Assessing protopectin transformation potential of plant tissue using a zoned criterion space

Vladimir V. Kondratenko1,* , Tatyana Yu. Kondratenko1, Andrey N. Petrov1, Georgy A. Belozerov2

1 Russian Research Institute of Canning Technology – branch of Gorbatov Federal Research Center for Food Systems at Russian Academy of Sciences, Vidnoye, Russia

2 Russian Scientific Research Institute of Refrigeration Industry – branch of Gorbatov Federal Research Center for Food Systems at Russian Academy of Sciences, Moscow, Russia

* e-mail: nauka@vniitek.ru

Received April 15, 2020; Accepted in revised form May 14, 2020; Published August 25, 2020

Abstract: Introduction. The existing diversity of plant raw materials and products predetermine the prospects of studying their potential as sources of pectin substances. However all current classifications are either fragmented or inconsistent. Study objects and methods. Our theoretical investigation aimed to develop an adequate classification for all taxa of plant origin, as well as their tissues and derivatives as pectin-containing materials. We developed criteria for assessing transformation potential of the protopectin complex based on the mass fractions of biologically active non-uronide components, native water-soluble pectin, the protopectin complex, and pectin substances. Individual boundary conditions were based on individual pectin potential, protopectin fragmentation potential, and pectin isolation potential. Results and discussion. Based on the boundary conditions, we defined an universal criterion space that included a set of points \( M \) in the coordinates expressed by three main criteria. According to individual boundary conditions, the criterion space was divided, or zoned, into four domains corresponding to protopectin fragmentation potential. They were characterized by: 1) lack of pectin potential, 2) ineffective protopectin fragmentation, 3) ineffective isolation of fragmentation products, and 4) effective isolation. Finally, we developed a generalized algorithm to determine the location of points \( M(\mu_1, \mu_2, \mu_3) \) in the zoned criterion space, characterizing the plant tissue. Conclusion. Our approach can be used to assess any plant tissue for its protopectin transformation potential, which determines the technological influence on its pectin potential. This approach is universal, i.e., applicable to both plant tissue and its derivatives.

Keywords: Protopectin complex, potential, transformation, evaluation system, criterion space

Funding: The materials were prepared as part of the government assignment to Gorbatov Federal Scientific Center for Food Systems at Russian Academy of Sciences.


INTRODUCTION

Food technology is currently striving to maximize the potential of raw materials and use new, non-traditional sources of essential nutraceuticals and food components with biological (antioxidants, enterosorbents, etc.) and/or technological (thickeners, stabilizers, etc.) functional activity [1, 2]. The most promising way to achieve that is a biotechnological approach that makes use of both living cultures of microorganisms and isolated enzyme systems. When using isolated enzyme systems, this approach involves a multiple stage fragmentation of a native supramolecular complex of plant and/or animal cell walls into target components with a wide range of physicochemical and/or technological properties [3–5].

One of the methods within this approach is to activate the potential of a multicomponent polymer matrix of cell walls and intercellular spaces. This method has a limited use in processing agricultural raw materials. It mainly consists in partial or complete
degradation (depolymerization) of its individual components to change the consistency or transparency of the final product, or to clear it of degradation products and improve its sensory characteristics. Most certainly, a targeted use of this polymer matrix is complicated by its highly heterogeneous components, a system of bonds between them, and highly entangled polymer chains [6]. Moreover, the heterogeneity of individual matrix components is a serious obstacle to controlling their properties during extraction [7, 8].

Pectin substances are among major carbohydrate biopolymers that have a wide variety of functional and technological characteristics [9, 10]. In a plant cell, they are represented by two main fractions – native water-soluble pectin and a native water-insoluble protopectin complex. The last one is the most valuable for transformation due to its molecular structure and composition [9].

The structure of cell walls in almost all terrestrial plants [6, 11, 12] makes them a potentially good resource for the industrial production of pectin. However, it is difficult to implement. Since the protopectin complex is a branched supramolecular structure incorporated into the cell wall, its transformation is mainly fragmentation into water-soluble polymers (soluble pectin). In addition, mass fractions of pectin substances and the protopectin complex may depend on the type, grade, and purpose of raw materials, their structure and phase of development, soil and weather conditions for their vegetation, as well as localization, duration and storage conditions, processing intensity, etc. [10, 13]. In this regard, the choice of a plant as a pectin-containing material should be determined by the purpose of its use.

Raw materials can be classified according to the size of their pectin potential – “high”, “medium,” and “small” (“low”, “insignificant”) [9, 10, 14]. The only fundamental approach to pectin production was offered by Donchenko in [15] and supplemented by Rodionova et al. in [19, 20] (works [16–18] are actually based on [15]). Although this approach is rather fragmented, it can be used as a basis for developing a universal system that takes into account the native pectin potential of plant tissue.

The protopectin complex is a key object whose fragmentation enables us to use the biomass of a plant material as a source of pectin substances. Due to the presence of certain plant organisms, mainly a natively soluble fraction of pectin, biomass can be attributed to potential sources of pectin. On the other hand, the biomass of certain taxonomic elements may contain a small amount of pectin, which makes its use ineffective.

Therefore, we found it relevant to develop a clear-cut classification of plant bio-resources into groups to determine the prospects of their use as pectin-containing raw materials.

In this regard, we aimed to develop a system of criteria for assessing the transformation potential of native complexes of plant carbohydrate biopolymers exemplified by pectin. To achieve this aim, we set the following objectives:

– working out criteria to assess the transformation potential of native plant biopolymers and the concept of their applicability, and

– developing a system of boundary conditions and an universal algorithm for classifying plant materials according to the transformation potential of their native pectin components.

