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## CORRELATION OF THE STRUCTURAL PECULIARITIES OF BIOACTIVE COMPOUNDS OF HERBAL REMEDY AND ITS PHARMACOLOGICAL VALUE

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Up to date a prominent place in the medical practice is occupied by herbal remedies due to such their characteristic as a combination of a wide spectrum of pharmacological action with low toxicity. This gives the opportunity for using them with the therapeutic or preventive purpose for many diseases, including dental [6].

Diseases of periodontal tissue widely distributed in the adult population of different countries. There is also their sharp increase among children and adolescents. Such inflammatory diseases as gingivitis and periodontitis prevail in the structure of dental diseases [5].

Antiseptic and antibacterial drugs are applied in complex therapy of these periodontal diseases. However, the long local application of synthetic antimicrobial agents can lead to the changes of properties of resident bacteria. As a result of which are the launching of the immune response and forming of primary inflammation. Bacterial strains develop resistance to the plant drugs much slower [3,6].

Numerous reports of scientists confirm a revival of interest to drugs of plant origin, noting a wide range of their pharmacological action and the effectiveness of assigning them to dental patients [1,2,6,14,16].

This underlines the timeliness of the search for new effective drugs of plant origin for the therapy of inflammatory periodontal diseases.

During previous works, possibility of using of licorice roots, sedge cane rootstocks as well as burnet rootstocks with its roots as components of a complex tincture for periodontitis treatment was experimentally substantiated, and an optimal raw material-extractant ratio, based on results of studying, was proved [16]. The composition of liquid medical form of the phyto-genous according to obtain experimental results has been proposed [8].

Qualitative and quantitative content of components of volatile fraction of complex tincture were analysed using method chromatography-mass spectrometry, 64 compounds were determined and 42 of them were identified. [9].

Activity of the new drug tincture for preventive dentistry was tested against the museum strains and the clinical ones of *Candida*'s genus. Submitted experimental data are precondition for considering the developed tincture as a potential plant drug for an oral candidiasis treatment [7].

Antimicrobial activity of fatty acids were demonstrated in scientific researches [4,10-13,15,17].

With the purpose of substantiation of expediency of use of herbal remedy for the therapy of inflammatory periodontal diseases we had to:

- carry out a study of fatty acid composition of lipophilic fraction of a mixture of herbal raw-materials-ingredients, from which the tincture was obtained;
- explore a composition of fatty acids in the herbal remedy after the extraction process;
- determine antimicrobial properties of the complex tincture in comparison with the herbal remedies, existing in the domestic pharmaceutical market, which are recommended for the treatment of inflammatory diseases in therapeutic stomatology.

### Materials and methods

Object of research is the liquid herbal remedy designed in the form of tinctures under the conditional name "Casdent".

The study of the composition of fatty acids was carried out with the help of the method of gas chromatography. Fatty acids were studied both in the lipophilic fraction of the base herbal mixture and in the final product, that is a complex tincture. Determination of methyl esters of fatty acids was performed on a gas chromatograph "Selmichrom-1" with a flame ionization detector.

The evaluation of antibacterial activity of the tinctures samples was carried out on test strains: *S. aureus* ATCC 25923, *E. coli* ATCC 25922, *P. aeruginosa* ATCC 27853, *S. pneumoniae* ATCC 49619, *B. anthracoides* DICK 1312 and *K. pneumoniae* K-7 NCTC 9127. The domestic herb preparation "Rotocan" ("Lubnifarm" JSC, Ukraine) and foreign preparation "Stomatophyt" ("Phytopharm Klenka S.A.", Poland) were used as medicines of comparison. The accepted method of diffusion into agar ("well" method) was applied. The determination of the antibacterial activity of tincture and of preparations of comparison was carried out according to the order № 167 of Ministry of Health of Ukraine (from 05.04.2007). All studies were conducted at the Mechnikov Institute of microbiology and immunology of AMSU in the laboratory of mediums and biochemistry of microorganisms under the direction of Osolodchenko T.P., chief of laboratory, Ph. D. in biol., senior scientist.

### Results and discussion

The results of the study of the component composition of fatty acid of lipophilic fractions of the herbal mixture and tincture are presented in Table 1.

Chromatograms of fatty acids of the investigated objects are shown in Fig. 1 and Fig. 2.

