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CONTENTS

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Analysis of trace elements accumulation in some landscape plants as an indicator of pollution in an urban environment: Case of Ankara

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Abstract: As a result of the increase in structure and population densities in urban areas, many problems arise in cities that need to be solved. With the effect of keeping the planned approaches to air pollution in the city's background, urban air pollution has started to feel serious with the adverse effects it has created on living things. Heavy metals, which are one of the components of air pollution, seriously threaten living things because they cannot be eliminated from metabolism. For this reason, heavy metal pollution should be monitored in order to make the necessary interventions. The research aims to interpret the trace element level by using *Cupressus sempervirens* L. *Thuja occidentalis* L. *Platanus orientalis* L. *Prunus cerasifera* Ehrh. and *Photinia serrulata* Lindl. plants in the city center of Ankara as biomonitors. In this context, variance analysis was performed on lead and cadmium concentration levels with the SPSS package program. The mean values were subjected to the Duncan test for multiple comparison purposes. The difference in the accumulation levels of plant species and organs was revealed due to the research.

Keywords: Urban Air Quality, Trace Elements, Accumulation, Biomonitoring, Ankara

Öz: Kentsel alanlarda yapı ve nüfus yoğunlukların zamanla artmasının bir sonucu olarak kentlerde pek çok çözülmesi gereken sorun ortaya çıkmaktadır. Kentlerde hava kirliliğine yönelik plan yaklaşımlarının geri planda tutulmasının etkisiyle kentsel hava kirliliği, kendini canlıların üzerinde yarattığı olumsuzluklar ile ciddi bir şekilde hissettirmeye başlamıştır. Hava kirliliği bileşenlerinden biri olan ağır metaller metabolizmadan tamamen atılamadığından canlı yaşamını ciddi bir şekilde tehdit eder. Bu nedenle gerekli müdahalelerin yapılabilmesi için ağır metal kirliliğinin izlenmesi gerekmektedir. Araştırmada Ankara kent merkezinde yer alan *Cupressus sempervirens* L. *Thuja occidentalis* L. *Platanus orientalis* L. *Prunus cerasifera* Ehrh. *Photinia serrulata* Lindl. Bitkilerinin biyomonitör olarak kullanılmasıyla trace element düzeyinin yorumlanması amaçlanmaktadır. Bu bağlamda kurşun ve kadmiyum konsantasyon düzeylerine SPSS paket programıyla varyans analizi yapılmıştır. Ortalama değerler çoklu karşılaştırma yapılması amacıyla Duncan teste tabi tutulmuştur. Araştırma sonucunda, bitki türü ve organların birikim düzeylerinin farklılığı ortaya konmuştur.

Anahtar Kelimeler: Kentsel Hava Kalitesi, Eser elementler, Birikim, Biyoizleme, Ankara

1. Introduction

Urban researches are studies that need to be handled multidimensionally, such as transportation [1-3], urban design [4-8], urban economy and development [9-11], landscape planning [12, 13], urban policy [14, 15] environment and infrastructure [16-18]. Increasing the quality of life in cities, which constitutes the main stage of daily activities in today's conditions, depends on determining the sources of the problems and interventions [19]. The main reasons for reducing the quality of urban life can be counted as population density, various industrial activities, use of poor quality fuel, the density of traffic, and the use of chemical products harmful to nature in many areas [20-23]. Problems such as climate change, global warming, and air pollution that arise from these problems affect all ecological systems [24, 25]. Air pollution, which is one of the problems that occur, is highly affected by the release from sources, the behavior of pollutants in the atmosphere, their transport by wind, and the silhouette and morphology of the city that cause their accumulation [26, 27]. In this context, air pollution research is of vital importance in terms of urban planning.

The accumulation of air pollutants on various living things can represent air quality on an urban scale. To determine the effect of air quality on living things, it has become very important to determine how far they have been moved and their accumulation levels, starting from their source [28]. However, the detection of pollutants in metropolitan cities is a complex research topic [29]. Among the main reasons, many externalities, such as the fact that it cannot be followed instantly, cannot be detected at the source, and the effect of weather events (such as meteorological movements) on the accumulation affects the atmospheric accumulation. Therefore, various studies are being carried out to use some species as biomonitors since it is difficult to monitor and the cost is high. Furthermore, heavy metals from these pollutants are

hazardous in high concentrations as they can have a toxic effect [30]. However, the direct measurement of heavy metals in the air does not provide enough information in terms of environmental impact and monitoring [31, 32].

Some materials such as mosses, indoor plant species, and the rings and organs of perennial trees used in landscape afforestation were used in some studies. High concentrations of metals that can accumulate in these species have been found. However, they have found that various heavy metals can get in multiple areas at a higher rate than others. For example, the differences between the element types found at the industrial sites and the metals found in the areas with high traffic indicate that passive sampling is appropriate in the search for a method. These papers have shown the absorption capacity of accumulation varies between species [33, 34]. Therefore, it is essential to investigate the suitability of the species that can be preferred as biomonitors for the selection of target pollutants. This study was aimed to determine the accumulation levels of Lead (Pb) and Cadmium (Cd) in the organs of 5 different landscape plants in areas with heavy traffic in the city center of Ankara.

2. Material and Method

This paper is conducted on the species grown in the urban center of Ankara, where the traffic is dense. In selecting the study area, the traffic's multi-port and low flow rate were taken into account. Samples were collected from *Cupressus sempervirens* L. (SCs), *Thuja occidentalis* L. (STo), *Platanus orientalis* L. (SPo), *Prunus cerasifera* Ehrh. (SPc) and *Photinia serrulata* Lindl. (SPs) plant, which is frequently used in landscape studies. Samples are from the last year's exile. They were collected in late October towards the end of the vegetation season of 2021, bagged and labeled, and brought to the laboratory. It was then dissected into organs without the use of metal tools. Some of the bark and leaves have been washed. After rinsing with distilled water, all samples were labeled.

In the next stages of the study, The US EPA 3052 was used to apply the method. Organs, leaf, bark and wood samples were also shown with their codes. Labeled samples were kept at room conditions for two weeks after pretreatment without being exposed to direct sunlight. It was then dried in an oven at 45°C for two weeks.

The dried plant samples were ground into powder and weighed 0.5 g, and placed in tubes designed for microwaving. 10 mL of 65% HNO_3 was added to the samples. The prepared samples were then burned in a microwave device at 280 PSI and 180 ºC for 20 minutes. After the processes were completed, the tubes were removed from the microwave and left to cool. Deionized water was added to the cooled samples to make up to 50 ml. After the prepared samples were filtered through filter paper, they were read at appropriate wavelengths in the ICP-OES device. The obtained values were multiplied by the dilution factor, and the element concentrations of the study were calculated.

SPSS program was used to compare the mean values of the analyses performed with three repetitions. Analysis of variance was applied to the data. Homogeneous groups were obtained by applying the Duncan test to statistically different groups, at least at the 95% confidence level. The analysis results are expressed with F values in terms of the storage capacity of the plants.

3. Results

When the high concentration Pb values obtained within the scope of the study were examined among the species, high values were obtained in SPc in Table 1. Although the lowest accumulation among the organs was in the wood, the accumulation level in SPc was relatively high with 6726 ppb. While the lowest value in wood was obtained with 877.66 ppb in SPo, it was found at 6995.2 ppb in outer bark and 6255.53 ppb in leaf. When ranking from high to low in terms of the values of Pb among the organs, they are listed as outer bark, leaf, and wood.

Table 1. Deposition of Pb concentrations (ppb) based on organs

Species	**Organ**			***F* value**
	Leaf	**Bark**	**Wood**	
SCs	8738.46 Cde	8881.60 De	2448.66 Ag	32.9***
STo	8702.00 Bcd	8808.40 Dd	1097.86 Ac	51.5***
SPo	6255.53 Cb	6995.20 Ea	877.66 Aa	1156.5***
SPc	9176.46 Ei	8806.33 Dd	6726.00 Ak	
SPs	8843.66 Eg	8688.33 Bc	2092.13 Af	
F value	9169.43***	2338.07***	16905.84***	

*** expresses p<0.001, lower case letters represent vertical directions, whereas capital letters represent horizontal directions.

When the concentration values in the leaf were compared, the highest value was obtained with SPs 28221.93 ppb, while the lowest value was obtained with STo 7953.20 ppb. Regarding values in the crust, the highest accumulation level was observed in SPo at 15712.86 ppb, while the minor accumulation was observed in SPc at 2940.06 ppb. When the accumulation levels in wood were compared, the accumulation in STo was analyzed, with 1842 ppb being the lowest.

Table 2. Deposition of Cd concentrations (ppb) based on organs

Species	Organ			*F* value
	Leaf	Bark	Wood	
SCs	9447.86 Ee	6525.33 Bd	2612.73 Ae	18034.62***
STo	7953.20 Dd	8805.86 Ei	1842.00 Ab	23105.08***
SPo	17015.13 El	15712.86 Dl	8109.20 An	8552.04***
SPc	19624.06 Dm	2940.06 Ba	2196.66 Ad	35244.1***
SPs	28221.93 Dn	7308.60 Bf	3185.46 Af	33703.61***
F value	44078.52***	13783.27***	30418.68***	

*** expresses p<0.001, lower case letters represent vertical directions, whereas capital letters represent horizontal directions.

4. Discussion and Conclusion

Heavy metal accumulation can cause serious health problems, a multidimensionality researched issue. For example, Conti et al. [35] determined the element levels in bees and edible hive products and interpreted the health risk status with reference doses. Another study analyzed the variation in Zn and Cd levels by exposing algae to cigarette smoke in the living area and investigated its effect on indoor air quality [36]. Therefore, the accumulation of toxic substances in living things can be handled in many contexts.

Heavy metal accumulation was investigated in 5 different plant species selected in the study. Isinkaralar [37] investigated the Cd concentration in the range of 120-250 ppb in *Ailanthus altissima* in his research conducted in another location in Ankara. In addition, the outer bark values of Cd are about twice that of wood. Similarly, a higher concentration was obtained in the bark than in the wood in all species in this study. However, *Thuja occidentalis* L. bark accumulation was approximately four times higher than in wood. Another study [38] compared the heavy metal uptake capacity of 14 species, which also followed the accumulation of Cd. *Chamaecyparis lawsoniana* was found to be quite suitable for monitoring. According to Turkyilmaz et al. [34], the change in Cd amounts according to traffic density was statistically significant at the 99.9% confidence only in the usage of *S. babylonica* according to their analysis of 4 different species. The highest Pb values were obtained in *A. hippocastanum*. Various studies reveal that traffic density and industrial emissions affect Pb and Cd concentrations [39]. Zinikovscaia et al. [40] used the algae biomonitoring technique in air pollution monitoring. Possible sources of air pollution in the case area, including Pb and Cd and other nine metals, have been identified as resuspension of soil particles, agricultural applications, vehicles, industry, and thermal power plants.

5. Suggestions

The most obvious result of the decrease in air quality in cities every day is seen in living things. Growth disorders, stress conditions, and early deaths, especially seen in landscape plants in urban areas, are the leading causes of toxic metals at very high levels. Although the ability of trees used in urban areas to absorb heavy metals in their bodies differs between species, it has been observed that all of them have the ability to absorb. The presence of Pb and Cd-containing metals, which are among the species' traffic-induced releases, is increasing due to the formation of both fuel-oriented and motor vehicles caused by wear and corrosion. More comprehensive information about the sources can be obtained by diversifying the locations in future studies.

Competing Interest / Conflict of Interest

The authors declare that they have no competing interests.

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Author Contribution

We declare that all Authors equally contribute.

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Determining the biocomfort zones in near future under global climate change scenarios in Antalya

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Abstract: Climate is a factor that affects the entire life of humans such as physiological development and characteristics, housing and house structures, food and cloth selections, and distribution on land. It is projected that global climate change would cause important changes in climate parameters in near future and affect the lives of all organisms on the earth directly or indirectly. It is estimated that these changes would cause significant changes in biocomfort zones. Thus, it is important to determine the biocomfort zones depending on the climate change scenarios and to use them in urban planning studies. In this study, it was aimed to determine the change in bioclimatic comfort zones in Antalya depending on the projected climate change scenarios. Within the scope of this study, considering the SSPs 245 and SSPs 585 scenarios of Coupled Model Intercomparison Project Phase 6, that is the 6th assessment report of IPCC, it was aimed to determine the current status and possible changes in biocomfort zones in Antalya in years 2040, 2060, 2080, and 2100. The results showed that the comfort zones in Antalya will generally shift from cold to hot towards the year 2100, that this shift will be at important level, and that the highest level of increase will be seen in southern regions with high population density and intense touristic activities.

Keywords: ETv, Radiation intensity, SSPs 245, SSPs 585, Temperature-humidity index.

Öz: İklim, fizyolojik gelişim ve özellikleri, barınma ve ev yapıları, yiyecek ve giysi seçimleri, karadaki dağılımı gibi insanın tüm yaşamını etkileyen bir faktördür. Küresel iklim değişikliğinin yakın gelecekte iklim parametrelerinde önemli değişikliklere neden olacağı ve yeryüzündeki tüm organizmaların yaşamını doğrudan veya dolaylı olarak etkileyeceği öngörülmektedir. Bu değişikliklerin biyokonfor bölgelerinde önemli değişikliklere neden olacağı tahmin edilmektedir. Bu nedenle iklim değişikliği senaryolarına bağlı olarak biyokonfor bölgelerinin belirlenmesi ve kentsel planlama çalışmalarında kullanılması önemlidir. Bu çalışmada, öngörülen iklim değişikliği senaryolarına bağlı olarak Antalya ilinde biyoklimatik konfor bölgelerindeki değişimin belirlenmesi amaçlanmıştır. Bu çalışma kapsamında, IPCC'nin 6. değerlendirme raporu olan Eşleştirilmiş Model Karşılaştırma Projesi Faz 6'nın SSPs 245 ve SSPs 585 senaryoları dikkate alınarak, Antalya'daki biyokonfor bölgelerindeki mevcut durum ve 2040, 2060, 2080 ve 2100 yıllarında olası değişimlerin belirlenmesi amaçlanmıştır. Sonuç olarak, Antalya'da konfor bölgelerinin 2100 yılına doğru genel olarak soğuktan sıcağa kayacağını, bu kaymanın önemli düzeyde olacağını ve en yüksek artışın nüfus yoğunluğunun yüksek ve turistik faaliyetlerin yoğun olduğu Antalya'nın güney bölgelerinde görüleceğini tespit edildi.

Anahtar Kelimeler: ETv, Radyasyon yoğunluğu, SSPs 245, SSPs 585, Sıcaklık-nem indeksi.

1. Introduction

In the rapid economic growth in the last 30-to-40 years in the world and the urbanization and industrialization process increased the need for energy and raw material and the activities performed for their production resulted in extraction of underground mineral resources and their use in industry as raw material [1-3]. As a result, the structure and composition of atmosphere have changed, and the CO_2 concentration has significantly increased in the atmosphere [4, 5]. This process caused global climate change through direct and indirect effects. Nowadays, the effects of global climate change can be seen everywhere, and it is estimated that the climatic anomalies would further increase [6-9]. As a result of climate change, the air temperature has been raised by almost 1 ºC in the 20th century and keeps increasing in this century [10], and environmental stresses and drought events have become more frequent and severe in natural habitat [11-15] arid and semi-arid regions, and marginal lands worldwide [16]. Urban areas are about 10 ºC warmer than adjacent rural surroundings because of heat islands [17].

Climate is a factor shaping the physiological development and characteristics, housing and house structures, food and cloth selections, and distribution of humans on the earth [18-20]. Since humans are warm-blooded organisms, they are significantly affected by external environmental conditions; the lives of humans depend on a specific range of climatic parameters [21, 22]. Humans feel comfortable at specific levels of climatic parameters such as temperature, humidity, and wind. The conditions meeting these criteria are named “bioclimatic comfort” or, in shortly, “biocomfort”. Climatic

parameters exceeding beyond these values considered comfortable may cause various problems such as anger, weariness, respiratory and circulatory problems, burning eyes, and dry throat [23, 24].

Hence, it is recommended for humans to live in places, which are suitable in terms of biocomfort, for health, performance, comfort, and peace. The peoples living in places, which are not suitable in terms of biocomfort, utilize various heating and cooling systems in order to adjust the microclimate conditions to the ranges that are suitable for humans. However, these systems cause important environmental damages and high levels of energy consumption. Thus, for the health, comfort, and happiness of humans and for energy efficiency, it is very important to determine the biocomfort zones and to plan the residential areas in this parallel [25-27].

Biocomfort conditions are shaped the climate parameters and the climate changes also alter the biocomfort zones. It can be stated that the global climate change might cause significant changes in biocomfort zones. Turkey, one of the countries to be affected by this change at most, is very sensitive to climate change and is one of the "countries under risk"; it is estimated that the annual temperatures will increase countrywide until year 2100 and the temperature increases might reach 6 ºC in several regions [9, 28, 29]. Hence, effort is made to calculate possible effects on the fields such as forestry, agriculture, and tourism and to develop strategies against future changes [30].

It is clear that climate change will cause important changes in climate parameters in near future and these changes will bring significant changes in biocomfort zones. However, no study examining how the biocomfort zones, which have an important role in urban planning studies, might change depending on the global climate change in the future. Thus, using the projected climate change scenarios, the present study aims to determine the changes in biocomfort zones in Antalya province, which is of significant important from both residential and touristic aspects.

2. Material and Method

Study Area

This study was carried out in Antalya, which is the fifth-largest city of Turkey. Antalya is a province that is widely preferred as a residential area for its geographical location and climatic and edaphic conditions. Besides that, since it is one of the most important hotspots for the tourists, it is considered as the capital city of tourism. For these reasons, population gradually increases, and it becomes a necessity to open new residential areas [31]. The geographical location of study area is illustrated in Figure 1.

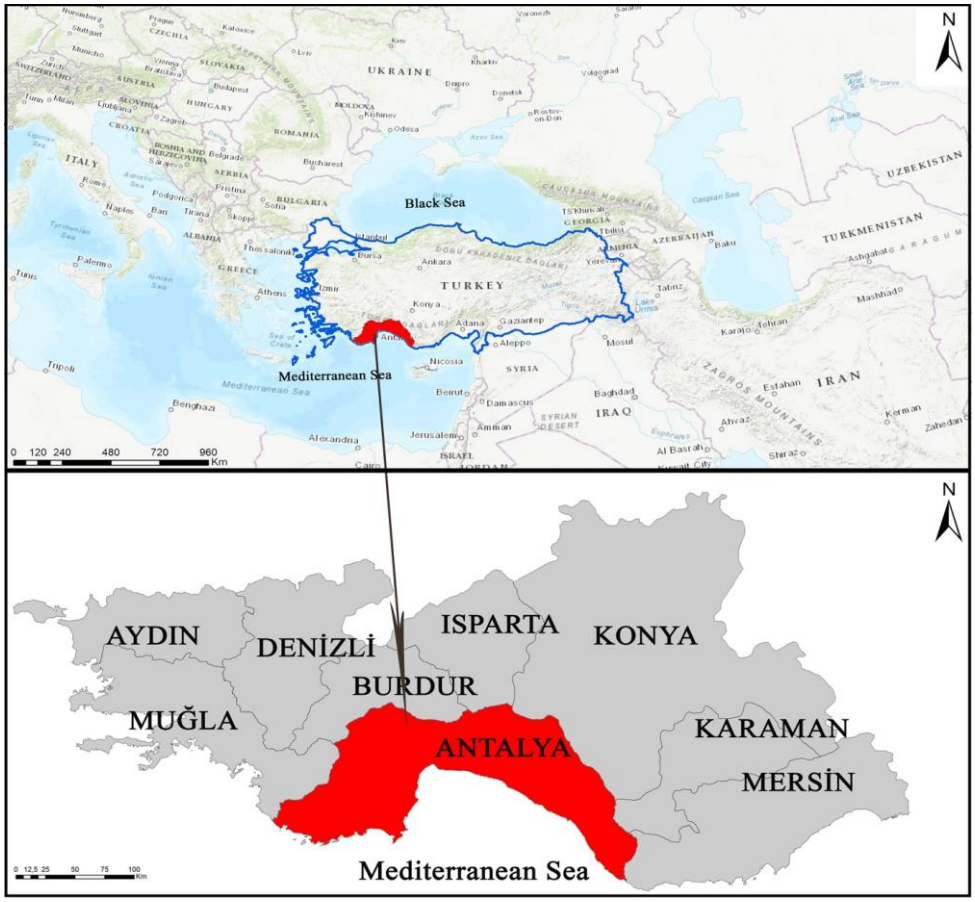

Figure 1. Geographic location of Antalya

Method

The global models among Coupled Model Intercomparison Project (Phase 6, CMIP6) that are prepared by the World Climate Research Programme (WCRP) are modified by IPCC in parallel with the recent events and used together with climate scenarios of IPCC [32]. CMIP6 in the 6th assessment report of IPCC (Intergovernmental Panel on Climate Change) was utilized in determining the scenarios used in this study.

The climate data obtained from the measurements made by 24 meteorology stations of the General Directorate of Meteorology between 2000 and 2020 were utilized in preparing the climate maps by using "Inverse Distance Weighted (IDW)" method. The future biocomfort maps were obtained by implementing the biocomfort indices formulas to the maps prepared using this method.

The base data to be used in such local or regional climate change and effect assessment studies were obtained from the data system of Department of Energy of Lawrence Livermore National Laboratory. These data allow the preparation of high-resolution (50 km resolution) climate projections. The climate data of CNRM-CM6-1 climate change model's SSPs 245 (an intermediate – radiative force is 4.5 W/m2) and SSPs 585 (the most extreme - radiative force is 8.5 W/m2) scenarios were downloaded in Netcdf file format. Then, these data were entered Arcmap 10.8 program and conversion procedures were performed. The mapping of data obtained was performed using the "Inverse Distance Weighted (IDW)" method which the simple equation of IDW is as follows:

$$z(x_0)=\frac{\sum_{i=1}^{n} z(x_i).d_{i0}^{-r}}{\sum_{i=1}^{n} d_{i0}^{-r}} \quad (1)$$

X0 location, where the estimations are made, is the function of n, which is the adjacent measurements, [z(X0i) and i=1,2,…,n]; r is the exponent that identifies the assigned range of every observation, whereas d indicates to the distance among observation location Xi and estimation location X0. The assigned weight of observations distant from the estimation location declines with the increase in exponent. The increasing exponent means that estimations are very similar to the nearest observations. The mathematical formulas are as explained above. The climate maps were prepared with calculations made using ArcGIS software [33, 34]. Then, by implementing two different biocomfort formulas to the climate maps of each scenario, the biocomfort maps were obtained. These maps were created throughout the projection period, from today and 20-year intervals (2020, 2040, 2060, 2080, and 2100) until 2100.

