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Adress:
17/19/28 Kamińskiego st.
90-229 Lodz, Poland

KRS: 0000628361
NIP: 7252139787
REGON: 364954217

e-mail: fundacja@promovendi.pl
www.promovendi.pl

ISBN: 978-83-967915-2-8

September, 2023

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September 16, 2023

PROMOVENDI

National Scientific Conference „Knowledge – Key to Success”

VII edition

January 21, 2023

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ASSESSMENT OF STATIC AND DYNAMIC BALANCE OF ACTIVELY DANCING CHILDREN

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Abstract:

The aim of this study was to assess the impact of active dance practice on dynamic and static balance among children aged 12 to 16 years. Total of 60 children were qualified for the study, and divided into two groups. The study group consisted of 30 children actively practicing dancing while the control group included 30 children not practicing dance. Static and dynamic balance was tested using the Zebris PDM stabilimetric platform. The conducted research showed statistically significant differences between the study groups in terms of static balance ($p<0.05$). Children actively practicing dance showed better static balance both with eyes open and closed in comparison to the control group. However, in the case of dynamic balance, there were no statistically significant differences between the groups. This research confirms that active dance practice has a positive effect on the static balance.

Keywords:
static balance, dynamic balance, children, dance

Introduction

In order for dance to exist, the human body had to poses the right features. One of them is balance, it means, the ability to maintain a stable posture with or without movement. Keeping the balance is a lifelong skill. As a small child, we learn how to keep and maintain it, we improve it during adulthood, but in old age we have to take particular care of it, because the loss of balance increases the risk of falls, which can lead to dangerous injuries. Balance has many sources of receiving stimuli in the human body - starting from sight, through touch and proprioception, to the sense of balance located in the inner ear [1-3].

There is a lack of literature describing the impact of dance on balance, its participation in exercise and the improvement it may provide. However, there are many studies focusing on rehabilitation with the help of dance in mental and neurodegenerative diseases, social disorders and self-acceptance [4-12]. The results of these studies indicate the positive impact of dance on the rehabilitation of patients. Unfortunately, there are no studies describing the impact of this physical activity on balance. The number of available, published studies is limited and they give different results, therefore many

researchers indicate the need for further exploration in this area [4-12]. This fact inspired the authors to carry out the research presented below, which would expand the literature on the subject. Researchers noticed a large improvement in balance depending on the length of the dancers' practice, the number of hours devoted to training, and the type of performed dance. Thanks to the multitude of styles and forms, dance has a wide range of technical aspects that can affect balance. The researchers focused on the dancers of a particular technique and style, which makes it difficult to establish a uniform result of the collected and developed data. The variety of research forms and differences in results indicate a constant need for further research and its deeper analysis [9-11,13-15]. Dance as a form of rehabilitation is a great example of how to mix business with pleasure. There are more and more established centers offering accessible opportunities for public dance rehabilitation. There are professional associations regularly publishing research results and uniting researchers, instructors, physiotherapists and dance therapists whose goal is to develop and support dance therapy [14, 15].

The aim of the study is to assess the impact of active dance practice on dynamic and static balance among children aged 12-16.

Material and methods

Study participants

The observation group consisted of 60 children, including 30 children from the study group and 30 children from the control group. Gender wise, in both subgroups the majority were girls (73.3% vs 53.3%), and the minority were boys (26.7% vs 46.7%). The control group was matched in terms of age and gender, and consisted of pupils of a primary school in the Podkarpackie County who did not practice dancing, while the study group consisted of active dancers, members of dancing clubs from the Podkarpackie County. The criterion for admission to the study group was conscious, voluntary consent to participate in the study, age from 12 to 16 years old, minimum 2 years long dance training and 4 to 5 hours of dance training per week. The control group consisted of age- and gender-matched healthy children who did not practice dancing. The criterion for exclusion from the study were musculoskeletal injuries, comorbidities that may disturb balance.

The average age of children in the study group is 14.1 years ± 1.4 and in the control group = 14.3 years ± 1.1, the average body height in the study group is 165.8. centimeters ± 7.4 and in the control group it was = 163.6. centimeters ± 6.9, body weight = 55.2 kilograms ± 8.9 vs. = 56.4 kilograms ± 8.2).

The study protocol was assessed and accepted by the Scientific Research Ethics Committee. All of the procedures were executed in full compliance with the principles set forth in the Declaration of Helsinki.

Procedure

The studies were conducted by one researcher in controlled conditions. Static and dynamic balance was tested using the Zebris PDM stabilimetric platform. The measurement was carried out with the eyes open and closed. Assessment on the platform involved continuous measurement of the Center of Foot Pressure (COP). By recording body sway deviations, it was possible to acquire accurate information on postural balance. COP movements corresponded to the Center of Mass movements (COM) in the frontal and sagittal planes. The measures taken into account in the analyzes

included the Average Load Point X, determining the lateral coordinates X (Devation X, in mm), the Average Load Point Y determining the anterior-posterior coordinates Y (Devation Y, in mm), Path Length (mm) of the COP during the trial, Average COP velocity (V average, in mm/s) and Area Circular, i.e., the area defined by the COP during the trial (mm^2).

Statistical analysis

The statistical analyzes of the collected material were computed using StatSoft's Statistica 13.3 package. To assess differences in the average level of a numerical feature, the student's t-test for independent samples was used, the t-test with independent estimation of variance. Due to the failure to meet the assumptions of the parametric test (lack of compliance of the distribution of the variable with the normal distribution verified by the Shapiro-Wilk test), a non-parametric test was used for two U Mann-Whitney population. The significance threshold level of $p < 0.05$ was assumed.

Results

First, the differences in the parameters of static balance between the test group and the control group were checked. Measurements were made on the left lower limb with eyes open. There were no statistically significant results between the studied variables in study and control groups. Detailed data are presented in Tab. 1.

Tab. 1. Relationship between the statistical balance between the study group and the control group (measurement on the left lower limb with eyes open)

Parameter/Group		Static balance (left lower limb – eyes open)								
		N	$\overline{X}$	Me	Min.	Max.	Q1	Q3	*SD*	*p*
95% Confidence ellipse area [mm²]	Study	30	795	854	292	1530	535	1030	323.8	**0.291****
	Control	30	1584	627	319	25953	409	952	4631.5	
COP path lenght [mm]	Study	30	743	722	408	1371	566	853	201.1	**0.501****
	Control	30	826	674	370	4594	489	866	746.3	
COP average velocity [mm/s]	Study	30	37	36	20	69	28	43	10.1	**0.478****
	Control	30	41	34	18	230	24	43	37.4	
Devation X [mm]	Study	30	2	1	-23	33	-11	12	14.6	**0.077***
	Control	30	9	9	-18	42	-2	17	13.7	
Devation Y [mm]	Study	30	-90	-90	-169	-32	-106	-74	26.6	**0.593***
	Control	30	-86	-84	-150	-36	-94	-66	27.3	

Source: own calculations

N – number of participants; $\overline{X}$ – mean; Me – median, Min. – minimum value, Max. – maximum value; Q1 – lower quartile; Q3 – upper quartile, SD – standard deviation;* T-student for independent samples-test results
** Mann-Whitney U-test results

The relationships between the parameters of statistical balance in children from the study group and the control group were checked when measured on the right lower limb and with eyes open. A higher deviation in the Y axis was observed in children from the control group compared to children from the study group. This was the only prominent difference that turned out to be statistically significant (p=0.006). Detailed data are presented in Tab. 2.

Tab. 2. Relationship between the static balance between the study group and the control group (measurement on the right lower limb with eyes open)

Parameter/Group		Static balance (right lower limb – eyes open)								
		N	$\overline{X}$	Me	Min.	Max.	Q1	Q3	*SD*	*P*
95% Confidence ellipse area [mm^2]	**Study**	30	1035	715	221	4321	588	1260	891,6	**0,291****
	Control	30	912	721	406	3982	596	942	653,5	
COP path lenght [mm]	**Study**	30	797	705	328	2337	569	864	383,3	**0,501****
	Control	30	726	694	392	1704	511	864	288,2	
COP average velocity [mm/s]	**Study**	30	40	35	16	117	28	43	19,2	**0,478****
	Control	30	36	35	20	85	26	43	14,3	
Devation X [mm]	**Study**	30	5	5	-36	33	-1	13	14,0	**0,077***
	Control	30	3	10	-87	42	-1	19	27,9	
Devation Y [mm]	**Study**	30	63	68	-3	105	45	81	26,7	**0,006****
	Control	30	87	85	11	222	69	104	36,8	

Source: own calculations

N – number of participants; $\overline{X}$ – mean; Me – median, Min. – minimum value, Max. – maximum value; Q1 – lower quartile; Q3 – upper quartile, SD – standard deviation;* T-student for independent samples-test results
** Mann-Whitney U-test results

In turns, when checking the relationships between the results of static balance of measurements carried out with eyes closed for both the left and right lower limbs, a higher deviation in the X axis was observed in people from the control group compared to children from the study group. The examined relationships turned out to be statistically significant at the level of p=0.004. Detailed data are presented in Tab. 3 and 4.

Tab. 3. Relationship between the static balance between the study group and the control group (measurement on the left lower limb with eyes closed)

Parameter/Group		Static balance (left lower limb – eyes closed)								
		N	$\overline{X}$	Me	Min.	Max.	Q1	Q3	*SD*	*P*
95% Confidence ellipse area [mm^2]	**Study**	30	3009	2037	428	13517	1752	3629	2453,3	**0,291****
	Control	30	7060	4454	1197	26801	3158	8941	6187,0	
COP path lenght [mm]	**Study**	30	1574	1604	1070	2641	1281	1724	365,1	**0,501****
	Control	30	2096	1973	748	4548	1272	2680	967,1	
COP average velocity [mm/s]	**Study**	30	80	82	53	132	64	90	18,7	**0,478****
	Control	30	100	91	37	227	56	131	49,1	
Devation X [mm]	**Study**	30	-0	4	-30	28	-12	9	15,2	**0,004***
	Control	30	11	10	-12	40	1	22	14,3	
Devation Y [mm]	**Study**	30	-78	-86	-170	62	-95	-63	45,1	**0,593***
	Control	30	-75	-75	-255	50	-89	-56	47,2	

Source: own calculations

N – number of participants; $\overline{X}$ – mean; Me – median, Min. – minimum value, Max. – maximum value; Q1 – lower quartile; Q3 – upper quartile, SD – standard deviation;* T-student for independent samples-test results
** Mann-Whitney U-test results

Tab. 4. Relationship between the static balance between the study group and the control group (measurement on the right lower limb with eyes closed)

Parameter/Group		Static balance (right lower limb – eyes closed)								
		N	$\overline{X}$	Me	Min.	Max.	Q1	Q3	*SD*	*p*
95% Confidence ellipse area [mm^2]	**Study**	30	3054	2451	1168	12818	1586	3167	2476,2	**0,291****
	Control	30	4361	2757	1216	14238	2087	5162	3564,7	
COP path lenght [mm]	**Study**	30	1386	1375	544	2537	1104	1525	405,6	**0,501****
	Control	30	1669	1516	872	3246	1152	2192	644,4	
COP average velocity [mm/s]	**Study**	30	71	70	49	127	56	77	18,7	**0,478****
	Control	30	84	76	44	162	58	110	32,2	
Devation X [mm]	**Study**	30	4	2	-23	35	-2	10	12,0	**0,004***
	Control	30	11	6	-15	91	-0	15	19,8	
Devation Y [mm]	**Study**	30	84	85	-21	135	71	106	30,5	**0,593***
	Control	30	56	60	-103	111	44	78	39,0	

Source: own calculations

N – number of participants; $\overline{X}$ – mean; Me – median, Min. – minimum value, Max. – maximum value; Q1 – lower quartile; Q3 – upper quartile, SD – standard deviation;* T-student for independent samples-test results
** Mann-Whitney U-test results

Subsequently, the relationships between the results for dynamic balance in the study group and the control group were examined in the measurements for the left and right lower limbs. No statistically significant differences were observed. Detailed data for the left lower limb are presented in Tab. 5. statistically significant differences were observed. Detailed data for the left lower limb are presented in Tab. 5.

Tab. 5. Relationship between the dynamic balance between the study group and the control group (measured on the left lower limb)

Parameter/Group		Dynamic balance (lower left limb)								
		N	$\overline{X}$	Me	Min.	Max.	Q1	Q3	*SD*	*p*
Time change heel to forefoot (s)	**Study**	30	0,29	0,30	0,16	0,47	0,24	0,33	0,07	**0,865*****
	Control	30	0,29	0,29	0,01	0,44	0,22	0,37	0,11	
Maximum Pressure - forefoot (N/cm^2)	**Study**	30	32,3	31,0	20,8	60,8	26,5	34,8	8,47	**0,695****
	Control	30	31,7	28,4	17,3	53,3	24,5	37,8	9,15	
Maximum Pressure - midfoot (N/cm^2)	**Study**	30	11,5	10,4	5,0	25,3	8,0	14,3	4,78	**0,137****
	Control	30	10,2	8,2	3,8	32,5	6,0	13,0	6,14	
Maximum Pressure - heel (N/cm^2)	**Study**	30	26,7	26,4	15,5	40,0	22,0	28,8	6,37	**0,273***
	Control	30	24,7	23,6	12,5	49,3	19,5	28,3	8,14	
Time maximum force % of stance time – forefoot	**Study**	30	73,8	74,9	47,5	80,6	72,4	76,1	5,74	**0,412****
	Control	30	72,6	74,0	57,9	82,6	68,4	76,3	6,16	
Time maximum force % of stance time – midfoot	**Study**	30	42,0	41,7	27,9	61,3	36,6	47,3	7,37	**0,549***
	Control	30	43,2	44,3	25,6	60,1	38,2	48,9	8,18	
Time maximum force % of stance time - heel	**Study**	30	19,6	19,8	7,0	25,7	16,4	22,9	4,17	**0,712****
	Control	30	20,2	20,1	14,2	26,4	17,3	23,8	3,52	

Source: own calculations

N – number of participants; $\overline{X}$ – mean; Me – median, Min. – minimum value, Max. – maximum value; Q1 – lower quartile; Q3 – upper quartile, SD – standard deviation;* T-student for independent samples-test results
** Mann-Whitney U-test results

Discussion

The aim of this study is to assess the impact of active dance practice on dynamic and static balance among children aged 12-16. The motivation to undertake these studies was the fact that in the literature the subject of the influence of dancing on balance sems to be neglected, especially concerning children. However, there are many centers and places where dance rehabilitation is being carried out, but it is still not very popular. It focuses mainly on the social aspect and mental disorders [4-12].

The conducted research has shown that dance is a training that improves static balance. Children actively practicing dance maintain better static balance both with eyes open and closed in comparison to the control group. However, as it happens with most therapies, it is important that the dance practice is done regularly, with the right commitment, usually over a long period of time. According to Sawicki et al. dancing has a positive effect on balance. Their research was carried out on 47 women who were students of the University of Poznań. 23 of them were active dancers while the other 24 were included in the control group. The authors point out that the conclusions of the conducted tests concern people with at least seven years of dance experience. Those conclusions prove that long-term and consistent dance practice affects the balance [13].

In our own research, in the case of dynamic balance, no statistically significant differences between the groups were found. We suppose that this may be related to the fact that there are many factors that affect balance. Among the children from the study groups, most are in puberty and undergo major growth, hormonal and structural changes, which also have a huge impact on static and dynamic balance what could have been reflected in our results. Moreover, our researched consisted of beginner dancers, which could also have influenced the obtained results.

The dance has many forms and styles. Depending on the needs and preferences of the dancer, one can always find something suitable and satisfying. From hip-hop, breakdance through ballet, stage dance to ballroom dancing. Each style requires different skills, muscle strength, balance and coordination. Ballroom dancing, for example, consists of 10 individual dances and each dance requires different skills from the dancers. This thesis was confirmed by research conducted by Bojanowska et al. who studied 34 dancers, including 17 women and 17 men, and 37 non-dancers. Participants in the study had to have at least one year of dance experience and attend at least two 1 hour long classes weekly. The groups were tested using the SIGMA platform, focusing on proprioception on an unstable surface. The results of the research indicated no improvement in balance in comparison to the non-dancing group. The study group, however, consisted of beginner dancers, which could have influenced the final results. The insufficient number of hours of weekly training could have also underestimated an impact on the of dance on the balance of the subjects. The authors point out that further research and follow up studies of this topic are required [14]. Dynamic and static balance in dance are needed when performing complex acrobatic figures, but unfortunately people who are just starting their adventure with dance are rarely provided with specialized training fully devoted to balance or coordination. Instead, they are provided with general development classes or so-called general practice, which main role is to copy known choreographies and to correct basic or later on more complicated errors.

According to the researchers, Crotts and his team conducted research on 15 dancers from the Dance Department of Temple University and 15 people from the Department of Physical Therapy of

the same university. Their static and dynamic balance was assessed. It was shown that the group of dancers had a much better statistical balance [9]. Adult dancers with long training experience participated in the study. However, the research does not specify the number of hours spent on training by the study group. While comparing the results to other researchers, it can be concluded that the dancers were training consistently for more than 1-2 hours a week. These results are consistent with our research, where we assessed children with a minimum of 2 years of training experience for a minimum of 4 hours a week. Other researchers also assessed balance in 25 dancers and 25 non-dancers. As in our study, the age of both groups was similar, averaging 21 years, and height and weight were also similar. The average dance experience was about 11 years long. The studies were conducted on women who were practicing dancing for a minimum of four hours daily, 3-4 days a week. Balance was assessed on the PRO Balance Master® platform. The study group showed much better results, which included better posture stabilization and the ability to maintain it while performing motor tasks [10]. Those results confirm the results of our research, that active dancing improves balance. However, they also indicate that if dance is supposed to have a noticeable effect on balance, it must be consistently practiced for a long time (according to the sources, at least for 5-6 years with constant intensity for 4-5 hours a week). This particular group included older and more experienced dancers, while the group we studied was a group of beginners in puberty that affects the development of posture, its balance and efficiency.

To sum up the above mentioned considerations, it can be concluded that the results of research conducted by other researchers, as well as the results of our own research, indicate a positive effect of dance on balance. Unfortunately, for this effect to be statistically significant, dance must be practiced for a long time and quite intensively, which can be considered one of the few disadvantages of this therapy. Dance is a therapy with a wide spectrum of activity and a large number of ways to influence the patient, therefore this therapy is very versatile - it can be adapted and adjusted to almost any age, gender, problem or need of the patient [9, 13-17]. However, the impact of dance has not yet been fully researched, so further studies are needed to obtain a full and reliable picture of dance and its therapeutic role.

Conclusions

The conducted research showed significant differences between the study groups in terms of static balance. Children actively practicing dance show and maintain better static balance both with eyes open and closed compared to the control group. However, in the case of dynamic balance, there were no statistically significant differences between both groups. This research confirms that active dance practice among children aged 12-16 has a positive effect on the static balance.

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CARBIMAZOLE – SYNTHESIS AND STRUCTURAL ANALYSIS OF THE TIAMAZOLE DERIVATIVE

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Abstract:

Carbimazole is a prodrug compound whose main function, in the human body, is to inhibit the overproduction of thyroid hormones of various origins. Its active form is thiamazole, which is formed upon precise delivery to the intended organ. Therefore, this paper attempts to comprehensively describe the efficient organic synthesis of the prodrug with its proposed reaction mechanism and to analyse its spatial structure using chromatographic and spectroscopic methods, verifying the data available in the literature. The work aims to better understand the chemistry of carbimazole in order to take greater advantage of its therapeutic capabilities, but also to be a starting point for further development efforts in the context of its modified derivatives.

Keywords:
carbimazole, methimazole, prodrugs, hyperthyroidism, synthesis

Introduction

As of 2001, as much as 22% of the Polish population was affected by hyperthyroidism, and three years later, the number of chronically ill patients reached 1 202 000 people according to the Central Statistical Office [1, 2]. Increased development and design of pro-drugs may be an effective response to this problem. Their aim was to overcome, in particular, pharmaceutical and pharmacokinetic barriers, i.e. chemical instability, poor oral absorption of the drug, poor patient acceptance, among others [3]. Therefore, protherapeutics are intended to be a group of inactive or partially pharmacologically inactive chemical derivatives that are expected to undergo enzymatic or non-enzymatic transformation to an active form under in vivo conditions [4]. The elimination of the derivatising group is intended to allow the initiation of therapeutic activity in a strictly enzymatically defined organ.

An example of a compound initially used for thyrotoxicosis (excessive production of thyroid hormones), preparation for thyroidectomy and supportive treatment of thyroid disorders, is thiamazole (thiamazole, methimazole) [5, 6]. According to the IUPAC nomenclature, it is a 2-mercapto-1-methylimidazole composed of a flat heterocyclic ring with one methyl substituent at the nitrogen atom. It has the ability to form tautomeric forms that are equimolar to each other,

which differ from each other by the presence of a thiol or thione group. This is related to the presence of two π-type electrons, which stabilise the aromatic thiamazole moiety (Fig. 1) [7].

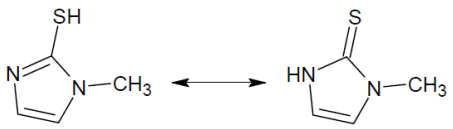

Fig. 1. Forms of thiol and thione tautomers of thiamazole
Source: own development

Its blocked derivative is carbimazole (carbimazole, neomercazole, basole), which is distinguished by the presence of an ethoxycarboxyl derivative that secures the active nitrogen from the heterocyclic ring [8]. Such a wide variety of elements present in the molecule allows the molecule to react versatilely in many microenvironments. For example, the presence of sulphur enhances ease of transport across biological membranes in the body, and the two nitrogens in the ring, after appropriate hydrolysis of the substituents, provide active reaction centres. It shows high sensitivity to sunlight, and its thermal decomposition is accompanied by the release of toxic nitroxide vapours and sulphoxides [9].

Carbimazole is a solid compound with a crystalline structure in the form of transparent or slightly whitish needles. It is odourless and has no flammable or explosive properties. In addition, it is soluble in water in small quantities and has sites that accept hydrogen bonding. It is a compound that, in addition to its thyroid importance, can be used as a free radical scavenger, i.e. an antioxidant. It reduces the intensity of the production of, among other things, hydroxyl radicals, which are formed by oxidation reactions [10]. Too much of this type of reaction could lead to numerous multi-organ damage at the tissue level, but also at the cellular level.

Initially, this compound, which is classified as a pro-drug, was tested, due to its thermal stability after dosing, as a therapeutic agent in the treatment of malaria [11]. However, after negative experimental results, it found its main use in thyroid disorders.

Material and methods

Reagents

The reagents that made it possible to carry out all the experiments are:

- standard:
  - carbimazole $C_7H_{10}N_2O_2S$ (≥ 98.0%), CAS 22232 – 54 – 8, *Sigma Aldrich (Germany);*
- derivatizing reactants:
  - methimazole $C_4H_6N_2S$ (≥ 99.0%), CAS 60 – 56 – 0, *Sigma Aldrich (Germany);*
  - etyl chloroformate $C_3H_5ClO_2$, CAS 541 – 41 – 3, *Sigma Aldrich (Germany);*
- solvents:
  - pyridine C_5H_5N (≥ 99.5%), CAS 110 – 86 – 1, *POCh (Poland);*
  - ethanol C_2H_6O (≥ 96%), CAS 64 – 17 – 5, *POCh (Poland);*
  - distilled water H_2O (100%), CAS 7732 – 18 – 5, *Maxima (Poland);*
- mobile phases:
  - used for high - performance liquid chromatography (HPLC):

- methanol: distilled water for HPLC with addition of phosphoric acid(V) with pH=2 in the following volume ratios: 90:10, 70:30;
- used for thin layer liquid chromatography (TLC):
  - formic acid: methanol (4:1);
  - acetone: butanol:sodium hydroxide (10%) (6:3:1);

- other reagents:
  - sodium chloride NaCl (≥ 99.0%), CAS 7647 – 14 – 5, *POCh (Poland);*
  - methanol – d_4 MeOD (≥ 99.8%), CAS 1849 – 29 – 2, *Sigma Aldrich (Germany);*
  - TLC Silica gel 60 F_{254} aluminium sheets, unmodified, aluminium reinforced, *Sigma – Aldrich (Kanada).*

Synthesis of carbimazole

2.00g of thiamazole was dissolved in 10ml of pyridine at 0°C and mechanical stirring was started until a homogeneous mixture was obtained. After 10 minutes, 3ml of ethyl chloroformate was introduced, maintaining a semi-liquid system. The reactants were stirred together for at least 30 minutes and then placed in a water bath with cooling medium for a further 30 minutes, controlling the temperature not to exceed 0°C. The resulting slurry was drained on filter paper under vacuum and washed with ethanol, followed by a mixture of ethanol and distilled water. After the procedure, the crystalline precipitate was placed in a paraffin-filled desiccators to dry.

HPLC, ^{1}H NMR, FTIR analysis

High Performance Liquid Chromatography analysis was made in two modes: with UV-DAD and MS detector.

HPLC-UV-DAD analysis was made on HP 1100 chromatograph, on non-polar C18 column (Thermo Scientific) 150 x 4.6mm, in isocratic condition, mobile phase was methanol: water in pH=2 (phosphoric(V) acid), flow rate 1ml/min.

LC-MS analysis was performed on a, Shimadzu high performance liquid chromatography quadrupole type tandem mass spectrometer, LCMS-8040, LC-20AD XR, SIL-20AC XR, LC-20AD XR, SPD-M20A, CTO-20AC, mobile phase was methanol: water, flow rate 1ml/min.

^{1}H NMR analysis was made on spectrometer NMR AVANCE II Bruker 400 MHz (9.39 T) with BBFO probe, Z-gradient, 5mm – broadband probe with X observation coil (X: 97Mo-31P + 19F) and 1H decoupling coil.

FTIR analysis was made on spectrometer FTIR JASCO LE 4600, standard construction: 7800-350 cm^{-1}, spectral resolution 0.4 to 16 cm^{-1}, standard detector: Peltier thermostated DLATGS (Mid-IR), standard beam splitter: Ge/KBr.

Results and discussion

Mechanism of carbimazole synthesis

The synthesis of carbimazole is the first stage of research. The active, main substrate is thiamazole, which undergoes an N-acylation reaction, i.e. the formation of an amide bond using an acylating agent (Fig. 2). Such a role in the reaction system is played by ethyl chloroformate, which is an ester of chloroformic acid and ethanol, which can act as a chlorinating agent,

a protective agent (blocking agent) or even an activating agent with catalytic properties, especially in metabolic transformations [12 – 14].

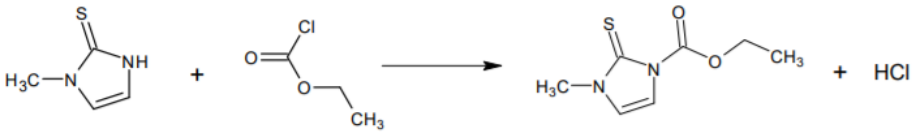

Fig. 2. Synthesis of carbimazole in structural terms [15, 16]
Source: own development

Such a selection of substrates and the type of reaction imply process requirements which, if adhered to, will increase yields. Therefore, the synthesis took place at 0°C in a pyridine solution. Desiccated thiamazole and laboratory equipment were used, with as little light as possible and constant air circulation achieved by means of an active fume cupboard. This is to limit the occurrence of downstream reaction stimulants that affect the activation of ethyl chloroformate decomposition, which can cause, at the very beginning of the test procedure, a reduction in production efficiency. The predicted side reactions are presented by Reaction (1) and Reaction (2).

$$C_3H_5ClO_2 + H_2O \rightarrow CHClO_2 + CH_3CH_2OH \quad (1)$$

$$CHClO_2 \rightarrow HCl + CO_2 \quad (2)$$

The main reaction of pro-drug synthesis in hyperthyroidism follows a mechanism that can be divided into two main steps. In the first, the transition of thiamazole into a de-derivatised form occurs as a result of dynamic contact with the blocking agent ethyl chloroformate. Electron pair displacements occur in the structures of these compounds, which consequently stabilise the main product. The second step is the uptake of the resulting hydrogen chloride by the pyridine molecules, forming the pyridine ion (Fig. 3 and Fig. 4). Depending on the conditions, the hydrogen chloride can partially volatilise, but also, by contacting the process water and steam, acidify the mixture.

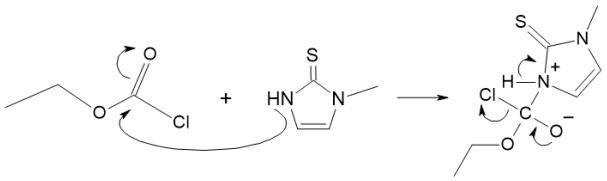

Fig. 3. Formation of the transition structure in the synthesis of carbimazole
Source: own development

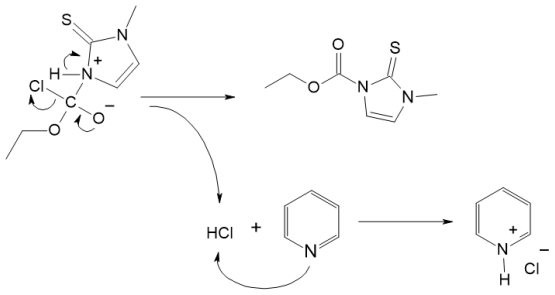

Fig. 4. Synthesis of carbimazole
Source: own development

Results of chromatographic analysis of carbimazole

The purity of the resulting mixture was confirmed by two types of liquid chromatography. Thin-layer chromatography was used first, which was performed on aluminium plates with a unmodified silica sorbent. Of the two sets of mobile phases used, the formic acid : methanol phase did not lead to component separation. Spot for thiamazole and carbimazole occurred at exactly the same distance from the start line, indicating a poorly chosen phase, in terms of separation, and exactly the same strength of the compounds' interactions with the stationary phase in such an environment. The second phase mixture allowed for a greater spread of compound spots and unambiguous analysis of the samples. From these, the high purity and homogeneity of the resulting product can be seen, particularly evident under the UV lamp at 254nm. This is evidenced by a single set of spots for a given line, which illustrate the presence of a molecule other than the active form, which is potentially the expected prodrug (Fig. 5).

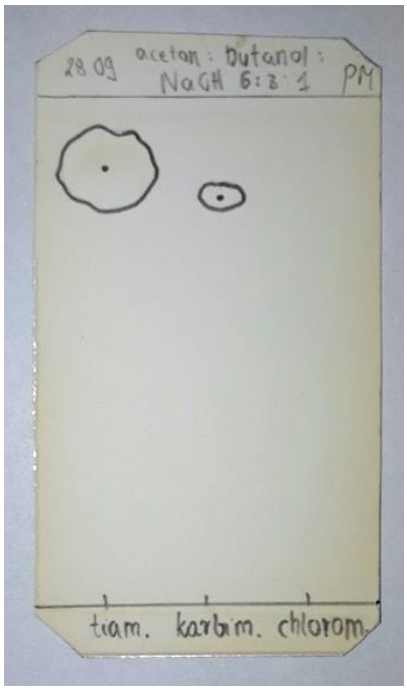

Fig. 5. TLC plate for acetone:butanol:sodium hydroxide (10%) phase (6:3:1)
Source: own development

Once measurements had been taken for each carbimazole synthesis sample in a given yield, it was possible to determine the retention factor, which allows the calculation of the retention factor for the main product. The identity of the compounds tested and the rapid transit time of the mixture components through the stationary phase were found. This means that the interaction with the polar stationary system is not strong and the analysed compounds stay long in the mobile phase, resulting in low retention factor values. This is a suggestion before performing an HPLC analysis in which thiamazole and carbimazole will actively adsorb on the non-polar stationary phase. Consequently peaks of the main components may appear relatively quickly on the chromatogram with much higher intensity, relative to possibly occurring minor impurities not observable by TLC. The relationships described are given in Tab. 1.

Tab. 1. Delay factor and retention for carbimazole in TLC analysis

Sample number	Synthesis yield [%]	Distance of the starting line from the front of the mobile phase – a [cm]	Distance of thiamazole spot from the start line – b [cm]	Distance of carbimazole spot from start line - c [cm]	R_f thiamazole [-] $R_f = \frac{b}{a}$	R_f carbimazole [-] $R_f = \frac{c}{a}$	Carbimazole retention factor – k [-] $k = \frac{1 - R_f}{R_f}$
1	44.27	6.80	5.80	5.40	0.85	0.79	0.26
2	61.66	6.40	5.10	4.80	0.80	0.75	0.33
3	87.63	6.40	5.30	4.90	0.83	0.77	0.31

Source: own calculations

Chromatographic analysis by HPLC focused on the determination of the characteristic retention times of thiamazole and carbimazole. By juxtaposing the commercial reagents with the compounds obtained, the presence of a prodrug or its close derivative in the precipitate studied, which was not thiamazole, was unambiguously noted. From the set of peaks obtained, it is possible to determine the relation that the higher the synthesis yield, the higher the soaring of the peak. The phenomenon of tailing or the proportion of smaller peaks, indicative of multiple impurities, is also not observed. This is presented in Tab. 2. The analysis was also performed on filtrates in which high contents of the main substrate and numerous small peaks of low soaring were recorded, which may be indicative of impurities resulting from the way the synthesis was performed, sample preparation or exposure of the mixture to the atmosphere. The higher the process yield, the complexity and intricacy of the chromatogram decreased.

Tab. 2. Retention time for samples in HPLC analysis of carbimazole

Sample number	Type of relationship tested	The origin of the relationship	Synthesis trial number	Retention times of the test compound [min]			Average compound retention time [min]	Standard deviation of retention time [min]
1	thiamazole	commercial	-	1.319	1.320	1.319	1.319	0.00058
2	carbimazole	commercial	-	1.406	1.401	1.406	1.404	0.00289
3	carbimazole	own synthesis	1	1.406	1.405	1.406	1.406	0.00058
4	carbimazole	own synthesis	2	1.411	1.406	1.406	1.408	0.00289
5	carbimazole	own synthesis	3	1.412	1.409	1.412	1.411	0.00173

Source: own calculations

When relating the chromatograms obtained to the chromatogram of the reference sample, note the presence of additional peaks of low intensity and complexity. These are not observed in samples of the own synthesis. They do not interfere with the reading of the data, but may indicate the presence of trace impurities or possible side compounds resulting from the small distribution of the carbimazole molecules (Fig. 6).

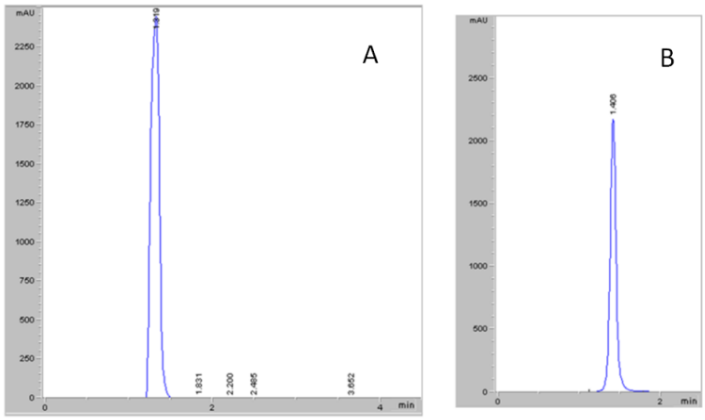

Fig. 6. Chromatogram of purchased thiamazole (A) and synthesised carbimazole (B)
Source: own development

Spectroscopic analysis of carbimazole

The first type of spectroscopic analysis, which was obtained using a DAD detector, with HPLC chromatography to determine the potential composition of the sample, was ultraviolet spectroscopy, which helped to identify characteristic groupings that distinguish the molecules from each other. Fig. 7 shows the spectrum of thiamazole (A) and carbimazole (B). In both cases, clear maximum can be seen at 210 nm and 240 nm, which are likely to originate from the transition from the non-bonding n to the anti-bonding σ* state, resulting from the excitation of carbon-sulphur and carbon-nitrogen bonds. In contrast, only in the case of the pro-drug spectrum is a discrete part from 279 nm observed, which is indicative of ester attachment and excitation from the non-bonding n to the anti-bonding π* state [17]. The analysis helps to provide an overview of the structure and confirms the attachment of the ethoxycarbonyl substituent.

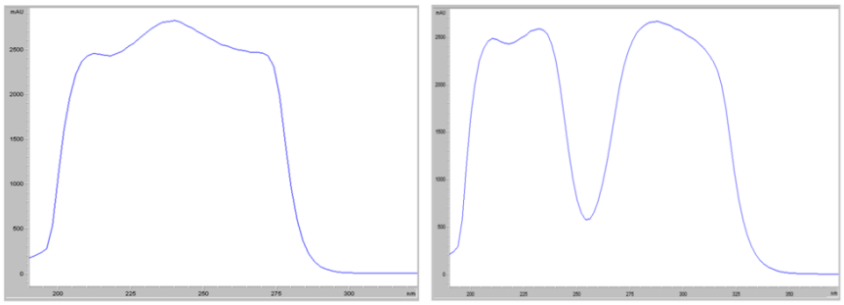

Fig. 7. Ultraviolet spectrum of thiamazole (A) and carbimazole (B)
Source: own development

The infrared spectrum complemented the acquired data with the determination of all functional groups for the carbimazole structure (Fig. 8.), which include the following vibrations:
- C - N bending vibrations in the range 1250 - 1000 cm^{-1},
- stretching vibrations C = S in the range 1220 - 1050 cm^{-1},
- bending vibrations C = C in the range 1900 - 1500 cm^{-1},
- stretching vibrations C = O in the range 1850 - 1600 cm^{-1},
- C - H stretching bond in the range 3000 - 2850 cm^{-1},
- bending for the - CH3 group in the range 1470 - 1430 cm^{-1},

- bending for group - CH2 - in the range 1485 - 1445 cm cm^{-1}[18].
Based on the comparison of all three post-synthetic samples, a greater stabilisation of the spectral lines and fewer perturbations are observed, which may have been due to the higher content of unreacted thiamazole, its derivatives or reaction by-products. However, the above spectral analysis do not fully confirm the presence of the therapeutic and do not exclude a mixture of substrates that may mimic effects similar to the spectra of pure reaction products.

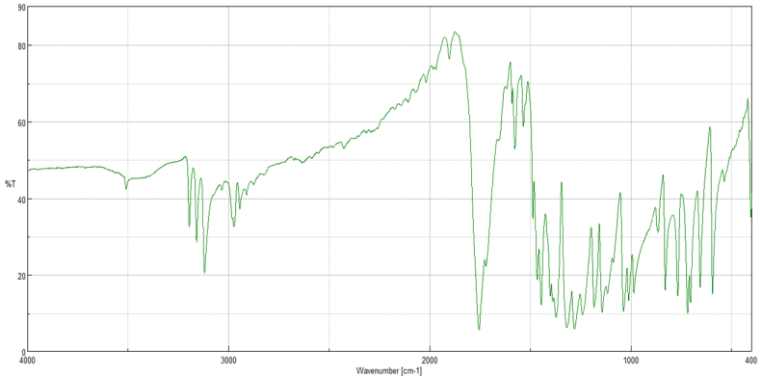

Fig. 8. Infrared spectrum of carbimazole
IR ν_{max} (cm^{-1}): 3511, 3196, 3159, 3120, 2983, 2975, 2946, 1756, 1720, 1488
Source: own development

To confirm the structure and presence of the inactive thiamazole derivative, proton magnetic resonance and mass spectrometer analyses were performed. From these, the mass of carbimazole (186g/mol) was confirmed in the form of a positive ion m/z = [M + H+]+ = 187. In the case of the product from the in-house synthesis, minor contents of the active form and the solvents or minor impurities used were detected (Fig. 9). Final confirmation of the spatial structure of carbimazole was provided by 1H NMR analysis. The correct positioning of the peaks and their multiplicity, together with their intensity coinciding with each other, fully substantiated the correct hydrogen distribution and their interrelationships in the carbimazole structure (Fig. 10) [19].

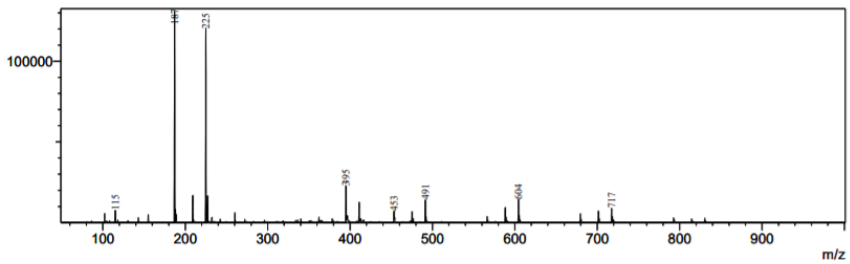

Fig. 9. Mass spectrum of carbimazole
Source: own development

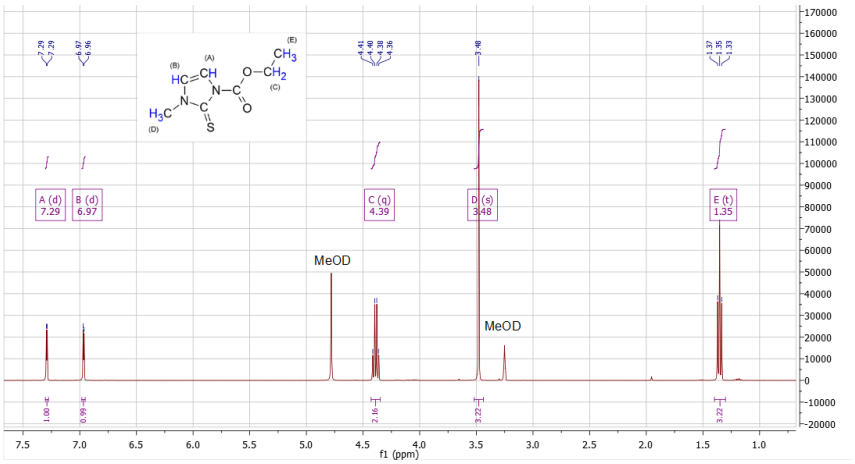

Fig. 10. ^{1}H NMR spectrum of carbimazole
Source: own development

Conclusion

The performed studies present an efficient and mechanistically predicted way to synthesise a therapeutic for hyperthyroidism. The nearly 90% reaction efficiency achieved is due to the use of an excess of a protecting agent, the frequency of reagent injection intervals and the selected experimental methodology. Along with the efficiency of the syntheses carried out, the vehemence of the reaction increased through the greater amount of energy released (exothermic reaction) and the overproduction of the gaseous mixture. This action led to the elimination of by-products and the performance of acylation with the migration of specific ions.

All synthesis effects were supported by comprehensive chromatographic and spectroscopic analysis. They enabled the precise determination of the mixture composition, purity and spatial structure of the main product, creating a modernised information base for the compound with all the analytical adjustments required when working with it.

On the basis of the physical and chemical stability obtained, further research could focus on making modifications to the structure of carbimazole, i.e. the introduction of an ethyl substituent instead of a methyl substituent (reduces harmfulness when dissociated), the replacement of sulphur with another macro- or micronutrient that would support thyroid function, e.g. zinc, or even a vitamin, e.g. B1 or B12. This could prove to be another step of medicinal chemistry towards solving the problems present in the world on a large scale.

Acknowledgements

This work was supported by the Polish Ministry of Education and Science.

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CHANGES IN TOURIST MOVEMENT IN TIMES OF PANDEMIC ON THE EXAMPLE OF OLESKO CASTLE IN THE OPINION OF LVIV REGION RESIDENTS

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Abstract:

The late start to the leisure and recreation season caused by the introduction of restrictive measures has also caused a cumulative effect that has negatively affected both the leisure and tourism industry and related industries - hotels and restaurants, transportation (passenger transport), retail trade, the entertainment industry and cultural institutions. Restrictions on movement that have been put in place by states to prevent the spread of COVID-19, declining incomes of citizens as a result of the economic crisis and recession are potentially increasing demand for recreation in Ukraine. The article deals with changes in tourist traffic during the COVID-19 pandemic on the example of Olesko Castle, according to residents of Lviv region. At the time of writing this article, significant differences in tourist traffic were observed, which the authors present and describe in detail. In addition, the authors specify the factors of tourist development limiting tourist movement during the COVID-19 pandemic in Olesko city. The research was conducted among 243 residents in the Lviv region between October-December 2021. According to given data, similar research has not been conducted in the study area to date.

Keywords:
tourism, COVID-19, Olesko Castle

Introduction

Tourism as an industry had its periods of greatest popularity, such as the Renaissance or the 17th and 18th centuries. Later, thanks to inventions and industrialisation, tourism became a mass phenomenon, but it is also worth mentioning periods when it faced many problems such as economic crises, epidemics and pandemics. A clear example of a crisis period in tourism can be observed today. Global tourist traffic has changed markedly. This has been influenced by, among other things, a reduction in the movement of tourists and a reduction in the activities of tourist facilities. According to WHO data, in April 2020. 96% of destinations worldwide could not provide tourism services due to pandemic-related restrictions. In the era of the COVID-19 pandemic, people have been trapped in their own homes. Since the start of the outbreak in November 2019, later recognised

as a pandemic in March 2020, global tourism traffic has changed markedly. The article deals with changes in tourist traffic during the COVID-19 pandemic using the example of Olesko Castle. It also deals with the collection of opinions of residents in the Lviv region. During the writing of the article, significant differences in tourist traffic during the pandemic period were observed, which the authors present and analyse in detail. In addition, the authors specify the factors limiting tourist traffic in the Olesko city area during the COVID-19 pandemic. The research discussed was conducted among 243 residents of the Lviv region in October-December 2021.

