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Ultrasound-assisted extraction of *Alhagi pseudalhagi* root and its mathematical modeling

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Abstract: Currently, research is being conducted to modify and improve extraction methods in several directions, including advancements in technical equipment, substitution of solvents, optimization of extraction conditions, and, in particular, the application of physical factors such as ultrasonic treatment. Among the innovative and promising approaches is the use of ultrasound to extract various biologically active compounds from natural materials.
This article presents the results of a scientific study on the ultrasound-assisted extraction of *Alhagi pseudalhagi* roots. The chemical composition of the extract was analyzed using gas chromatography–mass spectrometry (GC-MS). A total of 30 chemical compounds were identified, including several valuable biologically active substances. According to the GC-MS analysis, the major components were gentriacontane (18.83%), β-sitosterol (18.13%), and lupeol (11.85%).
The main factors influencing the diffusion of extractive substances from raw materials into the extractant - namely, ultrasonic power, sonication time, and temperature - have been investigated. These factors were used to design a full three-factor experimental plan. Consequently, a mathematical representation of the ultrasound-assisted extraction mechanism was established for further simulation and analysis. The resulting regression equation allows for the evaluation of the influence of these factors on extract yield.

Keywords: ultrasonic extraction; ultrasound power; sonication time; complete three-factor experiment; regression equation

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1. Introduction

Plant materials are valuable natural raw materials used in everyday life as food products, nutrient additives, aromatic components, and pharmaceuticals etc. The use of plant materials has a long history, and over the centuries, mankind has developed a large number of processing methods (Azmir et al., 2013). In the production of biologically active substances (BAS), plant extracts are widely used. Plant extracts are compounds or compound mixtures obtained from plants or their parts (leaves, flowers, seeds, roots). There are conventional methods for obtaining extracts from plant materials (maceration, percolation, and reflux extraction) (Orio et al., 2012), as well as non-conventional extraction methods (supercritical fluid extraction, pressurized liquid extraction, ultrasonic extraction, microwave-assisted extraction) (Mason et al., 2011; Li et al., 2017; Liu et al., 2018; Wen et al., 2018; Orio et al., 2012). Among modern methods of extracting components from plant materials, extraction using ultrasound takes a special place.

The ultrasound-assisted extraction method can significantly reduce the process duration and ensure a more complete extraction of substances (Vinatoru, 2001; Rostagno et al., 2003). When exposed to ultrasonic waves, the boundary diffusion layer is disturbed, and the penetration of the extractant into the material is improved. As a result, the raw material swells much faster, turbulent and vortex flows appear, which promote the transfer of masses and the dissolution of substances. The contents are intensively mixed even inside the cell (which cannot be achieved by other extraction methods). All this leads to a significant acceleration of the process of active substances transfer from raw materials to the extractant (Shah Buddin et al., 2018).

Ultrasonic extraction is an environmentally friendly and highly effective method for separating biologically active substances. This method is characterized by the use of very small amounts of organic solvents or their complete rejection, as well as an increase in the yield of target biologically active substances. Moreover, ultrasonic extraction can have a certain effect on the physicochemical properties of biologically active components. It has been established that ultrasonic treatment increases the yield of the most active substances of the plant, as polyphenols, which have a choleretic, anti-inflammatory, anti-allergic, antimicrobial, and vasodilatory effect compared to the traditional method. However, with an increase in the ultrasound power, the decomposition of some catechins and gallic acids begins (Zhu et al., 2018; Shen et al., 2023). This is due to the fact that at high ultrasound power, free radicals are formed in large quantities, which destroy polyphenols.

Optimal conditions for increasing the yield of polyphenols were observed in the ultrasound frequency range below 40 kHz (Dzah et al., 2020). Some studies have shown that under optimal conditions, not only does the amount of polyphenols increase, but also their antioxidant activity (Mehmood et al., 2019; Kwaw et al., 2018).

The following studies examined the effect of ultrasound on polysaccharides, which are an important group of biologically active substances. It was found that after such exposure, the molecular weight of these carbohydrates decreases, but the yield and biological activity increase.

Therefore, it is extremely important to select optimal conditions for ultrasound extraction to ensure the bioavailability of biocomponents.