In lipophilic fractions of all the samples determined the presence of both saturated and unsaturated fatty acids. 19 fatty acids were found in the herbal composition 13 of which were identified. 9 fatty acids were found in the "Casdent" tincture 8 of which were determined. We would like to note that among the identified substances content of fatty acids decreased in the order: linoleic > palmitinic > myristinic > linolenic > oleic (herbal mixture) and palmitinic > lauric > linoleic > oleic > stearic (complex tincture).

In general, in all the studied objects (Table 1) palmitinic acid dominated among the saturated acids (14,67% and 36,12%), and linoleic acid dominated among the unsaturated acids (40,33% and 19,86%).

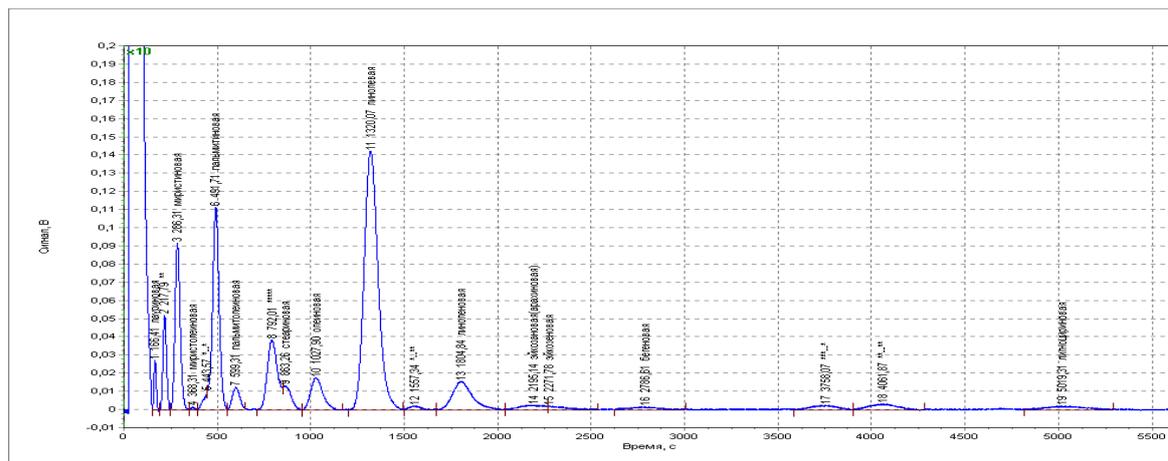
The amount of saturated fatty acids is 30,9% for the herbal mixture and 64,38% for the complex tincture,

and the amount of unsaturated fatty acids is 53,0% for the herbal mixture and 33,99% of the complex tincture among the identified fatty acids of lipophilic fractions of herbal objects.

**Table 1 – The results of the analysis of the composition of fatty acids of lipophilic fractions of the investigated objects**

N	Methylic esters of fatty acid	Carbon skeleton of the fatty acid	Samples	
			herbal mixture	complex tincture
			Content, % of the sum	
1.	Lauric acid	C 12:0	1,38	23,06
2.	*	–	3,91	–
3.	Myristinic acid	C 14:0	9,81	0,89
4.	Myristoleic acid	C 14:1	0,08	–
5.	**	–	0,87	–
6.	Palmitinic acid	C 16:0	14,67	36,12
7.	Palmitoleic acid	C 16:1	1,96	–
8.	***	–	8,44	1,63
9.	Stearic acid	C 18:0	2,25	4,31
10.	Oleic acid	C 18:1	4,28	12,48
11.	Linoleic acid	C 18:2	40,33	19,86
12.	****	–	0,35	–
13.	Linolenic acid	C 18:3	5,93	1,60
14.	Arachic acid	C 20:0	1,37	–
15.	Gondoic acid	C 20:1	0,42	0,05
16.	Behenic acid	C 22:0	0,34	–
17.	*****	–	0,97	–
18.	*****	–	1,56	–
19.	Lignocerylic acid	C 24:0	1,08	–
Total saturated fatty acids			<b>30,9</b>	<b>64,38</b>
Total unsaturated fatty acids			<b>53,0</b>	<b>33,99</b>
Total unidentified fatty acids			<b>16,1</b>	<b>1,63</b>
Ratio of unsaturated fatty acids to saturated			<b>1,72:1</b>	<b>0,53:1</b>

