сөздер:** су-дисперсиялы лак-бояу материалдары; акрил дисперсиясы; аминқұрамды қоспа; фазалар аралық өзара әрекеттесулер; беткі-көлемдік қасиеттер.

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## ИССЛЕДОВАНИЕ ПОВЕРХНОСТНО-ОБЪЕМНЫХ СВОЙСТВ АКРИЛОВОЙ ДИСПЕРСИИ В ПРИСУТСТВИИ АМИНОСОДЕРЖАЩЕГО АДДИТИВА

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**Резюме.** *Введение.* Водоразбавляемые лакокрасочные материалы на основе полимерных дисперсий рассматриваются как приоритетное направление развития покрытий вследствие снижения экологической нагрузки и повышения требований к безопасности производства и применения. Вместе с тем водные акриловые дисперсии сохраняют технологические ограничения, связанные с формированием плёнки, межфазными взаимодействиями и устойчивостью к воздействию влаги. Одним из перспективных путей улучшения свойств является введение аминоксодержащих поверхностно-активных веществ, способных регулировать зарядово-ассоциативные процессы и структуру межфазного слоя. *Целью работы* являлось установление влияния аминоксодержащей добавки на поверхностно-объёмные свойства водной акриловой дисперсии и выявление факторов, определяющих изменение межфазной активности и структурирования компонентов в объёме. *Задачи исследования* включали сопоставление поведения системы «вода–аддитив» и системы «акриловая дисперсия–вода– аддитив», а также анализ причин перераспределения протонизированных и менее ионизированных форм добавки между объёмом и границей раздела фаз. *Методы:* межфазные характеристики оценивали на установке серии приборов АСАМ с видеорегистрацией профиля капли и расчётом параметров межфазного состояния методом аппроксимации формы капли на основе уравнения Юнга-Лапласа. Объёмные свойства контролировали методами кондуктометрии (удельная электропроводность) и потенциометрии с измерением водородного показателя (рН) при варьировании содержания аминоксодержащей добавки полиэтиленполиамин. *Результаты и обсуждение:* показано, что в водной среде добавка

проявляет ограниченную межфазную активность. В присутствии акриловой дисперсии межфазный эффект усиливается, что указывает на вовлечение добавки в специфические взаимодействия с функциональными группами плёнкообразующего и на изменение её распределения между поверхностью и объёмом. *Заключение.* Полученные результаты обосновывают использование полиэтиленполиамина как инструмента управления межфазными и объёмными процессами в водных акриловых дисперсиях и могут быть применены при разработке водоразбавляемых покрытий.

**Ключевые слова:** водно-дисперсионные лакокрасочные материалы; акриловая дисперсия; аминоксодержащий аддитив; межфазные взаимодействия, поверхностно-объёмные свойства.

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## EXTRACTION OF BIODEGRADABLE SURGICAL THREADS BASED ON POLYLACTIDE

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**Abstract.** Conventional surgical sutures should be removed after wound healing, because they cause additional pain and discomfort for the patients. Polylactide (PLA) is an aliphatic polyester derived from the renewable resources, which is biocompatible and biodegradable; however, its relatively high stiffness can limit its surgical applications. This study has the purpose to develop biodegradable surgical sutures based, on PLA and poly(vinyl alcohol) (PVA), and to investigate their physicochemical, mechanical, and biodegradation properties. To reduce PLA stiffness, PLA has been blended with PVA to form composite fibers. The fibers have been prepared from the polymer blends, using ultrasonic treatment to improve mixing. The blend homogeneity has been assessed, using UV-Vis spectroscopy, chemical structure has been characterized by the IR spectroscopy, and surface morphology has been investigated by scanning electron microscopy (SEM). The SEM has revealed changes in the surface morphology and gradual degradation of the fibers over a 16- week period, which has also been supported by the mass-loss measurements in soil. The mechanical properties have been determined according to ASTM D2256. AN incorporation of PVA has increased fiber extensibility and elasticity, and the PLA-PVA composition (20:80 wt.%) has shown the most favorable mechanical performance among the tested formulations. Overall, the results suggest that the PLA-PVA composite fibers are promising candidates for absorbable surgical suture materials.

**Keywords:** polylactide, polyvinyl alcohol, surgical suture, biodegradable, composite fiber, surgical fibers

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**Citation:** R.K. Rakhmetullaeva, D. Beibit, A.K. Zholdasbayev, E.A. Tussupkaliyev, A.K. Toktabayeva, Z.N. Kainarbayeva. Extraction of biodegradable surgical threads based on polylactide. *Chem. J. Kaz.*, 2026, 1(93), 79-92. DOI: <https://doi.org/10.51580/2026-1.2710-1185.08>

## 1. Introduction

The biodegradable absorbable sutures have become essential in the surgical practice, since they eliminate the need to remove and minimize the tissue reaction. Polylactide (PLA) is a widely used biodegradable polymer, known for its biocompatibility and high strength. PLA-based sutures gradually hydrolyze into harmless products ( $\text{CO}_2$  and  $\text{H}_2\text{O}$ ) in vivo, avoiding the pain and complications of suture removal. They have been successfully applied in many types of surgeries, including internal organ operations and cosmetic procedures. However, monofilament PLA sutures can be relatively stiff and have a long resorption period, which may not meet all surgical requirements. To improve flexibility and performance, blending PLA with another biopolymer is a promising approach [1–5].

Polyvinyl alcohol (PVA) is a biodegradable, water-soluble polymer that has found use in medicine (e.g., as a component of absorbable surgical threads, implants, and drug delivery systems) due to its biocompatibility and flexibility. Combining PLA with PVA could yield a composite fiber that leverages the strength of PLA and the flexibility of PVA. A major challenge in creating a PLA/PVA blended fiber is the incompatibility of the two polymers – they do not share a common solvent and can interact to form complexes that cause phase separation. Recent research has explored multi-block copolymers and composite fibers to address such challenges. In this study, we employ an ultrasonic solution blending method to produce a PLA–PVA block copolymer fiber and investigate its physicochemical properties as a potential biodegradable surgical suture. The work focuses on developing improved PLA-based biodegradable fibers and examining their mechanical properties and biodegradability. [6–7].

## 2. Materials and Methods

Poly lactide (PLA) and polyvinyl alcohol (PVA) were used as the base polymers for fiber preparation. Tetrahydrofuran (THF) (as a solvent for PLA) and water (as a solvent for PVA) were used to dissolve the polymers. All reagents were of analytical grade [4–7].

**Preparation of PLA–PVA Solution:** To obtain a homogeneous polymer blend, a cosolvent approach was adopted. PLA was dissolved in THF to make a 1.5wt.% solution, and PVA was dissolved in water to make a 3wt.% solution. The PVA solution was gradually added to the PLA solution under continuous stirring. A preliminary solubility test was performed by mixing varying proportions of the two solutions and monitoring clarity (UV–Vis spectroscopy was used to monitor solution transmittance). It was found that adding up to approximately 10wt.% of the PVA solution (water content) to the PLA/THF solution did not cause turbidity. Therefore, the final PVA:PLA mass ratio was kept at 90:10 (i.e., 10wt.% PLA, 90wt.% PVA in the mixture) to ensure a homogeneous blend without precipitation [8,12].

**Ultrasonic Treatment and Block Copolymer Formation:** The combined PLA/PVA solution (at 90:10 ratio) was subjected to ultrasonic treatment to induce

block copolymer formation between PLA and PVA. Ultrasonication was carried out for a fixed duration (20minutes) at room temperature, using an ultrasonic bath (35kHz) to promote polymer-polymer interactions. This process yields a PLA–PVA block copolymer in the solution. The resulting mixture was then centrifuged to isolate any formed polymer complex (precipitate). The precipitate was collected and washed to remove the unbound homopolymer. [9–10].

**Isolation and Purification:** The synthesized PLA–PVA product was purified by the selective solvent extraction. The precipitated polymer was first soaked in the fresh THF for 24 hours to dissolve and remove any unreacted PLA homopolymer. Subsequently, the remaining solid was soaked in water for 24 hours to remove any unreacted PVA. The recovered solid block copolymer was dried to constant weight in a vacuum oven. The yield of the block copolymer was determined gravimetrically by comparing the dried mass of the product to the initial total polymer mass.

**Solubility and Swelling Tests:** To evaluate the behavior of the PLA–PVA material in various media (relevant to bodily fluids and processing solvents), the pieces of the dried copolymer sample were immersed in different liquids: distilled water, physiological saline (0.9% NaCl), dimethylformamide (DMF), ethanol, and n-hexane. Swelling or dissolution was observed qualitatively after 24 hours at the room temperature, and categorized as “no change (–)”, “slightly swollen”, or “fully swollen/dissolved.”

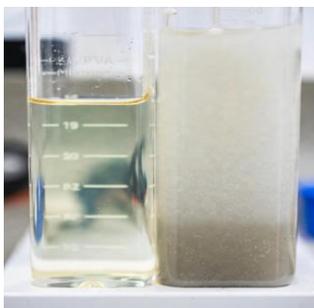
### 3. Results and Discussion

#### *Obtaining of biodegradable filaments, based on polylactide, and study of their physicochemical properties*

**The Formation of Homogeneous PLA/PVA Blends:** The initial challenge was to find a common solvent system for PLA and PVA. PLA is soluble in organic solvents like THF, whereas PVA is soluble in water, but not in THF. We gradually combined the two solutions while monitoring clarity. It was observed that up to 10wt.% of PLA (in THF) could be introduced into the PVA aqueous solution (or vice versa) without phase separation. Beyond a PLA fraction of about 10%, the mixture turned cloudy and a precipitate formed. This cloud point indicates the formation of an interpolymer complex between PLA and PVA when one polymer’s concentration becomes too high. Figure 1 shows the appearance of the polymer mixture: at a PVA:PLA ratio of 90:10 (by mass) the solution remains transparent, whereas higher PLA content leads to precipitation. The successful blending at 90:10 suggests that a block copolymer or complex forms in small amounts but remains colloiddally stable at lower PLA content [8, 11–13].

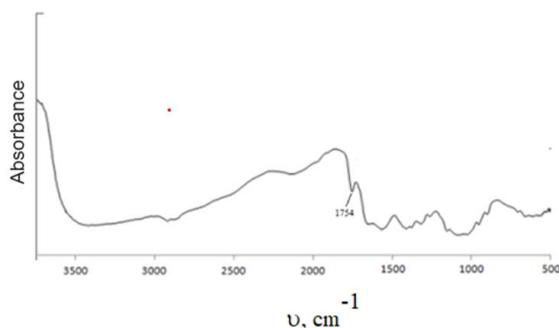
This finding guided the preparation of the fibers. The block copolymer formation during ultrasonication was further confirmed by FTIR spectroscopy. In the FTIR spectrum of the PLA–PVA precipitate (complex), the characteristic absorption bands of PVA (such as the O–H stretching around  $3300\text{cm}^{-1}$ ) were greatly diminished or no longer visible, and the intensity of the PLA carbonyl band ( $\sim 1750\text{cm}^{-1}$ ) was significantly reduced compared to pure PLA. This

suggests strong intermolecular interactions (likely hydrogen bonding) between PVA and PLA chains in the complex.



**Figure 1** - Visual appearance of the PLA/PVA polymer mixture. The solution remains clear up to the PLA fraction of ~10 wt.% (left), while in case of the higher PLA content (right) the mixture becomes cloudy due to the polymer-polymer complex formation.

The disappearance of the distinct PVA peaks in the blend spectrum indicates that the PVA hydroxyl groups are involved in bonding with PLA, contributing to the formation of the PLA–PVA block copolymer. Figure 2 displays the IR spectra of pure PVA, pure PLA, and the PLA–PVA complex. In the complex, absorption peaks unique to each homopolymer are attenuated, confirming the successful integration of the two polymers at a molecular level [8, 11, 13].



**Figure 2** - FTIR spectra of pure PVA, pure PLA, and the PLA–PVA block copolymer. The spectrum of the PLA–PVA product shows the reduction of PVA's O–H bands and PLA's C=O band, indicating the formation of a combined polymer complex.