**STUDY OBJECTS AND METHODS**

According to existing data, all plant materials can be classified into four main groups, namely:

– bio-resources with sufficient potential for protopectin fragmentation and subsequent isolation of its products as independent substances;

– bio-resources with sufficient potential for protopectin fragmentation, but with insufficient potential for isolation of its products;

– bio-resources with insufficient potential for protopectin fragmentation, but with sufficient potential for natively soluble pectin;

– bio-resources with no pectin potential.

On the one hand, this differentiation involves unifying plant characteristics and reducing them to certain generalized values. On the other hand, it involves dividing the domain of generalized values into four fixed zones. As we know, a universal tool for unifying an arbitrary set of source factors is a range of anonymized criteria reducible to a certain system with the use of boundary conditions [21, 22]. Thus, we can apply a criteria-based approach to fulfilling our objectives.

To be able to scale the criteria to determine clear boundary conditions, we used Harrington’s individual desirability function in its canonical form [23]:

$$d_i = e^{-x \cdot \phi(b_i)}$$  \hspace{1cm} (1)

where $d_i$ is the dimensionless value of Harrington’s individual desirability function; $b_i$ is the constant; $b_{i0}$ is the coefficient; and $\phi$ is the dimensionless operator of Harrington’s individual desirability function.

We introduced the first and second individual criteria for protopectin fragmentation potential among the main criteria to assess the native pectin potential.

Let us begin with the first criterion. According to [7, 8], the presence of pectin in the tissue or a certain amount of protopectin in the cell wall matrix is not sufficient for assessing the native pectin potential of plant tissue. The tissues of many plant organisms also contain a significant amount of organic and mineral components with valuable vitamins and antioxidant activity, pronounced aroma, micro- and macronutrient values, etc. [17]. They are also highly sensitive to active technological impact factors. During protopectin fragmentation, organic and mineral components can enter into uncontrolled interactions, resulting in a partial or complete loss of their biological potential. Therefore,
when assessing the native pectin potential, we should take into account the presence of these biologically active components among other significant factors.

Thus, we decided a complex operator as an independent variable, taking into account mass fractions of protepectin and biologically active components in the tissue:

\[ \phi_i = \frac{\omega_{pp}}{\omega_{pp} + \omega_{avp}} \]  
(2)

where \( \omega_{pp} \) is the mass fraction of protepectin, mg in 100 g; \( \omega_{av} \) is the mass fraction of the \( i \)-th biologically active component, mg/100 g; and \( \lambda \) is the number of biologically active components in the tissue (\( \lambda \in \mathbb{N} \)).

To apply this operator in practice, we transformed it as follows:

\[ \phi_i = \frac{1}{\sum_{i=1}^{\lambda} \frac{\omega_i}{\omega_{pp}}} = \frac{1}{\mu_i + 1} \]  
(3)

where

\[ \mu_i = \sum_{i=1}^{\lambda} \frac{\omega_i}{\omega_{pp}} \]  
(4)

Thus \( \mu_i \) is the first dimensionless individual criterion of protepectin fragmentation potential.

As we can see, with all possible values of \( \omega_{pp} \) and \( \sum_{i=1}^{\lambda} \omega_i \), this criterion has the following range of definition:

\[ \mu_i \in [0; \infty) \]  
(5)

In this case, Harrington’s individual desirability function can be expressed as:

\[ d_i = e^{-\left(b_{11} \cdot \frac{\omega_i}{\omega_{pp}} \right)} = e^{-\frac{\omega_i}{\omega_{pp}}} \]  
(6)

where \( d_i \) is the dependent dimensionless variable; \( b_{0} \) is the empirical dimensionless constant; and \( b_{11} \) is the empirical dimensionless coefficient.

To determine the numerical values of \( b_{0} \) and \( b_{11} \), we had to set the primary relations between the pairs \( \{\mu_i; d_i\} \) and \( \{\mu_{12}; d_{12}\} \), for which we proceeded from the following considerations.

If an \( i \)-th biologically active component has a specific measure of value \( p_i \), the total measure of value for all biologically active components under consideration is:

\[ v_{bac} = \sum_{i=1}^{\lambda} m_i \cdot p_i = \frac{m}{100} \sum_{i=1}^{\lambda} \omega_{np} \cdot p_i \]  
(7)

where \( v_{bac} \) is the total measure of value for all biologically active components, units; \( m_i \) is the mass of the \( i \)-th component, mg/100 g of plant tissue; \( m \) is the tissue mass, mg; \( p_i \) is the specific measure of value of the \( i \)-th component, units/mg; and \( \omega_{np} \) is the mass fraction of the \( i \)-th component in the plant tissue, %.

If specific measures of value for the components are expressed through some average specific measure of value then formula (7) looks as follows:

\[ v_{bac} = \frac{m}{100} \sum_{i=1}^{\lambda} \omega_{np} \cdot p_{av} \]  
(8)

where \( v_{bac} \) is the total measure of protepectin value, units; \( m_{pp} \) is the total mass of protepectin in the tissue, mg; \( p_{pp} \) is the specific measure of protepectin value, units/mg; and \( \omega_{pp} \) is the mass fraction of the \( i \)-th component in the plant tissue, %.