Comment: \* - \*\*\*\*\* - unidentified ingredients



**Fig. 1 – Chromatogram of fatty acids of the herbal mixture**

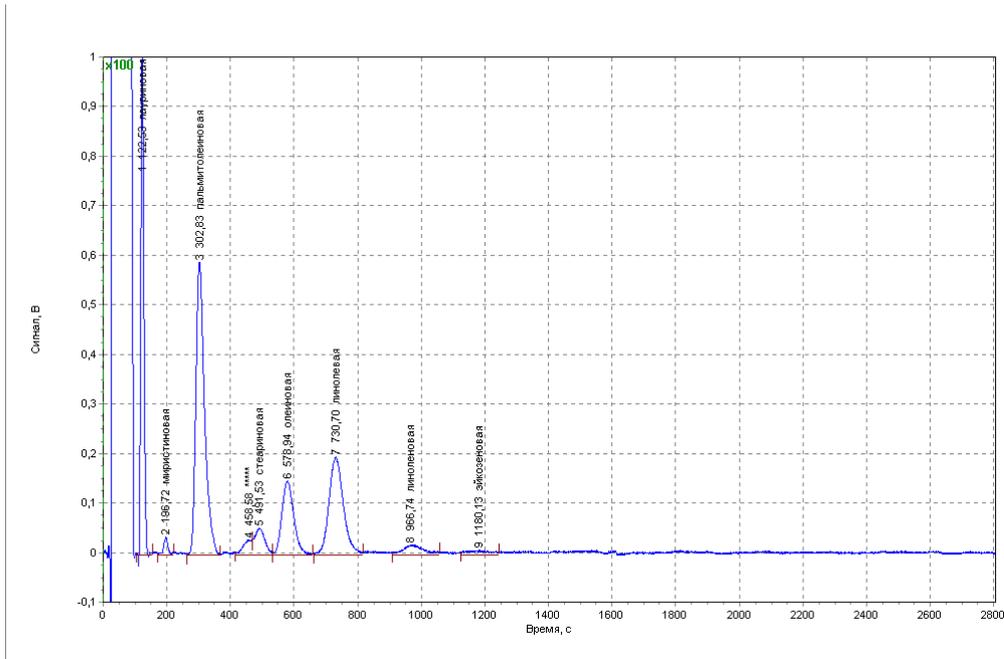


Fig. 2 – Chromatogram of fatty acids of the complex tincture

On the basis of the obtained values the ratios of unsaturated fatty acids to saturated fatty acids were calculated. This ratio is 1,72:1 for mixture and the ratio is 0,53:1 for “Casdent”. It should be noted that the content of the unidentified ingredients in the mixture is in 10 times more, than in the tincture.

The next stage of research is the study of antimicrobial properties the herbal remedy. Based on the obtained results macrocontours of spectrum of antimicrobial activity are plotted down for the tinctures under study and reference preparation

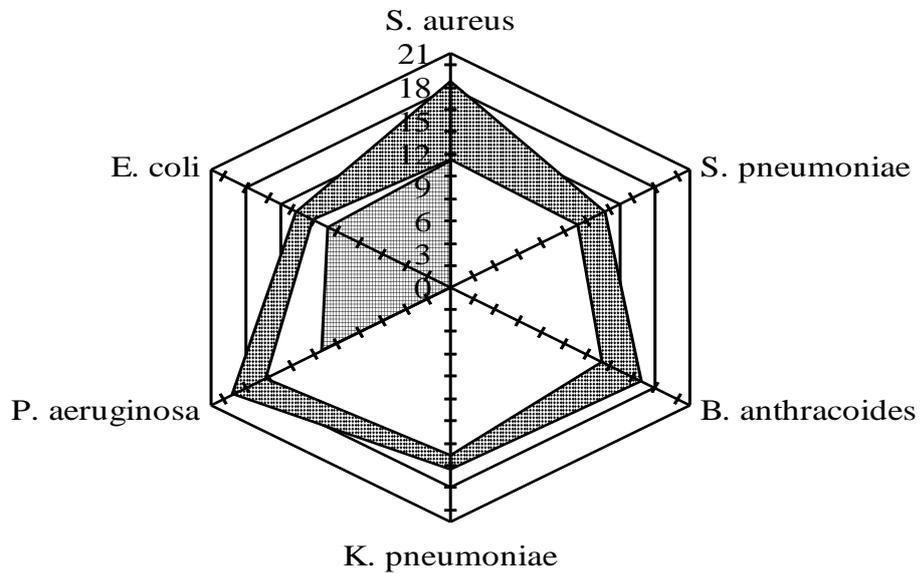


Fig. 3 – Macrocontour of spectrum of the antimicrobial activity of test specimens (diameters of the growth cessation zone the museum strains of microorganisms, mm), where:

- ◆◆◆◆ – tincture “Casdent”;
- – drug “Stomatophyt”;
- ▣ – drug “Rotocan”.

