WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 3, Issue 6, June, 2022

RESULTS OF COMPUTER STUDY OF BIOLOGICAL ACTIVITY OF GOSSIPOL PRODUCTS

Khakberdiev Shukhrat Mahramovich
Jizzakh Polytechnic Institute
E-mail: h.shyxrat81@gmail.com

Mullajonova Ziyodabonu Sayfula qizi
Jizzakh Polytechnic Institute

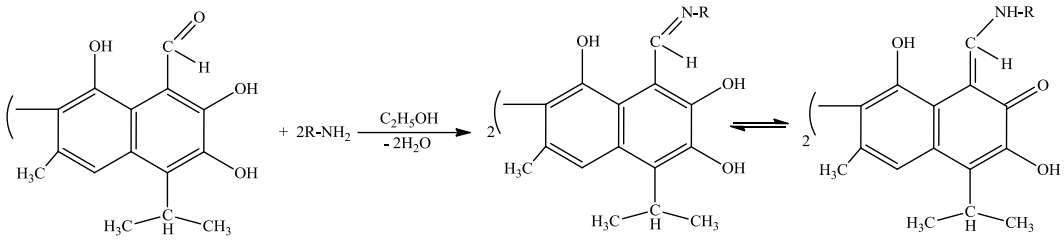
Annotation
Gossypol is a polyphenol substance, its structure is complex and its biological properties are unique. Its derivatives are now used in medical practice as a means of combating viral diseases due to their wide range of physiological activity. Schiff bases with heterocyclic amino compounds of Gossypol were obtained and their structure was studied using IQ, -UB spectra.

Keywords: Gossypol, heterocyclic, Shiff base, azometin, spectrum, solvent, reaction, computer program, PAS program.

Introduction

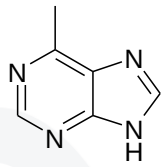
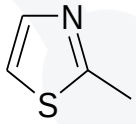
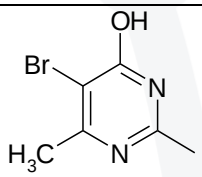
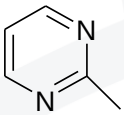
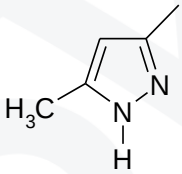
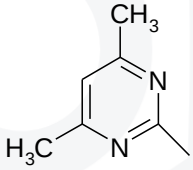
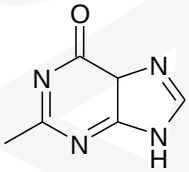
Gossypol, along with its chemical structure and diversity of biological activity, is a major source in the development of drugs against various viral diseases, colds, gastrointestinal ulcers and tumors. Some of the gossypol derivatives have strong interferon induction properties along with high biological activity [1-2].
One of the important tasks is to synthesize the new gossypol Shiff bases, study their biological activities and create drugs against immune diseases based on them.
The substances formed as a result of the reaction of substances containing an amino group with gossypol are called Schiff bases or azometin derivatives. In the synthesis of Schiff's bases, gossypol and primary amine are extracted in a ratio of 1: 2 mol, sufficient for its dissolution is poured 96% ethyl alcohol and stirred for three hours when heated in a magnetic stirrer (70-80°S), the reaction is controlled using YuQX [3-4-5]. Once the reaction is complete, the resulting substance is left for one day to completely precipitate, then filtered and washed 2-3 times with ethyl alcohol [6-7-8]. The resulting substance was dried in a place away from direct sunlight.
The reaction was carried out according to the following scheme:

WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 3, Issue 6, June, 2022

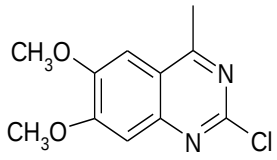
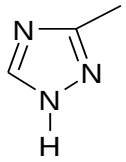


When the physicochemical properties of all the synthesized substances were studied, it became clear that all the substances formed were crystalline substances ranging from yellow to brown.

Some of the synthesized Shiff basicsphysicochemical quantities

№	Radical –R	Liquid °S	R_f			reaction yield %	pH	Color
			1	2	3			
1		261-63	0,51	0,52	0,63	36,5	7,6	orange
2		254-56	0,54	0,62	0,63	72,2	9	yellow
3		215-17	0,57	0,7	0,76	77,5	8,7	bright red
4		205-07	0.50	0,67	0,57	73,78	8,8	yellow
5		285-87	0,49	0,51	0,55	82,3	9,1	orange
6		228-29	0,51	0,74	0,69	72,4	7,8	brown
7		277-78	0,31	0,70	0,77	39	8	Light yellow