In the present work, the process of ultrasound-assisted extraction of the root of the *Alhagi pseudalhagi* (Bieb.) Desv. (*A. pseudalhagi*). The plant has been modeled mathematically for the first time. Notoriously, the substances contained in this plant, flavonoids and alkaloids, have a high biological activity and are used in both indigenous and official medicine (Srivastava et al., 2014).

2. Materials and methods

Ultrasound-assisted extraction was carried out on a Bandelin Sonoplus HD 2200 homogenizer (Germany). The weighed portions of raw materials in the experiments made 5.0 g, the ratio of raw materials: extractant (hexane) made 1:5.

The chemical composition of the obtained dry extract was analyzed using a gas chromatograph (Agilent 7890A) coupled with a mass-selective detector.

3. Results

3.1. *Gas chromatography–mass spectrometric analysis of* A. pseudalhagi *roots*

The chemical composition of the extract derived from *A. pseudalhagi* roots via ultrasonic extraction was analyzed by gas chromatography–mass spectrometry (GC-MS) (Lytovchenko et al., 2009). Out of the 30 peaks detected in the chromatogram, 17 compounds were qualitatively and quantitatively identified using the Wiley spectral database. The extract is predominantly composed of gentriacontane (18.83%), β-sitosterol (18.13%), and lupeol (11.85%). Gentriacontane is a saturated hydrocarbon (alkane) consisting of 31 carbon atoms. Gentriacontane is widely used in the cosmetic industry as a cream component, serving as both an emollient and a skin-protective agent. Additionally, it is employed in the production of organogels formulated with vegetable oils, functioning as a structure-forming agent and solid carrier. Experimental data confirm that gentriacontane forms a microcrystalline structure, creating a stable three-dimensional network in oil-based media, making it ideal for use as a filler and emollient.

β-Sitosterol is a phytosterol widely distributed in various plant sources (Figure 1). It exhibits a broad spectrum of pharmacological activities, including anti-inflammatory, hypocholesterolemic, neuroprotective, anticancer, and antibacterial effects (Awad et al., 2000).

