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# STRUCTURAL ANALYSIS OF SUPRAMOLECULAR COMPLEXES OF SCHIFF BASES

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**Abstract**
Gossypol Schiff bases were synthesized and water-soluble supramolecular complexes of monoammonium salt of glycyrrhizic acid (MSGA) in a ratio of 1:4 were obtained, taking into account the insolubility of these substances in water. Some physico-chemical parameters of the complexes, their structure were estimated using IR-, UV-spectra and computer software. These quantum-chemical calculations were carried out in the ChemOffice program using the molecular mechanics (MM2) method with an empirical force field.

**Keywords**: Gossypol, amino compound, Schiff's base, spectrum, polyphenol, triterpene, aldehyde, cotton plant, naphthalene, MSGA.

Gossypol is found in different concentrations in different parts of the cotton plant. Gossypol, together with the diversity of its chemical structure and biological activity, is the main source for the creation of drugs against various viral diseases, colds, gastrointestinal ulcers and swellings. Some of Schiff's bases have strong interferon-inducing properties along with high biological activity, but gossypol derivatives are not soluble in water [1-2].

Taking into account the insolubility of Schiff bases in water, it is aimed to obtain their supramolecular complexes with the monoammonium salt of glycyrrhizic acid (MSGA) [3-4-5]. Molecules in these complexes are formed not by covalent bonds, but by hydrogen bonds. In most cases, covalent bonding is the major part of this process.

MSGA is known to form clathrates with sparingly water-soluble drugs into a water-soluble form. MSGA is a major triterpene glycoside isolated from the root of the licorice plant and has a number of unique physicochemical properties, one of which is its solubilization property. Therefore, by forming supramolecular complexes with drugs, MSGA dramatically increases their solubility in water, reduces their toxicity, and at the same time provides an opportunity to maintain the effectiveness of action even in very small doses [6-7-8].

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To obtain supramolecular complexes, 4 mol of MSGA was dissolved in 50 % $C_2H_5OH$, 1 mol of Schiff's base was added to it, and the reaction was carried out at 50-60 °C for 6-8 hours with regular stirring. Ethyl alcohol was removed from the reaction mixture using a rotary evaporator, and the aqueous portion was lyophilized. Supramolecular complexes of thirty gossypol Schiff bases in 1:4 ratio were obtained. Some of their physico-chemical parameters were studied:

Supramolecular complexes were obtained according to the following scheme:

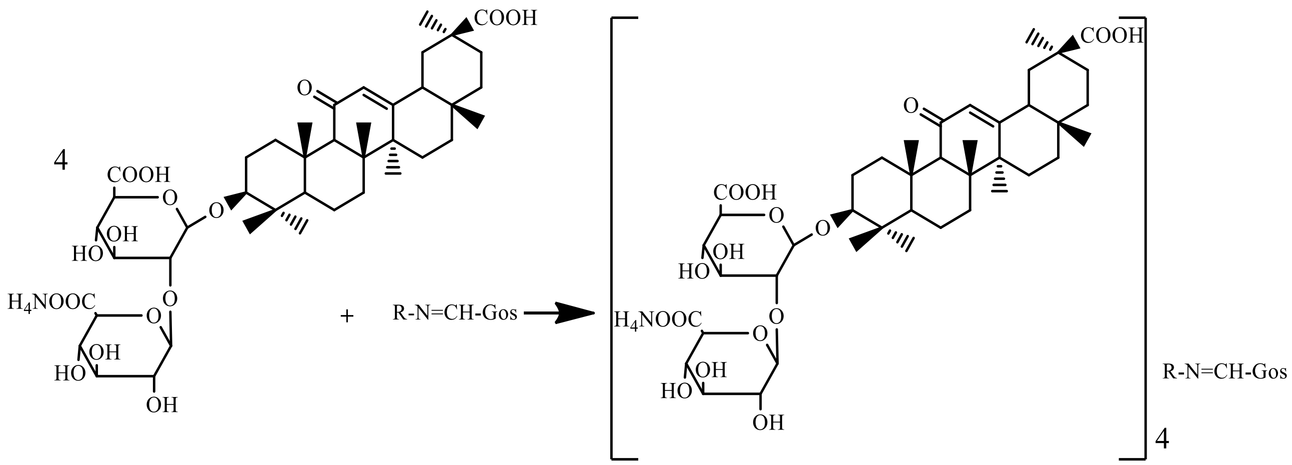


**Table 1**
**Some physicochemical constants of water-soluble supramolecular complexes of Schiff bases with MSGA**

| № | Supramolecular complex | Mol Ratio | Liquid °S | $R_f$ | Reaction yield, in % | Color |
|---|---|---|---|---|---|---|
| 1 | Di-(1-amino-2-bromoethane)gossypol + MSGA | 1:4 | 211-212 | $0.42^1$ $0.28^2$ | 91 | yellow |
| 2 | Di-(2-amino-2-methylpropane)gossypol + MSGA | 1:4 | 218-219 | $0.42^1$ $0.34^3$ | 93 | yellow |
| 3 | Di-(1-aminobutane)gossypol+MSGA | 1:4 | 214-215 | $0.38^1$ | 91 | yellow |
| 4 | Di-(phenylhydrazine)gossypol+MSGA | 1:4 | 189-190 | $0,70^2$ | 90 | yellow |
| 5 | Di-(2,4-dinitrophenylhydrazine)gossypol + MSGA | 1:4 | 239-240 | $0,64^2$ | 98 | yellow |
| 6 | Di-(o-nitroaniline)gossypol+MSGA | 1:4 | 212-213 | $0,46^3$ | 98 | yellow |
| 7 | Di-(4-amino-2-methylphenol)gossypol + MSGA | 1:4 | 221-222 | $0,30^2$ | 99 | yellow |
| 8 | Di-(solicylamine) gossypol+MSGA | 1:4 | 197-198 | $0,30^3$ | 94 | yellow |
| 9 | Di-(benzylamine)gossypol+MSGA | 1:4 | 218-219 | $0.58^1$ | 96 | yellow |

**Systems: 1)** Hexane-acetone 1:1 **2)** Hexane-acetone 1.5:1 **3)** Benzene-acetone 2:1
When MSGA forms supramolecular complexes, the -OH and -COOH groups in it form a hydrogen bond and allow joining. In addition, the hydrophobic part of GKMAT is affected by the hydrophobic parts of gossypol derivatives.When the UV and IR spectra of the obtained supramolecular complexes were analyzed, it was revealed that the signals in the spectrum of Schiff bases were broadened due to the hydrogen bonds in the complex compounds [9-10-11-12].

MSGA with di-(2,4-dinitrophenylhydrazine) gossypol When analyzing the IR spectrum of the supramolecular complex, we can see the change of the absorption maxima at 3091 cm$^{-1}$ due to the valence vibrations of the new –N=CH– bond and the absorption maxima at 3450.98-2873.94 cm$^{-1}$ due to the bonds in the MSGA supramolecular complex.

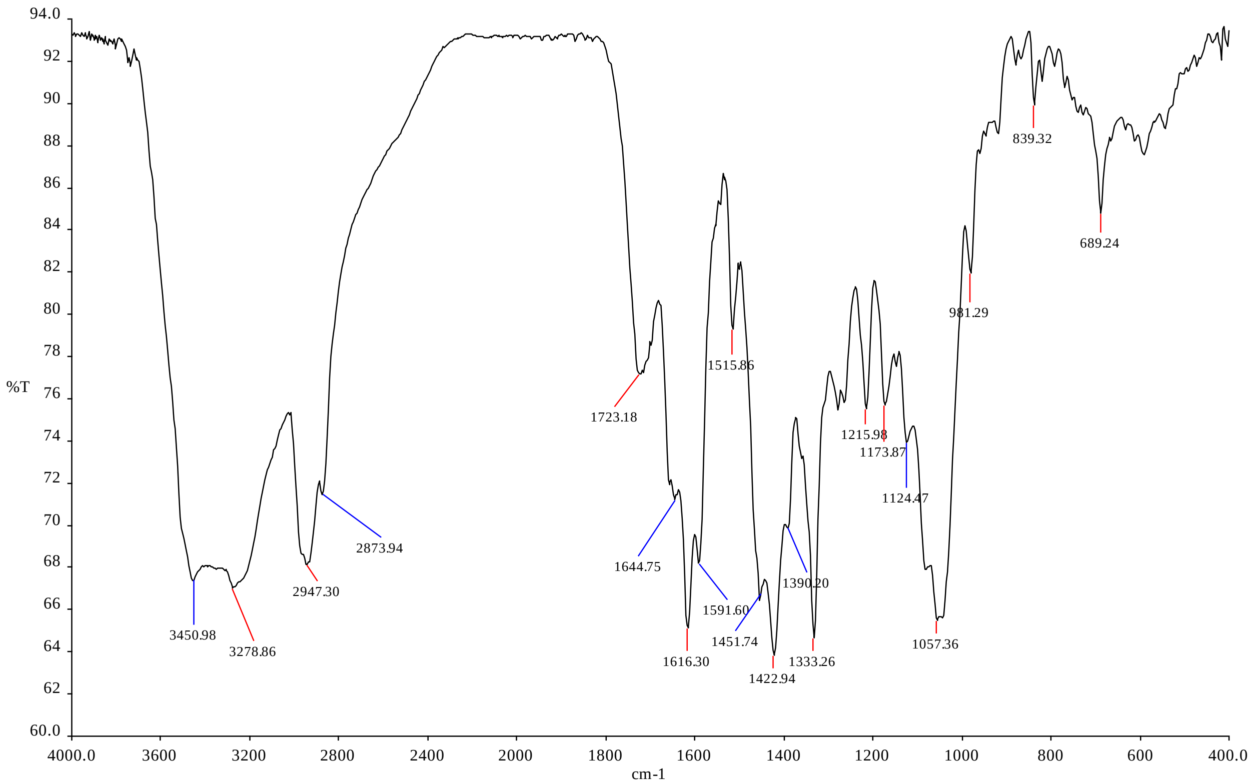


Figure 1. IR spectrum of di-(2,4-dinitrophenylhydrazine)gossypol+ MSGA

The UV spectrum of MSGA supramolecular complex with di-(2,4-dinitrophenylhydrazine)gossypol gave absorption maxima at 244.33-424.72 cm$^{-1}$ for this substance [13-14-15-16].