First of these indices was DI (Temperature-humidity index (discomfort indices)) and applied as reported by Cetin et al. (2019) [35].

$$DI = T-(0.55-0.0055 \times RH) \times (T-14.5) \quad (2)$$

Where;

DI: Temperature-humidity indices (discomfort index);

T: Monthly mean temperature (°C);

RH: Relative humidity (%).

This study was carried out in Antalya, which is the fifth-largest city of Turkey. Antalya is a province that is widely preferred as a residential area for its geographical location and climatic and edaphic conditions. Besides that, since it is one of the most important hotspots for the tourists, it is considered as the capital city of tourism. For these reasons, population gradually increases, and it becomes a necessity to open new residential areas [31]. The geographical location of study area is illustrated in Figure 1.

Table 1. Classification of indices and thermal comfort for people [35].

Thermal comfort category for people	Index values (DI)
Extremely ice	< − 40.0
Freezing cold	− 39.9 to − 20
Extremely cold	− 19.9 to − 10
Very cold	− 9.9 to − 1.8
Cold	− 1.7 to + 12.9
Cool	13.0 to + 14.9
Comfortable	15.0 to + 19.9
Hot	20.0 to + 26.4
Very hot	26.5 to + 29.9
Extremely hot	> + 30.0

The second index used in this study is Effective Temperature taking wind velocity (ETv) and its implementation was explained as follows [36]:

$$ETv = 37–(37-T)/[0.68–0.0014RH+1/(1.76+1.4v0.75)]-0.29T(1-RH/100) \quad (3)$$

Where; T is dry bulb temperature (°C); RH is relative humidity (%); and v is wind speed (m/s).

Table 2. Categories of ETv values [36].

ET (°C)	Degree of Physiological Stress	Thermal Sensation
ET < 5	Extreme cold stress	Very cold
5 ≤ ET < 10	Extreme cold stress	Cold
10 ≤ ET < 13	Shivering	Moderately cold
13 ≤ ET < 16	Cooling of the body	Quite cool
16 ≤ ET < 19	Slight cooling of the body	Slightly cool
19 ≤ ET < 22	Contraction of blood vessels	Mild
22 ≤ ET < 25	Thermal neutrality	Comfortable
25 ≤ ET < 28	Slight sweating, Dilation of blood vessels	Warm
28 ≤ ET < 31	Sweating	Quite hot
31 ≤ ET < 34	Profuse sweating	Hot
ET > 34	Thermoregulatory failure	Very hot

Within the scope of the present study, the biocomfort maps of Antalya province were prepared using the data of existing meteorology stations first. Then, the climate parameter changes projected according to SSPs 245 and SSPs 585 scenarios of CNRM-CM6-1 model were added to current data and how the biocomfort zones in Antalya province will be shaped if these scenarios take place was identified by making use of ID and ETv indices.

3. Results

Models Developed Using DI Method

The map illustrating the future situation of biocomfort zones of Antalya province in years 2020, 2040, 2060, 2080, and 2100 by using DI method according to SSPs 245 and SSPs 585 scenarios is presented in Figure 2. The numeric values of regions mapped in Figure 2 are presented in Table 3.

As a result of the calculations made using DI method, it was determined that the comfort zones will increase in the province in general according to both of SSPs 245 and SSPs 585 scenarios. Today, the province consists of 40.78% cold, 29.74% cool, and 29.39% comfortable zones but not hot zone. As a result of the calculations made using SSPs 245 scenario, the province in 2040 will consist of 27.92% cold, 35.36% cool, and 36.72% comfortable zones. In year 2060, the province will consist of 5.30% cold, 34.91% cool, 59.58% comfortable, and 0.21% hot zones. In year 2080, the province will consist of 16.80% cold, 36.65% cool, and 46.55% comfortable zones, whereas the projections made for the year 2100 indicate that the composition of province will be 6.28% cold, 36.27% cool, 57.29% comfortable, and 0.26% hot zones. Given the calculations made according to SSPs 245 scenario, it was determined that comfortable zones will constitute approx. 60% of the province.

Considering the SSPs 585 scenario, the calculations showed that the province in year 2040 will consist of 28.81% cold, 33.20% cool, and 37.99% comfortable zones, whereas the composition in year 2060 will be 6.90% cold, 35.62% cool, 57.13% comfortable, and 0.34% hot zones. In year 2080, the province is projected to consist of 1.14% cold, 13.95% cool, 81.27% comfortable, and 3.64% hot zones. For the year 2100, the province will consist of 1.53% cold, 76.61% cool, and 21.86% comfortable zones. As a result of the calculations performed, it is projected that there will be no cold zone in year 2100 in the province according to SSPs 585 scenario and comfortable zones will constitute approx. three-fourths of province and hot zones are projected to constitute one-fifth of province.

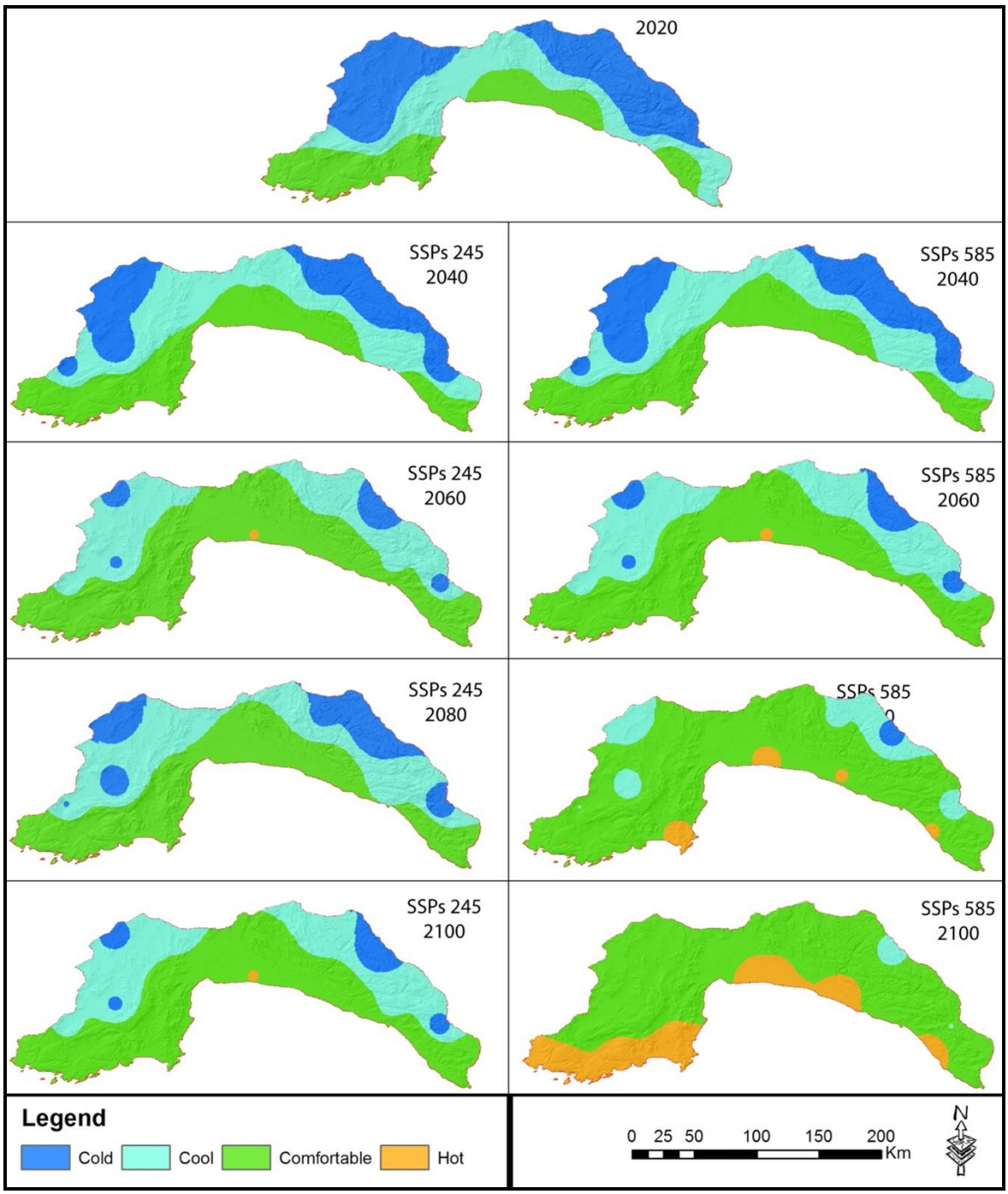

Figure 2. Models created using DI method

Table 3. The numeric values of current and future status of suitable areas mapped given in Figure 2 under the SSPs 245 and SSPs 585 scenarios.

Scenario	Spatial Distribution	Relevance	Years				
			Today	**2040**	**2060**	**2080**	**2100**
SSPs 245	Hectare (Ha)	Cold	28597.0	19539.0	3710.0	11753.0	4392.0
		Cool	20814.0	24743.0	24427.2	25648.0	25314.0
		Comfortable	20568.0	25697.0	41693.0	32578.0	40094.0
		Hot	-	-	149.0	-	179.0
	Percentage (%)	Not suitable	40.87	27.92	5.30	16.80	6.28
		Suitable	29.74	35.36	34.91	36.65	36.17
		Very Suitable	29.39	36.72	59.58	46.55	57.29
		Hot	-	-	0.21	-	0.26
SSPs 585	Hectare (Ha)	Cold	28597.0	20159.0	4830.0	801.0	-
		Cool	20814.0	23233.0	24930.0	9760.0	1071.0
		Comfortable	20568.0	26587.0	39979.0	56873.0	53610.0
		Hot	-	-	240.0	2545.0	15298.0
	Percentage (%)	Not suitable	40.87	28.81	6.90	1.14	-
		Suitable	29.74	33.20	35.62	13.95	1.53
		Very Suitable	29.39	37.99	57.13	81.27	76.61
		Hot	-	-	0.34	3.64	21.86

Models Created Using ET*v* Method

The map illustrating the future situation of biocomfort zones of Antalya province in years 2020, 2040, 2060, 2080, and 2100 by using ETv method according to SSPs 245 and SSPs 585 scenarios is presented in Figure 3. The numeric values of regions mapped in Figure 3 are presented in Table 4.

As with the DI method, the calculations made using the ETv method showed that, according to SSPs 245 scenario, the comfortable zones will increase until the year 2060 and, after a decrease in 2080, they will further increase in 2100. According to SSPs 585 scenario, it was determined that the comfortable zones will increase until 2060 but then decrease. The province currently consists of 0.19% moderate cold, 12.19% quite cold, 32.94% slightly cool, 43.06% mild, and 11.13% comfortable zones. Based on the calculations made according to SSPs 245 scenario, it is projected that the province in year 2040 will consist of 1.82% quite cool, 38.99% slightly cool, 44.52% mild, and 14.67% comfortable zones. In year 2060, the province is estimated to consist of 0.91% quite cool, 15.60% slightly cool, 45.40% mild, and 33.20% comfortable zones, whereas warm zones are projected to cover 4.89% of province. For the year 2080, the projected composition is 0.74% quite cool, 31.14% slightly cool, 44.84% mild, 23.07% comfortable, and 0.21% warm zones. In the year 2100, the province will have 19.13% slightly cool, 46.46% mild, 31.70% comfortable, and 2.71% warm zones.

Given the calculations made using SSPs 585 scenario, the province is projected to consist of 16.73% slightly cool, 44.55% mild, 37.59% comfortable, and 1.13% warm zones in 2040 and 9.36% slightly cool, 49.33% mild, 39.50% comfortable, and 1.80% warm zones in 2060. Moreover, the projections showed that the province will consist of 9.62% slightly cool, 46.75% mild, 37.54% comfortable, and 6.09% warm zones in 2080 and 28.91% comfortable, and 53.62% warm zones and 17.46% hot zones, which have not existed before, in year 2100. According to SSPs 585 scenario, there will be no moderate cool and quite cool zones until 2080 and the slightly cool and mild zones will disappear in until 2100.

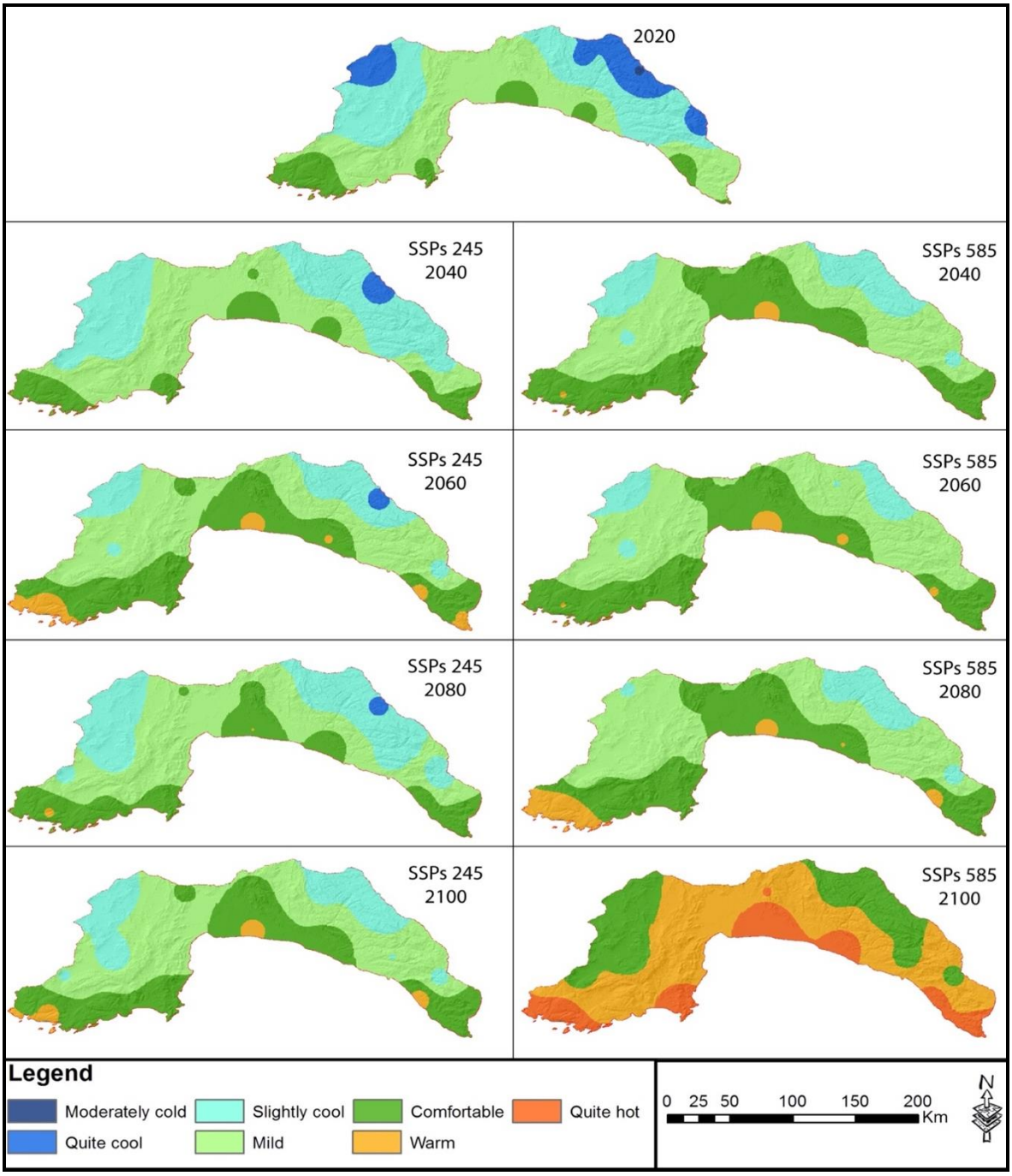

Figure 3. Models created using ET*v* method

Table 4. The numeric values of the current and future status of suitable areas mapped given in Figure 3 under the SSPs 245 and SSPs 585 scenarios

Scenario	Spatial Distribution	Relevance	Years				
			Today	2040	2060	2080	2100
SSPs 245	Hectare (Ha)	Moderate Cold	130.0	-	-	-	-
		Quite Cool	8602.0	1272.0	637.0	521.0	-
		Slightly Cool	23050.0	27282.0	10917.0	21790.0	13388.0
		Mild	30131.0	31157.0	31770.0	31376.0	32512.0
		Comfortable	8066.0	10286.0	23230.0	16142.0	22180.0
		Warm	-	-	3425.0	150.0	1899.0
	Percentage (%)	Moderate Cold	0.19	-	-	-	-
		Quite Cool	12.19	1.82	0.91	0.74	-
		Slightly Cool	32.94	38.99	15.60	31.14	19.13
		Mild	43.06	44.52	45.40	44.84	46.46
		Comfortable	11.53	14.67	33.20	23.07	31.70
		Warm	-	-	4.89	0.21	2.71
SSPs 585	Hectare (Ha)	Moderate Cold	130.0	-	-	-	-
		Quite Cool	8602.0	-	-	-	-
		Slightly Cool	23050.0	11708.0	6552.0	6731.0	-
		Mild	30131.0	31176.0	34520.0	32717.0	-
		Comfortable	8066.0	26306.0	27645.0	26269.0	20234.0
		Warm	-	789.0	1262.0	4262.0	37524.0
		Hot	-	-	-	-	12221.0
	Percentage (%)	Moderate Cold	0.19	-	-	-	-
		Quite Cool	12.19	-	-	-	-
		Slightly Cool	32.94	16.73	9.36	9.62	-
		Mild	43.06	44.55	49.33	46.75	-
		Comfortable	11.53	37.59	39.50	37.54	28.91
		Warm	-	1.13	1.80	6.09	53.62
		Hot	-	-	-	-	17.46

4. Discussion and Conclusion

Study results showed that, according to both methods and scenarios, significant changes would occur in the biocomfort zones of Antalya province due to global climate change. The temperature increase will cause a shift from cold to hot, and the hot zones will significantly increase in 2100. The temperature increase will be felt from north to south and reach a remarkable level on the southern side of province.

This study suggests that global climate change will significantly affect biocomfort. These findings show that a significant risk is coming. Given the maps created within the scope of this study, it can be stated that significant temperature increases will occur in Antalya, especially in the southern region, until the year 2100, and warm and hot zones will form in these regions. The first point drawing attention here is that the regions with a high level of temperature increase are those with high population density and are important, especially for summer tourism. Temperatures further increase in the city centers due to the buildings, hard surfaces, cooling systems, vehicles, and human activities, and the mean temperatures in heat islands show up to reach much higher levels [27, 37]. Hence, it can be stated that the mean temperatures will reach much higher levels in regions having the highest population density.

Another point to consider is that the values obtained here were calculated using the annual mean meteorological data. According to the mean values of the whole Antalya province for the period 1930-2020, the annual mean temperature was 18.8 °C, whereas the mean temperatures were 25.3 °C in June, 28.5 °C in July, and 28.4 °C in August [38]. Thus, the temperature increase will reach significant levels in the summer months, which are important for tourism, and it will negatively affect touristic activities.

The results obtained showed that the comfort zones will shift from cold to hot until the year 2100, that the change will be at a remarkable level, and that the highest level of changes will be observed in regions with both high population density and touristic activities. Considering that the temperatures are already very high in the summer, and people need air-conditioning systems in the summer season, it is projected that this need and use of air-conditioning systems will increase much more in the future. This will result in a high level of energy consumption. It is estimated that worldwide energy consumption will increase by 60% in 2030, and it will double in our country. Given the fact that the population will increase only by 1% in this period, it can be understood how high the increase in energy consumption will be [39-41]. The air-conditioning systems needed to adjust the microclimate conditions to levels suitable for humans are very important for energy consumption and costs. Moreover, the production to be made to meet the energy need may cause an increase in carbon release, and it may accelerate global climate change [25].

The temperature increase will cause changes affecting all the organisms, besides the changes in biocomfort zones for humans. Climate is one of the most important factors affecting the living conditions of organisms, and all the phenotypic characteristics of organisms are shaped by the mutual interaction between genetic structures [42, 43] and environmental variables [39, 44, 45]. The climatic factors are the most important factors influencing plant development and their distribution on the earth [43, 46, 47], and climate changes, directly and indirectly, affects all organisms. Hence, it is projected that the global climate change might have destructive and irreversible effects on the organisms and ecosystems, cause climate-dependent natural events such as forest fires, drought, floods, desertification, and erosion, and increase the ecological degradation rates and the most important effects will be the temperature increase and the decrease in water resources [18, 48-50]. Climate change is an effective result in the ecosystem's distribution and function and will shape the ecosystem's reactions to habitat changes [9, 51, 52]. The change in temperature and precipitation regime will increase the frequency of biotic damages such as insects and fungus and abiotic damages such as forest fires and floods [47, 53, 54].

It was reported that the most destructive effect of global climate change would be on the plants, which have no effective migration mechanism. Climate changes endangering the ecosystem continuity cause reactions among trees such as adaptation to climate, local adaptation, migration, and loss of life [55, 56]. Furthermore, besides the adverse effects such as invasion by foreign species, it was also reported that climate change would slow down the growth of several species, and it might have significant effects on the carbon balance of tropical forests [57]. It was stated that the projected increase in heavy rainfalls would bring uncertainties in food cycles, soil fertility, and food flows in the medium- and long-run [58]. Hence, it is emphasized that many plant species will not be able to adapt to the effects that occur depending on the climate change, and it might cause many problems such as the extinction of several species (especially the rare and endemic ones), ecosystem losses, and loss of biodiversity [9].

The negative effects of climate change on the ecosystem will also negatively affect the lives of humans, a part of the ecosystem, and the destructive effects of climate change on food and water resources, which are very important for the human life, will cause difficulties in access to those resources and it will significantly and irreversibly affect the lives of humans [8]. For this reason, considering the result of the present study from various perspectives, it can be stated that the results obtained for Antalya province will be observed in similar ways throughout the world, and the changes that will significantly affect the lives of all organisms in the world may occur in a short period.