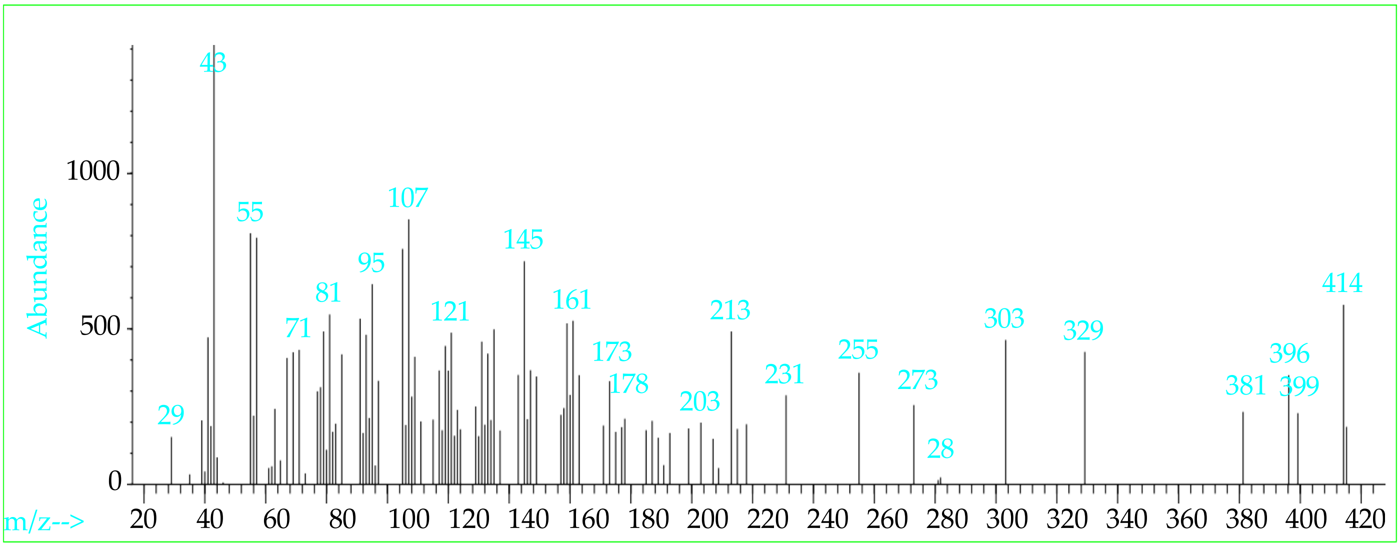

Figure 1. Mass spectrum of β-sitosterol

Lupeol is a pentacyclic triterpene, a natural organic compound with pronounced pharmacological activity **(**Figure 2**).** It is found in various medicinal plants, fruits, and resins. Lupeol exhibits anti-inflammatory activity (by inhibiting inflammatory mediators such as TNF-α, IL-β, and COX-2), as well as antimicrobial (effective against both Gram-positive and Gram-negative bacteria), antiprotozoal, antiproliferative, and anti-invasive effects (Liu et al., 2021).

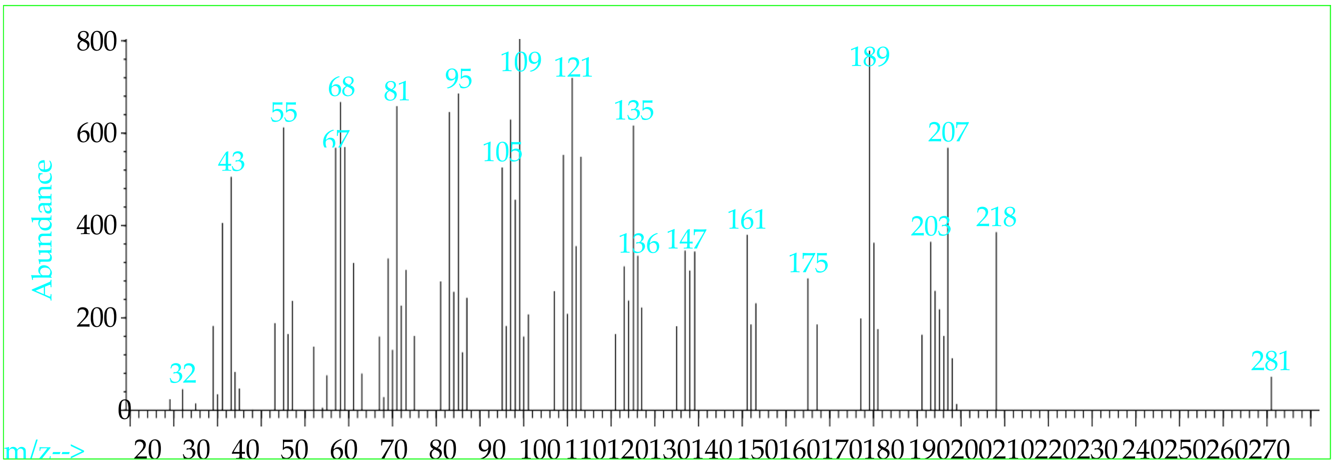

Figure 2. Mass spectrum of lupeol

The hexane extract contains fatty acids—a significant class of organic compounds with notable biological activity. Linolenic acid (5.79%) is an omega-3 fatty acid and an essential compound, as it is not synthesized by the human body (Sala-Vila et al., 2022). It supports cardiovascular, brain, and immune system health. Oleic acid (3.12%) lowers levels of "bad" cholesterol and improves the elasticity of cell membranes. Octadecanoic acid (0.83%) is used in the pharmaceutical industry as a base for ointments and suppositories.

Tetracosanoic acid (0.99%) is a component of the lipid membrane of cells. It is used in pharmaceuticals and cosmetics as an emollient, conditioning agent, and ointment base component.

3.2. Mathematical modeling of ultrasonic extraction of A. pseudalhagi roots

The effect of various factors (ultrasound power, sonication time, and temperature conditions) on the total extract yield obtained by ultrasonic extraction has been studied. The results are shown in Table 1.