After the ultrasonic synthesis and solvent extraction steps, the yield of the PLA–PVA block copolymer was high. Most of the PVA and PLA were successfully linked or entangled in the precipitated product. A small fraction of PLA remained unreacted (dissolved in THF and removed in the first extraction). The yields for different initial PLA ratios are presented in Table 1. As the initial PLA content in the mixture increased from 10% to 30%, the fraction of unreacted PLA also increased slightly (from 4.3% to 7.4%), and consequently the

copolymer yield decreased from 95.7% to 92.6%. This trend is expected because higher PLA content makes it more challenging for all PLA chains to find PVA partners to bond with, leaving some PLA homopolymer free [9–10].

Despite the slight decrease in yield at higher PLA content, the overall high yield (>92%) indicates the ultrasonic blending method is effective for creating PLA–PVA copolymers. The presence of any unreacted PLA (particularly at 30wt.% initial PLA) suggests that some PLA remained as separate phases or did not fully integrate, possibly due to its higher molecular weight fractions that were less susceptible to ultrasonic breakup and coupling.

**Table 1** - Unreacted PLA and block copolymer yield for different initial PLA fractions in the mixture

The proportion of PLA in the initial mixture, %	Unreacted homopolymer (PLA), %	block copolymer yield, %
10	4.3	95.7
20	5.8	94.2
30	7.4	92.6

Despite the slight decrease in yield at higher PLA content, the overall high yield (>92%) indicates the ultrasonic blending method is effective for creating PLA–PVA copolymers. The presence of any unreacted PLA (particularly at 30 wt.% of the initial PLA) suggests that some PLA remained as separate phases or did not fully integrate, possibly due to its higher molecular weight fractions that were less susceptible to the ultrasonic breakup and coupling.

**Solubility and Swelling Behavior:** The resulting PLA–PVA copolymer fibers were tested for solubility and swelling in various solvents, as it was summarized in Table 2. In water and in 0.9% saline (which simulate physiological conditions), the fibers did not dissolve. They showed only slight swelling in saline solution and essentially no swelling in pure water. This is a favorable result, indicating that the material is water-insoluble and would retain integrity when used as a suture in body fluids (saline represents blood or tissue fluid). In organic solvents, the fibers behaved differently: in dimethylformamide (DMF) and n-hexane, the material swelled significantly. These solvents can penetrate and plasticize or partly dissolve one of the components (DMF is a good solvent for PVA and moderate for PLA; n-hexane can swell PLA). Ethanol caused no swelling or dissolution, likely because neither PLA nor PVA is significantly soluble in ethanol at room temperature. The solvent resistance in aqueous media confirms that the PLA–PVA threads will remain intact during the wound-healing period, yet the material can still absorb some fluids (slight swelling) which might be beneficial for knot tightening and drug release if used as a delivery vehicle [6–7, 11, 13].

**Table 2** - Swelling behavior of PLA–PVA (5/95, 10/90, 15/85 by wt.%) block copolymers in different solvents

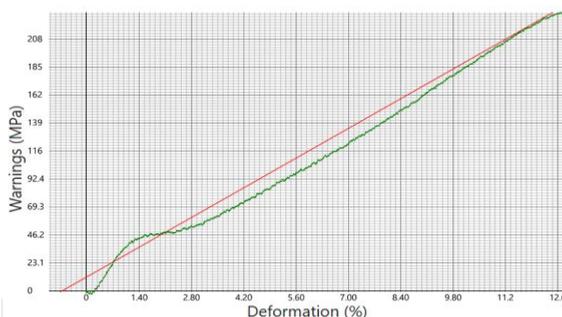
Solvents	Initial reaction mixture composition, PLA-PVS Mol, %		
	05-95	10-90	15-85
Water	-	-	-
NaCl(0,9%)	slightly swollen	slightly swollen	slightly swollen
Dimethylformamide	swollen	swollen	swollen
Ethanol	-	-	-
n-hexane	swollen	swollen	swollen

Note: “-” indicates no noticeable swelling or dissolution.

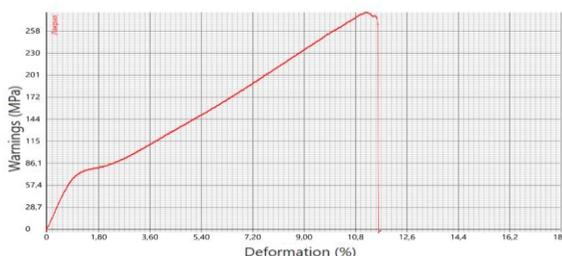
**Mechanical Properties of Fibers:** Tensile testing was performed on fibers with 10%, 20%, and 30% PLA content (balance PVA). The 10 wt.% PLA fiber had a breaking force of 40.5 N and an elongation at break of about 13%. However, this sample did not meet the ASTM D2256 requirements for surgical sutures (in terms of minimum strength for a given size). The 20 wt.% PLA fiber showed a breaking force of 49.9 N and elongation of 11.7%, which did meet the required standard. The 30 wt.% PLA fiber had a breaking force of 51.0 N and elongation of 17%, but interestingly this sample, despite a higher load capacity, did not meet the standard’s requirements either (likely due to an overly high elongation or other criteria such as knot security not measured here). The data indicate that incorporating a moderate amount of PLA (around 20%) into PVA yields the strongest fiber that still retains adequate flexibility without becoming too much stiff or brittle. [3, 18–19]

For all samples, the stress–strain curves indicated that the incorporating PVA into the blend markedly increased the fiber elasticity (strain at break), as compared with the neat PLA. PVA is a ductile polymer, and its inclusion improved the ultimate elongation. At the same time, the presence of PLA provided the reinforcement of strength. The 20% PLA fiber achieved the best balance of strength and flexibility. By adjusting the PLA/PVA ratio in the copolymer, it is possible to tune the mechanical properties of the suture fibers. This tunability is advantageous for meeting different surgical needs (e.g., some applications might prefer a higher stiffness, others - more elasticity). Figures 3–5 illustrate the stress–strain curves for the samples with 10%, 20%, and 30% PLA, respectively, demonstrating the differences in the tensile performance. [3, 18]

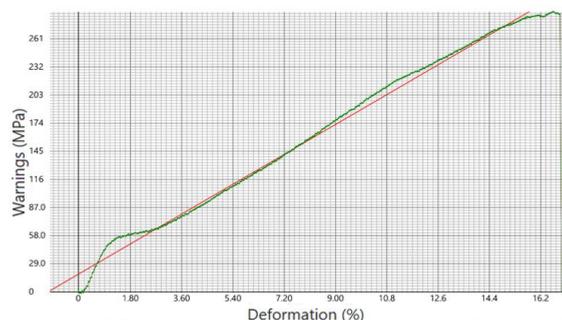
The improvements in the mechanical properties with the addition of PVA can be attributed to the formation of the PLA–PVA block copolymer which likely results in a phase-separated morphology of hard (PLA-rich) and soft (PVA-rich) domains. Such morphology can increase toughness. The presence of PVA (a flexible polymer) in the matrix helps to absorb energy and to prevent the crack propagation, while PLA provides reinforcement. In short, the PLA/PVA ratio effectively determines the tensile strength and ductility of the fibers [11, 13].



**Figure 3** – The stress–strain curve of the PLA/PVA 10/90 (wt.%) fiber sample. The fiber shows a moderate strength (breaking load ~40 N) and relatively a high elongation (~13%).



**Figure 4** – The stress–strain curve of the PLA/PVA 20/80 (wt.%) fiber sample. This composition exhibits the highest tensile strength (~50 N) with ~12% elongation, meeting the standard requirements for the surgical suture materials.

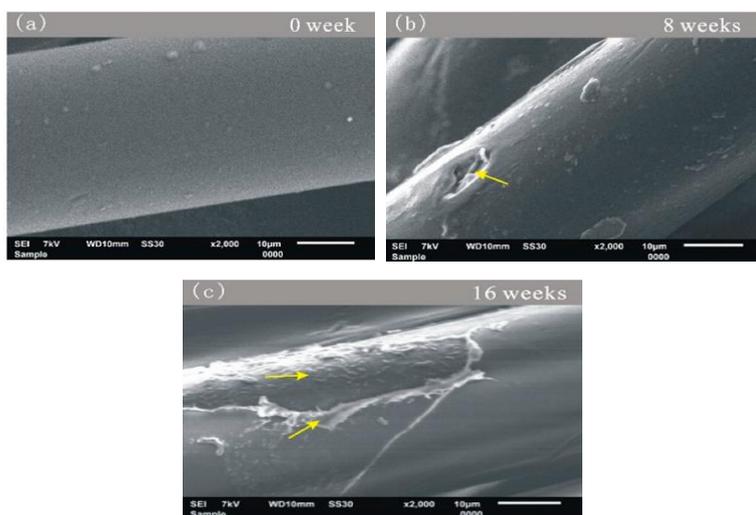


**Figure 5** – The stress–strain curve of the PLA/PVA 30/70 (wt.%) fiber sample. The strength (~51 N) is high, but the elongation (~17%) is larger; this sample did not meet one of the standard criteria (likely due to its mechanical profile outside the optimal range).

The Suture Handling Properties: In the practical surgical use, sutures should not only be strong, but also be well handled — they should tie securely into knots without slipping, and have sufficient flexibility. All the prepared PLA–PVA fiber samples were observed to tie knots easily. The 10% PLA fibers, being very pliable (due to high PVA content), were easiest to knot, but somewhat weaker. The 30% PLA fibers were the strongest, but slightly stiffer, which could make knot tying more difficult. The 20% PLA fiber struck a good middle ground,

maintaining flexibility while providing a high strength. These qualitative observations align with the quantitative tensile results. In general, modern surgical suture materials require a combination of strength, flexibility, knot security, and predictable absorption time. The PLA–PVA fibers developed here meet those general requirements: they are biocompatible, sufficiently strong, and have good handling characteristics due to the PVA component. [1–3]

**In Vitro Degradation (SEM Analysis):** Biodegradability is a critical feature of absorbable sutures. The PLA–PVA fibers were designed to gradually degrade in the body. SEM images of the fiber surface at different degradation times are presented in Figure 6. Initially (Figure 6a), the fiber surface is relatively smooth with slight texture from the extrusion process. After 8 weeks in phosphate-buffered saline (Figure 6b), the surface shows noticeable roughening: the smoothness has disappeared and small cracks or pits are evident. By 16 weeks (Figure 6c), the fiber surface is extensively eroded with many more cracks and some fragmentation visible. This progressive development of surface porosity and cracking confirms that the fibers biodegrade over time in a simulated physiological environment. The degradation appears to initiate at the surface and work inward, which is typical for hydrolytically degradable polymers like PLA (surface erosion is enhanced by water penetration into amorphous regions). The uneven degradation pattern (localized cracks) may be due to the two-phase nature of the material – PVA-rich domains might erode faster (being hydrophilic) leaving behind PLA-rich regions until they too break down. The SEM evidence supports that after several weeks, the structural integrity of the fiber will diminish as needed for absorption in tissue. [14–17]



**Figure 6** - SEM images of PLA–PVA fibers at different degradation times: (a) initial (no degradation), (b) after 8 weeks in PBS at 37 °C, and (c) after 16 weeks. The initially smooth fiber surface develops roughness and cracks over time, indicating the gradual biodegradation of the suture.