From Eq. (11), it follows that

\[ \omega_{pp} = \frac{v_{bac} \cdot 100}{m_{pp} \cdot p_{pp}} \]  
(9)

If we apply similar considerations to protepectin, then:

\[ v_{pp} = m_{pp} \cdot p_{pp} = \frac{m \cdot \omega_{pp} \cdot p_{pp}}{100} \]  
(10)

where \( v_{pp} \) is the total measure of protepectin value, units; \( m_{pp} \) is the mass of protepectin in the tissue, mg; \( p_{pp} \) is the specific measure of protepectin value, units/mg; and \( \omega_{pp} \) is the mass fraction of the \( i \)-th component in the plant tissue, %.

Respectively, if \( v_{bac} \) , protepectin fragmentation makes no sense, even with its significant amount in the tissue. Therefore, a prerequisite for protepectin fragmentation is:

\[ \mu_i \leq \frac{v_{pp}}{v_{bac}} \]  
(11)

If \( p_{av} \) is expressed as \( \bar{p}_{av} \) – in fractions of \( p_{pp} \) – then condition (15) looks as follows:

\[ \mu_i \leq \frac{1}{\bar{p}_{av}} \]  
(12)

When calculating \( \bar{p}_{av} \), it is advisable to use \( \bar{p}_i \) rather than \( p_i \), its value reduced to \( p_{pp} \):

\[ \bar{p}_{av} = \frac{p_{av}}{p_{pp}} = \frac{\sum_{i=1}^{\lambda} m_i \cdot \bar{p}_i}{\sum_{i=1}^{\lambda} m_i} \]  
(13)

Theoretically, \( \bar{p}_{av} \) can be determined using several approaches. However, we believe that the most appropriate approach is based on a daily human need for individual nutrients. This approach is least opportunistic (compared to the financial approach) and subjective (compared to direct expert assessments). Naturally, daily
Table 1 Specific measures of value for biologically active components and pectin in 100 g of plant tissue

<table>
<thead>
<tr>
<th>Component</th>
<th>Recommended daily requirement, units</th>
<th>Estimated daily requirement</th>
<th>Specific measure of value, mg⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mg</td>
<td>mg/kg</td>
<td>( n )</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Protein, g</td>
<td>800.00•</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Amino acids, mg/kg•</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>– essential amino acids:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>histidine</td>
<td>14</td>
<td>0.071428571</td>
<td>2.198</td>
</tr>
<tr>
<td>isoleucine</td>
<td>19</td>
<td>0.052631579</td>
<td>1.619</td>
</tr>
<tr>
<td>leucine</td>
<td>42</td>
<td>0.023809524</td>
<td>0.733</td>
</tr>
<tr>
<td>lysine</td>
<td>38</td>
<td>0.026315789</td>
<td>0.81</td>
</tr>
<tr>
<td>methionine</td>
<td>13.16•</td>
<td>0.075987842</td>
<td>2.338</td>
</tr>
<tr>
<td>phenylalanine + tyrosine</td>
<td>27</td>
<td>0.037037037</td>
<td>1.14</td>
</tr>
<tr>
<td>threonine</td>
<td>16</td>
<td>0.0625</td>
<td>1.923</td>
</tr>
<tr>
<td>tryptophan</td>
<td>4</td>
<td>0.25</td>
<td>7.692</td>
</tr>
<tr>
<td>valine</td>
<td>19</td>
<td>0.052631579</td>
<td>1.619</td>
</tr>
<tr>
<td>cysteine</td>
<td>5.84•</td>
<td>0.171232877</td>
<td>5.269</td>
</tr>
<tr>
<td>– non-essential amino acids</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>– other amino acids</td>
<td>87.85•</td>
<td>0.011383039</td>
<td>0.35</td>
</tr>
<tr>
<td>Lipids, g•</td>
<td>69.9</td>
<td>69 900</td>
<td>1 075.38</td>
</tr>
<tr>
<td>– saturated fatty acids</td>
<td>21.2</td>
<td>21 200</td>
<td>326.15</td>
</tr>
<tr>
<td>– monounsaturated fatty acids</td>
<td>25.4</td>
<td>25 400</td>
<td>390.77</td>
</tr>
<tr>
<td>– polyunsaturated fatty acids</td>
<td>23.3</td>
<td>23 300</td>
<td>358.46</td>
</tr>
<tr>
<td>Digestible carbohydrates, g•</td>
<td>275</td>
<td>275 000</td>
<td>4 230.77</td>
</tr>
<tr>
<td>Pectin, g•</td>
<td>2</td>
<td>2 000</td>
<td>30.77</td>
</tr>
<tr>
<td>Minerals•</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>– Ca, mg</td>
<td>1 000</td>
<td>1 000</td>
<td>15.3846</td>
</tr>
<tr>
<td>– Mg, mg</td>
<td>400</td>
<td>400</td>
<td>6.15385</td>
</tr>
<tr>
<td>– K, mg</td>
<td>2 500</td>
<td>2 500</td>
<td>38.46154</td>
</tr>
<tr>
<td>– Na, mg</td>
<td>1 300</td>
<td>1 300</td>
<td>20</td>
</tr>
<tr>
<td>– P, mg</td>
<td>800</td>
<td>800</td>
<td>12.30769</td>
</tr>
<tr>
<td>– Cl, mg</td>
<td>2 300</td>
<td>2 300</td>
<td>35.38462</td>
</tr>
<tr>
<td>– Fe, mg</td>
<td>14.4</td>
<td>14.4</td>
<td>0.22154</td>
</tr>
<tr>
<td>– Zn, mg</td>
<td>12</td>
<td>12</td>
<td>0.18462</td>
</tr>
<tr>
<td>– J, µg</td>
<td>150</td>
<td>0.15</td>
<td>0.00231</td>
</tr>
<tr>
<td>– Cu, mg</td>
<td>1</td>
<td>1</td>
<td>0.01538</td>
</tr>
<tr>
<td>– Mn, mg</td>
<td>2</td>
<td>2</td>
<td>0.03077</td>
</tr>
<tr>
<td>– Se, µg</td>
<td>63</td>
<td>0.063</td>
<td>0.00097</td>
</tr>
<tr>
<td>– Cr, µg</td>
<td>50</td>
<td>0.05</td>
<td>0.00077</td>
</tr>
<tr>
<td>– Mo, µg</td>
<td>70</td>
<td>0.07</td>
<td>0.00108</td>
</tr>
<tr>
<td>– Co, µg</td>
<td>10</td>
<td>0.01</td>
<td>0.00015</td>
</tr>
<tr>
<td>– Si, mg</td>
<td>30</td>
<td>30</td>
<td>0.46154</td>
</tr>
<tr>
<td>– F, mg</td>
<td>4</td>
<td>4</td>
<td>0.06154</td>
</tr>
<tr>
<td>Vitamins and provitamin•</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>– water soluble</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ascorbic acid (vitamin C), mg</td>
<td>90</td>
<td>90</td>
<td>1.38462</td>
</tr>
<tr>
<td>thiamine (vitamin B₁), mg</td>
<td>1.5</td>
<td>1.5</td>
<td>0.02308</td>
</tr>
<tr>
<td>riboflavin (vitamin B₂), mg</td>
<td>1.8</td>
<td>1.8</td>
<td>0.02769</td>
</tr>
<tr>
<td>vitamin B₆, mg</td>
<td>2</td>
<td>2</td>
<td>0.03077</td>
</tr>
<tr>
<td>vitamin B₁₂, µg</td>
<td>3</td>
<td>0.003</td>
<td>20000</td>
</tr>
<tr>
<td>niacin, mg</td>
<td>20</td>
<td>20</td>
<td>0.30769</td>
</tr>
<tr>
<td>pantothenic acid, mg</td>
<td>5</td>
<td>5</td>
<td>0.07692</td>
</tr>
<tr>
<td>biotin, µg</td>
<td>50</td>
<td>0.05</td>
<td>0.00077</td>
</tr>
<tr>
<td>folic acid and folates, µg</td>
<td>400</td>
<td>0.4</td>
<td>0.00615</td>
</tr>
<tr>
<td>– fat soluble</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>carotenoids, mg</td>
<td>5</td>
<td>5</td>
<td>0.07692</td>
</tr>
<tr>
<td>vitamin D, µg</td>
<td>10</td>
<td>0.01</td>
<td>0.00015</td>
</tr>
</tbody>
</table>