Dependence of antimicrobial actions on the test-strain of microorganism was ascertained by experimental studying of the antibacterial activity of the tincture.

It has been found that antimicrobial potential of tinctures "Casdent" exceeds the antimicrobial activity of such reference preparations as "Rotocan" and "Stomatophyt". It is proved insignificant antimicrobial effect of herbal preparation "Rotocan" against *S. aureus*, *E. coli* and *P. aeruginosa*.

The foreign preparation "Stomatophyt" shows antimicrobial activity against all studied strains of microorganisms, but its level is inferior to developed tincture "Casdent".

### Conclusion

1. The component composition and quantitative content of fatty acids in the mixture of herbal raw-materials-ingredients, from which the tincture was received, and in the herbal remedy "Casdent" were determined by the method of gas-liquid chromatography
2. Identified antimicrobial potential of the complex tincture exceeds mentioned feature of herbal medicines, represented in the domestic pharmaceutical market for the treatment of inflammatory periodontal diseases.
3. The presence, found out by the previous and this researches, of such groups of biologically active substances as volatile compounds, flavonoids, saturated and unsaturated fatty acids determines the expected pharmacological activities of tinctures "Casdent", among which an antimicrobial activity is confirmed. This is the basis for the inclusion of the developed herbal remedy in therapeutic regimen of inflammatory diseases in dentistry.

### References

1. Асилбекова, Д. Т. Полиненасыщенные жирные кислоты масла семян *Cortusa turkestanica* [Текст] / Д. Т. Асилбекова, Х. Р. Нуриддинов, А. М. Нигматуллаев и др. // Химия природных соединений. – 2010. – № 2. – С. 151-153.
2. Кашпур, Н. В. Дослідження антибактеріальної та антифунгальної активності хлороформних фракцій трави *Galium dasypodium* Klok. і *Galium salicifolium* Klok. [Текст] / Н. В. Кашпур, О. В. Горяча, Т. В. Ільїна та ін. // Актуальні питання фармацевтичної і медичної науки та практики. – 2012. – № 1(8). – С. 7-9.
3. Лобань, Г. А. Роль резидентної мікрофлори в розвитку патологічних процесів порожнини рота [Текст] / Г. А. Лобань // Український стоматологічний альманах. – 2009. – № 3. – С. 3-5.
4. Назаров, П. Е. Полиненасыщенные жирные кислоты как универсальные эндогенные биорегуляторы [Текст] / П. Е. Назаров, Г. И. Мягкова, Н. В. Гроза // Вестник МИТХТ. – 2009. – Т. 4, № 5. – С. 3-19.
5. Трифонов, Б. В. Об использовании фитопрепаратов в детской стоматологической практике [Текст] / Б. В. Трифонов, С. Н. Гонтарев, И. С. Гонтарева, Я. В. Луценко // Вестник АМГН. – 2010. – №1(4). – С. 42-44.