Accompanying the physical changes, there was measurable mass loss of the fibers over time. A higher PLA content generally slows the degradation because PLA is more hydrophobic and degrades slower than PVA. This effect was observed in the soil burial test results (which provide an environmental perspective on degradation) shown in Table 3. After 8 weeks being buried in soil, the sample with 10% PLA retained only about 17% of its original mass (0.0212g of 0.121g), whereas the sample with 30% PLA retained about 35% of its mass (0.05315g of 0.1503g). The 20% PLA sample was intermediate, with about 32% remaining (0.0532g of 0.1660g). The trend across 1, 3, and 8 weeks illustrates that all samples lose mass over time (indicating biodegradation), but higher PLA content yields slower mass loss. This is consistent with PLA's known slower biodegradability relative to PVA. Notably, even the 30% PLA sample lost more than 60% of its mass in 8 weeks, confirming that the block copolymer remains biodegradable despite the presence of a substantial fraction of the more recalcitrant PLA. The combination of PLA with PVA thus allows tuning the degradation rate: more PVA leads to faster degradation (which might be useful for fast-healing tissues), while more PLA prolongs the suture's presence (for wounds that need longer support). [8, 14–15]

**Table 3** - Biodegradation of PLA–PVA fibers under soil burial conditions (Remaining mass of samples over time)

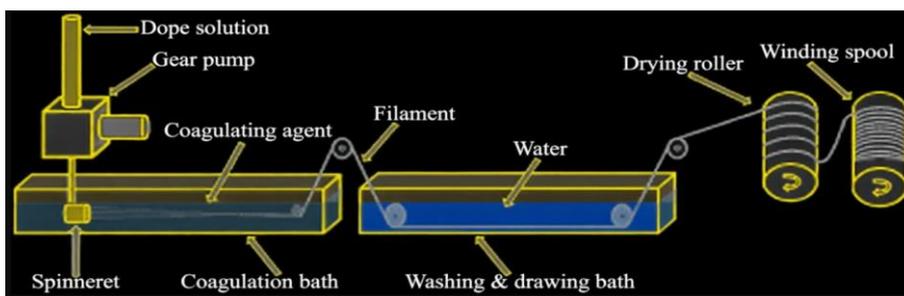
The proportion of PLA in the initial mixture, %	initial weight, g/g	1 pound, g/g	3 pound, g/g	7 pound, g/g
10	0.1215	0.0735	0.0357	0.0212
20	0.1660	0.1183	0.0728	0.0532
30	0.1503	0.1263	0.1135	0.05315

The loss of mass and structural integrity over time demonstrates that the PLA–PVA sutures are indeed biodegradable. In surgical terms, this means the suture will gradually weaken and be absorbed by the body, aligning with the healing timeline so that the suture's support is present only as long as needed. The differences between compositions suggest that by varying PLA content one can tailor how long the suture persists: e.g., 30% PLA might be used when a longer support period is desired, while 10% PLA might be suitable for faster-healing tissues. [14, 17]

The Proposed Production Technologies: Based on the experimental findings, we propose two approaches to produce the PLA-based sutures on a larger scale:

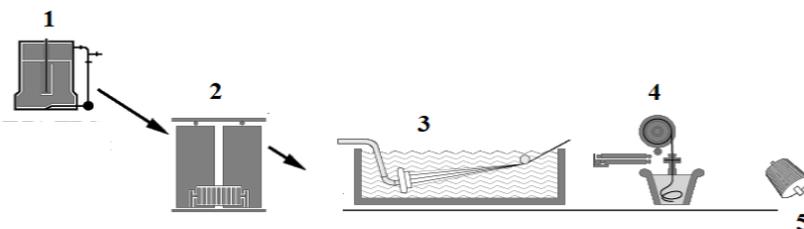
Method 1. Precipitation (Wet) Spinning of PLA: In this approach, a PLA solution of a relatively high concentration ( $\geq 25\%$  w/v in a suitable solvent) is prepared. This viscous solution is pumped through a spinneret (a nozzle with the fine orifices) into a coagulation bath, containing a nonsolvent (for example, ethanol or water). As the PLA solution jets enter the bath, PLA precipitates into solid filaments. These filaments are drawn out and wound onto a spool. The process may be aided by an applied electric field or just by the force of extrusion.

The fibers can then be washed and dried. This method is analogous to traditional wet spinning, where a polymer is precipitated from solution into fibers. Figure 7 illustrates this method: a reservoir holds the PLA solution, which is extruded through capillaries into a coagulation bath, and the resulting fiber is collected on a take-up roll. This method could produce pure PLA fibers; however, it may not directly yield a PLA–PVA blend fiber unless PVA is also integrated (which is challenging since PVA isn't soluble in the same solvent). Thus, this method is mainly considered for PLA alone or if a second polymer can be co-spun. [3, 12]



**Figure 7** - Schematic of precipitation (wet) spinning for PLA fibers: The PLA solution is extruded through a spinneret into a coagulation bath, forming fibers that are stretched and collected on a spool.

**Method 2: Solution Mixing and Wet Spinning of PLA–PVA:** This approach stems from our laboratory process. Here, calculated amounts of PVA solution and PLA solution are first mixed in a reactor (as we did in small scale) to form a homogenous spinning dope containing both polymers. This mixed solution is then fed to an extrusion system. (1) The mixed PLA/PVA solution is loaded into a spinning pump, (2) extruded through a multi-hole spinneret into a coagulation bath (water or another non-solvent that precipitates both polymers together), forming a fiber that contains intimately mixed PLA and PVA. (3) The fiber is drawn through the bath and can undergo stretching (to align polymer chains and improve strength) and washing. Finally, (4) the fiber is collected on a bobbin and dried. Additional post-treatments (like cross linking or coating) can be applied if needed. Figure 8 shows a proposed flow diagram: two input streams for PLA and PVA solutions combine, and then go through the spinneret into a bath, followed by rollers for stretching and a winding system. This method allows co-spinning of PLA and PVA, effectively implementing the laboratory synthesis in a continuous fiber production process. It is a wet-spinning variant tailored for two polymers. [3, 12]



**Figure 8** - Proposed technological scheme for producing PLA–PVA surgical suture fibers (Method 2: solution mixing and wet spinning). 1 – Mixing reactor for PLA and PVA solutions; 2 – holding tank for spinning dope; 3 – coagulation bath; 4 – stretching and washing rollers; 5 – take-up spool (bobbin).

Between these two methods, the second is directly related to our research outcome and is preferred for making PLA/PVA blend fibers. The first method (precipitation spinning) could be an alternative for pure PLA fibers or potentially used as a first step to create a core that is later coated with PVA. Further research and development would be required to optimize these processes, such as adjusting solvent choices, extrusion rates, coagulation bath composition, and draw ratios to achieve fibers with the desired diameter and properties.

In summary, the results demonstrate that a block copolymer approach to combining PLA with PVA is feasible and effective. The PLA–PVA fibers have achieved the high tensile strength (nearly 50N for 20% PLA content in our sample, which is comparable to, or better than some commercially available absorbable sutures), and they show the predictable degradation behavior. The ability to modulate the mechanical properties and degradation by simply changing the PLA/PVA ratio gives this material a versatility for various medical applications. The fibers also fulfill the general requirements for the suture materials in terms of knotting behavior and handling. The proposed manufacturing schemes provide a foundation for scaling up production of these fibers, bridging the gap between the laboratory samples and the mass-produced surgical sutures.

#### 4. Conclusion

A novel biodegradable surgical suture material, based on a polylactide/polyvinyl alcohol (PLA–PVA) block copolymer, has been developed and characterized. By using an ultrasonic solution blending technique, we have successfully combined PLA and PVA into a homogeneous fiber, overcoming the challenge of their incompatibility. The PLA–PVA fibers have shown excellent tensile properties, with the PLA 20% (wt.) content, yielding the strongest fiber (breaking load ~50 N) that meets the standard surgical suture requirements. A lower PLA content has increased flexibility, but reduced strength, while a higher PLA content has increased strength marginally, but at the cost of knot security and compliance. [1–3, 8, 11, 13–17]

The fibers have been found to be biocompatible and absorbable. They have remained intact in the aqueous environments, swelling only slightly in saline, which is advantageous for maintaining the wound support during the initial healing. The infrared spectroscopy has confirmed the formation of the intermolecular bonds between PLA and PVA in the copolymer. The scanning electron microscopy and mass loss measurements have demonstrated that the sutures biodegrade gradually: the surface erosion and mass reduction have occurred over weeks, and the rate of degradation can be tuned by adjusting the PLA/PVA ratio. In particular, the fibers with a higher PVA content degrade faster, which can be useful for the wounds that heal quickly, whereas those with a higher PLA content persist longer for the extended support. [1, 3, 8, 11, 14–17]

The study has also proposed practical methods for scaling up the production of the PLA-based sutures, including a co-spinning process for the PLA/PVA blends. These methods can be further refined to produce fibers with the consistent quality, suitable for medical use.

In conclusion, the developed PLA–PVA biodegradable sutures exhibit a combination of the desirable properties: high strength, flexibility, and controlled biodegradability. These threads are promising for surgical applications, potentially improving patient outcomes by eliminating the removal procedures and reducing the tissue reaction. The further studies will be focused on the *in vivo* performance and will refine the fabrication process, while the current findings support the potential of the PLA–PVA fibers as the next-generation absorbable suture materials. [1–3, 8, 11, 13–19].

**Acknowledgments:** The work was carried out within the framework of the project of the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan under the project: BR27101179.

**Conflict of interests:** The authors declare that there is no conflict of interest between the authors that requires disclosure in this article.

## ПОЛИЛАКТИД НЕГІЗІНДЕГІ БИОБЫДЫРАЙТЫН ХИРУРГИЯЛЫҚ ЖІПТЕРДІ АЛУ

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**Түйіндемe.** Дәстүрлі хирургиялық тігіс жіптері жара жазылғаннан кейін алып тастауды қажет етеді, бұл пациенттерге қосымша ауырсыну мен қолайсыздық тудырады. Полилактид (ПЛА) – жаңартылатын шикізат көздерінен алынатын, биоүйлесімді және биоыдырайтын алифатты полиэфир; алайда оның салыстырмалы түрде жоғары қаттылығы хирургиялық тәжірибеде қолданылуын шектеуі мүмкін. Осы зерттеудің мақсаты полилактид (ПЛА) және поливинил спирті (ПВС) негізінде биоыдырайтын хирургиялық тігіс жіптерін әзірлеу және олардың физика-химиялық, механикалық қасиеттері мен биоыдырау қабілетін зерттеу болды. ПЛА-ның қаттылығын төмендету үшін ПЛА ПВС- пен араластырылып, композиттік талшықтар түзілді. Талшықтар полимер қоспаларынан ультрадыбыстық өңдеу қолдану арқылы алынды, бұл компоненттердің біртекті араласуын жақсартуға мүмкіндік берді. Қоспалардың біртектілігі ультракүлгін-көрінетін спектроскопия әдісімен бағаланды, химиялық құрылымы инфрақызыл спектроскопия арқылы талданды, ал беткі морфологиясы сканерлеуші электрондық микроскопия (СЭМ) көмегімен зерттелді. СЭМ нәтижелері 16 апта ішінде талшықтардың беткі

морфологиясының өзгеруін және біртіндеп деградацияға ұшырауын көрсетті, бұл топырақта массаның жоғалуын өлшеу нәтижелерімен де расталды. Механикалық қасиеттер ASTM D2256 стандартына сәйкес анықталды. ПВХ енгізілуі талшықтардың созылғыштығы мен серпімділігін арттырды, ал ПЛА–ПВХ (20:80 мас.%) композициясы зерттелген құрамдар ішінде ең қолайлы механикалық сипаттамаларды көрсетті. Жалпы алғанда, алынған нәтижелер ПЛА–ПВХ композиттік талшықтарының сорылатын хирургиялық тігіс материалдары ретінде перспективалы кандидаттар екенін дәлелдейді.

**Түйінді сөздер:** полилактид, поливинил спирті, хирургиялық тігіс материалы, биоыдырайтын, композиттік талшық, хирургиялық талшықтар

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## ПОЛУЧЕНИЕ БИОРАЗЛАГАЕМЫХ ХИРУРГИЧЕСКИХ НИТЕЙ НА ОСНОВЕ ПОЛИЛАКТИДА

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**Аннотация.** Традиционные хирургические швы необходимо удалять после заживления раны, что вызывает дополнительную боль и дискомфорт у пациентов. Полилактид (ПЛА) - это алифатический полиэфир, получаемый из возобновляемых ресурсов, который является биосовместимым и биоразлагаемым; однако его относительно высокая жесткость может ограничивать его применение в хирургии. Целью данного исследования было разработать биоразлагаемые хирургические швы на основе ПЛА и поливинилового спирта (ПВХ) и изучить их физико-химические, механические свойства и биоразлагаемость. Для снижения жесткости ПЛА, ПЛА смешивали с ПВХ для образования композитных волокон. Волокна получали из смесей полимеров с использованием ультразвуковой обработки для улучшения смешивания. Однородность смесей оценивали с помощью ультрафиолетово-видимой спектроскопии, химическую структуру анализировали с помощью инфракрасной спектроскопии, а морфологию поверхности исследовали с помощью сканирующей электронной микроскопии (СЭМ). СЭМ выявила изменения морфологии поверхности и постепенную деградацию волокон в течение 16 недель, что также подтверждается измерениями потери массы в почве. Механические свойства определялись в соответствии со стандартом ASTM D2256. Включение ПВХ увеличило растяжимость и эластичность волокон, а композиция ПЛА–ПВХ (20:80 мас.%) показала наиболее благоприятные механические характеристики среди исследованных составов. В целом, результаты свидетельствуют о том, что композитные волокна ПЛА–ПВХ являются перспективными кандидатами для рассасывающихся хирургических шовных материалов.

