



# The Study of the Molecular Structure of the Nine -High, Depending on the Concentration of Hydrogen Peroxide by the Method of Spin Labels

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## Abstract

The spin labelling method was used to study the effect of hydrogen peroxide on the molecular structure of the medicinal plant elecampane. It is shown that the effect of hydrogen peroxide depends on the volume of its concentration. In the EPR spectra, with a sequential increase in the volume of hydrogen peroxide concentration, the line broadens, that is, the signal from a more disinhibited signal goes to a retarded form. It was found that with an increase in the spectral parameters ( $2A'z$  is the distance between the external extrema;  $\Delta H-1$  is the line width in a low field;  $\Delta H+1$  is the line width in a high field and  $\Delta H_0$  is the width of the central component of the EPR spectrum), samples in the medium (high elecampane root + hydrogen peroxide + nitroxyl radical) becomes: a more viscous solution, and with a large volume of hydrogen peroxide concentration (6.0 ml), a strong thick solution is obtained and structural transitions occur, accompanied by a noticeable increase in the rotational diffusion of the radical in the studied samples, which indicates an increase in the interaction between molecules and the spin label.

**Keywords:** Molecular dynamics; Spin label; Medicinal plant; Elecampane high; Hydrogen peroxide; Electron paramagnetic resonance (EPR); Nitroxyl radical

## Introduction

Medicinal plants are currently a valuable remedy for the treatment and prevention of chronic diseases. At the same time, the advantage of most plants is their low toxicity. In addition, it is believed that those medicinal plants that grow in environmentally friendly conditions are more effective [1,2]. The aim of this work is to study the effect of hydrogen peroxide on the structure of molecules as part of the drug plant of nine -high, the high, growing in the Khovlyigsky district of the Kulyab valley at an altitude of 1437 m.

above the sea of sea of the Republic of Tajikistan. Eleasil tall is one of the most popular medicinal plants used by almost all diseases [3,4]. The plant has the following therapeutic effect: anti-inflammatory; antimicrobial; expectorant; choleric; diuretic; Anthelmar (especially with ascariasis). The method of spin triggers is one of the effective methods of studying changes in the molecular dynamics of biological objects in the area of its connection and sensitive to molecular mobility of the macromolecules [5-7]. The study of the molecular structure and the

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properties of medicinal plants modified by the spin mark (I) makes it possible to explore the change in the structure of molecules and properties in the influence of external factors. The peculiarity of the spinning method of the labels is that a stable nitroxile radical is introduced into the matrix of the studied sample, the EPR of which

is sensitive to the conformational mobility of the macromolecule associated with the anisotropy of the G-factor and the ultra-thin interaction of the electronic back with nuclei of the nitrogen of nitrogen. The spectrum of the EPR of the radical depends on its orientation in the external magnetic field [8].

**Table 1:** Spin-lame spin-lace-laid derivatives of high-high dimensions of high hydrogen peroxide (PV).

№	The concentration of hydrogen peroxide in the root	Spectral parameters				
		$h_0/h_{-1}$	$h_{+1}/h_{-1}$	$\Delta H_0$ , Гайсс	$\tau_c$ calculated by $(h_0/h_{-1})$	$\tau_c$ calculated by $(h_{+1}/h_{-1})$
1	Tread. radical	1,5	1,7	5	$0,2 \cdot 10^{-9}$	$1,2 \cdot 10^{-10}$
2	1,5 % PV	1,7	1,9	5	$0,4 \cdot 10^{-9}$	$1,7 \cdot 10^{-10}$
3	3.0 % PV	1,7	1,7	6	$0,5 \cdot 10^{-9}$	$1,5 \cdot 10^{-10}$
4	6.0 % PV	1,7	1,8	6	$0,5 \cdot 10^{-9}$	$1,5 \cdot 10^{-10}$

Note: The correlation time is determined in two cases in which the pattern of change is the same.