\( n \) - Estimated daily requirement, \( P_f \) - Specific measure of value, mg⁻¹.
requirements for certain components depend on our knowledge of biochemical processes in the human body, as well as on the constantly changing environmental situation in the world [24]. However, these factors should not significantly affect \( p_{av} \).

The value of \( p_{av} \) was calculated in several stages.

At the first stage, we determined daily requirements for each of the biologically active components \( (u_i) \) and pectin \( (u_{ps}) \) based on a daily energy requirement of 2000 kcal and an average body weight of 65 kg. The differences in daily requirements for men and women were averaged. For comparability, all the values were presented in mg/kg of body weight.

At the second stage, we calculated specific measures of value for biologically active components \( (p_i) \) and pectin \( (p_{ps}) \):

\[
\begin{align*}
    p_i &= u_i^{-1} \\
    p_{ps} &= u_{ps}^{-1}
\end{align*}
\]  
(18)  
(19)

The specific measures of value for pectin \( p_{ps} \) and protopectin \( p_{pp} \) were numerically identical since protopectin is only valuable for the human body in the form of its fragmentation products. To simplify, we assumed that processing resulted in all protopectin fragmented in a targeted manner (i.e., into fragments that could be identified as pectin).

At the third stage, we determined specific measures of value in the fractions of the specific measure of pectin values \( p_{av} \).

The calculation results are shown in Table 1.

At the fourth stage, we calculated the value of \( p_{av}^{-1} \) (Table 2). Based on the data in [31], we determined the content of biologically active components in 100 g of tissue for 21 types of plant materials from the classification presented in [16]. For each type of raw material, formula (17) was used to calculate the values of \( p_{av}^{-1}(j) \) and \( p_{av}^{-1}(i) \), where \( j \in N \).

Some assumptions were made in the calculations. For example, the mass fractions of the components which were not available in the database were assumed as equal to zero [31]. The amount of carotenoids was calculated based on the biological potential of each type of raw material as \( m_{av} = m_{\beta - car} + \frac{1}{2} \sum m_{n - com} \) where \( m_{\beta - car} \) is the mass fraction of \( \beta \)-carotene, mg/100 g; \( \sum m_{n - com} \) is the sum of mass fractions of other carotenoids, mg/100 g [24]. The amount of tocopherols was also calculated taking into account the biological potential of each type of raw material as \( m_{av} = m_{\alpha - toc} + m_{\gamma - toc} \) where \( m_{\alpha - toc} \) and \( m_{\gamma - toc} \) are the mass fractions of \( \alpha \) - and \( \gamma \)-tocopherols, respectively; mg/100 g [24]. To determine the sum of the remaining amino acids, we subtracted the mass fractions of essential and non-essential amino acids from the mass fraction of protein.

The calculation results are shown in Table 2.