**Ключевые слова:** полилактид, поливиниловый спирт, хирургический шовный материал, биоразлагаемый, композитное волокно, хирургические волокна

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## ASSESSMENT OF THE BIOLOGICAL EFFECT OF 2,2-PROPAGYLOXY BENZOIC ACID ON GRAINS OF SINGLE AND DICOTYLEDONOUS PLANTS

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**Abstract:** *Introduction.* Oxygen heterocyclic compounds occupy an important place in modern organic and medical chemistry. Tetrahydropyran derivatives in particular are widely studied due to their structural diversity and biological activity. In this regard, the problem of agronomy and phytochemistry is to determine the biological activity of propargyloxybenzoic acid, an oxygenated derivative of 2,2-dimethyltetrahydropyran-4 — on and propargylated salicylic acid in the grains of single and dicotyledonous plants by the reaction of Favorsky. *The purpose and objectives of the work* is to study the biological activity of seeds of single and dicotyledonous plants with the synthesis of a new oxygenated heterocyclic compound based on 2,2-dimethyltetrahydropyran-4-on and propargylated salicylic acid. *Tasks* obtaining the original compound by The Prince reaction, synthesizing a new derivative using the Favorsky reaction, and studying its biological activity. *Conclusion* (conclusions). The oxygen heterocycle 2,2-dimethyltetrahydropyran-4-on was obtained with dimethylvinyl-ethylcarbinol in a sulfuric acid medium and using mercury sulfate as a catalyst, with a yield of 70% through the Prince reaction mechanism. By reacting the resulting 2,2-dimethyltetrahydropyran-4-on with the acetylene derivative of salicylic acid by the Favorsky reaction, the acetylene derivative of 2,2-dimethyltetrahydropyran-4-on was synthesized with a 57% yield of 2,2-propagyloxy benzoic acid. The physicochemical properties of the obtained oxygen heterocycle compounds were determined and studied by IR spectroscopy. According to the results of a study of the biological activity of 2,2-propagyloxy benzoic acid on single and dicotyledonous plant grains, it was found that it significantly inhibited the growth of dicotyledonous plants in high concentrations, and was effective as a growth stimulant for single dicotyledonous plants.

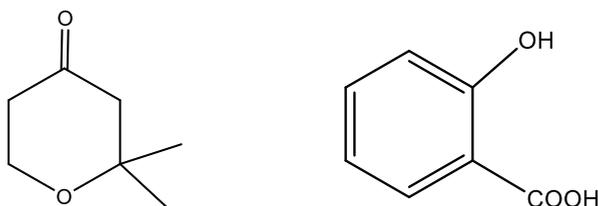
**Key words:** oxygen heterocycles, 2,2-dimethyltetrahydropyran-4-on, 2,2-propagyloxy benzoic acid, single and dicotyledonous plants.

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**Citation:** Duisenali A.M., Yelibaeva N.S., Burasheva G.Sh., Umbetova A. K., Litvinenko Y.A., Asylkhanov Zh. S. Assessment of the biological effect of 2,2-propagyloxy benzoic acid on grains of single and dicotyledonous plants. Chem. J. Kaz., 2026, 1(93), 93-100. DOI: <https://doi.org/10.51580/2026-1.2710-1185.09>

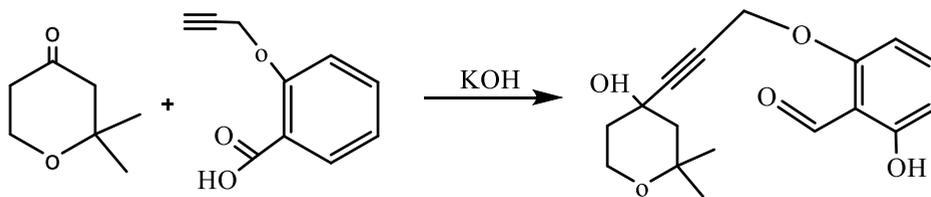
## 1. Introduction

Oxygen-containing heterocyclic compounds are widely studied in modern organic and pharmaceutical chemistry, as they form an important basis for drugs, agrochemical agents, and functional materials due to their synthetic flexibility and biological activity [1]. In recent years, special reviews have been published on oxygen-containing heterocycles, discussing recent advances in their innovative synthesis methods and biological applications [2]. 2,2-Dimethyltetrahydropyran-4-one is a six-membered saturated heterocycle. It has two methyl groups in 2,2-dimethyl on one carbon, and a carbonyl group in the 4-position. Due to this, the molecule resembles the structure of a  $\gamma$ -keto ester, which plays an intermediate role in the synthesis of  $\gamma$ -lactones and  $\gamma$ -lactams [3].



**Figure 1** - Structural formula of 2,2-dimethyltetrahydropyran-4-one and salicylic acid.

The propargyl group is widely used in organic synthesis and is an effective reagent for the preparation of complex heterocycles. The introduction of this group is considered an important tool in current research to expand the construction of heterocycles; a review of the synthesis and applications of propargyl derivatives has been published in recent years [3]. In addition, salicylic acid is an important phytohormone in plant physiology, regulating growth and stress responses, its role including the root system and growth [4].



**Scheme 1** - Preparation of 2,2-propargyloxybenzoic acid.

Based on these studies, it is clear that new methods for the synthesis of oxygenated heterocycles and the study of their effects on plants are relevant in science and applied chemistry - this demonstrates the integration of modern chemical synthesis and biological testing [5].

## 2. Experimental part

### 2.1. Experimental chemical section

The progress of the reactions and the purity of the obtained products were monitored by thin-layer chromatography (TLC) using Sorbifil (Sorbpolymer, Krasnodar, Russia) coated with CTX-1A silica gel, with a UV-254 indicator, particle size 5–17  $\mu\text{m}$ . The eluent for the TLC analysis was a benzene-EtOH mixture in a ratio of 1:3. Solvents for recrystallization and solvents for synthesis were purchased from Merck KGaA with a purity of  $\geq 99\%$ . Infrared (IR) spectra of the compounds were recorded on a Bruker Avance III 400 MHz spectrometer, on KBr tablets.

The synthesis of 2,2-Propargyloxybenzoic acid was obtained in 72% yield according to the literature [6].

### 2.2. Experimental biological section

To study the effect of 2,2-propargyloxybenzoic acid on grains, first, homogeneous and clean grains were selected in the experimental work, which were soaked for 24 hours in distilled water or in 2,2-propargyloxybenzoic acid solutions at concentrations of 0.01%, 0.05% and 0.1%; then, the grains were placed in soil or Petri dishes, and their growth was monitored at a temperature of 22–25  $^{\circ}\text{C}$  and a 12-hour light/12-hour dark cycle, and the germination percentage, root and shoot length, number of primary leaves and biomass were measured daily for 48 hours and 60 hours compared with the control group (grains soaked only in distilled water), thus determining the effect of the acid on plant growth [7–10].

## 3. Results and discussion

In the present study, to determine the effect of 2,2-propargyloxybenzoic acid on grains, grains of monocot and dicot plants were soaked in solutions of different concentrations for 12 hours. *Triticum aestivum* (wheat) was selected as monocot grains, and *Pisum sativum* (pea) as dicot grains. Five concentrations of 2,2-propargyloxybenzoic acid were prepared for the study: 0.1%; 0.01%; 0.001%; 0.0001%; 0.00001%. 25 grains were taken for each experiment, and three replicates were performed for each concentration. *Triticum aestivum* grains soaked in solutions of different concentrations are shown, the number of grains in each beaker is the same, and the concentration of the solution is indicated at the bottom. This figure depicts the initial stage of the experiment, i.e., the process of soaking the grains for 12 hours.



**Figure 2** - Appearance of wheat and pea seeds after 12 hours of exposure to 5 different concentrations of 2,2-propargyloxybenzoic acid.

According to the results of the study, the effect of 2,2-propargyloxybenzoic acid varied depending on the plant species and concentration. In all glasses, the pea seeds were wet, and some showed swelling. This is a sign of water absorption and initial physiological activity due to the solution.



**Figure 3** - Appearance of wheat and pea seeds placed in a solution of 2,2-propargyloxybenzoic acid after 48 hours.



**Figure 4** - Appearance of wheat and pea seeds placed in a solution of 2,2-propargyloxybenzoic acid after 60 hours.

The results of 48 and 60-hour germination of wheat grains showed that 2,2-propargyloxybenzoic acid has a concentration-dependent effect on the initial growth of grains. Compared with the control, changes in the length of roots and shoots were observed in grains treated with acid solutions. At low concentrations (0.001–0.01%), relatively normal development or slight stimulation of shoots was observed, while at high concentrations (0.05–0.1%), a shortening of the root system, poor development of the shoot and general morphological disorders of the shoots were clearly observed.

At high concentrations (0.01% and above), germination was inhibited in most grains, and normal development of the roots and shoots was clearly

observed or they did not appear at all. This indicates that the acid has an inhibitory effect in high doses.

It is observed that the germination process in grains placed in a solution of 2,2-propargyloxybenzoic acid changes in a concentration-dependent manner. In the control (0%) grains, germination signs were weak or not observed at all. At low concentrations (0.0001–0.001%), embryo rupture and the formation of the first radicle were observed in some grains, indicating the beginning of the germination process.

**Table 1** – Wheat seeds placed in solutions of different concentrations of 2,2-propargyloxybenzoic acid

Concentration, C (%)	12 h., (cm)	48 h., (cm)	60 h. (cm)
0.1	3.5	7	13.8
0.01	4.5	10	15.5
0.001	2.5	8	10.5
0.0001	4.5	9	16
0.00001	5	10	15.9
Control (water)	4	11	15

**Table 2** – Pea seeds placed in solutions of different concentrations of 2,2-propargyloxybenzoic acid

Concentration, C (%)	12 h., (cm)	48 h., (cm)	60 h. (cm)
0.1	1	1.4	1.8
0.01	1	2	2.5
0.001	0.5	0.6	0.7
0.0001	0.4	0.5	0.5
0.00001	0.1	0.4	0.6
Control (water)	0.5	0.5	0.5

The results of the study of the effect of 2,2-propargyloxybenzoic acid showed that this compound acts as a growth stimulant in monocots, but has a negative effect on dicots. As is known, the growth of dicots such as common bean (*Phaseolus vulgaris*) is significantly inhibited at high concentrations, which makes it possible to use 2,2-propargyloxybenzoic acid against weeds. In addition, the effect on the development of fungi in common bean seeds is low, which indicates that this compound has high herbicidal activity and insufficient fungicidal activity, i.e., additional modification is required for its use as a fungicidal agent.

#### 4. Conclusion

The results of the conducted studies showed that the biological activity of 2,2-propargyloxybenzoic acid depends on the plant species. While this compound has a growth-stimulating effect on monocotyledonous plants, it significantly inhibits the growth of dicotyledonous plants, including cowpea, at high concentrations. This property indicates the possibility of using 2,2-propargyloxybenzoic acid as a selective herbicide. In addition, the observation of fungal development on cowpea seeds indicates that the fungicidal activity of this

compound is insufficient and that structural modification or additional studies are necessary for its use as a fungicide.

**Funding:** The work was supported by the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan (project № AP23485116).

**Conflict of interest:** The authors declare that there is no conflict of interest between the authors that requires disclosure in this article.