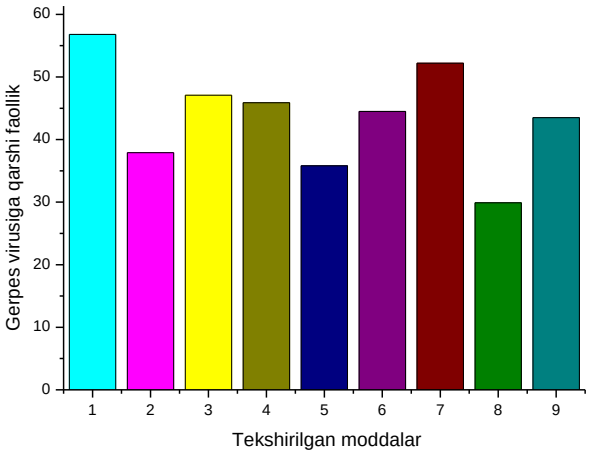
WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 3, Issue 6, June, 2022

8		200-01	0,78	0,55	0,37	71	7,7	brown
9		250-51	0,35	0,62	0,75	73,3	7,6	yellow

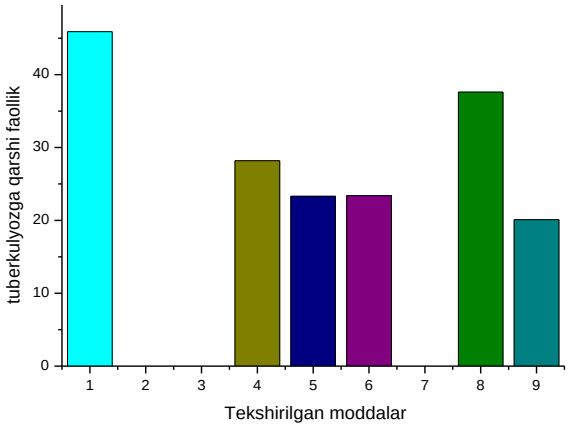
Systems:
1Hexan-acetone(3:2.5), 2Benzene-acetone(5:1.5) 3Benzene-alcohol (3:1)
Absorption peaks in the range of 270–350 nm were observed in the UV spectra of the obtained gossypol Shiff bases. When analyzing the IR spectra, the valence oscillations at 1720-1750 cm-1 belonging to the -SNO group disappeared and were replaced by the -CH = NH- and = CH-NH- groups of 1602.8-1672.9.
valence oscillations in the range of cm-1 were observed [9-10-11].
The approximate biological properties of Schiff's bases were studied using computer modeling PAS software to determine the biological activity of substances in order to save substances and implement a targeted approach in the study of biological properties of synthesized substances. The results of biological activity studied in a computer program differ by 15-20% compared to the practical results. Accordingly, the activity of the obtained substances against a number of diseases and disease viruses was determined.
A) Herpes Virus **B)** Tuberculosis Virus **C)** Bacteria **D)** Antioxidant
E) Immunomodulatory **F)** Interferon Induction

1. Di- (adenine) gossypol
2. Di- (2-aminothiazole) gossypol
3. Di- (2-amino-4-methyl-5-bromine-6-hydroxopyrimidine) gossypol
4. Di- (2-aminopyridine) gossypol
5. Di- (3-amino-5- methyl pyrazole) gossypol
6. Di- (2-amino-4,6-dimethyl pyrimidine) gossypol
7. Di- (guanine) gossipol
8. Di- (4-amino-2-chloro-6,7-dimethoxy quinolizidine) gossypol
9. Di- (3-amino-1,2,4-triazole) gossypol

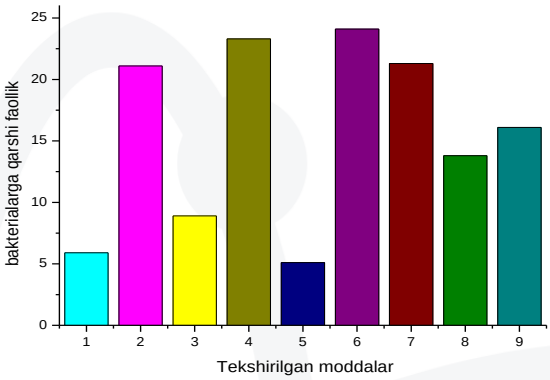
WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 3, Issue 6, June, 2022



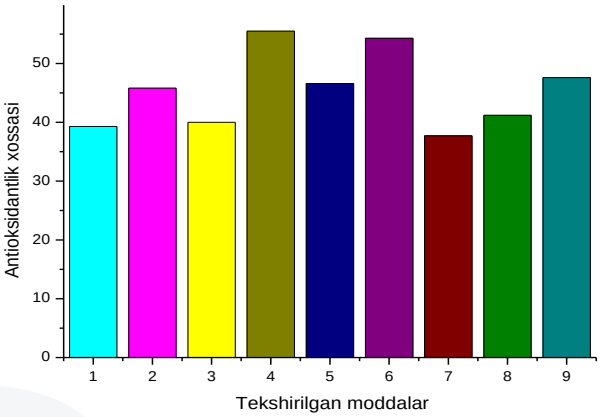
A)