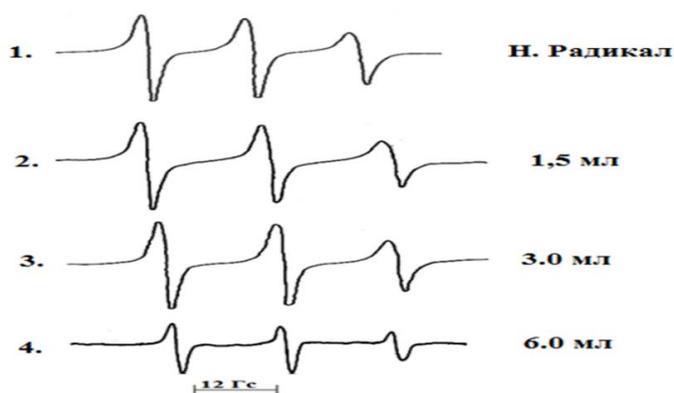
The studied samples of the drug plant of nine -high in powder form modified with a spin mark (I) according to the method [9]. EPR spectra recorded on the REP radio spectrometer-1306 in standard molybdenum ampoules with an internal diameter of 3.0 mm, in which they placed 25 mg of spin-laughter sample. The process of manufacturing studied samples was carried out as follows: they took 50 mg of the peeled nine of the high (DV) to the test tubes and added 1.5 ml of hydrogen peroxide (PV), the mixture was left for 5 days as a result, a viscous solid mixture was obtained, and then added 1.5 ml The nitroxyl radical (HP) in ethanol solution is obtained by sample №1, which in the future we call PV = 1.5 ml with the concentration of PV. Sample № 2 - all the same, but added 3.0 ml of PV, it turned out a thicker mixture: Pv = 3.0 ml concentration. Sample №3- all the same, but added 6.0 ml of PVs a strong dense mixture: the volume of concentration PV = 6.0 ml the correlation of the rotation of the spin labels in the studied samples were determined by the formulas: [6]

$$\frac{1}{\tau_c} = \frac{3,64 \cdot 10^9}{\left( \sqrt{\frac{h_0}{h_{-1}}} - 1 \right) \Delta H_0};$$

$$\nu = \frac{1}{\tau_c} = \frac{1,2 \cdot 10^{10}}{\left( \sqrt{\frac{h_{+1}}{h_{-1}}} - 1 \right) \Delta H_0} \text{сек}^{-1},$$

Where  $\Delta H_0$  is the width of the central component in the Gausses;  $H_0$ ,  $H+1$  and  $H-1$ -the intensity of the components of the spectrum with  $M=0, +1$  and  $-1$ ,  $\square = 1/\tau$ - the value, conditionally called the "rotation frequency" of the radical. Figure 1 shows the EPR -spectra of stable nitroxile radical (I) in ethanol solution with a concentration of  $4 \cdot 10^{-3}$  m / l, with the correlation time ( $\tau_c < 10^{-7}$  p.) And the spin -the mild medicinal plant of the high of the high

when influence Hydrogen peroxide (PV) with various voluminous concentrations. As can be seen from Fig. 1, with an increase in the concentration in the spectra of EPR, the line is observed between the components, that is, inhibition. It indicates that, with large values of the concentration of hydrogen peroxide concentration in the test sample, the process of dissolution occurs, that is, a structural change accompanied by a noticeable increase in rotational diffusion of the radical in the studied samples, which indicates an increase in the interaction between molecules and spin marking (Figure 1). And with low values of the volume of PV concentration in the samples of the spin -smeared nines high, the process of dissolution occurs, but very little and so it turns out, a little viscous solution (Table 1).



**Figure 1:** EPR spectors of free nitroxile radical (I) in ethanol solution with a concentration of  $4 \cdot 10^{-3}$  m/l with correlation time ( $TC < 10^{-8}$ С.)-1; and spin - swordsurous nine -high in among (DV+PV+HP) with the influence of various volumes of concentration of hydrogen peroxide: 2 - 1.5 ml; 3 - 3.0 ml; 4 - 6.0.

In Figure 1 and Table 1, the following parameters of the spin-laughter spin-laeled derivatives of the high-me-laughter at different concentrations of hydrogen peroxide: 2A'Z-the distance between



external extremes;  $\Delta H_0$  – width Central component in Gausses;  $h_0$ ,  $h_{+1}$ ,  $h_{-1}$  -intensity and  $\Delta H_0$ ,  $\Delta H_{+1}$ ,  $\Delta H_{-1}$  -the width of the central, low -floor and high -floor components of the EPR spectrum;  $h_0/h_{-1}$  -the intensity of the central and high -floor lines of immobilized labels;  $h_{+1}/h_{-1}$  - the ratio of the intensities of high -floor and low -floor lines of immobilized marks for the studied samples.

Thus, the experimental results obtained by the method of spin triggers indicate that:

- In a solution of hydrogen peroxide with the presence of a medicinal plant of nine -high and in ethanol solution of nitroxyl radical, that is, in a mixture containing hydrogen peroxide, affects the molecular structure of drugs;
- With a large volume of concentration of hydrogen peroxide (6.0 ml), a strong thick solution is obtained, and structural transitions occur, accompanied by a noticeable increase in rotational diffusion of the radical in the studied samples.

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