Mathematical Modeling of Biological Activity of Plant Growth Regulators

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Abstract. The paper dwells upon asymmetrical triazines as plant growth regulators. It presents in vitro and in vivo tests of 1,2,4-triazine compounds. The authors have developed a mathematical model to predict growth promotion, which serves as the basis of the proposed algorithm for projecting the biological efficacy of nitrogen-containing heterocycles.

1. Relevance

In today’s world, plant growth regulators are a popular solution that guarantees early harvest, improves survival, accelerates fruiting, and enables crops to better sustain adverse weather. These agents are versatile and equally efficient in horticulture and vegetable farming.

As a plant grows, it becomes irreversibly larger by generating new organs, cells, or cellular elements. Thus, plant growth is a quantitative increase in mass. Development, on the other hand, concerns the qualitative changes in plant morphology and physiology. The processes are tied to one another; plant growth is susceptible to external factors, which makes plants sensitive to any adverse environmental conditions [1,2].

The physiology of a plant is affected by the agents that some of the plant cells synthesize and others are receptive to. These agents are referred to as phytohormones, and they are designed to control plant growth. Some of them promote growth while others inhibit it.

The idea of using phytohormones has led to the laboratory synthesis of agents that have the same effect. Plant growth regulator (PGR) is an umbrella term that refers to phytohormones and their synthetic counterparts.

PGRs are a popular solution in agriculture, as they help maximize plant life and productivity. PGRs can boost productivity when fertilizers, pesticides, or agricultural machinery are not options or are useless. Since PGRs are applied as very low-concentration solutions, they are also environmentally safe [5,6].

There are several classifications applicable to PGRs; in general, these agents fall into:

– auxins, which control foliage, stem, branch, and shoot growth;
– gibberellins, which enable seeds to germinate;
– cytokinins, which trigger the natural cell division processes while also causing older shoots to age and die;
– brassinosteroids, which enable fruits and seeds to reap normally [7].
PGRs are not uniform in terms of chemical structure; rather, they belong to multiple different classes of chemical compounds. Some are indole compounds, others are derivatives of aromatic carboxylic acids, succinic acid, or organophosphorus compounds [8–16].

Nitrogen-containing heterocycles, in particular symmetrical and asymmetrical triazines, are of particular interest in terms of plant growth promotion efficacy. Symmetrical derivatives are a good solution, hence their popularity; however, such derivatives are barely exposed to biogradation. This is why the easily biodegradable asymmetrical triazines are a more promising solution [17–20].

2. Statement of problem and experimentation

The research team has developed methods for synthesizing a variety of asymmetrical triazine derivatives. This paper presents the results of testing the biological activity of two 1,2,4-triazine compounds: 1-hexahydro-1,2,4-triazinone-3 (plant growth-promoting agent 1) and 4-amino-1,4,5,6-tetrahydro-1,2,4-triazinone-5 (plant growth-promoting agent 2) [21,22].

The team tested the synthesized plant growth-promoting agents (PGPA) in vitro and modeled the data mathematically by applying an algorithm that identified the most biologically active PGR at low concentrations.

In vitro experiments were designed as follows. Wheat, cucumber, radish, and vetch seeds were placed in Petri dishes and soaked in 4 ml of standard solution. Then the dishes were placed in a thermostatic chamber and remained there for two days at 27°C; preparations were made in concentrations of 0.1, 1, and 10 mg/l. Each experiment was run four times. The efficacy of tested compounds was assessed two days later by measuring the length (l) and mass (m) of the etiolated sprouts. Results are shown in Table 1.