5. Suggestions

The results of present study suggest that significant changes will occur in the biocomfort zones in Antalya province in near future, that this change will be in form of general warming, that the comfort zones will shift from cold to hot towards 2100, and that the highest level of temperature increase will occur in the regions with the highest population density and intense touristic activities. This finding can be interpreted in the way that the use and cost of cooling systems in order to ensure the suitable comfort conditions will increase. Cooling systems are systems that contribute to the increase in global climate change due to their energy consumption and use of gases and the increase in temperature will cause these systems to be used more and the higher level of use of these systems will cause a higher level of temperature increase.

Many studies reported that the global climate change will have direct or indirect effect on the entire world. Of course, the most effective method for avoiding these effects is to slow down the climate change first and then to stop it. However, it seems not possible. In this case, the most effective defense mechanism against the global climate change is to predetermine the possible changes and to take the required measures. Local and regional measures play an important role in the conflict with negative effects of global climate change. In this study, it is projected that, throughout the province of Antalya, the comfort zones will shift from south to north. Hence, the northern settlement areas should be planned for the new settlement plans in this province.

The results obtained in this study suggest that the uncomfortable zones will increase in the areas with high population density. Considering that the buildings, impermeable surfaces, vehicles, and human activities and, consequently, the mean temperature will be at a higher level in these regions, the regulations should be immediately made in accordance with these factors. It might be recommended to increase the green areas within the city, replace the hard grounds reflecting the light with grass or any more suitable hard grounds, establish rooftop gardens, sheath the outer surfaces of buildings with suitable materials, and prioritize the green-building problem. In order to minimize the effects of global climate change in medium- and long-run, it can be recommended to minimize the fossil fuel consumption, take measures decreasing the use of vehicles (developing public transportation systems, planning cycle roads, and increasing electric vehicles, etc.), and increase the use of renewable energy resources. Furthermore, it is known that the most significant effects of this process will be on the water, which is an essential source for life. Hence, it is necessary to save water, decrease the factors polluting the waters, and use wastewaters for agricultural purposes by recycling them.

Competing Interest / Conflict of Interest

The authors declare that they have no competing interests.

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Change of B and Ag concentrations due to traffic density in some plants growing in Samsun city center

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Abstract: Increasing population and industrialization have brought air pollution, air pollution has increased to a level that threatens human health in some cities and has become one of the most important agenda topics of today. In the city, many pollutants arise from exhaust gases, car wheels, vehicles, and vehicle wear. Because heavy metals can remain in nature for a long time without deterioration and their concentration in the environment is constantly increasing. Therefore, the determination of heavy metal concentration is of great importance in terms of determining the risky areas and risk level. Biomonitors are the most important indicators that show the change in the concentration of heavy metal pollution in the atmosphere. In this study, it was tried to determine the changes in the concentrations of B and Ag elements based on organ washing and traffic density in *Euonymus japonica* (Ej), *Juniperus sabina* (Js), and *Buxus sempervirens* (Bs), which can be used to monitor traffic-induced heavy metal concentration. Leaf and branch samples were collected from the individuals of the plant species that are the subject of the study, grown in areas with heavy traffic, low density, and no traffic, washing process was carried out in some of the samples, and heavy metal analyzes were made in the prepared samples, and the concentrations of B and Ag elements were determined. It was determined that different species accumulate heavy metals at different levels, and the changes in the concentrations of the elements vary depending on the organ and traffic density on the species basis.

Keywords: Heavy metal, Biomonitor, Traffic, B, Ag

Öz: Artan nüfus ve sanayileşme, hava kirliliğini de beraberinde getirmiş, hava kirliliği bazı şehirlerde insan sağlığını tehdit edecek düzeyde artmış ve günümüzün en önemli gündem konularından birisi haline gelmiştir. Kent içerisinde egzoz gazları, araba tekerleri, araçlar ve araç aşınmalarından kaynaklanan pek çok kirletici madde ortaya çıkmaktadır. Bunlar arasında özellikle ağır metaller büyük öneme sahiptir. Zira ağır metaller doğada bozulmadan uzun süre kalabilmekte ve çevredeki konsantrasyonu da sürekli artmaktadır. Ayrıca biyobirikme eğilimindedir. Bundan dolayı ağır metal konsantrasyonunun belirlenmesi, riskli bölgelerin ve risk düzeyinin tespit edilmesi açısından büyük öneme sahiptir. Ağır metal kirliliğinin atmosferdeki konsantrasyonunun değişimini gösteren en önemli belirteçler biyomonitörlerdir. Bu çalışmada da trafik kaynaklı ağır metal konsantrasyonunun izlenmesinde kullanılabilen *Eonymus japonica* (Ej), *Juniperus sabina* (Js) ve *Buxus sempervirens* (Bs) türlerinde B ve Ag elementlerin konsantrasyonlarının organ bazında yıkama durumu ve trafik yoğunluğuna bağlı değişimi belirlenmeye çalışılmıştır. Çalışma kapsamında çalışmaya konu bitki türlerinin, trafiğin yoğun olduğu, az yoğun olduğu ve trafiğin bulunmadığı alanlarda yetişen bireylerinden yaprak ve dal örnekleri toplanmış, örneklerin bir kısmında yıkama işlemi gerçekleştirilmiş ve hazırlanan örneklerde ağır metal analizleri yapılarak B ve Ag elementlerinin konsantrasyonları belirlenmiştir. Çalışma sonucunda farklı türlerin ağır metalleri farklı düzeyde biriktirdiği, elementlerin konsantrasyonlarındaki değişimin de tür bazında organ ve trafik yoğunluğuna bağlı olarak değişiklik gösterdiği belirlenmiştir.

Anahtar Kelimeler: Ağır metal, Biyomonitor, Trafik, B, Ag

1. Introduction

In addition to the increase in the world population in recent years, the gradual increase in the population living in urban centers has brought along many problems [1-25]. In this process, as a result of traffic and other anthropogenic activities, especially in urban centers, various elements, many of which are dangerous for life, are found in soil [26-30], water [31-38] and air [39-56] concentrations in various organs of animals [57] and plants [58-73] growing in these environments are constantly increasing. As a result, nature is destroyed and indirectly problems such as global climate change arise [3, 6, 8, 43, 71, 74-77].

Air pollution is considered the most dangerous among environmental pollution [46, 52, 53, 54, 56, 61, 78]. Air pollution is one of the most important problems of today [46, 47-49, 52-56, 61, 74-76]. It is stated that approximately 7 million people in the world die every year due to air pollution-related reasons [46, 52-56, 79]. It is stated that even in Turkey,

whose air is considered quite clean compared to many countries, 29 thousand people lost their lives due to air pollution in 2016 [56].

Among the components of air pollution, heavy metals have a special importance because they tend to bioaccumulate and can be toxic to human health even at low concentrations [80-82]. Studies show that almost all metals have a toxic effect when taken above a certain amount [83]. Since heavy metals are so important for human health, it is extremely important to determine the heavy metal concentration in the air and to monitor its change, to determine the risky areas and the risk level [42].

The change of heavy metal pollution in the atmosphere can be determined by direct and indirect methods. However, direct measurement of heavy metal pollution in the atmosphere; has disadvantages such as being expensive, not being able to determine the direct effect of atmospheric pollution on the ecosystem, and not providing data for the periods before the measurement time [59]. In addition, these methods usually require expensive measuring instruments and carry a higher risk of contamination compared to bioindicators. One of the most effective methods used to detect air pollution is bioindicators. In addition to being cheap and easy, this method can provide more reliable data on the periodic change of heavy metal concentration [39].

Landscape plants, which are most exposed to air pollution, are the best indicator of this pollution. It shows the course of the increase in the heavy metal concentration in the air over time by accumulating heavy metal pollution caused by fossil fuels on its stem, leaves, and needles, especially in areas with heavy traffic [34, 65, 84]. Therefore, instead of directly detecting heavy metal pollution, bioindicators or biomonitors are often used as an indicator of pollution [68, 69]. This study, it was aimed to determine the change of heavy metals B and Ag concentrations in some landscape plants grown in Samsun city center depending on plant type, plant organ, washing status, and traffic density.

2. Material and Method

Material

The study was carried out on samples collected from the city center of Samsun. Within the scope of the study, it is grown in areas with heavy traffic, low density, and no traffic (at least 100 m near there is no highway) and frequently used in landscaping; Samples were collected from plant species *Euonymus japonica* (Ej), *Juniperus sabina* (Js) and *Buxus sempervirens* (Bs). The samples were taken from the last year's shoot, that is, the one-year-old part, by cutting with pruning shears, and packaged, labeled, and brought to the laboratory.

Method

The samples brought to the laboratory after being collected and labeled were laid on cardboard and subjected to the separation process. Leaves and branches are separated, grouped, and labeled. Then half of the samples were separated and subjected to the washing process. In the washing process, firstly the samples were washed with tap water, then they were placed in a bottle, water was added, and the particulate matter adhering to the surface of the samples was tried to be removed by shaking rapidly. Afterward, the process was repeated by draining the dirty water and filling it with clean water. After the color of the water became clear, the same procedure was performed three times with distilled water, and the samples, which were taken out of the last bottle, were washed again with distilled water. Within the scope of the study, the samples that were washed were coded with (+) and the samples that were not washed were coded with (-) signs. Afterward, the samples were broken into pieces for easy drying and placed in glass petri dishes, and labeled again. The samples prepared in this way were kept for 15 days to become room-dry, and the laboratory was ventilated every day during this period. The air-dried samples were dried in an oven at 45°C for one week to dry them completely.

Statistical Analysis

The data obtained as a result of the study were entered into the excel program and evaluated with the help of the SPSS 22.0 statistical package program. Analysis of variance was applied to the data with the help of the SPSS program and homogeneous groups were obtained by applying the Duncan test to the data with $p<0.05$, that is, at least 95% confidence level differences. The obtained data were simplified, processed into tables, and interpreted.

3. Result

In the samples subject to the study, the variation of the B concentration in the areas where there is no traffic, where there is little or no traffic, analysis of variance and Duncan test was applied to the data, the average values obtained, the F value and significance level obtained as a result of the analysis of variance, and the homogeneous groups formed as a result of the Duncan test is given in Table 1.

Table 1. Variation of B (ppm) concentration depending on species, organ, and washing condition

Species	Organ	Washing	TRYOK	TRAZ	TRCOK	F Value
Ej	leaf	+	23,78 gB	21,65 hA	32,48 hC	2151,1***
		-	30,80 hC	23,97 iA	25,96 gB	702,5***
	Branch	+	23,68 gB	35,34 jC	15,46 fA	5201,2***
		-	30,35 hC	9,85 eA	12,17 dB	15161,8***
Js	leaf	+	10,97 dA	10,46 fA	14,17 eB	90,6***
		-	17,51 eC	4,53 cAB	14,77 ef	12422,1***
	Branch	+	5,34 bB	1,74 aA	6,62 bC	226,4***
		-	8,27 cB	3,55 bA	10,06 cC	779,1***
Bs	leaf	+	67,58 iC	48,96 lA	51,97 jB	1234,5***
		-	69,95 jC	46,40 kA	47,28 iB	3761,8***
	Branch	+	18,71 fC	12,84 gB	9,97 cA	107,1***
		-	3,48 aB	7,75 dC	1,57 aA	1736,6***
F Value			13286***	10541***	4630***	

***: p<0,001; **: p<0,01

When the results of the analysis of variance are examined, it is seen that the traffic density in all organs subject to the study and the change in B concentration based on organs in all traffic densities is statistically significant at the 99.9% confidence level. When the average values are examined; The B concentration is between 3.48 ppm and 69.95 ppm in the area where there is no traffic; between 1.74 ppm and 48.96 ppm in low traffic areas; and it is seen that it varies between 1.57 ppm and 51.97 ppm in areas with heavy traffic. It is very difficult to say that there is a linear relationship between traffic density and B concentration.

In the samples subject to the study, the Ag concentration was not trafficked; the change was determined in the areas where it is less dense and dense. Analysis of variance and Duncan test were applied to the data, mean values obtained; F value and significance level obtained as a result of variance analysis, and homogeneous groups formed as a result of Duncan test are given in Table 2.

Table 2. Variation of Ag concentration depending on traffic density based on species, organ, and washing

Species	Organ	Washing	TRYOK	TRAZ	TRCOK	F Value
Ej	leaf	+	719,0 eA	1113,3 bB	604,6 cdA	39,6***
		-	723,3 eB	255,3 aA	306,3 abcA	23,0***
	Branch	+	148,0 aA	2374,3 cdC	414,3 abcdB	274,9***
		-	351,6 abcA	2237,6 cB	2103,3 eB	32,022**
Js	leaf	+	209,3 abc	228,3 a	199,6 ab	0,337 ns
		-	607,0 deA	1051,0 bB	716,0 dA	16,095**
	Branch	+	415,3 bcdA	2613,0 deB	319,6 abcA	243,2***
		-	181,3 abA	2739,6 eB	2239,3 eB	69,8***
Bs	leaf	+	230,3 abc	188,0 a	333,0 abc	1,801 ns
		-	431,6 cd	516,3 a	511,0 bcd	1,892 ns
	Branch	+	1989,0 fB	2683,6 deC	161,6 aA	926,7***
		-	2795,6 g	2174,0 c	2303,6 e	4,391 ns
F Value			126,5***	86,6***	69,8***	

***: p<0,001; **: p<0,01

According to the results of the analysis of variance regarding the change in Ag concentration, the change in Ag concentration based on organs is statistically significant in all traffic densities. However, the change of Ag concentration in washed Js leaves, Bs leaves and unwashed Bs rafts depending on traffic density is not statistically significant. When the Duncan test results are examined; Ag concentration is between 148.0 ppb and 2795.6 ppb in the area where there is no traffic; between 188.0 ppb and 2739.6 ppb in low traffic areas; and it is seen that it varies between 161.6 ppb and 2303.6 ppb in areas with heavy traffic. It is noteworthy that, in general, the highest concentrations were obtained in the Bs branches.

4. Discussion and Conclusion

Within the scope of the study, the change of B and Ag elements depending on the traffic density based on species, organ, and washing status was determined. Although many studies have been carried out on heavy metals to date, many studies have been carried out on elements such as Pb, Cd, Ni, Co, Cr [66, 67], and the elements subject to the study

have been largely neglected. However, it is stated that when all heavy metals are taken above a certain rate, they can be harmful to health, and especially heavy metals taken by inhalation can be much more harmful.

The results of the study show that the changes in both heavy metals based on organs are at a statistically significant level at all traffic densities, and there can be great differences in heavy metal concentrations between species and organs. In the studies carried out to date, it has been revealed that the heavy metal concentration varies significantly based on species, and it has been stated that the changes based on species can be tens of times [85, 86]. The change of heavy metal concentrations based on organs has also been the subject of many studies, and in these studies, it has been revealed that the heavy metal accumulation potentials of different organs of different species differ significantly [87].

The significant variation in heavy metal concentrations on both species and organ basis is primarily related to the anatomical structure of the plant organ [88]. Heavy metal accumulation in organs; The physical and chemical properties of metals vary depending on factors such as forms, the morphology of organs, surface area, surface texture, exposure time to heavy metals, environmental conditions, and gas exchange [60]. In addition, heavy metal accumulation in plant organs varies greatly depending on the plant habitus [62]. Plant habitus is formed under the mutual interaction of plant genetics [45, 89-91] and environmental conditions [73, 92-94]. Therefore, environmental conditions that affect plant life conditions also greatly affect heavy metal accumulation in plant organs [59]. Within the scope of the study, it was determined that there could be a significant difference between the washed and unwashed samples. It is reported that heavy metals can adhere to various particles in the atmosphere after leaving their source, and thus most of the metals coexist with the particles in the atmosphere [83]. Particulate matter (PM) contains a complex mixture of various heavy metals in the atmosphere, many of which are harmful. Therefore, particulate matter contaminated with heavy metals can cause serious problems in terms of human and environmental health [63]. Therefore, many studies have been conducted on PM [95]. Another factor evaluated within the scope of the study is traffic density. It is stated that one of the most important sources of heavy metal pollution is traffic activities [42]. In many studies, it has been determined that heavy metal concentrations in plant organs vary significantly depending on traffic density [88]. In this study, it is very difficult to say that there is a linear relationship between the concentrations of the elements in the study and the traffic density. This result can be interpreted as the elements in the study are not emitted from traffic-related pollutants. Traffic is one of the important sources of heavy metal pollution, and there are many sources, especially industrial activities [40, 41].

Studies carried out to date have shown that the diffusion of heavy metals in the atmosphere and their entry into the plant body is a very complex mechanism [59]. The mutual interaction of plants with heavy metals and therefore heavy metal accumulation in the plant is closely related to plant metabolism [96]. Therefore, the stress level of the plant [97-99], plant origin [61, 63, 65], hormone applications [90, 91, 100] and genetic structure [101] affect heavy metal absorption and thus heavy metal concentration in plants [60]. Some of researches with landscape architecture mentioned the planning and management for selecting plants [102-129]. These research explained the landscape plants for use.

As a result, the change of heavy metal concentration in plants is the result of a complex mechanism depending on the interaction of many factors. However, this mechanism has not been fully resolved. Information on the uptake of heavy metals from aboveground organs is very limited [96].

5. Recommendations

One of the most important problems of today is air pollution. Air pollution has gained special importance with the increase in the level of awareness on this issue as well as the population density in the city centers, and many studies have been carried out on the importance of this issue and the solution of the problem. Among the solution proposals, increasing green areas is seen as one of the most effective methods. Because plants can significantly reduce air pollution.

However, the effects of different species on different pollution factors are at different levels. Although a large number of plant species have been studied in studies carried out so far, these studies are not yet at a sufficient level. There is no information about the potential of many plant species to accumulate heavy metals. However, as in this study, it has been determined that there are great differences between the heavy metal accumulation potential of plant species in many studies. Therefore, it is necessary to use the species that are not included in the studies in similar studies and to identify plants that can be more effective in monitoring and reducing heavy metal pollution. Therefore, it can be suggested that similar studies be continued by diversifying.

The importance of heavy metals in terms of human health is known and there are many studies on this subject. However, studies mostly focus on elements such as Pb, Ni, Cr, Co, Cd. However, it is necessary to intensify studies and identify risky areas on elements such as B, Ag, Ga, As, which can be extremely harmful to human health, but have not been given much importance and studied so far.

Competing Interest / Conflict of Interest

The author declare that they have no competing interests

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6. References

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Investigation of structure-activity relationships with molecular docking for some antiepileptic drugs and voltage-gated calcium (CaV) channels

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Abstract: In the study, the active drugs molecules used in the treatment of convulsive seizures occurring in epilepsy disease were used. These molecules; Vigabatrin, Lokosamidin, Zonisamide, Oxcarbazepine, Levetiracetam, Tiagabin, Topiramate, Lamotrigine, Gabapentin, Felbamate, Ethosuximide, Valproic Acid, Mesuximide, Ethotoin, Primidone, Trimethadion, Phenytoin, Remasemide, Mephenytoin. These molecules have been selected considering the physiopathological mechanisms of action of epilepsy. Since the selected molecules are used as a potential antiepileptic agent, they were deemed suitable for molecular insertion studies. In addition, voltage-gated calcium channels, which play an important role in epilepsy, are emphasized. Voltage-gated calcium channels (CaV) act by providing the flow of Ca+ ions during the action potential that triggers seizure formation, and among the ten subtypes of voltage-gated calcium (CaV) channels, CaV3.1- CaV3.3, T-type or abnormal activities are associated with epilepsy, psychiatric form the associated low-voltage-activated subfamily. For this reason, the PDB ID: 6KZP receptor, which acts as an antagonist according to its activity on the channel in the formation of epileptic seizures, was chosen for the molecular insertion study. As a result of molecular placement studies; Oxcarbazepine and Phenytoin gave the best binding affinity for 6KZP with a value of -7.5 kcal/mol. Other results are in descending order (in kcal/mol); Tiagabine (-7.4), Mesuximide (-7.3), Primidone (-7.1), Remacemide (-7.0), Topiramate (-6.9) Mephenytoin (-6.7), Lomotrigine and Ethotoin (-6.4), Locosamide and Zonisamide (-6.1) , Felbamate (-6.0), Levetiracetam and Gabapentin (-5.4), Esuximide (-5.1), Valproic Acid (-4.9), Trimethadione (-4.7), Vigabatrin (-4.4) determined as.

Keywords: Calcium Channels, Epilepsy, Moleculer Docking, Ligand, Receptor, Drug

Öz: Çalışmada epilepsi hastalığında ortaya çıkan konvülsif nöbetlerin tedavisinde kullanılan etken ilaç molekülleri kullanılmıştır. Bu moleküller; Vigabatrin, Lokosamidin, Zonisamid, Okskarbazepin, Levetiracetam, Tiagabin, Topiramat, Lamotrijin, Gabapentin, Felbamat, Ethosuximide, Valproic Asit, Mesuximid, Ethotoin, Primidon, Trimethadion, Phenitoin, Remasemide, Mephenytoin. Bu moleküller epilepsinin fizyopatolojik etki mekanizmaları dikkate alınarak seçilmiştir. Seçilen moleküller potansiyel bir antiepileptik ajan olarak kullanıldığından moleküler yerleştirme çalışmaları için uygun görülmüştür. Ayrıca epilepside önemli rol oynayan voltaj kapılı kalsiyum kanalları üzerinde durulmuştur. Voltaj kapılı kalsiyum kanalları (CaV), nöbet oluşumunu tetikleyen aksiyon potansiyeli sırasında Ca+ iyonlarının akışını sağlayarak hareket eder ve voltaj kapılı kalsiyum (CaV) kanallarının on alt tipi arasından CaV3.1- CaV3.3, T- tipini veya anormal aktivitelerden epilepsi ve psikiyatri ile ilişkili düşük voltajla aktive edilen alt familyayı oluşturmaktadır. Bu nedenle moleküler yerleştirme çalışması için epileptik nöbetlerin oluşumunda kanal üzerindeki aktivitesine göre antagonist görevi gören PDB ID:6KZP reseptörü seçilmiştir. Moleküler yerleştirme çalışmaları sonucunda; Okskarbazepin ve Fenitoin, -7.5 kcal/mol değeri ile 6KZP için en iyi bağlanma afinitesini vermiştir. Diğer sonuçlar azalan sıradadır (kcal/mol olarak); Tiagabin (-7.4), Mesuximide (-7.3), Primidon (-7.1), Remasemide (-7.0), Topiramat (-6.9) Mefenitoin (-6.7), Lomotrigin ve Ethotoin (-6.4), Locosamide ve Zonisamide (-6.1), Felbamat (-6.0), Levetiracetam ve Gabapentin (-5.4), Esuximide (-5.1), Valproik Asit (-4.9), Trimethadion (-4.7), Vigabatrin (-4.4) olarak belirlendi.