Since \( p_{av}^{-1}(j) \) values were significantly different for different types of raw materials, we calculated the average \( p_{av}^{-1}(av) \) and the margin of error \( \Delta \) to determine boundary values \( (\mu_1, \mu_2) \):

\[
\begin{align*}
    p_{av}^{-1}(av) &= \sum_{j=1}^{\zeta} p_{av}^{-1}(j) \\
    \Delta &= \left( \mu_1, \mu_2 \right) \sqrt{\sum_{j=1}^{\zeta} \left( p_{av}^{-1}(j) - p_{av}^{-1}(av) \right)^2} \\
    &= \left( \mu_1, \mu_2 \right) \left( \zeta - 1 \right)
\end{align*}
\]

(20)  
(21)

where \( \zeta \) is the number of raw material types; \( t(\alpha; \zeta - 1) \) is Student’s t-test; and \( \alpha \) is the probability of error (0.05).

Based on the above, the value of \( \mu_1 \) for the first pair \( \{\mu_1; d_{11}\} \) was calculated as:
The value of $\mu_{12}$ for the second pair $\{\mu_{12}; d_{12}\}$ was calculated as the second order of $\mu_{11}$:

$$\mu_{12} = \left(\bar{p}_{av(1)} - \Delta \right)^2$$

(23)

The critical (boundary) values of $\mu_i$ were based on the analysis of Harrington’s desirability function, using $\mu_{11}$ and $\mu_{12}$ as reference values. Since they are preset, the calculated values were rounded to the nearest whole number.

Despite the rigor of expression (16), its right-hand side is an empirical value based on the chemical composition of a finite number of plant raw materials and, therefore, it cannot be considered a priori. To make up for this feature, we further determined the critical values of $\mu_i$ on the basis of Harrington’s desirability function, using $\mu_{11}$ and $\mu_{12}$ as reference values.

Since a smaller reference value corresponded to a larger value of Harrington’s individual desirability function, we defined a condition $\text{Cond}_{d_i}$ that determined the individual form of the function as:

$$\text{Cond}_{d_i} = \left[ \frac{d_{11}}{\mu_{11}} < \frac{0.60}{3}; \frac{d_{12}}{\mu_{12}} < \frac{0.40}{10} \right]$$

(24)

Based on $\text{Cond}_{d_i}$, we calculated the values of the constant and the coefficient: $b_{h1} = -0.246; b_{h1} = 3.673$.

The critical values of the first criterion for the protopectin fragmentation potential at the points with standard critical values of the desirability function can be calculated using Eq. (6) with the variable $\mu_i$:

$$\mu_i[D_i] = -1 - \frac{h_1}{h_{h0} + \ln[-\ln(d_{11})]}$$

(25)

where $\mu_i[D_i]$ is the value of the criterion $\mu_i$ at the critical
point $D_i$ of Harrington’s individual desirability function determined by Eq. (6) and corresponding to $d_i$; and $d_i$ is the standard $i$-th critical (canonical) value $d_i$ of Harrington’s individual desirability function.

The graphic interpretation of Harrington’s individual desirability function corresponding to the condition $Cond_{d_i}$ is given in Fig. 1. For each value of $d_i$, we determined the corresponding values of $\mu_i[D_i]$.

As we can see, the $\mu_i$ range of definition includes four domains separated by the critical values of $\mu_i[D_i]$, where $i = 1, 2, 3$. By definition, domain IV includes those $\mu_i$ values at which the fragmentation of the protopectin complex makes no sense due to a low value of the individual function of desirability.

Domain III covers those $\mu_i$ values at which the individual desirability function is large enough for protopectin fragmentation to make sense, but insufficiently large to neglect non-uronide bioactive components and isolate the products of fragmentation.

In domains I and II, the individual desirability function is so large that the content of non-uronide bioactive components in plant tissue can be completely ignored.

Based on the physical meaning of the boundary conditions for $\mu_i$, we established two individual boundary conditions that partially determined the native pectin potential of plant tissue.

Boundary condition I:
- $\mu_i > \mu_i[D_i]$ means the absence of the first individual potential for protopectin fragmentation;
- $\mu_i \leq \mu_i[D_i]$ means the presence of the first individual potential for isolation of protopectin fragmentation products.

Boundary condition II:
- $\mu_i[D_i] \geq \mu_i[D_1]$ means the absence of the first individual potential for isolation of protopectin fragmentation products;
- $\mu_i \leq \mu_i[D_2]$ means the presence of the first individual potential for isolation of protopectin fragmentation products.

Next, we determined the structure and properties of the second dimensionless individual criterion for the protopectin fragmentation potential.

The second independent variable was a complex operator based on the mass fraction of protopectin in the tissue:

$$\varphi_2 = \frac{\sigma_{pp}}{100} = \mu_2$$  \hspace{1cm} (26)

where $\varphi_2$ is the dimensionless operator of Harrington’s individual desirability function; and $\mu_2$ is the second dimensionless individual criterion for the protopectin fragmentation potential.

Harrington’s individual desirability function was expressed as:

$$d_2 = e^{-e^{-(\varphi_2+b_{12})}} = e^{-e^{-(b_{20}+b_{21} \varphi_2)}}$$  \hspace{1cm} (27)

Thus, the condition $Cond_{d_2}$ that determined the individual function was set as:

$$Cond_{d_2} = \begin{bmatrix} d_{21} \equiv 0.35 \\ d_{22} \equiv 0.65 \\ \mu_{21} \equiv 0.001 \\ \mu_{22} \equiv 0.05 \end{bmatrix}$$  \hspace{1cm} (28)

Based on $Cond_{d_2}$, we calculated the values of the constant and the coefficient: $b_{20} = -6.68 \times 10^{-2}$ and $b_{21} = 18.179$. The critical values of the $\mu_2$ criterion were calculated as:

$$\mu_2[D_i] = \frac{b_{20} + \ln\left[\left(-\ln(d_{2i})\right)\right]}{b_{21}}$$  \hspace{1cm} (29)

where $\mu_2[D_i]$ is the value of $\mu_2$ at the critical point $D_i$ of Harrington’s individual desirability function calculated by Eq. (6) and corresponding to $d_{2i}$; $d_{2i}$ is the standard $i$-th critical (canonical) value $d_i$ of Harrington’s individual desirability function.