## ДАРА ЖӘНЕ ҚОС ЖАРНАҚТЫ ӨСІМДІКТЕР ДӘНДЕРІНЕ 2,2-ПРОПАГИЛОКСИ БЕНЗОЙ ҚЫШҚЫЛЫНЫҢ БИОЛОГИЯЛЫҚ ӘСЕРІН БАҒАЛАУ

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**Түйіндемe:** *Kіріспе.* Оттекті гетероциклді қосылыстар қазіргі органикалық және медициналық химияда маңызды орын алады. Әсіресе тетрагидропиран туындылары олардың құрылымдық әртүрлілігі мен биологиялық белсенділігіне байланысты кеңінен зерттелуде. Осыған байланысты 2,2-диметилтетрагидропиран-4-он мен пропаргилденген салицил қышқылы Фаворский реакциясы арқылы оттекті туынды — пропаргилоксибензой қышқылын алып оны дара және қос жарнақты өсімдіктер дәндерінде биологиялық белсенділігін анықтау агробиология мен фитохимияның өзекті мәселе болып табылады. Жұмыстың *мақсаты мен міндеттері* 2,2-диметилтетрагидропиран-4-он мен пропаргилденген салицил қышқылы негізінде оттекті гетероциклді қосылысты синтездеп, дара және қос жарнақты өсімдік дәндеріне биологиялық белсенділігін зерттеу. *Міндеттері* бастапқы қосылысты Принс реакциясы арқылы алу, Фаворский реакциясы көмегімен жаңа туынды синтездеу және биологиялық белсенділігін зерттеу. *Қорытынды (тұжырымдар).* Оттекті гетероцикл 2,2-диметилтетрагидропиран-4-он диметилвинил-этинилкарбинолмен күкірт қышқылы ортасында және сынап сульфатын катализатор ретінде қолдану арқылы, Принс реакция механизмі арқылы 70 % шығыммен алынды. Алынған 2,2-диметилтетрагидропиран-4-онды Фаворский реакциясы арқылы салицил қышқылының ацетиленді туындысымен әрекеттестіру арқылы 2,2-диметилтетрагидропиран-4-онның ацетиленді туындысы 2,2-пропагилокси бензой қышқылы 57 % шығыммен синтезделді. Алынған оттекті гетероцикл қосылыстарының физико-химиялық қасиеттері анықталды және ИҚ спектроскопиясымен зерттелді. 2,2-пропагилокси бензой қышқылының дара және қос жарнақты өсімдік дәндеріне жүргізілген биологиялық белсенділігін зерттеу нәтижелері бойынша қос жарнақты өсімдіктердің өсуін жоғары концентрацияларда айтарлықтай тежеді, ал дара жарнақты өсімдіктерге өсу стимуляторы ретінде ықпалды екені анықталды.

**Түйінді сөздер:** оттекті гетероциклдер, 2,2-диметилтетрагидропиран-4-он, 2,2-пропагилокси бензой қышқылы, дара және қос жарнақты өсімдіктер

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## ОЦЕНКА БИОЛОГИЧЕСКОГО ВОЗДЕЙСТВИЯ 2,2-ПРОПАРГИЛОКСИ БЕНЗОЙНОЙ КИСЛОТЫ НА СЕМЕНА ОДНОДОЛЬНЫХ И ДВУДОЛЬНЫХ РАСТЕНИЙ

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**Резюме.** *Введение.* Кислородсодержащие гетероциклические соединения занимают важное место в современной органической и медицинской химии. Особое внимание уделяется производным тетрагидропирана, которые широко исследуются благодаря их структурному разнообразию и биологической активности. В связи с этим получение кислородсодержащего производного — пропаргилоксибензойной кислоты — из 2,2-диметилтетрагидропиран-4-она и пропаргилированной салициловой кислоты с использованием реакции Фаворского, а также определение его биологической активности на семенах однодольных и двудольных растений является актуальной задачей агробиологии и фитохимии. *Цель и задачи работы.* Целью работы является синтез кислородсодержащего гетероциклического соединения на основе 2,2-диметилтетрагидропиран-4-она и пропаргилированной салициловой кислоты, а также изучение его биологической активности на семенах однодольных и двудольных растений. *В задачи исследования* входили получение исходного соединения с применением реакции Принса, синтез нового производного с помощью реакции Фаворского и исследование его биологической активности. *Заключение (выводы).* Кислородсодержащий гетероцикл 2,2-диметилтетрагидропиран-4-он был получен с выходом 70 % при взаимодействии диметилвинилэтинилкарбинола в среде серной кислоты с использованием сульфата ртути в качестве катализатора по механизму реакции Принса. В результате взаимодействия полученного 2,2-диметилтетрагидропиран-4-она с ацетиленовым производным салициловой кислоты в условиях реакции Фаворского было синтезировано ацетиленовое производное — 2,2-пропаргилоксибензойная кислота — с выходом 57 %. Были определены физико-химические свойства полученных кислородсодержащих гетероциклических соединений и проведены их исследования методом ИК-спектроскопии. По результатам изучения биологической активности 2,2-пропаргилоксибензойной кислоты установлено, что при высоких концентрациях она существенно ингибирует рост двудольных растений, тогда как в отношении однодольных растений проявляет стимулирующее действие.

**Ключевые слова:** кислородсодержащие гетероциклы, 2,2-диметилтетрагидропиран-4-он, 2,2-пропаргилоксибензойная кислота, однодольные и двудольные растения.

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Правила оформления статей в журнале  
«ХИМИЧЕСКИЙ ЖУРНАЛ КАЗАХСТАНА»

### 1. ОБЩИЕ ПОЛОЖЕНИЯ

Журнал «Химический журнал Казахстана» (ISSN 1813-1107, eISSN 2710-1185) выпускается ордена Трудового Красного Знамени АО «Институтом химических наук им. А.Б. Бектурова» 4 раза в год и публикует работы по широкому кругу фундаментальных, прикладных и инновационных исследований в области химии и химической технологии.

Языки публикации: казахский, русский, английский. Журнал индексируется Казахстанской библиометрической системой и включен в Перечень изданий, рекомендуемых Комитетом по контролю в сфере образования и науки Министерства образования и науки Республики Казахстан для публикации основных результатов научной деятельности.

Издание имеет следующие рубрики:

1. Обзорные статьи до 20 печатных страниц
2. Оригинальные статьи (до 8–10 печатных страниц)
3. Краткие сообщения (до 4–5 печатных страниц)

### 2. ПРЕДСТАВЛЕНИЕ СТАТЕЙ

Редакция принимает статьи от казахстанских и зарубежных авторов. В целях популяризации Журнала, редакционной коллегией приветствуется прием статей на английском языке.

**Для регистрации и публикации статьи** материал статьи представляется в редакцию через систему электронной подачи статьи на сайте Журнала (<https://www.chemjournal.kz/>) в комплекте со следующими документами:

1. Электронная версия статьи в форматах Word и PDF со встроенными в текст таблицами, схемами, рисунками (файл должен быть назван по фамилии первого автора на английском языке).

2. Сопроводительное письмо, адресованное в Редакцию Химического журнала Казахстана от организации, в которой данное исследование выполнено, с утверждением, что материал рукописи нигде не публиковался, не находится на рассмотрении для опубликования в других журналах и в материалах статьи отсутствуют секретные данные. В сопроводительном письме указываются сведения об авторе для корреспонденции: Фамилия, имя и отчество автора, служебный адрес с указанием почтового индекса, адрес электронной почты, телефон и ORCID.

3. Все статьи, опубликованные в Химическом журнале Казахстана (ISSN 1813-1107, eISSN 2710-1185) публикуются в открытом доступе. Чтобы обеспечить свободный доступ читателям и покрыть расходы на экспертную оценку, редактирование, поддержание сайта журнала, долгосрочное архивирование и ведение журнала, взимается плата за обработку статьи. Правила оплаты за опубликование принятой к печати статьи находятся в отдельном документе на сайте Журнала «Оплата за опубликование».

4. Статье присваивается регистрационный номер, который сообщается авторам в течение недели после получения указанного перечня документов; на этот номер необходимо ссылаться при переписке.

5. Принятым к печати статьям присваивается цифровой идентификатор (DigitalObjectIdentifier – DOI).

6. Учитывая невозможность проводить статьи на казахском языке через систему антиплагиат, будут учитываться формулировки рецензентов и решение издательской коллегии.

7. Статьи должны быть оформлены согласно шаблону, который можно скачать в разделе «Отправка материалов» на сайте Химического Журнала Казахстана.

### 3. СТРУКТУРА ПУБЛИКАЦИЙ

3.1. В начале **обзоров, оригинальных статей и кратких сообщений** на первой строке указывается номер по Универсальной десятичной классификации (УДК или UDC), соответствующий заявленной теме. Дается прописными буквами в верхнем левом углу. Также на первой строке справа прописными буквами полужирным шрифтом № 14 указывается название журнала **ХИМИЧЕСКИЙ ЖУРНАЛ КАЗАХСТАНА (ҚАЗАҚСТАННЫҢ ХИМИЯ ЖУРНАЛЫ, CHEMICAL JOURNAL OF KAZAKHSTAN)**, год, номер.

3.2. Далее через строку приводится международный стандартный сериальный номер журнала (ISSN 1813-1107, eISSN 2710-1185) и на следующей строке слева приводится DOI: который будет иметь значение после принятия статьи к печати.

3.3. Далее, после отступа строки указывается **заглавие статьи** прописными буквами, шрифт № 14 – полужирный, выравнивание текста по центру. Название должно максимально полно и точно описывать содержание статьи, включать ключевые слова, отражающие направление и/или основной результат исследования, но в то же время быть коротким и ясным и не содержать сокращений.

3.4. Далее, после отступа строки, указываются **инициалы и фамилии автора(-ов)** строчными буквами, шрифт № 12 полужирный, курсив, выравнивание текста по центру. Фамилия автора, с которым следует вести переписку, должна быть отмечена звездочкой (\*): *С.С. Сатаева\**, *А.М. Джубаналиева*.

3.5. Через строку шрифтом № 12, строчными буквами, курсивом с выравниванием текста по центру следуют **наименование(я) организации(й)** с указанием части названия организации, которая относится к понятию юридического лица (в английском тексте необходимо указывать официально принятый перевод названия), город, страна. В английском варианте адресные сведения должны быть представлены на английском языке, в т.ч. город и страна.

Строки с фамилиями авторов и названиями организаций содержат надстрочные индексы (после фамилии и перед названием организации), указывающие на место работы авторов.

На следующей строке курсивным начертанием, шрифт № 12, с выравниванием текста по центру указывается электронный адрес для переписки.

3.6. **Резюме (Abstract, Түйіндеме)** состоит из краткого текста (не менее 150–250 слов, шрифт № 12) на языке статьи. **Abstract** публикуется в международных базах, данных в отрыве от основного текста. Резюме должно быть автономным, все вводимые обозначения и сокращения необходимо расшифровать здесь же.

Приветствуется структурированное резюме, повторяющее структуру статьи и включающее: *введение, цели и задачи, методы, результаты и обсуждение, заключение (выводы)*. В то же время, цели и задачи описываются, если они не ясны из заглавия статьи, методы следует описывать, если они отличаются новизной. В резюме включаются новые результаты, имеющие долгосрочное значение, важные

открытия, опровергающие существующие теории, а также данные, имеющие практическое значение. Следует использовать техническую (специальную) терминологию вашей дисциплины.

Резюме дается без абзацного отступа строчными буквами; оно не должно содержать номера соединений, экспериментальные данные и ссылки на литературу.

**Резюме** только одно – в начале текста.

3.7. Далее на языке статьи без абзацного отступа строчными буквами шрифтом № 12, выравнивание текста по левому краю приводятся **ключевые слова** (от 5 до 10 шт.), обеспечивающие наиболее полное раскрытие содержания статьи.

3.8. В **кратких сообщениях** приводится резюме (150–200 слов), ключевые слова, но деления на разделы не требуется. Дается текст краткого сообщения на одном из трех языков с выполнением требований к УДК, названию статьи, перечню авторов, наименований организаций, в которых они работают, указанию автора для переписки. В тексте краткого сообщения приводятся конкретные **существенно новые результаты, требующие закрепления приоритета** с необходимыми экспериментальными подробностями. Затем следуют: информация о финансировании, благодарности, сведения о конфликте интересов, информация об авторах и список литературы.

3.9. Статья начинается с **введения**, в котором формулируется цель и необходимость проведения исследования, кратко освещается состояние вопроса со ссылками на наиболее значимые публикации с избеганием ссылок на устаревшие результаты. Излагаются открытия, сделанные в ходе данного исследования. Указывается структура статьи.