Literature review

Both the tourist and the day visitor are the subject of tourism studies. The term tourist first appeared in literature in Stendhal's novel Memoirs of a Tourist in 1838 (Memoires d'un touriste). The tourist of the title is a young man who wanders the world in order to have interesting adventures and for pleasure. He wishes to find the meaning of life in travel [1]. Travelling, a person always gains some kind of experience, positive or negative it depends on various internal and external factors. The Law of Ukraine "On Tourism" presents a tourist as a person who travels within Ukraine or to another country for a purpose not prohibited by the law of the country of permanent residence for a period of 24 hours to one year without performing any gainful activity and with the obligation to leave the country or the place of permanent residence within a certain period of time. According to Article 25 of the Law of Ukraine "On Tourism", tourists and same-day visitors are covered by the law of protection of consumer rights, the norms of the Law of Ukraine "On Protection of Consumer Rights" apply to tourists and same-day visitors, while tourists and same-day visitors meet certain criteria that distinguish them on the basis of making different volumes of consumption of services related to the concepts of "tourism", "tourism activities" or the possibility to engage in tourism without receiving tourism services at all (own translation) [2].

Taking into account the dominant motive for the trip, tourism can be divided into three types: leisure tourism, sightseeing (excursion) tourism and specialised (qualified) tourism. Considering the duration of the migration (trip), two types of tourism can be distinguished: holiday (long-term) tourism and holiday (short-term) tourism. In order to increase income from tourism, it is necessary to invest in the development of tourism infrastructure and to intensify tourist visits. According to K. Czech and A. Nitkiewicz-Jankowska, tourism infrastructure is a set of facilities, equipment and institutions necessary for the proper functioning of a tourism area. Tourism infrastructure consists of:

- accommodation base,
- catering facilities,
- communication (transport) base,
- accompanying facilities [3].

The emergence of the deadly COVID-19 disease has caused huge financial losses and triggered a global health and economic crisis around the world. The most frightening news of seasonal flu epidemics, pandemics and disasters, result in a sharp decline in travel and tourism, the dominant factor in the service industry. Pandemics have a negative impact on tourists' behaviour and mental wellbeing. As a result, they cancel planned trips for fear of contracting the disease, as avoiding virus transmission during travel seems impossible [4]. In total, the losses to the tourism industry in Ukraine are estimated at more than US$1.5 billion (own translation) [5].

The Lviv region offers a tourist product which is the "Golden Horseshoe". It is one of the most famous routes of defensive architectural monuments. The sites are currently in good condition unlike many others. It includes such famous sites as the castle in Olesko, Stary Siole, Svirzh, Zloczow and Podhorce [6]. Olesko Castle is one of the oldest castles in Ukraine. At one time its location was right on the border of two states - Lithuania and Poland, so the rulers of both countries fought over the appropriation of the stone palace (own translation) [7]. There are references to the castle in the literature from 1366 onwards. It can be assumed that it even existed under the rule of the Galician-Volyn principality and was the residence of a prince or nobleman. In 1605, the Olesko castle became the property of Voivode Jan Danilovich (own translation) [8]. In the middle of the 17th century, Jan Sobieski, the king of Poland, was born here (own translation) [9]. From the second half of the 17th century the castle began to decline (own translation) [8]. In 1951, Olesko Castle was struck by lightning, which caused a massive fire. For most of its existence, the castle walls were severely damaged. The castle was restored almost from ruin only a few decades ago (own translation) [7].

Today, the Olesko Castle grounds house a museum-branch of the Lviv Art Gallery and an open-air museum. The museum's exhibits include a painting by the Italian painter M. Altomonte, "The Battle of Vienna", dating from 1692, and a table on whose lid a "map" of religious pilgrimages was depicted. This table is one of the castle's most unique exhibits as it is considered to be the rarest cartographic exhibit among Ukraine's museum collections (own translation) [9].

Purpose of the study

The writing of the article was undertaken by the authors in October 2021. The aim of writing the article is to answer the questions:

- To what extent has the frequency of visits to Olesko Castle, by residents of the Lviv region, changed?
- To what extent has the frequency of visits to Olesko Castle by domestic tourists changed in the subjective opinion of local residents?
- To what extent has the frequency of visits to Olesko Castle by foreign tourists changed in the subjective opinion of local residents?

The answers to these questions will help the authors of the paper to specify to what extent tourism has changed during the pandemic on the example of Olesko Castle.

In addition, the author of the paper aims to obtain answers to the following questions:

- In which tourist base did the changes introduced during the pandemic have the strongest impact on changes in the frequency of visits to Olesko Castle?
- Which limiting factor will have the strongest impact on changes in the frequency of visits to Olesko Castle in each tourist development base?

The writing of the article was undertaken by the authors in October 2021. The aim of writing the article is to answer the questions:

- Has the frequency of visiting sites on the "Golden Horseshoe" trail changed in the present (2020-2021) compared to the frequency of visiting before 2020?
- To what extent has the frequency of visits to the 'Golden Horseshoe' tourist trail by domestic tourists changed in the subjective opinion of local residents?

- To what extent has the frequency of visiting the "Golden Horseshoe" tourist trail by foreign tourists changed in the subjective opinion of local residents?
- Does the Zolota Pidkova tourist route encourage domestic and foreign tourists to visit the Lviv region?

Research material and methods

Scientific research serves the purpose of cognition of reality, i.e. describing it, explaining the state and causes of phenomena, forecasting (predicting) future phenomena, as well as the possibility of influencing them. Various tools and methods are used in cognition - observation, experiment, surveying, testing, statistical analysis, etc. The primary tool of description is language, and the description must therefore meet the criteria of being unambiguous, comprehensible, concise and without redundancy of information. The scientific description must allow the study in question to be replicated. Accurate, linguistically and logically correct definitions of the concepts under study are essential, as well as the correct formulation of conclusions [10].

In the research in question, the subjective method was used. A survey questionnaire created by the author of the study was used as a research tool to collect relevant data. Before starting the survey, each respondent was able to read brief information regarding the purpose of the research and the results obtained, which will be used exclusively for the thesis. Participation in the survey was voluntary. A questionnaire consisting of three substantive parts was used in the research. After verification of all questionnaires, it was found that the study group consisted of 99 inhabitants of the town of Zloczów comprising 40.7% of all surveyed persons, 75 inhabitants of the town of Podhorce comprising 30.9% of all surveyed persons and 69 inhabitants of the town of Olesko comprising 28.4% of all surveyed persons. In terms of gender, 138 women, accounting for 56.8% of all people surveyed, and 105 men, making up 43.2% of all people surveyed respectively, took part in the study (Fig. 1).

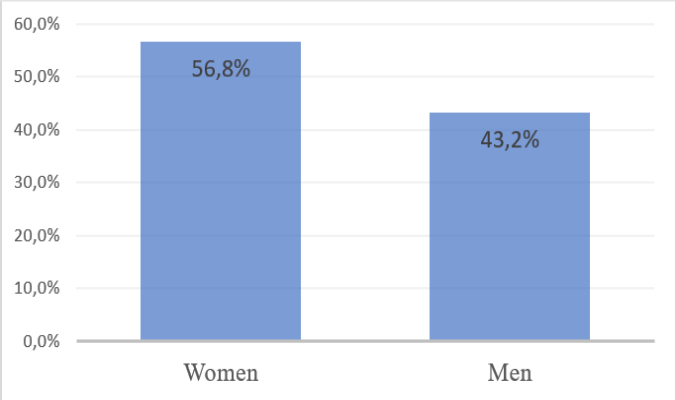


Fig. 1. Structure of the study group in relation to gender
Source: own research

The research was conducted electronically using the web-based survey system "Microsoft Forms". The link to the survey questionnaire was made available to residents of the Lviv region through the social networking site Facebook on the groups "ОЛЕСЬКО - РІДНА СТОРОНА Олеський Фейсбук", "Шукаю Золочів", "ZOLOCHIV. NET", "Барахолка смт ОЛЕСЬКО.",

"Підгірцівська громада", additionally on the information portal "ZOLOCHIV.NET" and through other people willing to help. The survey lasted from October to December 2021.

Results of the study

Fig. 2 shows visits to Olesko Castle by residents of the Lviv region before and during the pandemic (Fig. 2). The chart shows that visiting the castle before the pandemic and during the pandemic is not clearly different, because just as before the pandemic most people 24.3% of respondents declared that they had not visited the castle in Olesko, so during the pandemic this percentage only "increased" to 77.0%, but the answer "I have not visited" remained dominant.

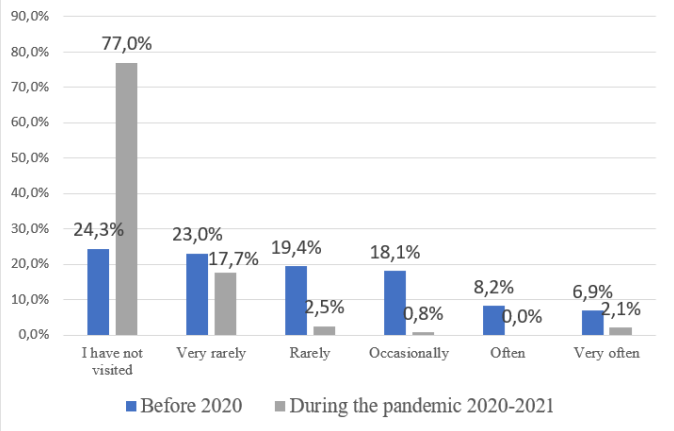


Fig. 2. Frequency of visits to Olesko Castle by respondents before and during the pandemic
Source: own research

Fig. 3 presents the perceptions of residents of the Lviv region about domestic tourists visiting Olesko Castle before and during the pandemic (Fig. 3). 23.0% of respondents declared that they had never met domestic tourists in the Olesko Castle area before the pandemic, 17.8% of people met domestic tourists rarely. During the pandemic, the difference in results is insignificant, only more respondents (81.1%) never met domestic tourists, while 17.8% rarely met tourists.

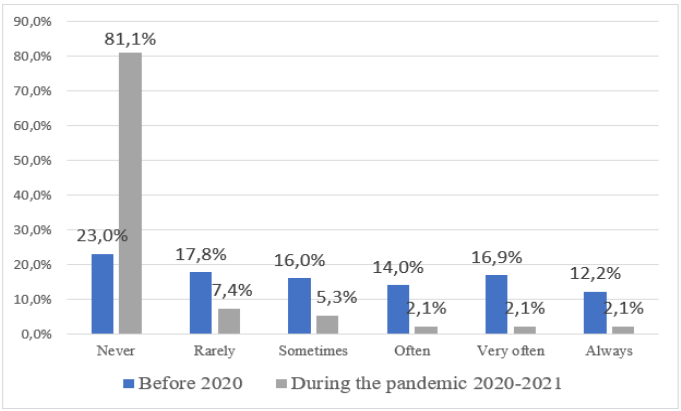


Fig. 3. Frequency of visits to Olesko Castle by domestic tourists before and during the pandemic
Source: own research

Fig. 4 presents the perceptions of residents of the towns of Złoczów, Podhorce and Olesko about foreign tourists visiting Olesko Castle before and during the pandemic (Fig. 4). The chart shows that

before the pandemic 26.3% of the people surveyed had never met or rarely (18.6%) met foreign tourists, while during the pandemic 86.4% declared that they had never met foreign tourists and 7.4% rarely met foreign tourists in the Olesko castle grounds.

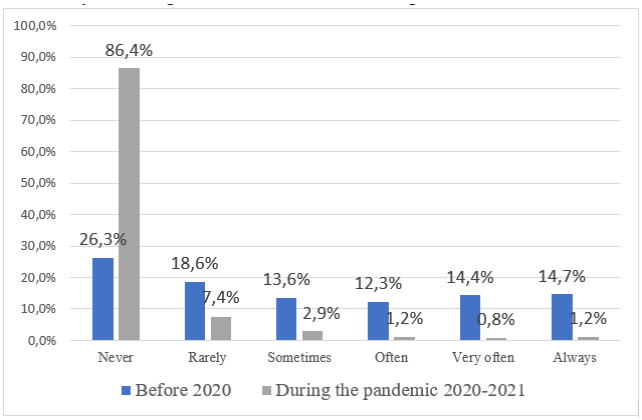
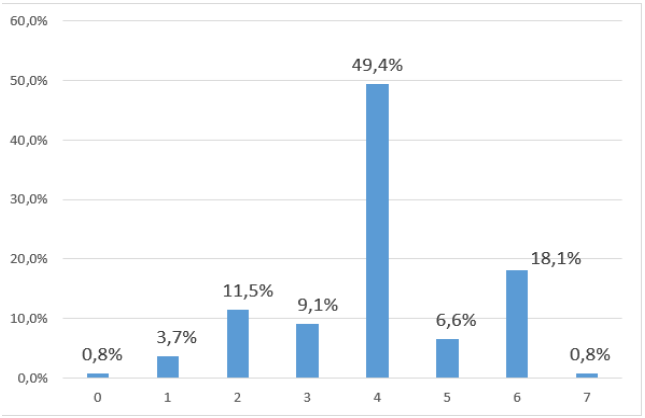


Fig. 4. Frequency of visits to Olesko Castle by foreign tourists before and during the pandemic
Source: own research

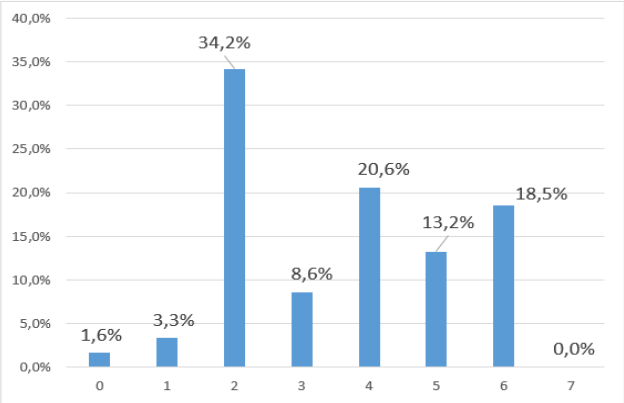
Fig. 5 shows that in Olesko the decisive factor limiting tourist traffic concerning the hotel base during the COVID-19 pandemic is the underdeveloped network of hotel facilities, 49.4% declared this, followed by the temporary or complete suspension of operations (18.1%) (Fig. 5).



Legend: 0 - no answer;
1 - price not commensurate with quality of services provided;
2 - distance from the visited attraction;
3 - limitations on use of accommodation services
4 - underdeveloped network of hotel facilities;
5 - reduction in facilities providing accommodation services;
6 - temporary or total suspension of activities;
7 - other.

Fig. 5. Factors limiting tourism in Olesko during the pandemic concerning the hotel base
Source: own research

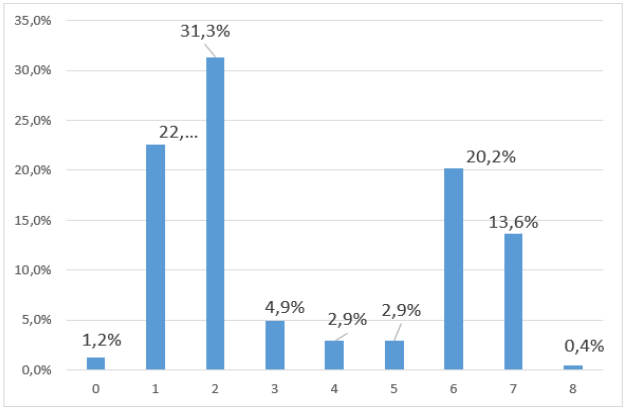
Fig. 6 presents the results on the subjective opinion of the residents of Lviv region on the factors limiting tourist traffic concerning the catering facilities during the COVID-19 pandemic (Fig. 6). The chart shows that the large distance from the visited attraction (32.1%) and the reduction of facilities providing catering services (20.6%) are decisive factors in the changes of tourist traffic in Olesko.



Legend: 0 - no answer;
1 - price not commensurate with quality of services provided;
2 - distance from the visited attraction;
3 - restrictions on the use of catering services;
4 - poorly developed network of catering facilities;
5 - reduction of facilities providing catering services;
6 - temporary or total suspension of activities;
7 - other.

Fig. 6. Factors limiting tourism in Olesko during the pandemic concerning the catering base
Source: own research

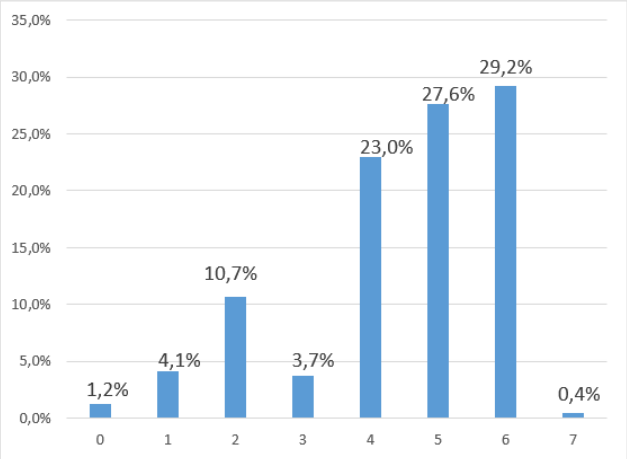
As can be seen from Fig. 7 in the Olesko area, the highest percentage of respondents declare that the poor condition of access roads is the main factor limiting tourist traffic in the transport base (31.3%), followed by the temporary suspension of domestic and foreign transport links (22.6%) (Fig. 7).



Legend: 0 - no answer;
1 - temporary suspension of domestic and foreign transport links
2 - poor condition of access roads;
3 - temporary suspension of domestic and foreign airlines;
4 - high prices for tickets;
5 - increased epidemiological control at borders;
6 - introduction of different epidemiological zones in the country;
7 - limitation of the permitted number of persons in transport;
8 - other.

Fig. 7. Factors limiting tourism in Olesko during the pandemic concerning the transport base
Source: own research

Fig. 8 presents the results on the subjective opinion of the inhabitants of the towns of Zloczów, Podhorce and Olesko on the factors limiting tourism concerning the accompanying base during the COVID-19 pandemic (Fig. 8). In the township of Olesko, the most important factors are the poorly developed accompanying base (29.2%) and the long distance from the visited attractions (27.6%).



Legend: 0 - no answer;
1 - introduction of curfews;
2 - temporary suspension of activities of places of entertainment and recreation (theatres, cinemas, galleries, markets, etc.)
3 - introduction of a senior citizens' hour in shops;
4 - restriction of the number of people allowed in public places;
5 - distance from the attraction to be visited;
6 - poorly developed accompanying facilities;
7 - other.

Fig. 8. Factors limiting tourism in Olesko during the pandemic concerning the accompanying base
Source: own research

Discussion

Research on changes in tourism during the pandemic on the example of Zloczow castle in the opinion of residents of the Lviv region has not yet been conducted. In the discussion, the author relies, inter alia, on similar marketing research on the territory of the above-mentioned cities conducted before the start of the COVID-19 pandemic.

In 2012 N. Mandiuk conducted marketing research on the territory of the castle in Olesko. One of the objectives of the research was the segmentation of tourists. The research of N. Mandiuk shows that visits to the castle in the town of Olesko had an upward trend from 2006 to 2010. The study of tourist flows by territorial structure shows that in 2006-2010 the main territory of demand for Olesko castle services is Lviv region (32.3%). This is followed by Kiev (14.6%), Ternopil (8.9%) and Volyn (8.4%). It should also be noted that around 10% of all museum visitors are foreign tourists, but this figure has increased by 2% over the last three years (2010-2012) (with the exception of 2010). A significant jump occurred in 2008, when the number of foreign tourists more than doubled. The main country showing demand for castle services is Poland (own translation) [11]. In our own research, the tourist traffic in 2020-2021 has a decreasing trend, which is a different result from the

results presented in the 2012 research. The difference of castle visits in the years before the pandemic and during the pandemic is 58.1 p.p. in domestic traffic and 60.1 p.p. in foreign traffic.

On the other hand, L. Borysenko, in his research conducted in 2021, states that Ukrainians mainly travel abroad during their travels. Thus, in 2019. 3.3 million tourists purchased tourist packages for a total of UAH 69 million, of which only UAH 237.9 thousand for domestic travel and the remaining UAH 2.2 million for tourist trips abroad, i.e. the vast majority of Ukrainians in 2019 preferred to rest outside Ukraine. Most tourists are residents of the city of Kyiv (252,000 within the country). The next largest number of domestic tourists are residents of Lviv, Ivano-Frankivsk and Odesa regions. The vast majority of domestic tourists travel for leisure purposes, with a significant proportion also occupied by business and training and spa trips. Sport and specialised tourism is something of an exception and is not popular among domestic tourists (own translation) [12]. Compared to the works presented above including the author's own research, it can be inferred that L. Borysenko presents a different angle on the intensity and trends of tourism in the time before the COVID-19 pandemic.

Both the author of their own study among a group of 243 respondents and M. K. Rahman, A. I. Gazi et al. in their 2021 study among a group of 731 respondents highlight the limiting factors affecting travel decisions and destinations during the COVID-19 pandemic. Rahman, Gazi et al. state that the COVID-19 pandemic significantly affected risk management, service delivery, travel model, distribution channel, avoidance of overcrowded destinations and hygiene and safety. Tourists believe that the COVID-19 pandemic has contributed to travel risk and management, as well as reducing their travel to destinations. Analysis of the data in this study found that tourists' perceptions of travel risk and management are highly related to risk management (self-translated) [13]. In our study, we found that the changes in tourism development introduced under the pandemic had a negative impact on the intensity of visits to the Golden Horseshoe Trail. The most significant impact of limiting factors is observed in the transport base, which is considered the basis for the realisation of any tourism activity, since, according to the definition of a tourist, "is a person who came to a given destination for the following purposes: leisure, medical, sightseeing, religious, sports, business, family, social, political and other (except for profit motives) and who spent at least one night at the place of temporary stay in public or private accommodation [14].

Conclusions

The aim of writing the paper was to analyse the changes that took place in tourist traffic during the COVID-19 pandemic on the example of the frequency of visits to Olesko Castle. The stated aim of the paper was fulfilled. Thanks to the reliable answers of the respondents taking part in the study, answers to the research questions posed earlier were obtained. After an in-depth analysis of the research results, the author formulated the following conclusions:

1. Residents of the Lviv region significantly reduced their visits to Olesko Castle during the COVID-19 pandemic.
2. Domestic tourists visited Olesko Castle to a significant extent less frequently during the COVID-19 pandemic than before it began.
3. Foreign tourists visited Olesko Castle to a lesser extent during the COVID-19 pandemic than before it began.

4. Changes made during the pandemic to the hotel base had the strongest impact on changes in the frequency of visits to Olesko Castle.
5. The smallest impact of changes introduced during the pandemic in tourism development in Olesko is seen in the accompanying base.
6. The greatest importance as a limiting factor in the hotel base of the city of Olesko during the pandemic has an underdeveloped network of hotel facilities.
7. The greatest importance as a limiting factor in the catering base of the city of Olesko during the pandemic is the distance from the visited attraction and the underdeveloped network of catering facilities.
8. The greatest significance as a limiting factor in the transport base of Olesko during the pandemic is the poor condition of access roads and the temporary suspension of domestic and foreign transport links.
9. The greatest importance as a limiting factor in the accompanying base of the town of Olesko during the pandemic is the poorly developed accompanying base and the long distance from the visited attraction.

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IX edition

April 15, 2023

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ASSESSMENT OF BODY COMPOSITION AND FITNESS LEVEL OF WOMEN IN A 3 LEAGUE CLUB

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Abstract:

The paper dealt with the consideration of the issue of physical fitness and body mass composition. In addition to the analysis of the literature, the paper conducted a study on a group of female volleyball players in the III league, allowing the evaluation of their body mass composition and physical fitness. The purpose of the study was to determine the physical fitness of female volleyball players in a III league club and their body mass composition. Fifteen female volleyball players participated in the research conducted in this regard. The study included analysis of body mass composition and performance of three fitness tests. The study used the case analysis method. The study had a two-stage character. First, the players' body mass composition was analyzed using a TANITA BC418 device. Then they performed tests to determine the level of their: agility, speed and power. The results suggest the existence of a relationship between the various parameters of body mass composition and physical fitness and performance.

Keywords:
physical fitness, bioelectrical analysis, body mass, volleyball, volleyball players, 3rd league club

Introduction

Physical fitness is the result of many relationships and variables. Nevertheless, both the habits formed from an early age and factors described as biological, genetic and psychological have a great influence and importance in its formation. Biological factors are extremely important, especially age, gender, body structure and motor skills. In the literature, it is possible to find positions according to which the concept of physical fitness is equated with the term motor skills. However, according to the position presented, among others, by Singier or Roth Willimczik, physical fitness is a much narrower concept in its scope, somewhat related to health promotion and positive habits in this respect [1]. Therefore, in this case, it is important to address issues related to structure, the description of body mass composition and the methods used to measure individual indicators.

One of the basic conditions for assessing an individual's health is to analyse their physical fitness. Commonly, the absence of ailments or visible disabilities allows a person to be considered physically fit. Increasingly, physical fitness is being subjected to various analyses, studies that make it possible to indicate the characteristics of fitness in various groups, such as social, age and occupational groups. In 1968, an attempt to define this concept was made by the World Health Organisation, which defined this term as "the ability to perform muscular work efficiently" [2]. Physical fitness is regarded as a key element and sign of health, and is relevant to developmental age. The level of physical fitness depends on factors such as gender, age, physique, level of development of motor skills, etc., which in turn is influenced by training and lifestyle [3].

Physical fitness allows the potential stored in the human body to be realised. It encompasses the work of individual systems, muscles, but also influences and, in a way, results from emotional stability and state of mind. Physical fitness is best assessed and understood by analysing its individual components, including aerobic fitness, muscular fitness, flexibility, stability and balance. The use of complex and appropriate exercise tasks is key in making an assessment. It is also important to remember when assessing physical fitness that it is significantly influenced by the body's characteristics, genetic background, but also by habits, exercise or dietary practices [4].

Physical fitness is the ability to perform muscular work economically and efficiently. Physical fitness refers to the ability to undertake a specific physical activity. However, common characteristics can be seen in them. We define physical fitness as the ability to perform motor activities and to develop motor characteristics (agility, speed, strength and other motor abilities) [5].

Physical fitness is genetically predetermined, and is improved naturally during an individual's life. Children improve their physical fitness at school during physical education classes or during spontaneous physical play. Adults can improve and maintain fitness potential through various forms of physical activity (running, swimming, team sports such as volleyball, football, handball, etc.), as well as tourism and recreation (cycling, rollerblading, walking, skiing, etc.) [6].

Physical fitness has a positive impact on a person's well-being. Fitness also enables people to engage in activities of daily living. Physical fitness and motor skills are factors that shape the quality of personal life - they influence interpersonal relationships. The efficiency of the cardiovascular, thermoregulatory and respiratory systems, a correct body build, a healthy lifestyle, the correct functioning of the secretion system and a good range of learned exercises determine the level of physical fitness [7]. They enable the analysis of representative samples of activities under standardised conditions and facilitate the assessment of a given trait or function. The results obtained from motor tests form the basis for training plans in athletes and for therapeutic recommendations in the case of individuals with impaired motor function [8].

By body weight, is meant the parameter that determines our weight. Awareness and self-control in maintaining a healthy body weight, to a large extent, implies our behaviour and eating habits and lifestyle. Body mass is a holistic concept encompassing many different factors, but the most important ones are: body fat, muscle tissue, body water content, bone tissue.

From the point of view of the field of physical education and sport, indirect methods, in which body mass is considered as the sum of 2 to 4 components, are the most relevant. In the vast majority of methods, factors such as body fat mass (FM - German: Fat Mass) and fat-free mass (FFM - German: Fat Free Mass) are assessed. Both of these components added together constitute total body mass. Fat mass includes lipids and the tissues that make up the fat cells. Fat Free Mass, refers to the sum of

the weight of skeletal and non-skeletal muscles, organs, skeleton and other soft tissues. It includes the body's protein reserves, which if these are upset, i.e. disease or physical inactivity, leads to a negative protein balance [9].

To determine the range of normal body weight, empirical tables of its values are established, which are dependent on age, height and division into body types. Then, based on these data, an average value is determined, which is labelled as normal. Based on anthropometric studies, norms of physical development are created. One-time or repeated measurements of this type reflect the level and rate of development of children, adolescents and adults. Measurement results are obtained as a result of the application of well-known and widely used weight and height indices (BMI, Cole's index - LMS - Least Mean Square), indices depicting the ratio of body circumferences to each other (WHR - Waist to Hip Ratio) or the ratio of waist circumference to body height (WHtR - Waist to Height Ratio), make it possible to calculate the quotient of individual measurable features and to relate the obtained result to gender- and age-appropriate norms. In addition to the above-mentioned indices, it is also possible to assess the thickness of the skin-fat folds using a fold-meter or to measure waist circumference alone (WC - Waist Circumference).

Measurement of body circumferences includes crude measures of relative fatness and muscularity. The skin-fat fold measurement technique, is used in epidemiologic studies. Hydrodensitometry, electrical bioimpedance and densitometry methods analyse the distribution of fluids in the body and the mass of tissue components. Computed tomography and magnetic resonance imaging, allow assessment of the mass and distribution of body fat and non-fat components, as well as bone mass.

One of the team sports associated with a significant energy load on the body and the possession of certain predispositions and characteristics of the players is volleyball. The originator of the volleyball rules was William G. Morgan - by day a physical education teacher at the Young Men's Christian Associaton (YMCA) in Holyoke, Massachusetts. On 9 February 1895, the premiere demonstration of the sport he created, which was then called Minonette, took place in the local gymnasium. Volleyball came to Poland through the YMCA, and the first demonstration match took place in Warsaw in 1919.

The aim of the work

The aim of this study is to assess the level of physical fitness and body composition, taking into account the interpretation of selected indices of nutritional status and body fat and muscle content, using a group of women playing in a third league club as an example.

Research questions:

1. What is the body composition of women playing in a third league club?
2. Does practising regular physical activity affect fitness and body composition?
3. What is the overall assessment of the fitness level of the women playing in the 3rd league club?
4. To what extent does physical fitness imply changes in body fat and muscle composition in female players?

Material and method

The study conducted on 08.12.2021, which took place in the sports hall of the University of Rzeszów, involved 15 players playing in a third league club. The group of 15 players surveyed was between 19 and 31 years of age. The players were divided into two groups, i.e. younger (19-22 years of age) - 8 people, and older (23-31 years of age) - 7 people. The average age of the female athletes surveyed was 22 years. The female athletes were between 162 cm and 186 cm tall. The average height of the female athletes was 172.5 cm. The weight of the female athletes was between 53.5 kg and 84.6 kg. The average weight was 70.1 kg. The BMI of the athletes ranged from 19.9 to 30.5, with a mean of 23.5 for the whole group. The athletes did not exercise intensively 12 hours before the study. The subjects showed no symptoms of infectious diseases that could affect electrolyte and fluid content.

The study was a two-stage procedure. Firstly, the body composition of the athletes was analysed using the TANITA BC418. The Tanita body mass analyser analyses body composition using the BIA or body bioimpedance method. The analyser is designed for adults and children over 7 years of age with active, inactive or moderate lifestyles. To ensure the most accurate measurement, the test should be carried out under appropriate hydration conditions.

Statistical analysis of the results obtained within the framework of the study was carried out using the Statistica 13.1 program. Using this program, an analysis of basic descriptive statistics was also performed.

The normality of the distribution was verified using the Shapiro-Wilk test. This test is considered to be one of the strongest tests for testing the normality of a distribution, especially when testing 'small-college' samples. The test is used to verify the hypothesis that the distribution of the random variable under study follows a normal distribution. The null hypothesis is verified on the basis of the calculated value of the W statistic:

$$W = \frac{(\sum_i a_i\,(n) * (X_{n-i+1} - X_i))^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2} \quad (1)$$

Where:

X_{n-i+1}-X_i are striae of order „i".

The coefficients $a_i(n)$ are constants that depend on „i" and the sample size „n". The coefficients are read from tables, which were developed by the test authors.

Once the test statistic W has been calculated, a check is made to ensure that its value is within the assumed critical area. The two-sided critical area is determined by the values of W(α/2, n) and W(1-α/2, n). The values are read from the tables of the W distribution. The null hypothesis that the distribution of the data is normal is rejected if the value of the W statistic is within the critical area in two variants:

$W \geq W(1-\alpha/2, n)$

$W \leq W(\alpha/2, n)$

However, if the value of the W statistic is outside the critical area, the null hypothesis (H0) should be accepted and the empirical distribution should be found to be consistent with the normal distribution.

The tests carried out did not show a normal distribution. Therefore, non-parametric tests were used. In order to assess the significance of differences between groups, the Mann-Whitney Test was used. It is used to verify the hypothesis of non-significance of differences between the medians of the variable under study in the two populations (where we assume that the distributions of the variable are close to each other). The Mann- Whitney test assumes the significance of differences below a $p < 0.05$.

In the study carried out, the variables did not have a convergent normal distribution. Therefore, values were described as median, lower and upper quartile. Correlations were verified using the Spearman test.

Results

Using measurements taken on a Tanita scale, results were obtained for the following indices: body weight, body fat %, body water %, muscle mass, BMR (kcal/kJ), visceral fat level. The results obtained were then grouped, into an older group and a younger group, according to the variable defined as the age of the athletes. The study showed no significant differences between the weights of the younger athletes and the older athletes. The difference between the medians was 1.1 kg, with a significance p of 0.093. The average weight of the different groups of female athletes is almost on the same level (Tab. 1).

Tab. 1. Comparison of the weights of a group of younger female athletes and older female athletes

Parameter	**Younger female athletes**			**Older female athletes**			**D (Me)**	**m**
	Me	Lq	Uq	Me	Lq	Uq		
Weight	68.2kg	57.3kg	71.6 kg	70.6kg	69.3kg	82.2 kg	1.1 kg	0.093

Legend: Me-Median; Lq-Lower quartile; Uq-Upper quartile; d- difference between medians, m- materiality level

Source: own research

The second variable investigated was body fat levels. For women, the normal parameters in this range should be 21-33% for women aged 20-39 years. The study showed no significant differences between the levels of body fat in the younger female athletes and the older female athletes. The difference between the medians of the groups was 4.15 kg, with a significance p of 0.1045. This difference was considered non-significant. The level of body fat, for the different groups of female athletes, is almost at the same level, and this is within the standard limit. The body fat weight for the younger female athletes averaged 15.9 kg, while for the older female athletes it was 19.8 kg (Tab. 2).

Tab. 2. Comparison of the weights of a group of younger female athletes and older female athletes

Parameter	**Younger female athletes**			**Older female athletes**			**D (Me)**	**m**
	Me	Lq	Uq	Me	Lq	Uq		
Level of body fat	23.5	21.85	26.35	27.5	23.3	28.6	4.15	0.1045

Legend: Me-Median; Lq-Lower quartile; Uq-Upper quartile; d- difference between medians, m- materiality level

Source: own research

With regard to the data obtained within the individual parameters, it was also decided to analyse their pattern in female athletes of a certain age. The data collected allowed the following conclusions to be drawn. The data collected include medians calculated for individual age groups. The level of adipose tissue mass in the total body mass, is at a similar level in female athletes of different ages. In the study group, female athletes aged 23 and 31 years had the highest weight. The highest levels of body fat in relation to total body weight were found in athletes aged 22, 23 and 31. The athletes aged 21 had the lowest weight and % body fat and total body fat mass.

As part of the body composition analysis carried out, information was also obtained on lean tissue mass in female athletes. The analysis of the fat-free tissue level, in the different groups of athletes, showed no significant statistical differences .It ranged between 45.3-58.5 for the younger athletes and 49.65-59.7 for the older athletes. The difference between the medians of the different groups was 1.3 (Tab. 3).

Tab. 3. Fat-free tissue levels in a group of female athletes

Parameter	**Younger female athletes**			**Older female athletes**			**D (Me)**	**m**
	Me	Lq	Uq	Me	Lq	Uq		
Level of fat-free tissue	51.6	45.3	53.85	52.9	49.5	59.7	1.3	0.2230

Legend: Me-Median; Lq-Lower quartile; Uq-Upper quartile; d- difference between medians, m- materiality level

Source: own research

The level of fat-free tissue was significantly higher than the level of body fat in the individual female athletes. The smallest difference in this regard was for female athletes aged 21 (difference of 18 kg) and 26 years (25.05 kg). In percentage terms, the proportion of lean tissue mass in relation to total body weight in ranged from 69% to 75%. For female athletes aged 19 years, fat-free tissue accounted for 74% of their body weight. The highest percentage of fat-free tissue was in female athletes aged 22 (77%), 20 and 24 (75%).

Another parameter that was examined as a result of the body composition analysis was muscle mass.The average value of muscle mass in the case of the younger athletes was 48.95 kg, while in the case of the older athletes it was 50.2 kg. The difference between the average values was 1.25 kg, meaning that the older athletes had 1.25kg more muscle mass than the younger athletes.

Another value that was verified during the tests was body hydration. The hydration level of the athletes in each age group. The athletes in the older group had 4.15 per cent less body hydration than the younger athletes. From a statistical point of view, this was a significant difference, although the body hydration score itself in both the older and younger groups was at a very high level. When divided into age-specific athletes, the parameters were highest for athletes aged 21 years, while the lowest were for athletes aged 23 years. The body water level of the individual athletes was at the upper limit of the norm for women of a given age.

The Tanita study also provided information on the bone mass of the athletes.

The next indicator analysed referred to the calorific requirements of the body in female athletes. Both the older and younger female athletes had a similar calorific requirement. The average requirement of the younger female athletes was 5853 kJ and that of the older female athletes was 6874 kJ. The younger female athletes on average require 1582 kcal, while the older female athletes require 1643. Female athletes aged 31 years require 1826 kcal, which corresponds to 7640 kJ.

The youngest athletes, aged 19, need 6761 kJ per day, which is equivalent to 1616 kcal. The average BMR value was set at 1 kcal/kg body weight/ 1 hour. For a woman weighing, for example, 60 kg, this ratio is 1440 kcal per day. The BMI of the female athletes is adequate for both their body weight and physical activity.

The verification of the data on the visceral measurements showed that there was a deviation which could be considered significant, albeit at a negligible level in relation to the norm in this area.

As a result of the physical performance tests , data was obtained to assess the overall physical performance of the younger and older female athletes. In the long jump, the older girls were 11.66 cm behind the younger girls.

In the shade to agility test, however, the senior athletes performed better. Their result was 0.32 s. better than the younger athletes (Tab. 4).

Tab. 4. Results from the agility test of the senior and junior female athletes

Parameter	**Junior female athletes**			**Senior female athletes**			**D (Me)**	**m**
	Me	Lq	Uq	Me	Lq	Uq		
Agility	8.880	8.650	9.070	8.560	7.980	9.210	-0.320	0.772338

Legend: Me-Median; Lq-Lower quartile; Uq-Upper quartile; d- difference between medians, m- materiality level

Source: own research

When assessing the power of the female athletes, the older athletes performed slightly better,scoring 0.5 s better than the younger athletes (Tab. 5).

Tab. 5. Results of the power test junior female athletes and senior female athletes

Parameter	**Junior female athletes**			**Senior female athletes**			**D (Me)**	**m**
	Me	Lq	Uq	Me	Lq	Uq		
Power (n/30s)	14.500	13.500	16.000	15.000	15.000	17.000	0.500	0.316920

Legend: Me-Median; Lq-Lower quartile; Uq-Upper quartile; d- difference between medians, m- materiality level

Source: own research

Relating the fitness data obtained to the two variables determining body mass composition, which showed significance, the following relationships are found.

The younger athletes, who had better hydration levels and less visceral tissue, performed worse than the older athletes in two of the three tests. The athletes included in the younger group were between 19 and 22 years old. Within the group, athletes who were better hydrated performed better than those with lower hydration levels. In addition, in the power test, female athletes with a high muscle mass, i.e. 53.50, performed significantly better than athletes with a lower level of muscle mass, e.g. an athlete with a muscle mass of 38.5 kg performed 2 seconds worse in this test than an athlete one year older but with a higher muscle mass. The athletes with the highest muscle mass in the group also performed much better in the agility test and the long jump than the younger athletes, whose body composition parameters were lower.

In the case of the athletes in the older group, the weakest results in the power test were achieved by athletes aged 23, who had the highest levels of body fat and relatively high levels of muscle mass within the group. For agility, the best result in the group was achieved by a female athlete with one of the lower levels of body hydration and muscle mass. For the long jump, the best result was achieved

by an athlete whose muscle mass was the highest and body fat level was average, in relation to the results obtained within the group as a whole.

Discussion

The main aim of the study was to assess the body mass composition and physical fitness of female athletes in a third league club. Sports clubs have become an integral part of the social infrastructure, offering organised sports activities and thus building skills and promoting the health of individuals. Internationally popular sports such as tennis, basketball and volleyball also require varying levels of competence, a high level of technical and tactical skills and appropriate anthropometric characteristics for successful participation. Anthropometric measurements, include body composition parameters e.g. muscle mass, body fat, hydration level. Somatic characteristics and body composition are influenced by training and the type of sport practised. Fat-free mass compared to total body mass is closely related to physiological parameters [11].

Female volleyball players were found to be generally taller than players of other games. In addition, average height and weight, body fat content and lean mass differ from players in other group sports [12].

This is due to the specific nature of the game that is volleyball. The players must be well prepared to cope with the intense demands of the game. Moderate to high intensity endurance training is crucial for the players to reach a higher level of fitness. They need to be fast, agile but also have strength and power. These factors are crucial for the game itself. Torque transfer, i.e. serves or groundstrokes in volleyball depends not only on technique but also, flexibility, muscle strength, speed and power [13].

In sport, there has often been interest in the subject of sports performance monitoring and analysis. One of the most well-known methods of body composition analysis is electrical bioimpedance analysis or BIA. This extremely simple, non-invasive and safe method is widely used in dietetic practices, doctors' offices and even fitness clubs. It involves measuring the electrical resistance of tissues (impedance) through which a low current is passed. By using the components of impedance, i.e. resistance (specific resistance) and reactance (capacitive resistance of cell membranes), and taking into account anthropometric parameters (age, weight, height, gender), it is possible to determine the amount of water in the body and then, using formulas, calculate the remaining components of the body. Depending on the number of electrodes used, it is possible to obtain accurate calculations even for the limbs and trunk separately (usually 2 - 4 electrodes are sufficient, but there are also 8-electrode devices). Monophasic or multiphasic current is used, with the former, mainly at 50kHz, being completely sufficient for dietary diagnostics, allowing reliable and reproducible results. BIA measurement can be an excellent basis for the prevention and treatment of modern civilisation diseases such as overweight, obesity, diabetes, hypertension and atherosclerosis. It is also an excellent tool for monitoring the effectiveness of dietary intervention or nutritional treatment.

Monitoring the body composition of elite volleyball players has been analysed in several studies including Malý et al. in 2011[14]; or Malý et al. in 2010 [15], Tsunawake et al. (2003) compared the body composition of junior basketball volleyball players and their physical fitness. The level of the studied parameters, measured by multi-frequency bioimpedance, is indicative of the quality of BC in both teams. LBM - lean body mass (active mass with a low proportion of fat), was almost identical

in the samples studied. According to research sources, volleyball players show significantly higher LBM values than non-athletes.

This parameter, which encompasses all body tissues except fat, is considered a major prerequisite for good volleyball performance. A higher LBM value provides a better predisposition for athletic performance based on physical fitness. Melrose, w and his team in their study, report a close correlation between LBM recorded in young female volleyball players (n = 29, mean age = 14.30 ± 1.37 years) with isometric arm strength (r = 0.90), isometric leg extension strength (r = 0.62) and ball speed after passing (r = 0.58) [16].

An important BC parameter is body target mass - BCM as a component of LBM, which is represented by metabolically active aerobic cells of skeletal muscle and cardiac muscle, internal organs, bone tissue, blood cells and the central nervous system, the central nervous system. According to Andreol, BCM assessment is among the best implications of muscular fitness to predict sports performance, of an individual. For top-performing athletes, BCM can increase up to 60% of LBM.

In the study carried out for this thesis, it was shown that the female athletes are among those who engage in regular physical activity. Their body mass parameters are appropriate for their age, with a body fat percentage within the normal range for women of their age, i.e. between 23% and 32%. The same is true for visceral tissue, the level of which varies significantly in the study group, but is within the lower limits of normal parameters (1 to 12). In the case of muscle mass, 93 % of the athletes have it at an intermediate level (14 athletes have a muscle mass between 48 and 67), only 7 % of the athletes have a muscle mass rated as low on the scale (i.e., below 47). The TBW range is also within the normal range defined for healthy individuals (the healthy range for women is 45-60%). The level of bone tissue in female athletes is also within the normal range defined for women of a certain weight 9for ladies weighing between 50-70 kg it is supposed to be 2.4 kg, for ladies over 70 kg-2.95 kg). The BMI for female athletes is also normal. It can therefore be concluded that regular physical fitness has a positive effect on body composition. The difference in values between the study groups was statistically insignificant, but moderate from the point of view of the magnitude of the test results.