Table 1. Effect of various factors on the extract yield of *A. pseudalhagi* roots

№	**Ultrasound power, W**	**Sonication time, min.**	**Temperature conditions, ^{0}C**	**Extract yield, mg**
1.	30	30	46	14.5
2.	60	30	47	13.4
3.	100	30	52	15.4
4.	30	10	40	12.7
5.	35	10	44	15.5
6.	40	20	42	14.5
7.	50	30	46	16.5
8.	60	20	47	17.2
9.	60	10	45	11.0
10.	70	20	46	18.5

To compile the regression equation of the extract, depending on the selected factors, methods of the experiment planning theory were used. Experiment planning is a procedure for choosing the number and conditions of experiments to solve the problem (creating a mathematical model of the object under study) (Anaya-Esparza et al., 2023).

In general, the mathematical description of the process can be presented as follows. Let the property (Y) of the object (in our case, the extract yield in mg) depends on several (n) independent variable factors ($x_1, x_2, ..., x_n$). The nature of this dependence is denoted as

$$Y=F(x_1, x_2, \dots, x_n) \quad (1)$$

The ‘’Y’’ value is called “response”, and the dependence itself, $Y = F(x_1, x_2, ..., x_n)$ - “response function”.

Independent variables $x_1, x_2, ..., x_n$ - otherwise factors, must be quantified. Factors can be of different dimensions and differ sharply in quantity.

The mathematical model of the process is a regression equation that connects the response function with factors (Assunção et al., 2023).

In our experiment, the regression equation is considered as the following polynomial:

$$Y = b_0 + \sum_{i=1}^{n} b_i X_i + \sum_{i,j=1}^{n} b_{ij} X_i X_j \quad (2)$$

Where b_0 is the free coefficient of the regression equation;

b_i – is the linear coefficient of the regression equation;

b_{ij} – matching coefficients or pairwise interaction effects.

Regression model coefficients are important in experiment design. Their absolute value indicates the degree of this factor’s effect on the response function, and the sign before the coefficient indicates the direction of the factor's action. Coefficients are determined as partial derivatives of the response function with respect to the corresponding variables (factors):

$$b_i = \frac{\partial Y}{\partial x_i}, \qquad b_{ij} = \frac{\partial^2 Y}{\partial x_i \partial x_j}, \qquad b_{ii} = \frac{\partial^2 Y}{\partial x^2} \tag{3}$$

Mathematical formalization and coding of variables (factors) are given below in Tables 2 and 3.

Table 2. List of factors included in the experiment

№	**Factor**	**Designations**	**Measurement unit**	**Variation range**
1	Ultrasound power	x_1	W	30÷100
2	Sonication time	x_2	min.	10 ÷30
3	Temperature	x_3	∘C	40 ÷52

The full factorial experiment starts with the coding operation. To begin with, the intervals of variation are selected (Table 3). Further, the coordinates of the plan center and the variation intervals are found, and then the encoding operation is performed.

Table 3. Factors coding

Factors	x_i	x_1	x_2	x_3
Upper level	x_i upper	100	30	52
Lower level	x_i lower	30	10	40
Basic level	$x_{i\,0}$	65	20	46
Variation interval	Δx_i	35	10	6

A three-factor experiment was carried out, where each factor has two levels. The main advantage of a factorial experiment is that all factors in the experiment are varied simultaneously. This leads to the fact that the variance in the estimation of the regression coefficients is *N* times less than the experimental error.

The algorithm for calculating a full factorial experiment of type 2^n (in this case, n = 3) is as follows:

1. Building a planning matrix
2. Calculation of the regression equation coefficients
3. Calculation of experimental error (repeatability variance)
4. Checking the significance of the regression coefficients
5. Choice of the form of the mathematical model