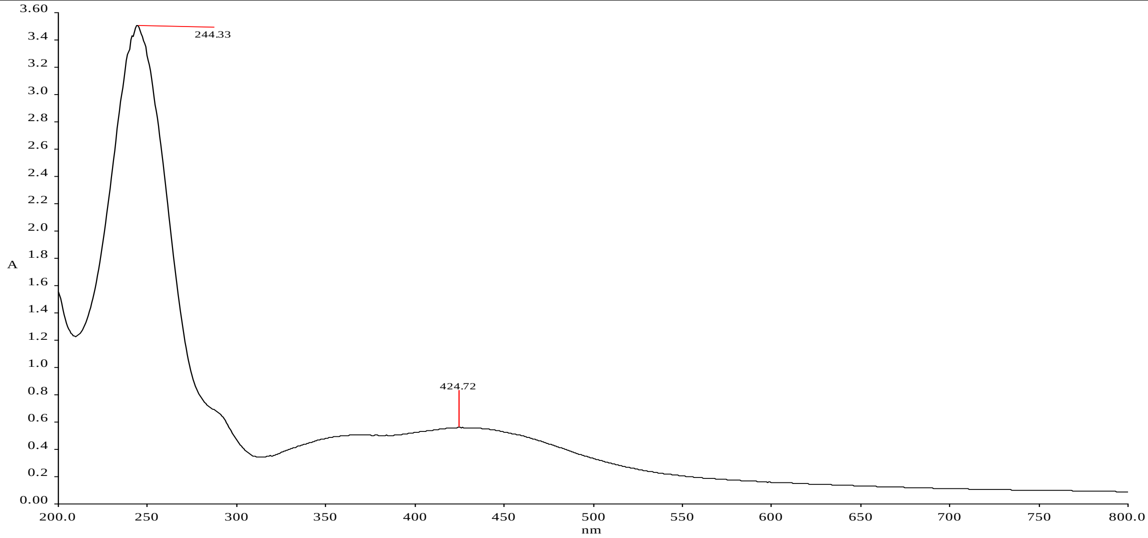


Figure 2. UV spectrum of di-(2,4-dinitrophenylhydrazine) gossypol+GKMAT

When analyzing the IR-spectrum of the Schiff base formed by p-toluidine with gossypol, we can see the absorption maxima at 3240-3430 cm$^{-1}$ belonging to the –$NH_2$ group at 3091 cm$^{-1}$ due to the valence vibrations of the new –N=CH– bond [17-18-19-20].

When analyzing the IR-spectrum of the supramolecular complex with MSGA based on the obtained Schiff base, it was found that the absorption maxima at 3091 cm$^{-1}$ were due to the valence vibrations of the new –N=CH– bond and at 3467.50-2920.22 cm$^{-1}$ were due to hydrogen bonds. we can see absorption maxima [21-22-23].

Model of MSGA supramolecular complexes with gossypol derivatives based on computer calculation

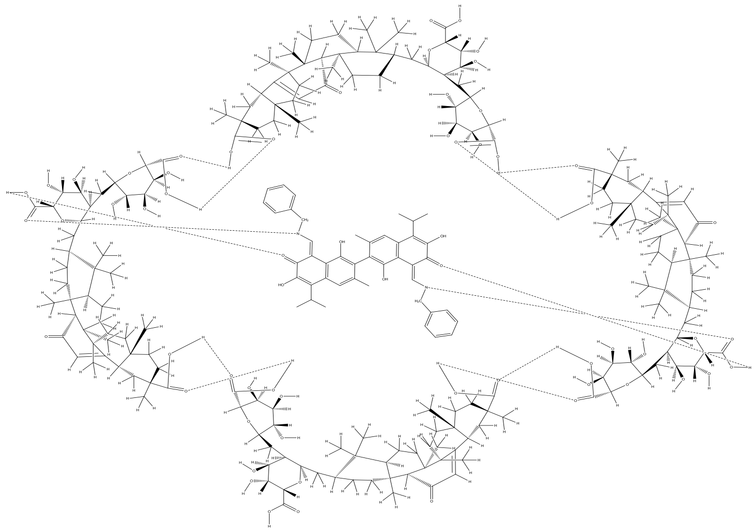

Figure 3. 1:4 with MSGA of gossypolidene benzylamine
model of the supramolecular complex in proportion

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