3.10. **Экспериментальная часть** содержит описание хода и результатов эксперимента, характеристику полученных соединений. В начале экспериментальной части приводятся названия приборов, на которых зарегистрированы физико-химические характеристики веществ и указываются условия измерения; также указываются либо источники использованных нетривиальных реагентов (например, «коммерческие препараты, название фирмы»), либо даются ссылки на методики их получения.

Каждый параграф экспериментальной части, описывающий получение конкретного соединения, должен содержать его полное наименование по номенклатуре ИЮПАК и его порядковый номер в статье. В методиках обязательно указывать количества реагентов в мольных и массовых единицах (для катализаторов – массу и мольные проценты), объемы растворителей. Методика эксперимента излагается в *прошедшем* времени.

Для известных веществ, синтезированных опубликованным ранее методом, необходимо привести ссылку на литературные данные. Для известных веществ, полученных новыми или модифицированными методами, должны быть представлены их физические и спектральные характеристики, использованные для подтверждения идентичности структуры, метод синтеза и ссылка на литературные данные.

Для всех впервые синтезированных соединений необходимо привести доказательства приписываемого им строения и данные, позволяющие судить об их индивидуальности и степени чистоты. В частности, должны быть представлены данные элементного анализа или масс-спектры высокого разрешения, ИК спектры и спектры ЯМР  $^1\text{H}$  и  $^{13}\text{C}$ .

Данные рентгеноструктурного анализа представляются в виде **рисунков и таблиц**. Все **новые соединения**, данные PCA которых приводятся в статье, должны быть **зарегистрированы в Кембриджской базе структурных данных** и иметь соответствующие **CCDC номера**.

Если, по мнению рецензента или редактора, новые соединения не были удовлетворительно охарактеризованы, статья не будет принята к печати.

**Пример методики:** *3-(2-Amino-6-methylpyridino)-3-carbonyl-3,4-dihydrocoumarin (12)*. To the alcoholic solution of 2.18 g (0.01 mol) of 3-carbethoxycoumarin, 1.08 g (0.01 mol) of 2-amino-6-methylpyridine was added with stirring. The mixture was boiled for 10 h. The solution was cooled, the precipitate was filtered. Then it was washed with cold EtOH. After the drying and recrystallization of the residue from i-PrOH yield of the product **12** was 2.05 g (63%), mp 226–228 °C, Rf 0.82 (1/2, EtOAc/hexane as eluent). Calculated, %: C 68.56; H 4.32; N 9.99 for C<sub>16</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>. Found, %: C 68.41; H 4.22; N 9.83. *Spectral data*.

**Внимание!** В статьях, посвященных синтезу новых соединений, допускается размещение **экспериментальной части** за разделом **Результаты и обсуждение**.

3.11. В разделе **Результаты и обсуждение**, который является наиболее важным, следует обсудить и объяснить полученные в работе **результаты**, проанализировать особенности синтеза, продемонстрировать и указать возможные ограничения. Провести сравнение полученных результатов с опубликованными ранее. Все новые соединения должны быть полностью охарактеризованы соответствующими спектральными и другими физико-химическими данными. В тексте обобщаются и разъясняются только те спектральные данные, которые используются для подтверждения структуры полученных соединений. Перечисление одних и тех же данных в тексте, таблицах и на рисунках не допускается. Для новых методов синтеза желательно обсудить механизм реакции. Для обобщения данных необходимо использовать понятные рисунки и таблицы. Представленные данные должны поддаваться интерпретации.

При обсуждении результатов следует придерживаться официальной терминологии IUPAC. Результаты рекомендуется излагать в прошедшем времени.

**Обсуждение** не должно повторять описание результатов исследования. В тексте должны быть использованы общепринятые в научной литературе сокращения. Нестандартные сокращения должны быть расшифрованы после первого появления в тексте. Единицы измерений должны быть указаны в Международной системе СИ.

3.12. Затем рекомендуется сформулировать **закключение**, в котором указать основные достижения, представленные в статье, и основной вывод, содержащий ответ на вопрос, поставленный во вводной части статьи, а также возможность использования материала статьи в фундаментальных или прикладных исследованиях.

3.13. Приводится информация о **финансировании** исследований.

3.14. Выражается **благодарность** тем, кто помог вам в подготовке вашей работы.

3.15. В рукописи должно быть заявлено о том, имеется ли **конфликт интересов**

3.16. В **информации об авторах** указываются: ученая степень, звание, должность, e-mail, ORCID.

3.17. Статя заканчивается **списком литературы** со ссылками на русском (или казахском) языке и ссылками на языке оригинала. Ссылки на литературные источники в тексте приводятся порядковыми арабскими цифрами в квадратных скобках по мере упоминания. Каждая ссылка должна содержать только одну литературную цитату. Список литературы должен быть представлен наиболее свежими и актуальными источниками без излишнего самоцитирования (не более 20 процентов). Для статей желателен список из не менее 10 ссылок со строками доступа в интернете.

3.18. Обязательна **информация об авторах**. В ней указываются: ученая степень, звание, должность, e-mail, ORCID, **фамилия, имя, отчество** полностью на трех языках.

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Список цитируемой литературы оформляется в соответствии с нижеприведенными образцами библиографических описаний (4.8.).

3.19. В конце статьи после списка литературы *дополнительно* приводится перевод **Резюме** на казахский (**Түйіндеме**) и на английский языки (**Abstract**). Слово **Резюме (Abstract, Түйіндеме)** дается по центру. На следующей строке с выравниванием по левому краю прописными буквами полужирным шрифтом № 12 приводится название статьи. Через строку без абзацного отступа курсивом, полужирным шрифтом № 11 даются инициалы и фамилии авторов.

На следующей строке без абзацного отступа курсивом, строчными буквами, шрифтом № 11 приводятся места работы авторов с надстрочными индексами (после фамилии и перед названием организации), указывающие на место работы авторов. Затем через строку с абзацного отступа с выравниванием текста по ширине идет текст резюме, набранный строчным шрифтом № 12.

Далее через строку с абзацным отступом строчными буквами шрифтом № 12, с выравниванием текста по ширине приводятся **ключевые слова** (от 5 до 10 шт.), обеспечивающие наиболее полное раскрытие содержания статьи.

3.20. Для статей, подаваемых на языке, отличном от английского (на казахском или русском языке), в конце статьи находится английский блок (**Abstract, Information about authors, References**).

3.21. Все страницы рукописи следует пронумеровать.

#### 4. ТРЕБОВАНИЯ К ОФОРМЛЕНИЮ РУКОПИСЕЙ

4.1. Объем статьи, включая аннотацию и список литературы: до 8–10 страниц. Обзорные статьи могут быть до 20 страниц. Статья должна быть напечатана на одной стороне листа А4 шрифтом Times New Roman, размер кегля 14 пт; межстрочный интервал – одинарный и полями: верхнее – 2.0 см, нижнее – 2.0 см, левое – 3.0 см, правое – 1.5 см; расстановка переносов не допускается; абзацный отступ – 1.0 см; форматирование – по ширине. Должен быть использован текстовый редактор *Microsoft Word for Windows*, в виде *doc*-файла, версия 7.0 и более поздние.

Для краткости и наглядности обсуждения соединения, упоминаемые более одного раза, следует нумеровать **арабскими** цифрами в сочетании со строчными **латинскими** буквами (для обозначения соединений с переменным заместителем). При упоминании полного названия соединения шифр дается в скобках.

Стереохимические символы и приставки, характеризующие структурные особенности или положение заместителя в молекуле, следует набирать курсивом (*italic*): (*R*)-энантиомер, *трет*-бутил, *пара*-ксилол. Вместо громоздких названий неорганических и часто употребляемых органических соединений следует давать их формулы: NaBr, TsOH вместо бромид натрия и толуолсульфоновая кислота. При использовании терминов и обозначений, не имеющих широкого применения в литературе, их значения поясняются в тексте при первом употреблении: например, полиэтилентерефталат (ПЭТФ).

Для изображения структурных формул химических соединений необходимо использовать редактор химических формул **ChemDrawUltra**. Все надписи на схемах приводятся на английском языке. В схеме необходимо указывать все условия реакций: над стрелкой – реагенты, катализаторы, растворители, под

стрелкой – температура, время, выход. Если условия реакций сильно загружают схему, их можно перенести в конец схемы, расшифровывая буквенными индексами, например,  $i$ :  $\text{HCl}$ ,  $\text{H}_2\text{O}$ ,  $80\text{ }^\circ\text{C}$ ,  $5\text{h}$ . Такой же буквенный индекс должен быть указан над стрелкой соответствующей реакции.

4.2. Уравнения, схемы, таблицы, рисунки и ссылки на литературу нумеруются в порядке их упоминания в тексте и *должны быть вставлены в текст статьи* после первого упоминания. Таблицы и рисунки должны сопровождаться подписью; заголовки к схемам даются при необходимости.

4.3. По возможности следует готовить **рисунки** с помощью компьютера. Однотипные кривые должны быть выполнены в одинаковом масштабе на одном рисунке. Кривые на рисунках нумеруются арабскими цифрами, которые расшифровываются в подписях к рисункам. Для всех **рисунков** необходимо представить графические файлы в формате *jpeg* с минимальным разрешением 300 dpi. Надписи на рисунках должны быть на английском языке и по возможности заменены цифрами, расшифровка которых дается в подписи к рисунку.

Одиночные прямые, как правило, не приводят, а заменяют уравнением линии регрессии. Пересечение осей координат следует располагать в левом углу рисунка, стрелки на концах осей не ставятся, линии, ограничивающие поле рисунка не приводятся, масштабная сетка не наносится. Малоинформативные рисунки, не обсуждаемые в статье спектры, вольтамперограммы и другие зависимости не публикуются. **Рисунки спектров не должны быть выполнены от руки**. Все рисунки должны иметь нумерацию арабскими цифрами (если рисунок не один). Слово «Рисунок» и наименование помещают после пояснительных данных и располагают следующим образом: Рисунок 1 – Детали прибора.

4.4. Каждая **таблица** должна иметь тематический заголовок и порядковый арабский номер (без знака №), на который дается ссылка в тексте (таблица 1). Название таблицы располагается над таблицей слева без абзацного отступа в одну строку с ее номером через тире без точки после названия. Графы в таблице должны иметь краткие заголовки, отражающие параметры, численные значения которых приведены в таблице; они пишутся в именительном падеже единственного числа с прописной буквы и через запятую сопровождаются соответствующими единицами измерения (в сокращенной форме). Рисунки или структурные формулы в графах таблиц не допускаются. Пропуски в графах при отсутствии данных обозначают тремя точками, при отсутствии явления – знаком «тире». Примечания к таблицам индексируются арабскими цифрами и помещаются в границах таблицы под материалом таблицы. Слово «Примечание» следует печатать с прописной буквы с абзаца. Если примечание одно, то после слова «Примечание» ставится тире и примечание печатается с прописной буквы. Несколько примечаний нумеруют по порядку арабскими цифрами без проставления точки и печатают с абзаца. В таблицах используют тот же шрифт, что и в тексте статьи; допускается уменьшенный (не менее № 10 шрифт TimesNewRoman).

4.5. При выборе единиц измерения рекомендуется придерживаться системы СИ: г, мг, м, см, мкм (микрометр, микрон); нм (нанометр, миллимикрон); пм (пикометр); Э (ангстрем); с (секунда); мин, ч (час), Гц (герц); МГц (мегагерц); Э (эрстед); Гс (гаусс); В (вольт); эВ (электронвольт); А (ампер); Ом, Па (паскаль); МПа (мегапаскаль); гПа (гектопаскаль); Дж (джоуль); К (кельвин),  $^\circ\text{C}$  (градус Цельсия); Д (Дебай).

**В десятичных дробях целая часть отделяется от дробной не запятой, а точкой.**

Используются следующие сокращения: т.кип. и т.пл. (точки кипения и плавления) – перед цифрами; конц. (концентрированный перед формулой соединения); М – молекулярная масса); моль, кал, ккал, н. (нормальный), М. (молярный); концентрация растворов обозначается (г/см<sup>3</sup>, г/л, моль/л).