6. Чаленко, Ю. Применение фитотерапевтических средств в комплексном лечении заболеваний пародонта [Текст] / Ю. Чаленко // Ліки України. – 2003. – № 1. – С. 24-27.
7. Шульга, Л. І. Вивчення антифунгальної дії стоматологічного фітозасобу [Текст] / Л. І. Шульга // Клінічна фармація. – 2011. – Том 15, № 2. – С. 52-55.
8. Шульга, Л. І. Розробка складу рідкої лікарської форми для терапевтичної стоматології [Текст] / Л. І. Шульга // Клінічна фармація, фармакотерапія та медична стандартизація. – 2011. – № 1-2. – С. 161-165.
9. Шульга, Л. І. Хромато-мас-спектрометричний аналіз компонентного складу легкої фракції настою «Касдент» [Текст] / Л. І. Шульга, В. С. Кисличенко, О. Ф. Пімінов // Український медичний альманах. – 2011. – Том 14, № 4. – С. 186-189.
10. Calder, P.C. Polyunsaturated fatty acids and inflammatory processes: New twists in an old tale [Text] / P. C. Calder // Biochimie. – 2009. – Vol. 91, № 6. – P. 791-795.
11. Carballeira, N. M. New advances in fatty acids as antimalarial, antimycobacterial and antifungal agents – a review [Text] / N. M. Carballeira // Progress in Lipid Research. – 2008. – Vol. 47. – P. 50-61.
12. Cunnane, S. C. Problems with essential fatty acids: time for a new paradigm? [Text] / S. C. Cunnane // Prog. Lipid Res. – 2003. – Vol. 42, № 6. – P. 544-568.
13. Desbois, A. P. Antibacterial free fatty acids: activities, mechanisms of action and biotechnological potential [Text] / A. P. Desbois, V. J. Smith // Applied Microbiology and Biotechnology. – 2010. – T. 85, № 6. – P. 1629-1642.
14. Maggi, F. Chemical composition and antimicrobial activity of *Hypericum hircinum* L. Subsp. *majus* essential oil [Text] / F. Maggi, C. Cecchini, A. Cresci et al. // Химия природных соединений. – 2010. – № 1. – С. 106-109.
15. Řiháková, Z. Antifungal activity of lauric acid derivatives against *Aspergillus niger* [Text] / Z. Řiháková, M. Plocková, V. Filip // European Food Research and Technology. – 2001. – Vol. 213. – P. 488-490.
16. Shulga, L. I. Experimental substantiation of herb material selection in the making of complex tincture for periodontics [Електр.] / L. I. Shulga, S. V. Biriukova, O. F. Piminov // Annals of Mechnikov Institute. – 2011. – № 1. – P. 30-33.
17. Sylvain, L. S. Effect of  $\alpha$ -linolenic, capric and lauric acid on the fatty acid biosynthesis in *Staphylococcus aureus* [Text] / L. S. Sylvain, V. M. Lucia, G. Elisabetta // International Journal of Food Microbiology. – 2009. – Vol. 129. – P. 288-294.

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**КОРЕЛЯЦІЯ СТРУКТУРНИХ ОСОБЛИВОСТЕЙ**  
**БІОЛОГІЧНО АКТИВНИХ СПОЛУК**  
**РОСЛИННОГО ЗАСОБУ ТА ЙОГО**  
**ФАРМАКОЛОГІЧНОЇ ЦІННОСТІ**  
**Шульга Л.І.**

Методом газової хроматографії підтверджено вміст та ідентифіковано жирні кислоти в ліпофільних фракціях як рослинної композиції, так і одержаної на

її основі настоянки. Наявність означеної групи біологічно активних сполук доповнює біологічну цінність фітопрепарату, оскільки жирні кислоти відповідають за прояв антимікробних властивостей поряд з флавоноїдами та леткими сполуками. Експериментально визначено протимікробну активність екстракційного засобу по відношенню до грампозитивних та грамнегативних мікроорганізмів.

**Ключові слова:** рослинний збір, настоянка, жирні кислоти, протимікробна активність.

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**КОРРЕЛЯЦИЯ СТРУКТУРНЫХ**  
**ОСОБЕННОСТЕЙ БИОЛОГИЧЕСКИ**  
**АКТИВНЫХ СОЕДИНЕНИЙ РАСТИТЕЛЬНОГО**  
**СРЕДСТВА И ЕГО ФАРМАКОЛОГИЧЕСКОЙ**  
**ЦЕННОСТИ**

**Шульга Л.И.**

Методом газовой хроматографии подтверждено присутствие и идентифицированы жирные кислоты в липофильных фракциях как растительной композиции, так и полученной из нее настоянки. Наличие данной группы биологически активных соединений дополняет биологическую ценность фитопрепарата, поскольку жирные кислоты отвечают за проявление антимикробных свойств наряду с флавоноидами и летучими соединениями. Экспериментально определена противомикробная активность экстракционного средства по отношению к грамположительным и грамотрицательным микроорганизмам.

**Ключевые слова:** растительный сбор, настоянка, жирные кислоты, противомикробная активность.

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Fatty acids in lipophilic fractions of the herbal composition as well as of the tincture obtained from it were detected and identified by the method of gas chromatography. The presence of this group of biologically active compounds supplements the biological value of the herbal medicine since fatty acids are responsible for the manifestation of antimicrobial properties along with flavonoids and volatile compounds. An antimicrobial activity of extraction agents was experimentally determined in regard to grampositive and gramnegative microorganisms.

**Key words:** mixture of officinal plants, tincture, fatty acids, antimicrobial activity.