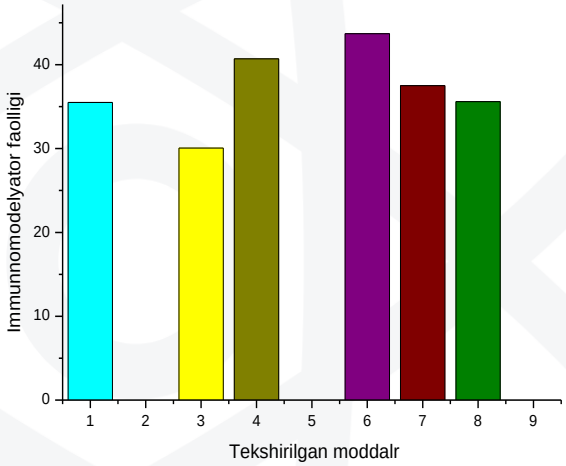
B)



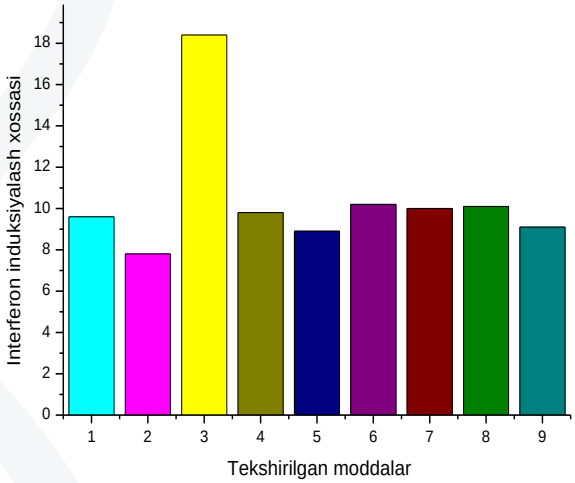
C)



D)



E)



F)

According to the results, the best activity against the herpes virus is based on adenine gossypol Shiff, against tuberculosis is also based on adenine gossypol Shiff, antibacterial gossypol 2-amino-4,6-dimethyl pyrimidine-based Shiff, antioxidant properties gossypol-based 2-amino pyrimidine Based on Shiff, the immunomodulatory property of gossypol is based on 2-amino-4,6-dimethyl pyrimidine. demonstrated.In some substances, for example, the Schiff base formed by gossypol with 2-aminothiazole and the Schiff base formed by gossypol with 3-amino-5-methyl pyrazole, the Shiff base formed by gossypol with 2-aminothiazole, the Schiff base formed by gossypol with 2-aminothiazole, the 2-amino-4-methyl-5 of gossypol -brom-6-hydroxopyrimidine-formed Schiff base and gossypol found to show no anti-tuberculosis activity in guanine-formed Schiff bases.

Фойдаланилган адабиётлар

1. Baram N.I., Ziyaev X.L., Ismailov A.I., Ziyamov Yu.S., Novye azoproizvodnye gossipola // XPS.2000. 145.
2. Glushenkova A.I., Nazarova I.P. Gossipol ego proizvodnыe i ix ispolzavanie. Tashkent: Izdatelstvo Fan, 1993. 86.p
3. Hakberdiev, S. M., Talipov, S. A., Dalimov, D. N., & Ibragimov, B. T. (2013). 2, 2′-Bis {8-[(benzylamino) methylidene]-1, 6-dihydroxy-5-isopropyl-3-methylnaphthalen-7 (8H)-one}. *Acta Crystallographica Section E: Structure Reports Online*, *69*(11), o1626-o1627.
4. Khamza, Toshov, Khakberdiev Shukhrat, and Khaitbaev Alisher. "X-ray structural analysis of gossypol derivatives." *Journal of Critical Reviews* 7.11 (2020): 460-463.
5. Khakberdiyev, S. M. (2021). Study of the structure of supramolecular complexes of azomethine derivatives of gossipol. *Science and Education*, *2*(1), 98-102.
6. Khaitbaev A. K., Khakberdiev S. M., Toshov K. S. Isolation of Gossypol from the Bark of Cotton Roots //Annals of the Romanian Society for Cell Biology. – 2021. – С. 1069-1073.
7. Хакбердиев Ш. М. и др. Синтез госсипольных производных орто, мета, пара толуидина и их строение //Science and Education. – 2021. – Т. 2. – №. 10. – С. 195-200.
8. Khakberdiev, Sh M., et al. "Synthesis and structure of gossypol azomethine derivatives." *Young Scientist,(4)* (2015): 42-44.
9. Хакбердиев Ш. М. и др. 3-аминопропанол-1 билан госсиполнинг турли комплекслари синтези ва макрофаглар миқдорига таъсири //Журнал естественных наук. – 2021. – Т. 1. – №. 1.

10. Хакбердиев, Ш., Қодир, Д., Маматова, Ф., & Муллажонова, З. (2022). Госсипол асосида ациклик аминобирикмаларнинг ҳосилалари синтези. *Журнал естественных наук*, *1*(2 (7)), 12-16.
11. Mahramovich, K. S., Sattarovna, K. F., & Farangiz, M. (2022). Synthesis of Gossipy Products of Pyrimidine Bases and Getting Their Water-Solved Complexes. *Eurasian Scientific Herald*, *8*, 118-121.