The requirements for physical predisposition for professional volleyball are getting higher and higher, as their weaknesses have to be compensated by other qualities (experience, foresight and volleyball intelligence). The highest level of sporting performance can only be achieved through the synergistic interaction of all components (factors influencing sporting performance). However, BC must not only be monitored selectively, but continuously. This type of information can allow the coach or the athletes themselves to identify their own changes in BC. When they are measured regularly they allow an assessment of the body's response to applied stimuli in sports training, during recovery from injury or appropriate supplementation.

Conclusions

1. The average weight of women in a third-league club is 69.3 kg. The players are on average 173 cm tall. Their BMI is 23.5. The average age of the players is 22 years. The average third-league player has 26% body fat, which corresponds to 18.4 kg of fat. In addition, the weight of fat-free tissue is 52.5 kg. Female athletes on average have 49.8 kg of muscle. Their body hydration is 49.2%. Their daily calorie requirement is 1603 kcal.

2. The female athletes are among those who engage in regular physical activity. The body mass parameters they possess are adequate for their age. The range of body fat they have is within the norms set for women of their age, i.e. between 23% and 32%. Similarly, for visceral tissue, the level of which in the study group shows significant differences, but in relation to the normal parameters (from 1 to 12) is within the lower limits of the norm. With regard to muscle mass, 93 % of the athletes have it at an intermediate level (14 athletes have a muscle mass between 48 and 67), with only 7 % of the athletes having a muscle mass rated as low on the scale (i.e. below 47). The TBW range is also within the normal range defined for healthy individuals (the range for women is 45-60%). The level of bone tissue in female athletes is also within the limits of the norm defined for women of a certain weight 9 for ladies between 50-70 kg it is to be 2.4 kg, for ladies over 70 kg-2.95 kg). The BMI for female athletes is also normal. It can therefore be concluded that regular physical fitness has a positive effect on body composition.

3. Female athletes perform well in agility, power and jumping tests. Their results show that regularly practised physical activity influences the overall fitness of the body. The players in the third league club are physically fit to a fairly good degree, in the opinion of the author of this paper.

4. Taking into account the results obtained within the framework of the conducted research, it should be concluded that the level of adipose tissue and muscle tissue can have a moderate influence on the achievement of higher or lower parameters of physical fitness assessment.

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DESIGNING POLYMERIC DRUG DELIVERY SYSTEMS – POLYMER PRODRUGS

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Abstract:

Prodrugs are inactive derivatives of active substances of therapeutic importance, which undergo biotransformation at the target site of the in vivo system, realizing their therapeutic potential. The combination of such a compound with a polymer chain makes it possible to obtain a polymer prodrug with a varied spatial structure and therapeutic effect. Currently, these types of compounds are used as a revolutionary group of anticancer drug carriers, but their design is burdened with many requirements in terms of bioavailability and biocompatibility, which future synthetic approaches must consciously meet.

Keywords:
polymer prodrugs, polymer-drug conjugate, hyperbranched polymer, HPMA

Introduction

In 1958, A. Albert described for the first time a pharmacologically inactive derivative that underwent selected transformations that improved their physicochemical properties. Such a compound has been termed a prodrug or proagent [1]. His concept was developed in later years by Harper, who introduced the term latency of a drug, i.e. a time-delay component or compound. Then, in order to solve many design problems, another important element of the prodrug's functioning was added. This was the aspect of non-enzymatic regeneration of the parent compound. On this basis, medicinal substances of this type began to be defined in various ways, e.g. bioreversible derivative, congener or latent drug [2].

A prodrug can be described as a pharmacologically inactive or partially inactive chemical derivative that is enzymatically or non-enzymatically converted to the active form in vivo [3]. After reaching the programmed position in the body and the rapid elimination of the derivatising group, it gains healing properties. Typically, the term is used for systems having a covalent bond between a drug and a chemical moiety. However, some researchers use this definition in the context of a salt of an active drug.

Each therapeutic agent is able to produce the desired pharmacological effects only when it reaches its intended place of action. Three main phases involved with bioavailability

or drug receptor interaction include the pharmaceutical, pharmacokinetic and pharmacodynamic phases. These phases determine specific properties of the drug substance, which should be achieved at the prodrug design stage. The pharmaceutical phase is responsible for improving the dissolution of the compound and its chemical stability. It tries to reduce the pain-producing effects or irritating, in terms of taste, smell and dosing [4]. The pharmacokinetic phase, on the other hand, is intended to increase the selectivity of a given substance, to make absorption more effective in various spheres, i.e. after oral administration, but also in the place of circulation of the drug outside the upper digestive and respiratory tracts. An important aspect is the time profile, which determines the release time of a given preparation in the tissue or target organ [5]. It should be as short as possible, which results in a faster healing effect. It is achievable when the presystemic metabolism is lowered.

Many barriers are believed to be of pharmacokinetic origin, which is one of the most common programming problems. The last phase that is taken into account in the drug-body contact is the pharmacodynamic phase. It is based on the appropriate activation of the drug into a biologically active compound and increasing the therapeutic index [4]. In addition, this phase tries to minimize cytotoxicity, i.e. toxicity to individual cells of the body caused by in situ factors of internal or external origin.

Tab. 1. Classification of prodrugs

Classification	Class	Subclass	Description
Chemical	Prodrugs associated with the operator	-	-
	Bioprecursors	-	-
	Macromolecular produgs	-	The carrier is a macromolecule, e.g. glycol.
	Drug-antibody conjugates	-	A carrier such as an antibody directed against the relevant antigen.
Due to the site of conversion of the prodrug into the active drug	Type 1 (intracellular activation)	Subtype IA	Conversion in target cells.
		Subtype IB	Transformation in the cells of the organs of basic metabolism.
	Type 2 (extracellular activation)	Subtype IIA	Activation in the enviroment of gastro - intestinal fluids.
		Subtype IIB	Activation in the circulatory system or in the compartment of other extracellular fluids.
		Subtype IIC	Activation near the target cells.
	Type 3 (mixed)	-	Prodrugs belonging to several categories.

Source: Guzik U., Hupert – Kocurek K., Nieć A., Wojcieszyńska D., *Areny jako proleki*, Katowice: Wiadomości chemiczne 2015

Protherapeutics with strictly defined properties are divided according to two general classification criteria. The first is a historical criterion and divides prodrugs into intentional and accidental. This illustrates the way of discovering individual healing forms. Most of them can be included in the target group, which was the result of a planned chemical interaction with a thorough knowledge of the mechanism of the target organ [6]. A more common and more detailed method of classification is that based on a chemical criterion. It divides all known prodrugs in terms of their structure, mechanisms of action and places of transformation into the active form (Tab. 1). In relation to this material, five most important classes

can be selected, belonging to the Wermuth classification and chemical classification. They are characterized by a complete structural and functional difference and they are:

- prodrugs associated with the operator,
- mutual prodrugs,
- bioprecursors,
- tripartite (three-element) prodrugs,
- polymer prodrugs [5].

Polymer prodrugs

The combination of a polymer chain with a therapeutically active substance is called a polymeric prodrug. These are systems for precise drug delivery to the target site by cleaving the drug-polymer bond [7]. They are aimed at improving the use of therapeutic agents in therapeutic applications. They are biocompatible, which means lack of toxicity, antigenicity and teratogenicity.

The successful assembly of such systems depends on the molecular weight, chemical structure, possible spatial obstacles, and the reactivity of the polymer and the biomolecule. Such synthesis is possible when both molecules have appropriate functional groups. Although the presence of a large number of organic groups increases the complexity of the system. Therefore, such a prodrug requires, in addition to the presence of a polymer backbone and a therapeutic substance, such elements as:

- biodegradable separator (protects against drug-polymer interaction),
- soluble group (supports intermembrane transport),
- target moiety (contacts the particle with the receptor) [5].

The scheme of such construction is shown in the Ringsdorf model (Fig. 1).

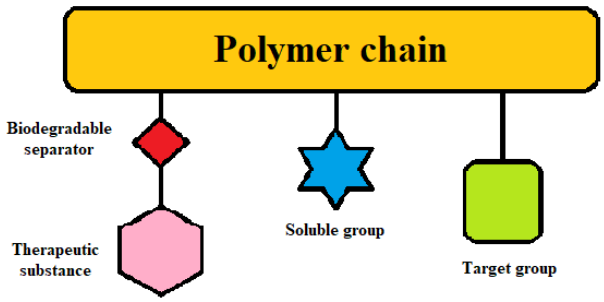

Fig. 1. Model of a polymer prodrug according to Ringsdorf [8]

The selected polymer, which is part of the prodrug structure, should show high biodegradability, biocompatibility and low toxicity. On this basis, several categories of classification of polymers used for therapeutic derivatization are distinguished, such as:

- origin:
  a) synthetic - widely used due to their possibility of structural modification; these include polyethylene glycol (PEG) and vinyl polymers;
  b) pseudosynthetic, e.g. polyglycolic acid (PGA), synthetic poly(α-amino acids);
  c) natural e.g. proteins, chitosan, dextran;
- molecular weight - due to the degree of complexity, oligomers or polymers are distinguished;

- chemical nature - acrylic or vinyl polymers, polyamino acids, polysaccharides;
- durability - stable polymers and biodegradable polymers [7, 9, 10].

The classification formulated in this way also translates into the division of the polymer prodrugs themselves. Within them, one more category can be distinguished. It is a type of factor that leads to the biotransformation of the drug, transforming it into a therapeutically active form. There are prodrugs sensitive to enzymes, the pH value of the environment, the presence of redox reactions and the temperature of the system [7]. Such sensitivity results from the specific selection of components that affect the high selectivity of the therapeutic.

Characteristics and functioning of polymer-drug conjugates

The basic component of a polymeric prodrug is the presence of a polymer-drug conjugate, which is formed by a covalent bond based on selected reactive or functional groups, which most often include: carboxyl, hydroxyl, thiol or amino groups. Relationships of this type should also be characterized by:

- a molecular weight below the renal excretion limit,
- lower solubility in water compared to the pure drug,
- low polydispersity to ensure structural homogeneity,
- stability in different physiological pH systems,
- reduced penetration into cells (limitation of accidental accumulation in undesirable systems) [10, 12].

Thanks to such properties, polymer prodrugs protect active substances against accelerated deactivation during circulation in intercellular and intracellular systems. They support the improvement of pharmacokinetics and create the possibility of delivering a complex set of ingredients that can support the specific therapeutic activity. As a result, they are regarded as one of the more promising models of drug delivery, called polymer drug delivery systems (PDDS) [13]. Examples of this type of colligates are presented in Tab. 2.

Tab.2. Selected polymer-drug conjugates

Nr.	Polymer - drug conjugate	Indication	Year of market introduction
1	SMANCS (Zinostatin, Stimalamer)	Hepatocellular carcinoma	1993
2	PEG - adenosine deaminase	SCID syndrome	1990
3	PEG - asparaginase	Acute lymphoblastic leukaemia	1994
4	PEG - growth hormone receptor antagonist	Acromegaly	2002
5	Branched PEG - anti-VEGF aptamer	Age - related macular degeneration	2004
6	PEG - anti-TNF Fab	Rheumatoid arthritis and Crohn's disease	2008

Source: Rohini N.A., Anupam J., Alok M., *Polymeric prodrugs: recent achievements and general strategies*., Journal of Antivirals and Antiretrovirals 2013

The functioning of such conjugates focuses primarily on two aspects. It is the process of targeted delivery as well as the release of the drug at the destination.

Targeting the therapeutic process can be achieved through active and passive means. The former are the result of chemical interference in the structure of the prodrug during synthesis.

Such a compound must have a specific ligand that will bind to the selected receptors. An example of this may be the HPMA-doxorubicin-galactosamine system intended for the treatment of liver cancer. In this system, galactosamine is the ligand that binds to asialoglycoprotein receptors located in hepatocytes. Only after active attachment, the polymeric structure of HPMA (N-(2-hydroxypropyl)methacrylamide) is desorbed, allowing doxorubicin to begin its anticancer activity.

Passive agents, on the other hand, are based on an extended transport time in the body, which generates passive accumulation in cancerous tumor. This is due to the increased permeability of the tumor vessels, as well as insufficient lymphatic drainage that occurs within it. This phenomenon is referred to as the EPR effect, which is the effect of increased permeation and retention. This task is valid for all solid tumors. However, such therapeutic targeting is fraught with limitations due to the heterogeneity of the vascular system and irregular blood flow in the tumor. As a result, such therapy loses its effectiveness.

The second aspect of the functioning of polymer prodrugs focuses on the precise release of the therapeutic compound. This process can be mediated by enzymatic or non-enzymatic hydrolysis. In both cases, a frequent design procedure is the use of a separator which, under selected environmental conditions, e.g. during contact with a specific catalysing enzyme starts the release mechanism. First, the polymer component is detached, which will activate a rapid intramolecular reaction towards the drug. The separator thus acts as a compound distancing the polymer from the therapeutic agent, deactivates the therapeutic agent itself (prolongs its usefulness in vivo), but is also a release trigger that initiates the healing process (Fig. 2.) [11].

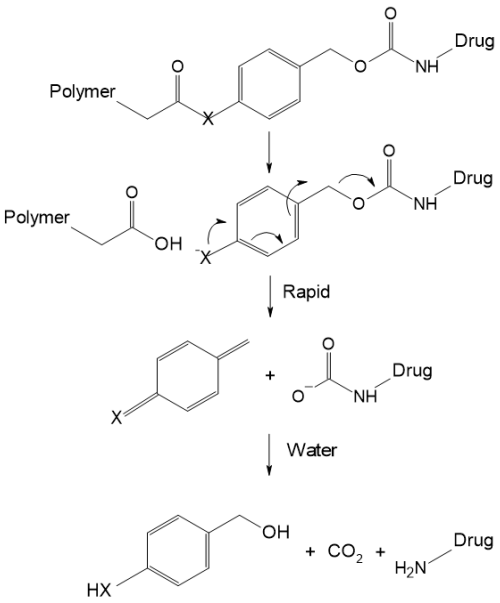

Fig. 2. Release of the active substance from polymer prodrugs [16]

Such a complicated and multidirectional functioning encounters many problems during the synthesis. This is due to the presence of numerous spatial obstacles to covalent conjugation. The introduction of an active separator may result in accelerated activation of the molecule prior to its delivery. Due to the high passivity and lack of drug release in the gastrointestinal tract, the prodrug is absorbed by endocytosis (Fig. 3), which is associated with

limited intercellular distribution. Therefore, it is recommended to direct the polymeric prodrug to the designated cell, tissue or organ, e.g. by means of a precise external injection [10].

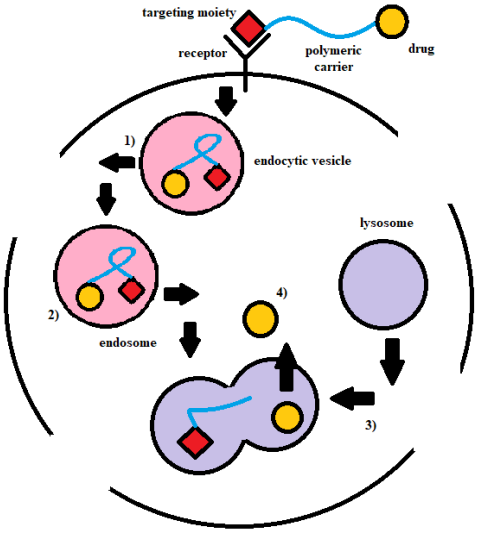

Fig. 3. Scheme of endocytosis of polymer prodrugs
1) interaction of the target moiety with the receptor and internalization of the drug delivery system;
2) transport in membrane-bound organelles;
3) fusion with lysosomes;
4) degradation of the prodrug and release of the active substance.

Spatial design of polymer prodrugs

The formation and modification of a chemically stable polymer prodrug is possible by forming stable amide, disulfide or ester bonds. Their presence prevents premature release of the drug, but at the same time catalyzed amides or esters can quickly unblock the therapeutic agent. They are also the basis for creating spatially complex structures that can increase the amount of a drug introduced into a cell or tissue at a time.

Their shape and form depend on the expression and type of receptor, the composition of the prodrug itself and the affinity between its elements, and the environmental conditions in which they are to operate. At the level of considering single polymer chains, a classic prodrug with a targeting agent and a conjugate of a hyperbranched polymer can be distinguished (Fig. 4.). The latter is characterized by several chains distributed radially, at the ends of which there are active compounds, targeting groups, which may intensify the response and speed of the therapy. Such a structure, in order to maintain its spatial position, is supported by the presence of hydrogen bonds, disulfide bridges and hydrophobic interactions. They are most often used in the case of spatially extended target sites or in the case of a large dispersion of the factor catalysing the biotransformation of the prodrug in the in vivo system [12, 14].

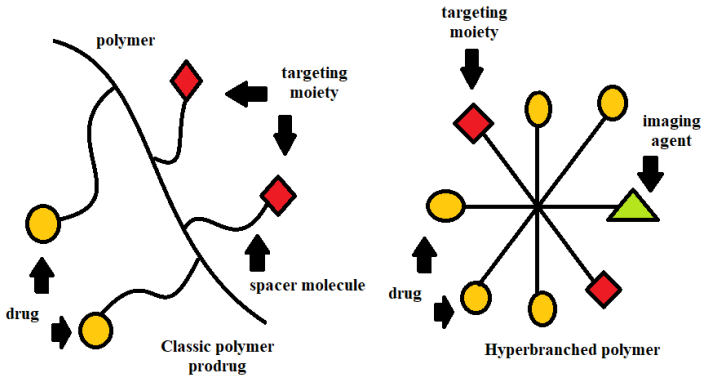

Fig. 4. Scheme of classical and hyperbranched polymers

Versatile use of polymer prodrugs

Polymer therapeutics is defined as a group of compounds, which include, among others, polymer prodrugs. One of their practical applications is to support the transport of medicinal substances through the blood-brain barrier, through which the transport of the drug in a traditional way is impossible or highly difficult. The use of such a solution makes it possible to reduce fluctuations in the therapeutic concentration, prevents drug degradation, and increases the permeability of proteins and peptides. The most commonly used polymer systems for this problem are:

- spherical single- or multi-layer liposomes, consisting of natural phospholipid polymers, inside which the active substance is enclosed;
- polymer capsules or surfaces impregnated with an active substance with a size of 1 to 1000 nm;
- polymeric microemulsions and micelles, consisting of amphiphilic copolymers with hydrophobic cores, e.g. a polymer of hydrophobic polypropylene glycol and hydrophilic PEG (poly(ethylene oxide)) [15].

Another example is a prodrug called bixalomer (cross-linked N,N,N,N-tetrakis (3-aminopropyl)butane-1,4-diamine), which helps treat hyperphosphatemia. Its great advantage is that it shows fewer side effects from the digestive system compared to conventionally used drugs. The functioning of this protherapeutic consists in binding phosphates, which are present in the lead in the case of this disease. It shows high selectivity in relation to other anions. Thanks to the presence of numerous amino groups in its structure, bixalomer is able not only to combine with phosphate anions, but also with protons, which avoids the occurrence of metabolic acidosis [17].

Vinyl polymers are one of the most commonly used components of polymer prodrugs, which can be obtained by radical polymerization of selected vinyl monomers. However, these types of polymers are not biodegradable, so the requirement is to maintain the weight of the polymer at least below the kidney filtration limit (40 - 50kDa), which is to prevent the retention of toxins in the body and the formation of harmful radicals. The most commonly used copolymer is HPMA (N-(2-hydroxypropyl)methacrylamide), which in combination with adriamycin

by means of the peptide chain Gly-Phe-Leu-Gly creates an anticancer agent used in the treatment of colon, lung and breast cancer [9].

There are also compounds that are candidates for this title of polytherapeutics, the current clinical use of which is highly limited for safety reasons. Synthetic antimicrobial peptides (AMPs) belong to this group, despite showing therapeutic potential in the context of neoplastic lesions. They have a wide spectrum of activity in the interaction of neuroma, leukemia and sarcoma cells. Their ability is based on selectively exerting cytotoxicity on cancer cells by penetrating them and destabilizing the plasma membrane. Currently, numerous works are being carried out on their modification in order to direct their actions and change their physicochemical properties through the use of a pro-drug approach. Derivatives are being designed that would additively or synergistically increase the effect of AMP compounds. One way is to compile with commonly used chemotherapeutic agents. Fig. 5 presents a synthetic path for the synthesis of a prodrug based on antimicrobial peptide compounds, which uses the PEG polymer as a carrier and blocking agent, which would ultimately increase the bioavailability of the molecule [18].

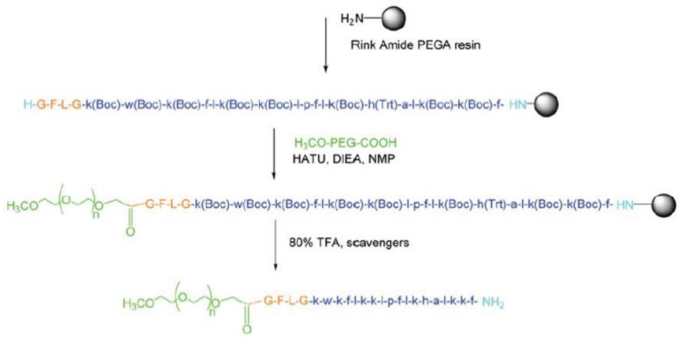

Fig. 5. Proposed synthesis pathway for AMP-based polymer prodrug

Conclusions

Polymer prodrugs are a revolutionary group of compounds that combine a biologically active substance with a polymer chain in its structure. Contrary to the classical reasoning of pro-drugs, this group of compounds is a kind of carrier of a protected active compound. Their construction can be based on natural and synthetic materials. Upon reaching its destination, the molecule undergoes biotransformation by exposure to an enzymatic or non-enzymatic factor, i.e. redox transformation, temperature or cellular pH. The released active therapeutic can then begin its therapeutic effect in the structure intended for this purpose. Their diversity and complexity result from the possibility of composing countless polymer systems, which are also burdened with the criteria of bioavailability and biocompatibility. Nevertheless, polymeric prodrugs find their use in anti-cancer therapies, becoming compounds whose continuous modification and improvement may affect the solution of many medical and pharmacological issues of the modern world.

Acknowledgements

This work was supported by the Polish Ministry of Education and Science.

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USE OF CLUSTERING FOR THE SALESMAN PROBLEM

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Abstract:

The salesman is to visit n cities. The order of the cities must be arranged so that the road is the smallest. When the number of cities is large, there are trillions of possible permutations of cities. Cities are divided into groups that are close to each other. We use the clustering method for this. Matlab has a ready CLUSTER procedure and we use it to create city groups. In each group of cities (in a cluster) we find the shortest route. We use iterative methods to find the shortest path in a cluster. Then we combine these routes into one route for the seller. This is an approximate solution to the seller's problem.

Keywords:
Clustering, salesman, route, matlab

Introduction

One of the important management issues is transport management. Transportation of materials should be planned in such a way that the cost of transport or the total transport route is the smallest. When the number of suppliers and recipients is small, this is not a problem. When the number of places (cities) to be reached is large, there is a problem with determining the route.

To date, the „traveling salesman problem" for a large number of cities he is supposed to visit has not been solved [1]. There are some methods to approximate the traveling salesman problem. Arora in his work [2] considered a polynomial time approximation scheme for the traveling salesman problem. Bellman in [3] applied dynamic programming to the traveling salesman problem. The branching and cutting algorithm for the symmetric traveling salesman problem was applied in [6]. In paper [5], the simulated annealing method was used to find an approximate solution to the traveling salesman problem. Serdyukov [7] used an estimation algorithm for the traveling salesman problem with a maximum. Steinerberger in his work [8] dealt with the following issue. For random points X_1, ..., X_n arranged in a unit square, the traveling salesman path length is denoted by $L(X_1, ..., X_n)$. For this path there is a constant β that $\lim_{n\to\infty} \frac{L(X_1, ..., X_n)}{\sqrt{n}} = \beta$. The limits of this constant have been estimated at $0.625 \leq \beta \leq 0.922$. The author in his work slightly improves these limits.

However, we are never sure whether we have received the best solution or only one close to the optimal one.

In this paper, we present another method of obtaining an approximate solution to the traveling salesman problem.

Presentation of the traveling salesman problem

We have *n* cities that salesman has to visit. Distance (or travel costs or travel time) between each pair of cities are known. The goal is to find the shortest (or cheapest or fastest) road that connects all the cities beginning with and ending at a given point (the city) [11, 13]. Symmetric travelling salesman problem will be considered in this study. In this problem, for any of the cities *A* and *B*, the distance from *A* to *B* is the same as that from *B* to *A*. In asymmetric travelling salesman problem the distance may be different [10, 13].

Traveling Salesman Problem is often defined in the language of graph theory. The travelling salesman problem is the issue of optimization which consists in finding a minimum Hamiltonian cycle in a weighted complete graph. We define a set of cities as a full graph *G*, which has *n* vertices. We associate a weight of distance (or the cost of travel or, travel time) between the two cities from each edge of the graph. The problem boils down to determining the minimum Hamiltonian cycle in graph *G*. Hamiltonian cycle is a cycle, which includes all the vertices of the graph *G*. Definition of the problem is simple, but it is difficult to solve. For a small number of cities we apply the algorithm relies on a complete review of all possible Hamiltonian cycles in *G* and choosing the shortest. If the number of cities is a large browsing of all possible Hamiltonian cycles in a graph *G* is unrealistic. This leads to an exponential computational complexity(*n*!). The practical application of this algorithm for more than a dozen cities is therefore impossible [12]. We have a (*n*-1)!/2 solutions to the traveling salesman problem with n cities. For the 20 towns is the number so high (more than 60 trillion) that the implementation of such an algorithm takes an incredibly long time (one thousand years). We are able to find a solution that is not the best (optimal), but it is not good enough and in addition it will be found within a reasonably short period of time. We can either use approximate algorithms [14].

Description of the calculation method

The set of n cities is divided into smaller groups, the so-called clusters. The idea behind the calculations is that in small clusters it is easier to find the shortest route connecting individual cities. Then we combine these roads into one whole and treat it as an approximate solution to the traveling salesman problem. The order of clusters, i.e. the order of connecting individual sections of the route, should be determined in advance. In addition, you must specify the start city and end city for each cluster. These cities should lie at the junction of clusters. These are places where clusters connect.

To create clusters, we will use the „cluster” procedure from Matlab.

Depending on how many clusters we divide the set of n cities into, we get different clusters. As a consequence, we can obtain another approximate solution to the traveling salesman problem. Different clustering methods and different distance calculation metrics can be used to create clusters. This also yields various approximate solutions to the traveling salesman problem. So what's the benefit of clustering if we can get different solutions? The advantage is that we don't have to compute the length of a traveling salesman's route for millions of permutations of different possible routes. We get one approximate path and optimize it, i.e. we correct only this one path to get a shorter one.

We will discuss clustering in the following chapters. Next, we will present a calculation example.

Clustering

Clustering is a data mining and machine learning concept derived from the broader concept of patternless classification.

Cluster analysis is a method of the so-called unsupervised learning. It is a method that groups elements into relatively homogeneous classes. The basis of grouping in most algorithms is the similarity between elements - expressed by the similarity function (metrics).

The purpose of cluster analysis is to organize the observed data into meaningful structures or groups by analyzing similarities in the elements subjected to research according to assumed criteria. In other words, the essence here is to search for elements (results of experiments, variables, objects) in the studied community in such a way as to create groups (clusters) in which, in terms of a specific feature, these elements are as similar as possible to each other and at the same time maximally different from in other groups.

Grouping can also solve problems like discovering structure in data and making generalizations. Grouping consists in separating groups (classes, subsets).

The selected targets for grouping are as follows:

- obtaining homogeneous test objects, facilitating the identification of their essential characteristics,
- reducing a large amount of primary data to a few basic categories that can be treated as objects of further analysis,
- reducing the workload and time of analyzes aimed at obtaining the classification of typical objects,
- discovery of an unknown structure of the analyzed data,
- comparing multi-feature objects [17].

Matlab's CLUSTER, PDIST and LINKAGE procedures

CLUSTER procedure

There is a CLUSTER procedure ready in Matlab that allows you to group elements in a set. Before using it, you must specify the metric by which to calculate the distance between the elements of the set. This is what the PDIST procedure is for. You must also specify the method by which clustering is to be performed. This is what the LINKAGE procedure is for.

The set of these three statements in Matlab is as follows:

```
y = pdist(x, 'metrics');
z = linkage(y, 'grouping method');
t = cluster(z, number of groups);
```

As a result of the CLUSTER procedure, a vector *t* with a length equal to the number of points to be grouped is obtained. The elements of this vector are numbers from 1 to number_groups. These numbers indicate the number of the group (cluster) to which the given point will be assigned.

PDIST procedure

The coordinates of the points to be grouped should be given in the set *x*. The second input parameter is 'metrics'. You can use the following metrics: 'euclid', 'seuclid', 'cityblock', 'mahal', 'minkowski' [15].

a) metric 'euclid' – euclidean metric

This is the Euclidean distance given by the formula

$$d(X,Y)=\left(\sum_{i=1}^{n}(x_i-y_i)^2\right)^{1/2}, \tag{1}$$

where *X*, *Y* are the points of the set in *n*-dimensional space, and x_i and y_i are the coordinates of these points.

For the points *X*(1,2), *Y*(9,8) and *Z*(2,6) it is *d*(*X*,*Y*)=10, *d*(*X*,*Z*)=4.1231, *d*(*Y*,*Z*)=7.2801.

b) metric 'seuclid' – standardizet euclidean metric

This is the standardized euclidean distance given by the formula

$$d(X,Y)=\left(\sum_{i=1}^{n}\frac{1}{\hat{s}_i^2}(x_i-y_i)^2\right)^{1/2}, \tag{2}$$

where $\hat{s}_i^2$ is the variance for the *i*-th coordinate of the points.

For the points *X*(1,2), *Y*(9,8) and Z(2,6) it is *d*(*X*,*Y*)=2.6880, *d*(*X*,*Z*)=1.3293, *d*(*Y*,*Z*)=1.7342.

c) metric 'cityblock' – city-block metric or Manhattan distance

This is the so-called „urban distance" defined by the formula

$$d(X,Y)=\sum_{i=1}^{n}|\,x_i-y_i\,|. \tag{3}$$

For the points *X*(1,2), *Y*(9,8) and Z(2,6) it is *d*(*X*,*Y*)=14, *d*(*X*,*Z*)=5, *d*(*Y*,*Z*)=9.

d) metric 'mahal' – Mahalanobis metric

This is the Mahalanobis distance given by the formula

$$d(X,Y)=\left((X-Y)\cdot C^{-1}\cdot(X-Y)^T\right)^{1/2}, \tag{4}$$

where *C* is the covariance matrix

$$C=\mathrm{cov}(X,Y). \tag{5}$$

This distance is also called the weighted Euclidean distance.

For the points *X*(1,2), *Y*(9,8) and Z(2,6) it is *d*(*X*,*Y*)=2, *d*(*X*,*Z*)=2, *d*(*Y*,*Z*)=2.

e) metric 'minkowski' – Minkowski metric, distance in an absolute Minkowski power metric

This is the Minkowski distance given by the formula

$$d(X,Y)=\left(\sum_{i=1}^{n}|\,x_i-y_i\,|^p\right)^{1/p}. \tag{6}$$

The quantity p is given as the third parameter of the „pdist" routine: y=pdist(x,'minkowski',p). If only the first two parameters are used without specifying „*p*", this parameter is assumed to be *p*=2.

For the points *X*(1,2), *Y*(9,8) and Z(2,6) and *p*=4 it is *d*(*X*,*Y*)= 8.5691, *d*(*X*,*Z*)=4.0039, *d*(*Y*,*Z*)=7.0116.

In newer versions of Matlab you can also use metrics: ‘chebychev’, ‘cosine’, ‘correlation’, ‘spearman’, ‘hamming’, ‘jaccard’. Description of these metrics can be found in the documentation of newer versions of Matlab.

LINKAGE procedure

The LINKAGE procedure is used to specify the method by which to cluster.

The input parameters of the LINKAGE procedure are: vector *y* obtained earlier from the PDIST procedure and „grouping method”. The following grouping method names can be used: ‘single’, ‘complete’ , ‘average’, ‘centroid’, ‘ward’.

a) ‘single’ method – single linkage

This method is called the nearest neighbor method or the single bond method.

In this method, the distance between the newly created cluster and the external unit is set as the smallest distance from the distance between the units in this cluster and the external unit [15]. If we assume that we have a set $X=\{x_i\}$ in *n*-dimensional space, where xi are members of this set and a point *P* not belonging to the set *X*, then the distance of the point *P* from the set *X* is given by the formula

$$d(P,X)=\min_i d(P,x_i). \tag{7}$$

The distance between two clusters is determined as the shortest distance from the distance between units from one and the other cluster [15].

If we assume that in n-dimensional space we have a set $X=\{x_i\}$, where x_i (i=1, …, k) are elements of this set, and a set $Y=\{y_j\}$, where y_j (j=1, …, m) are elements of the set *Y*, then the distance of the set *X* from the set *Y* is given by the formula

$$d(X,Y)=\min_{i,j} d(x_i,y_j). \tag{8}$$

In this method, group merging is based on the distance between the closest elements belonging to the clusters being joined. The groups with the shortest distance between their nearest elements are combined first. We start with groups of size 1 (each object creates one cluster), and then, after each connection, we reduce the number of groups by 1 [16].

b) ‘complete’ method – complete linkage

This method is called the furthest neighbor method or the full bond method.

In this method, the distance between the newly created cluster and the external unit is set as the greatest distance from the distance between the units in this cluster and the external unit [15].

For a point *P* not belonging to the set *X*, the distance of the point *P* from the set *X* is given by the formula

$$d(P,X)=\max_i d(P,x_i), \tag{9}$$

where xi are elements of this set X in n-dimensional space.

The distance between two clusters is set as the greatest distance from the distance between units in one of the other clusters.

For two sets *X* and *Y*, the distance between them is given by the formula

$$d(X,Y)=\max_{i,j} d(x_i,y_j). \tag{10}$$

In this method, we use the distance between the most distant elements belonging to the groups to decide which of the two clusters to connect first [16].

c) 'average' method – average linkage

This is the medium connection method. The distance between the newly created cluster and the external unit is determined as the arithmetic average of the distance between the units in this cluster and the external unit [15].

For a point P and a set X defined above, the distance between them is

$$d(P,X)=\frac{1}{k}\sum_{i=1}^{k}d(P,x_i), \tag{11}$$

where m is the number of elements of the set X.

The distance between two clusters is determined as the arithmetic mean of the distance between units from one of the other clusters [15].

For two sets X and Y defined as above, the distance between them is

$$d(X,Y)=\frac{1}{k\cdot m}\sum_{i=1}^{k}\sum_{j=1}^{m}d(x_i,y_i). \tag{12}$$

In this case, the distance between clusters is defined as the average distance between all pairs of elements belonging to both groups. This method is abbreviated as UPGMA (unweighted pair group method with arithmetic mean). If we use weights in the form of cluster sizes (the number of elements contained in them), we obtain the WPGMA method (weighted pair group method with arithmetic mean) [16].

d) 'centroid' method [16]

For each group, we calculate the centroid - as the average value of all objects (vectors) belonging to a given group. The inter-cluster distance is defined as the distance between the centroids of these clusters. This method is abbreviated as UPGMC (unweighted pair group method centroid). There is also a method that takes into account the size of clusters in the form of appropriate weights. It is abbreviated as WPGMC (unweighted pair group method centroid).

The main idea of the algorithm is to determine k centroids – one for each group. Then each of the given objects is assigned to the nearest centroid. This is how the k-clusters we want to obtain are created. As part of the algorithm, for each of the initially obtained clusters, we recalculate the centroids and redistribute the objects in the manner already discussed.

We repeat this operation until none of the objects changes the cluster.

In general, the k-means algorithm can be presented in the following points [17]:

1) we determine k points in the space represented by the objects that will be grouped. These points will be the initial centroids of the groups,
2) we assign each object to a group for which the distance between its centroid and a given object is the smallest (according to a specific measure),
3) when all points are assigned, we calculate new centroid positions in the resulting clusters,
4) we repeat steps 2 and 3 until the changes in the position of the centroids (in subsequent steps) are small enough, or until a certain number of iterations are performed.

e) Ward's method [15]

In this method, two groups of objects are combined into one group so as to minimize the sum of squared deviations of all objects from these two groups from the center of gravity of the new group, which will be created as a result of combining these two groups.

At each stage of combining groups of objects, out of all groups of objects that can be combined,

those groups are combined into one group, which as a result form a group of objects with the smallest differentiation due to the variables describing them.

The Ward method is one of the agglomeration clustering methods, which is distinguished from the others by the use of the analysis of variance approach to estimate the distance between clusters.

The procedure in the Ward method is similar to that in other agglomeration methods [16]. The procedure is as follows:

1) determination of the $n \times n$ taxonomic distance matrix, which contains the distance of each pair of objects. This matrix is symmetrical about the main diagonal, which is all zeros,
2) finding pairs of objects (and then clusters) for which the mutual distance is the smallest. It should be assumed that these objects have the numbers „*p"* and „*q"*, where $p<q$,
3) joining „*p*" and „*q*" into one new cluster, which occupies the position with the number „*p*". At the same time, the object (cluster) with the number „*q*" is removed, and the numbers of clusters with a number higher than it are reduced by one. Thus, the dimension of the matrix is reduced by 1.

An example of clustering

In order to illustrate, we will use the coordinates of one hundred points (coordinates of cities) distributed on a plane. The coordinates of these points are listed in Tab. 1.

Tab. 1. Point numbers and coordinates

nr	*X*	*y*	*nr*	*x*	*y*	*nr*	*x*	*y*	*Nr*	*x*	*Y*
1	3878	656	26	1789	958	51	380	818	76	1922	690
2	993	934	27	3404	1501	52	2940	340	77	3817	902
3	1250	1003	28	3518	1081	53	2521	137	78	380	1051
4	2622	1491	29	1262	59	54	2946	1618	79	1180	99
5	1291	536	30	1419	1731	55	2632	1483	80	2653	809
6	832	245	31	3908	189	56	2100	403	81	3417	141
7	2721	1441	32	3802	173	57	896	1847	82	614	1387
8	751	820	33	3090	1531	58	2142	1811	83	3115	887
9	1262	1820	34	2568	1972	59	2478	1187	84	930	1680
10	2714	1687	35	459	1668	60	2419	1012	85	2599	1827
11	3601	1324	36	3877	601	61	2288	1807	86	2588	1292
12	1235	1932	37	1812	1709	62	2591	305	87	164	909
13	128	859	38	302	1509	63	330	262	88	1431	136
14	1222	1939	39	3481	823	64	239	344	89	745	1023
15	3350	1520	40	3957	1741	65	951	273	90	1622	1649
16	251	1253	41	1318	279	66	2988	789	91	1787	1009
17	622	681	42	3450	1832	67	2570	602	92	24	993
18	2581	1665	43	1617	1826	68	22	677	93	2957	1401
19	930	1711	44	3368	1651	69	3700	1201	94	3638	45
20	47	862	45	1389	1372	70	1112	1056	95	3757	886
21	281	1430	46	2539	240	71	869	1563	96	782	389
22	2569	938	47	3873	1321	72	2858	561	97	1721	1638
23	182	25	48	940	963	73	841	619	98	201	1814
24	447	355	49	3020	473	74	3897	105	99	3945	1561
25	2681	1819	50	3853	919	75	2180	1622	100	1550	1202

Source: own calculations

One hundred points distributed on the plane are shown in Fig. 1.

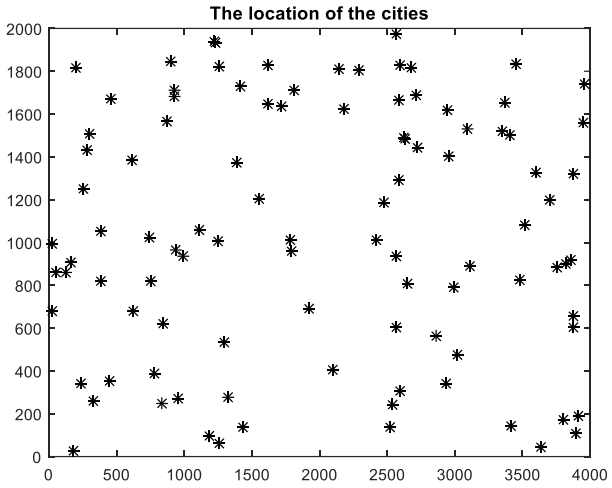

Fig. 1. Distribution of one hundred points (cities) on a plane
Source: own calculations

The length of the traveling salesman's route was calculated by counting the sections from the first to the last hundredth. This route is shown in Fig. 2.

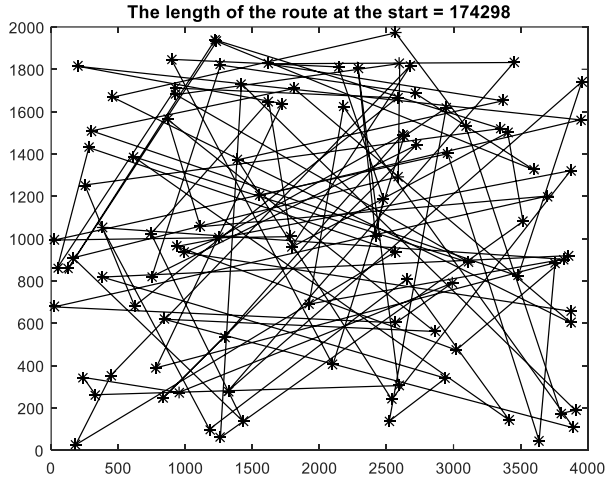

Fig. 2. Length of the traveling salesman route in order of cities from 1 to 100
Source: own calculations

The following commands were used in the computer program in Matlab:

```
y = pdist(x, 'euclid');
z = linkage(y, 'centroid');
t = cluster(z, 14);
```

This means that the euclidean distance and the centroid method were chosen.

The following clusters were obtained, shown in Fig. 3.

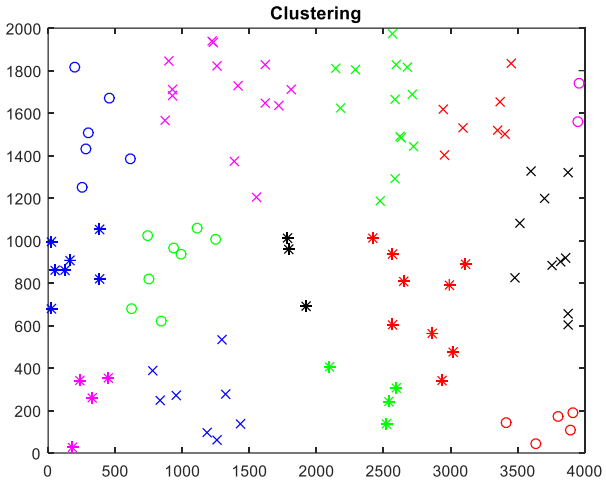

Fig. 3. Division of 100 points into 14 clusters
Source: own calculations

Individual clusters are marked in the figures with the following colors:
Cluster 1 – green stars – *
Cluster 2 – red stars – *
Cluster 3 – blue stars – *
Cluster 4 – pink stars – *
Cluster 5 – green circles – ○
Cluster 6 – blue x – x
Cluster 7 – red x – x
Cluster 8 – green x – x
Cluster 9 – pink circles – ○
Cluster 10 – black x – x
Cluster 11 – black gwiazdki – *
Cluster 12 –red circles – ○
Cluster 13 – blue circles – ○
Cluster 14 – pink x – x

The city numbers assigned to the individual clusters are as follows:
Cluster 1: 46 53 56 62
Cluster 2: 22 49 52 60 66 67 72 80 83
Cluster 3: 13 20 51 68 78 87 92
Cluster 4: 23 24 63 64
Cluster 5: 2 3 8 17 48 70 73 89
Cluster 6: 5 6 29 41 65 79 88 96
Cluster 7: 15 27 33 42 44 54 93
Cluster 8: 4 7 10 18 25 34 55 58 59 61 75 85 86
Cluster 9: 40 99
Cluster 10: 1 11 28 36 39 47 50 69 77 95
Cluster 11: 26 76 91
Cluster 12: 31 32 74 81 94
Cluster 13: 16 21 35 38 82 98
Cluster 14: 9 12 14 19 30 37 43 45 57 71 84 90 97 100

Now we define the start and end points of the routes in each cluster. We do it on the basis of Fig. 3. To find the shortest path in the cluster, the following method was used: two numbers from the range 2 ÷ *k*-1 were drawn, where *k* means the size of the cluster. Then the cities (city numbers) were swapped in the reverse order from this range. The length of the obtained route in the cluster was calculated. This was repeated 400 times for each cluster. The shortest routes in each cluster were stored. Additional calculations were made. For each found cluster route, three successive cities were cyclically swapped. Cities with numbers nr_{i-1}, nr_i, nr_{i+1} were changed to nr_{i+1}, nr_{i-1}, nr_i. Each time the length of the path in the cluster was calculated and the smaller one was stored. The shortest paths found in the clusters are shown in Fig. 4.