Anahtar Kelimeler: Kalsiyum Kanalları, Epilepsi, Moleküler Docking, Ligand, Reseptör, İlaç

1. Introduction

Epilepsy is a neurological disease that affects the majority of the world's population and is characterized by sudden, irregular or excessive neuronal excitation in the gray matter of the brain due to high excitability of the brain and presents symptomatically with seizures [1, 2]. Although there is not much information about the cellular and molecular mechanisms of epileptic seizures, the most well-known mechanism is excessive neuronal firing, which is caused by the disruption of the balance between excitatory and inhibitory voltage-dependent/synaptic transmission. Neurotransmitters are divided into excitatory neurotransmitters and inhibitory neurotransmitters. Excitatory neurotransmitters are acidic amino acids that cause depolarization of the cell by increasing the passage of Na+ and Ca2+ into the cell. Inhibitory neurotransmitters are amino acids that cause hyperpolarization of the cell by increasing the passage of Cl- into the cell

or increasing the outflow of K+ and closing the Na+ and Ca2+ channels in the cell membrane and reducing the entry of Na+ and Ca2+ into the cell. This imbalance in the nervous system causes the development of epilepsy in a certain region of the brain, due to functional disorders in macromolecules involved in excitatory and inhibitory transmission in the epileptic brain [3].

Another mechanism is neuronal membrane and molecular channel changes in ionic conduction [4]. The movement of ions in these synaptic transmissions, which occur in the nervous system through neurotransmitters, creates an action potential in the cell membrane that causes epileptic seizures. The cell membrane has a certain negative voltage (membrane potential) depending on the intracellular and extracellular ion concentration. A nerve cell in the resting phase is polarized and has a membrane potential of about -70 mV to -80 mV. This potential is balanced by ion pumps and ion channels, creating a concentration gradient across the membrane with a greater negative charge inside the cell. With the positive shift of the membrane voltage, the depolarized membrane action potential (AP) is formed, and nerve and muscle cells are stimulated by this potential (Figure 1). AP transmitted along the axon in neurons is transferred to the next neuron via neurotransmitters at the axon tip and neuronal firing is provided. After depolarization, the membrane becomes hyperpolarized by reaching a voltage below the resting potential [5]. This is a response to prevent excessive excitability as a result of successive firings in a healthy nervous tissue, and the membrane quickly returns to the resting phase (polarization). Therefore, the state of extreme excitability; increased excitatory synaptic neurotransmission, decreased inhibitory synaptic neurotransmission, or a change in ion concentration on both sides of the membrane causing depolarization or multiple synchronized sub-threshold excitatory stimuli [6].

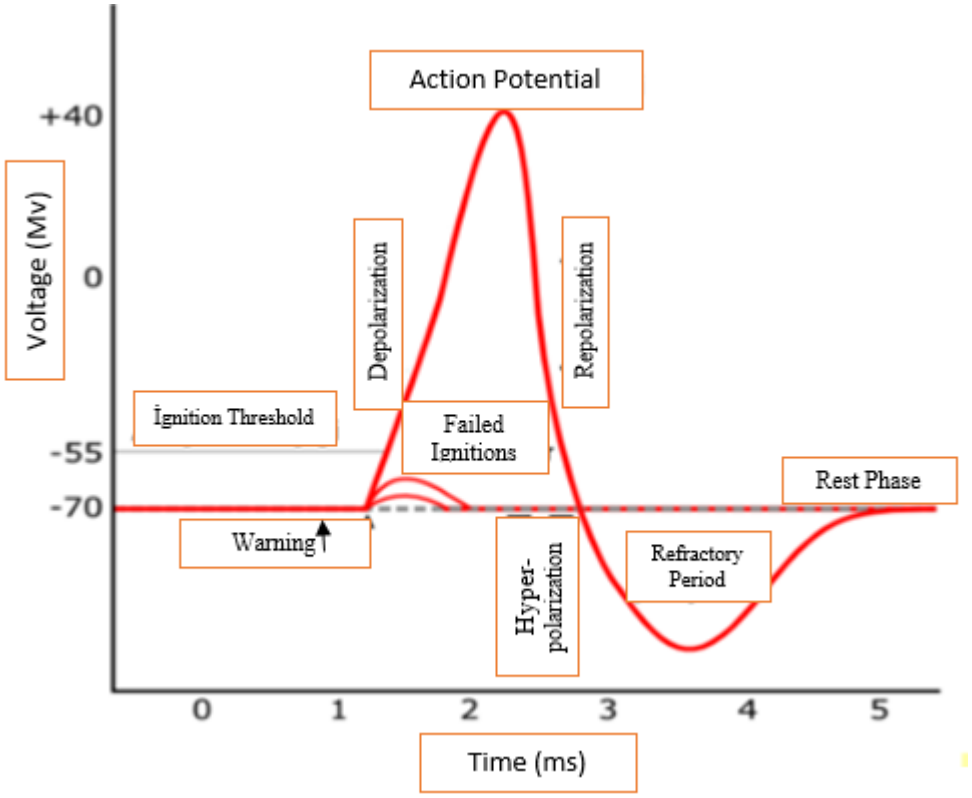


Figure 1. Voltage change during membrane action potential [6]

Treatment methods of epilepsy aim to terminate seizures or reduce the number of seizures with the mentioned mechanisms. Despite the availability of several successful AEDs, some AEDs show toxicity and clinically important drug-drug interactions. Therefore, there is still a need for new drugs with better efficacy and tolerability [7, 8]. Therefore, quantitative structure-activity relationship techniques (QSAR and 3D-QSAR) have been widely used approaches in resolving the action mechanisms of known AEDs or in the design and efficacy of new compounds. These techniques help to predict and improve the activities of different compounds and to identify new compounds with less side-effect profiles [9, 10].

Epilepsy Treatment-Antiepileptic Drugs

The first discovered antiepileptic drugs (bromide, phenobarbital) that suppress the occurrence, spread and severity of seizures have negative properties in terms of keeping seizures under control and side effects [11]. AEDs are classified as first and second generation antiepileptics based on their availability before and after 1990 [12]. Until 1990, only six classical drugs (carbamazepine, ethosuximide, phenobarbital, valproic acid, phenytoin, primidone) could be used for the

treatment of epilepsy, while second generation AEDs (vigabatrin, felbamate, gabapentin, lamotrigine, topiramate, tiagabine, oxcarbazepine, levetire) pregabalin, lacosamide) treatment options have increased [13]. New AEDs have advantages such as higher tolerability, less drug interactions, and no inducing effects on hepatic metabolism enzymes [14]. Sodium channel blockers, calcium channel blockers, glutamate receptor antagonists, GABA receptor agonists and carbonic anhydrase inhibitors are used in the treatment of epilepsy. The part discussed in this study is calcium channels.

Calcium channel blockers; Calcium channels are very important for rhythmic brain activity, especially in the thalamus region. L, N, and T-type calcium channels, especially T-type calcium channels, play a role in absence seizures and their inhibition is important in absence seizures [15]. Voltage-gated calcium channels (CaV) contribute to the general excitability of neurons by transmitting Ca2+ and a small amount of Na+ and play an important role in neuronal firing. It also controls neurotransmitter release from presynaptic nerve endings. In CaV, which has α1, α2, δ1, β subunits, the α1 subunit is functional. The CaV-α1 subunit, four homologous regions (DI-IV), and the selectivity filter with six transmembrane segments (S1-6) forming each region are important components of this subunit. There are several types of the CaV-α1 subunit, and CaV is classified according to the α1 subunit it contains (L-type, P/Q-type, N-type, R-type, T-type). For example, high voltage-dependent channels (type N, P/Q, and R) respond to strong depolarization and control presynaptic neurotransmitter release. Low voltage coupled channels (T-type) respond to normal depolarization and lead to transient currents [16]. Excessive levels of intracellular Ca2+ can lead to neuronal dysfunction (dysfunction) and cell death [17]. Excessive functionality of voltage-gated T-type calcium channels has a negative effect on epilepsy. Calcium ions entering the cell cause excitability and cause seizures. With calcium channel blockade, the formation of epileptic seizures is suppressed by preventing the penetration of Ca2+ ions in high concentrations into the cell.

In the light of the information given in the introduction, the interaction of a total of 19 antiepileptic substances selected according to their active mechanisms with CaV was examined using the computer aided drug design module. These active substances have mechanisms to suppress epileptic seizures. With the molecular docking method, the preferred conformations of one molecule (ligand) to bind to another molecule (receptor) to form a stable complex have been tried to be predicted. Obtained binding energies and resulting bond structures provide important information about the resulting conformations. When we look at the docking studies of known antiepileptics in the literature; Piplani et al. (2016) Homology modelling and molecular docking studies of human placental cadherin protein for its role in teratogenic effects of anti-epileptic drugs article named in the docking study with PDB-1Q55 protein in their anti-epileptic drugs; -5.06 for ethosuximide, -5.27 for felbamate, -6.3 for gabapentin, -5.15 for lacosamide, -6.59 for lamotrigine, -5.00 for leviteracitam, -5.36 for mesuximide, -6.59 for phenytoin, -6.14 for primidone, -9.17 for remacimide, -6.5 for tiagabin, -6.32 for topiramate, -4.63 for valproic acid, -6.13 for vigabatrin and -6.37 Kcal/ for zonisamide , they obtained the mole values [18]. When we compare the results we obtained, it is seen that the values obtained for ethosuximide are almost the same. Felbamate, levetiracetam, mesuximide, phenytoin, primidone, tiagabine, topiramate, valproic acid values gave higher binding affinity in our study; Lower values were obtained for gabapentin, lacosamide, lamotrigine, remacemide, vigabatrin and zonisamide values. In another study, Kundaikar et al. (2015) obtained an affinity value of -3.93 for phenytoin and -3.11 kcal/mol for lamotrigine [19]. Compared to our study, it was seen that our results gave higher binding affinities for both antiepileptics. Results may vary depending on binding sites and target proteins.

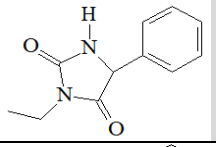
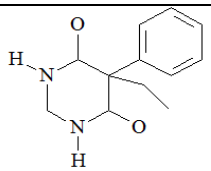
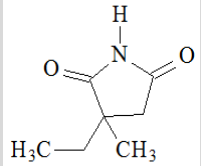
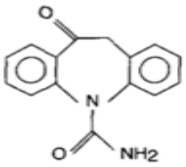
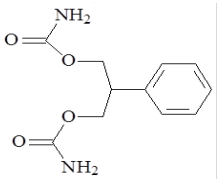
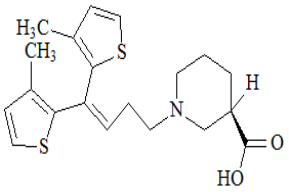
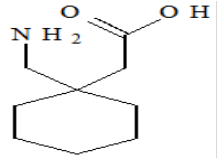
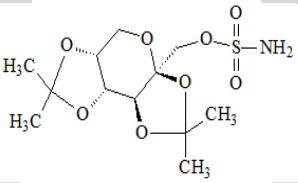
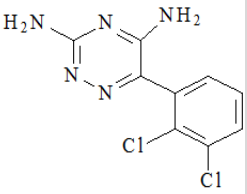
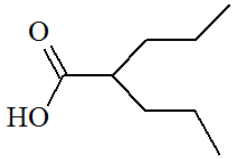
2. Material and Method

Material

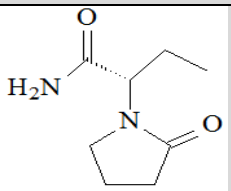
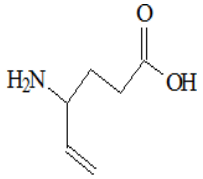
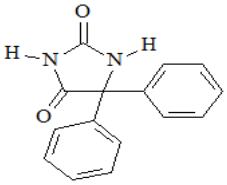
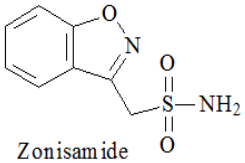
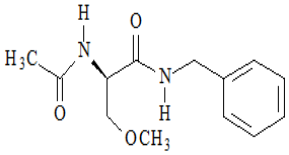
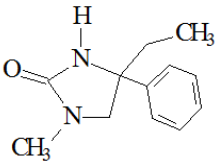
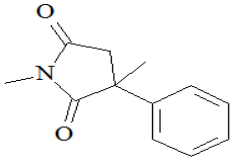
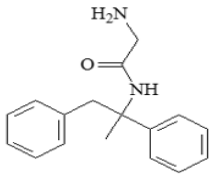
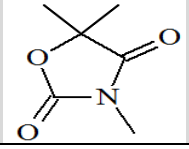
Active Substances Used (Ligand Files)

The 19 active substances selected for the study are listed in Table 1 according to their mechanism of action and their molecular structures are given. The chemical structures of the selected ligand molecules are important. In the results section, it is shown in detail which compound of the ligand molecule and which amino acid structure of the selected macromolecule dock and bond. The molecular structures of 19 active ingredients are listed below. These active ingredients are; Ligands for free download from the database ıt can be listed as [20] It can be listed as; Ethotoin, Primidon, Ethosuximide, Oxcarbazepine, Felbamate, Tiagabine, Gabapentin, Topiramate, Lamotrigine, Valproic acid, Levetiracetam, Vigabatrin, Pheytoin, Zonisamide, Lacosamide, Mephenytoin, Mesuximide, Remadicemide and Trimethadione.

Table 1. Compounds and their action mechanisms of antiepileptic drugs

Compounds	Action Mechanisms	Moleculer Structure
Ethotoin	Na^+ channel inhibition	
Primidone	GABA increase, Glutamate decrease, Na^+, Ca^{2+} channel inhibition, K^+ channel opening	
Ethosuximide	T-type Calcium (Ca^{2+}) channel inhibition	
Oxcarbazepine	Sodium channel inhibition, N, P, R type Ca^{2+} channel inhibition	
Felbamate	Glutamate inhibition, NMDA receptor blockage, increases GABA levels, Na^+ channel blockade, blockade of voltage-gated Ca^{2+} channels	
Tiagabine	Increases GABA concentrations and inhibits GABA-AT	
Gabapentin	Increases GABA levels, Calcium channel modification	
Topiramate	Glutamate reduction, voltage-transition sodium channel inhibition, activation of potassium currents, AMPA and glutamate inhibition, voltage-transition calcium channel inhibition, NMDA inhibition, increase of GABA concentration, inhibition of carbonic anhydrase isoenzyme	
Lamotrigine	Voltage-gated sodium channel inhibition, glutamate reduction, Ca^{2+} channel inhibition	
Valproic acid	Na^+ and T type Ca^{2+} channel inhibition, GABA increase, K^+ channel activity	

continue table….

Compounds	Action Mechanisms	Moleculer Structure
Levetiracetam	Modulation of synaptic vesicle proteins, N, T-type Ca^{2+} Channel inhibition, increases voltage-gated potassium channel conductivity, increases GABA concentration, and inhibits glutamate system by stimulating	
Vigabatrin	GABA increase opens K^+ (potassium) channels, increases Cl^- channel opening, GABA-AT inhibition effect	
Phenytoin	Sodium and calcium channel inhibition activates K^+ channel transmission, increases GABA concentration	
Zonisamide	T-type Calcium channel inhibition, Inhibit Carbonic Anhydrase isoenzyme, voltage-gated Na^+ channel inhibition, inhibit glutamate release	 Zonisamide
Lacosamide	It increases the slow inactivation phase of the Na^+ channel and is responsible for blocking the voltage-gated sodium channel.	
Mephenytoin	Inhibits voltage-gated Na^+ channel conduction	
Mesuximide	T-type Ca^{2+} channel inhibition, partial NMDA inhibition	
Remacemide	Blocks NMDA responses, inhibits voltage-gated Na^+ channel conduction	
Trimethadione	T-type Ca^{2+}, Na^+ channel inhibition, partial NMDA inhibition	

Selected Macromolecule (Receptor Files)

PDB ID: 6KZP was chosen as the receptor in the research conducted with the molecular docking method. It was chosen because it acts as an antagonistic molecule for voltage-gated calcium channels [21]. 6KZP; 3.1 Cryo-EM structures of human CaV bound to Apo and antagonist with its calcium channel ligand structure is a macromolecule studied (Figure 2). Voltage-gated calcium channel subunit 3.1 (CaV3.1) is a macromolecule that will act as a blockade antagonist of epileptic seizures. Among the ten subtypes of voltage-gated calcium (CaV) channels, CaV3.1-CaV3.3 constitute the T-type, or low voltage-activated subfamily, whose abnormal activities are associated with epilepsy, psychiatric.

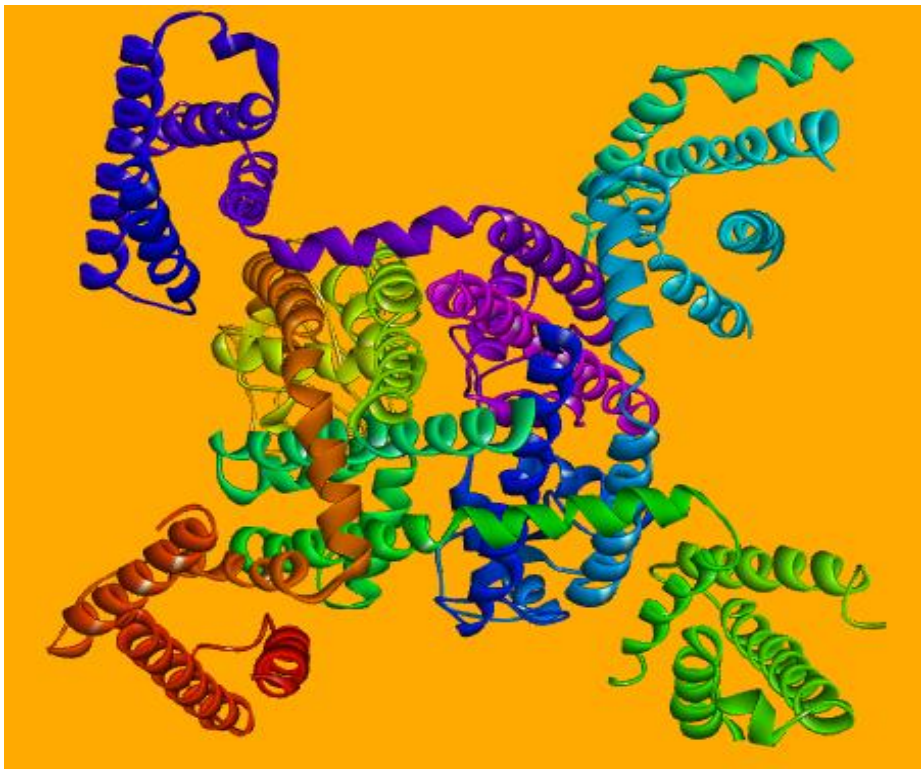


Figure 2. 3D image of 6KZP macromolecule

Method

Working Stages

Firstly, the macromolecule obtained from the databases was saved in the receptor.pdb format by removing the previously studied ligands in the Discovery Studio program, and the ligands were recorded in the same format as ligand.pdb. Afterwards, water is removed from macromolecules in Autodock Tolls program, only polar hydrogens are added and the molecule is saved in receptor.pdbqt format. Then, after the torsion root and the number of rotatable bonds were determined in the ligands, they were recorded in ligand.pdbqt format.

In the next step, the grid was applied to the molecules and the grid dimensions and coordinates were recorded in the configuration file. From the calculated RMSD (root-mean-square deviation) values, the conformation less than 2Å is attributed to the effective binding with the receptor. In the Discovery Studio program, which is a modeling program, 2D and 3D images are obtained, the best value conformation from the out file is placed into the macromolecule. By leaving the conformation with the lowest RMSD value inside the molecule, bond properties and lengths were examined.

Moleculer Docking Analysis

Preparation of Target Protein

As explained in the introduction 6KZP coded molecular structure were selected according to their effect potentials on ligands and active site amino acids were determined by using the DSV (Discovery Studio) [22] program for chelating calculations. After this prepared structure was optimized, it was saved in receptor.pdb format for use in clamping calculations, and the prepared structure was opened with the Autodock Vina Tolls (ADT) program and all crystalline waters in the active region were deleted. Finally, polar hydrogens were added to the structure and saved in .pdbqt format. At the end of the preparation process, active region coordinates were selected to determine the grid structure and conf. saved to file.

The 6KZP macromolecule was selected according to its mechanism of creating an antagonistic effect for neurotransmitters in epilepsy disease, and it shows the potential to interact well on the action mechanisms of certain ligands in the study. In this study, the active binding sites of the 6KZP macromolecule consisting of only the A chain were determined for the docking study and the following amino acid active sites were selected for the binding sites; GLU 354, PHE 917, LEU 920, GLN 922, GLY 951, ASN 952, PHE 956, LYS 1462, ASP 1463, VAL 1505, THR, 1777. The research area was determined as 375Å interval, the grid size was determined as 56Å×54Å×52Å for all ligands. The location of this search area is set for all ligands, the X, Y and Z coordinates of the center are set as

172.839, 171.636 and 186.780 and recorded for each in the conf.txt file. The data obtained for all pdb files are shown later in the results section in the form of tables and figures.

Preparation of Selected Ligands

The 19 ligands in the study were selected according to the features that can convulse seizures in epilepsy disease. First of all, 19 of our substances to be used as ligands were downloaded as .sdf files from the database specified in the material method section. The .sdf file downloaded with the Discovey Studio program has been optimized [20] and the structure saved as ligand.pdb has been prepared for clamping with the help of the ADT user interface. After determining the torsion root of the ligands prepared in DSV in Autodock Vina Tolls program, the number of rotatable ligaments was determined and the file was saved in ligand.pdbqt format.