**Для всех впервые синтезированных соединений обязательны данные элементного анализа либо масс-спектры высокого разрешения.**

В *брутто-формулах* элементы располагаются в следующем порядке: С, Н и далее согласно латинскому алфавиту. Формулы молекулярных соединений и ониевых солей даются через точку (например, С<sub>5</sub>Н<sub>5</sub>Н.НCl). Пример записи констант и данных элементного анализа: т.кип. 78°C (100 мм рт. ст.), т.пл. 50°C (EtOH), d<sub>4</sub><sup>20</sup>0.9809, n<sup>20</sup>1.5256; Найдено, %: С 59.06; Н 7.05; I 21.00; N 8.01. С<sub>a</sub>Н<sub>b</sub>I<sub>c</sub>N<sub>d</sub>O<sub>e</sub>. Вычислено, %: С 59.02; Н 7.01; I 21.20; N 8.22.

**ИК и УФ спектры.** В экспериментальной части для ИК и УФ спектров должны быть указаны характеристические частоты полос, длины волн максимумов поглощения, коэффициенты экстинкции (или их логарифмы) и условия, при которых записан спектр.

**Примеры записи:** ИК спектр (тонкий слой),  $\nu$ , см<sup>-1</sup>: 1650 (C=N), 3200–3440 (O–H). УФ спектр (EtOH),  $\lambda_{\max}$ , нм (lg $\epsilon$ ): 242 (4.55), 380 (4.22).

Спектры ЯМР <sup>1</sup>H и <sup>13</sup>C. Должны быть указаны рабочая частота прибора, использованный стандарт и растворитель. Протоны в составе сложных групп, к которым относится сигнал, следует подчеркнуть снизу – 3.17–3.55 (4H, м, N(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>); для положения заместителей использовать обозначения 3-CH<sub>3</sub>; для обозначения положения атомов – C-3, N-4 и т.д. Если какой-нибудь сигнал в спектре описывается как дублет, триплет или дублет дублетов и т.п. (а не синглет или мультиплет), необходимо привести соответствующие КССВ. Если проведены дополнительные исследования для установления строения или пространственных взаимодействий атомов, должны быть указаны использованные двумерные методы. В описании спектров ЯМР <sup>13</sup>C отнесение конкретного сигнала к конкретному атому углерода приводится только тогда, когда определение проведено на основе двумерных экспериментов.

**Примеры записи:**

Спектр ЯМР<sup>1</sup>H (400 МГц, CDCl<sub>3</sub>),  $\delta$ , м. д. ( $J$ , Гц): 0.97 (3H, т,  $J=7.0$ , CH<sub>3</sub>); 3.91 (2H, к,  $J=7.0$ , COOCH<sub>2</sub>); 4.46 (2H, д,  $J=6.1$ , NCH<sub>2</sub>); 7.10–7.55 (6H, м, H-6,7,8, NHCH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>); 7.80 (1H, с, HAr); 7.97 (1H, с, H-5'); 8.13 (1H, д, д,  $J=8.2$ ,  $J=2.3$ , H-5); 11.13 (1H, с, NH).

Спектр ЯМР<sup>13</sup>C (100 МГц, DMSO-*d*<sub>6</sub>),  $\delta$ , м. д. ( $J$ , Гц): 36.3 (CH<sub>2</sub>CH<sub>3</sub>); 48.5 (C-5); 62.3 (CH<sub>2</sub>CH<sub>3</sub>); 123.0(CAr); 125.8 (д, <sup>2</sup> $J_{CF}=26.1$ , C-3',5' Ar); 128.9 (CPh); 134.4 (C-5a); 168.3 (C=O).

**Масс-спектры** приводятся в виде числовых значений  $m/z$  и относительных значений ионного тока. Необходимо указывать метод и энергию ионизации, массовые числа характеристических ионов, их интенсивность по отношению к основному иону и по возможности их генезис. В случае химической ионизации при описании прибора необходимо указать газ-реагент. В масс-спектрах высокого разрешения найденные и вычисленные значения  $m/z$  приводятся с четырьмя

десятичными знаками; если найденное значение  $m/z$  соответствует не молекулярному иону, брутто-формула и вычисленное значение  $m/z$  также приводится для того же иона.

**Пример записи данных масс-спектра:** Масс-спектр (ЭУ, 70 эВ),  $m/z$  ( $I_{\text{отн}}$ , %): 386  $[M]^+$  (36), 368  $[M-H_2O]^+$  (100), 353  $[M-H_2O-CH_3]^+$  (23).

Масс-спектр (ХИ, 200 эВ),  $m/z$  ( $I_{\text{отн}}$ , %): 387  $[M+H]^+$ (100), 369  $[M+H-H_2O]^+$  (23).

**Пример записи данных масс-спектра высокого разрешения:**

Найдено,  $m/z$ : 282.1819  $[M+Na]^+$ .  $C_{17}H_{25}NNaO$ .

Вычислено,  $m/z$ : 282.1828.

4.6. **Данные рентгеноструктурного исследования** следует предоставлять в виде рисунка молекулы с пронумерованными атомами, например, С(1), N(3) (по возможности в представлении атомов эллипсо и дамителиловых колебаний). Полные кристаллографические данные, таблицы координат атомов, длин связей и валентных углов, температурные факторы в журнале не публикуются, а депонируются в Кембриджском банке структурных данных (в статье указывается регистрационный номер депонента).

4.7. По требованиям международных баз данных Scopus, Clarivate Analytics, Springer Nature при оценке публикаций на языках, отличных от английского, библиографические списки должны даваться не только на языке оригинала, но и на латинице (романским алфавитом). Поэтому авторы статей, подаваемых на русском и казахском языке, должны предоставлять список литературы в двух вариантах: *один на языке оригинала (Список литературы)*, а другой — *в романском алфавите (References)*. Последний список входит в английский блок, который расположен в конце статьи.

Если в списке есть ссылки на иностранные публикации, они полностью повторяются в списке **References**. При цитировании русскоязычного журнала, переводимого за рубежом, в русскоязычной версии Списка литературы необходимо привести полную ссылку на русскоязычную версию, а в **References** – на международную.

Список источников в **References** должен быть написан только на романском алфавите- латинице (при этом он должен оставаться полным аналогом Списка литературы, в котором источники были представлены на оригинальном языке опубликования).

Для написания ссылок на русскоязычные источники (и источники на иных, не использующих романский алфавит, языках) следует использовать ОФИЦИАЛЬНЫЙ ПЕРЕВОД и ТРАНСЛИТЕРАЦИЮ (см. Требования к переводу и транслитерации).

В **References** требуется следующая структура библиографической ссылки из русскоязычных источников: авторы (транслитерация), перевод названия статьи или книги на английский язык, название источника (транслитерация – для тех изданий, которые не имеют установленного редакцией английского названия), выходные данные в цифровом формате, указание на язык статьи в скобках (in Russian или in Kazakh). Транслитерацию можно выполнить на сайте <http://www.translit.ru>.

Условные сокращения названий русскоязычных журналов и справочников приводятся в соответствии с сокращениями, принятыми в «Реферативном журнале Химия». англоязычных и других иностранных журналов – в соответствии с сокращениями, рекомендуемыми издательством «Springer and Business Media»:

<http://chemister.ru/Chemie/journal-abbreviations.htm>. Для статей на русском и казахском языках название журнала «Химический Журнал Казахстана» следует сокращать: «Хим. Журн. Каз.» и «Каз. Хим. Журн.» соответственно, а для статей на английском языке: «Chem. J. Kaz.». Приводятся фамилии и инициалы **всех авторов** (сокращения и др. и *et al* не допускаются).

В Списке литературы и в **References** все работы перечисляются **В ПОРЯДКЕ ЦИТИРОВАНИЯ**, а **НЕ** в алфавитном порядке.

**DOI.** Во всех случаях, когда у цитируемого материала есть цифровой идентификатор, его необходимо указывать в самом конце описания источника. Проверять наличие doi у источника следует на сайте <http://search.crossref.org> или <https://www.citethisforme.com>.

Для формирования списка литературы (всех без исключения ссылок) в Журнале принят библиографический стандарт без использования разделителя «//»:

Author A.A., Author B.B., Author C.C. Title of article. Title of Journal, **2005**, 10, No. 2, 49–53.

Для казахско- или русскоязычного источника:

Author A.A., Author B.B., Author C.C. Title of article. Title of Journal, **2005**, 10, No. 2, 49– 53. (In Kazakh or In Russian).

Ниже приведены образцы оформления различных видов документов, которых необходимо придерживаться авторам при оформлении романского списка **References**.

**Описание статьи из журналов:**

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Нежелательно оставлять одно переводное название конференции (в случае если нет переведенного на английский язык названия конференции), так как оно при попытке кем-либо найти эти материалы, идентифицируется с большим трудом.

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4.9. Пример англоязычного блока для представления статьи, написанной на языке, отличном от английского:

**Abstract**

**DETERMINATION OF THE HAZARD CLASS OF OIL-CONTAMINATED AND NEUTRALIZED SOIL**

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*Introduction.* Pollution by oil has a negative effect on chemical, physical, agrophysical, agrochemical and biological properties of soils. Sorption methods of cleaning the soil with the help of humic preparations from oil pollution are of great importance. *The purpose* of this work is to study the composition and properties of the contaminated and neutralized soil, the determination of the toxicity indexes of all components of oil waste, the calculation of the hazard class of waste according to their toxic-ecological parameters. *Methodology.* Samples of the contaminated and neutralized soil were treated with the use of humate-based energy-accumulating substances. The metal content in the contaminated soil was determined by spectrometry using an AA 240 instrument using the method of decomposing the sample with a mixture of nitric, hydrofluoric and perchloric acids until the sample was completely opened. *Results and discussion.* Fractional composition of oil products of all samples is stable: the content of complex acetylene hydrocarbons is ~ 70.0% of the total mass of oil products, the content of resins and paraffin-naphthenic group of hydrocarbons is 27.3%, the content of bitumens is 2.6%. In the neutralized soil, paraffin-naphthenic fractions, resins, bitumens and asphaltenes were mainly found; complex acetylene hydrocarbons are not present. *Conclusion.* It has been established that the contaminated soil belongs to the substances of the 3rd hazard class. Neutralized soil became less toxic and according to the total toxicity index, it was classified as hazard class 4 (low hazard). Neutralized soil can be used as construction and road materials, at the improvement of boreholes and at land reclamation.

**Keywords:** oil, contaminated soil, neutralized soil, humate-based energy storage substance, toxicity, radioactivity, hazard class.

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### Ғылыми жарияланымның этикасы

«Қазақстанның химиялық журналы» (бұдан әрі – Журнал) баспасының алқасы мен бас редакторы «Жариялану этикасы жөніндегі комитет – (Committee on Publication Ethics – COPE)» (<http://publicationethics.org/about>), «Еуропалық ғылыми редакторлардың қауымдастығы» (European Association of Science Editors – EASE) (<http://www.ease.org.uk>) және Ғылыми жарияланым этикасының комитетінде (<http://publicet.org/code/>) қабылданылған халықаралық талаптарды ұстанады.

Баспа қызметіндегі әдепке сай емес іс - әрекеттерді (плагиат, жалған ақпарат және т.б.) болдырмауға және ғылыми жарияланымдардың жоғары сапасын қамтамасыз ету үшін, қол жеткізген ғылыми нәтижелерді жұртшылыққа жариялау мақсатында редакция алқасы, авторлар, рецензенттер, сондай-ақ баспа үдерісіне қатысатын мекемелер этикалық нормалар мен ережелерді сақтауға міндетті және олардың бұзылмауына барлық шараларды пайдалануы тиіс. Осы үдеріске қатысушылардың барлығының ғылыми жарияланымдар этикасының ережелерін сақтауы, авторлардың зияткерлік меншік объектілеріне құқықтарын қамтамасыз етуге, жарияланымдар сапасын арттыруға және авторлық құқықпен қорғалған материалдарды жеке тұлғалардың мүддесі үшін пайдалану мүмкіндігін жоюға көмектеседі.