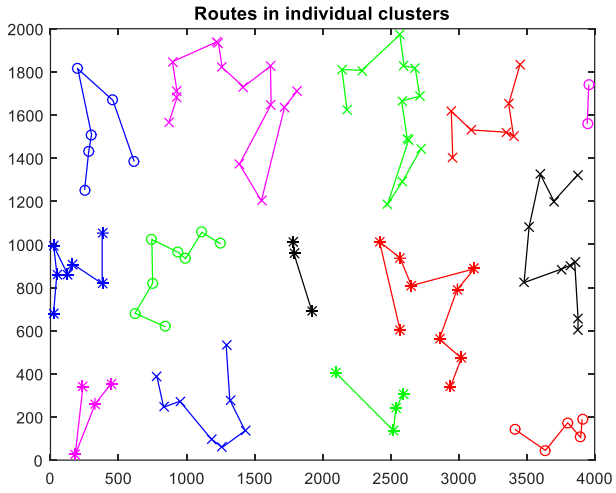

Fig. 4. Calculated routes in each cluster
Source: own calculations

After combining all the routes in the clusters, we get an approximate total traveling salesman route. It is shown in Fig. 5.

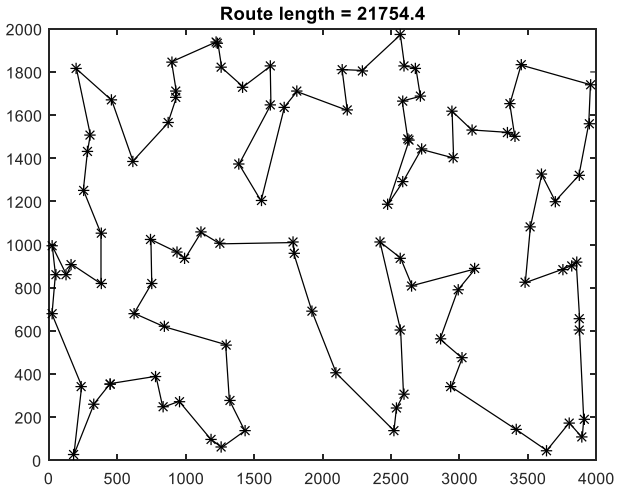

Fig. 5. Approximate route of a traveling salesman
Source: own calculations

The route found, as we mentioned earlier, depends on how the clustering is done. With a different number of clusters, for different length counting metrics, for different methods of finding clusters, the route will be different. We suppose that our received route is not optimal. Using Figs. 4 and 5, we correct the received route. From cluster 14 we move two points numbered 45 and 100 to cluster 11. The coordinates of these points are (1389, 1372) and (1550, 1202). Also from cluster 8 we move two points numbered 59 and 86 to cluster 2. The coordinates of these points are (2478, 1187) and (2588, 1292). The new clusters after correction are shown in Fig. 6.

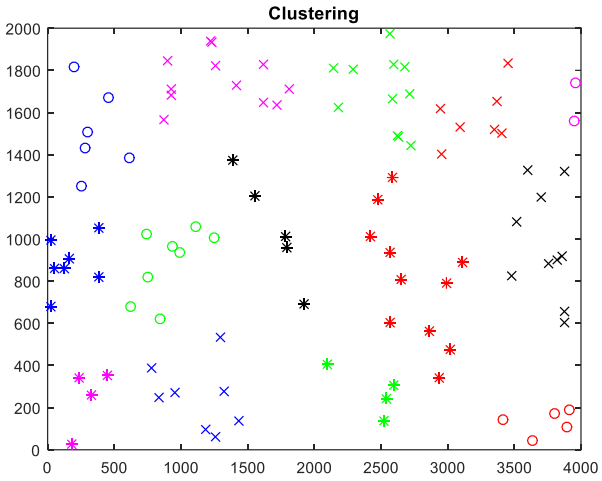

Fig. 6. New clusters after correction
Source: own calculations

The routes in these clusters are shown in Fig. 7.

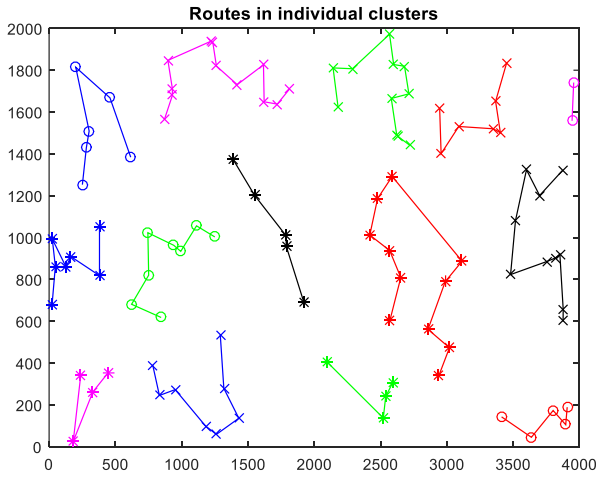

Fig. 7. New routes in clusters after correction
Source: own calculations

After combining these routes, we get an approximate total traveling salesman route. It is shown in Fig. 8.

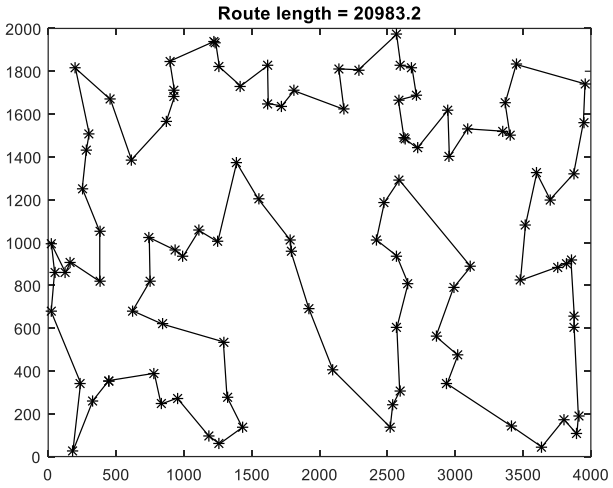

Fig. 8. Approximate traveling salesman route after correction
Source: own calculations

It turned out that the total length of the traveling salesman's path is shorter. It is 20983.2. In Fig. 5, it was 21754.4.

We will make another correction of the route. We will move three points numbered 4, 7, 55 from cluster 8 to cluster 2. The coordinates of these points are (2622, 1491), (2721, 1441) and (2632, 1483). In addition, we will move one point number 93 from cluster 7 to cluster 2. The coordinates of this point are (2957, 1401). The new division into clusters is shown in Fig. 9.

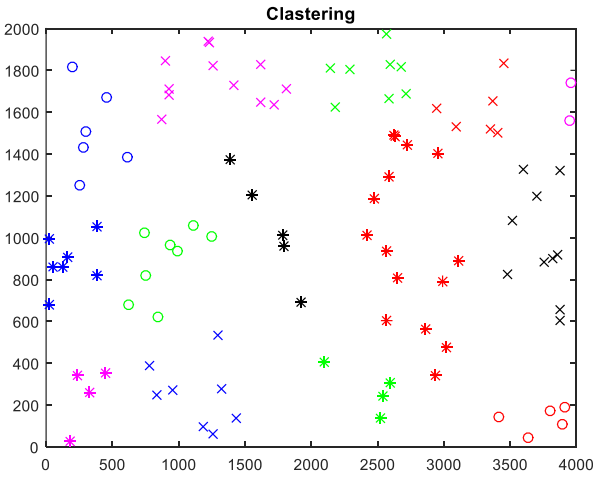

Fig. 9. New clusters after the second correction
Source: own calculations

The routes in these clusters are shown in Fig. 10.

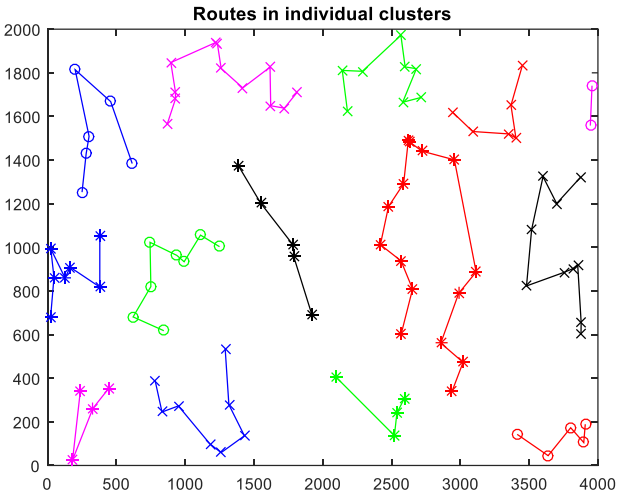

Fig. 10. New routes in clusters after second correction
Source: own calculations

After combining these routes, we get the total traveling salesman route. It is shown in Fig. 11.

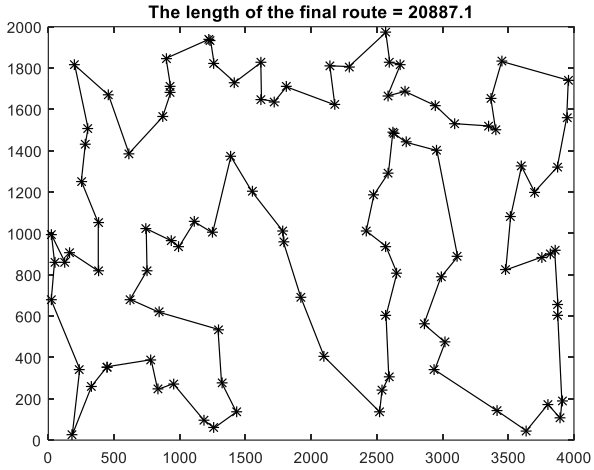

Fig. 11. A designated traveling salesman route
Source: own calculations

It turned out that the total length of the traveling salesman's path is shorter. It is 20887.1. In Fig. 8, it was 20983.2. The consecutive city numbers are as follows:

24 63 23 64 68 20 92 13 87 51 78 16 21 38 98 35 82 71 84 19
57 14 12 9 30 43 90 97 37 75 58 61 34 85 25 18 10 54 33 15
27 44 42 40 99 47 69 11 28 39 95 77 50 1 36 31 74 32 94 81 52
49 72 66 83 93 7 55 4 86 59 60 22 80 67 62 46 53 56 76 26 91
100 45 3 70 2 48 89 8 17 73 5 41 88 29 79 65 6 96.

If we wanted the traveling salesman to leave city number 1 first, we move the initial 53 numbers from this set to the end. We get the following route:

1 36 31 74 32 94 81 52 49 72 66 83 93 7 55 4 86 59 60 22
80 67 62 46 53 56 76 26 91 100 45 3 70 2 48 89 8 17 73 5 41
88 29 79 65 6 96 24 63 23 64 68 20 92 13 87 51 78 16 21 38 98

35 82 71 84 19 57 14 12 9 30 43 90 97 37 75 58 61 34 85 25 18 10 54 33 15 27 44 42 40 99 47 69 11 28 39 95 77 50.

This completes the route planning for the traveling salesman.

It turns out that we got exactly the same route as in [4]. In paper [4], the city numbers are arranged in reverse order.

Conclusion

The paper presents a new method of solving the traveling salesman problem. Clustering was used for this. The cities to be visited by the traveling salesman were divided into groups of so-called clusters. Cities were divided into 14 clusters. This was done using ready-made Matlab procedures PDIST, LINKAGE and CLUSTER. The 'euclid' metric and the 'centroid' clustering method were selected. The shortest path was found in each cluster. With a small number of elements in the cluster, it was possible. The order of occurrence of the clusters had to be determined. These roads were then clustered together into a single route. In this way, an approximate solution to the traveling salesman problem was obtained.

Using other metrics and other methods of clustering and a different number of clusters, a different approximate solution to the traveling salesman problem is obtained.

Since the obtained solution was not satisfactory, it was decided to correct it. Several elements from one cluster were transferred to others. A significant improvement of the solution was obtained. The traveling salesman's final route was much shorter.

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TIN-117m ISOMER AS A REPLACEMENT FOR TECHNETIUM- 99M FOR DIAGNOSTIC APPLICATIONS

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Abstract:

In this work tests of production of the new radioisotope ^{117m}Sn were performed by means of a typical medical linear accelerator used in radiotherapy treatment. This isomer of tin is a promising radioisotope for its application for diagnostic purposes in nuclear medicine because of emitted energy of 158.56 keV close to that emitted by ^{99m}Tc. Its provides possibilities to use the same collimators system in gamma camera as it is for ^{99m}Tc. The appropriate half-life of 13.6 days and only the gamma transition to the stable state of ^{117m} Sn with very small amount conversion electrons make the considered isomer an ideal alternative to ^{99m}Tc. Presently, most of reactors using to produce radioisotopes for nuclear medicine are approaching the end of their life. As a consequence, the regression of ^{99m} Tc production is becoming more and more current. However, it can be produced in nuclear reactors by using two nuclear reactions ^{118}Sn(γ,n)^{117m} Sn as well as in the neutron capture reaction ^{116} Sn(n,γ)^{117m}Sn.

Keywords:
radioizotops, nuclear medicine, radiopharmaceutics, tin-117m

Introduction

This article focuses on how the medical tin isomer ^{117m}Sn can be produced and used in the context of its wider application in nuclear medicine and, in particular, in diagnostics. Up to now, the ^{117m}Sn tin isomer has been used as an effective pain reliever after bone metastases. However, the gamma- ray energy emitted by ^{117m}Sn is optimal for scintigraphy and, in addition, this tin isomer can also be combined with a wide variety of ligands. Tin ^{117m}Sn can be efficiently produced in many nuclear reactions without the use of research reactors, which is a great advantage, especially in light of the perceived crisis in technetium ^{99m}Tc production. The aim of this paper is to review the applications of the tin-117m isomer and how it can be produced, in the context of the replacement of technetium- 99m by tin-117m.

Nuclear medicine

Nuclear medicine is one of the specialties of medicine, involving the administration of radiopharmaceuticals to patients, i.e. substances with radioactive isotopes that emit

ionizing radiation (photons, electrons and positrons) for use in the diagnosis and treatment of disease. Two imaging techniques are used in diagnosis. The radioisotopes commonly used in scintigraphic imaging are technetium-99m, iodine-123 [1, 2]. The second main diagnostic technique is positron emission tomography (PET). It uses β+ emitters such as fluorine-18, gallium-68 and many others [1, 4-9]. A good example of a radionuclide used in radioisotope therapy, is iodine-131 [1, 10], used to destroy thyroid tissue in the treatment of hyperthyroidism and cancer. Recently, nuclear medicine has strongly supported advanced research in immunology. This branch of nuclear medicine is called radioimmunology [11]. An example of such research is in vitro diagnostics, which determines the amount of various substances such as drugs, hormones and antibodies in the blood [12-14]. In vitro diagnostics is based on radioisotopes ^{125}J, ^{14}C and ^{3}H [15].

Production of medical radioisotopes

Due to the rapid development of nuclear medicine, there is an increasing demand for radioactive isotopes used in diagnosis and therapy. Currently, most medical radionuclides are produced by irradiating uranium targets (fission reactions) or targets enriched in the parent isotope (simple capture reactions (n.γ) also called radiological neutron capture), in research reactors [16, 17]. The main suppliers of radioisotopes produced in reactors are Belgium, Canada, Netherlands, France and South Africa [16]. Radioisotopes with excess neutrons (β- emitters) are mainly produced in research reactors, while those with excess protons are produced in cyclotrons [18] in various reactions (p,n), (p,pn), (d,n) and (γ,n). Nuclei with excess protons disintegrate by β+ decay. Therefore, most cyclotron radionuclides are suitable for use in positron emission tomography.

Technetium-99m

As already mentioned, technetium-99m is the primary radioisotope used in nuclear medicine. This radionuclide has a relatively short half-life of $T_{1/2}$ = 6 hours, which prevents its use in medical centers away from research reactors. Therefore, ^{99}Mo/^{99m}Tc generators powered by fission production (^{99}Mo, $T_{1/2}$ = 65.94 hours [19]) are used. 85% of all nuclear medicine studies use ^{99}Mo/ ^{99m}Tc generators for liver, lung, bone diagnostics [20]. The ^{99m}Tc shortage caused by the unexpectedly prolonged closure of the Chalk River (Canada) and Petten (Netherlands) reactors and the permanent cessation of ^{99}Mo production at Chalk River in 2016 have contributed to the search for alternative methods of ^{99m}Tc production [21-24]. Non-reactor technetium-99m can be produced in small quantities directly using cyclotrons and accelerators, in a cyclotron by bombarding a molybdenum-100 target with an 18 MeV proton beam (in a (p,2n) reaction) to produce technetium-99m [21], or in a linear accelerator to produce molybdenum-99 in a ^{100}Mo(γ,n)^{99}Mo photo-fusion reaction induced by high-energy X-rays [22, 23]. The IAEA recommends the use of medical cyclotrons for the production of ^{99m}Tc [24]. There has also been considerable interest in the search for new radioisotopes that could be an alternative to technetium-99m. A good candidate is the tin-117m isomer.

Characterisation of tin-117m

^{117m}Sn is the nuclear isomer in the second initial state of tin. This state is characterized by an 11/2 spin, negative parity, an excitation energy of 314.6 keV and a half-life of $T_{1/2}$ = 13.6 days [19, 25].

It decays by cascade gamma decay and internal conversion. The cascade conversion energies of all ^{117m}Sn decay products are shown in Tab. 1.

Tab 1. Decomposition characteristics of ^{117m}Sn

Product	Energy [KeV]	Emission intensity (transition probability) in [%]
Gamma radiation	158.6	86.4
	156.0	2.1
Electrons	126.8	64.9
	151.6	26.2
	129.4	11.7

Source: Nigel Stevenson, Clear Vascular, Inc. , Production of Commercial High Specific Activity Sn-117m Radiochemical and Chelates

Production of tin-117m

Tin isomer can be produced in a research reactor by two reactions, the neutron radiation capture (n,γ) of enriched tin-116 (abundance 14.54%) and by an inelastic neutron reaction (n,n) on enriched tin-117 (7.68%). The latter reaction is most efficient in reactors with higher fluxes, as specific activity values of about twice that of the radiative capture reaction can be achieved [26]. Production using uranium targets is not efficient due to the very small amounts of tin-117m in the fission products. However, ^{117m}Sn can be produced in cyclotrons and linear accelerators. The characteristics of the nuclear reactions leading to the formation of tin-117m are shown in Tab. 2.

Tab. 2. List of nuclear reactions leading to the formation of ^{117m}Sn.

Reaction	Cross section
115-In(α,pn)	16 mb at 31.5 35.4 MeV [27]
117S(p,p'ϒ)	0.37 mb at 23.6 MeV [28]
114Cd(α,n)	480 mb at 20 MeV [29]
116Cd(α,3n)	1.2 at 36 MeV [30]
121Sb(p, α)	Several hundred mb at 30-42 MeV [28]
118Sn(n, ϒ)	290 mb at 15 MeV [30]
116Sn(n, ϒ)	6 mb at thermal energies [31]
118Sn(n,n')	Over 317.2 keV [31]

Source: [27-31]

Discussion of the uses of tin-117m.

To date, ^{117m}Sn has been used as an effective means of relieving pain caused by bone metastases [32-34]. Such radionuclide therapy leads to a significant improvement in the quality of life of patients. This use is due to the desirable half-life of tin-117m, the energy of the emitted electrons and the emission intensity of the internal transformations. To date, tin-117m has not been widely used in radiopharmaceuticals. Currently, the only radiopharmaceutical is tin(IV)-117m DTPA (pentitic acid) [33] used for bone pain relief. Tin-117m can also be combined with other ligands such as PyP (pyrophosphate), EHDP (disodium ethylenedodehydroxydiphosphonate) and MDP (methylene standard gamma camera imaging system, for example, to use the same collimator system as for technetium - 99m. Thus, the energy of the gamma rays emitted by ^{117m}Sn is optimal for

scintigraphy.diphosphonate) [33]. ^{117m}Sn is also a diagnostically promising radioisotope, as it emits gamma radiation of 158.6 keV, which is close to the energy of ^{99m}Tc. This allows the use of an existing Technetium-99m emits gamma radiation during decay, which is used in diagnostics, in addition X-rays, Auger electrons and internal conversion electrons are emitted (Tab. 3).

Tab. 3. Energy emitted during decay of technetium ^{99m}Tc

Radiation type		**Energy [KeV]**
Electrons	IC-M	1.82
	Auger L-1	2.05
	Auger M	2.32
	Auger L	2.66
	Auger KL	15.3
	Auger K-1	17.8
	IC 3k	122.0
	IC 2L	137.0
	IC 2 M	140.0
	IC 3L	140.0
X radiation	X-ray K2	18.3
	X-ray K1	18.4
	X-ray K1	20.6
	X-ray K2	21.0
Gamma radiation	Gamma	141.0

Source: A. Taborda et al. / Applied Radiation and Isotopes 108 (2016) 58–63

The decay of tin-117m also emits gamma radiation of similar energy to that emitted during the decay of technetium-99m, and internal conversion electrons and Auger electrons are emitted (Tab. 4).

Tab. 4. Energy emitted during decay of tin Sn-117m

Radiation type		**Energy [KeV]**
Electrons	Auger-L	3
	Auger-K	21
	CE-K1	126.8
	CE-K2	129.4
	CE-L1	151.6
	CE-L2	154.1
	CE-M1	155.1
Gamma radiation	Gamma	158.6

Source: Nigel Stevenson, Clear Vascular, Inc. , Production of Commercial High Specific Activity Sn-117m Radiochemical and Chelates

Summary

The dose at the cellular level (micrometer range) from tehnet- 99m decay is greater than that from tin-117m decay. Doses at the 10-2 cm level are virtually the same. It should be noted that some particles from technetium decay have a range of a few centimeters, which is not the case for tin decay. The doses from gamma radiation are almost identical, due to similar energies. The energy from Auger electrons from technetium-99m decay is deposited locally and cannot be counted on a macroscopic

scale [36]. Virtually all of the energy is deposited in the cytoplasm, so that cells are not damaged, with only a trace amount reaching the cell nucleus.

Tin-117m is one of the few medical radioisotopes that can be used in radiotherapy as well as in diagnostics. Due to its relatively long half-life, the tin isomer does not require a radionuclide generator. Consequently, the problem of contamination of radiopharmaceuticals with the parent radioisotope disappears. In diagnostics, contaminated radiopharmaceuticals are a source of additional dose to patients. Tin-117m can be efficiently produced in many nuclear reactions without the use of research reactors, which is a very big advantage especially in light of the perceived crisis in technetium-99m production.

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ADVANTAGES OF USING THE TRANSLATION METHOD IN FOREIGN LANGUAGE LEARNING

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Abstract:

This article examines the advantages of the translation method (TM), also known as the grammar-translation method, in the context of foreign language teaching. Despite the emergence of innovative language teaching approaches such as the direct method, the audiolingual method, and the communicative approach, TM remains relevant in various educational contexts. The article provides an overview of the history of the translation method, dating back to ancient Rome, and its evolution over the centuries. It then delves into the benefits of TM, including facilitating the learning of vocabulary and grammatical structures, enhancing cultural understanding, fostering creativity and problem-solving skills, and increasing student motivation and engagement. Furthermore, the article explores how the translation method can support students with learning difficulties by examining various strategies and techniques employed in instructional practice. In conclusion, the article highlights the merits and limitations of the translation method in foreign language teaching and suggests directions for future research on the optimal use of this method in educational practice.

Keywords:
translation method, language learning, teaching, TM

Introduction

This article explores the advantages of the translation method (TM), also known as the grammar-translation method, in the context of foreign language teaching. Despite the emergence of innovative language teaching methods, such as the direct method, the audio-lingual method, or the communicative approach, TM remains relevant in various educational contexts. The article presents a review of the history of the translation method, dating back to ancient Rome, and its evolution over the centuries. The article then delves into the benefits of TM, such as facilitating vocabulary and grammatical structures learning, enhancing cultural understanding, fostering creativity and problem-solving skills, as well as increasing student motivation and engagement. Furthermore, the article investigates how the translation method can support students with learning difficulties, analyzing various strategies and techniques used in teaching practice. In conclusion, the article highlights the advantages and limitations of the translation method in foreign language teaching and suggests directions for future research on the optimal use of this method in educational practice.

In the era of globalization and the growing need for intercultural communication, the translation method (TM) plays a significant role in foreign language teaching. Despite the existence of innovative language teaching methods, such as the direct method, the audio-lingual method, or the communicative approach, TM still finds application in many educational contexts. In this article, we will present the history of the translation method, its advantages, and how it can support students with diverse needs.

The translation method, also known as the grammar-translation method, focuses on teaching grammar, vocabulary, and language structures through the analysis and translation of texts. The article will present the history of this method, which dates back to ancient Rome, and its evolution over the centuries.

In the subsequent parts of the article, the benefits of the translation method will be discussed, including facilitating the learning of vocabulary and grammatical structures, as well as enhancing cultural understanding. The impact of the method on developing creativity and problem-solving skills will also be presented, along with research indicating the potential of this method in increasing student motivation and interest.

The article will then focus on the ways in which the translation method can support students with learning difficulties, taking into account various strategies and techniques employed in teaching practice.

The conclusion will draw insights related to the application of the translation method in foreign language teaching, pointing out its advantages and limitations, as well as possible directions for further research on the optimal utilization of this method in educational practice.

History of the Translation Method

The translation method, also known as the grammar-translation method, has a long and rich history in foreign language teaching. Its roots go back to ancient Rome, where education was mainly based on learning Latin, the language of science, law, and religion. Teaching Latin was based on translating texts from Greek into Latin [1].

In the Middle Ages, when Latin was the dominant language of science in Europe, the translation method was widely used in language teaching. Students learned Latin through the analysis and translation of literary and philosophical texts from ancient languages, such as Greek or Hebrew, into Latin [2].

During the Renaissance, the translation method continued to be used in teaching Latin, but it also began to be applied in teaching modern European languages, such as French, German, or Italian. During this period, greater emphasis was placed on learning foreign languages due to contact with other cultures and the development of trade and diplomacy [3].

In the 19th century, the translation method became the dominant method of teaching foreign languages in Europe, and then spread to other continents. Students learned a foreign language through the translation of literary and scientific texts, with teaching focusing on grammar, vocabulary, and written translation [4].

Although many innovative language teaching methods emerged in the 20th century, such as the direct method, the audiolingual method, or the communicative approach, the translation method still plays a significant role in foreign language teaching. Nowadays, it is often used as a complement to

other methods and as a tool for teaching specialized language, such as in legal or medical translations [5].

The translation method has its advantages, such as developing reading comprehension, writing, and metalinguistic awareness skills of students. However, in recent years, this method has also faced criticism, mainly for its lack of emphasis on developing speaking and listening skills, as well as its limited engagement of students in the learning process [6].

Despite these limitations, the translation method still finds its place in foreign language teaching, especially in the context of students with learning difficulties. Contemporary research shows that a properly adapted translation method can contribute to effective foreign language teaching, especially if used in combination with other, more communicative methods [7].

ADVANTAGES OF THE TRANSLATION METHOD

Facilitating vocabulary and grammatical structures learning, as well as understanding culture

The translation method significantly facilitates the learning of vocabulary and grammatical structures, which results from the active participation of students in the translation process, leading to a better understanding of the material [8]. Moreover, this method supports language acquisition through exposure to various texts and contexts, allowing students to more effectively master the language [9].

Introducing translation as a teaching tool facilitates the understanding of complex grammatical structures and allows for the verification of correct rule application [10]. Students learn how to apply grammar and various language structures in practice, leading to more effective communication [7].

Using the translation method also enables a better understanding of differences between languages and learning vocabulary in context. As students translate texts from one language to another, they have the opportunity to confront different grammatical and lexical constructions [1]. This approach facilitates the acquisition of words and their meanings, as students perceive them in context, rather than as separate units [11].

One of the important aspects of learning vocabulary and grammar in a translation context is developing pragmatic competence. Students learn how to appropriately use language in various situations and how to adapt their communication to the cultural context [12]. Therefore, the translation method becomes an effective tool in language teaching, as it allows students to learn not only words and grammar but also the culture in which the language operates.

In the context of language teaching, the translation method can be used in various ways, such as an element of homework, classroom exercises, or group projects. As a result, students have the opportunity to use translation as both an individual and group learning method, allowing for the development of cooperation and communication skills among participants [13]. Additionally, translation can be applied in language teaching at various levels of proficiency, making this method universal and adaptable to the needs of different students [14].

In light of the growing interest in foreign language teaching, the translation method is gaining increasing popularity among teachers and students [15]. It supports the learning process not only by providing students with in-depth knowledge of grammar and vocabulary but also by enabling them to establish connections with the culture in which the language operates [16].

Fostering creativity and problem-solving skills

The translation method, with its approach to teaching foreign languages, can also contribute to the development of students' creativity and problem-solving skills. Supporting these aspects is particularly important in the context of contemporary society, which increasingly appreciates creativity and the ability to adapt to various situations and challenges [17].

Unlike learning based on memorizing rules and patterns, the translation method emphasizes acquiring knowledge through practice, giving students more freedom to explore the language and develop creativity. For example, students can experiment with various translation strategies to find the best solutions for a given context or communication goal [13].

Translation as a process often requires students to perform various tasks that engage multiple language and cognitive skills, such as analysis, synthesis, or evaluation. Consequently, students learn to make decisions based on their own judgment and intuition, which in turn influences the development of their problem-solving skills [18].

The translation method also allows students to acquire teamwork and time management skills, which further contribute to the development of problem-solving abilities [14]. Collaborating with other students can help identify potential problems and generate various solutions, which is essential in the context of a dynamic professional world [19].

It is also worth noting that the enrichment of the learning process with a cultural aspect, which the translation method provides, can also impact the development of students' creativity [20]. Understanding and comparing different cultures can stimulate students' creative thinking and encourage them to seek innovative solutions at the intersection of cultures [21].

In conclusion, the translation method not only supports the learning of vocabulary and grammar structures but also fosters creativity and problem-solving skills among students. By incorporating cultural aspects and emphasizing practical application, this approach offers a well-rounded and engaging learning experience that prepares students for the challenges of today's diverse and interconnected world.

Increasing motivation and interest among students

In foreign language learning, motivation and interest play a crucial role in the process of acquiring knowledge and language skills [22]. The application of the translation method (TM) in foreign language teaching can contribute to increasing motivation and interest among students at various stages of learning [23]. This subsection will discuss the advantages of the translation method in the context of student motivation and analyze how TM can increase interest in learning a foreign language.

1) Greater language awareness

By analyzing language structures, students learn to recognize differences and similarities between their native language and the foreign language [24], which increases their language awareness. This heightened language awareness can lead to increased motivation among students who begin to appreciate the richness of the foreign language and the complexity of its structures [25]. Understanding these aspects of the language can also contribute to increased self-confidence among students, which in turn affects their motivation for further learning [26].

2) Greater autonomy in learning

One of the goals of foreign language teaching is for students to achieve independence in learning and communication in the foreign language [27]. The translation method, requiring students to independently translate texts and interpret sentences and expressions, can contribute to the development of skills necessary for achieving autonomy in learning [7]. For example, students learning through the translation method may be more inclined to independently search for information about grammar and vocabulary, which in turn can lead to greater engagement and motivation to learn the foreign language [5].

3) Greater understanding of culture

Translating texts related to the culture of a given country allows students to gain knowledge about the traditions, customs, and values of the culture of that language [28]. This knowledge can increase students' interest in the foreign language and contribute to the understanding that learning a language is not only about acquiring language skills but also broadening horizons and developing intercultural competencies [29]. Understanding the culture of countries where the foreign language is used can also help students better establish relationships with native speakers of that language, which translates into greater motivation and engagement in the learning process [20].

4) Practical applications

The translation method can be particularly interesting for students who have specific professional or educational goals related to translation [30]. Students who plan to work as translators, foreign language teachers, or individuals involved in international business may appreciate the practical application of the translation method in their future professional life [18]. This awareness of practical benefits can increase students' motivation to learn a foreign language, as they will perceive learning as an investment in their future [31].

5) Diversification in teaching

Introducing the translation method into the foreign language teaching program can contribute to diversifying classes and increasing student interest [32]. Translating texts, analyzing grammar, or solving translation tasks are just some of the activities that can be engaging and interesting for students [33]. A variety of tasks can help maintain a high level of student engagement, which is essential for success in learning a foreign language [34].

In summary, the translation method can contribute to increasing motivation and interest among students in learning a foreign language by developing greater language awareness, promoting autonomy in learning, fostering cultural understanding, providing practical applications, and diversifying teaching. Although this method may not be suitable for all students and teachers, its application can bring benefits in the context of motivation to learn a foreign language.

Support for Students with Learning Difficulties

The translation method, which involves teaching foreign languages by comparing and translating grammatical structures, vocabulary, and idioms from the native language to the target language, can provide many benefits to students with learning difficulties. Support for these students can include various strategies that enable better understanding and assimilation of learning content.

Firstly, the translation method helps students with learning difficulties understand the material by referring to their native language. Comparing grammatical structures between languages allows for a better understanding of the rules governing the target language, which can be helpful for students

with learning difficulties who may need additional explanations and simplifications [35]. Moreover, using the native language can increase students' motivation to learn, as they perceive translation as something more accessible and understandable [36].

Another advantage of the translation method is that it can be adapted to the individual needs of students with learning difficulties. Teachers can provide additional materials and exercises that help students understand complex grammatical and lexical issues, taking into account their specific educational needs [37]. Various translation techniques, such as written or oral translation, can also be applied depending on the needs and abilities of the student [15].

For students with learning difficulties, such as dyslexia, the translation method can be helpful in improving the reading and writing process. The practice of translating texts allows for the refinement of reading comprehension skills, as students must understand the meaning of the message in one language in order to translate it into another [38]. Additionally, written translation requires students to use vocabulary and grammar precisely, which can lead to an improvement in the quality of their written statements [39].

It is also worth noting that the translation method can support the development of metalinguistic skills in students with learning difficulties. These skills include language awareness, the ability to reflect on one's own language and foreign languages [40]. Through translation, students with learning difficulties have the opportunity to analyze and compare different language aspects, leading to a deeper understanding of the structures and rules governing languages [41]. This, in turn, can contribute to better mastery of a foreign language.

In the context of multilingualism, the translation method can also contribute to the development of interlanguage competence in students with learning difficulties. This competence refers to the student's ability to use knowledge and skills from one language for learning and communication in another language [42]. The practice of translation can help students with learning difficulties transfer language knowledge and skills between different languages, thus enhancing their overall language competence [43].

In conclusion, the translation method can bring many benefits to students with learning difficulties, such as better understanding of the material, adapting teaching to individual needs, improving the reading and writing process, developing metalinguistic skills, and interlanguage competence. It is important for teachers to use this method in a flexible and tailored way to meet the specific needs of students in order to achieve optimal results in foreign language teaching.

Summary

The academic article discussing the advantages of the translation method (TM) in the context of foreign language teaching begins with an introduction in which the author presents the historical context and evolution of this method, dating back to ancient Rome. They indicate that despite the emergence of modern teaching methods such as the direct method, the audiolingual method, or the communicative approach, TM still plays an important role in language education.

The discussion of the advantages of the translation method leads to several conclusions. First, it is worth noting that TM enables students to gain a solid grasp of vocabulary and grammatical structures, which is crucial for mastering a foreign language at a high level. Students acquire

knowledge of words and their meanings, learn how to form grammatically correct sentences, and how to apply various grammatical forms, which ultimately leads to a better understanding of the language. Secondly, the translation method allows students to understand the cultural context and connections between language and culture. This is extremely important, as language is closely related to the culture and values of the society in which it operates. Knowledge of the culture of the country whose language we are learning allows for a better understanding and assimilation of the language, as well as enables its use in practical situations, such as conversations or correspondence.

Thirdly, the translation method fosters creativity and problem-solving skills. Students learn to analyze texts, identify language problems, and seek solutions. TM forces students to think in two languages simultaneously and encourages experimentation with form and content, which in turn leads to the development of creative thinking skills.

Fourthly, the author indicates that TM can increase motivation and interest in students, especially when applied in an engaging and appropriate manner for the learners. It is important to pay attention to the selection of suitable texts for translation that will be interesting for students, and to apply various teaching techniques that take into account the individual needs and interests of the students. By adapting their approach to the translation method, teachers can effectively increase students' motivation to learn a foreign language.

Fifthly, the article includes a section dedicated to supporting students with learning difficulties, in which the author analyzes various strategies and techniques used in teaching practice in the context of the translation method. The findings from this chapter suggest that TM can be helpful for students with various needs, as it allows for tailoring the material to individual predispositions and capabilities of students. Teachers can utilize the translation method to help students with learning difficulties overcome barriers and achieve success in learning a foreign language.

These conclusions suggest that the translation method, although it has its drawbacks, can be an effective tool in language teaching if properly adapted to the needs of students and educational goals. The introduction of innovative teaching techniques and adapting the translation method to individual student needs can make this method even more effective and user-friendly. As a result, teachers can exploit the advantages of the translation method to contribute to the improvement of their students' language skills and prepare them for effective functioning in a multilingual and multicultural environment.

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SYNTHESIS OF NEW INDOLE-URACIL BIOCONJUGATES WITH POTENT BIOLOGICAL ACTIVITY

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Abstract:

New indole and uracil derivatives with triazole rings were obtained. All of them were synthesized by the CuAAC procedure and were characterized by spectral methods. Additionally, theoretical calculations were carried out, showing that newly synthesized compounds could be concerned as a potential pharmaceuticals.

Keywords:
indole, gramine, uracil, click chemistry, spectroscopic analysis

Introduction

Indole (Fig. 1), specifically 2,3-benzopyrrole, is an aromatic, heterocyclic organic compound. In its structure, indole contains a six-membered benzene ring connected to a five-membered pyrrole ring [1]. Moreover, this chemical compound contains 10 delocalized π electrons [2]. Indole derivatives are commonly found in various natural products or plants but are sometimes present in animals or marine organisms [1]. Many of these compounds exhibit various pharmacological properties, which is why they are intensively studied worldwide for their biological activity. A large group of indole derivatives is the indole alkaloids. They reveal anticancer, antibacterial, antiviral, anti-inflammatory, analgesic, antifungal, antidiabetic, and antidepressant properties [2]. For example, derivatives of lysergic acid, more widely known as ergot alkaloids, are very toxic. However, on a small doses, they exhibit an oxytocic effect [3]. Strychnine (Fig. 1), an ergot alkaloid, is a strong poison – it paralyzes the central nervous system. Nonetheless, in small doses, it can be used as a stimulant [4]. Another example of an indole alkaloid is Gramine (Fig. 1) – (1-(1H-Indol-3-yl)-N,N-dimethylmethanamine) [5]. It exhibits a pharmaceutical effect similar to ephedrine – it causes relaxation of bronchial smooth muscles, vasodilation, increases blood pressure, kidney inflammation, and bronchial asthma. It is also an important chemical compound since it is used to synthesize new indole derivatives [6, 7].

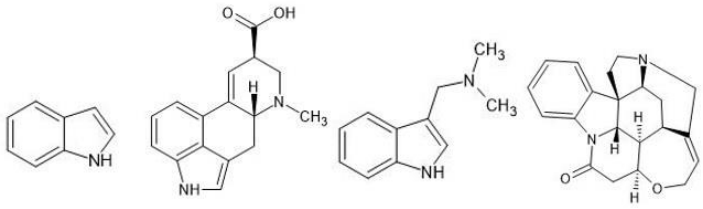

Fig. 1. The structures of indole, lysergic acid, gramine and strychnine

One of the most important derivatives of indole alkaloids, due to their anti-cancer activities, is indole-3-carbinol (I3C). It occurs in many plant organisms – in the tissues of vegetables from the brassica family – for example, cauliflower or cabbage. What is important, is that many studies have shown that people who consume more cruciferous vegetables have a lower risk of developing cancer than those who do not [8-9]. Many indole derivatives, specifically indolyl-3-acetic acid derivatives, are also used as drugs. For example, acemetacin is used as an analgesic and anti-inflammatory drug, and sumatriptan is used as an anti-migraine drug [8, 10].

Uracil (Fig. 2) is a common, natural pyrimidine derivative. It is one of the four nucleobases in the nucleic acid – RNA. In RNA, it binds to adenine through two hydrogen bonds. Due to their wide range of biological activity, uracils are used in drug development processes. Antiviral and antitumor activity are two of the important properties of uracil analogs, but they also exhibit herbicidal, bactericidal, and insecticidal activity. The best-known uracil analog is 5-Fluorouracil (Fig. 2). It is a well-known anticancer agent widely used to treat solid tumors such as colon and breast cancer [11].

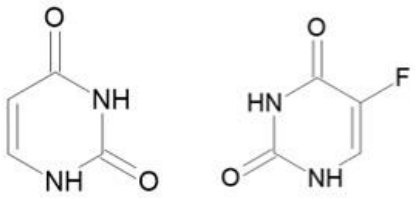

Fig. 2. The structures of uracil and 5-Fluorouracil

The term “click chemistry” refers almost exclusively to the CuAAC reaction – Copper (I) catalyzed Azide-Alkyne Cycloaddition) [12]. The general characteristics of this type of reaction are simplicity, mild conditions, wide range, less cytotoxicity of by-products, and high stereospecificity and chemoselectivity. The reaction product should be easily isolated. This type of reaction is widely used to modify biomolecules such as nucleic acids, lipids, and proteins. It is also used in drug research [13,14]. Moreover, in 2022, three chemists were awarded the Nobel Prize in Chemistry for developing click chemistry and bioorthogonal chemistry. Barry Sharpless and Morten Meldal (they laid the foundations of click chemistry) and Carolyn Bertozzi (she used click chemistry to map the glycan complex, and she developed the process which is currently used in the development of anti-cancer drugs) [15].

In our previous work, we synthesized conjugates containing indole and uracil moiety. Additionally, we synthesized new gramine with phthalimide derivatives containing a triazole ring using the CuAAC procedure. What is more, these conjugates were screened for antioxidant and

hemolytic activities. All of the obtained conjugates efficiently protect the human erythrocytes against hemolysis which is caused by oxidative stress [16, 17]. These results encouraged us to continue researching new gramine and uracil derivatives using click chemistry.

Experimental

In Fig. 3 and Fig. 4 are shown the schemes of synthesis of all new conjugates.

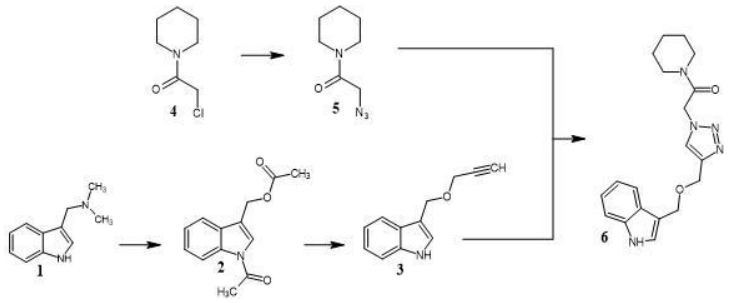

Fig. 3. The synthesis scheme of the compound 6

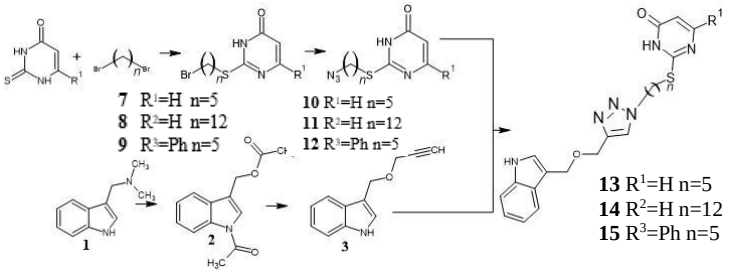

Fig. 4. The synthesis scheme of the compounds 13-15

3-Propargyloxymethylindole (3) was obtained according to [17].
2-Azido-1-(piperidin-1-yl)ethan-1-one (5) was obtained according to [18].

Synthesis of compound 6

2-Azido-1-(piperidin-1-yl)ethan-1-one (0,5 mmol) was dissolved in *tert*-Butyl alcohol (1mL) by mixing. 3-propargyloxymethylindole (0.5 mmol) was dissolved in *tert*-Butyl alcohol (2,5 mL) and (0,5 mL) methanol. Both aqueous solutions were mixed together and stirred at room temperature on a magnetic stirrer. $CuSO_4 \cdot 5H_2O$ (5 mg, catalytic amount) and sodium ascorbate (13 mg, catalytic amount) dissolved in 1 mL distilled water was added. Four catalyst portions were added until the aqueous layer of reaction mixture turned bluish-green. The reaction was monitored by TLC (PhMe: EtOAc 1:1). The reaction mixture was extracted with ethyl acetate (3 x 10 mL). The organic layer was washed with distilled water (30 mL) and brine (30 mL). Then it was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. Orange-brownish oil was obtained.