Modeling Work with Discovery Studio Visualizer After ADT

It has been stated above that ligands are set in ligand.pdbqt format and macromolecules are set in receptor.pdbqt format with the ADT program, which acts as an interface in the Autodock Vina clamping study. In the Discovery studio program, after calling the receptor.pdb file, which was purified from water in the first stage, the out.pdbqt file containing the conformations obtained from the molecular dockingstudy with ADT was opened and the conformation with the lowest affinity value and RMSD value below 2Å was copied from the out.pdbqt file and pasted into the receptor. By performing 3-dimensional and 2-dimensional modeling, bonding properties, bond type and bond lengths were obtained and the data are shown in the results section.

3. Result and Discussion

In the Discovery Studio 2020 Client program, the conformation that gives the best value was placed inside the 6KZP macromolecule to see 2D and 3D structures. The binding affinity values obtained for ligands as a result of this calculation are summarized in Table 2.

Table 2. The binding affinity values of ligands placed in 6KZP at the best conformation

Ligand's	Best Binding affinity (kcal/mol)	Distance from best mode (Å)	
		RMSD l.b	RMSD u.b
Vigabatrin	-4.4	0.000	0.000
Lacosamide	-6.1	0.000	0.000
Zonisamide	-6.1	0.000	0.000
Oxcarbazepine	-7.5	0.000	0.000
Levatiracetam	-5.4	0.000	0.000
Tiagabine	-7.4	0.000	0.000
Topiramate	-6.9	0.000	0.000
Lamotrigine	-6.4	0.000	0.000
Gabapentin	-5.4	0.000	0.000
Felbamate	-6.0	0.000	0.000
Ethosuximide	-5.1	0.000	0.000
Valproic acid	-4.8	0.000	0.000
Mesuximide	-7.3	0.000	0.000
Ethotoin	-6.4	0.000	0.000
Primidone	-7.1	0.000	0.000
Trimethadione	-4.7	0.000	0.000
Phenytoin	-7.5	0.000	0.000
Remacemide	-7.0	0.000	0.000
Mephenytoin	-5.7	0.000	0.000

When the results were examined, Oxcarbazepine and Phenytoin gave the best binding affinity with 6KZP macromolecule -7.5 kcal/mol. Oxcarbazepine and Phenytoin gave the best binding affinity for 6KZP with a value of -7.5 kcal/mol. When the other ligand results are examined, we can rank the results in descending order (as kcal/mol); Tiagabine (-7.4), Mesuximide (-7.3), Primidone (-7.1), Remasemide (-7.0), Topiramate (-6.9) Mephenytoin (-6.7), Lomotrigine and Ethotoin (-6.4), Locosamide and Zonisamide (-6.1), Felbamate (-6.0), Levetiracetam and Gabapentin (-5.4), Esuximide (-5.1), Valproic Acid (-4.9), Trimethadione (-4.7), Vigabatrin (-4.4). The bond types, bond lengths, binding energies and 3D structures of ligand-receptor conformations are presented in detail below.

Vigabatrin

According to the results of the molecular docking analysis, the vigabatrin macromolecule was embedded in 6KZP. The binding affinities and RMSD values for the ligand vigabatrin embedded in the macromolecule 6KZP (Figure 2) are given in Table 2. The binding affinity value at the best binding position of the ligand vigabatrin placed on the macromolecule 6KZP was obtained as -4.4 kcal/mol. The 2D and 3D pictures of the intermolecular interactions between the conformation of vigabatrin in the best binding mode and the macromolecule 6KZP are shown in Figure 3. In this and all other ligands hereafter, the A chain is used for the docking process of the 6KZP macromolecule, and the amino acid active sites for the binding sites are as follows; GLU 354, PHE 917, LEU 920, GLN 922, GLY 951, ASN 952, PHE 956, LYS 1462, ASP 1463, VAL 1505, THR 1777. The ligand-protein interactions obtained were as follows; The LYSA1462 amino acid binding site formed a double bonded oxygen atom with a 3.97 Aº alkyl bond interaction. GLUA354 and GLNA922 amino acid binding sites formed a conventional hydrogen bond interaction with the hydroxyl group of 2.36 Aº and 2.12 Aº lengths, respectively. GLNA922 amino acid active site are 2.55 Å length of with amine they formed a conventional hydrogen bond interaction. And GLNA923 amino acid active site respectively are 2.30 Å and 2.73 Å with amine they formed a conventional hydrogen bond interaction with a length of (Table 3).

Table 3. Interactions, types and distances between vigabatrin and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
LYS_A1462	O atom in Vigabatrin	3.97	Alkyl
GLU_A354	Hydroxyl group in Vigabatrin	2.36	Conventional hydrogen bond
GLN_A922	Hydroxyl group in Vigabatrin	2.12	Conventional hydrogen bond
GLN_A922	NH_2 compound in Vigabatrin	2.55	Conventional hydrogen bond
GLN_A923	NH_2 compound in Vigabatrin	2.30	Conventional hydrogen bond
GLN_A923	NH_2 compound in Vigabatrin	2.73	Conventional hydrogen bond

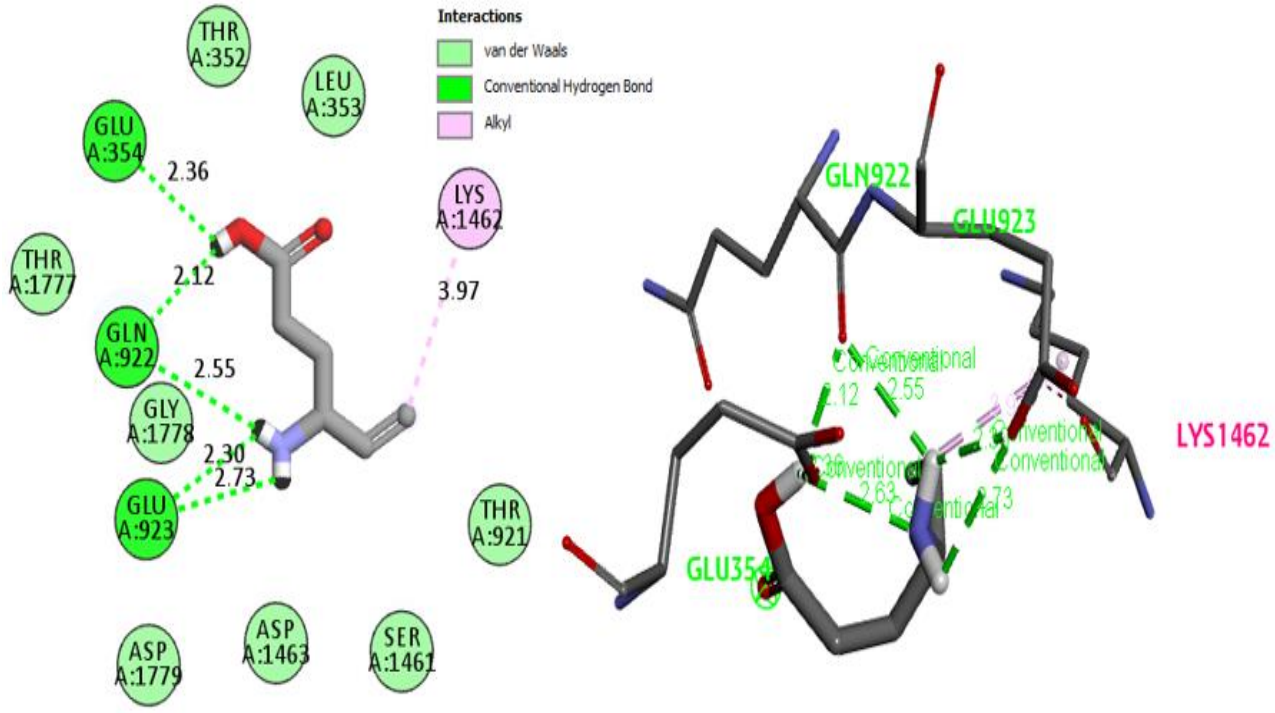


Figure 3. 2D and 3D representation of Vigabatrin and 6KZP macromolecules by molecular docking method

Lacosamide

The binding affinities and RMSD values for the ligand locosamide embedded in the macromolecule 6KZP are given in Table 2. The binding affinity value of the ligand locosamide placed in the macromolecule 6KZP at the best binding position was -6.1 kcal/mol, and the 2D and 3D visualizations of the intermolecular interactions between the locosamide's best binding mode position and the macromolecule 6KZP are shown in in appendix 1. The resulting ligand-protein interactions were as follows; The amino acid active site LEUA1819 formed a 3.79Å long pi-sigma bond interaction with the benzene group (Table 4).

Table 4. Interactions, types and distances between lacosamide and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
LEU_A1819	Benzen group in Lacosamide	3.79	Pi-Sigma

Zonisamide

The binding affinity value at the best binding position of ligand zonosamide placed on the macromolecule 6KZP was -6.1 kcal/mol, and the 2D and 3D visualizations of the intermolecular interactions between the zonosamide best binding mode position and the macromolecule 6KZP are shown in in appendix 2. The resulting ligand-protein interactions were as follows; The THRA921 amino acid binding site formed a 2.37Å-long conventional hydrogen bond interaction with the amine group. The LEUA920 amino acid active site formed a 4.51Aº long pi-alkyl bond interaction with the benzoxoazalin compound. The amino acid active sites of PHEA956 and LEUA872 formed a pi-pi T-shaped and pi-alkyl bond interaction with the benzene group with a length of 5.06Aº and 4.69Aº. Additionally, the types and distances of interactions are summarized in Table 5 in detail.

Table 5. Interactions, types and distances between zonisamide and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
THR_A921	NH_2 compound in Zonisamide	2.37	Conventional hydrogen bond
LEU_A920	Benzaxazoline group in Zonisamide	4.51	Pi-Alkyl
PHE_A956	Benzen group in Zonisamide	5.06	Pi-Pi T- shaped
LEU_A872	Benzen group in Zonisamide	4.69	Pi-Alkyl

Oxcarbazepine

The binding affinity value at the best binding position of the ligand oxcarbazepine placed in 6KZP was obtained as -7.5 kcal/mol. 2D and 3D visualizations of the intermolecular interactions between the oxcarbazepine best binding mode position and the macromolecule 6KZP are shown in appendix 3 and the resulting ligand-protein interactions were as follows; The amino acid active sites ALAA1502 and LEUA872 formed pi-alkyl and pi-sigma bond interactions with the benzene group of 4.52Å and 3.41Å lengths (Table 6).

Table 6. Interactions, types and distances between oxcarbazepine and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ALA_A1502	Benzen group in Oxcarbazepine	4.52	Pi-Alkyl
LEU_A872	Benzen group in Oxcarbazepine	3.41	Pi-Sigma

Levatiracetam

The binding affinity value of levatiracetam at the best binding position of the ligand inserted into 6KZP was -5.4 kcal/mol, and 2D and 3D visualizations of the intermolecular interactions between the levatiracetam best binding mode position and the macromolecule 6KZP are shown in appendix 4. The resulting ligand-protein interactions are as follows; The amino acid binding sites ASNA926, GLUA324 and ASPA924 formed a conventional hydrogen bond interaction with the amine group of 2.67Aº- 2.26Aº and 1.98Å lengths, respectively. ASPA924 amino acid active site formed a carbon-hydrogen bond interaction with the nitrogen atom with a length of 3.73Å, respectively. LYSA927 amino acid active site formed a 3.77Å long carbon hydrogen bond interaction with the O atom (Table 7).

Table 7. Interactions, types and distances between levatiracetam and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ASN_A926	NH_2 compound in levatiracetam	2.67	Conventional hydrogen bond
GLU_A354	NH_2 compound in levatiracetam	2.26	Conventional hydrogen bond
ASP_A924	NH_2 compound in levatiracetam	1.98	Conventional hydrogen bond
ASP_A924	Nitrogen atom in levatiracetam	3.73	Carbon hydrogen bond
LYS_A927	O atom in levatiracetam	3.77	Carbon hydrogen bond

Tiagabine

The binding affinity value at the best binding position of ligand tiagabine placed in 6KZP was -7.4 kcal/mol, and 2D and 3D visualizations of the intermolecular interactions between the position in the best binding mode of tiagabine and the macromolecule 6KZP are shown in Appendix 5. The resulting ligand-protein interactions were as follows; The PHEA1817 amino acid active site formed a 5.52Å alkyl bond interaction with the S atom. The amino acid binding sites VALA1820 and VALA1505 formed an alkyl bond interaction with the methyl group, with a length of 3.77Aº and 4.92Aº, respectively. The benzene group and VALA1505, LEUA1813 and ALAA1460 amino acid active sites formed 5.49Å-5.25Å and 5.29Å long alkyl bond interactions, respectively. The amino acid binding sites VALA1820, VALA1512 and META1508 formed pi-alkyl, pi-alkyl, pi-sulfur and pi-alkyl bond interactions with the methylthiaphene group in lengths of 4.82Å-5.31Aº- 5.58Å and 5.26Aº, respectively. The amino acid active sites VALA1505 and META1508 formed an alkyl bond interaction of 3.77Å and 4.70Å with the methylene group (Table 8).

Table 8. Interactions, types and distances between tiagabine and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
VAL_A1820	Methyl group in Tiagabine	3.77	Alkyl
VAL_A1820	Methylthiophene group in Tiagabine	4.82	Pi-Alkyl
VAL_A1512	Methylthiophene group in Tiagabine	5.31	Pi-Alkyl
PHE_A1817	S atom in Tiagabine	5.52	Pi-Sulfur
VAL_A1505	Methyl group in Tiagabine	4.92	Alkyl
VAL_A1505	CH_2 group in Tiagabine	3.77	Alkyl
VAL_A1505	Benzen group in Tiagabine	5.49	Alkyl
LEU_A1813	Benzen group in Tiagabine	5.25	Alkyl
ALA_A1460	Benzen group in Tiagabine	5.29	Alkyl
MET_A1508	CH_2 group in Tiagabine	4.70	Alkyl
MET_A1508	Methylthiophene group in Tiagabine	5.58	Pi-Sulfur
MET_A1508	Methylthiophene group in Tiagabine	5.26	Pi-Alkyl

Topiramate

The binding affinity value of the ligand topiramate placed in 6KZP at the best binding position was obtained as -6.9 kcal / mol. The 2D and 3D visualizations of the intermolecular interactions between the position in the best binding mode of topiramate and the macromolecule 6KZP are shown in appendix 6, and after the molecular docking study, the interactions were as follows; The amino acid active sites PHEA362, PHEA362 and TYRA361 formed an alkyl bond interaction with the methyl group of 4.92Aº- 4.64Aº and 5.33Å lengths. The TYRA361 amino acid binding site formed a 5.05Å long pi-sulfur bond interaction with the S atom (Table 9).

Tablo 9. Interactions, types and distances between topiramate and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
PHE_A362	CH_3 compound in Topiramate	4.92	Alkyl
PHE_A362	CH_3 compound in Topiramate	4.64	Alkyl
TYR_A361	CH_3 compound in Topiramate	5.33	Alkyl
TYR_A361	S atom in Topiramate	5.05	Pi-Sulfur

Lamotrigine

The binding affinity value at the best binding position of the ligand lamotragine placed in 6KZP was obtained as -6.4 kcal/mol. 2D and 3D pictures of the intermolecular interactions between the position in the best binding mode of lamotragine and the macromolecule 6KZP are shown in appendix 7. The resulting ligand-protein interactions are as follows; SERA1461, GLYA1778, GLNA922, THRA352, LEUA353 and GLUA354 amino acid active sites formed a conventional hydrogen bond interaction of 2.45Aº-2.59Aº-2.97Aº-2.27Å-2.88Å and 2.13Å lengths, respectively, with the amine compound. LYSA1482 amino acid active site formed a 3.86Aº alkyl bond interaction with the methyl group (Table 10).

Table 10. Interactions, types and distances between lamotrigine and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
SER_A1461	NH_2 compound in Lamotrigine	2.45	Conventional hydrogen bond
GLY_A1778	NH_2 compound in Lamotrigine	2.59	Conventional hydrogen bond
GLN_A922	NH_2 compound in Lamotrigine	2.97	Conventional hydrogen bond
THR_A352	NH_2 compound in Lamotrigine	2.27	Conventional hydrogen bond
LEU_A353	NH_2 compound in Lamotrigine	2.88	Conventional hydrogen bond
GLU_A354	NH_2 compound in Lamotrigine	2.13	Conventional hydrogen bond
LYS_A1482	CH_3 compound in Lamotrigine	3.86	Alkyl

Gabapentin

The binding affinity value at the best binding position of the ligand gabapentin placed in 6KZP was obtained as -5.4 kcal/mol. 2D and 3D pictures of the intermolecular interactions between the position in the gabapentin best binding mode and the macromolecule 6KZP are presented in appendix 8. The resulting ligand-protein interactions were as follows; The amino acid active sites ASNA952 and LEUA920 formed a conventional hydrogen bond interaction with the amine compound with a length of 2.01Aº and 2.90Aº, respectively. The amino acid active sites LEUA920 and LEUA872 formed an alkyl bond interaction with the benzene group of 5.05Å and 4.88Å lengths, respectively. The GLYA951 amino acid active site formed an unfavorable acceptor-acceptor bond interaction of 2.77Aº with the carbon monoxide group (Table 11).

Table 11. Interactions, types and distances between gabapentin and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ASN_A952	NH_2 compound in Gabapentin	2.01	Conventional hydrogen bond
LEU_A920	NH_2 compound in Gabapentin	2.90	Conventional hydrogen bond
LEU_A920	Benzen group in Gabapentin	5.05	Alkyl
LEU_A872	Benzen group in Gabapentin	4.88	Alkyl
GLY_A951	Carbon monoxide group in Gabapentin	2.77	Unfavorable Acceptor-Acceptor

Felbamate

The binding affinity value at the best binding position of the ligand felbamate placed on the macromolecule 6KZP was obtained as -6.0 kcal/mol. The 2D and 3D visualizations of the intermolecular interactions between the felbamate best binding mode position and the macromolecule 6KZP are shown in appendix 9 and the interactions after the molecular docking study are as follows; The amino acid active sites ILEA387, ASNA388, SERA383, SERA383 and ILEA351 formed a conventional hydrogen bond interaction with the amine group of 2.75Aº-2.01Aº-2.66Aº-2.34Å and 2.74Aº lengths, respectively. PHEA956 amino acid active site formed a 4.53Aº long pi-pi stacked bond interaction with the benzene group. THRA352 amino acid active site formed a 3.57Å long carbon hydrogen bond interaction with the O atom (Table 12).

Table 12. Interactions, types and distances between felbamate and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ILE_A387	NH_2 compound in Felbamate	2.75	Conventional hydrogen bond
ASN_A388	NH_2 compound in Felbamate	2.01	Conventional hydrogen bond
SER_A383	NH_2 compound in Felbamate	2.66	Conventional hydrogen bond
SER_A383	NH_2 compound in Felbamate	2.34	Conventional hydrogen bond
ILE_A351	NH_2 compound in Felbamate	2.74	Conventional hydrogen bond
THR_A352	O atom in Felbamate	3.57	Carbon hydrogen bond
PHE_A956	Benzene group in Felbamate	4.53	Pi-Pi Stacked

Ethosuximide

The binding affinity value at the best binding position for the ligand ethosuximide inserted in 6KZP was -5.1 kcal/mol, and 2D and 3D visualizations of the intermolecular interactions between the best binding mode position and the macromolecule 6KZP in ethosuximide are presented in Appendix 10. After the study, the interactions were as follows; The amino acid active sites ASNB952 and LEUA920 formed a conventional hydrogen bond interaction with the amine group of 2.30Å and 2.28Å lengths, respectively. The amino acid active sites LEUA920 and LEUA872 formed an alkyl

bond interaction with the methylene group of 4.27Å and 4.22Å lengths, respectively. The PHEA956 amino acid active site formed a 5.30Å long pi-alkyl bond interaction with the methyl group (Table 13).

Table 13. Interactions, types and distances between ethosuximide and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ASN_B952	NH_2 compound in Ethosuximide	2.30	Conventional hydrogen bond
LEU_A920	NH_2 compound in Ethosuximide	2.28	Conventional hydrogen bond
LEU_A920	CH_2 compound in Ethosuximide	4.27	Alkyl
LEU_A872	CH_2 compound in Ethosuximide	4.22	Alkyl
PHE_A956	CH_3 compound in Ethosuximide	5.30	Pi-Alkyl

Valproic Acid

The binding affinity value of the ligand valproic acid placed in the 6KZP in the best binding position was obtained as -4.8 kcal/mol, and the 2D and 3D pictures of the intermolecular interactions between the position of the valproic acid in the best binding mode and the macromolecule 6KZP are presented in appendix 11. After molecular chelation, the interactions are as follows; ILEA380 amino acid active sites formed alkyl bond interactions with the methylene group of 4.39Aº and 4.53Aº lengths, respectively. The amino acid active sites PHEA384, PHEA385, PHEA1727 and PHEA1773 formed a pi-alkyl bond interaction with the methylene group of 4.36Å-4.75Å-4.84Aº and 5.12Aº lengths, respectively. The ILEA379 amino acid active site formed a classical hydrogen bond interaction with the hydroxyl group of 2.54Å (Table 14).

Tablo 14. Interactions, types and distances between valproic acid and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ILE_A379	Hydroxyl group in Valproic acid	2.54	Conventional hydrogen bond
ILE_A380	Methylene group in Valproic acid	4.39	Alkyl
ILE_A380	Methylene group in Valproic acid	4.53	Alkyl
PHE_A384	Methylene group in Valproic acid	4.36	Pi-Alkyl
PHE_A1727	Methylene group in Valproic acid	4.84	Pi-Alkyl
PHE_A1773	Methylene group in Valproic acid	5.12	Pi-Alkyl
PHE_A385	Methylene group in Valproic acid	4.75	Pi-Alkyl

Mesuximide

The binding affinity value at the best binding position of the ligand mesuximide placed in 6KZP was obtained as -7.3 kcal/mol. 2D and 3D visualizations of the intermolecular interactions between the mesuximide best binding mode position and the macromolecule 6KZP are presented in appendix 12. The resulting ligand-protein interactions are as follows; Amino acid active sites of ILEA380, LEUA1819 and PHEA1773 formed pi-alkyl, pi-alkyl and pi-pi stacked bond interactions with the benzene group in lengths of 5.01Å-5.08Å and 5.91Å, respectively. PHEA1727, META1728 and GLYA1724 amino acid active sites formed pi-alkyl, alkyl and carbon hydrogen bond interactions with the methyl group of 4.65Å-4.83Å and 3.69Å lengths, respectively. The GLYA1724 amino acid active site formed a 3.29Aº long carbon hydrogen bond interaction with the O atom (Table 15).