6. Checking the adequacy of the regression equation
7. Making decisions

As a result of three-factor planning of Full Factorial Design (FFD) 2^3 type (number of experiments - 8, factors change at two levels: upper and lower), a mathematical model of the process, taking into account the interaction of factors with each other, is obtained in the following form:

$$y=14.9+0.55x_1-0.5x_2+0.9x_3+1.5x_1x_3-0.55x_2x_3 \quad (4)$$

It should be emphasized that when performing a passive experiment, when replicates were not carried out, and an additional experiment in the planned centre was not set, obtaining the repeatability variance becomes practically impossible. In this case, the quality of approximation of the experimental data obtained by the approximate regression equation can be estimated by comparing the residual variance S^2_{res} and the ratio of the mean S^2_y by the Fisher criterion (Rashad et al., 2023), i.e.:

$$F_{cal}=\frac{S^2_y}{S^2_{res}} \quad (5)$$

where,

$$S^2_y=\frac{1}{N-1}\sum_{j=1}^{N}(y_{jэ}-y_э)^2 \quad (6)$$

$$y_э=\frac{1}{N}\sum_{j=1}^{N}y_{jэ} \quad (7)$$

$$S^2_{res}=\frac{1}{N-K-1}\sum_{j=1}^{N}(y_{jэ}-y_j)^2 \quad (8)$$

$f_1= N-1$ is the number of freedom degree in the ratio of the mean S^2_y,
$f_2= N-h$ is the number of freedom degree of the residual variance, $h=k+1$

Estimation of the equation coefficients (4) was carried out by formulas (5) - (8). Equation (4) includes significant regression coefficients that ensure its adequacy. Verification of the adequacy of the obtained equation is carried out by the standard method of comparing the tabular and calculated values of the Fisher criterion.

From equation (4), it follows that the extract yield is most affected by such factors as ultrasound power and temperature conditions. Sonication time has the least effect, and the nature of this effect is negative, i.e., with an increase in the sonication time, the extract yield decreases.

4. Discussion

Currently, work on the mathematical modeling of ultrasonic extraction is being carried out. For example, in this work (Uvidia Armijo et al., 2025), mathematical modeling of the process of ultrasonic extraction of *Annona muricata* L. leaves was carried out using the Elovich model. For this purpose, ultrasonic extraction was carried out at three temperatures (30, 40, and 50 °C) and six different time intervals (2, 5, 10, 20, 30, and 40 minutes). The kinetics of this process is described by the Elovich equation, i.e., the kinetics of the process are mathematically modeled. The accuracy of this model is estimated by the Pearson correlation coefficient between the experimental results and the predicted model. The Elovich model fits the experimental data, and the Pearson correlation coefficients correspond to the range of 0,997 and 0,998. This indicates that the model correctly predicts the extraction kinetics in the case under study.

In the following study (Reche et al., 2021), mathematical modeling of ultrasonic extraction of biologically active components from artichoke is carried out. The modeling is based on a quantitative description of the effect of temperature and ultrasound power density on the yield of biologically active substances, taking into account the simultaneous effect of diffusion and convection during ultrasonic extraction It was found that the effective diffusion coefficient increases with increasing temperature and the external mass transfer coefficient and the equilibrium yield of the extract depend on both the temperature and the ultrasound power.

In this paper (Abazi Bajrami et al., 2023), the kinetics of the extraction of biologically active compounds from the plant *Helichrysum arenarium* under the influence of ultrasound were investigated. Modeling of the extraction kinetics in two phases was carried out on the basis of mathematical interpretation of kinetically and diffusion-controlled processes.

This paper presents mathematical modeling of ultrasonic extraction of *Alhagi pseudalhagi* roots using the Full Factorial Design method. Mathematical modeling is based on a systematic, complex study of the influence of three factors (sound power, temperature, and time) on the yield of biologically active substances. This allows us to predict the results obtained with various combinations of factors, i.e., the yield of biocomponents, without prior experience.

5. Conclusion

The mathematical apparatus of a complete factorial experiment, i.e., when in the course of one experiment the values of all factors are varied simultaneously, allows for carrying out a computer experiment instead of costly full-scale ultrasonic extraction for production purposes (time, material costs, sometimes impossible) and to obtain a mathematical model of the process under consideration.

6. Supplementary Materials: No supplementary material.

7. Author Contributions

Conceptualization - G.B.; methodology - A.K.; software - A.T.; validation - B.T.; formal analysis - G.B.; investigation - A.K.; resources - S.S.; data curation - R.S.; writing - original draft preparation - B.T.; writing - review and editing - G.B.; visualization - P.K.; supervision - B.T.; project administration - R.S.; funding acquisition - G.B. All authors have read and agreed to the published version of the manuscript.