General procedure for the preparation of compounds 7-9

Thiouracil (2 mmol for compounds 7,8) and 6-Phenyl-2-thiouracil (2 mmol for compound 9) were dissolved in 0,1 M methanolic solution of NaOH. 1,5-dibromide (6 mmol) for compounds 7,9 and 1,12-dibromide (6 mmol) for compound 8 was added to the reaction mixture. The colorless solution

was stirred on a magnetic stirrer at room temperature for four days. The reaction was monitored by TLC (PE: EtOAc 3:7). After this time mixture was white and was acidified with dilute hydrochloric acid (~1 M) to about 3 pH. After concentration under reduced pressure and overnight in the refrigerator, a precipitate formed. The crude product was filtered off and purified over column chromatography using $CHCl_3$:EtOAc 5:1 as an eluent. The precipitate was dried at room temperature.

General procedure for the preparation of compounds 10-12

2,5-bromopetylthiouracil (0,58 mmol for compound 10), 2,12-bromododecylthiouracil (1 mmol for compound 11), 2,5-bromopetylthio-6-phenyluracil (1,15 mmol for compound 12) were dissolved in DMF (2 mL). Sodium azide was dissolved in distilled water (2 mL). Both substrates were mixed in a ratio of 1:5. Both solutions were mixed together. The reaction mixture was stirred for 36 hours on a magnetic stirrer and heated for about 8 hours with a water bath (65^{o}C). The reaction was monitored by TLC (PE: EtOAc 3:7). After this time, distilled water (5 mL) was added. The reaction mixture was extracted with diethyl ether (3 x 10 mL). The organic layer was washed with distilled water (30 mL) and brine (30 mL). The solution was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. A white precipitate was obtained.

General procedure for the preparation of compounds 13-15

2,5-azidopetylthiouracil (0,44 mmol for compound 13), 2,12-azidododecylthiouracil (0,27 mmol for compound 14), and 2,5-azidopetylthio-6-phenyluracil (0,32 mmol for compound 15) were mixed with 3-propargyloxymethylindole (0,44 mmol for compound 13, 0,27 mmol for compound 14 and 0,32 mmol for compound 15) and dissolved in DMSO (5 mL). The reaction mixture was stirred on a magnetic stirrer at room temperature. $CuSO_4 \cdot 5H_2O$ (5 mg, catalytic amount) and sodium ascorbate (13 mg, catalytic amount) dissolved in 1 mL distilled water was added. Catalyst portions were added consistently until the aqueous layer of reaction mixture turned bluish-green. The reaction was monitored by TLC (PhMe: EtOAc 1:1). Then distilled water was added (5 mL), and the reaction mixture was extracted with chloroform. The organic layer was washed with distilled water (30 mL) and brine (30 mL). The colution was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. A greenish oil was obtained. The crude product was purified over a chromatography column using gradient elution, starting from eluent chloroform/methanol 10:1 and finishing on chloroform/methanol 10:1 for compound 13. In a case of compound 14, starting eluent was chloroform/ethyl acetate 5:1, and the final eluent was ethyl acetate. Compound 15 was stared with chloroform/ethyl acetate 10:1 as an eluent and ended up with ethyl acetate. The thick, brownish oils were obtained.

Results and discussion

The structures of the newly obtained compounds were confirmed by spectroscopic methods (FT-IR spectroscopy ^{1}H NMR, ^{13}C NMR, and mass spectrometry – EI-MS and ESI-MS). The most characteristics bands for FT-IR spectroscopy are shown below (Fig. 3). In the representative IR spectrum of conjugate 13, we can see the characteristic band at 1665.20 cm^{-1} which is related to the carbon-oxygen bond from the thiouracil molecule. Moreover, we can see the band with the maximum at 3409.71 cm^{-1} corresponding to the carbon-hydrogen bond from the indole. A small band of about

3050 cm^{-1}, which is not stated, is related to the carbon-hydrogen bond from the triazole ring. We can also see the bonds at 2916.63 cm^{-1} and 2849.50 cm^{-1}, characteristic of carbon-hydrogen bonds from an aliphatic chain.

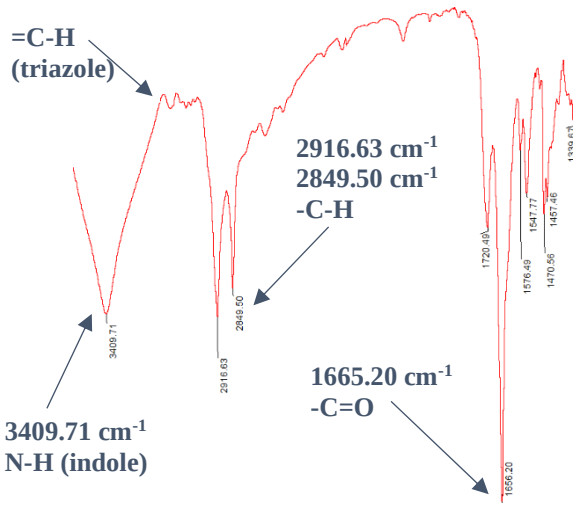

Fig. 5. FT-IR spectrum of the compound 13

Nuclear Magnetic Resonance also allows confirmation structures of new, obtained derivatives. The ^{1}H NMR spectra of all new derivatives (Fig. 4 and 5) show characteristic signals from 8.59 ppm to 6.17 ppm, corresponding to an indole moiety and hydrogen atoms from the triazole ring. For compound 15 in this range also occur protons from the benzene ring. We can see signals from the ether group in the 5.11 – 4.69 ppm range for the all compounds. The singlet at 3.9 ppm corresponds to an alpha proton of compound **6**. At the lower chemical shift values, from 3.53 ppm to 1.26 ppm, signals from protons in the piperidine ring are observed (compound **6**). Signals diagnostic for protons from methylene groups from an aliphatic chain for the compounds **13-15** appear from 3.14 to 1.26 ppm.

Regarding ^{13}C NMR spectrum, the number of signals corresponds to the number of carbon atoms in the molecule. Signals about 164 ppm (Fig. 5) are characteristic of a carboxyl group of compound 14. In general, spectra for all newly obtained derivatives show characteristic signals from 154.82 ppm to 110.86 ppm assigned to carbon atoms from the indole moiety, thiouracil, and triazole rings. Signals at the lower chemical shift values, 64.43-25.33 ppm range, belong to aliphatic chain carbon atoms.

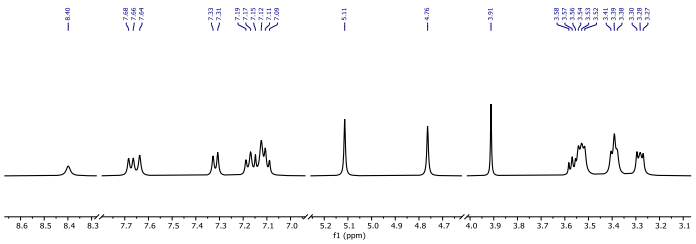

Fig. 6. ^{1}H NMR spectrum of the compound 6

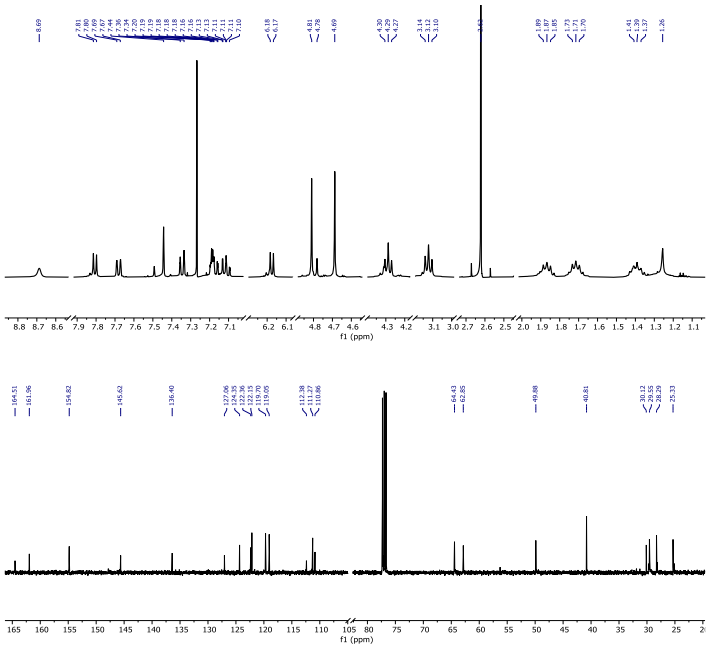

Fig. 7. ^{1}H NMR and ^{13}C NMR of the compound 14

For compounds 13 and 14, the ESI-MS spectra were recorded. In the case of derivative 13 (Fig. 6), the domination ion at m/z = 447 corresponds to the protonated ion $[424 + Na]^+$, where 424 refers to its molecular mass. The dominations ion peaks at m/z = 353 and m/z = 523 are assigned to the protonated ions $[353+Na]^+$ and $[500+23]^+$ for the compounds 6 and 15, respectively. However, compound 14 was characterized by EI-MS spectrometry, and molecular ion peak appeared at m/z = 522.

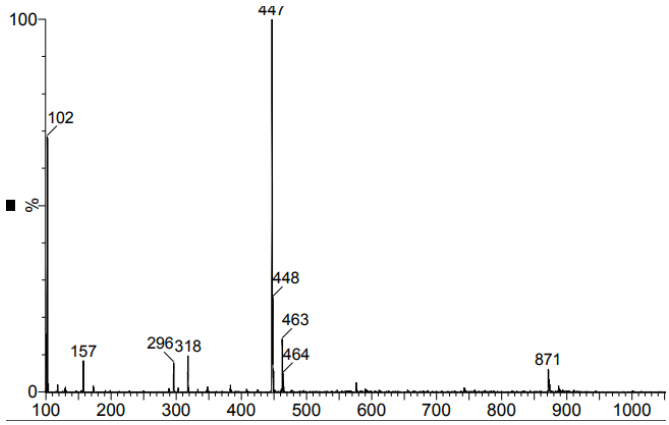

Fig. 8. ESI-MS spectrum of the compound 13

Theoretical calculations

SwissADME is a freely available web tool and one of the most recent sites by the Swiss Institute for Bioinformatics. Drug development concerns the assessment of absorption, distribution, metabolism, and excretion – in short, ADME – especially in the early stages of the discovery. Thus, this program helps verify if new compounds can be concerned as potential drugs.

Moreover, this program shows if the compound fulfills the Lipinski rule of 5, which evaluates the drug-likeness of chemical compounds. Lipinski's rule of 5 specifies the following criteria: no more than 5 hydrogen bond donors (HBD) and no more than 10 hydrogen bond acceptors (HBA). Also, the molecular mass has to be less than 500 daltons, a calculated octanol-water partition coefficient (log P) cannot exceed 5, and the polar surface area cannot exceed 140 A^2 (TPSA) [19, 20].

All new, obtained derivatives (6, 13-15) were examined using SwissADME. The results are shown in the table below (Tab. 1).

Tab. 1. The criteria of the Lipinski rule of 5 of derivatives 6, 13-15

Compound	MW	HBD	HBA	log P	TPSA
6	353.42	1	4	1.17	76.04
13	424.52	2	5	1.64	126.78
14	522.71	2	5	3.15	126.78
15	500.62	2	5	2.74	126.78

Source: own calculations

Data presented in the table above shows that two of the newly obtained compounds (6 and 13) fulfill Lipinski's rule of 5 criteria. The other two (14 and 15) show one violation – their molecule weight is higher than 500 Da. Inferring from the data, compounds 6 and 13 can be considered potential pharmaceuticals.

Conclusions

Results indicate that click chemistry is very useful method for obtaining new indole derivatives. Spectroscopic analysis confirms the structures of all new conjugates. The theoretical calculations show that two of the obtained compounds could be considered potential pharmaceuticals.

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VII edition

June 03, 2023

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IMPORTANCE OF PANORAMIC X-RAY IN THE MAXILLOFACIAL REGION

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Abstract:

Panoramic x-ray is an overview picture because it allows a visual of all teeth as well as surrounding bone structures. In this article; we would like to present how important a routine x-ray is in catching a variety of asymptomatic diagnoses. This article is based on the results of examinations of patients who reported to the Clinic of Maxillofacial Surgery, UCK in Gdańsk. There were people aged 20-50 with male prevalence. Annually there are 300 people with this issue. The histopathological diagnoses were mostly Odontogenic Cysts or Odontogenic Keratocyst (OKC). As a matter of fact, maxillofacial radiological examinations are capable of detecting these changes at earlier stages resulting in less invasive surgical treatment. In return, we would receive faster healing and smaller loss of bone structure. A multicystic lesion can be treated microsurgically, as opposed to a more invasive surgical procedure.

Keywords:
Odontogenic Cysts, OKC, panoramic x-ray, maxillofacial surgery, oral health

Introduction

Panoramic radiography is a two-dimensional (2-D) dental x-ray examination that captures as we said before the entire mouth in a single image, including the teeth, upper and lower jaws, surrounding structures and tissues [1,12]. X-ray imaging helps doctors diagnose and treat medical conditions. It exposes you to a small dose of ionizing radiation to produce pictures of the inside of the body. X-rays are the oldest and most often used form of medical imaging [1]. A panoramic x-ray is a commonly performed examination by dentists and oral surgeons in everyday practice and is an important diagnostic tool. It covers a wider area than a conventional intraoral x-ray and, as a result, provides valuable information about the maxillary sinuses, tooth positioning and other bone abnormalities. This examination is also used to plan treatment for full and partial dentures, braces, extractions and implants [1]. This form of imaging can also reveal dental and medical anomalies such as: advanced periodontal disorder, tumor and oral cancer, temporomandibular joint or TMJ disorders, impacted teeth including wisdom teeth, sinusitis, cysts in the bone.

Pathological lesions

Odontogenic cysts are the most common osteolytic lesions (90% to 97% of reported cysts) in the oral region. Its growth is slow, formed from remnants of odontogenic epithelium of Malassez [9]. As we said before, they are mostly identified on routine examinations with head and neck imaging such as orthopantomograms and computed tomography (CT). In which case they can be differentiated from inflammatory odontogenic cysts (periapical cyst, residual cyst, paradental cyst) [2, 3, 9], development odontogenic cysts (dentigerous cyst, gingival cyst, orthokeratinizing odontogenic cyst, eruption cyst [11], lateral periodontal cyst [4], glandular cyst, odontogenic keratocyst (OKC)) [2, 9]. Inflammatory odontogenic cysts and odontogenic keratocysts (OKC) are among the most common lesions diagnosed in relation to articles and patients from the Clinic of Maxillofacial Surgery, UCK in Gdańsk [5].

Inflammatory odontogenic cysts

Inflammatory odontogenic cysts are benign, osteolytic, asymptomatic lesions however, left untreated, can spread and affect surrounding bone and tissue [9]. They are classified into periapical or lateral radicular cyst, residual cyst and paradental cyst, which need a source of infection to proliferate [12]. We also must remember that inflammatory odontogenic cysts look similar to periapical granuloma, periapical scar, early stages of periapical cemento-osseous dysplasia, lateral periodontal cyst, glandular odontogenic keratocyst, unicystic ameloblastoma, periapical cyst, residual cyst, lateral radicular cyst [9].

Fig. 1. Patient female, age 42, inflammatory odontogenic cysts
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

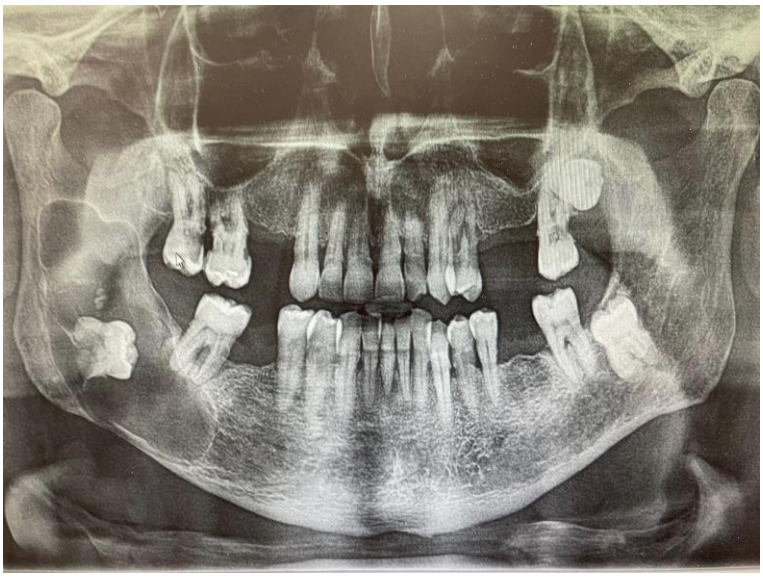

Fig. 2. Patient male, age 65, inflammatory odontogenic cysts
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

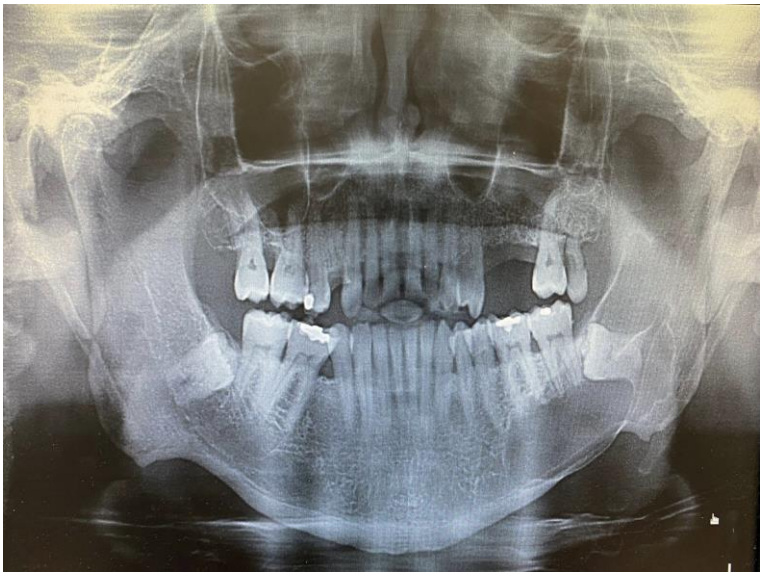

Fig. 3. Patient male, age 41, inflammatory odontogenic cysts
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

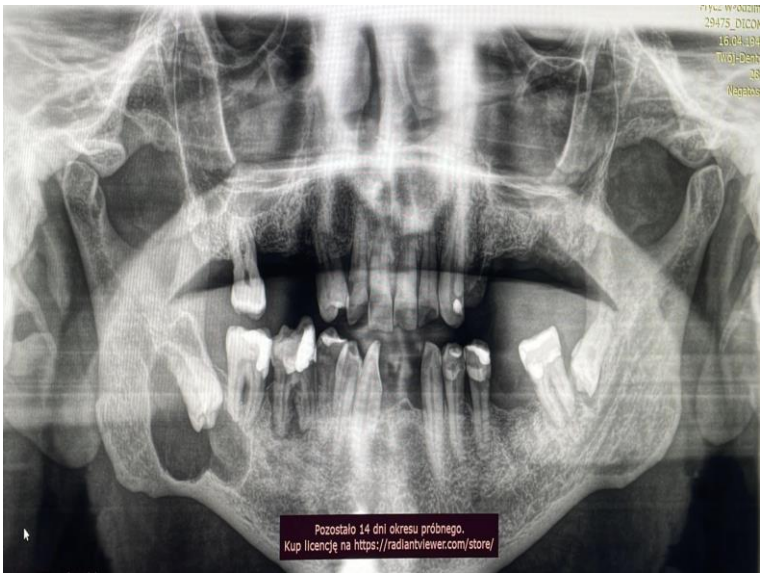

Fig. 4. Patient, male age 76, inflammatory odontogenic cysts
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

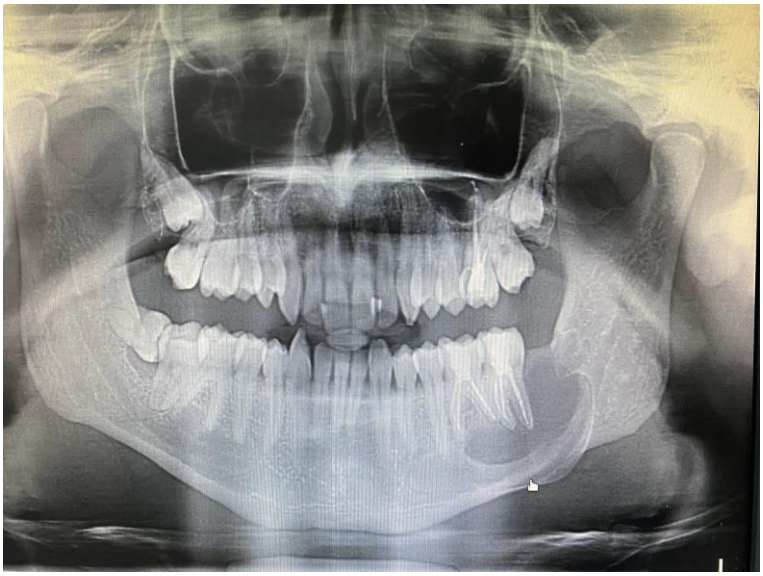

Fig. 5. Patient, male age 27, inflammatory odontogenic cysts
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Odontogenic Keratocyst (OKC)

Odontogenic Keratocyst is an expansional type of cyst of epithelial origin. First described by Philipsen in 1956. Since then, this lesion has been of particular interest due to its high recurrence rate and aggressive nature [10]. The prevalence of OKC (also known as KCOT) ranges from 3% to 11% of odontogenic tumors. It has an increased incidence in men usually within the second/third decade of life. The most popular area affected in the posterior part of the mandible [6, 10, 13]. When diagnosing it is important to remember odontogenic keratocyst (OKC) look similar to dentigerous cyst, ortho-keratinizing odontogenic cyst and even ameloblastoma due to their aggressive nature [10].

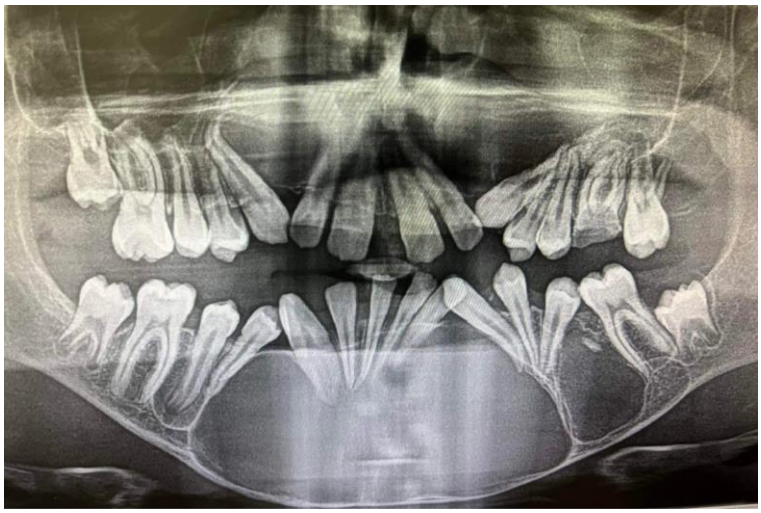

Fig. 6. Patient male, age 14, odontogenic keratocyst (OKC)
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Fig. 7. Patient female, age 15, odontogenic keratocyst (OKC)
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Treatment

There are a range of treatment possibilities. In most cases when caught early, a periapical cyst, which presents as a small circular lesion around the apex of a tooth, can be treated by way of endodontics, known more commonly today as a root canal [9]. Some cases where root canal treatment is not advised or unsuccessful, the only form of treatment is removal of the given tooth. Few periapical cysts linger and form a residual cyst post extraction. In this case, enucleation of the lesion is required. Treatment is often varied depending on the size of the lesion as well as location. Referring back to when we spoke of treating cysts of the first and second molars, removing the cyst alone would suffice [9]. However, when treating the third molar, the entirety of the tooth and cyst are excised [7, 15]. In this case of treatment, constructive techniques of the region affected by the bone defect should be considered to minimize further abnormalities. Furthermore, odontogenic keratocysts, when found in later stages, may require marsupialization or resection as opposed to earlier stage OKC's which are manageable by way of enucleation and possible peripheral ostectomy to achieve healthy bony

margins. [9] Most importantly, following up after treatment of such lesions with pre as well as post procedure x-ray imaging is vital. [8, 14].

Conclusion

Most of the odontogenic cysts have an excellent prognosis with no reports of recurrence even when the development is notable in size (as we could see on previous photos). The key is to remove the entire area of affected tissue and bone structure to allow for adequate bone recovery and advantageous results. Treatment options should include conservative management, such as extracting impacted teeth with biopsy to rule out other lesions. It is important to note that long-term developing maxillary bone cysts can become infected resulting in bone inflammation. Incidentally, neoplastic transformation of the lining epithelium from such cysts may also occur. When a developing maxillary bone cyst occurs and grows within the alveolar processes can lead to a displacement and/or loosening of teeth resulting ultimately in malocclusion. Vital for recovery is the patient's involvement in post procedure care; this involves good oral hygiene, routine examinations along with follow-up x-ray imaging. Every patient, including younger patients should have routine radiological examinations to allow for early detection of pathological lesions.

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ARTERIOVENOUS MALFORMATION OF THE ORAL CAVITY INCLUDING DESTRUCTION OF THE BODY AND BRANCH OF THE MANDIBLE

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Abstract:

A hemangioma is a tumor of vascular origin. One third of newborn babies are burdened with hemangiomas, but only about 75% of these changes are found at birth or in the first months of a child's life. Hemangiomas are twice as common in girls. In 70- 90% of cases, they are localized in the skin, less often on the mucous membranes, only occasionally in internal organs and the skeleton. In our paper, we present a description of an extremely rare arteriovenous malformation of the floor of the oral cavity of such size, involving the destruction of the body and branch of the mandible on the right side, as a result of which a pseudoaneurysm lesion was formed in the submental area. The patient first came to the Clinic of Maxillofacial Surgery of the University Clinical Center of the Medical University of Gdańsk 14 years ago. In the meantime, she underwent numerous malformation embolization procedures. Acrylic glue, spirals, ethyl alcohol with a concentration of 96% were used.

Keywords:
vascular malformation, magnetic resonance, arteriography, computer tomography, lower jaw

Introduction

The basic proliferative element in an hemangioma is a budding endothelial cell, resulting in a primitive vascular lumen. Hemangioma (haemangioma) is the most common, whereas lymphatic (lymphangioma) or mixed lymphatic and blood (lymphohemangioma). Malignant hemangioma (angiosarcoma) is very rare.

Hemangiomas in the face, neck and oral cavity, unlike those located in other parts of the body, are characterized by a separate symptomatology and pathomechanism and cause aesthetic and functional multi-organ disorders. In their advanced form, they cause significant distortions, and depending on their location, they lead to visual, speech, swallowing and breathing disorders. Developing in the vicinity of the bones or intraosseously, they distort the bone skeleton of the face, leading to disturbances in the eruption of teeth or their significant displacement. The rich blood supply

in this area causes rapid growth of angiomas and a relatively high risk of bleeding and haemorrhages [1].

Case presentation

In 2009, a 14-year-old patient with her mother came to the Oral and Maxillofacial Surgery Clinic of the University Clinical Center of the Medical University of Gdańsk.
Medical history: the patient suffers from Hashimoto's - takes Letrox and has no allergies. The patient was referred from a dentist because of a lesion in the right submandibular area that had persisted for 6 months. Clinically: painless to palpation, a soft lesion measuring 2.5 x 2 cm. There was no skin discoloration. The patient reported a steady growth of the lesion. Intraorally visible shallowing of the vestibule in the range of teeth 44- 47. From radiological examination, thinning of the bone structure was visible in the area of tooth 46. An extraction was performed, followed by intense bleeding [2, 3]. The tooth was replanted. Direct pressure on the area was placed with gauze. An attempt was made to collect a specimen for histopathological examination. The procedure was abandoned due to intense bleeding. A hemangioma lesion was found.

The patient did not report to the Oral and Maxillofacial Surgery Clinic of the University Clinical Center in Gdańsk for another year.

In 2010, a double angiography was performed with embolization of the tributaries from the maxillary artery. The vessels were sealed with acrylic glue. The procedures were performed at the Clinical Hospital in Warsaw.

Magnetic resonance imaging was performed in 2011.

In the description of the examination: the lesion involves the right hyoid- glossus, mylohyoid and partly the anterior belly of the digastric muscle. Anteriorly, it reaches the sublingual gland, downwards it descends below the lower edge of the mandible and reaches the anterior outline of the submandibular gland. The area occupied by pathological vessels measures 28 x 37 x 35 mm.

Magnetic resonance imaging was performed in 2014. In the description of the examination: on the right side, pathologically dilated vessels are visible in the area of the parotid gland, the masseter muscle, in the enlarged submandibular gland, in the branch and body of the mandible and in the periosteum, in the vestibule of the oral cavity, where it forms a conglomerate of about 33 x 9 mm near the mandible, and in the bottom oral cavity with the involvement of the hyoid-lingual and mandibular-hyoid muscles. In the floor of the oral cavity, dilated vessels are visible on both sides. The mandibular body and branch on the right side thickened to about 13 mm, about 38 mm long (correct image of the mandibular body from tooth 5), with an abnormal signal with a thickened cortical layer.

In 2014, embolization of the branches of the facial artery using 3 spirals and embolization of the branches coming from the right lingual artery.

Fig. 1. Magnetic resonance, 07.2011
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

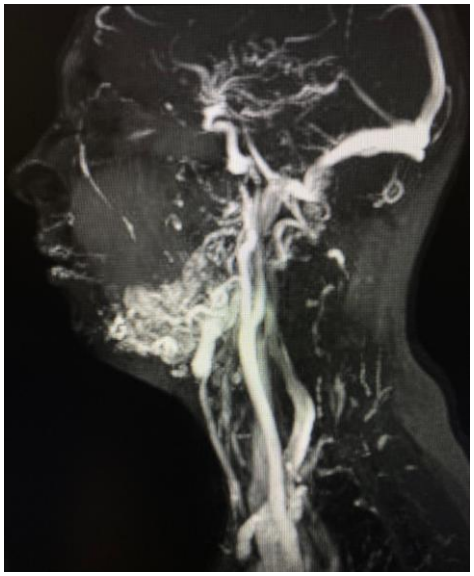

Fig. 2. Arteriography, 03.2014
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Magnetic resonance imaging was performed in 2015. In the description of the study: compared to the 2014 study, the extent of the vascular malformation on the right side supplied from the branches of the right external carotid artery is comparable. Wide veins surround the right submandibular gland, visible in the parapharyngeal space. The right retromandibular vein is also wider.

In 2015, embolization of the right external carotid artery.

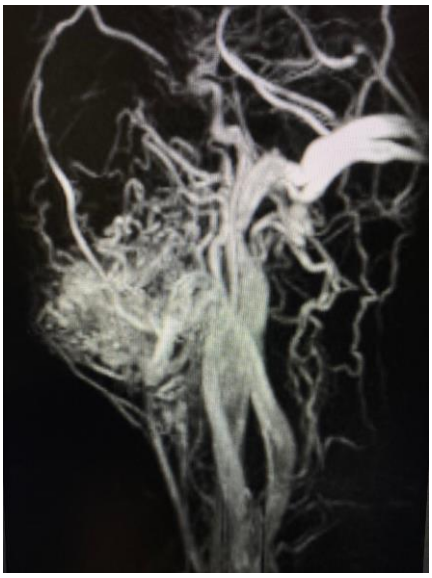

Fig. 3. Magnetic resonance, 09.2015
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

In 2016, reembolization and implantation of 4 spirals into the branch of the maxillary artery. In 2017, the next stage of closing the branches from the facial artery with the help of 3 spirals. The above procedures were performed in the Clinical Hospital in Poznań.

Fig. 4. Panoramic radiography, 03.2020
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Computed tomography was performed in 2020. The examination shows a hypodense focus (probably filled with fluid) between the roots of tooth 46 with a disruption of the cortex of the mandibular body at the mesial root from the vestibular side. The lesion in the mandible measures 6 x 10 mm.

In 2021, the Patient reported to the Oral and Maxillofacial Surgery Clinic of the University Clinical Center in Gdańsk due to an injury to tooth 46, 3 days earlier. Since then, persistent bleeding from the tooth pocket, mobile mesial wall of the tooth. The tooth was treated by a dentist.

In January 2023, at the University Clinical Center in Gdańsk, an arteriography of the superior thyroid, lingual and facial arteries, the final section of the ECA on the right side was performed, followed by embolization. The next stage of the procedure is planned for June 2023.

Fig. 5. Computer tomography, 09.2020
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

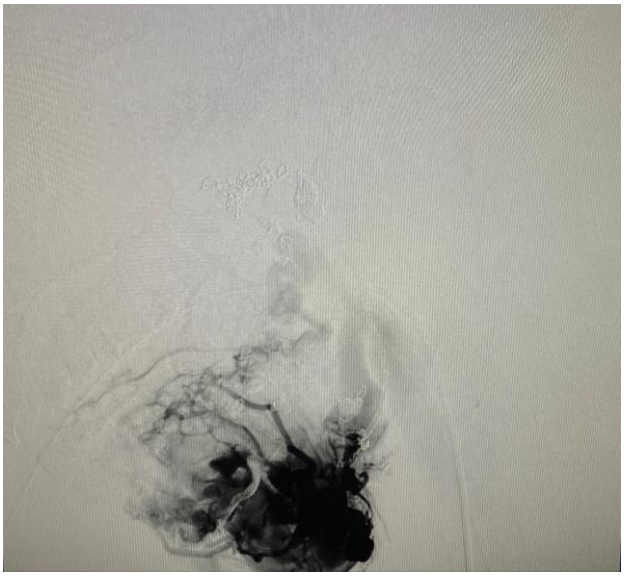

Fig. 6. Arteriography, 01.2023
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

In May 2023, there was a sudden progression of the change, which is why the Patient reported to the Maxillofacial Surgery Clinic. Clinically, apart from edema in the right submandibular area, there was also an exaggeration in the submental area. It was decided to hospitalize the patient.

Fig. 7. Hospitalisation, 05.2023
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Fig. 8. Hospitalisation, 05.2023
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Fig. 9. Hospitalisation, 05.2023
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Ultrasound of the chin area was performed: a centrally visible lesion of 23 x 37 mm in the nature of an aneurysm with the "Pepsi sign" visible. The examination was extended with CT angiography, which showed: an extensive facial AV malformation supplied from both external carotid arteries with a nidus in the submental area of 33 x 27 mm [4]. Vessels enter the body of the mandible on the right side, causing thinning of the bone structure.

It was decided to perform a tracheotomy and then partial embolization of the outflow malformation and the nidus of the lesion in the body of the mandible on the right side with 96% ethyl alcohol (60 ml).

The next stage is planned for June 2023, where several percutaneous punctures of the enlarged outflow part of the malformation were performed with its partial embolization using 95% ethyl alcohol (60 ml).

Control arteriography showed no significant reduction of venous outflows.

Another treatment is scheduled for July 2023.

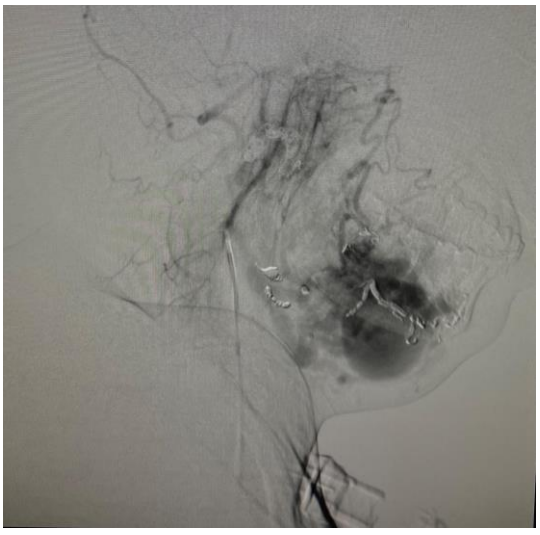

Fig. 10. Arteriography, 06.2023
Source: Department of Maxillofacial Surgery, Medical University of Gdansk

Treatment

Treatment of hemangiomas is often very difficult, hence the variety of methods used in the treatment of these tumors. We can distinguish conservative, destructive, surgical and combined methods. The choice of method depends on the form, location and size of the hemangioma [5].

Conservative treatment includes pharmacological treatment (intratumoral administration of steroid hormones) and selective embolization [6, 7]. Destructive methods include obliteration, electrodessication, cryotherapy and laser therapy. Surgical treatment includes intratumoral puncture, complete excision, ligation of the arteries [1, 8].

The patient underwent numerous malformation embolization procedures in various clinics, e.g. Gdansk, Poznan, Warsaw. Acrylic glue, spirals, ethyl alcohol with a concentration of 96% were used [9].

Conclusions

Hemangiomas, although they are classified as benign tumors, can even be life-threatening (massive hemorrhages). The tactics of treatment must be determined individually, taking into account both the selection of the right time and the method of treatment, which is not always easy. The planned treatment must take into account the risk of local general complications, sometimes very dangerous, as well as the final result of treatment, both functional and aesthetic [10].

Despite the progress in medicine, the treatment of hemangiomas is still difficult and it seems that the best results can be obtained by combining various therapeutic methods adapted to the form, location, extent of the tumor and the age of the patient [1].

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WORK RELATED TO THE DEVELOPMENT OF A NEXT-GENERATION POWER BANK

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Abstract:

The demand for power banks has significantly increased in the past decade with the proliferation of mobile devices such as smartphones, tablets, and laptops. Depending on the customer's requirements and the intended applications for which the devices are intended, power banks vary in terms of capacity, charging standard support, output power, and connectors. This paper presents experimental development work related to designing a portable power bank with high capacity and high power while maintaining small size. The design process involved identifying user requirements and necessary technical parameters such as capacity, charging current, and build quality. The designed power bank features a capacity of 26800mAh and four USB ports with a combined power of 128 W. The device underwent a series of experiments to test its performance and efficiency. The results of the research and development work showed that the proposed solution meets the technical requirements and is capable of providing long-lasting power to electronic devices. The power bank is portable and can be carried on board an airplane, allowing for charging of all USB-compatible devices, including laptops.

Keywords:
power bank, development, quality, battery, Li-ion

The Power Bank Market

The power bank market is highly diverse in terms of capacity, power, price, and quality. Currently, there are numerous brands offering portable power banks, including both electronics manufacturers and companies specializing in phone and tablet accessories. The majority of power bank manufacturers originate from China and produce their products there.

This market exhibits steady growth, driven by the increasing popularity of mobile devices and the corresponding demand for portable power sources. According to a report by Report Ocean, The global power bank market size was US$ 18.1 billion in 2021. The global power bank market is forecast to reach US$ 29.34 billion by 2030 by growing at a compound annual growth rate (CAGR) of 5.9% during the forecast period from 2022 to 2030 [1].

In recent years, power banks equipped with fast charging technology have emerged in the market, accelerating the charging process of mobile devices. With technological advancements,

manufacturers are increasingly incorporating USB-C ports with Power Delivery protocol, enabling rapid charging of larger devices such as laptops.

The power bank market is saturated with cheap and low-quality products, which can pose safety risks to users. It is therefore recommended to purchase devices from reputable manufacturers and avoid suspiciously cheap offers that promise capacities that are physically impossible to achieve with currently available technologies.

What do consumers expect from power banks

The key feature that customers pay attention to is the battery capacity. The larger the capacity, the more times the device can be charged before the power bank needs to be recharged. Many people also look for devices with compact sizes that are easy to carry while traveling, thus ensuring peace of mind and eliminating the need to conserve battery power in their mobile devices.

The second aspect is the power output of the device. For most users, a device capable of charging a phone is sufficient, hence the abundance of affordable solutions providing a maximum of 10 W of power. However, the current standard is becoming a minimum of 18 W of power, allowing for the use of quick charge profiles such as 9 V/2A. On the other hand, users who want to charge a laptop require a power bank with a minimum power output of 45 W.

Customers also pay attention to the reliability, durability, and longevity of power banks. They want their devices to be resistant to mechanical damage and equipped with electronic safeguards that protect both the power bank and the devices connected to it.

Other features that customers value include ease of use, charging time, and the number of USB ports. Many people look for devices with one or multiple ports that allow charging multiple devices simultaneously [2].

How does the development of the mobile device market and their energy demand look like

The market for mobile devices such as smartphones, tablets, laptops, and smartwatches is evolving rapidly. Over the past decade, there has been a significant increase in the popularity of these devices, and thanks to technological advancements, they have become more advanced and versatile. Along with this rise in popularity, the energy demand required to power these devices has also significantly increased [3-5].

The energy demand of mobile devices is a variable factor and depends on various factors such as screen size, processor power, type and number of applications used, as well as usage patterns and users themselves. Consequently, mobile device manufacturers face the challenge of ensuring battery performance and durability to meet the growing demands of users.

With the increasing energy demand, there is a growing need to charge mobile devices, which becomes a greater challenge for users. In the case of smartphones and tablets, charging can be done through USB ports, wall chargers, car chargers, or wireless charging. For larger devices like laptops, the use of larger and more advanced chargers with USB-C ports and Power Delivery protocol is necessary.

How is the USB-C charging standard developing

The USB-C charging standard is continuously evolving and improving. Below are some of the key changes and enhancements:

USB Power Delivery (USB PD) - This technology allows for the transmission of higher amounts of power through the USB-C port. USB PD enables charging of devices with higher power requirements, such as laptops, and even powering small electrical devices like flashlights.

Increasing charging power - The original USB-C standard allowed for power delivery up to 100 W, but newer standards now support charging of devices with higher power requirements, even up to 240 W. This allows for the replacement of outdated barrel connectors with the versatile USB-C port [6].

What are the fast charging standards for mobile devices

Modern mobile devices such as smartphones and tablets are typically equipped with lithium-ion batteries. Fast charging standards for mobile devices define how these batteries can be charged more efficiently than traditional charging through a wall socket.

Quick Charge (QC) - A standard developed by Qualcomm. It allows for charging compatible devices up to 50% in 15 minutes and full charging within 1 hour [7].

USB Power Delivery (USB PD) - A standard developed by the USB Implementers Forum. It enables charging of mobile devices using a USB-C cable, supporting power delivery of up to 240 W in the revision 3.1 [8]. In comparison, standard charging through a USB-A port delivers 5W. The higher power in this standard is achieved through two factors:

Increasing the voltage from the standard 5 V to, depending on the profile, 9 V, 12 V, 15 V, 20 V, 28 V, 36 V, or 48 V.

Increasing the charging current to a maximum of 5 A. These factors allow us to achieve the mentioned 240 W as shown in formula (1.1.).

(1.1.)

$$P = U * I \tag{1}$$

$$P = 48 * 5 = 240\ [W] \tag{2}$$

where:

P – Power [W];

U – Voltage [V];

I – Current [A].

Super VOOC - A standard developed by Oppo. It enables charging battery in just 35 minutes from 0% to 100%. The standard focuses on delivering higher current at the standard voltage of 5 V. For example, VOOC 3.0 offers 5 V at 4 A [9].

Dash Charge - A standard developed by OnePlus. It allows for more efficient charging of OnePlus devices by lowering the temperature at which the device heats up during charging. This was achieved by transferring voltage and current control to the charger. Lowering the cell temperature allows for increased charging power, which is utilized by this standard [10].

Adaptive Fast Charging (AFC) - A standard developed by Samsung. It enables more efficient charging for Samsung devices compared to standard charging [11].
It's worth noting that not all mobile devices support all fast charging standards [12].

What standards must power banks meet

Power banks are portable devices used to charge other mobile devices such as smartphones, tablets, or laptops. In order to ensure safe and efficient charging, they should comply with specific standards and possess appropriate certifications.

As a standard practice for devices introduced into the European market, power banks require the CE marking [13].

To affix this marking, the manufacturer must meet the requirements set by European directives:

Battery Directive 2006/66/EC establishes rules for the placing on the market and management of batteries and accumulators to protect the environment and public health [14].

EMC Directive 2014/30/EU establishes principles for the electromagnetic compatibility of electrical and electronic devices to ensure their proper operation and minimize electromagnetic interference [15, 16].

RoHS Directive 2011/65/EU restricts the use of certain hazardous substances, such as lead and cadmium, in electrical and electronic products to protect the environment and public health [17].

WEEE Directive 2012/19/EU (Waste Electrical and Electronic Equipment) establishes principles for the collection, processing, and recycling of electrical and electronic waste to protect the environment and promote sustainable waste management [18].

These directives imply the need to meet the requirements set by standards such as:

IEC 62133 - This standard specifies safety requirements for lithium-ion batteries, including power banks. It defines requirements regarding temperature, voltage, current flow, and other parameters [19].

CISPR 35:2016 - This standard pertains to electromagnetic field emissions from electrical and electronic devices [20].

In addition, to enable air transportation of batteries, compliance with the requirements related to the UN 38.3 standard is necessary.

The UN 38.3 standard defines requirements for the safe transportation of lithium-ion batteries, including durability tests, resistance to temperature and pressure changes, to ensure protection against the risks associated with transportation accidents.