| Experiment          | Concentration, mg/l | Wheat | Cucumber | Radish | Vetch |
|---------------------|---------------------|-------|----------|--------|-------|
| control sample      | water               | 100   | 100      | 100    | 100   |
| prototype           | 1                   | 117   | 114      | 108    | 109   |
|                     | 10                  | 117   | 112      | 102    | 100   |
| plant growth-       | 0.1                 | 124   | 125      | 122    | 110   |
| promoting agent 1   | 0.5                 | 124   | 124      | 110    | 115   |
|                     | 0.1                 | 120   | 119      | 120    | 119   |
|                     | 1.0                 | 118   | 117      | 118    | 111   |
|                     | 2.5                 | 115   | 115      | 107    | 120   |
|                     | 5.0                 | 115   | 114      | 113    | 118   |
|                     | 10.0                | 116   | 112      | 110    | 117   |
|                     | 20.0                | 90    | 100      | 98     | 100   |
| plant growth-       | 0.1                 | 114   | 127      | 110    | 115   |
| promoting agent 2   | 0.5                 | 116   | 126      | 111    | 113   |
|                     | 0.75                | 118   | 124      | 114    | 117   |
|                     | 1.0                 | 120   | 124      | 115    | 117   |
|                     | 2.5                 | 121   | 123      | 120    | 119   |
|                     | 5.0                 | 122   | 121      | 121    | 121   |
|                     | 10.0                | 127   | 120      | 124    | 121   |
|                     | 20.0                | 100   | 98       | 100    | 96    |

As indicated by laboratory tests, plant growth-promoting agent 2 had greater biological efficacy. To confirm the results, the researchers constructed mathematical models that would predict the biological efficacy of plant growth-promoting agents as a function of their concentration; the integral biological efficacy metric was calculated and ranked by value.
The following mathematical models were developed to analyze the biological efficacy of plant growth-promoting agents:

\[ l(x) = a_1 x^2 + a_2 x + a_3 \]  
\[ m(x) = b_1 x^2 + b_2 x + b_3 \]

where \( l \) (mm) is the length in two days; 
\( M \) (mg) is the mass of etiolated sprouts; 
\( x \) (mg/l) is the PGPA concentration for experiments 1 and 2; 
\( a_1 \left( \frac{l^2}{mg^2} \cdot mm \right), b_1 \left( \frac{l^2}{mg} \right), a_2 (mm), b_2 (l), a_3 (mm), b_3 (mg) \) are the model parameters.

Table 2 presents the parameters of the models (1) and (2) calculated by the least squares method.

### Table 2. Calculated model parameters for plant growth-promoting agent 1.

| Parameters of the model (1) | Coefficient of correlation | Parameters of the model (2) | Coefficient of correlation |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| \( a_1 \) | \(-0.071\) | \(-0.064\) | \( 0.016 \) | \(-1.375\) | \( 121.510 \) | \( 0.94\) |
| \( a_2 \) | \( 0.022 \) | \(-1.453\) | \( 0.006 \) | \(-0.726\) | \( 110.370 \) | \( 0.98\) |
| \( a_3 \) | \( 0.163\) | \( 120.590 \) | \( 0.99 \) | \(-0.054 \) | \( 0.215 \) | \( 117.020 \) | \( 0.89\) |
| \( R \) | \( 0.97\) | \( 0.98 \) | \( 0.99 \) | \( 0.81\) | \( 0.99 \) | \( 0.98\) |

### Table 3. Calculated model parameters for plant growth-promoting agent 2.

| Parameters of the model (1) | Coefficient of correlation | Parameters of the model (2) | Coefficient of correlation |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| \( a_1 \) | \(-0.178\) | \( 2.819 \) | \(-0.061 \) | \(-0.096\) | \( 124.960 \) | \( 0.99\) |
| \( a_2 \) | \( 3.203 \) | \( 110.930 \) | \( 0.98 \) | \(-0.067 \) | \( 0.616 \) | \( 110.280 \) | \( 0.73\) |
| \( a_3 \) | \( 2.443 \) | \( 112.480 \) | \( 0.98 \) | \(-0.153 \) | \( 2.0 \) | \( 115.750 \) | \( 0.99\) |
| \( R \) | \( 0.98\) | \( 0.97\) | \( 0.97 \) | \( 0.97\) | \( 0.99 \) | \( 0.98\) |

The calculations can also be visualized, see Figure 2.

![Figure 1](image-url)
Where $l$ is the length of an etiolated wheat sprout, mm; $x$ is the PGPA concentration; $a_1=-0.178$; $a_2=2.819$; $a_3=115.07$.

In laboratory tests, PGPA concentration never exceeded 20 mg/l, as higher dosage would trigger herbicidal effects.