Tablo 15. Interactions, types and distances between mesuximide and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ILE_A380	Benzen group in Mesuximide	5.01	Pi-Alkyl
LEU_A1819	Benzen group in Mesuximide	5.08	Pi-Alkyl
PHE_A1773	Benzen group in Mesuximide	5.91	Pi-Pi Stacked
PHE_A1727	CH_3 group in Mesuximide	4.65	Pi-Alkyl
MET_A1728	CH_3 group in Mesuximide	4.83	Alkyl
GLY_A1724	CH_3 group in Mesuximide	3.69	Carbon hydrogen bond
GLY_A1724	O atom in Mesuximide	3.29	Carbon hydrogen bond

Ethotoine

The binding affinity value at the best binding position of the ligand ethotoin placed in 6KZP was obtained as -6.4 kcal/mol. The 2D and 3D pictures of the intermolecular interactions between the position in the best binding mode of ethotoin and the macromolecule 6KZP are shown in appendix 13. After the study, the interactions were as follows; The amino acid active sites of ILEA380, LEUA1819 and PHEA384 formed pi-alkyl, pi-alkyl and pi-pi t-shaped bond interactions with the benzene group of 4.67Aº-5.29Aº and 4.98Å lengths, respectively. GLYA1724 amino acid active site formed a carbon hydrogen bond interaction with the O atom of 3.49Å length (Table 16).

Tablo 16. Interactions, types and distances between ethotoine and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
ILE_A380	Benzen group in Ethotoine	4.67	Pi-Alkyl
LEU_A1819	Benzen group in Ethotoine	5.29	Pi-Alkyl
PHE_A384	Benzen group in Ethotoine	4.98	Pi-Pi T- shaped
GLY_A1724	O atom in Ethotoine	3.49	Carbon hydrogen bond

Primidone

The binding affinity value at the best binding position of the ligand primidone placed in 6KZP was obtained as -7.1 kcal/mol, and the 2D and 3D pictures of the intermolecular interactions between the position in the best binding mode of the primidone and the macromolecule 6KZP are presented in appendix 14. The resulting interactions were as follows; The amino acid active sites PHEA384, PHEA385 and VALA1822 formed pi-alkyl, pi-alkyl and alkyl bond interactions with the methylene group in lengths of 4.33Å-4.93Å and 4.37Å. GLYA1724 amino acid active site formed a carbon hydrogen bond interaction with the O atom of 3.60Å length. The amino acid active sites of ILEA380 and LEUA1819 formed a pi-alkyl bond interaction with the benzene group of 4.66Å and 5.15Å lengths, respectively (Table 17).

Tablo 17. Interactions, types and distances between primidone and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
PHE_A384	CH_2 compound in Primidone	4.33	Pi-Alkyl
PHE_A385	CH_2 compound in Primidone	4.93	Pi-Alkyl
VAL_A1822	CH_2 compound in Primidone	4.37	Alkyl
GLY_A1724	O atom in Primidone	3.60	Carbon hydrogen bond
ILE_A380	Benzen group in Primidone	4.66	Pi-Alkyl
LEU_A1819	Benzen group in Primidone	5.15	Pi-Alkyl

Trimethadione

The binding affinity value at the best binding position of the ligand trimethadione placed on the macromolecule 6KZP was obtained as -4.7 kcal/mol. The 2D and 3D visualizations of the intermolecular interactions between the position in the best binding mode of trimethadione and the macromolecule 6KZP are shown in appendix 15. After the molecular docking process, the interactions were as follows; VALA1512, VALA1512, ILEA1824, ILEA1389, VALA1820, VALA1820, VALA1505, VALA1508 and PHEA1509 amino acid binding sites with methyl group whit respectivly 3.96Å-4.85Å-5.47 Å-4.84Å-4.22Å-4.51Å-4.53Å- 4.65Å and 5.32Å a length of they have formed alkyl, alkyl, alkyl, alkyl, alkyl, alkyl, alkyl and pi-alkyl bond interactions with. The PHEA1817 amino acid active site formed a 3.19Å long carbon hydrogen bond interaction with the O atom (Table 18).

Tablo 18. Interactions, types and distances between trimethadione and 6KZP macromolecule

Resude	**Ligand group**	**Distance (Å)**	**Interaction**
VAL_A1512	CH_3 compound in Trimethadione	3.96	Alkyl
VAL_A1512	CH_3 compound in Trimethadione	4.85	Alkyl
ILE_A1824	CH_3 compound in Trimethadione	5.47	Alkyl
ILE_A1389	CH_3 compound in Trimethadione	4.84	Alkyl
VAL_A1820	CH_3 compound in Trimethadione	4.22	Alkyl
VAL_A1820	CH_3 compound in Trimethadione	4.51	Alkyl
VAL_A1505	CH_3 compound in Trimethadione	4.53	Alkyl
MET_A1508	CH_3 compound in Trimethadione	4.65	Alkyl
PHE_A1509	CH_3 compound in Trimethadione	5.32	Pi-Alkyl
PHE_A1817	O atom in Trimethadione	3.19	Carbon hydrogen bond

Pheytoin

The binding affinity value of the ligand phenytoin placed on the macromolecule 6KZP at the best binding position was obtained as -7.5 kcal/mol. 2D and 3D visualizations of the intermolecular interactions between the position in the best binding mode of phenytoin and the macromolecule 6KZP are shown in appendix 16 and the interactions after the study were as follows; The amino acid active sites of VALA1822, LEUA1723, PHEA384 and ILEA380 are pi-alkyl, amide pi-stacked, pi-pi t-shaped and pi-alkyl with the benzene group in the lengths of 4.47Å-4.67Å-5.21Å and 4.43Å, respectively they formed a bond interaction (Table 19).

Tablo 19. Interactions, types and distances between phenytoin and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
VAL_A1822	Benzene group in Phenytoin	4.47	Pi-Alkyl
LEU_A1723	Benzene group in Phenytoin	4.62	Amide-Pi Stacked
PHE_A384	Benzene group in Phenytoin	5.21	Pi-Pi T- shaped
ILE_A380	Benzene group in Phenytoin	4.43	Pi-Alkyl

Remacemide

The binding affinity value at the best binding position of the ligand remasemide placed in 6KZP was obtained as -7.0 kcal/mol. 2D and 3D visualizations of the intermolecular interactions between the position in the best binding mode of remasemide and the macromolecule 6KZP are shown in appendix 17 and the interactions after the study are as follows; The amino acid regions VALA1802, VALA1505 and PHEA1817 formed a pi-sigma, pi-alkyl and pi-pi t-shaped bond interaction with the benzene group, with a length of 3.40Å-4.75Å and 5.15Å, respectively. The META1508 amino acid regions formed an alkyl bond interaction with the methyl group of 4.48Aº and 4.05Aº lengths, respectively. Additionally, the types and distances of interactions are summarized in Table 20 in detail.

Tablo 20. Interactions, types and distances between remacemide and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
VAL_A1820	Benzene group in Remacemide	3.40	Pi-Sigma
VAL_A1505	Benzen group in Remacemide	4.75	Pi-Alkyl
PHE_A1817	Benzen group in Remacemide	5.15	Pi-Pi T- shaped
MET_A1508	CH_3 compound in Remacemide	4.48	Alkyl
MET_A1508	CH_3 compound in Remacemide	4.05	Alkyl

Mephenytoin

The binding affinity value of the ligand mephenytoin placed in the macromolecule 6KZP at the best binding position was obtained as -6,7 kcal/mol. 2D and 3D visualizations of the intermolecular interactions between the position in the best binding mode of mephenytoin and the macromolecule 6KZP are shown in appendix 18, and the interactions after molecular docking are as follows; The PHEA1727 amino acid region formed a 3.18Aº long pi-donor hydrogen bond interaction with the amine group. Amino acid regions ILEA308, PHEA384 and LEUA1819 formed pi-alkyl, pi-pi t-shaped and pi-alkyl bond interactions with the benzene group in length of 4.47Å-5.17Å and 5.45Å, respectively. The amino acid regions PHEA384, LEUA1819 and VALA1822 formed pi-alkyl, alkyl and alkyl bond interactions with the methylene group of 4.93Å-5.33Å and 4.40Aº lengths, respectively (Table 21).

Tablo 21. Interactions, types and distances between mephenytoin and 6KZP macromolecule

Resude	Ligand group	Distance (Å)	Interaction
PHE_A1727	NH_2 compound in Mephenytoin	3.18	Pi-Donor hydrogen bond
ILE_A308	Benzene group in Mephenytoin	4.47	Pi-Alkyl
PHE_A384	Benzen group in Mephenytoin	5.17	Pi-Pi T- shaped
LEU_A1819	Benzene group in Mephenytoin	5.45	Pi-Alkyl
PHE_A384	CH_2 compound in Mephenytoin	4.93	Pi-Alkyl
LEU_A1819	CH_2 compound in Mephenytoin	5.33	Alkyl
VAL_A1822	CH_2 compound in Mephenytoin	4.40	Alkyl

The results of molecular coupling of 19 ligand molecules obtained by their receptor interactions are combined. It was seen that the oxcarbazepine and phenytoin molecule gave the best affinity value, but when we look at the type of bonds it formed, it formed a pi-alkyl, pi-sıgma, pi-pi T shaped and amide-pi T stacked bonds instead of the desired hydrogen bond or van der Waals bond. Hydrogen bond types such as carbon hydrogen bond and classical hydrogen bond are desired bond types. because the stronger the bond between the molecules, the better the interaction. The best interactions in molecular interactions are van der Waals and hydrogen bonding, while the least important interactions are covalent and ionic bonds. One reason is that while cysteine is the only amino acid that will form the covalent disulfide bond, there are many amino acids that will interact with each other through hydrogen bonding and van der Waals interactions. The other reason is that the number of amino acids capable of forming ionic bonds is very few, and the number of units capable of forming hydrogen bonds or van der Waals interactions is innumerable. Although vigabatrin gave the lowest affinity value with the 6KZP macromolecule among 19 molecules, it gave the conventional hydrogen bond with the amino acid GLUA354, GLUA922 and GLUA923. The controversial issue is whether it is the type of bond emerging or the affinity value obtained that matters in docking studies.

When we look at the results, if we compare the bond types formed by the active substances that give the closest or the same affinity values; When the phenytoin (-7.5kcal/mol) and oxcarbazepine (-7.5kcal/mol) ligands were examined, it

was seen that they gave the same affinity values. Although they gave the two highest results among 19 protein-ligand structures, they could not form the desired hydrogen and van der Waals bonds. there are only a few pi bonds, and phenytoin interacted with the four amino acids of the 6KZP protein, while oxcarbazepine interacted with two types of interactions with the two amino acid structures of 6KZP. Then the following ligands with the highest binding affinity are tiagabine (-7.4kcal/mol) and mesuximide (-7.3kcal/mol), respectively. Tiagabin combined the 12 ligand groups in its structure with the 6KZP protein to form various pi and alkyl bonds, while Mesuximide combined the 7 ligand groups and the 6KZP protein in its structure to form the hydrogen bond, which is one of the strong bond structures for various pi bonds, alkyl bonds and molecular interactions.

When we compare primidone (-7.1kcal/mol) and remacamide (-7.0kcal/mol), we see that only a ligand group in the structure of primidone forms hydrogen bonds with the 6KZP macromolecule. Primidone formed hydrogen bonds with 1 of the 6 ligand groups, while remacemide did not form hydrogen bonds with any of the 5 ligand groups. Only various pi and alkyl bonds have occurred. When Topiramate and mephenytoin were compared, it was seen that Topiramate gave -6.9 kcal/mol mephenytoin -6.7kcal/mol. Although ligand-receptor structures gave low results in close binding affinity, only mephenytoin gave the desired hydrogen bond structure with the macromolecule. While mephenytoin interacted with 7 ligand groups, topiramate interacted with 4 ligand groups. And various pi and alkyl bonds are formed. When looking at lamotrigine and ethotoin, it is seen that they give the same binding affinity (-6.4 kcal/mol). Although they showed the same value, lamotrigine formed much more conventional hydrogen bonds with the 6KZP macromolecule than ethotoin. There were 7 types of interactions between the lamotrigine-receptor, and 6 of them were hydrogen bonded. According to this result, we can say that there is a strong interaction. Ethotoin, on the other hand, formed 1 hydrogen bond from 4 types of interactions with the receptor. Among the 19 ligands, we can say that the structure that forms the most hydrogen bonds in ligand-receptor interactions compared so far is the lamotrigine-6KZP structure. The comparison in the total will be made when all results are compared.

Although locasamide and zonisamide (-6.1 kcal/mol) gave the same binding affinity, locasamide formed a single interaction with the 6KZP macromolecule and formed the pi-sigma bond. Zonisamide, on the other hand, formed 4 types of interaction with the receptor and formed 1 hydrogen bond. The conclusion to be drawn from here is that even if they have the same binding energies, the types of bonds, their numbers and strengths can be very different from each other. We can say the following for felbamate (-6.0 kcal/mol) and levetiracetam (-5.4 kcal/mol); Felbamate induced more interactions than levetirecetam through ligand addition to the macromolecule, but appears to form hydrogen bonds to the same extent as levetiracetam. Felbamate formed hydrogen bonds with 6 out of 7 ligand groups, while levetirecetam formed hydrogen bonds with all 6 ligand groups. When gabapentin (-5.4 kcal/mol) and ethosuximide (-5.1 kcal/mol) are examined, it is seen that both ligand structures create 5 types of interaction with the receptor, and both ligand-receptor structures give 2 conventional hydrogen bonds. Considering the bond types made with valproic acid (-4.9 kcal/mol) and trimethadione (-4.7 kcal/mol), which have low binding affinity, it is seen that valproic acid combines 7 ligand groups and trimethadione 10 ligand groups with amino acid sites. The desired hydrogen bond structure was revealed between the 6KZP macromolecule and both ligand structures, and it was observed that various pi and alkyl bonds were also formed.

In addition to the bond structures and interaction types, the IC50 values and protein binding rates of the studied antiepileptic drugs were also examined. The IC50 is the concentration of inhibitor that inhibits 50% of the enzyme, and a low IC50 indicates a high inhibition value. The lower the IC50 concentration values for a drug molecule, the better it inhibits. In the light of this information, when the IC50 and protein binding rates obtained from the Pubchem database for 19 antiepileptic drugs were examined in Table 22, it was seen that the protein binding rate was not suitable for vigabatrin, which gave the lowest affinity value, and the IC50 value on calcium channels could not be determined. For oxcarbazepine, one of the ligands with the highest value, the IC50 value appeared inactive, while the plasma protein binding rate was 40%. For Phenytoin, on the other hand, the IC50 value is 21.9, while the protein binding rate is 90%. Other rates are detailed in the table. As a result of the information given above, since it is known that the high inhibition potential of the drug is proportional to the low IC50 concentration level, the determined IC50 concentration of phenytoin, which gives the best binding affinity and percentage, gave the highest value. Gabapentin, which gave the lowest IC50 concentration, showed lower values for docking affinity and protein binding compared to phenytoin and oxcarbazepine. According to these results, in addition to the inhibitory effect of gabapentin, it know that the bond types and interactions with protein are better than phenytoin and oxcarbazepine.

Table 22. Docking, IC50 and protein binding values of antiepileptics

Ligand's	Best Binding affinity (kcal/mol)	IC50 (μM)	Protein Binding(%)
Vigabatrin	-4.4	-	Protein binding is not amenable
Lacosamide	-6.1	Undefined	<%15
Zonisamide	-6.1	3.3	%40
Oxcarbazepine	-7.5	İnactive	%40
Levatiracetam	-5.4	İnactive	%40
Tiagabine	-7.4	-	%96
Topiramate	-6.9	10	%9-17
Lamotrigine	-6.4	8.1	%55
Gabapentin	-5.4	0.14	<%3
Felbamate	-6.0	İnactive	%20-36
Ethosuximide	-5.1	Undefined	Protein binding is not amenable
Valproic acid	-4.8	Undefined	%10-18.5
Mesuximide	-7.3	-	Protein binding is not amenable
Ethotoin	-6.4	İnactive	Protein binding is not amenable
Primidone	-7.1	Undefined	%10.78-13.70
Trimethadione	-4.7	Undefined	%90
Phenytoin	-7.5	21.9	%90
Remacemide	-7.0	-	Protein binding is not amenable
Mephenytoin	-5.7	-	Protein binding is not amenable

As a result, it was more meaningful to compare the drugs with higher IC50 values -zonisamide, topiramate, lamotrigine, gabapentin, phenytoin-included in Table 22 and whether the ligands showing the desired bond types or the ligands with high chelate affinity had higher IC50 values. Such that, while zonisamide gave an affinity value of -6.1 kcal/mol, it showed inhibition with a value of 3.3 μM. When the binding interaction of zonisamide was examined, it was seen that it made conventional hydrogen bonds, which is one of the desired bond structures. For topitramate, while it showed a binding affinity of -6.9 kcal/mol, it gave an inhibition value with 10 μM, but it did not show a strong interaction. When the lamotrigine ligand was examined, it gave its affinity with a value of -6.4 kcal/mol, and its IC50 value was found to be 8.1 μM. Considering the intermolecular interaction, it was seen that it formed more than one strong interaction. For gabapentin, the binding affinity was -5.4 kcal/mol, while the inhibition value was 0.14 μM, and it is seen that it forms strong bonds in the interaction between the structures. For phenytoin, chelate value was -7.5 kcal/mol, while the IC50 value was found to be 21.9 μM and they did not create a strong and much interaction in the intermolecular interaction. The conclusion to be drawn from this is that having high binding affinity alone is not sufficient. The interpretation we can make according to the data we have is that ligands with an IC50 value of <10 μM can form one or more strong interactions even if they have low affinity, and complex structures with an IC50 value higher than >10 μM show high affinity but do not give the desired bond types.

When looking at the total, it was seen that those with the best affinity values did not make the strongest bonds, while those with the lowest affinity gave the desired hydrogen bond types. And besides, the IC50 values of the structures giving the best affinity were high, while gabapentin, which gave the lowest IC50 concentration value, did not exhibit high binding affinity. The conclusion to be drawn as we discuss it here is that the degree of binding affinity, the number of bonds obtained, and the bond structures are not parallel. And it has been observed that the drug can exhibit low affinity even if the protein binding rates are high or they show the best inhibition concentration..

4. Conclusion

In the study, Discovery Studio 2020 program and AutoDOCK Vina energy scoring were used, and there are various scoring functions. The results show that PDB ID: 6KZP macromolecule, which has an antagonistic effect on voltage-gated calcium channels, also gave good affinity values in studies with 19 active substances. The IC50 values and protein binding rates, as well as the types of bonds that result from the docking study, are important to us. Because even if the affinity value obtained in the ligand-protein docking study is low, considering the low IC50 value and high protein binding rates, we can say that the stronger the bond they establish, the better the interaction.

Competing Interest / Conflict of Interest

The authors declare that they no conflict of interest. The none of the authors have any competing interests in the manuscript.