Furthermore, the energy of a power bank must not exceed 100 Wh to be allowed on board an aircraft [21].

Research and Development (R&D) Work

The primary objective was to construct a high-power and high-capacity power bank. The target power value for a single USB-C port was set at 65 W, allowing efficient charging of laptops. Additionally, the power bank was intended to enable charging multiple devices simultaneously, leading to the decision to incorporate two USB-C ports and two USB-A ports.

In the development phase, the initial iteration aimed to achieve a power output of approximately 45 W. To accomplish this, the Power Delivery charging standard with a 20 V 2.25 A profile was

utilized. Power Delivery was chosen due to its popularity and clear trend in mobile device charging technology.

Considering price, availability, and specifications, it was assumed that an optimal power supply would consist of a cell pack with a capacity of at least 20,000 mAh in a 3S2P configuration.

The objectives were based on the idea of allowing a laptop to be charged once. In mobile devices, the upper limit of accumulated energy is typically around 100 Wh. Therefore, the proposed 72 Wh pack, the relationship between voltage, energy and capacitance is shown in formula (1.2), would enable charging up to approximately 70% of laptops equipped with the highest energy. In standard laptops with battery energy ranging from 40 to 60 Wh, it would provide a single charge, while in ultrabooks with energy ranging from approximately 30 to 50 Wh, it could even allow for two charges. (1.2.)

$$E = (Q * U) / 1000 \tag{1}$$

$$E = (20000mAh * 3.6V) / 1000 = 72000\ [Wh] \tag{2}$$

where:

E – Energy [Wh];

Q – Capacity [mAh];

U – Voltage [V].

To carry out the device development work, an experimental method was employed. Taking into account the issues described above, an initial specification was developed with the following parameters:

Maximum output power: 45 W.

2 USB-A ports with support for Quick Charge 2.0/3.0 on all outputs.

USB-C port In/Out - Max input power: 45 W (2 x 1.5 A x 15 V), Quick Charge 2.0/3.0.

Capacity: 20,100 mAh.

Battery configuration: 3S2P (20,100 mAh).

Nominal voltage of a single cell: 3.63 V.

Charging voltage: 4.2 V (12.6 V for the 3S2P battery).

Charging current: 0.3 C / 975 mA (1950 mA for the 3S2P battery).

Maximum discharge current: 0.5 C / 1625 mA (3250 mA for the 3S2P battery).

Based on the above, it was decided to use the INR18650F1L LG cell for the initial battery packs.

Device Schematic

When the R&D work began, device was divided into according to (Fig. 1) and then began searching for and selecting solutions that would help us achieve specific functionalities. These blocks can be expanded as follows:

- BMS - Battery Management System - is a block responsible for monitoring the operation of cells and protecting them within the battery. A Battery Management System is any electronic system that manages the battery, for example, by protecting the battery from operating outside its safe operating area, monitoring its state, calculating secondary data, and reporting this data.

- MCU - microcontroller, its task is to manage the device's operation and communication between other blocks.
- DC-DC - this block is responsible for converting the input voltage to the appropriate output voltage, depending on the information from the controller.
- PD Controller - the system is responsible for communication with the connected device and appropriate driving of the converter.
- USB QC controller - similarly to the PD controller, it is responsible for driving the output voltage.
- USB-C block represents the connector of the same name, used for connecting the receiving device.
- USB-A block represents the connector of the same name, used for connecting the receiving device.

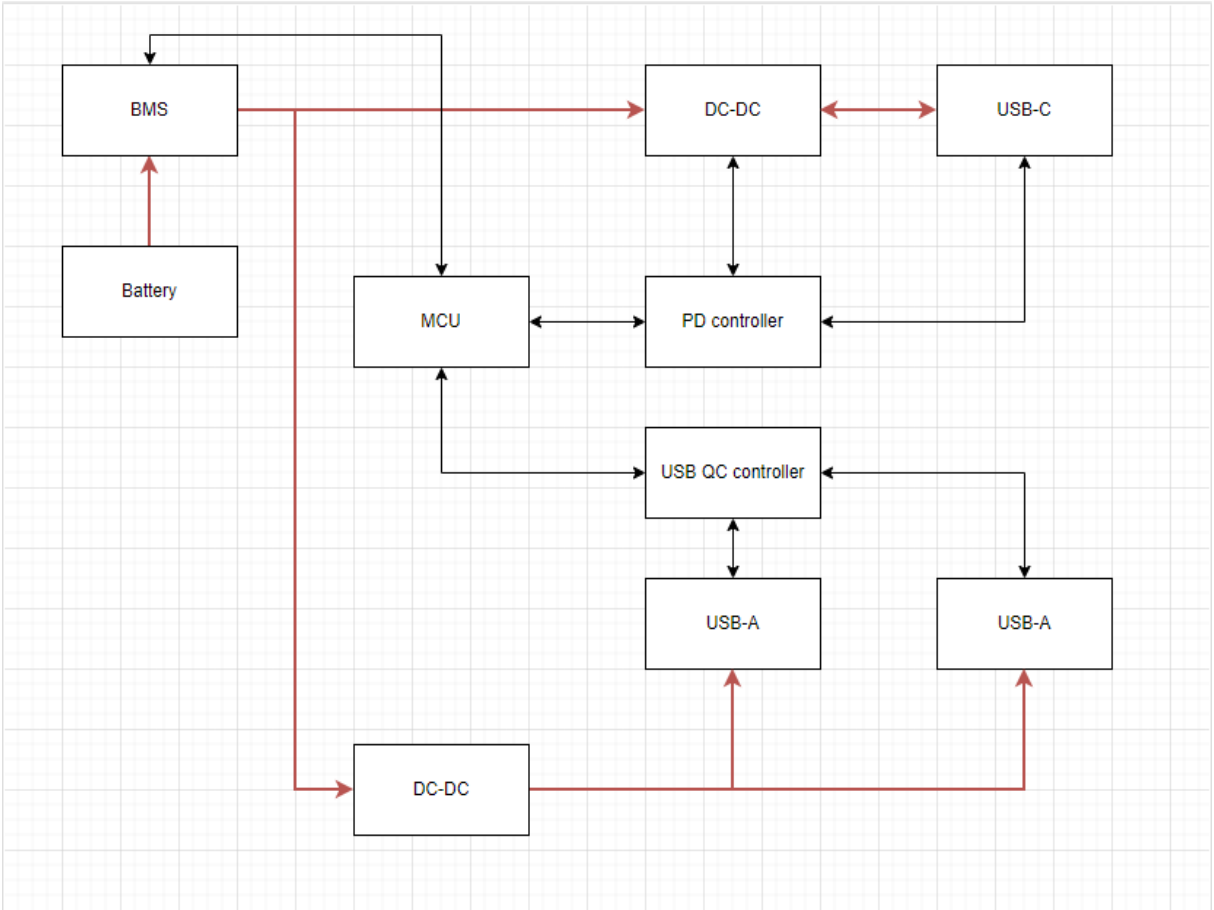

Fig. 1. Block diagram of the device

Charging and Discharging Circuit

The key elements in this device are the PD controller, converter, and battery. Therefore, team started selects appropriate solutions. The following components have been choose for this solution:

PD Controller IP2716 and STUSB1602.

Converters SC8815 and SC8802.

All selected solutions have successfully passed tests and demonstrated charging and discharging efficiency often exceeding 90%. Due to the varying number of profiles, poor documentation, and lack of technical support, it was decided to reject the IP2716 circuit. Among the remaining available solutions, the CYPD3171 in combination with SC8802 proved to be the best fit and worked well together, so the decision was made to focus only on the development of this branch. the designed solution is shown in (Fig. 2).

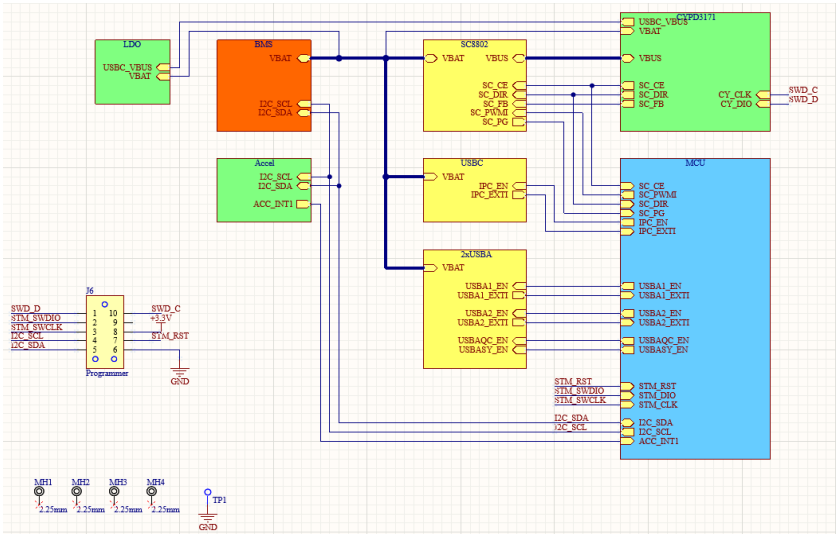

Fig. 2. Block diagram with electrical connections

At the stage of the project, noticed the components used in the device could operate with higher voltages. According to the initial configuration, the basic setup is 3S2P, which translates to a fully charged pack voltage of 12.6 V and a discharged voltage of 9 V. Increasing the voltage was achieved by adding one module in series, resulting in a 4S2P configuration and corresponding voltages of 16.8 V when fully charged and 12 V when discharged. The new solution is shown in (Fig. 3) higher voltage results in increased power at the same current. A sample built for testing purposes, discharged under full load, demonstrated improved efficiency and lower operating temperatures. This allowed for an increase in the overall power of the device.

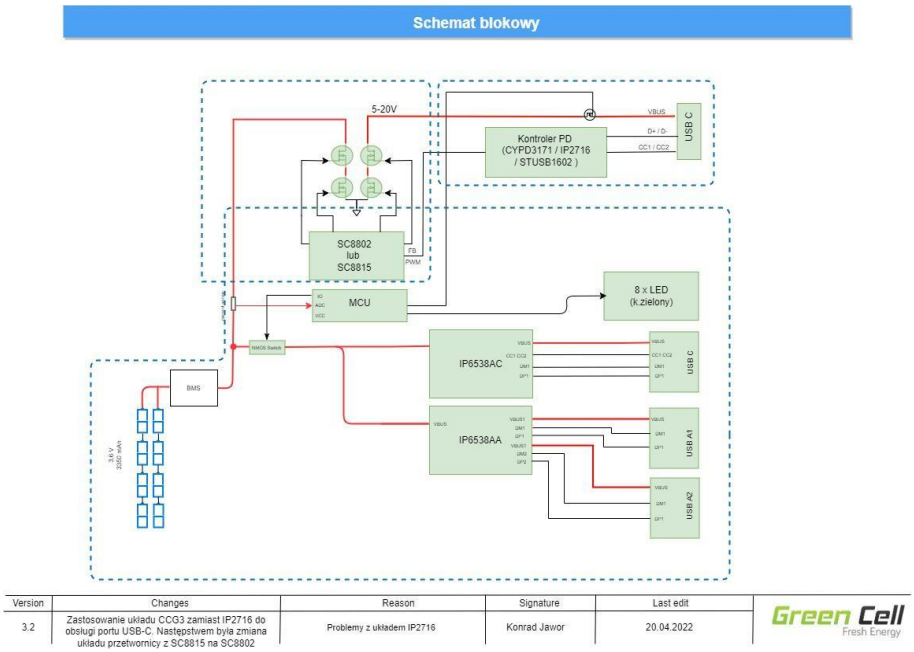

Fig. 3. Block diagram with assigned circuit solutions

Battery Pack

The operation of the entire device focuses on efficient and safe energy storage. Therefore, the selection and proper design of the cell pack are factors that directly impact the device's parameters, lifespan, safety, and reliability. To ensure that the choice is correct, carried out a series of tests aimed at simulating various operating conditions, shown in (Fig. 4). Tests included simulation of working temperatures, loads, and capacity degradation due to the number of cycles.

Fig. 4. Aging test

The test results in the form of capacitance decay curves are shown in (Fig. 5.)

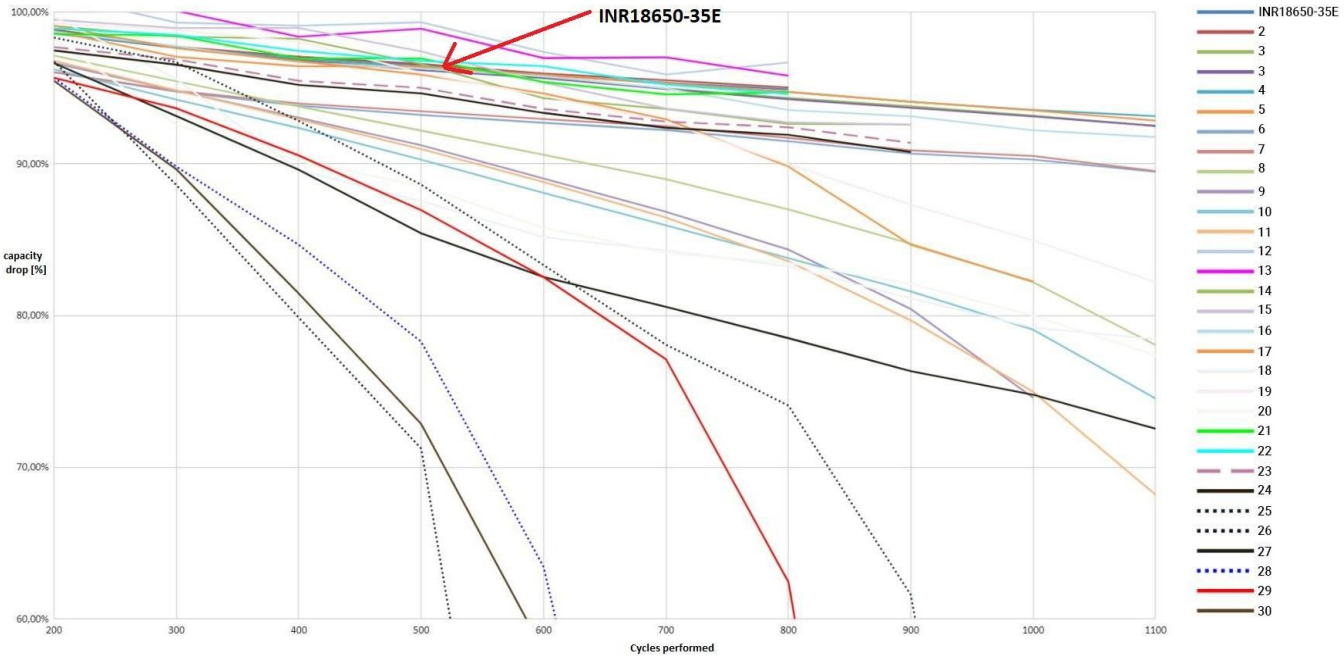

Fig. 5. Percentage decrease in capacitance due to the number of cycles performed

Based on tests and documentation, the Samsung INR18650-35E cell was selected. It showed very good consistent results, good price-to-quality ratio, and good availability. By conducting synthetic and nonsynthetic tests, research team obtained results that met our requirements and allowed us to propose the final specification, which is as follows:
Capacity: 26,800 mAh (3.6 V) 96.48 Wh.
Input:
USB-C1 Power Delivery 5 V⎓3 A / 9 V⎓3 A / 12 V⎓3 A / 15 V⎓3 A / 20 V⎓3 A (Max 60 W).
Output:
USB-C1 Power Delivery 5 V⎓3 A / 9 V⎓3 A / 12 V⎓3 A / 15 V⎓3 A / 18 V⎓3 A / 20 V⎓3.25 A (Max 65 W).
USB-C2 Power Delivery 5 V⎓3 A / 9 V⎓3 A / 12 V⎓2.25 A / PPS 3.3-11V⎓3 A (Max 27 W).
USB-A1 Ultra Charge 5 V⎓2.4 A / 9 V⎓2 A / 12 V⎓1.5 A (Max 18 W).
USB-A2 Ultra Charge 5 V⎓2.4 A / 9 V⎓2 A / 12 V⎓1.5 A (Max 18 W).

Compatibility

The ability to fast charge connected devices is one of the key factors determining the commercial success of such devices. To utilize such features, it is necessary to provide the appropriate communication protocol for device connection.

There are specialized circuits responsible for handling communication with the receiving device and negotiating charging profiles. In the project, the CYPD3171 circuit was used, which is a microcontroller integrated with a USB Type-C controller (USB-C) that supports Power Delivery (PD) standards. The circuit was chosen due to its significant reduction in the time required for device implementation and the reliability it demonstrated in tests.

The testing of this solution involved laboratory and user tests. The laboratory tests included reading the available list of charging profiles, triggering each profile individually, and subjecting the circuit to rated current load. Such a test allows us to conclusively determine not only the correctness of the controller's programming but also whether the converter's response is correct and whether the device is capable of delivering the power communicated in the profile.

The user tests involved practical tests where device samples were given to testers, whose task was to test the devices in various usage scenarios and with a wide range of different devices.

Construction

The design concept, battery pack size, PCBA, and regulatory requirements were guiding factors in the selection of materials and device construction.

The external casing is made of extruded and milled aluminum, which is then anodized. Aluminum provides rigidity, impact resistance, and efficient heat dissipation for the product. The anodized coating further protects the aluminum from corrosion and increases its resistance to damage and scratches. An additional advantage of the anodizing process is the ability to control the surface color. However, the color may have a certain tolerance range.

The remaining structural elements are made of UL94 V0 flame-retardant polycarbonate. Polycarbonate was chosen for its mechanical properties, particularly its impact resistance, which is crucial for the device's durability against falls.

The plastic construction was designed to prevent contact between the aluminum casing and the battery cells or current-carrying wires. Along the aluminum profile, there is a cutout where a transparent polycarbonate element is inserted to guide the light. The desired aesthetics of the emitted light were achieved by also using a second plastic element, this time made of frosted material, which is responsible for diffusing the light. This approach allows the LED strip to have an aesthetic and diffused appearance, without showing individual points of light intensity emitted by specific diodes. The initial prototypes were produced using SLA 3D printing. This allowed for the validation of device dimensions and component distribution. To verify the strength of the aluminum profile, a similar profile was notched and subjected to bending and drop tests. The results obtained were satisfactory, allowing for the refinement of 3D models for specific production processes and the creation of injection molds and an extruder for the aluminum profile.

Components from the injection molds and extruded aluminum were used for further product testing, such as drop tests of the final product. Ultimately, the entire construction underwent testing according to the UN38.3 standard, where the strength and reliability of the designed solution were confirmed.

During testing, overheating problem was diagnosed due to high power output of 128W. This problem was addressed by adding thermal pads that provide high thermal conductivity between the converters and the aluminum casing. During testing, the casing itself did not exceed temperature ranges specified by standards. However, as a safety measure, three overheating protection stages were added to the device, cutting off power from the USB ports to limit the device's power, with prioritization given to the USB-C port.

Wake-up Mechanism

Various solutions for waking up the device from sleep mode were tested. Typically, to wake up a power bank, it is needed to press a dedicated button. Among the possible alternative methods, two possible solutions have been selected: an accelerometer and a capacitive sensor. Since this component was not difficult to prototype and would be a particularly important element in actual use, immediately proceeded to testing with a group of several individuals. The test results indicated that the capacitive sensor was too susceptible to interference generated by the converters. Therefore, first solution was rejected during the testing phase due to the lack of a straightforward resolution in our case.

The performance of the accelerometer pleasantly surprised us as it was predictable and benefited from the hardware support of the BMA280 module's "double tap" feature. After a series of tests, the research team decided to use this solution in the final product.

Testing of the Finished Product

After completing the development work, it was time to conduct testing and verification of the finished product to determine if the desired result had been achieved. Ready device shown in (Fig. 6).

Fig. 6. Ready device
Source: [22]

The initial production samples already met all the parametric requirements, the test report is shown in (Tab. 1). T0 Samples demonstrate efficiencies exceeding 90% under full load. The product exhibited excellent compatibility and operational stability. No unexpected issues related to its functionality were observed.

Tab. 1. Summary of tests for PBGC04 T0 device sample

Parameter	Value
Dimensions	184,7 x 80,15 x 22,2 (mm)
Weight	590,3g (prototyp)
Charging time: 0-100%	110min 24C dg.
Max. charging power	60W
Max. discharging power (on a single port)	65W
Total discharging power (all ports)	128W
Input Efficiency:	5V/69% more than 5V -> 91-95%
Output Efficiency:	63,13% - 93,62%
Output energy:	58,8Wh - 88,2Wh
QC / PD support	YES / YES
Actual cell max. charging current / Specification. max. charging current	2,5A / 2A
Chip applied	CYPD3171+SC8802, IP6538, 2xSY8813+2xFP6601
Date	11.03.2020
Sample index	PBGC04v6

Conclusions

Research on various types of cells, charging technologies, and functionalities has led to the development of a power bank with previously unavailable solutions in the market. This has contributed to its popularity due to its versatility of use.

Durability tests conducted on the power bank have increased its resistance to mechanical damage, thus extending its lifespan.

The introduction of features such as fast charging, overvoltage protection, and short circuit protection has enhanced the safety of using the power bank and improved its overall performance quality.

Device at the time of its premiere stood out from the competition with its unique functions and functionalities. This contributed to a good reception on the market and finding a large group of users.

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INSOMNIA AND ITS RELATIONSHIP WITH SELECTED PERSONALITY TRAITS

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Abstract:

Sleep is very important for the proper functioning, however, personality traits and some sociodemographic characteristics may be associated with a higher risk of insomnia. The aim of this study was to investigate the relationship between insomnia and personality traits (emotionality and extraversion) and sociodemographic characteristics. Data were collected from 305 adult Poles (232 women, 73 men), aged 18 to 65. Two subscales from the HEXACO Personality Inventory – Revised (60-item version) and the Athens Insomnia Scale were used for measurements. Insomnia was significantly related to extraversion (negatively) and emotionality (positively) but not to age. There were no differences in the level of insomnia by gender or educational level. It is important to consider personality traits when dealing with the problem of insomnia.

Keywords:
insomnia, extraversion, emotionality, personality

Insomnia - Characterization of the Problem

Insomnia, considered the predominant form of sleep disorders, is one of the more common health problems among adults. It is characterized by subjective feelings of poor sleep quality and impaired functioning during the day [1]. The International Statistical Classification of Diseases and Health Problems (ICD-10) distinguishes non-organic insomnia. It involves a persistent lack of sufficient quantity and quality of sleep at least three times a week for at least a month, and its symptoms primarily include difficulties in falling asleep, maintaining sleep, or waking up too early. Insomnia can exist as a separate disease - primary insomnia, or be the result of another existing somatic or mental disease - secondary insomnia [2]. Sleep-related difficulties can be a serious problem, considering the important role sleep plays in human functioning. It is described as a state of rest for the body and serves a regenerative function. Its deficiency disrupts proper psychophysical functioning, primarily negatively affecting consciousness and reasoning abilities [3].

Insomnia and Selected Personality Traits

The HEXACO personality structure model, authored by Ashton and Lee [4], consists of the following factors: honesty/humility, emotionality, extraversion, agreeableness, conscientiousness,

and openness to experience. Among the traits that may correlate with insomnia are emotionality and extraversion.

Emotionality is described as a tendency to experience anxiety in response to stress and fear of threat. Highly emotional individuals feel the need for emotional support from others and sentimental attachment. Research conducted on the relationship between insomnia and neuroticism (a trait included in the Five-Factor Model of Personality, which is very similar to Emotionality in the HEXACO Model) confirms that these two variables are significantly positively related [5-7]. The strength of this relationship may vary when considering the gender of the participants. For example, in the study by Biegańska [5], the correlation between neuroticism and mental and physical health, including insomnia, was strong among women and moderate among men. Lachowska's study [6] on 159 women and 154 men, which explores the significance of neuroticism for various consequences of occupational stress among working parents, including anxiety and insomnia, also presents similar conclusions. Anxiety and insomnia occur much more frequently in individuals with higher levels of neuroticism. The authors of a study conducted on a sample of 400 individuals also indicate that emotional stability (emotionality) is a predictor of insomnia [7]. Similarly, Krizan et al. [8] show in the results of their study that a high level of neuroticism can predict insomnia. Likewise, in a study conducted on Finnish and Australian populations by Hintsanen et al. [9], a high level of neuroticism was associated with greater sleep problems. The results of the study by Kim et al. [10] indicate that neuroticism is the most important factor influencing overall scores on the insomnia scale. The findings obtained so far are also confirmed by a longitudinal study conducted among 327 shift workers [11], which suggests a moderate relationship between neuroticism and insomnia [5-11].

Extraversion, on the other hand, can be defined as a sense of self-assurance or perceiving oneself in a positive way. Individuals with high levels of extraversion are energetic and derive joy from social interactions. In the study by Biegańska [5], a weak negative correlation between extraversion and mental and physical health, including insomnia, was found among women, while among men, this correlation was moderate. A study conducted on a sample of 400 individuals revealed a negative correlation between extraversion and insomnia [7]. Similarly, in a study conducted on Finnish and Australian populations by Hintsanen et al. [9], a high level of extraversion was associated with fewer sleep problems, unlike neuroticism. The results of the study by Kim et al. [10] showed a small negative correlation between extraversion and the level of insomnia. A longitudinal study conducted among 327 shift workers [11] also demonstrated a negative relationship between insomnia and extraversion, although the strength of this relationship was weak. Similarly, the findings from the study by Krizan et al. [8] indicate that low extraversion can be a predictor of insomnia.

Insomnia and sociodemographic variables

Research on insomnia takes into account comparisons based on the gender of the participants. Many studies indicate that women are more likely than men to experience insomnia, as exemplified by the study by Biegańska [5]. In the study by Nowicki et al. [12] on a sample of 1245 women and 1168 men aged 18-79, the results show that women more frequently report insomnia, especially difficulties in falling asleep, particularly in older age groups. However, some results suggest that gender is not a differentiating factor in terms of insomnia outcomes [13].

Regarding age, insomnia generally occurs more frequently among the older age group [1, 12]. This may be due to increasing health problems that come with age. Bidzan [14] emphasizes that in the older age group, the body becomes more sensitive to various factors such as hormonal changes and environmental factors like noise and temperature. The human body in old age is also more susceptible to various disorders, such as dementia syndromes or depressive disorders. This is also influenced by a higher frequency of consuming chemical substances, such as medications.

The last demographic factor that may influence insomnia is education. A study conducted by Kiejna et al. [15] showed that both men and women with lower education levels experience sleep problems more frequently, while those with higher education levels experience them less often. Similar results were obtained in a study by the Center for Public Opinion Research, which reported that 33% of individuals with basic education suffer from sleep disorders, including insomnia, compared to only 17% of those with higher education [1]. However, the study by Robert Stewart and others presented higher values, with 43% of individuals with low education levels experiencing insomnia, compared to 35% among those with higher education [16]. There are also conflicting reports suggesting no relationship between education level and insomnia [12].

Research aim and research hypotheses

Based on the literature review and observed regularities regarding insomnia, a study was conducted with the aim of verifying the relationship between insomnia and the described psychological factors, namely extraversion and emotionality, as well as demographic factors such as gender, age, and education level. Based on the results of previous studies, the following hypotheses were formulated:

H1: There is a positive correlation between the level of emotionality and insomnia.
H2: There is a negative correlation between the level of extraversion and insomnia.
H3: The level of insomnia is higher in women than in men.
H4: The level of insomnia increases with age.
H5: The level of insomnia is lower in individuals with higher education.

Method

Sample description

The study, conducted in March and April 2023, included 305 participants, with 73 being male and 232 being female. The age of the respondents ranged from 18 to 65 years (M = 31.34). Among the participants, 24 individuals reported having primary education, 13 had vocational education, 128 had secondary education, and 140 had higher education. The study was conducted using a questionnaire method, utilizing a Google form. The questionnaire link was posted in several Facebook groups. The study was fully anonymous and voluntary, and participants were informed that they could withdraw from participation at any time.

Tools

HEXACO-PI-R

The HEXACO-PI-R Personality Inventory (60-item version), developed by Kibeom Lee and Michael C. Ashton, and adapted into Polish by Piotr Szarota [17], was used to measure selected

psychological variables. Two factors from the entire scale were utilized: emotionality and extraversion. Each factor consisted of 10 statements. Participants were required to respond to each statement using a five-point Likert scale, where 1 indicated "strongly disagree" and 5 indicated "strongly agree." The internal consistency, measured by Cronbach's alpha, was 0.74 for emotionality and 0.85 for extraversion in the current study.

Athens Insomnia Scale

Insomnia was measured using the Athens Insomnia Scale (AIS) in the Polish adaptation by Małgorzata Fornal-Pawłowska, Dorota Wołyńczyk-Gmaj, and Waldemar Szelenberger [18]. This tool assesses insomnia symptoms and consists of 8 statements. Participants had to rate each statement on a scale of 0 to 3 points, where 0 indicated the absence of the symptom and 3 indicated its severe presence. The total score ranged from 0 to 24 points. The first five items pertain to sleep-related symptoms, while the remaining three items relate to daytime functioning. The original studies demonstrate high reliability and validity of this tool. In the current study, the internal consistency, measured by Cronbach's alpha, was 0.83.

Sociodemographic data were collected using a self-designed questionnaire, which included information regarding gender, age, and education level.

Statistical analyses

The calculations were performed using the SPSS software. The Shapiro-Wilk test was used to assess the normality of the distribution of the analyzed variables. Correlation analysis was conducted using the Spearman's rho coefficient. Gender comparisons were made using the Mann-Whitney U test, while groups distinguished by education level were compared using the Kruskal-Wallis ANOVA.

Results

The first step involved checking the normality of the distribution for the quantitative variables included in the analyses, namely insomnia, emotionality, extraversion, and age. Among these variables, only emotionality followed a normal distribution. The normality of the insomnia variable's distribution was also examined within gender and education level groups. In the female group, emotionality showed a distribution in line with normality, while in the male group, both emotionallity and extraversion exhibited normal distributions. However, insomnia did not follow a normal distribution in the groups distinguished by education level.

To verify hypotheses H1 and H2, a correlation analysis was conducted. Detailed data on descriptive statistics and correlation coefficients are presented in Tab. 1. Insomnia was significantly positively correlated with emotionality, while it had a negative correlation with extraversion.

Hypothesis H3 was tested using the Mann-Whitney U test, which revealed no significant differences in insomnia between genders ($U = 9584$; $Z = 1.814$; $p = 0.077$; female $M = 8.24$; male $M = 7.11$).

Next, the correlation between age and the level of insomnia (H4) was examined. The correlation analysis showed no statistically significant result ($R = -0.07$, $p = 0.219$).

To test hypothesis H5, a Kruskal-Wallis ANOVA was performed, which indicated no statistically significant differences in the level of insomnia among groups distinguished by education level ($H =$

1.916; df = 3; p = 0.590; primary M = 9.13, vocational M = 8.62, secondary M = 7.91, higher M = 7.77).

Tab. 1. Descriptive statistics of the analyzed variables and values of Spearman's rho correlation coefficients

	Variables	M (SD)	Me	Skewness	Kurtosis	Min-Max	W	1	2	3	4
1	**Insomnia**	7.97 (4.40)	7	.59	-.23	0 - 22	0.96***	-			
2	**Emotionality**	31.38 (7.59)	31	-.05	-.33	13 - 49	0.99	.25***	-		
3	**Extraversion**	30.65 (8.61)	31	-.19	-.58	10 - 48	0.99**	-.36***	-.19***	-	
4	**Age**	31.34 (10.96)	29	.77	-.07	18 - 65	0.93***	-.08	-.02	.28***	-

W = Shapiro-Wilk test statistic
*p<0,05; **p<0,01; ***p<0,001

Source: own calculations

Discussion

The conducted study and statistical analyses have allowed for the verification of the hypotheses. The results showed a positive relationship between emotionality and insomnia, confirming the assumption in hypothesis H1. Similar findings have been reported in numerous studies in the literature [5-7, 11]. There was also a correlation between extraversion and insomnia, with increased extraversion associated with decreased insomnia, thus supporting hypothesis H2. This is consistent with the results of studies by Biegańska [5], Fabbri et al. [7], and Kim et al. [10]. However, no statistically significant differences in insomnia levels were found between genders, similar to the findings of Andrzejewska et al. [13]. Hypothesis H3, suggesting higher levels of insomnia in women compared to men, was not confirmed. Additionally, the analysis did not find a statistically significant correlation between age and the level of insomnia, thus hypothesis H4 was not supported. The results obtained in this study contradict findings from other research [1, 12]. Education level was not found to be a differentiating factor in the severity of insomnia, and therefore, hypothesis H5 was not confirmed. Similar results were presented by Nowicki et al. [12] in their study.

The conducted study is not without limitations. The sample selection was not random, which hinders the generalization of the results to the entire population. The online survey format, especially for older individuals who may not commonly use computers, the internet, or Facebook, may have favored the participation of individuals who do not represent the typical demographic of that age group. Additionally, the relatively small number of respondents above the age of 35 may have influenced the verification of the hypothesis regarding the increase in insomnia with age. Another limitation concerns the gender disproportion among the participants, with a predominance of females.

In summary, the study results confirmed the association between insomnia and psychological variables such as emotionality and extraversion. However, no relationship was found between insomnia and age or differences in its level based on sociodemographic variables such as gender or education level. When considering the application of the research findings in supporting individuals experiencing insomnia and in its prevention, it is important to consider the level of extraversion and

emotionality. Further research on this topic is recommended, with particular emphasis on verifying the role of sociodemographic variables, as research reports often provide conflicting data. Future studies should aim to increase the sample size and ensure its representativeness. Additionally, including questions about the use of electronic devices emitting blue light may provide a better understanding of the insomnia problem. The respondents' diet and lifestyle may also be important factors to consider. Insomnia is a socially significant problem that affects various aspects of human functioning, so it is crucial not only to understand its causes but also to implement interventions that can alleviate its effects or prevent its occurrence.

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CORROSION PROTECTION – CORROSION INHIBITORS

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Abstract:

Corrosion, which most often refers to the electrochemical oxidation of the metal, is the degradation of a material's qualities brought on by a chemical and/or electrochemical interaction with the environment. Anti-corrosion fluids are one of the many techniques used to stop the corrosion of metals, and they are frequently employed to offer temporary corrosion protection during production, storage, and transit activities.

Keywords:
inhibitors, corrosion, fluids

Introduction

Corrosion inhibiting fluids are made by combining corrosion inhibitors, film-forming agents, and other additives with a base fluid [1]. Depending on the kind of base fluid, these fluids can be classed as solvent-, oil-, or water-based corrosion inhibitors. Corrosion inhibitors are unquestionably essential to achieving excellent performance. The two primary categories of corrosion inhibitors are inorganic and organic. In different base fluids and for various metals, inorganic inhibitors like nitrite, nitrate, chromate, dichromate, and phosphate are frequently utilized. Organic inhibitors include sulfonates, alcohols, ethers, amines, amides, amine salts, carboxylates, heterocyclic nitrogen compounds, phosphates, polymers, natural products, and others based on their account of the polar groups [2-4].

Electrochemical mechanism of metal oxidation

In electrochemical corrosion, two processes take place simultaneously: oxidation (dissolution of the metal) and reduction (release of hydrogen, reduction of oxygen, release of metal from solution and others). In addition, the process of metal dissolution in electrochemical corrosion is accompanied by the exchange of electrons and ions between the metal and the electrolyte.

The rate of corrosion of metals in electrolyte solutions depends largely on the properties of the solution: the process proceeds equally in acidic, basic or neutral environments.

Precisely because of the mechanism of electrochemical action of the inhibitors forming protective barriers on the metal surface, corrosion inhibitors can be classified as anodic, cathodic or mixed based on the method of corrosion inhibition [5, 6].

Anodic inhibitors, often referred to as passivation inhibitors, reduce the anodic reaction by blocking it and promoting the metal's natural passivation reaction as a result of the development of a film adsorbed on the metal. In general, inhibitors interact with the corrosion product that has already developed to create a cogent and soluble coating on the metal surface. The concentration of the anodic inhibitors in the solution must be high enough to have the desired effect [7]. When inhibitors are used in an insufficient amount, the film protection is affected since the metal is not entirely covered, leaving exposed areas of the metal that can corrode. Nitrates, molybdates, sodium chromates, phosphates, hydroxides, and silicates are a few instances of anodic inorganic inhibitors [8].

Cathodic corrosion inhibitors stop the metal's cathodic reaction from happening while corrosion is taking place. These inhibitors include metal ions that can initiate a cathodic reaction because of their alkalinity, resulting in the formation of insoluble compounds that precipitate only at cathodic sites. They leave behind a thick, adherent coating on the metal that prevents the diffusion of reducible species in these regions. This raises surface impedance and restricts the diffusion of reducible species, such as oxygen and conduction electrons, in these regions. The cathodic inhibition caused by these inhibitors is strong. Magnesium, zinc, and nickel ions are a few examples of inorganic cathodic inhibitors. These ions interact with the hydroxyl groups (OH^-) in water to create insoluble hydroxides ($Mg(OH)_2$, $Zn(OH)_2$, and $Ni(OH)_2$), which are then deposited on the cathodic site of the metal surface to shield it. Other substances that exhibit the similar chemical process include polyphosphates, phosphonates, tannins, lignins [8].

Organic substances known as mixed inhibitors attach to metal surfaces where they form a coating and obstruct both cathodic and anodic processes. Organic chemicals that are utilized as mixed inhibitors occasionally operate as cathodic, anodic, or combined cathodic and anodic inhibitors, on the whole, they work through a surface adsorption process known as film formation. Strongly adsorbing naturally occurring molecules on compound metal surfaces exhibit effective inhibition and little environmental danger. This inhibits the metal from dissolving in the electrolyte by creating a protective hydrophobic coating on the metal surface. They must be soluble or dispersible in the medium surrounding the metal. Examples of organic substances include amines, urea, aldehydes, heterocyclic nitrogen compounds, sulphur-containing compounds, caffeine and extracts of natural substances [8-10].

Influence of various factors on the effectiveness of inhibitors

The effectiveness of inhibitors depends on a number of factors that can either positively or negatively affect the effectiveness of protection. The most important of these factors are the concentration of the inhibitor, the pH of the solution, the temperature, the flow rate of the aggressive environment, the type and concentration of the aggressive components, and the presence of various metals in the system.

Chemistry of corrosion inhibitors

Nitric and chromate compounds

Nitrites are anodic inhibitors, just as chromates, and they block the system by producing a passive iron oxide layer [11]. They are eco-friendly environmental inhibitors. At pH values of 9 to

10, nitrites also prevent the corrosion of copper, tin, and nickel alloys in addition to steel. Nitrites shouldn't be employed in open systems since, in the presence of oxygen, they oxidize to nitrates. Nitrites do not function as good inhibitors. The shield that nitrites generate can be harmed by the presence of chloride and sulfate ions. In a closed recirculation system, they are frequently used with borax. Chromate is a very powerful inhibitor that keeps aluminum alloys from corroding. Chromates are the most powerful inhibitors, but they are poisonous, their usage is restricted and not advised. If the systems to be blocked include bimetallic connections or high chloride concentrations, a high concentration is necessary. As oxidizers, they increase anodic current density over the threshold required for passivity. Examples of chromate inhibitors include Na_2CrO_4 or $Na_2Cr_2O_7$. Iron oxide and chromium oxide are present in the passive protective layer that is created, making chromate inhibitors particularly effective. The use of metalworking fluids that contain nitrite and/or chromate is restricted due to safety and environmental concerns, and there is a high demand for alternatives to these inhibitors that are both environmentally responsible and water-soluble and can offer comparable corrosion prevention efficacies to solvent-based and oil-based corrosion inhibitors [12].

Sulfonates

The most often applied corrosion inhibitors in anti-corrosion compositions are metal sulphonates. Given the metal cations, they can be categorized as Ba, Mg, Ca, or Na salts; they can also be split into petroleum or manufactured sulfonates. The choice of cations, together with the size of the cation, affected the charge separation and dipole strength of the sulfonate groups, according to early research. This was true for the adsorption of several sulfonates from an anhydrous oil solution. The sequence of Na < Mg < Ca < Ba was shown to be the most efficient for reducing corrosion. Because of their special rust-prevention and water displacement qualities, barium and calcium sulphonates are particularly popular in industrial formulations, whereas sodium sulphonates are more frequently utilized to create rust preventatives that emulsifies in water. By serving two purposes – forming a protective layer and neutralizing acidic components that might promote rusting – calcium sulphonates, in addition to neutral salts, are also good rust preventatives [13-17].

Amines

Amines are organic versions of ammonia derivatives where one or more hydrogen atoms have been swapped out for hydrocarbon chains with various structures and carbon atom counts. Their subclass is determined by how many hydrocarbon chains are connected to the N atom. $-NH_2$, -NHR, and $-NR_1R_2$ groups are present in primary, secondary, and tertiary amines, which are distinguished by having one, two, or three hydrocarbon chains connected to the N atom. The protective effect of amines, which is correlated with the molecular charge of the N atom, is demonstrated to increase with the amount of hydrocarbon chains in earlier research. The solubility of the amine and the strength (durability) of the amine-metal coordination link produced are what determine how effective its anti-corrosion characteristics are. The foundation of amine compounds' anticorrosive properties is their ability to adhere to surfaces of protected metals, creating a hydrophobic layer that significantly restricts the access of water and aggressive ions while delaying the metal's anodic electrochemical corrosion processes. The primary drawbacks of utilizing amine corrosion inhibitors are their short duration of action, irritable odor, and toxicity. Problematic is how selectively amines function to shield metal structures from corrosion. The usage of a particular amine

for a certain metal is necessary for the creation of corrosion inhibitors. For instance, certain amines may shield steel while accelerating the corrosion of copper or bronze. The undesirable characteristics of the inhibitors can be overcome with recently synthesized, improved amine compounds. Without losing the inhibitors' anti-corrosion qualities, their undesirable traits can be avoided or at the very least greatly minimized [18]. One of the simplest film-forming amine compounds, octadecylamine (ODA), $CH_3(CH_2)_{17}NH_2$, has long been employed in nuclear and fossil fuel power plants to shield steel. The molecule contains a hydrophilic head and a hydrophobic tail. Once the film is produced, this physical barrier inhibits iron dissolution (anodic and cathodic actions) and makes it impossible for water, oxygen, or other corrosive chemicals to access the metal surface [19].

Amides

In the case of amides in anti-corrosion fluids, the high electron structure of the amide group will promote adhesion to the electropositive metal surface, while the hydrocarbon chains will repel water and then inhibit corrosion. Many amides have been proposed for altered corrosion with more advanced environmental regulations. N-oleoyl sarcosine is one of the few oil-soluble amide corrosion inhibitors that can be derived from gasoline, mineral oil, and silicone lubricants. Subsequent studies receive a synergistic effect of a mixture of sodium nitrite and N-acyl sarcosine as corrosion inhibitors in lubricants, as well as a synergistic rust-inhibiting composition consisting of N-acyl sarcosine and a dicarboxylic acid amine salt. Solubility of corrosion inhibitors in both oil and water is desirable in return for application. In addition, the acylamino acid derivative in the triazole derivative test can be part of the corrosion inhibition in both the organic hydrocarbon component and the water. If the preparation is used for water, the antibacterial properties are also used for the application. The N-alkylcarboxylic acid amide reacts with the reactions of the cyclic acid anhydride and the fatty amine, showing good anti-corrosion and antimicrobial activity [20-25].

Amine salts

Amine salts, particularly amine salts of carboxylates, have long been used to stop metals from corroding. Because they are created on-site by the interaction of an amine and a carboxylic acid, they are practical to utilize. In metalworking fluids, neutralized amine carboxylates offer lubricity, emulsification, detergency, as well as corrosion inhibition. According to studies, the amount of carbon atoms has an impact on performance, and carboxylic acids in the C18 to C22 range, including tall oil fatty acid (TOFA), which neutralizes TEA, are the best possibilities. Additionally, the usage of alkyl ammonium carboxylate salt-ethoxylated trimer, acid dimer, or acid dimer esters of alkylphenol as corrosion inhibitors in hydrocarbon fuels or oil. Alkyl ammonium carboxylate salt-ethoxylated trimer, acid dimer, or acid dimer esters of alkylphenol are additionally powerful corrosion inhibitors that may be added to hydrocarbon fuels or oil formulations. Alkenylsuccinic acid semi-amides can also be used as corrosion inhibitors with a low tendency to foam in aqueous solutions to increase water solubility [25-28].

Carboxylates

By adsorbing a carboxylate group (Lewis base) on the metal surface (Lewis acid), carboxylates can prevent corrosion by generating a hydrophobic layer. Oleic acid, soybean fatty acid, TOFA, and polymerized fatty acids like dimer acids are examples of long-chain fatty acids that have long been

recognized as corrosion inhibitors in a variety of applications. Short-chain fatty acids, on the other hand, can actually encourage corrosion. using dicarboxylic acid and dicarboxylic esters acids as composition additives to effectively stop metal corrosion. Tetra propenyl succinic acid derivative, succinic anhydride derivatives, and succinic amine derivatives work together to reduce rust development in lubricating oils. It is important to keep in mind, though, that dicarboxylic acids have a tendency to precipitate in the presence of Ca^{2+} or Mg^{2+} ions, which would negate their rust-prevention abilities [25].