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Alhagi pseudalhagi-дің тамырын ультрадыбысты экстракциялау және оны математикалық модельдеу

Айжүз Көкораева, Ғалия Байсалова, Расул Сергибаев, Абзал Талтенов, Бикамила Торсықбаева, Пернегүл Құжатова, Сымбат Сансызбай

Аңдатпа. Қазіргі уақытта экстракция әдістерін өзгертуге және жетілдіруге бағытталған зерттеулер белсенді жүргізілуде. Бұл бағыттар кең ауқымды міндеттерді қамтиды -

техникалық жабдықты оңтайландыру мен экстрагенттерді таңдаудан бастап, үдерісті жүргізу шарттарын нақтылауға дейінгі аралықты қамтиды. Әсер етудің физикалық факторларын, атап айтқанда, ультрадыбысты қолдануға ерекше назар аударылады. Ультрадыбыстық экстракция табиғи шикізаттан биологиялық белсенді заттарды алудың болашағы зор әдістерінің бірі ретінде қарастырылады.
Бұл мақалада *Alhagi pseudalhagi* өсімдігінің тамырларын ультрадыбыстық әдіспен экстракциялау бойынша жүргізілген ғылыми зерттеудің нәтижелері ұсынылған. 30 химиялық қосылыс анықталды, олардың арасында бағалы биологиялық белсенді заттардың бар екені анықталды. GC-MS талдауының нәтижелері бойынша компоненттердің ең үлкен үлесі гентриаконтан (18,83%), β-ситостерол (18,13%) және лупеолға (11,85%) тиеселі болды.
Өсімдік шикізатынан экстрагентке диффузияланатына экстрактивті заттардың шығымына әсер ететін негізгі факторлар анықталды: ультрадыбыстың қуаты, ультрадыбыстық өңдеу ұзақтығы және температуралық режим. Осы факторлардың негізінде толық үш факторлы эксперимент жүргізілді. Нәтижесінде ультрадыбыстық экстракция процесінің математикалық моделі жасалды. Алынған регрессия теңдеуі экстракт шығымына көрсетілген факторлардың әсерін сандық бағалауға мүмкіндік береді.

Түйін сөздер: ультрадыбысты экстракция; ультрадыбыс қуаты; ультрадыбыстық өңдеу ұзақтығы; толық үш факторлы эксперимент; регрессия теңдеуі

Ультразвуковая экстракция корней *Alhagi pseudalhagi* и ее математическое моделирование

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Аннотация: В настоящее время активно проводятся исследования, направленные на модификацию и совершенствование методов экстракции. Эти направления охватывают широкий спектр задач - от оптимизации технического оснащения и выбора экстрагентов до уточнения условий проведения процесса. Особое внимание уделяется применению физических факторов воздействия, в частности, ультразвука. Ультразвуковая экстракция рассматривается как один из перспективных методов извлечения биологически активных веществ из природного сырья.
В данной статье представлены результаты научного исследования, посвящённого ультразвуковой экстракции корней *Alhagi pseudalhagi*. Химический состав экстракта, полученного методом ультразвуковой экстракции, изучен с использованием газ-хроматографии-масс-спектрометрии. Выявлено 30 химических соединений, среди которых установлено наличие ценных биологически активных веществ. По результатам ГХ-МС анализа наибольшую долю среди компонентов составили гентриаконтан (18,83%), β-ситостерол (18,13%) и лупеол (11,85%).
Определены основные факторы, влияющие на диффузию экстрактивных веществ из растительного сырья в экстрагент: мощность ультразвука, продолжительность ультразвуковой обработки и температурный режим. На основе этих факторов проведён полный трёхфакторный эксперимент. В результате разработана математическая модель процесса ультразвуковой экстракции. Полученное уравнение регрессии позволяет количественно оценить влияние указанных факторов на выход экстракта.

Ключевые слова: ультразвуковая экстракция; мощность ультразвука; время обработки ультразвуком; полный трехфакторный эксперимент; уравнение регрессии