![Figure 2](image-url)  \hspace{1cm} Figure 2 Graphic interpretation of Harrington’s individual desirability function given condition $Cond_{d_2}$ and variable $\mu_2
The graphic interpretation of Harrington’s individual desirability function corresponding to the condition \( \text{Cond}_{d_i} \) is presented in Fig. 2. For each value of \( d_{2i} \), we calculated the corresponding values of \( \mu_2[D_i] \).

Just like with \( \mu_1 \), the \( \mu_2 \) range of definition includes four domains separated by the critical values of \( \mu_2[D_i] \), where \( i = 1, 2, 3 \).

By definition, domain IV covers those values of \( \mu_2 \) at which the fragmentation of the pectin complex makes no sense. This led us to formulate the third individual boundary condition:

- \( \mu_2 < \mu_2[D_i] \) means the absence of the second individual potential for pectin fragmentation;
- \( \mu_2 \geq \mu_2[D_i] \) means the presence of the second individual potential for pectin fragmentation.

We should note that fragmentation potentials I and II are categorical, i.e., if one of them is absent, the total fragmentation potential is absent as well.

Domains I, II, and III include such values of \( \mu_2 \) that ensure not only pectin fragmentation, but also the isolation of fragmentation products. Based on the canonical reference values of the individual desirability function, we formulated the fourth boundary condition:

- \( \mu_2 \geq \mu_2[D_i] \) means the absence of the second individual potential for isolation of pectin fragmentation products;
- \( \mu_2 < \mu_2[D_i] \) means the presence of the second individual potential for isolation of pectin fragmentation products.

Similar to the first and the second fragmentation potentials, the individual isolation potentials are categorical.

The third independent variable was a complex operator based on the mass fraction of pectin substances in the tissue:

\[
\phi_3 = \frac{\omega_{ps}}{100} = \mu_3 \tag{30}
\]

where \( \phi_3 \) is the dimensionless operator of Harrington’s individual desirability function; \( \omega_{ps} \) is the total amount of pectin substances, %; and \( \mu_3 \) is the third dimensionless individual criterion for the pectin fragmentation potential.

In this case, the condition \( \text{Cond}_{d_i} \) that determined the individual function was calculated as:

\[
\text{Cond}_{d_i} = \left[ \frac{d_{3i} \geq 0.40}{0.01} \frac{d_{32} \geq 0.65}{0.07} \right] \quad \tag{31}
\]

Based on expression (31), we calculated the constant and the coefficient as \( b_{30} = -3.8367 \times 10^{-2} \) and \( b_{31} = 12.5788 \), respectively, and the critical boundaries of \( \mu_3 \) as:

\[
\mu_3[D_i] = -\frac{b_{30} + \ln[-\ln(d_{3i})]}{b_{31}} \tag{32}
\]

where \( \mu_3[D_i] \) is the value of \( \mu_3 \) at the critical point \( D_i \) of Harrington’s individual desirability function calculated by (6) and corresponding to \( d_{30} \); and \( d_{3i} \) is the standard \( i \)-th critical (canonical) value \( d_i \) of Harrington’s individual desirability function.

Figure 3 shows the graphic interpretation of Harrington’s individual desirability function given \( \text{Cond}_{d_i} \). For each value of \( d_{4i} \), we calculated the corresponding values of \( \mu_4[D_i] \).

Here, we can clearly see domain IV with no pectin potential in the plant tissue.

As a result, we formulated the fifth individual boundary condition:

- \( \mu_4 < \mu_4[D_i] \) means the absence of pectin potential;
- \( \mu_4 \geq \mu_4[D_i] \) means the presence of pectin potential.

Thus, the pectin potential is categorical.

The fourth independent variable was a complex operator based on the ratio of the mass fractions of pectin and pectin substances in the tissue:

\[
\phi_4 = \frac{\omega_{pp}}{\omega_{sp}} = \frac{1}{\mu_4 + 1} \tag{33}
\]

where \( \phi_4 \) is the dimensionless operator of Harrington’s individual desirability function; \( \omega_{pp} \) is the mass fraction of natively soluble pectin substances, %; and \( \mu_4 \) is the third dimensionless individual criterion for the pectin fragmentation potential calculated as:

\[
\mu_4 = \frac{\omega_{pp}}{\omega_{sp}} \tag{34}
\]

Then, the condition \( \text{Cond}_{d_i} \), which determined the individual function, was calculated as:

\[
\text{Cond}_{d_i} = \left[ \frac{d_{4i} \geq 2.50}{0.65} \frac{d_{42} \geq 1.25}{0.80} \right] \quad \tag{35}
\]

Based on expression (35), we calculated the constant and the coefficient \( b_{40} = -0.3419 \), \( b_{41} = 4.1441 \).

Based on \( \text{Cond}_{d_i} \), the critical boundaries of \( \mu_4 \) were calculated as:

\[
\mu_4[D_i] = -1 - \frac{b_{41}}{b_{40} + \ln[-\ln(d_{4i})]} \tag{36}
\]

where \( \mu_4[D_i] \) is the value of \( \mu_4 \) at the critical point \( D_i \) of Harrington’s individual desirability function calculated by (6) and corresponding to \( d_{4i} \); and \( d_{4i} \) is the standard \( i \)-th critical (canonical) value \( d_i \) of Harrington’s individual desirability function.