Heterocyclic nitrogen compounds

Numerous heterocyclic nitrogen compounds, including imidazolines, thiazoles, triazoles, benzotriazoles, and pyrazoles, have demonstrated their efficacy as corrosion inhibitors for a variety of metals without producing ash. By bonding with the metal via the N-electron pair and/or -electron cloud, they can adsorb on the surface of the metal, blocking active sites on the surface and preventing corrosion. A corrosion inhibitor that contains at least one carboxylic acid and a certain family of pyridine derivatives can synergistically improve the corrosion inhibition and defoaming properties of a lubricating oil. In contrast to pyridine, imidazoline-based inhibitors have a five-atom ring with two nitrogen atoms in the structure. When paired with a long hydrocarbon chain, this structure will in some way alter the inhibitory effectiveness [29-31].

Phosphates

The group of phosphate inhibitors includes a wide variety of compounds with relatively simple structures, such as ortho-phosphates, triphosphates, pyrophosphates and compounds of higher condensed phosphates with more complex structures. Polyphosphates, complex compounds of metaphosphates, belong to a large group of substances containing chains or rings consisting of phosphorus and oxygen atoms. They are complex-forming compounds and with divalent metals form positively charged molecules. Of the phosphates, polyphosphates are the most important and most widely used inhibitors. They are used successfully as corrosion inhibitors primarily for iron and steel in inert or almost inert waters (e.g. cooling, natural, tap water). Polyphosphates then have a dual role, namely to reduce scale formation and inhibit corrosion. Polyphosphates of the hexaphosphate type show the ability to form well-soluble compounds with many ions, including those found in natural waters: Ca^{2+}, Mg^{2+}, Fe^{2+}, Zn^{2+}. Therefore, polyphosphates contained in waters in higher concentrations act as a strong depolariser of anodic iron dissolution and markedly increase corrosion. Polyphosphates also show the ability to strongly adsorb on the metallic surface and make the surface hydrophilic to water. These inhibitors are very attractive for several reasons, they are non-toxic, they are effective even in the presence of significant amounts of chlorides, a small amount is sufficient to inhibit corrosion of iron and steel, and they can also be used to protect other metals, e.g. Al, Cu. Polyphosphates, however, also exhibit disadvantageous characteristics, namely during their use they decompose with the formation of orthophosphates, which with calcium give a loose calcium phosphate precipitate. This conversion to orthophosphate occurs much faster at elevated temperatures. Pitting corrosion can occur at insufficient concentrations of this inhibitor. Despite the widespread usage of phosphate-based corrosion inhibitors, there are rising worries about their long-term toxicity and detrimental effects on the environment [5, 32, 33].

Polymers

There is now a hunt for safer corrosion inhibitors, such as green corrosion inhibitors and other more ecologically friendly corrosion inhibitors. The majority are biodegradable and contain no heavy metals or other hazardous substances. Studies of the corrosion-inhibiting properties of polymeric substances, such as plant gums, have demonstrated that plant products are affordable, easily accessible, and renewable sources of materials. They are also ecologically acceptable and environmentally favorable. According to research, certain polymers can be utilized as corrosion inhibitors because they form complexes with metal ions and on metal surfaces thanks to their functional groups. These complexes take up a lot of surface area, covering the metal's surface and shielding it from the corrosive chemicals in the solution. Different cationic polymers, including polyethyleneimine derivatives, polyacrylamide derivatives, polydicyanediamide derivatives, and anionic polymers such polymaleic acid derivatives, polyacrylic acid derivatives, and polyacrylic acid, can suppress corrosion. It was discovered that COOH-group-containing polymers are powerful polymer systems that can function as corrosion inhibitors. The anticorrosion properties of polymethacrylic acid and the copolymer of styrene and maleic acid on zinc pigments in aqueous alkaline [34].

Natural products

Another extremely intriguing alternative are plant extracts, which include a group of organic substances that aid in inhibiting the rusting process. The benefit of such extracts is that creating such an extract from any plant is thought to be an easy operation, allowing for improved efficiency in both extraction and the application of these chemicals for various research. An extract is a mixture made up of a plant's or a plant's active ingredients and a solvent-containing media. The polarity of the solvent employed, as well as other factors like Soxhlet extraction procedures, affect the extraction efficiency. These extracts are mostly recognized for their anti-inflammatory, antiviral, antioxidant, and antibacterial properties. Extracts are frequently made from the entire plant or from sections of it that have greater quantities of active compounds, or phytochemicals. The literature suggests that active chemicals found in extracts from plants, fruits, seeds, flowers, and leaves have the potential to prevent corrosion in conditions that are hostile. Additionally, these substances are emerging as affordable, accessible, and sustainable corrosion inhibitor substitutes. Plant extracts have gained importance as an easily accessible, renewable, and ecologically acceptable source for a variety of inhibitors. They are significant sources of compounds with excellent inhibitory efficiency. Numerous of these plant extracts exhibit corrosion inhibitory action that may be caused by the presence of heterocyclic components such alkaloids, flavonoids, etc. [35]. Due to its horizontal adsorption on the steel surface, guar gum, a polysaccharide component derived from guar beans, can operate as a corrosion inhibitor of carbon steel [36].

Conclusion

One of the greatest methods to stop the negative effects of corrosion on a metal substrate is to utilize corrosion inhibitors. Additionally, the application of an appropriate inhibitor can offer long-term protection against corrosion, particularly lowering the significant maintenance expenses of a damaged or corroded surface. The efficiency of corrosion inhibition is determined by how the

adsorbed inhibitor affects subsequent metal finishing processes and film-forming capacity. The chemical composition and physicochemical characteristics of the inhibitor compounds, their adsorption at anodic and/or cathodic sites, their suppression of the cathodic and/or anodic reaction, and the formation of protective films as a result of interactions between the available surface charge, metal ions, and other molecules are typical factors that affect inhibition mechanisms.

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APPLICATION OF FEDERATED LEARNING IN HIGHER EDUCATION IN POLAND

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Abstract:

The subject of the article is to check the usefulness of federated learning in higher education. The main thesis of the work is the statement that federated learning is able to accurately indicate the chances of timely graduation. The study is based on the analysis of the timeliness of graduation using a neural network using federated learning. The first step was to prepare the data, the next step was to create 10 architectures that were checked for accuracy. After creating the architectures, a solution was created that tested each created neural network and performed tests on it. The tests were carried out by determining values such as accuracy and loss functions, which then determined the selection of the best network.

Keywords:
federated learning, neural network, fuzzy sets

Introduction

With the rise of machine learning, privacy and legal issues began to arise. Traditional neural networks use datasets stored on centralized servers, which can cause concern [1]. In some cases, the law doesn't allow the storage of certain kinds of data. This kind of regulation can be applied in medicine, where most of the data is sensitive [2]. Federated learning comes to solve these problems. The main difference between this approach and the traditional approach is focus on decentralization and data privacy. In a federated network, every device has their own model, which is trained with local data. Then models are sent to a central server which the main purpose is to aggregate models and share them to clients (if aggregated model is better than previous) [1]. Federated learning can be divided according to the type of problem being solved. To this end, we distinguish: Federated Transfer Learning (FTL), Horizontal Federated Learning, Vertical Federated Learning.

- Federated Transfer Learning - a special type when clients data sets contains different kind of data (only in small extent they are overlapping). Using overlapping data, it is possible to predict results for all clients (Fig. 1) [3].

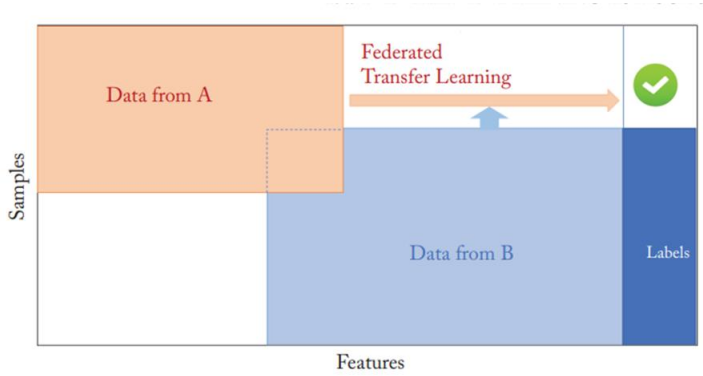

Fig. 1. Diagram of federated transfer learning
Source: Yang Q. i in., Federated Learning. Synthesis Lectures on Artificial Intelligence and Machine Learning, Berlin: Springer, 2020

- Horizontal Federated Learning – in this type every client shares similar features, but they apply to different users, ex. Hospitals can store similar type of data about different patients (Fig. 2) [4].

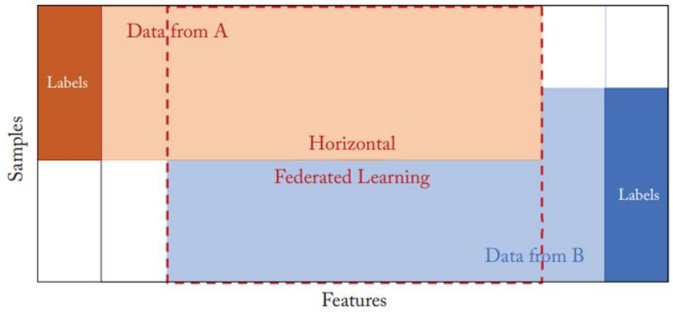

Fig. 2. Diagram of horizontal federated learning
Source: Yang Q. i in., Federated Learning. Synthesis Lectures on Artificial Intelligence and Machine Learning, Berlin: Springer, 2020

- Vertical Federated Learning – in this type, only one client stores labels of data. This client is named as a guest or active client. Other clients are named passive client or host. Additionally, labels have to be the same for all clients, otherwise predictions won't be correct (Fig. 3) [5].

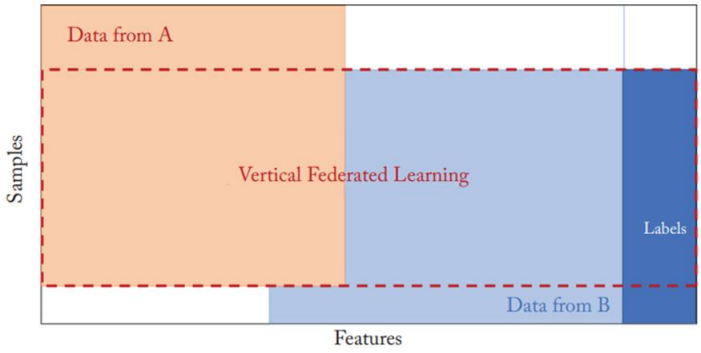

Fig. 3. Diagram of vertical federated learning
Source: Yang Q. i in., Federated Learning. Synthesis Lectures on Artificial Intelligence and Machine Learning, Berlin: Springer, 2020

Nowadays, education have a problem with not only small amount of candidates, but also with unsuccessfully graduations. More and more defence of diploma theses are postponed, or it is not always successful. To resolve this problem, federated learning can be used to provide student information about probability of his successful graduation. The system could use data from many universities (which will be a client in terms of federated learning) and provide students' information suited for their university and help them to successfully graduate. Also with this system candidates could check which university could give them the highest probability of successful graduation. The main goal of this work is to propose optimal neural network structure to find the most accurate model for predicting successfulness of graduation.

Fuzzy sets theory

Every not empty fuzzy set A has membership function (2), which determines the degree of object membership in the fuzzy set A [6],

$$A : X \to [0,1]. \tag{2}$$

In federated learning, an aggregation is intended to be used. An aggregation is a process by which data is merged to produce a new set of data. For $n \in N$, where $n \geq 2$ function $A : [0, 1]^n \to [0, 1]$, is growing (3). For $x_i, y_i \in [0, 1]$, where $i = 1, \dots, n$ A is an aggregation function if satisfies condition (4) [7],

$$x_i \leq y_i \Rightarrow A(x_1, \dots, x_n) \leq A(y_1, \dots, y_n), \tag{3}$$

$$A(0, \dots, 0) = 0, A(1, \dots, 1) = 1\,. \tag{4}$$

Aggregation can be used in various forms, ex.: arithmetic mean (5), geometric mean (6), harmonic mean (7) and OWA (8) [8],

$$A(x) = \frac{1}{n}(x_1 + x_2 + \cdots + x_n), \tag{5}$$

$$A(x) = \sqrt[n]{x_1 x_2 \dots x_n}, \tag{6}$$

$$A(x) = \frac{n}{\frac{1}{x_1} + \cdots + \frac{1}{x_n}}, \qquad x_i > 0, \tag{7}$$

$$OWA(x_1, \dots, x_n) = \sum_{i=1}^{n} w_i x_{(i)}. \tag{8}$$

Federated learning process

Of all the types of federated learning, Horizontal Federated Learning was used in this paper. The main reason for this choice is the fact that each client has the same set of attributes in the data. Based on the type adopted, the federated learning process consists of the following steps:

1. Create three clients.
2. Training of the shared model on selected clients using user data with using neural network.
3. Send local model parameters to the server.
4. Aggregate updates by the server using the arithmetic mean.

5. Resend the model to clients, with the changes included.
6. Update local model parameters if they do not degrade model performance.

Neural network theory

The fundamental neural network is a single perceptron, which can be used in linear separable set classifications. It consists of multiple inputs (labelled as x_1, x_2, …, x_n) and one output. Every input has weight (labelled as w_1, w_2, …, w_n), which determines impact of inputs. The weighted sum of inputs (7) is passed to the activation function, which result is an output [9],

$$x = \sum_{i=0}^{n} w_i x_i \,, \tag{7}$$

$$y = f(x). \tag{8}$$

Activation function can be used to apply nonlinearity to neuron [10]. The following activation functions are used in the work: sigmoid function and ReLu function. Sigmoid function values in range from 0 to 1,

$$f(x) = \frac{1}{1 + e^{-x}}. \tag{9}$$

In case of ReLu function values are in 0 to positive infinity range. (10). In case of passing values less than 0, the result of the function will be 0 [11],

$$f(x) = \max(0, x). \tag{10}$$

Individual perceptron's can be combined to create a net, where all neurons are connected to each other. By adding layers to the network, formula for network output are changed. Changed version calculated output of individual neuron in net in the following way:

$$y_j = f\left(\sum_{i=0}^{n} w_{ji} x_i + w_{0i}\right). \tag{11}$$

The process of learning the net are made by weights modification. To do this, a backpropagation algorithm and cost function are used [12]. The cost function calculates how much prediction (labelled as y_i) differs from real data (labelled as Y_i). In case of logistic classifier, the cost function will be log loss function [13], which is calculated by the following formula:

$$L(y_i) = -\frac{1}{n}\sum_{i=1}^{n} [Y_i \ln y_i + (1 - Y_i) \ln(1 - y_i)] \,. \tag{12}$$

Backpropagation algorithm passes over every neuron and calculates by the gradients how much change the weight [14], which is calculated by the following formula:

$$w_{ji} = w_{ji} + \alpha * \nabla_{w_{ji}} L(y_j). \tag{13}$$

Data preparation

The received data was in the form of an Excel file, which contain separated sheet for every course. At an early stage of data transformation, data has been merged to a single CSV (comma-separated values) file. The main purpose of that was to prepare data for transformation. In the next stage, duplicates were removed and converted to desired data format. The last phase was data normalization, in this step min-max function for normalization was used. Every value were from 0 to 1 range. 0 meant no grade, 1 meant highest grade. The created dataset contained 22 columns with courses and matura exam results, and one column with information whether the student successfully graduated. Amount of students were 2862, where, 2027 successfully graduated while 835 not. The data were imbalanced, to resolve this, objects which didn't successfully graduated were duplicated.

Solution preview

The solution was created using Python language, which has great support for machine learning libraries. In federated learning area it's required to have client set which has unique dataset. In this particular scenario, the network would consist of 3 clients. That's mean the entire dataset was split by 3 clients. To develop the best model, the solution was created to try different combinations of parameters and architectures. Every architecture was checked how behaves with different client amount and dataset repeat count. For each combination, the model was created 3 times to calculate average accuracy. Every model was trained for 1000 rounds to check when they are overfitting.

To find the best architecture, 10 architectures were created (Tab. 1). Every architecture contained a sigmoid layer as a last layer to predict likelihood of successful graduation.

Tab. 1. Architectures

No.	No. of layers	No. of neurons in each layer
1	3	18, 9, 1
2	3	24, 12, 1
3	4	18, 18, 9, 1
4	4	24, 24, 12, 1
5	4	64, 32, 8, 1
6	3	15, 10, 1
7	3	10, 5, 1
8	4	10, 10, 5, 1
9	4	64, 10% dropout, 16, 1
10	5	64, 64, 10% dropout, 16, 1

Source: own elaboration

Results

Of all the architectures, the seventh (Fig. 4), the fourth and the first had the greatest accuracy (Tab. 2). While others architectures overfit or had not that high accuracy.

Tab. 2. Accuracy matrix for: first, fourth and seventh architecture

Client no.	Architecture no. 1	Architecture no. 4	Architecture no. 7
1	55%	53%	57%
2	74%	77.5%	76%
3	60%	62%	64%
Federated	74%	74%	77%
Entire data set	75%	74%	78.5%

Source: own elaboration

Depending on the actual client, the same architecture could have different accuracy and loss function values (Tab. 3). However, if all clients were federated, much better results were obtained. Compared to a network that used an entire dataset, federated learning came very close to accuracy.

Tab. 3. Loss function matrix for: first, fourth and seventh architecture

Client no.	Architecture no. 1	Architecture no. 4	Architecture no. 7
1	2.4	3	2.2
2	2.3	0.79	0.6
3	5.5	1.8	1.5
Federated	0.75	0.6	0.5

Source: own elaboration

Additionally, the seventh architecture has been chosen the best because of low loss function values and better accuracy for one and three used clients.

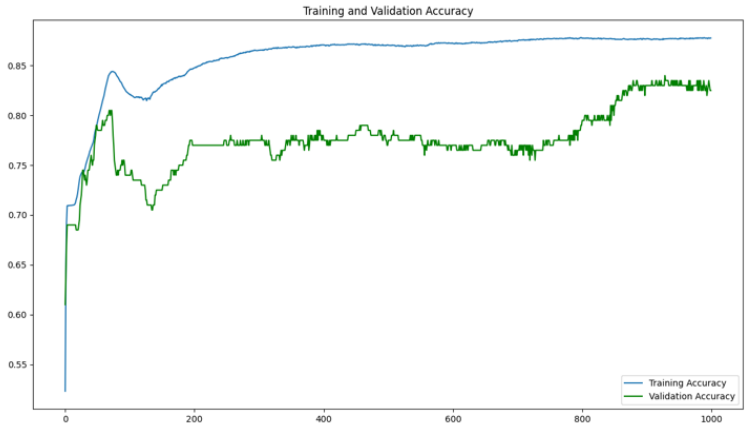

Fig. 4. Training and validation accuracy graph for seventh architecture
Source: own elaboration

The last step in evaluating architectures was determination of the AUROC value. For the seventh architecture, the value was 0.794. Where if AUROC = 0, it means random classifier, AUROC = 1 means ideal classifier.

Conclusions and future works

From all the created architectures, the seventh was the best, which consist of: layer with 10 outputs and ReLu as an activation function, layer with 5 outputs and ReLu as an activation function and layer with 1 output and sigmoid as an activation function. This architecture has 77% accuracy, which is a good result considering the amount of data gaps.

The accuracy could be higher if data contained fewer data gaps or if data sets from more universities would be available. Data gaps were filled with 0 as a value, but it could be done differently, such as arithmetic mean for course. Future research will attempt to analyse the effectiveness of the model using various techniques for overwriting deficiencies.

Another problem that occurred during the creation of the solution was the choice of the aggregation operator. The arithmetic mean was chosen, but this is not the only way. As part of future research, an attempt will be made to analyse the effectiveness of the model using different aggregation operators.

The third problem that arose during the design of the solution was the choice of artificial intelligence method, as part of future research, an analysis of other available methods will be performed.

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REACTION BETWEEN SYNTHETIC FIBERS (POLYESTER) AND WATER SOLUTIONS OF VARIOUS pH VALUES UNDER THE INFLUENCE OF THE UV-A RADIATION

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Abstract:

The increasing awareness of the risks associated with the use of plastics calls into question their safety when stored in the open space. Under these conditions, plastics are exposed to physical and chemical factors, such as UV radiation (sunlight) and changing pH conditions caused for example by precipitation. Therefore, the question arises whether the described conditions do not lead to the depolymerization of plastics and do not lead to a chemical reaction in which by-products of the decomposition of plastics are formed. Another important question that arises in the discourse is whether these factors can help in the disposal of plastics. This paper presents the effects of UV-A radiation and extreme pH values on polyester fibers. The test results clearly show that polyester fibers are characterized by high resistance to physical and chemical factors, and thus their decomposition as a result of their operation is negligible. No decomposition reaction results in no reaction by-products.

Keywords:
environmental protection, chemical sciences, polyester, degradation of synthetic fibers, plastics

Introduction

Polymers are chemical compounds synthesized in the reaction of polymerization occurring between monomers. The monomer is a chemical compound that has two or more functional groups. Polymers are widely implemented in all kinds of industries, for instance, the clothing industry, which sees an increase in yearly production. In 2015, worldwide clothing production was 84 million tons, of which 52 million tons comprised synthetic materials (the most common being polyester) [1-3].

The increase in the production of clothes, one of the ingredients of which is polyester, results in a simultaneous increase in polyester waste. The increasing quantity of waste is a cause of the increased quantity of products of polyester decomposition. This product is an environmental hazard. The depolymerisation is set under the influence of UV radiation and pH changing due to the precipitations. The question is how products made of polyester behave during depolymerization under UV and pH.

In Poland in 2021 were used 106.50 tons of synthetic materials and were produced 13 674k. tons of municipal waste. 34 % of municipal waste was a plastic. It shows, that a big problems is production of plastics on a global scale. Thats fact make a problem with waste going to landfill sites and compels to search for methods of faster degradation materials [4-5].

Plastic does not biodegrade, that is in arrears in landfill sites for a long time. The one of the degradation methods of polymers are photodegradation. Exposition of UV radiation leads to overcome the bonds between carbon atoms. This fact causes a change physical properties of the polymers. Therefore, research to determine the rate of polymer degradation is a major challenge [6].

Materials and methods

Pre-experimental part included: the preparation of the Microclima 1000 (Snijders, BV, Netherlands) chambre to storage the sample, installation of UV lamps, compilation and preparation of laboratory equipment. The stage of preparation and execution of the research lasted from December 13, 2022, until April 19, 2023, and included the research planning stage, during which the experiment was designed. The following stage included the preparation of the polyester samples with dimensions of 2.5 x 3.0 cm and weighing all sample with analytical balance for testing and the preparation of solutions of hydrochloric acid (HCl) and sodium hydroxide (NaOH) with a concentration of 0.1; 0.0001 mol/dm³. More concentrated solution (0.1 mol/dm^3) was prepared of a weighted amount of an acid and made up to volume with deionization water. Preparing dilutions is method, that make less concentrated solution (0,0001 mol/ dm^3). All solutions were prepared in a glass volumetric flask.

The samples prepared in this way were placed in glass Petri dish with previously prepared solutions of volume 0.02 dm^3. The prepared polyester samples were submerged in solutions of hydrochloric acid (HCl) with a concentration of 0.1 mol/dm³ and 0.0001 mol/dm³, which respectively corresponds to pH = 1.0 and 4.0, and in solutions of sodium hydroxide (NaOH) with a concentration of 0.1 mol/dm³ and 0.0001 mol/dm³, which respectively corresponds to pH = 13.0 and 10.0, as well as in deionized water with an approximate pH = 6.0. At last, all sample series were protected with Parafilm in order to restrict evaporation of solutions.

In the second stage of the research, the samples were placed inside a Microclima 1000 (Snijders, BV, Netherlands) chamber, where they were exposed to UV- A radiation of various intensity (Tab. 1), in series, alternately with the period without irradiation. The chamber had a constant temperature of 25.0 ºC in the first period of irradiation and 30.0ºC in the remaining periods.

In the last stage, the samples were taken out of the Microclima 1000 (Snijders, BV, Netherlands) chamber and the acid and alkali solutions in which they were located during the previous stage of the study, washed with deionized water and drained. The samples were examined on spectroscopy ATR-FTIR (Attenuated Total Reflactance-Fourier Transform Infrared) on a Spectrum Two (PerkinElmer, USA) spectroscope . During the tests, a wavenumber of 400 to 4000 cm^{-1} and a pressure of the sample of the diamond crystal of approximate value of 100 N/m was applied.

Tab. 1. Solar irradiation period

Date	Hight [cm]	Temperature [°C]	UV intensity [W/m]
23.12.2022- 04.01.2023	darkness	25.0	-
04.01.2023- 24.01.2023	12.30	30.0	8.898
24.01.2023- 25.01.2023	darkness	30.0	-
25.01.2023- 01.02.2023	14.60	30.0	8.120
01.02.2023- 14.02.2023	17.70	30.0	7.485
14.02.2023- 21.02.2023	20.70	30.0	6.686
21.02.2023- 27.02.2023	23.70	30.0	6.652

Source: own elaboration

Results

Based on the tests of polyester samples, it was shown that no new chemical bonds appeared on the surface of the polymers, and therefore no new chemical compound was found, contrary to the material control. The material control was polyester, which was not susceptible to various chemical and physical factors.

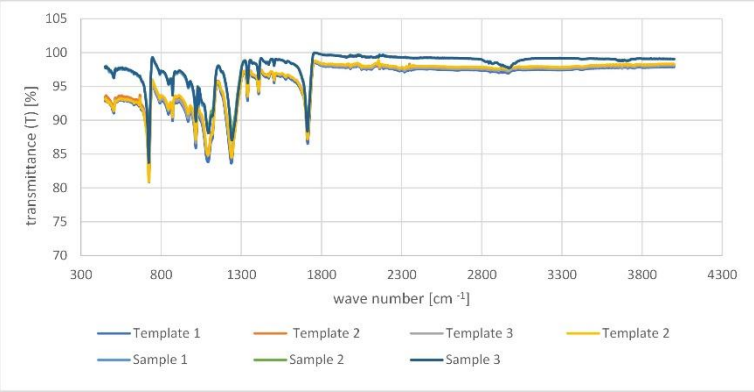

Fig. 1. FTIR spectrum reaction polyester fibers and deionisation water
Source: own elaboration

According to the information one can extract from the FTIR spectrum (Fig. 1), one can see no exception from all the four patterns used as a reference material.

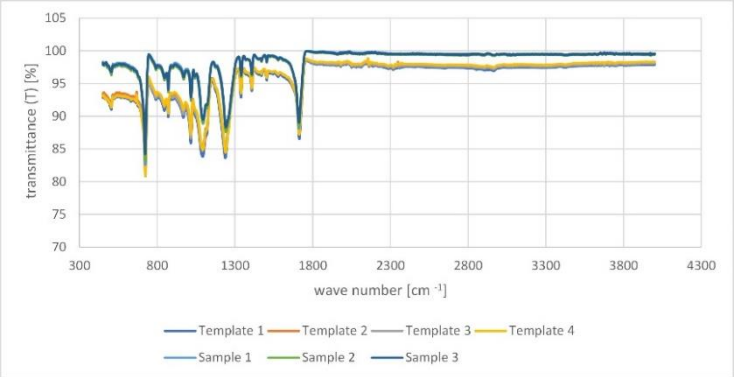

Fig. 2. FTIR spectrum reaction polyester fibers and aqueous solution of hydrochloric acid (HCl) with a concentration of 0.1 mol/dm^3
Source: own elaboration

The spectrum of the reaction of polyester with an aqueous solution of hydrochloric acid (HCl) with a concentration of 0.1 mol/dm^3 (Fig. 2) does not allow to identify the reaction symptoms of the used compounds under the influence of UV-A radiation.

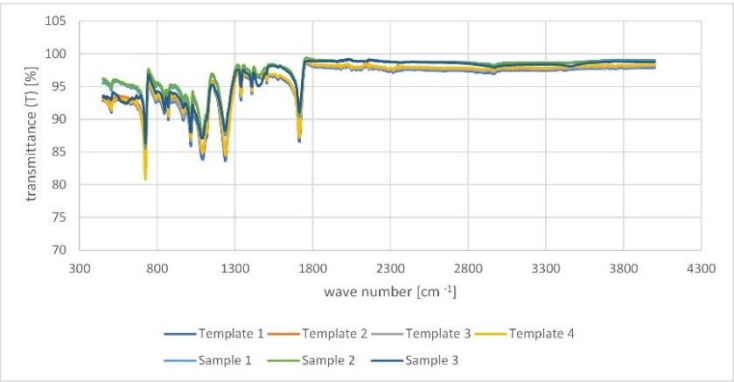

Fig. 3. FTIR spectrum reaction polyester fibers and sodium hydroxide (NaOH) with a concentration of 0.1 mol/dm^3
Source: own elaboration

The spectroscopic FTIR spectrum (Fig. 3) gives a picture which indictes no symptoms of the reaction between the tested sample of polyester and water solution of the sodium hydroxide (NaOH) with a concentration of 0.1 mol/dm^3 under the influence of UV-A radiation.

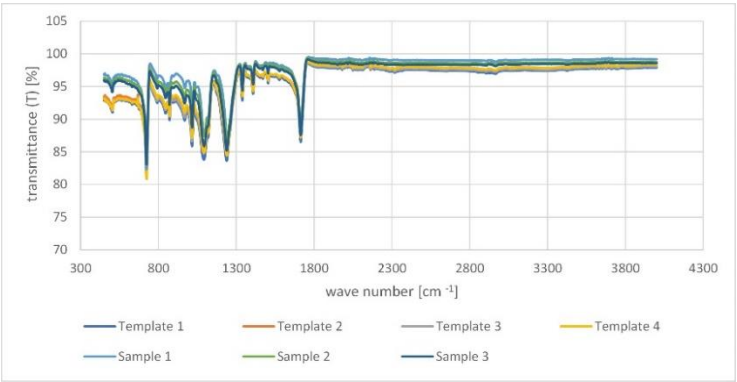

Fig. 4. FTIR spectrum reaction polyester fibers and aqueous solution of hydrochloric acid (HCl) with a concentration of 0.0001 mol/dm^3
Source: own elaboration

No visible change in Fig. 4 (FTIR spectrum) shows that the reaction between synthetic fibers (polyester) and an aqueous solution of hydrochloric acid (HCl) under the influence of UV-A radiation does not take place even with a lower concentration of the solution (0.0001 mol/dm^3).

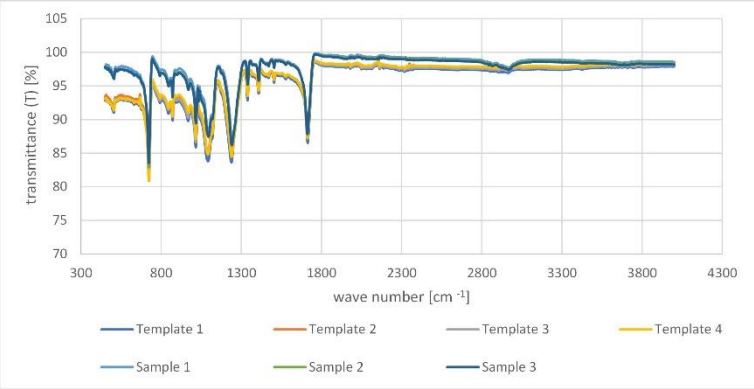

Fig. 5. FTIR spectrum reaction polyester fibers and aqueous sodium hydroxide (NaOH) with a concentration of 0.0001 mol/dm^3
Source: own elaboration

The last presented FTIR spectrum (Fig. 5) presents the approximate reaction between test sample of polyester fibers and aqueous sodium hydroxide (NaOH) (0.0001 mol/dm^3) under the influence of UV-A radiation.

Discussions

The synthetic materials used in the textile industry have a various resistance to photodegradation. Data mentioned in Salerno-Kochan's study [7] show a high UV resistance of polyester fibers, which is later confirmed in the conducted research. Polyester fibers in the our experiments that were carried out, are not damaged, which may be confirmed by the lack of changes in FTIR spectrum of the tested sample.

In her research, Salerno-Kochan [7] paid attention to the hydrolysis reaction. The hydrolysis reaction can do in an inert environment, in alkaline environments and acidic environments too. That fact gives an impression that the depolymerisation reaction should take place in all samples of polyester that were used in tests. No apparent signs of chemical reaction may be caused by new technology production of synthetic fibers or their modification by the production of clothes. Salerno-Kochan [7] ran her test in 2002. From that time, all technology has undergone large-scale modernization. Another important thing is that the chemical reaction of hydrolysis polyesters should be implemented in the minimal temperature of 100 ºC which is highlighted in the report of Salerno-Kochan [7]. We are therefore able to draw useful lessons and acknowledge that lower temperature (30 ºC) does not initiate depolymerization reaction of polyester or significantly slows the reaction down.

Another card relationship we can see in the chemical reaction between the solution of sodium hydroxide (NaOH) and polyester fibers. That reaction can be initiated in the superficial layers of polymers and cannot work in deep polymers fibers. The polymers fibers due to the actions of sodium hydroxide are dissolved. Ellison's [8] test shows the sodium hydroxide (concentration 10.00%) in temperature 60 ºC can dissolve polyester fibers. That chemical reaction suggests that may arise as

a by-product of the reaction. During the test we do not see such dependence. We must know that the environment of the experiment was different in both tests. The concentration of sodium hydroxide and temperature in the environment of reaction are different widely. The differences of the results could be a result of a time difference between tests (40 years). Technological progress may result in a different method of fibre production. That are the factors contributing to a difference between the materials samples.

It should be acknowledged that the conducted research may not be sufficient enough to determine the resistance of polyester fibres to the factors such as the extreme pH indications or UV radiation. The research was time-restricted to 4 months which might have been an insufficient period to indicate an alternation that might have taken place on the surface of the material. This being said, the necessity of further research on that topic is acknowledged.

Conclusions

Based on the obtained results, it can be concluded that synthetic fibers (polyester) do not react with hydrochloric acid with a concentration of 0.1 and 0.0001 mol/dm^3 under the influence of UV-A radiation with the formation of the by-products of its disintegration within 4 months.

The obtained results also confirm that polyester fibers do not produce decomposition by-products as a result of the action of an aqueous solution of sodium hydroxide with a concentration of 0.1 mol/dm^3, and under the influence of a solution with a concentration of 0.0001 mol/dm^3, under the influence of UV-A radiation over a period of 4 months.

It's a chemical process that does not take place between polyester fibers and deionized water by the UV-A radiation per 4 months. It means that in that reaction, the by-products do not arise. During the 4 months discussed, chemical reaction did not occur.

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THE RELATIONSHIP BETWEEN ASSERTIVENESS AND SELECTED PSYCHOLOGICAL AND SOCIO-DEMOGRAPHIC TRAITS

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Abstract:

Assertiveness is an important social competence that significantly contributes to the proper functioning of an individual. The aim of this study was to investigate the relationship between assertiveness and extraversion, shyness, self-esteem, as well as sociodemographic characteristics. A total of 252 adult citizens of Poland (193 females, 59 males), aged 18 to 69, were examined. The Rathus Assertiveness Schedule (RAS), the HEXACO Personality Inventory - Revised subscale for extraversion, a revised shyness scale, and the SES self-esteem scale were used to measurements. Assertiveness was significantly related to extraversion (positive), shyness (negative), self-esteem (positive), and age (positive). A higher level of assertiveness was observed among women, individuals in relationships, and older individuals. The obtained results suggest the importance of fostering assertiveness development among young people, particularly considering its association with self-esteem.

Keywords:
assertiveness, extraversion, shyness, self-esteem, gender

Assertiveness - Problem Characterization

Andrew Salter is recognized as the founder of the assertiveness issue today. Assertiveness is a type of skill that enables social functioning in line with one's own interests without fear. An assertive individual openly expresses their opinions and thoughts while simultaneously respecting the opinions of others. This skill allows a person to live in harmony with themselves and maintain positive relationships with others [1]. Assertiveness has been contrasted by Spencer Rathus with aggression and submissiveness. The result of aggression is the construction of negative relationships with others, despite achieving the goal. Submissiveness, on the other hand, leads to considering others' opinions more often than one's own. Assertiveness strikes a balance between these two attitudes, as it enables the defense of one's own interest without infringing on someone else's dignity [1].

Assertiveness and Selected Psychological Traits

The HEXACO personality structure model, developed by Ashton and Lee, defines extraversion as self-assurance. Individuals with high levels of extraversion are energetic, perceive themselves positively, and derive pleasure from interacting with others [2]. In a study by Averett and McManis [3] involving 103 students, a significantly positive relationship between assertiveness and extraversion was demonstrated. The strength of this relationship was moderate. Similar results were obtained in a study by Hernandez and Mauger [4] using two samples. The first sample consisted of 12 psychiatric hospital patients, 67 students, and 69 state prisoners, while the second sample comprised exclusively 50 psychiatric hospital patients. In both samples, a very similar and significant positive correlation between assertiveness and extraversion was found. In a study involving 84 undergraduate students, including 65 females, 17 males, and two individuals who did not disclose their gender, the results significantly indicated that higher levels of assertiveness were associated with higher levels of extraversion [5]. Similarly, in T. Lobel's study, extraversion showed a significant positive correlation with assertiveness [6]. This same relationship between extraversion and assertiveness was confirmed by a study conducted on 573 pairs of twins by J. Rushton et al. [7].

Shyness, during interactions with others, can manifest as inhibition and restraint in words, negative self-perception, or a general sense of tension. Shy individuals may experience fear and anxiety about being negatively judged by others, which can result in physiological symptoms of distress [8]. Molen distinguishes three components of the shyness syndrome: the emotional arousal component (fear, anxiety), the behavioral component (withdrawal, inhibition, or a deficit in social skills), and the cognitive component (irrational thoughts) [8]. A study by Kirst [5] showed that high levels of assertiveness were associated with low levels of shyness, thus indicating a negative correlation between these two variables. A study conducted on a sample of 336 high school students revealed a strong negative correlation between assertiveness and shyness, both in a group of 212 females and a group of 124 males [9]. Similarly, in a study conducted on a sample of 419 high school students by Ezer [10], shyness emerged as a significant negative predictor of assertiveness.

Self-esteem, as conceptualized by Rosenberg, is a person's positive or negative attitude towards their own self, a global self-evaluation. Individuals with high self-esteem perceive themselves as "good enough" and valuable. Those with low self-esteem exhibit dissatisfaction with themselves [11]. In a study involving 84 undergraduate students, the results confirmed the hypothesis of a positive correlation between assertiveness and self-esteem [5]. The results of a study by Camargo et al. [12] on first-semester students aged 15 to 42 indicated a positive and linear correlation between assertiveness and self-esteem. Similar results were obtained among nursing students, confirming a significant positive correlation of moderate strength between assertiveness and self-esteem [13]. Similarly, findings from a study by Hamraoui et al. [14] on medical students suggest a strong positive relationship between assertiveness and self-esteem.

Age and gender

Crassini et al. [15] conducted a study whose results indicated that men exhibit a higher level of assertiveness than women. Similar conclusions were drawn from the study by Kimble et al. [16], who also pointed out that older individuals have higher levels of assertiveness. Similarly, a study by Onyeizugbo [17] involving 214 married individuals demonstrated that both age and gender differentiate the level of assertiveness. The results showed that younger men have a higher level of

assertiveness compared to younger women. However, older men exhibited lower levels of assertiveness than older women. Eskin's study [18] also confirms that assertiveness increases with age. In a study conducted on a sample of 282 women by H. AlDeghaishem and N. Alsahoo [19], an increase in assertiveness with age was also observed. Gender differences in assertiveness were also noted in the study by Mueen et al. [20]. Their results indicated that men achieve higher assertiveness scores. However, the findings of Ezer's study [10] suggest that women are more assertive than men. Conversely, Hamraoui et al. did not confirm that age and gender differentiate the level of assertiveness in their study on a sample of 336 individuals [14].

Relationship Status

The aforementioned study by H. AlDeghaishem and N. Alsahoo [19] on a sample of women showed that relationship status significantly differentiates the level of assertiveness. Married women exhibited a higher level of assertiveness compared to women without a partner. Hamraoui et al. [14] conducted a study that confirmed that individuals in relationships are more assertive than singles. On the other hand, Devanesam and Saral [21] conducted a study on a sample of 156 women and did not find that relationship status differentiated the level of assertiveness. Similarly, in the previously mentioned study by Mueen et al. [20], conducted on a sample of 100 individuals, the significant role of relationship status in differentiating assertiveness levels was not confirmed.

Siblings

Having siblings can influence the development of various psychological traits. Spending time with siblings allows individuals to learn certain behaviors and how to function in different situations. Siblings can provide an environment that fosters the development of social functions, including assertiveness. In a study conducted by Lasota et al. [22], the positive impact of having siblings on socio-emotional competencies was confirmed. However, the results of Shrestha's study [13] did not confirm that having siblings differentiated the level of assertiveness.

Research Purpose and Hypotheses

Based on the analysis of available literature and observed patterns related to assertiveness, a study was conducted to confirm the relationship between assertiveness and the described psychological factors such as extraversion, shyness, and self-esteem, as well as sociodemographic factors like gender, age, relationship status, and having siblings. Based on the results of previous studies, the following hypotheses were formulated:

H1: There is a positive correlation between the level of extraversion and assertiveness.
H2: There is a positive correlation between the level of self-esteem and assertiveness.
H3: There is a negative correlation between the level of shyness and assertiveness.
H4: Assertiveness levels increase with age.
H5: Assertiveness levels are higher in men than in women.
H6: Assertiveness levels are higher in individuals in relationships.
H7: Assertiveness levels are higher in individuals with siblings.

Method

Sample Description

The study was conducted in July 2023, involving 252 participants, of which 59 were male and 193 were female. The age of the participants ranged from 18 to 69 years (M = 29; Me = 27). Based on the median age, two groups were determined: the "*younger*" group ranging from 18 to 27 years and the "*older*" group ranging from 28 to 69 years. Out of the respondents, 214 individuals reported having siblings, while 38 individuals were only children. Among the participants, 160 were currently in a relationship, 53 had been in a romantic relationship at some point but were single at the time of the study, and 39 had never been in a relationship. The study was conducted using a questionnaire via the Google Forms platform. The questionnaire link was shared on several Facebook groups. The study was fully anonymous and voluntary. Each respondent had the option to discontinue their participation at any time, as they were informed.

Tools

HEXACO-PI-R

To measure the variable of extraversion, the HEXACO Personality Inventory-Revised (60-item version) by Kibeom Lee and Michael C. Ashton was used in its Polish adaptation by Szarota [23]. This factor consists of 10 statements. Participants had to respond to each statement using a five-point Likert scale, where 1 indicated "Strongly disagree" and 5 indicated "Strongly agree". In the present study, the Cronbach's alpha reliability coefficient for extraversion was 0.845.

Self-Esteem Scale (SES)

Self-esteem measurement was conducted using the SES (Self-Esteem Scale) by Morris Rosenberg in its Polish adaptation by Łaguna, Lachowicz-Tabaczek, and Dzwonkowska [11]. This tool consists of 10 statements. Participants had to respond to each statement using a four-point scale, where 1 indicated "Strongly disagree" and 4 indicated "Strongly agree". The internal consistency of the tool, measured by Cronbach's alpha, was 0.916 in the current study.

Revised Cheek and Buss Shyness Scale

The level of shyness was measured using the Revised Cheek and Buss Shyness Scale in its Polish adaptation by Kwiatkowska, Kwiatkowska, and Rogoza [24]. This tool consists of 13 statements. Participants had to respond to each statement using a five-point Likert scale, where 1 indicated "Strongly disagree" and 5 indicated "Strongly agree". The Cronbach's alpha reliability coefficient for this tool in the present study was 0.890.

Rathus Assertiveness Schedule (RAS)

To measure assertiveness, the RAS (Rathus Assertiveness Schedule) by Spencer Rathus was used in its Polish translation by Bogdan Wojciszke [25]. This scale consists of 30 statements. Participants had to respond to each statement using a six-point rating scale, where -3 indicated "Definitely does not apply to me" and 3 indicated "Definitely applies to me". In the current study, the Cronbach's alpha reliability coefficient for this tool was 0.644.

Self-designed questionnaire

Sociodemographic data were collected using a self-designed questionnaire, which included questions about gender, age, relationship status ("currently in a relationship"; "currently not in a relationship, but I have been"; "I have never been in a relationship"), and having siblings.

Statistical Analyses

The statistical software SPSS was used for calculations. The normality of the distribution of analyzed variables was checked using the Shapiro-Wilk test. Correlation analysis was conducted using the Pearson correlation coefficient and the Spearman's rho. The level of assertiveness between genders was compared using the t-test. The same test was employed to check for differences between age groups and between only children and individuals with siblings. Groups categorized by relationship status were compared using the Kruskal-Wallis ANOVA.