Редакцияға жіберілген барлық ғылыми мақалалар міндетті түрде екі жақты құпия сараптамаға жіберіледі. Журналдың редакциялық алқасы мақаланың журнал тақырыбына және талаптарына сәйкестігін анықтайды, журналға тіркеу үшін оны алдын ала саралауға журналдың жауапты хатшысына жібереді. Ол қолжазбаның ғылыми құндылығын анықтап, мақала тақырыбына жақын ғылыми мамандықтары бар екі тәуелсіз сарапшыны анықтайды. Мақалаларды редакциялық алқа және редакциялық алқа мүшелері, сондай-ақ басқа елдерден шақырылған рецензенттер сараптайды. Мақаланы сараптау үшін рецензенттерді таңдау туралы шешімді бас редактор қабылдайды. Сараптау мерзімі 2-4 апта және рецензент өтініші бойынша оны 2 аптаға ұзартуға болады.

**Редакция мен рецензент** қарауға жіберілген жарияланбаған материалдардың құпиялығына кепілдік береді. Жариялау туралы шешім журналдың редакциялық алқасы тексергеннен кейін қабылданады. Қажет болған жағдайда (редактор(лар) және/немесе рецензент(лер) тарапынан ескертулердің болуы) қолжазба авторларға қосымша түзетулерге жіберіледі, содан кейін ол қайта қаралады. Этика нормалары бұзылған жағдайда, мақаланы жариялаудан бас тарту құқығын Редакция өзіне қалдырады. Жауапты редактор мақалада плагиат деп есептеуге жеткілікті ақпарат болған жағдайда оны жариялауға рұқсат бермейді.

**Авторлар** редакцияға жіберілген материалдардың жаңа, бұрын жарияланбаған және түпнұсқа екендігіне кепілдік береді. Авторлар ғылыми нәтижелердің сенімділігі мен маңыздылығына, сондай-ақ ғылыми этика қағидаттарының сақталуына, атап айтқанда, ғылыми этиканы бұзылмауына (ғылыми деректерді қолдан жасау, зерттеу деректерін бұрмалауға әкелетін бұрмалау, плагиат және жалған бірлескен авторлық, қайталау, басқа адамдардың нәтижелерін иемдену және т.б.) тікелей жауапты.

Мақаланы редакцияға беру авторлардың мақаланы (түпнұсқада немесе басқа тілдерге немесе тілден аудармада) басқа журналға(ларға) жібермегенін және бұл материалдың бұрын жарияланбағанын білдіреді. Олай болмаған жағдайда мақала

авторларға «Авторлық құқықты бұзғаны үшін мақаланы жарияламау» деген шешіммен қайтарылады. Басқа автордың туындысының 10 пайыздан астамын, оның авторлығын және дереккөзге сілтемелерді көрсетпей сөзбе-сөз көшіруге жол берілмейді. Алынған үзінділер немесе мәлімдемелер автор мен дереккөзді міндетті түрде көрсете отырып ресімделуі керек. Шамадан тыс өзге материалдарды пайдалану, сондай-ақ кез келген нысандағы плагиат, соның ішінде дәйексіз дәйексөздер, басқа адамдардың зерттеулерінің нәтижелерін иемдену этикаға жатпайды және қабылданбайды. Зерттеу барысына қатынасқан барлық тұлғалардың үлесін мойындау қажет және мақалада зерттеуді жүргізуде маңызды болған жұмыстарға сілтемелер берілуі керек. Бірлескен авторлар арасында зерттеуге қатыспаған адамдарды көрсетуге жол берілмейді.

Автор(лар) жұмыстарында қателіктер байқалса, бұл туралы дереу редакторға хабарлап, түзету туралы ұсыныс беруі тиіс.

Қолжазбаны басып шығарудан бас тарту туралы шешім рецензенттердің ұсыныстарын ескере отырып, редакция алқасының отырысында қабылданады. Редакциялық алқаның шешімімен жариялауға ұсынылмаған мақала қайта қарауға қабылданбайды. Жариялаудан бас тарту туралы хабарлама авторға электрондық пошта арқылы жіберіледі.

Журналдың редакциялық алқасы мақаланы жариялауға рұқсат беру туралы шешім қабылдағаннан кейін редакциялық алқа бұл туралы авторға хабарлайды және жариялау шарттарын көрсетеді. Мақалаға берілген пікірлердің түпнұсқасы Журнал редакциясында 3 жыл сақталынады.

## Этика научных публикаций

Редакционная коллегия и главный редактор научного журнала «Химический журнал Казахстана» (далее – Журнал) придерживаются принятых международных стандартов «Комитета этики по публикациям» ([Committee on Publication Ethics – COPE](http://publicationethics.org/about)) (<http://publicationethics.org/about>), «Европейской ассоциации научных редакторов» (European Association of Science Editors – EASE) (<http://www.ease.org.uk>) и «Комитета по этике научных публикаций» (<http://publicet.org/code/>).

Во избежание недобросовестной практики в публикационной деятельности (плагиат, изложение недостоверных сведений и др.) и в целях обеспечения высокого качества научных публикаций, признания общественностью, полученных автором научных результатов, члены редакционного совета, авторы, рецензенты, а также учреждения, участвующие в издательском процессе, обязаны соблюдать этические стандарты, нормы и правила и принимать все меры для предотвращения их нарушений. Соблюдение правил этики научных публикаций всеми участниками этого процесса способствует обеспечению прав авторов на интеллектуальную собственность, повышению качества издания и исключению возможности неправомерного использования авторских материалов в интересах отдельных лиц.

Все научные статьи, поступившие в редакцию, подлежат обязательному двойному слепому рецензированию. Редакция Журнала устанавливает соответствие статьи профилю Журнала, требованиям к оформлению и направляет ее на первое рассмотрение ответственному секретарю Журнала, который определяет научную ценность рукописи и назначает двух независимых рецензентов – специалистов, имеющих наиболее близкие к теме статьи научные специализации. Рецензирование статей осуществляется членами редакционного совета и редакционной коллегии, а также приглашенными рецензентами других стран. Решение о выборе того или иного рецензента для проведения экспертизы статьи принимает главный редактор. Срок рецензирования составляет 2-4 недели, но по просьбе рецензента он может быть продлен, но не более чем на 2 недели.

Редакция и рецензент гарантируют сохранение конфиденциальности неопубликованных материалов присланных на рассмотрение работ. Решение о публикации принимается редакционной коллегией Журнала после рецензирования. В случае необходимости (наличие замечаний редактора(-ов) и/или рецензента(-ов)) рукопись направляется авторам на доработку, после чего она повторно рецензируется. Редакция оставляет за собой право отклонить публикацию статьи в случае нарушения правил этики. Ответственный редактор не должен допускать к публикации информацию, если имеется достаточно оснований полагать, что она является плагиатом.

Авторы гарантируют, что представленные в редакцию материалы являются новыми, ранее неопубликованными и оригинальными. Авторы несут ответственность за достоверность и значимость научных результатов, а также соблюдение принципов научной этики, в частности, недопущение фактов нарушения научной этики (фабрикация научных данных, фальсификация, ведущая к искажению исследовательских данных, плагиат и ложное соавторство, дублирование, присвоение чужих результатов и др.)

Направление статьи в редакцию означает, что авторы не передавали статью (в оригинале или в переводе на другие языки или с других языков) в другой(-ие) журнал(ы) и что этот материал не был ранее опубликован. В противном случае статья немедленно возвращается авторам с формулировкой «Отклонить статью за нарушение авторских прав». Не допускается дословное копирование более 10 процентов работы другого автора без указания его авторства и ссылок на источник. Заимствованные фрагменты или утверждения должны быть оформлены с обязательным указанием автора и первоисточника. Чрезмерные заимствования, а также плагиат в любой форме, включая неоформленные цитаты, перефразирование или присвоение прав на результаты чужих исследований, неэтичны и неприемлемы. Необходимо признавать вклад всех лиц, так или иначе повлиявших на ход исследования, в частности, в статье должны быть представлены ссылки на работы, которые имели значение при проведении исследования. Среди соавторов недопустимо указывать лиц, не участвовавших в исследовании.

Если автором(-ами) обнаружена ошибка в работе, необходимо срочно уведомить редактора и вместе принять решение об исправлении.

Решение об отказе в публикации рукописи принимается на заседании редакционной коллегии с учетом рекомендаций рецензентов. Статья, не рекомендованная решением редакционной коллегии к публикации, к повторному рассмотрению не принимается. Сообщение об отказе в публикации направляется автору по электронной почте.

После принятия редколлекцией Журнала решения о допуске статьи к публикации редакция информирует об этом автора и указывает сроки публикации. Оригиналы рецензий хранятся в редакции Журнала в течение 3 лет.

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## Scientific Publication Ethics

**The Editorial Board and Editor-in-Chief of the scientific journal the “Chemical Journal of Kazakhstan” (hereinafter referred to as the Journal) adhere to the accepted international standards of the “Committee on Publication Ethics” (Committee on Publication Ethics – COPE) (<http://publicationethics.org/about>), the “European Association of Science Editors” (European Association of Science Editors – EASE) (<http://www.ease.org.uk>) and the “Committee on Scientific Publication Ethics” (<http://publicet.org/code/>).**

To avoid unfair practices in the publishing activities (plagiarism, false information, etc.) and in order to ensure the high quality of the scientific publications and public recognition of the scientific results, obtained by the author, the members of the Editorial Board, authors, reviewers, as well as institutions, involved in the publishing process, are obliged to comply with ethical standards, rules and regulations, and take all measures to prevent their violation. The compliance with the rules of the scientific publication ethics by all process participants contributes to ensuring the rights of authors to intellectual property, improving the quality of the publication and excluding the possibility of misuse of the copyrighted materials in the interests of the individuals.

All scientific articles submitted to the editors are subject to mandatory double-blind peer reviewing. The Editorial Board of the Journal determines the compliance of the article with the specificity of the Journal, the registration requirements and sends it for the first reviewing to the Executive Secretary of the Journal, who determines the scientific value of the manuscript and appoints two independent reviewers – the specialists with the scientific specializations closest to the topic of the article. The articles are reviewed by the members of the Editorial Board and the Editorial Staff, as well as the invited reviewers from the other countries. The decision to choose one or another reviewer for reviewing the article is made by the Editor-in-Chief. The reviewing period is 2-4 weeks, though at the request of the reviewer, it can be extended, but no more than for 2 weeks.

**The editors and the reviewer** guarantee the confidentiality of the unpublished materials submitted for reviewing. The decision to publish is made by the Editorial Board of the Journal after reviewing. If necessary (the presence of comments by the editor(s) and/or reviewer(s)) the manuscript is sent to the authors for revision, after which it is re-reviewed. The editors reserve the right to reject from the publication of the article in case of violation of the rules of ethics. The Executive Editor should not allow the information to be published if there is sufficient reason to believe that it is plagiarism.

**The authors** guarantee that the materials, submitted to the editors are new, previously unpublished and original. The authors are responsible for the reliability and significance of the scientific results, as well as compliance with the principles of scientific ethics, in particular, the prevention of violations of scientific ethics (fabrication of the scientific data, falsification leading to distortion of the research data, plagiarism and false co-authorship, duplication, appropriation of other people's results, etc.).

The submission of an article to the editor means that the authors did not submit the article (in the original or translated into or from the other languages) to the other Journal(s), and that this material was not previously published. Otherwise, the article is immediately returned to the authors with the wording “Reject the article for the copyright infringement.” The word-for-word copying of more than 10 percent of the work of another author is not allowed without indicating his authorship and references to the source. The borrowed fragments or statements should be drawn-up with the obligatory

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If the author(s) finds an error in the work, it is necessary to immediately notify the editor thereof, and together decide on the correction.

The decision to refuse from the publication of the manuscript is made at a Meeting of the Editorial Board, taking into account the recommendations of the reviewers. An article, which is not recommended by the decision of the Editorial Board for the publication, is not accepted for re-consideration. A notice of the refusal to publish is sent to the author by e-mail.

After the Editorial Board of the Journal makes a decision on the admission of the article for the publication, the Editorial Board informs the author thereof, and specifies the terms of the publication. The original reviews are kept in the Editorial Office of the Journal for 3 years.

Технический редактор: *Ж.Б.Узакова*

Подписано в печать 27.03.2026г.  
Формат 70x100 <sup>1</sup>/<sub>16</sub>. 7.68. п.л. Бумага офсетная. Тираж 300.

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