Figure 4 shows the graphic interpretation of Harrington’s individual desirability function given \( \text{Cond}_{d_i} \), with \( d_{4i} \) values corresponding to \( \mu_4[D_i] \) values.

Based on the logical content of \( d_{4i} \) and the numerical values of \( \mu_4[D_i] \), the range of definition can be divided into four domains that determine the fragmentation potential of the pectin complex and the isolation potential of fragmentation products.

According to Fig. 4, domain IV covers those values \( \mu_4 \) at which the mass fraction of water-soluble pectin exceeds that of the pectin complex so much that there is practically no reason for its individual fragmentation. Thus, we determined the sixth boundary condition as follows:

- \( \mu_4 > \mu_4[D_i] \) means the absence of the third individual potential for pectin fragmentation;
- \( \mu_4 \leq \mu_4[D_i] \) means the presence of the third individual potential for pectin fragmentation.
Following the same pattern, we determined the seventh boundary condition (VII), namely:

- \( \mu_3[D_3] < \mu_4 \leq \mu_3[D_3] \) means the absence of the third individual potential for isolation of protopectin fragmentation products;
- \( \mu_3 \leq \mu_4[D_3] \) means the presence of the third individual potential for isolation of protopectin fragmentation products.

In addition, boundary conditions VI and VII are based on:

\[
\mu_4 \leq \mu_4[D_i]
\]  

where \( i = 3 \) for condition VI and, \( i = 2 \) for condition VII. However, \( \mu_4 \) can be expressed as:

\[
\mu_4 = \frac{\omega_{ps}}{\omega_{pp}} = \frac{\omega_{ps} - \omega_{pp}}{\omega_{pp}} = \frac{\mu_3 - \mu_2}{\mu_2}
\]

Then, given the presence of the third individual fragmentation potential:

\[
\mu_3 \leq \mu_2 \cdot (\mu_4[D_i] + 1)
\]  

Thus, the third individual potentials of fragmentation and isolation are relative since they are involved in the formation of respective total potentials indirectly,
through expressions in which they act as one of the variables.

If we assume that there is a certain criterion space with coordinates \( \mu_1, \mu_2 \) and \( \mu_3 \), the pectin potential of any plant material can be clearly determined as a geometrical location of the point \( M[\mu_1, \mu_2, \mu_3] \) corresponding to the material under analysis.

Based on the \textit{a priori} assumption that

\[
\omega_{ps} + \sum_{j=1}^{4} \omega_j \leq 100 \quad (40)
\]

we can establish the eighth boundary condition (VIII): the top boundary of the range of definition for all possible values of \( M[\mu_1, \mu_2, \mu_3] \) is determined by the following basic proposition:

\[
\mu_{3(top)} = 1 - \mu_2 \quad (41)
\]

In addition, since a part cannot be larger than a whole, it is also true that:

\[
\omega_{pp} \leq \omega_{ps} \quad (42)
\]

which leads to the following condition:

\[
\mu_3 \geq \mu_2 \quad (43)
\]

i.e., the bottom boundary of the range of definition for all possible values of \( M[\mu_1, \mu_2, \mu_3] \) is determined by the second basic proposition:

\[
\mu_{3(bot)} = \mu_2 \quad (44)
\]

The last formula is an expression of boundary condition IX.

**RESULTS AND DISCUSSION**

Thus, according to boundary conditions VIII and IX, a set \( A \) of all points \( M[\mu_1, \mu_2, \mu_3] \) can be defined as

\[
M[\mu_1, \mu_2, \mu_3] \in [\mu_{3(bot)}, \mu_{3(top)}] \bigg|_{\mu_3 \geq \mu_2; \mu_3 \geq 0; \mu_3 \leq 100} \quad (45)
\]

graphically presented in Fig. 5.

The logic of assessing plant bioresources for the presence of pectin substances determines general boundary conditions for defining a set of points \( M[\mu_1, \mu_2, \mu_3] \) as the following hierarchy: “individual pectin potential \( \rightarrow \) individual fragmentation potential of the protopectin complex \( \rightarrow \) individual isolation potential of protopectin fragmentation products”. Thus, the entire set of points \( M[\mu_1, \mu_2, \mu_3] \) can be divided into four subsets:

- subset \( A_1 \) characterized by the absence of a common pectin potential in all the elements;
- subset \( A_2 \) where \( A_1 \cap A_2 = \emptyset \) and all the elements have a common pectin potential, but lack a common potential for protopectin fragmentation;
- subset \( A_3 \) where \( A_2 \cap A_3 = \emptyset \) and all the elements have common pectin and protopectin fragmentation potentials, but lack a common isolation potential for fragmentation products; and
- subset \( A_4 \) where \( A_3 \cap A_4 = \emptyset \) and all elements have common pectin and protopectin fragmentation potentials, as well as isolation potential for fragmentation products.

By definition, the following is true for all the subsets:

\[
A_1 \cap A_2 \cap A_3 \cap A_4 = \emptyset \quad (46)
\]

Based on the above, the existence of \( A_j \) corresponds to:

\[
\mu_2 \leq \mu_3 < \mu[M[D_1]] \quad (47)
\]

The area of definition for all \( A_j \) elements is partially presented in Fig. 6.