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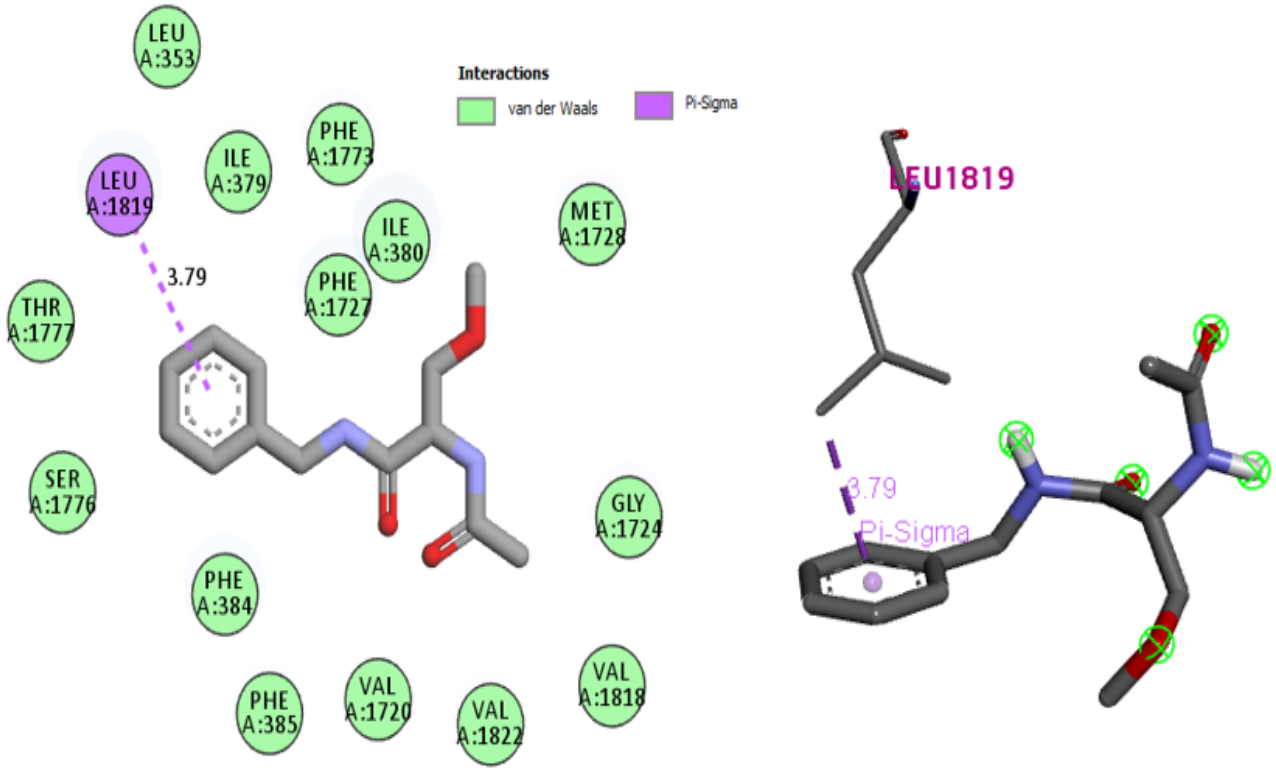
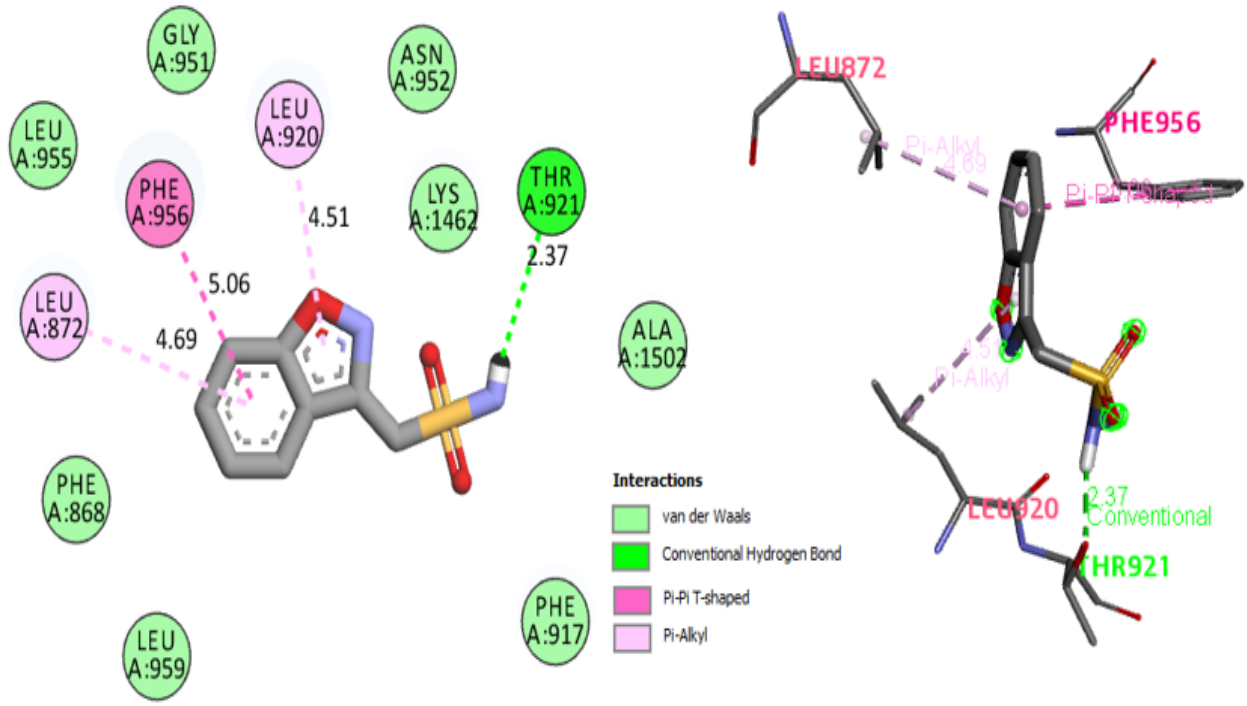
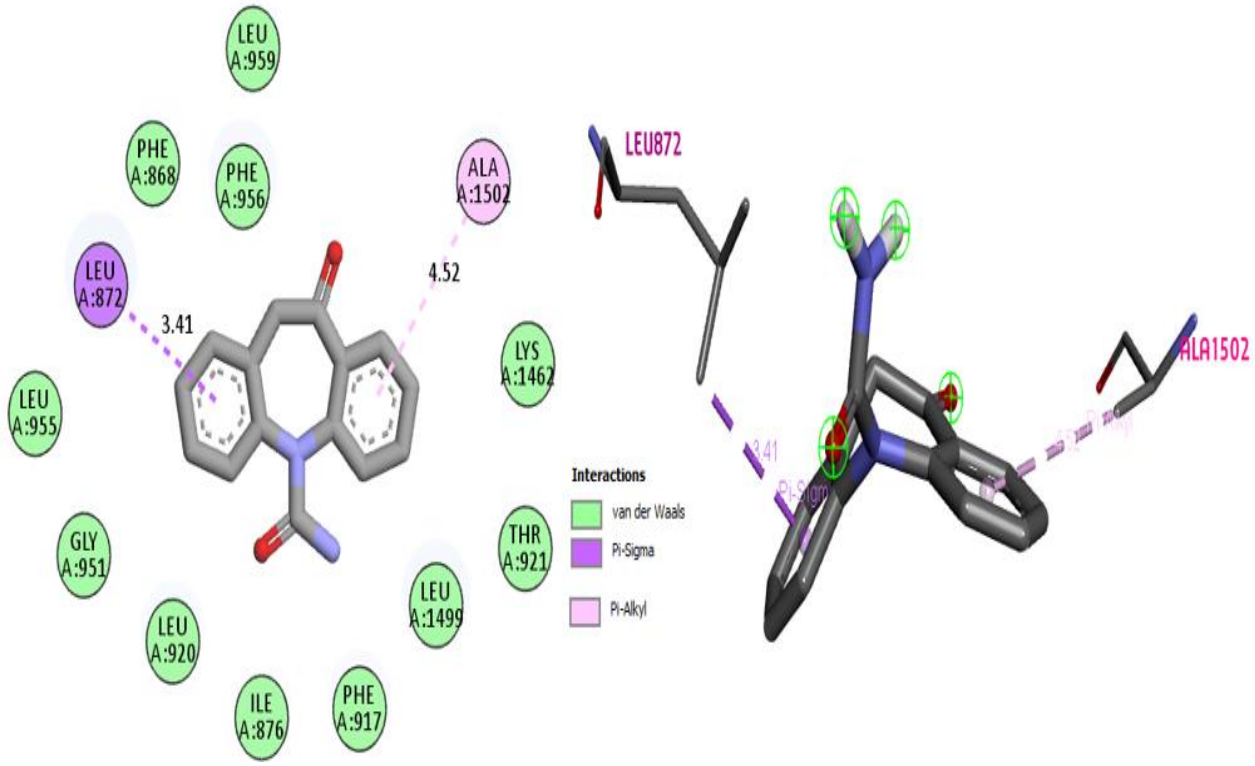
Appendix



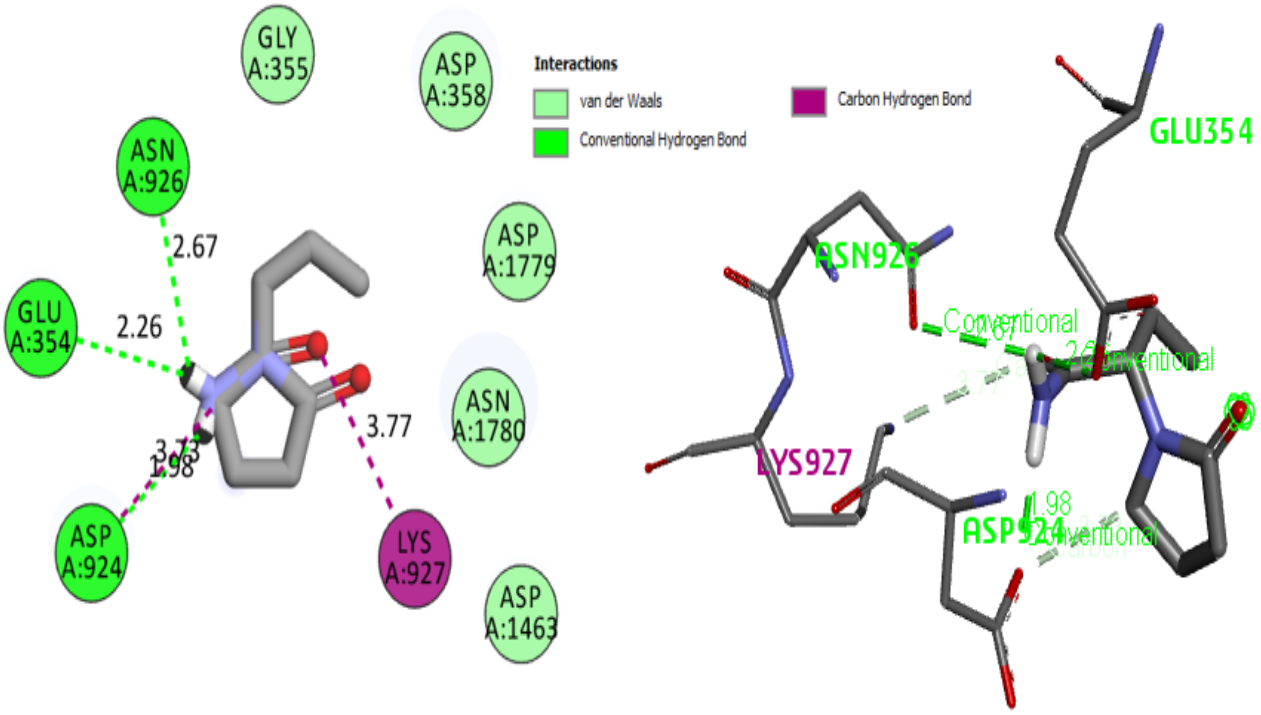
Appendix 1. 2D and 3D display of the interaction of locasamide and macromolecule (6KZP)



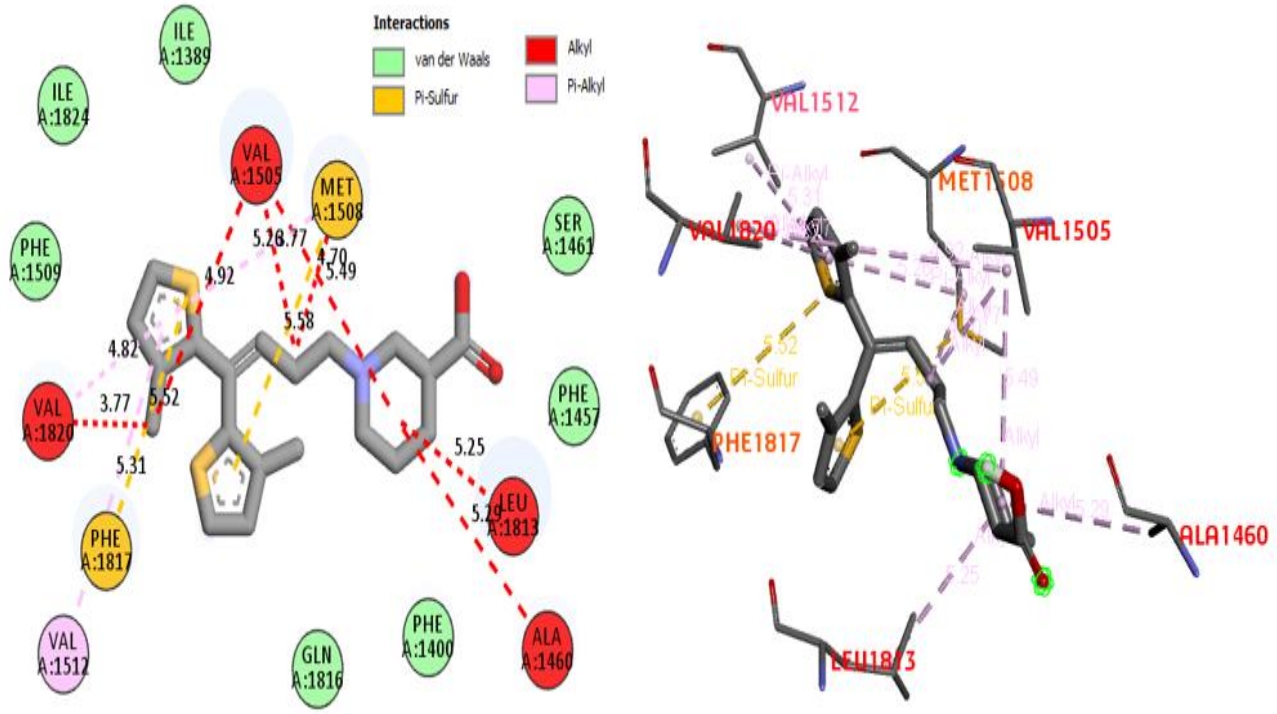
Appendix 2. 2D and 3D display of the interaction of zonisamide and macromolecule (6KZP)



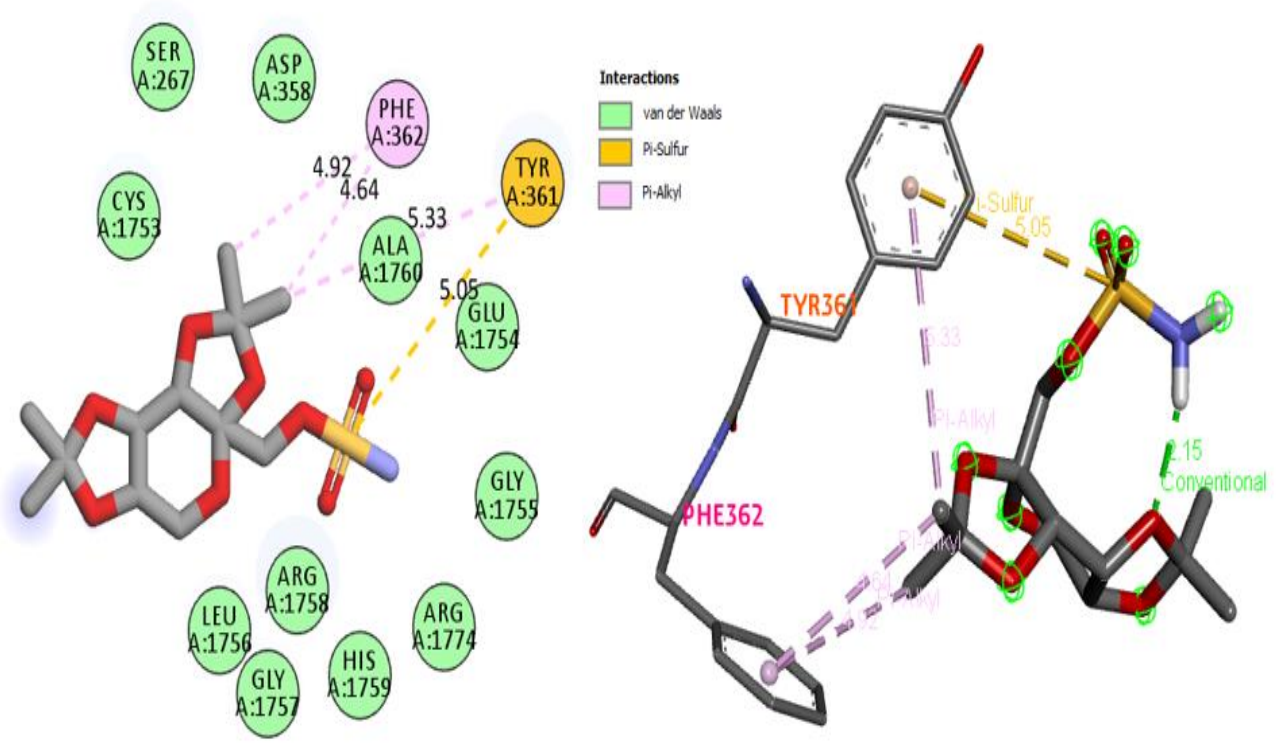
Appendix 3. 2D and 3D display of the interaction of oxcarpazepine and macromolecule (6KZP)



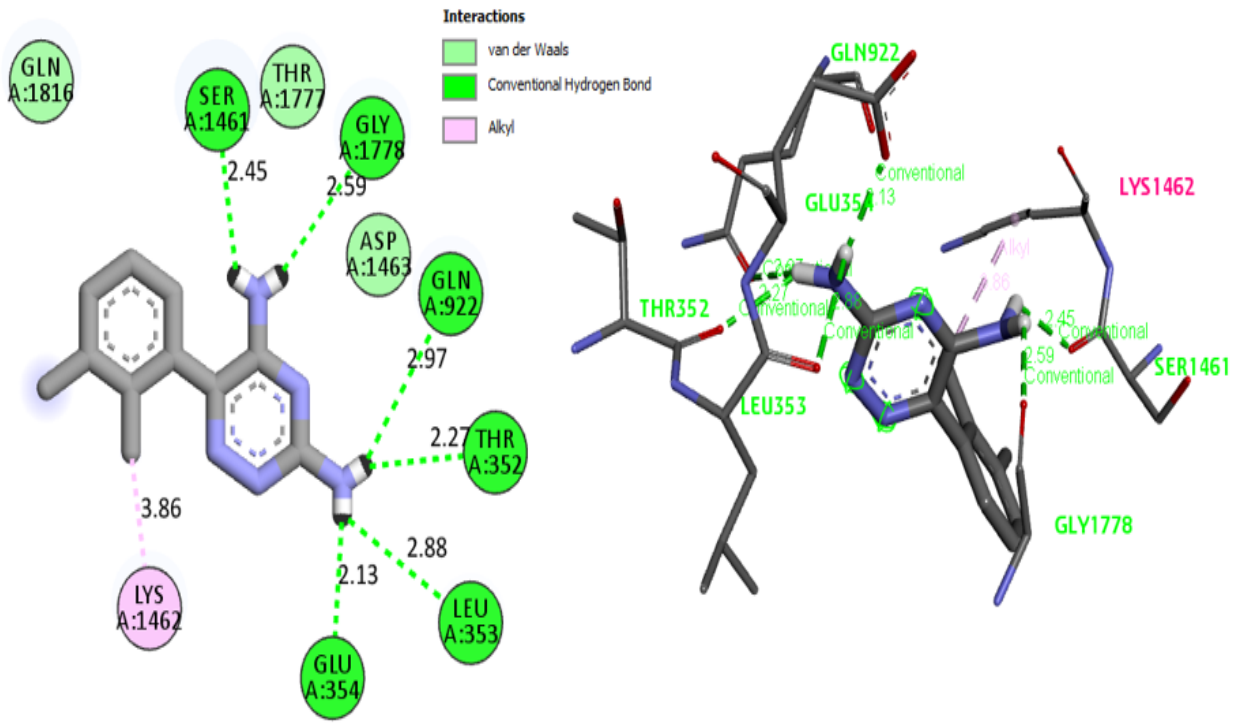
Appendix 4. 2D and 3D display of the interaction of levatiracetam and macromolecule (6KZP)



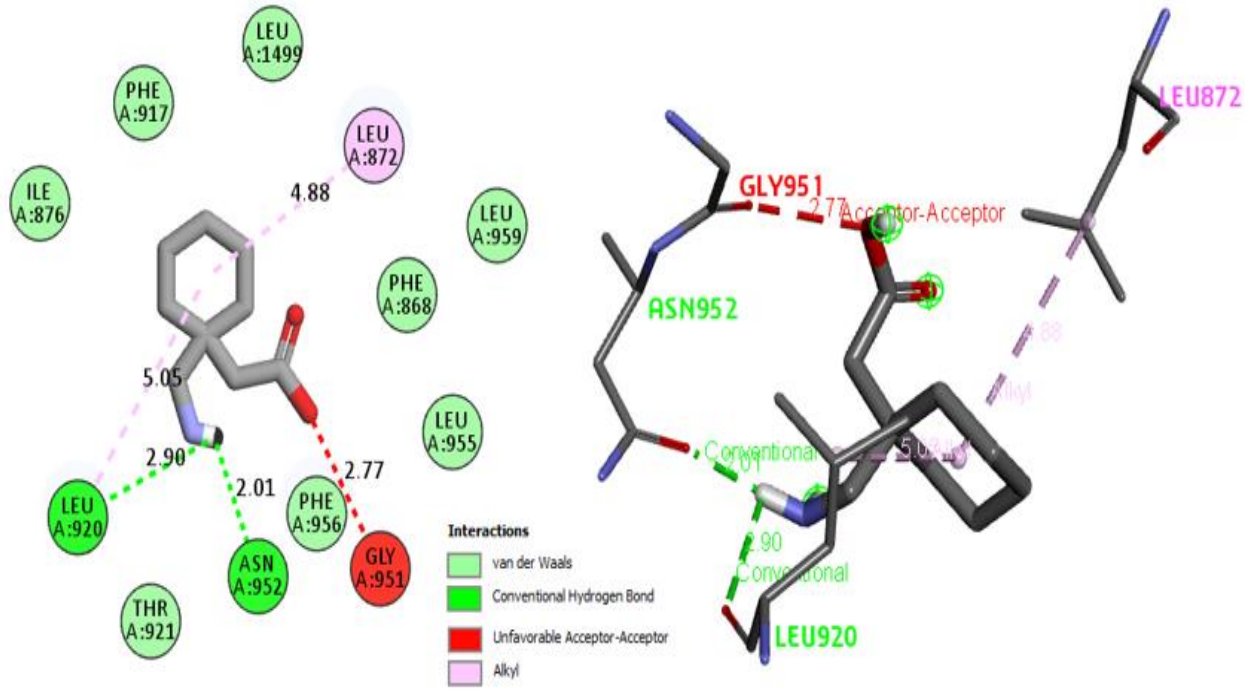
Appendix 5. 2D and 3D display of the interaction of tiagabine and macromolecule (6KZP)