The researchers also calculated the coefficient of correlation, or $R$-normalized correlation. As shown in Table 2, this coefficient exceeded 0.7, which means the efficacy of a PGPA strongly correlated with its concentration. Besides, this proved the models (1) and (2) adequate, effectively making them applicable to predicting the efficacy of the PGPAs under consideration at any concentration; hence the research team did not have to run extra in vitro tests and was able to analyze the process as a continuous process for concentrations ranging from 0.1 to 20.0 mg/l. The continuity meant the process status could be retrieved for any point.

Autocorrelation function, which defines the rate of change in biometric parameters as a function of concentration, was applied to describe the dynamics of the biological process under consideration [23]:

$$R_{cor}^1 = \frac{1}{\Delta c} \int_{c_1}^{c_2} l(x) l(x + \Delta x) dx$$

$$R_{cor}^2 = \frac{1}{\Delta c} \int_{c_1}^{c_2} m(x) m(x + \Delta x) dx$$

where $R_{cor}^1$ and $R_{cor}^2$ are autocorrelation functions of biometric parameters expressed as (1) and (2); $x$ and $x + \Delta x$ are two cross-sections spaced at $\Delta x$; $\Delta c = c_2 - c_1$ is a change in the PGPA concentration. Table 3 presents the calculations.

**Table 4. Calculated biometric parameters.**

| Experiment | Wheat | Cucumber | Radish | Vetch |
|------------|-------|----------|--------|-------|
|            | $R_{cor}^1$ | $R_{cor}^2$ | $R_{cor}^1$ | $R_{cor}^2$ | $R_{cor}^1$ | $R_{cor}^2$ | $R_{cor}^1$ | $R_{cor}^2$ |
| 1          | 11,869.75 | 11,839.00 | 11,679.63 | 10,132.00 | 12,249.38 | 11,727.25 | 10,328.50 | 9,947.75 |
| 2          | 12,318.50 | 12,927.13 | 11,712.25 | 10,676.63 | 11,683.13 | 12,001.00 | 10,757.75 | 11,700.38 |

### 3. Experimental results

As can be seen in the tables above, plant growth-promoting agent 2 was more efficient; it could be used to raise the biometric parameters (length and mass of sprouts) to their appropriate values.

The agents analyzed herein were compared to the conventional agent (prototype) in terms of mean biological efficacy at 1 mg/l, see Figure 1.

**Figure 2.** Mean biological efficacy for the conventional PGPA and PGPGs under consideration. Measured at 1 mg/l.
1- conventional plant growth-promoting
2- plant growth-promoting agent 2
3 plant growth-promoting agent 1

As can be seen in the tables, the model output was close to the actual values found in the lab. Indeed, 4-amino-1,4,5,6-tetrahydro-1,2,4-triazinone-5 (PGPA 2) had higher biological efficacy at minimum concentrations as found from the length (l) and mass (m) of sprouts.

To further confirm this finding, the team tested it in vivo. Plant growth-promotion analysis used sunflower and corn and covered a 20-hour timeframe. Seeds were soaked in the working media at 0.1 to 20 mg/l Then the agent-treated corn and sunflower seeds were planted in pots, each of which was 25 cm in diameter; each experiment was run four times. Two weeks after seeding, the team measured the mass of the aerial portions of plants and used this metric to find how efficient the compound was in comparison with the prototype and the control, see Table 4.

| Table 5. Plant mass, in vivo tests, %.
| Experiment | Concentration, mg/l | Sunflower | Corn |
|------------|---------------------|-----------|------|
| control sample | water | 100 | 100 |
| prototype | 1 | 109 | 112 |
| | 10 | 117 | 113 |
| plant growth-promoting agent 1 | 1 | 121 | 123 |
| | 10 | 120 | 119 |
| plant growth-promoting agent 2 | 1 | 119 | 122 |
| | 10 | 127 | 126 |

4. Conclusion
Sunflower and corn had the largest gain in mass when using 4-amino-1,4,5,6-tetrahydro-1,2,4-triazinone-5; the two-staged test of these new compounds as plant growth and development regulators returned the same values as a priori mathematical screening, which means the algorithm is recommendable for predicting the biological activity of these compounds.

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