The existence of subset \( A_j \) corresponds to:

\[
\begin{align*}
1 - \mu_1 \cdot \mu_2 & \geq \mu_3 \\
\mu_2 \cdot (\mu_4[D_1] + 1) & \geq \mu_3 \\
\mu_1[D_1], \mu_2 < \mu[M[D_1]] & \geq \mu[M[D_1]]
\end{align*}
\]

\[
\mu_2 \cdot (\mu_4[D_1] + 1) \geq \mu[M[D_2]]
\]

Figure 7 shows a partial area of definition for all \( A_j \) elements.

The existence of \( A_j \) corresponds to:

\[
\begin{align*}
1 - \mu_1 \cdot \mu_2 & \geq \mu_3 \\
\mu_2 \cdot (\mu_4[D_1] + 1) & \geq \mu_3 \\
\mu_1[D_1], \mu_2 < \mu[M[D_1]] & \geq \mu[M[D_1]]
\end{align*}
\]

\[
\mu_2 \cdot (\mu_4[D_2] + 1) \geq \mu[M[D_2]]
\]

Figure 8 presents the area of definition for all \( A_j \) elements.

The existence of subset \( A_j \) corresponds to:

\[
\begin{align*}
1 - \mu_1 \cdot \mu_2 & \geq \mu_3 \\
\mu_2 \cdot (\mu_4[D_2] + 1) & \geq \mu_3 \\
\mu_1[D_1], \mu_2 < \mu[M[D_1]] & \geq \mu[M[D_1]]
\end{align*}
\]

\[
\mu_2 \cdot (\mu_4[D_2] + 1) \geq \mu[M[D_2]]
\]

The area of definition for all \( A_j \) elements is presented in Fig. 9.

Thus, the specific value \( M[\mu_1, \mu_2, \mu_3] \) that shows its belonging to one of the subsets \( A \) (where \( i = 1, 2, 3, 4 \)) in the zoned criterion space clearly determines the plant tissue’s overall potential for protopectin fragmentation.

Our approach to classifying plants as pectin-containing materials, which is based on a system of criteria and a zoned criterion space, has clear advantages over existing methods due to its objectivity determined by the boundary conditions.

However, when analyzing this approach, we can easily see that the \( \mu_1 \) and \( \mu_2 \) values corresponding to \( d_1 \) and \( d_2 \) in the conditions \( Cond_{1,2,3,4} \) were set \textit{a priori}, based on general assumptions regarding the degree of acceptability of certain \( \mu_j \) values within Harrington’s individual desirability functions in accordance with the boundary (canonical) values of \( d \).

Yet, the conditions \( Cond_{1,2,3,4} \) determine the coefficients and constants, and, consequently, individual desirability
functions, as well as numerical values of $\mu_j[\Omega_j]$. Therefore, at this stage, our approach has a general, conceptual form requiring further research.

Based on the results, we developed a generalized algorithm to determine the geometric location of plant tissue in the zoned criterion space, or $\mathcal{M}[\mu_1, \mu_2, \mu_3]$ belonging to one of the subsets (Fig. 10). We can use this algorithm to assess any plant tissue’s potential for transformation of the protopectin complex, which determines the influence of any technological impact on its pectin potential.

The approach that we used to determine the criterion space and boundary conditions for its zoning explicitly suggests that this algorithm is universal for classifying plant tissue or its derivatives as pectin-containing materials. Thus, the algorithm is applicable to any type of plant material for which the $\mu_1$, $\mu_2$ and $\mu_3$ criteria can be numerically expressed.

**CONCLUSION**

To sum up, our investigation showed the following results.

1. We developed a system of criteria to assess the transformation potential of the protopectin complex in plant tissue. This system is based on the geometrical
Figure 10 Algorithm for plant tissue classification according to protopectin fragmentation potential based on the geometric location in the zoned criterion space

location of $M[\mu_1, \mu_2, \mu_3] -$ the point that corresponds to the material under analysis – in a zoned criterion space with coordinates in the form of dimensionless individual criteria for protopectin fragmentation potential.

2. The dimensionless individual criteria for protopectin fragmentation potential included the ratio between the mass fractions of biologically active components and protopectin in plant tissue, the mass fraction of the protopectin complex expressed in unit fractions, and the mass fraction of total pectin substances expressed in unit fractions.

3. We established nine individual boundary conditions, individual pectin potential, two individual fragmentation potentials, and three individual isolation potentials for pectin substances, which altogether determine a system of zoning the criterion space.

4. The boundary conditions in the definition area for a set of points $M[\mu_1, \mu_2, \mu_3]$ had the following hierarchy: individual pectin potential $\rightarrow$ individual
fragmentation potential of the protopectin complex → individual isolation potential of protopectin fragmentation products.

5. We developed an algorithm to classify plant tissues according to protopectin fragmentation potential based on the geometric location in the zoned criterion space.

CONTRIBUTION
All the authors were equally involved in writing the manuscript and are equally responsible for plagiarism.

CONFLICT OF INTEREST
The authors state that there is no conflict of interest.

REFERENCES


28. MR 2.3.1.2432–08 Normy fiziologicheskikh potrebnostey v ehnergii i pishchevykh veshchestvakh dlya razlichnykh grup naseleniya Rossiyskoy Federatsii [Norms of physiological requirements for energy and nutrients for various population groups of the Russian Federation]. Moscow: Federal Center for Hygiene and Epidemiology of Rospotrebnadzor; 2009. 36 p.


ORCID IDs
Vladimir V. Kondratenko https://orcid.org/0000-0002-0913-5644
Tatyana Y. Kondratenko https://orcid.org/0000-0001-8237-0774
Andrey N. Petrov https://orcid.org/0000-0001-9879-482X
Georgy A. Belozerov https://orcid.org/0000-0002-8152-146X