Results

The analysis began by checking the normality of the distribution of quantitative variables included in the analyses, namely assertiveness, extraversion, shyness, self-esteem, and age. The variables of assertiveness and extraversion were found to have a distribution consistent with normality. The normality of the distribution of assertiveness and extraversion variables was also checked within groups categorized by gender, age group, relationship status, and having siblings. In each analyzed group, a normal distribution was observed.

To test hypotheses H1, H2, and H3, a correlation analysis was conducted. Assertiveness was significantly positively correlated with extraversion and self-esteem, and significantly negatively correlated with shyness. Descriptive statistics and correlation coefficients are provided in Tab. 1.

To verify hypothesis H4, a correlation analysis was also performed. Assertiveness was significantly positively correlated with age. A comparison between the *younger* and *older* groups was carried out using the t-test, revealing significant differences in assertiveness levels ($t = -3{,}172$; $p < 0{,}001$; *younger* $M = -1{,}31$; *older* $M = 2{,}64$).

The t-test was conducted to verify hypothesis H5, comparing assertiveness levels between genders. Significant differences were found, with higher assertiveness observed in women compared to men ($t = -3{,}137$; $p < 0{,}001$; male $M = -3{,}12$; female $M = 1{,}45$).

Verification of hypothesis H6 required a one-way ANOVA. Differences in assertiveness levels were found between groups categorized by relationship status. Post-hoc tests were conducted, indicating differences between Group I (currently in a relationship) and Group III (never been in a relationship), as well as between Group II (not currently in a relationship but have been in one before) and Group III. The highest level of assertiveness was observed in Group II ($M = 1.21$), slightly lower in Group I ($M = 1.07$), and the lowest in Group III ($M = -3.56$).

A t-test was performed to compare groups with and without siblings in terms of assertiveness levels. The results did not show significant differences.

Tab. 1. Descriptive statistics of the analyzed variables and values of correlation coefficients.

	Variables	M(SD)	Me	Skewness	Kurtosis	Min-Max	W	1	2	3	4	5
1	**Assertiveness**	0.38 (0.627)	0	0.171	0.123	-26-31	0.995	-				
2	**Extraversion**	30.12 (0.558)	30	0.079	-0.572	10-50	0.990	.148*	-			
3	**Shyness**	36.84 (0.744)	38	-0.066	-0.862	13-62	0.979**	-.187**	-.769***	-		
4	**Self-esteem**	28.21 (0.508)	28.5	-0.272	-0.927	10-40	0.958***	.163**	.84***	-.578**	-	
5	**Age**	29 (0.646)	27	1.087	1.137	18-69	0.896***	.185**	.247***	-.259***	.240***	-

W = Shapiro-Wilk test statistic
*p<0.05; **p<0.01; ***p<0.001

Source: own calculations

Discussion

The conducted study and the performed statistical analyses allowed for the verification of the formulated hypotheses. The analysis of the results revealed a statistically significant positive correlation between assertiveness and extraversion, confirming the assumption made in hypothesis H1. This is consistent with the findings of other studies, including Averett and McManis [3], Hernandez and Mauger [4], Kirst [5], and Lobel [6]. Hypothesis H2, which suggests that self-esteem increases with assertiveness, was also confirmed. Similar results are presented in other studies in the literature [5, 12-14]. Hypothesis H3, stating a negative correlation between shyness and assertiveness, was confirmed. This is also in agreement with the results of studies by Kirst [5], Bratko et al. [9], and Ezer [10]. Hypothesis H4, asserting that assertiveness increases with age, was confirmed. The analyses showed a statistically significant correlation. Similar results were obtained in the study by Onyeizugbo [17], Eskin [18], and AlDeghaishem and Alsahoo [19]. As for the assumption that assertiveness would be higher in men than in women, the study yielded different results than expected. Higher assertiveness was observed in women than in men, thus hypothesis H5 was not confirmed. The obtained results contradicted some research findings [15, 20], but were consistent with others [10, 17]. Hypothesis H6, suggesting a higher level of assertiveness in individuals in relationships, was partially confirmed. The highest level of assertiveness was observed in the group of individuals who were not currently in a relationship but had been in one before, while slightly lower in the group of individuals currently in a relationship. The lowest level of assertiveness was observed in the group of individuals who had never been in a relationship. The difference between the group of individuals who were previously in a relationship but not currently and the group currently in a relationship is not statistically significant. However, significant statistical differences were observed between these two groups and the group that had never been in a relationship. The results of the study by Hamraoui et al. [14] also partially align with the hypothesis, showing that individuals in relationships are more assertive than singles. Regarding the assumption of higher assertiveness in individuals with siblings, the analyses showed no statistically significant difference. Therefore, hypothesis H7 was not confirmed. Similar results were obtained in a study conducted by Shrestha [13].

The conducted study, however, does have limitations. Generalizing the results may be challenging due to the non-random nature of the sample. There was a significant gender imbalance among the participants, with a much larger number of women than men. Similarly, there was a significant disparity between individuals with siblings and only children, with more than five times fewer only children. Similar imbalances were present among individuals currently in a relationship, those who were in a relationship before but not currently, and those who had never been in a relationship. Another limitation could be the online survey format, which might have favored younger individuals due to better internet access.

Further research on the topic of assertiveness is warranted, given its impact on an individual's daily functioning. In future studies on assertiveness, it would be valuable to analyze more variables such as lifestyle, quality of interpersonal relationships, or the number of friends. Such data could provide a more comprehensive understanding of the issue of low assertiveness and potentially inform the development of appropriate psychological training programs to enhance assertiveness. Low assertiveness can be a significant problem as it restricts an individual's social functioning and is additionally associated with low self-esteem, as confirmed in this study. Therefore, gaining a better understanding of this issue and developing methods to support assertiveness development is crucial.

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DEVELOPMENT OF POPULATION PATTERNS IN ORDER TO CREATE A SERIES TYPES OF ORTHOSES MADE BY 3D PRINTING

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Abstract:

The currently used methods of supplying patients with forearm injuries is the use of a classic, white plaster cast. Work is underway on the use of 3D printing technology for the production of forearm orthoses. Due to the size of the population, standards should be introduced to unify the sizes of forearm orthoses based on application of 3D printing. This case study presents the implementation of measurement methods and 3D scanning technology to create a 3D model of a forearm brace. The presented concept is based on the performance of population research, the development of a series of types of forearm orthosis sizes as well as the preparation of a 3D model of the forearm to design a 3D printed orthosis in a specific size. It is expected that the developed method will become a solution in the production of standard sizes of orthoses with the help of 3D scanning technology using for this purpose an industrial 3D printing system in the field of production of orthopedic supplies intended for the treatment of forearm injuries.

Keywords:
3D printing, 3D scanning, CAD, 3D model, forearm orthosis

Introduction

Forearm injuries account for more than 1/6 of all injuries in the human body. The approximate number of forearm injuries in the European Union is almost 3 million per year [1]. In Poland, it is about 250,000 injuries per year [2]. These numbers are constantly increasing due to the aging of the population, which is related with an increased risk of fracture. In addition, according to Eurostat data for 2021, the average number of doctors per 1,000 patients in the European Union is 3.9, and nurses are 8.4, which transfers to the time devoted to a patient admitted to hospital [3]. The total duration of the procedure of supplying a patient after a forearm injury lasts more than 2 hours (mainly due to the time-consuming application and drying of the plaster cast), requires the involvement of at least

two medical personnel (doctor, nurse) and the use of a emergency room during this time. The Globenewswire report "Casting and Splinting Market Size To Reach USD 4,052.0 Million By 2027" indicates a CAGR of -6.1% and the value of the orthopedic supply market at over $4 billion by 2027 [4].

Currently, the path of a patient with an orthopedic injury at the Hospital Emergency Department, including in Poland looks like this: after providing personal data by the patient, establishing his medical history, he is assessed in the triage system, which means how quickly help will be provided. The patient is then consulted by an orthopedist - interview, physical examination, ordering basic tests and X-rays, possible administration of painkillers depending on the needs. In temporary supplies, e.g. in a triangular bandage, he goes to the radiology department, which is located on the premises of the hospital (often the distance is several hundred meters and is related with the need to move to another building), there he waits in the queue to enter the X-ray machine. After taking the X-ray picture, he returns to the hospital's emergency department. This all takes time, usually about an hour, often much longer. Then the patient goes for another visit to the orthopedic doctor, where, based on the X-ray image, a decision on further treatment is made:

- attempt to set the upper limb (applying a plaster cast, i.e. non-surgical treatment). If everything went well, the patient is discharged home and continues treatment.
- decision on surgery - if there is a fracture multi-fragment or X-ray image obtained is of poor quality, or the bone fragments have moved after setting the upper limb, it is possible to order a Computed Tomography or a decision on surgery is made.

In the course of these activities, there are added costs related to the application of orthopedic equipment (usually white classic plaster), labor costs of medical personnel, operating costs of the treatment room, costs related to the application and removal of the cast, costs of medical staff tools, patient treatment costs, related to the X-ray, the costs of disposing of the plaster cast, which range from PLN 1,200 - 2,000 per patient, and the exclusion of the patient from full activity for a period of up to 12 weeks.

Therefore, attempts are being made to replace the plaster cast with alternative solutions, such as forearm orthosis made in 3D printing technology. Such a product is characterized by high durability, fit to the patient's forearm, easy to put on and photos of the orthosis, easy diagnosis of the patient due to the translucency of the structure (if an X-ray is taken in the orthosis, it is possible to see all bone fragments and assess the patient's condition); water resistance, lightweight construction (up to 3x lighter than white plaster cast); creating holes to ventilate the skin, which transfers to monitoring the patient's forearm, e.g. checking whether the hand swells. In the projected expenses, the procedure based on the use of 3D printing technology (creating forearm orthosis) would reduce the patient's service costs to PLN 800 and exclude the patient from full activity for a period of up to 6-8 weeks.

In the case of personalized orthoses made by 3D printing, the patient must be 3D scanned and the orthosis is designed based on the 3D model of the forearm (STL model), this process can take up to several hours [5], and then the patient waits for the orthosis to be made, which takes several up to several dozen hours [6].

Therefore, attempts have been made to standardize the process of creating orthoses based on 3D printing technology [5].

In order to use size groups, it was necessary to determine the size of the outer structure of the orthosis for the patient's forearm. It was decided how many different sizes of outer sizes of orthoses to prepare. To determine the size of the outer orthosis, measurements near the wrist, such as wrist circumference, hand length, and forearm length, were measured based on body size measurement data conducted by the Korean government in 2010 [7].

This study was limited to adults between the ages of 20 and 30 and limited the measurement area to wrists only. As shown in Tab. 1, average size close to the wrist in men, it varies by about 12 mm in standard deviation by age and by less than 10 mm for women. Other dimensions, such as outer hand size, hand length, and forearm length, were also analyzed from the measurement data. For the size of the outer hand, the standard deviation difference for men it was 9 mm and for women it was also 9 mm. Based on this data, it was expected that if the outer case could accommodate a 20 mm difference in wrist size, it would be sufficient. If the wrist radius has been established in the range of 28 mm to 32 mm, the outer wrist size would be 175.8 mm to 200.9 mm, and the difference would be 25.1 mm. Therefore, it was decided that the radius of the outer casing would differ by a maximum of 4 mm. In other words, three sizes of outer casings that are perpendicular to the direction of the section, plus and minus 2 mm from the standard, are acceptable in the case of a difference in wrist sizes.

Accordingly, the size of the outer case is divided into three types (large, medium, small). The difference between each type was 2 mm in this case. The difference in the size of the outer casing created a gap in the inner frame. This gap acted as a buffer for personal differences in the size of wrists, hands and forearms.

Tab.1. Measurement of forearm parameters carried out in Korea in 2010 [5]

Sex	Age	N	Mean	S.D.
Male	20-24	133	171	8.22
	25-29	122	181	10.95
	30-34	100	179	11.41
	35-39	103	178	11.87
	All	438	178	11.28
Female	20-24	108	160	9.18
	25-29	100	160	8.29
	30-34	101	158	8.07
	35-39	101	159	10.09
	All	410	159	8.95

(Source : 6th Report of Size Korea 3D-scan Measurement Project)

Similarly, in the case of faces, an update of existing data was carried out because it was based on anthropometric data collected more than 30 years ago. In order to reflect the diversity of the current U.S. employment relationship, it was necessary to adapt these patterns to current demographics.

Anthropometric studies were conducted on a group of 3,997 respirator users in order to collect data on the current population of employees. 1,013 people were examined using a 3D scanner, which allowed for accurate facial dimensions for each category.

Five digital 3D head models were developed that represent the categories of small, medium, large, long/narrow and short/wide. These models can be used in respirator research, certification standards and design to reduce the risk of injury or illness from hazardous substances inhaled by workers [8].

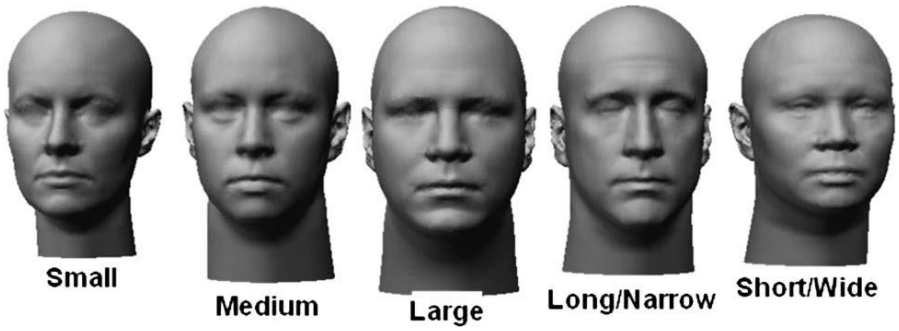

Fig.1. 5 digital head models created as part of research done in the USA
Source:[8]

Therefore, it is necessary to develop more accurate population patterns that allow the development of size standards for orthoses made by 3D printing. Then after measuring the circumference of the patient's forearm, they will allow you to choose the right size of the orthosis, which can be put on the patient instead of the traditional white cast. The new orthosis concept should have features that ensure easy size selection and an adjustment system in the circumference of the forearm and have a light and airy structure that allows you to monitor the patient's condition.

Methodology

The study was carried out as part of the research and development project of Mediprintic sp. z o. o. in which the main author is pursuing an industry doctorate in order to collect data for designing forearm orthoses made by 3D printing. The study was conducted in two parts.

The first part of the study concerned the measurements of forearm circumferences made with a tailor's meter to collect numerical data of the measured forearm parameters. The study measured thumb circumference, thumb circumference at base, knuckle metacarpal circumference, diagonal metacarpal circumference, wrist circumference, hand length, length from fingertips to shoulder joint, circumference in front of forearm, elbow circumference, bicep circumference, length from wrist to the elbow joint, circumference in the middle of the forearm, circumference in front of the shoulder. For statistical purposes, measurements were taken of both the left and right forearms. The key parameter that was taken into account was also the patient's height.

The second part concerned the performance of a 3D scan of the forearm in the straightened and bent position.

Fig. 2. the position of the forearm during the examination, on the left an example of the forearm in a straightened position, on the right an example of the forearm in a bent position

The study was conducted on a group of 73 volunteers - 56 men and 17 women. The age of the people taking part in the study was in the 17 - 81 age group. The study was conducted on healthy people. In the past, 3 people on whom measurements were taken suffered forearm injuries in the past, however, this did not affect the measurement results in any way.

As part of the manual measurements of the forearm, measurements were taken on 73 people using a tape measure on their left and right forearms, which resulted in the collection of 146 measurements. The measurements are presented in the following figures:

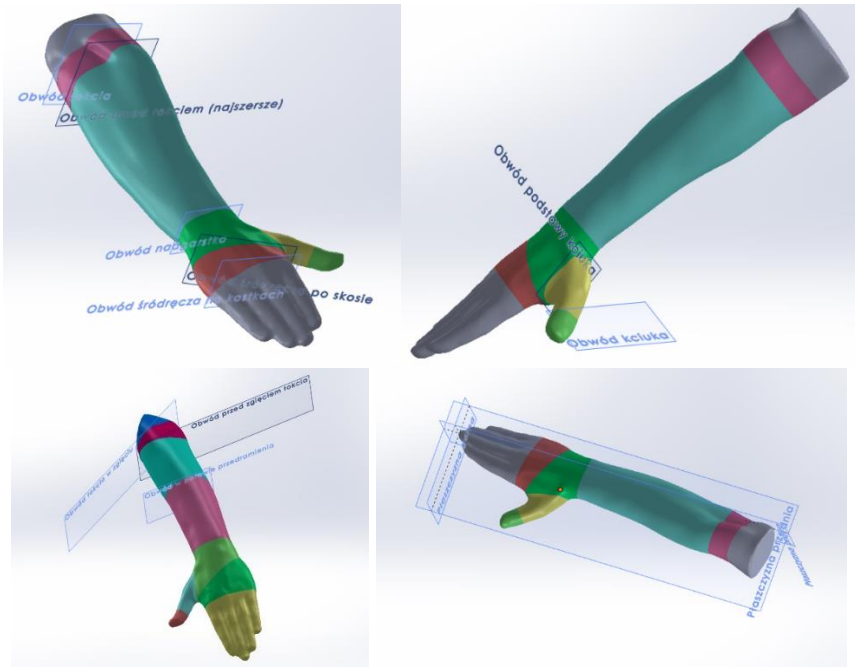

Fig. 3. designated areas for measuring circumferential parameters of the forearm

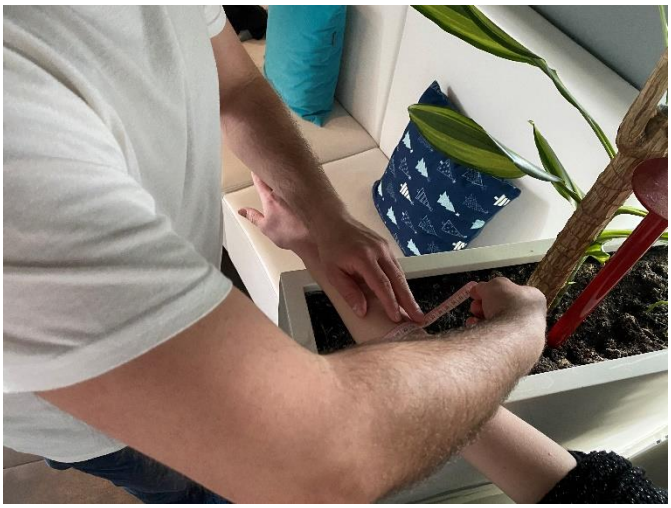

Fig. 4. Taking measurements of the forearm using a tailor's tape measure

For the 3D scans of the forearms, a handheld 3D Artec EVA scanner was used, using white structured light with resolution parameters up to 0.2 mm, accuracy up to 0.3 mm/m, exposure time 0.0002 s, working distance in the range of 0.4 - 1 m to the measured object [9].

The procedure of 3D scanning of the people subjected to the study consisted in the first place in preparing the station for scanning the forearm:

1. Chair/armchair/stool without armrests;
2. A tripod supporting the patient's hand in a stable position;
3. Safety glasses/sunglasses due to the white flashing light coming from the 3D scanner;
4. A laptop connected with a USB cable to a 3D scanner;
5. 3D scanner.

Fig. 5. 3D scanning station

The scanning process was performed in the following order:

1. Preparation of the patient (presentation of forearm positions in which the scanning process took place);

Fig. 6. Forearm positions during 3D scanning

2. Connecting the 3D scanner to the computer and checking the correct operation of the software:
    a. Scanner software settings:
        i. Real-Time Fusion - recommended on (preliminary point cloud merge into a grid of triangles on the real-time scan preview);
        ii. Maximum scan speed - 16 fps (for Artec EVA);
        iii. Geometry & texture – the software is based on texture, so it is worth choosing this option for better scan quality.
    b. The actual 3D scanning process for both hands of the patient:
        i. The scanner should be in the range of 40 - 70 cm from the scanned surface;
        ii. During the scan, manipulate the distance from the scanned surface in such a way that the histogram is in the middle of the vertical graph (green);
        iii. It is recommended to scan the patient's hand first to minimize interference caused by vibration of the patient's hand muscles (mainly fingers).
    c. Checking the correctness of mapping the patient's hand geometry (especially the hand). Repeat the scan if necessary.
    d. Saving data from 4 scans (left straightened forearm, left flexed forearm, right straightened forearm, right flexed forearm);
    e. Data archivization.
3. Importing the project with a set of scans (point clouds) of the patient to the 3D scanner software (Artec Studio 15 Professional).
4. In the case of several fragments of scans showing the same position of the forearm, they should be synchronized with each other:
    a. Function - "Align" (enables automatic alignment of fragments relative to each other, setting scans based on common points, if any, or manual positioning);

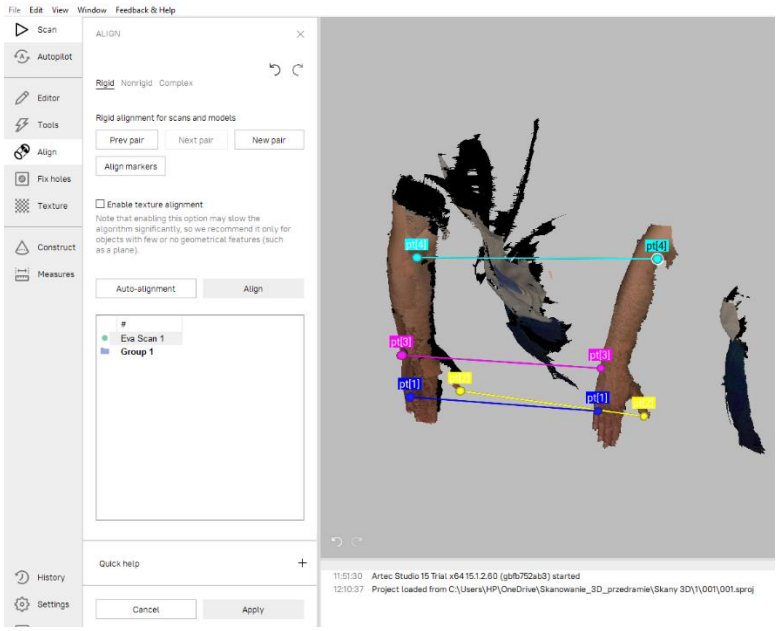

Fig. 7. An example of positioning forearm scans based on common points

5. Then, with an active complete/synchronized scan, go to the "Tools" tab, where you should proceed to align the registered scan frames (Registration):
    a. Rough serial registration;
    b. “Fine registration”;
    c. Global registration (“Global registration”);
        i. The “Downsampling” value should be between 0.3 and 1.
        ii. In the case of several fragments of scans, it is possible to deteriorate the synchronization of point cloud components using the "Global registration" option. In this case, it is recommended to undo the process and skip the global frame registration.
6. The alignment level of the scan frames reflects the "Error" parameter in the right side panel with the list of available scans. The optimal values for this parameter should be within in the range of 0 to 1.

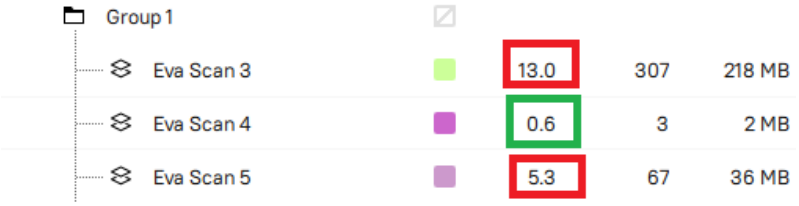

Fig. 8. Example of "Error" parameter value

7. Removal of points from the cloud that are considered interference (not integrated with a larger whole) - "Outlier removal" function with default parameters;
8. Merging a point cloud into a triangle mesh using Sharp Fusion:
    a. "Fill holes" parameter set to "All (watertight)";
    b. In the case of an unsatisfactory effect of merging the point cloud, it is recommended to use the "Smooth Fusion" function with the same value of the "Fill holes" parameter;
9. The actual post-processing of the merged triangle mesh:

a. Separating the hand from the place of arm support - "Eraser" option in the "Editor" tab
b. Depending on the quality of the obtained mesh (scan), various steps are recommended in the final post-processing: cutting out the "traps" of the mesh ("Eraser"), filling holes ("Fix holes" tab), smoothing the surface ("Smoothing brush" tool), filling gaps and removing unwanted geometry ("Defeature brush" tool):

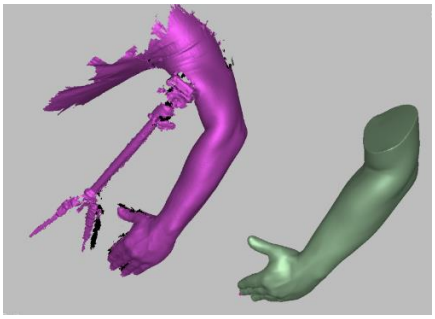

Fig. 9. Triangle mesh before post-processing (left) and the same mesh after post-processing (right)

c. Placement of the scan in the defined coordinate system on the basis 3 points located on the tips: olecranon, thumb and ring finger ("Rough positioning" tool):

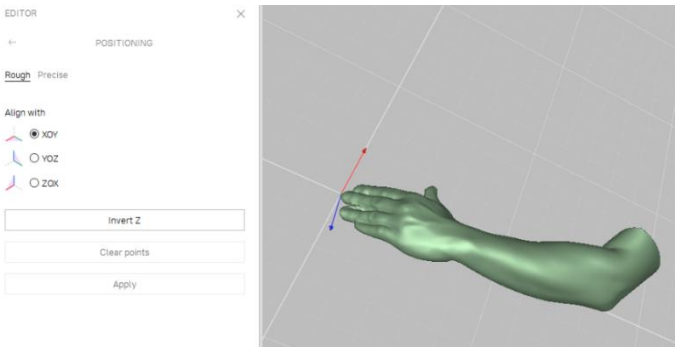

Fig. 10. An example of placing a finished scan in a fixed coordinate system

10. Before exporting the scan, it is recommended to simplify the triangle mesh in order to limit the size of the final file ("Fast mesh simplification" tool)
11. Exporting the finished scan to '.STL' format.

Results

Among the collected data from the measurements of the forearm, the key parameters were distinguished in the preparation of the standard sizes of the orthosis are: metacarpal circumference, wrist circumference, circumference in the middle of the forearm, circumference in front of the shoulder. Among the people taking part in the study, the height of people taking measurements was in the range of 150 - 196 cm.

As part of the conducted research, it was assumed that the main criterion is the dependence of the height parameter of the examined person, which is presented on the X axis, with respect to the circumferential parameters of the forearm, which are presented on the Y axis. For the analysis of these cases, trend lines were used, which reflect the general direction of changes in the data in to

identify patterns and trends in the data. A linear trend line was used to indicate that the dependent value is proportional to changes in the independent value.
In the analyzed cases of dependencies:

1. Height from metacarpal circumference,
2. Height from wrist circumference,
3. Height from the circumference in front of the arm,
4. Height from mid-forearm circumference,

it follows that the above data show a linear upward trend. Thus, it can be indicated that the higher the height, the larger are the circumferences in the forearm of the tested person.

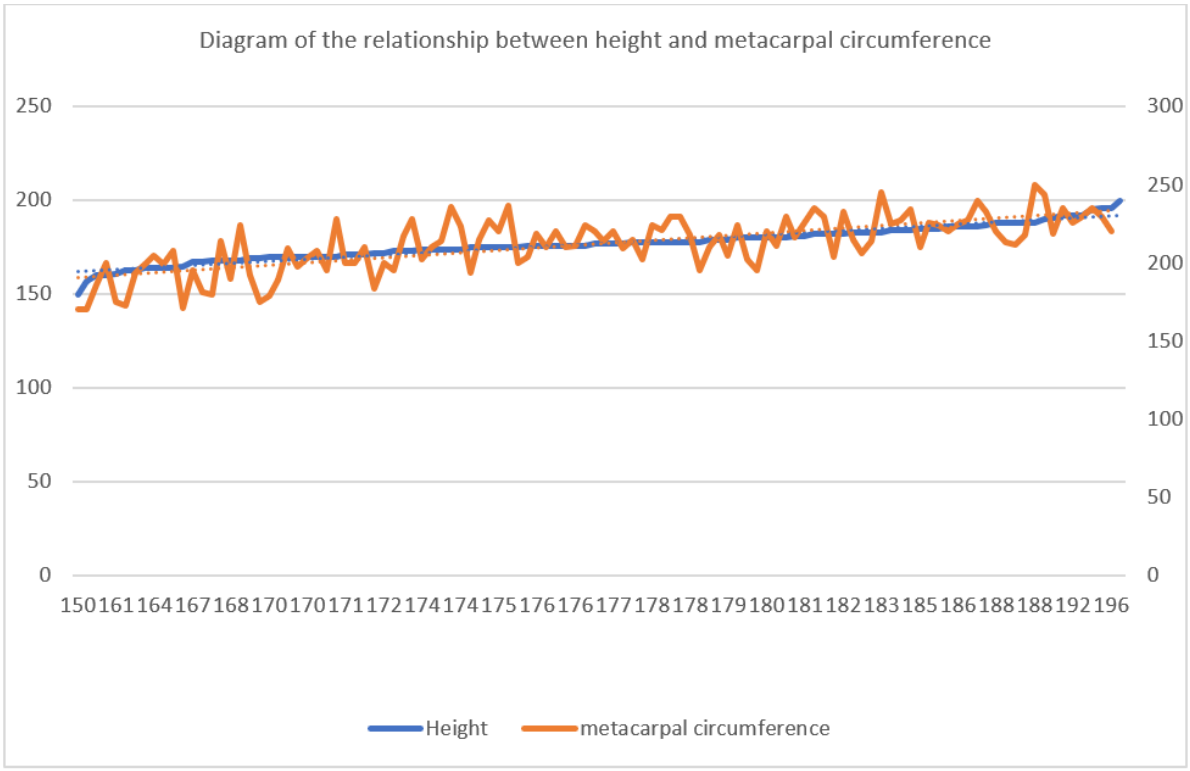

Fig. 11. Graph of growth to metacarpal circumference

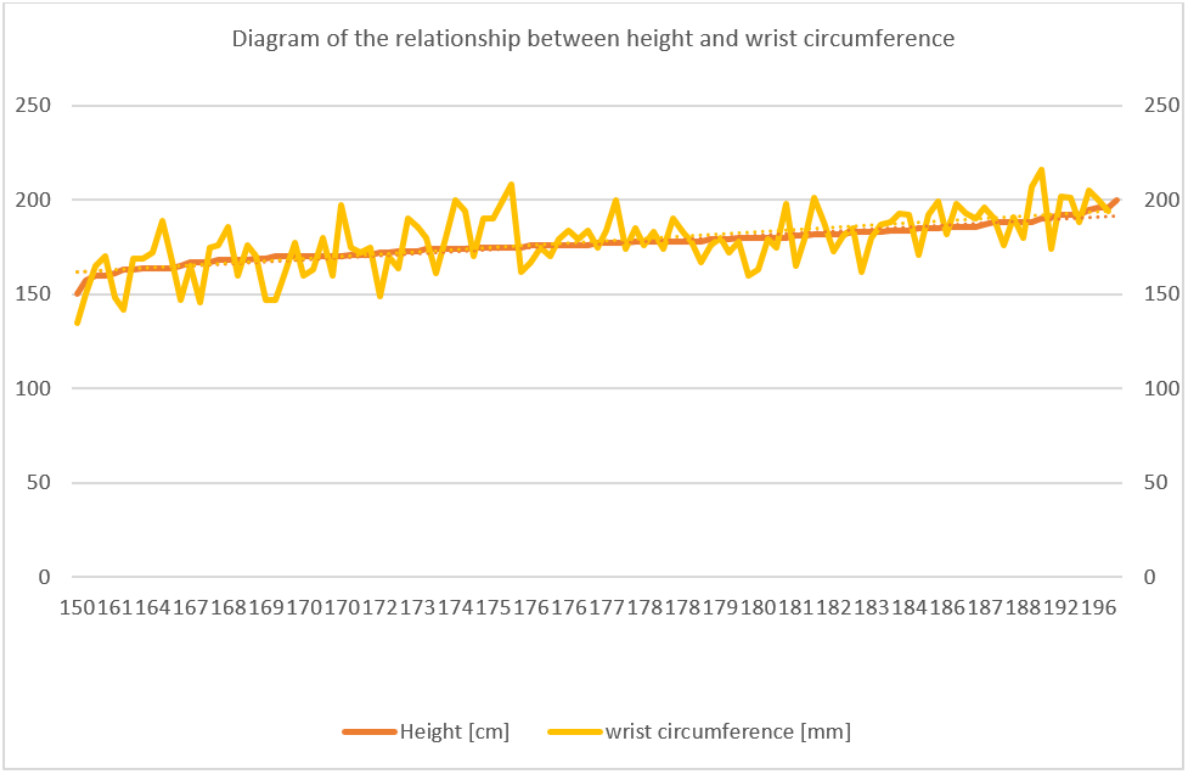

Fig. 12. Growth to wrist circumference chart

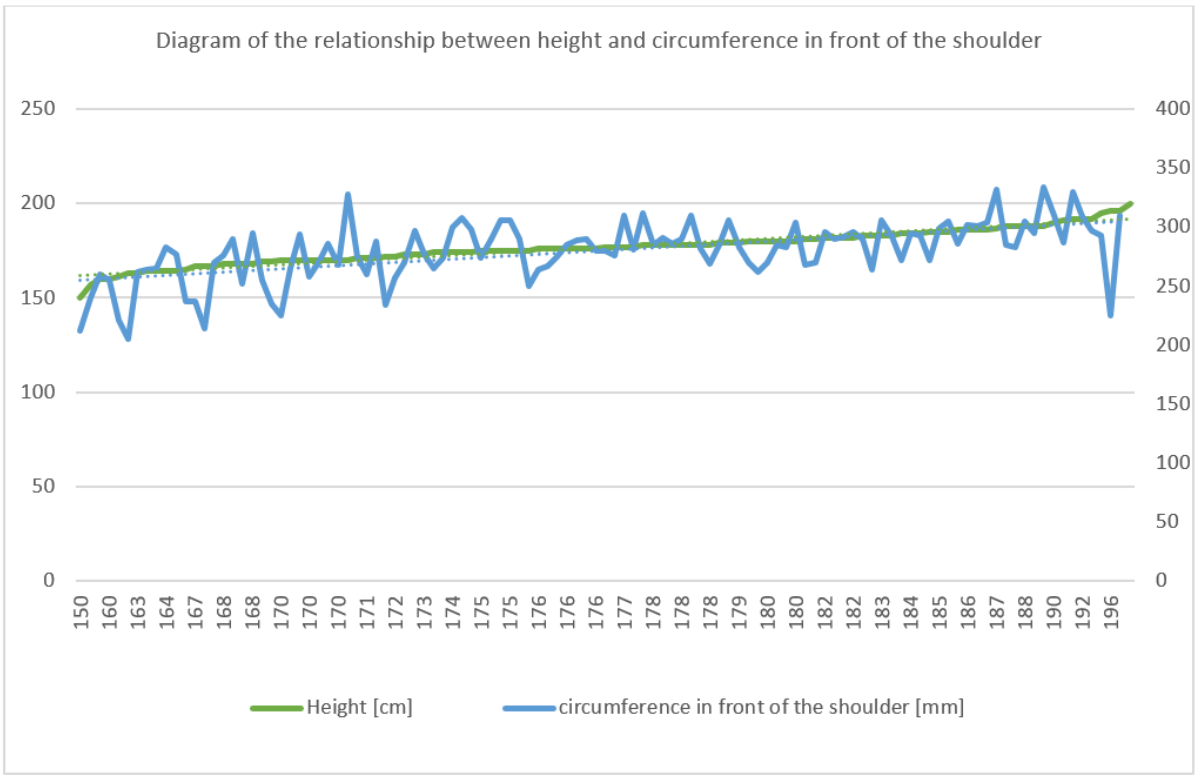

Fig. 13. Graph of the relationship between height and circumference in front of the shoulder

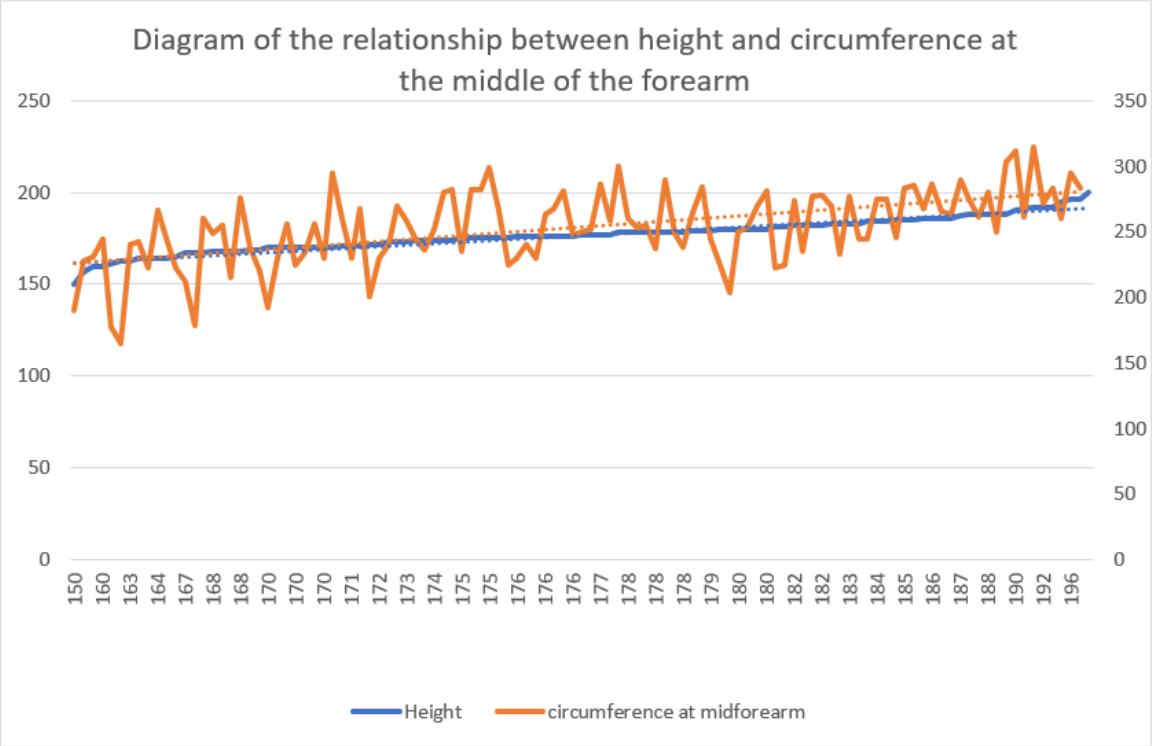

Fig. 14. Graph of the relationship between height and circumference in the middle of the forearm

By analyzing the presented dependences of height on circumferential parameters, a division into three size groups was made, in which the main criterion was the patient's height. The division was based on height up to 166 cm, in the range of 166 - 185 cm and above 185 cm due to significant differences in the circumferential sizes of patients. In addition, it was assumed that for each indicated size group, a circumferential adjustment system of the orthosis should be used in the range of 2 to 3 cm on each side of the forearm circumference.

Tab.2. Division into size groups

Number of people tested		73	
The height range of the examined persons		150-200 cm	
3 basic groups (length division)	**height < 165.9 cm**	**166 < height < 184.9**	**height > 185**
Number of people in the group	11	50	12
Group percentage	14%	69%	17%
Survey numbers	3, 4, 19, 21, 28, 55, 60, 61, 63, 66, 68	1, 2, 5, 6, 7, 8, 9, 13, 16, 18, 20, 22, 23, 24, 25, 26, 27, 29, 30, 31, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 51, 53, 56, 57, 58, 59, 64, 65, 67, 69, 70, 71, 72, 73	10, 11, 12, 14, 15, 17, 32, 48, 50, 52, 54, 62
Size groups	**1 size group**	**2 size group**	**3 size group**

Based on the collected information on size groups, representative examples were selected from each size group, on the basis of which it was possible to proceed to the orthosis design stage. On the basis of selected surveys, 3D scans were selected for the indicated people to design forearm orthoses

based on them. Size S was created for survey 61, size M was selected for survey 7, and size L was selected for survey 12.

Tab.3. selection of representative patients for the development of size groups

Survey number		**Survey 61**		**Survey 7**		**Survey 12**	
parameters	**Forearm**	RIGHT	LEFT	RIGHT	LEFT	RIGHT	LEFT
sex		woman		man		man	
Height [cm]		164		174		188	
metacarpal circumference [mm]		199	191	236	225	212	215
wrist circumference [mm]		169	167	200	200	191	183
circumference in front of the arm (just before the elbow) [mm]		264	262	308	303	305	302
mid-forearm circumference [mm]		242	220	280	270	280	271

Then, the results of measurements from the analysis of individual size groups (group 1, group 2, group 3) for the left and right forearm were compared. A correlation of approximately 0.99 was calculated for each size group. In the case of a correlation of 0.99, it can be concluded that there is a very strong positive relationship between these variables. This means that the variables are very closely related, and when one variable changes, the other variable is likely to change in a similar way.

Tab.4. Correlation of measurement results between the left and right forearms

CORRELATION	GROUP 1 - LEFT AND RIGHT FOREARM
	0.9961
	GROUP 2 - LEFT AND RIGHT FOREARM
	0.9988
	GROUP 3 - LEFT AND RIGHT FOREARM
	0.9991

Based on the collected information, it can be concluded that after designing an orthosis on either side of the hand (left or right), it is possible to create an orthosis design, and then using the mirror image, create a design for the opposite forearm orthosis.

Fig. 15. Example 3D scan of the forearm

Based on selected 3D scans from individual size groups, it is possible to develop a forearm orthosis design for each size group.

Fig. 16. An exemplary designed forearm brace in size S

Discussion

The study indicated the use of forearm measurements in order to collect data on the design of forearm orthoses in relation to the presented publications related to the development of a series of types of orthoses and standardization of sizes. The use of a 3D scanner in the preparation of a 3D model of the forearm in order to create a model of the orthosis in CAD software was evaluated. The problem is the optimal preparation of the station for 3D scanning in order to fully map the forearm in order to match the created 3D model to the real patient's forearm. Implementation is an important factor in the designed forearm orthoses using the 3D printing method, a system that allows adjusting the fit of the orthosis to the circumference of the forearm. The applied solution based on the collection of biometric data allowed for the development of a series of types of orthoses for people between 150 - 200 cm tall in size S, M, L.

However, there are a few things that need to be improved through future research. Firstly, measurements should be made among a larger group of people to confirm the effect of height on the circumference of the forearm. Secondly, it is necessary to verify other solutions in the field of 3D scanning, e.g. use of the 3D Structure Sensor Pro, Curatio Instant 3D Handscanner. In the future, it is necessary to cooperate with various medical clinics to expand research among children and adolescents.

Conclusion

Based on the conducted research, the following conclusions regarding the measurements of the forearm were presented:

1. Measuring with a tailor's meter is hardly reproducible.
2. Due to the width of the tape measure, it is not very accurate when measuring parameters on the bends of the arm or complex surfaces, e.g. the base of the thumb.
3. The value of the measurement depends to a large extent on the force of tightening the tailor's measuring tape around the measured circumference. It is impossible to choose a constant value for this force.
4. The measurement in and around the bends of the arm depends on the angle of the bend of the forearm relative to the upper arm. A measuring station should be developed that will ensure the stability of this parameter and the repeatability of measurements.

5. It is recommended to use in the future, e.g. a digital measuring line (small contact surface with the tested surface).

In the case of using the Artec EVA 3D scanner, the following conclusions were presented:

1. The Artec EVA scanner emits light from LEDs that can cause epileptic seizures in sensitive patients, therefore, it was necessary to wear sunglasses during the measurement.
2. After using a tripod, which was a 1-point support in the middle of the arm (biceps or triceps, depending on the position of the hand), arm tremors were largely eliminated, the patient did not feel discomfort associated with the need to hold the hand in an uncomfortable position for a long time and the scanning process itself per person has been significantly shortened to 5-10 minutes.
3. Thanks to the partial stabilization of the patient's scanned hand, the time needed for post-processing of a single scan was also reduced (less disturbances and inaccuracies in the geometry mapping).
4. Despite the improvement in the accuracy of scans using the 1-point hand support, hand tremors were common, causing inaccuracies and anomalies in the area of the entire hand (even the wrist).
5. Despite the use of 1-point stabilization of the arm, it is recommended to use a second support point in the future (e.g. in the region of the 2nd phalanx of the little finger for a straight hand).
6. When scanning the forearm, it is recommended to map the hand with the fingers first in order to reduce hand muscle tremors to some extent (the longer the scan, the greater the chance of disturbances related to the movement of the hand in relation to the initial position).
7. It is not recommended to scan objects against bright light.
8. The patient should not wear checkered clothes during the scan.

Funding

1. 1.1.2 PARP Startup Platform POPW.01.01.02-18-0084/20 "Application of personalized orthoses, medical setter and 3D scanner in a modified method of treating forearm injuries"
2. Activity 1.3: R&D works financed with the participation of capital funds sub-activity 1.3.1: Support for research and development projects in the preseed phase by proof of concept funds - BRIdge Alfa "Development of a functional prototype of a device for setting the forearm and a medical scanner allowing for the collection of biometric data for the design of forearm orthoses".

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PROMOVENDI

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