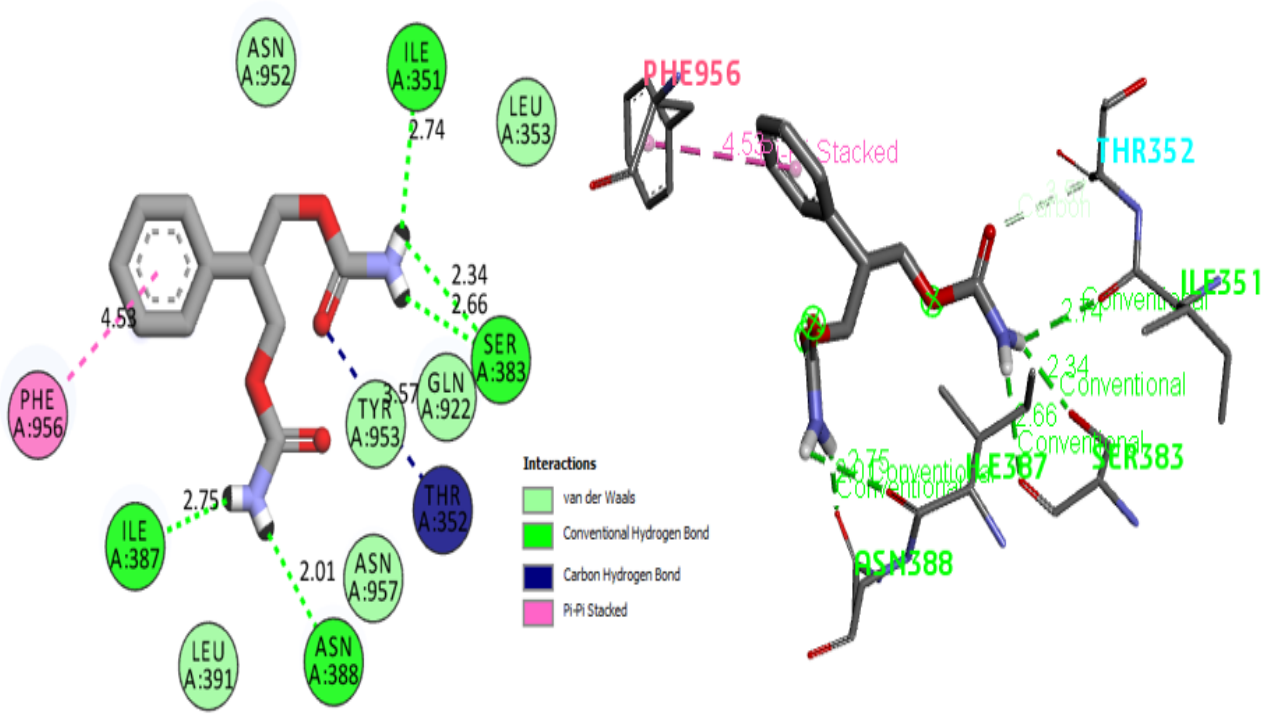
Appendix 6. 2D and 3D display of the interaction of topiramate and macromolecule (6KZP)



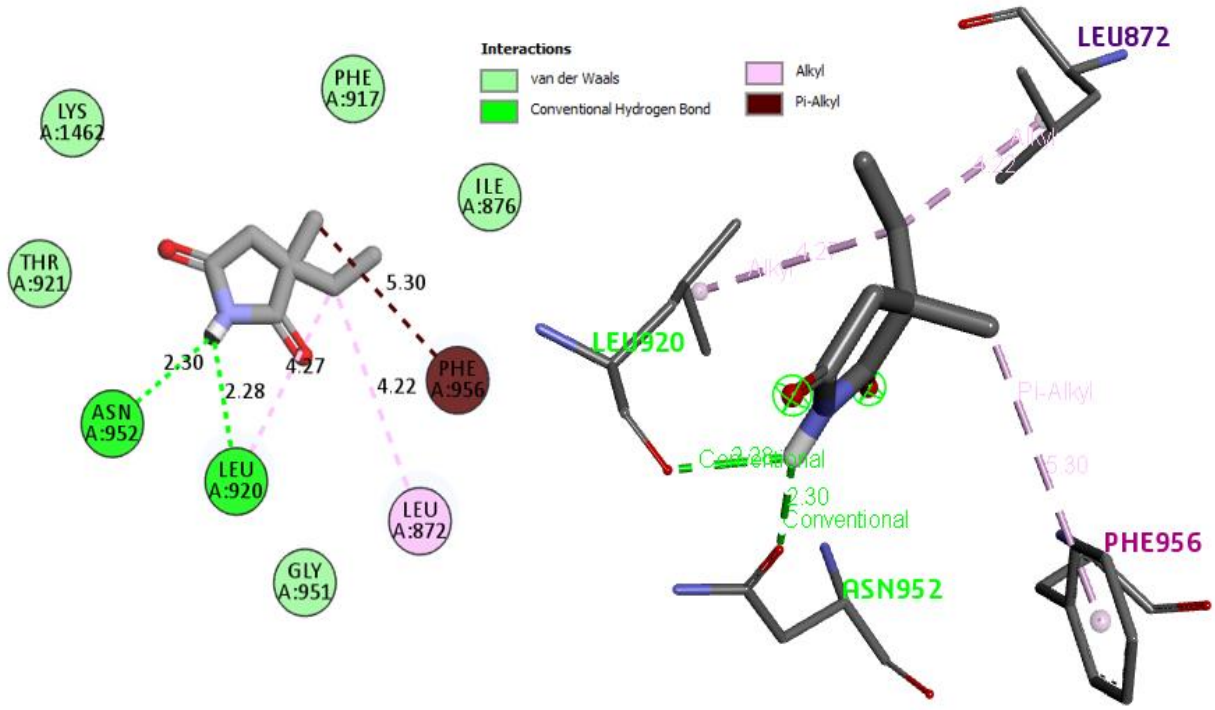
Appendix 7. 2D and 3D display of the Interaction of lamotrigine and macromolecule (6KZP)



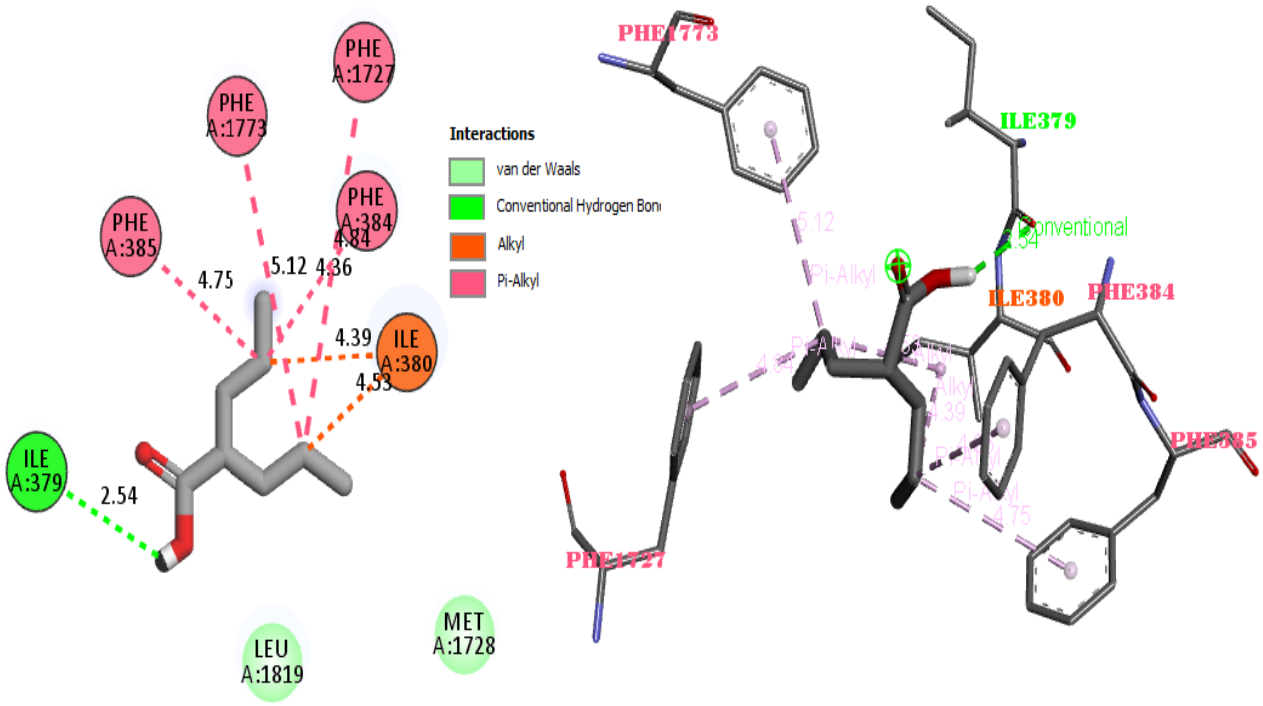
Appendix 8. 2D and 3D display of the interaction of gabapentin and macromolecule (6KZP)



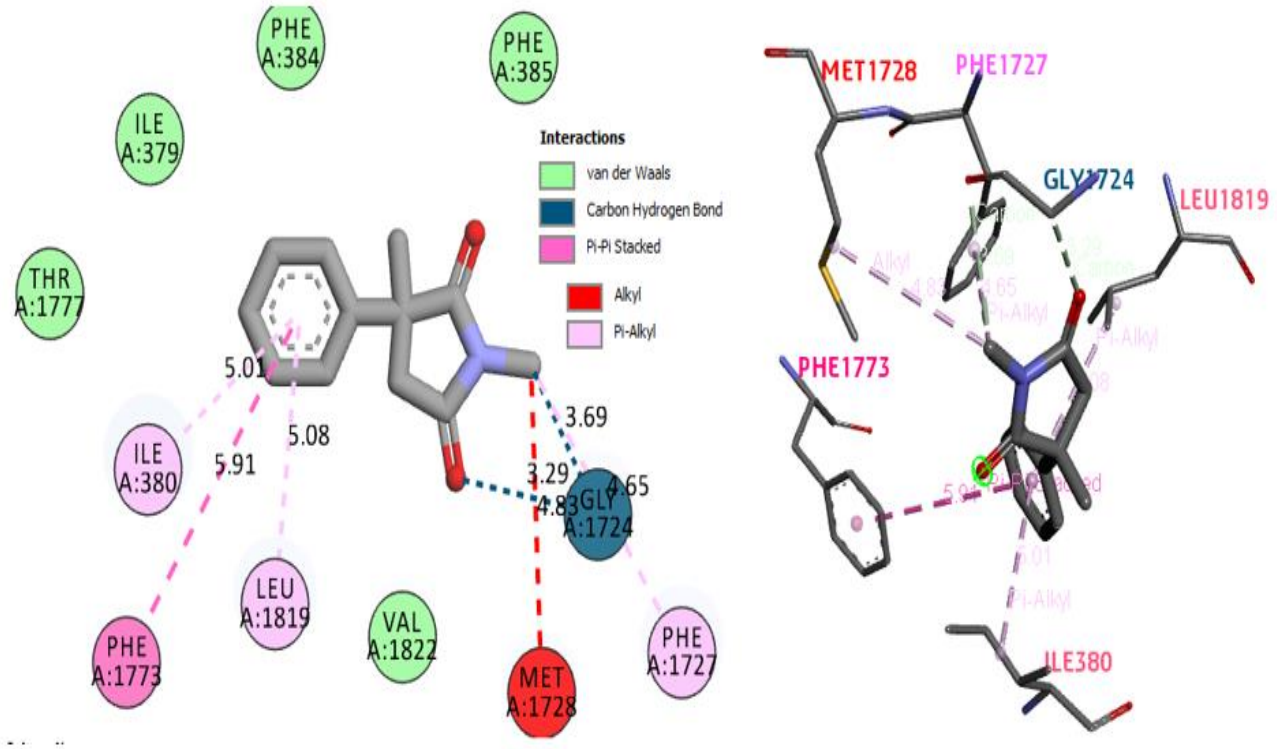
Appendix 9. 2D and 3D display of the interaction of felbamate and macromolecule (6KZP)



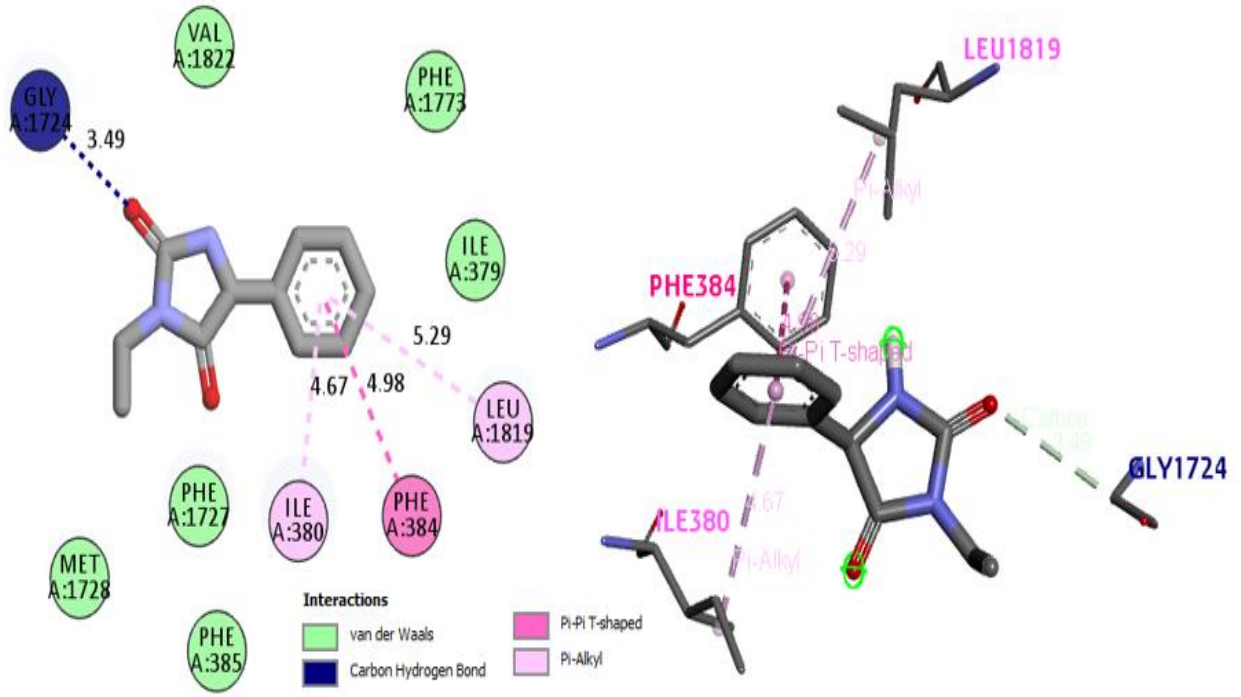
Appendix 10. 2D and 3D display of the interaction of ethosuximide and macromolecule (6KZP)



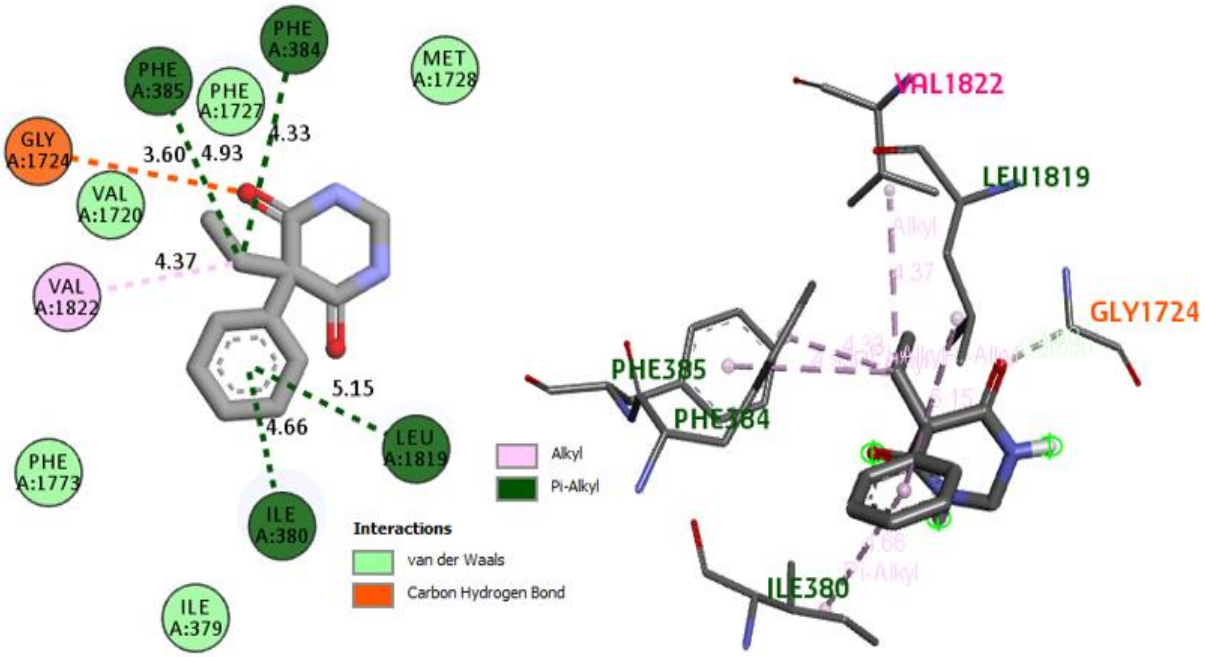
Appendix 11. 2D and 3D display of the interaction of valproic acid and macromolecule (6KZP)



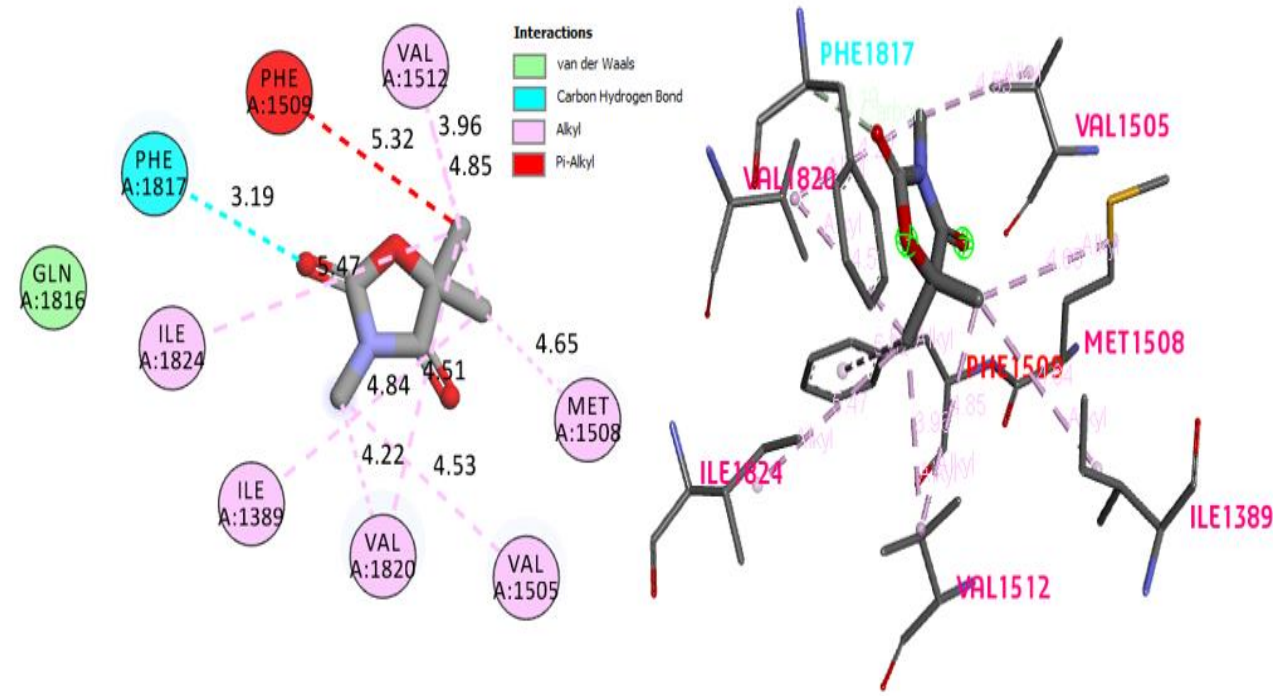
Appendix 12. 2D and 3D display of the interaction of mesuximide and macromolecule (6KZP)



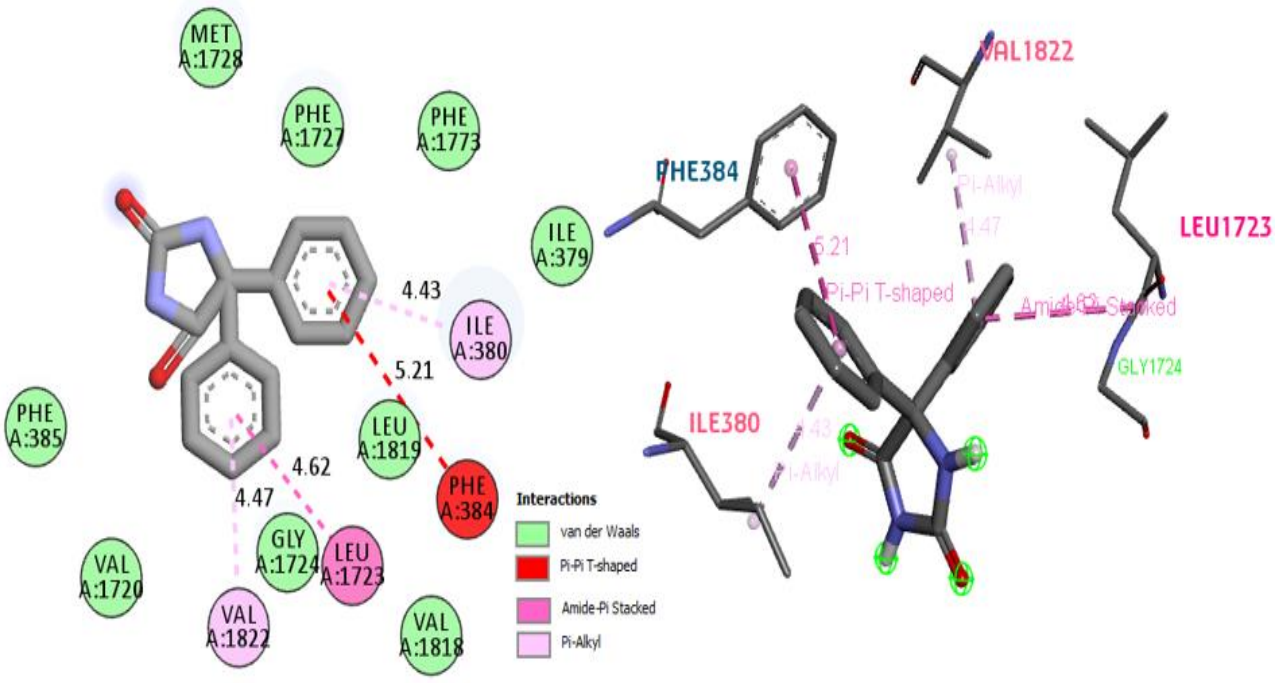
Appendix 13. 2D and 3D display of the interaction of ethotoine and macromolecule (6KZP)



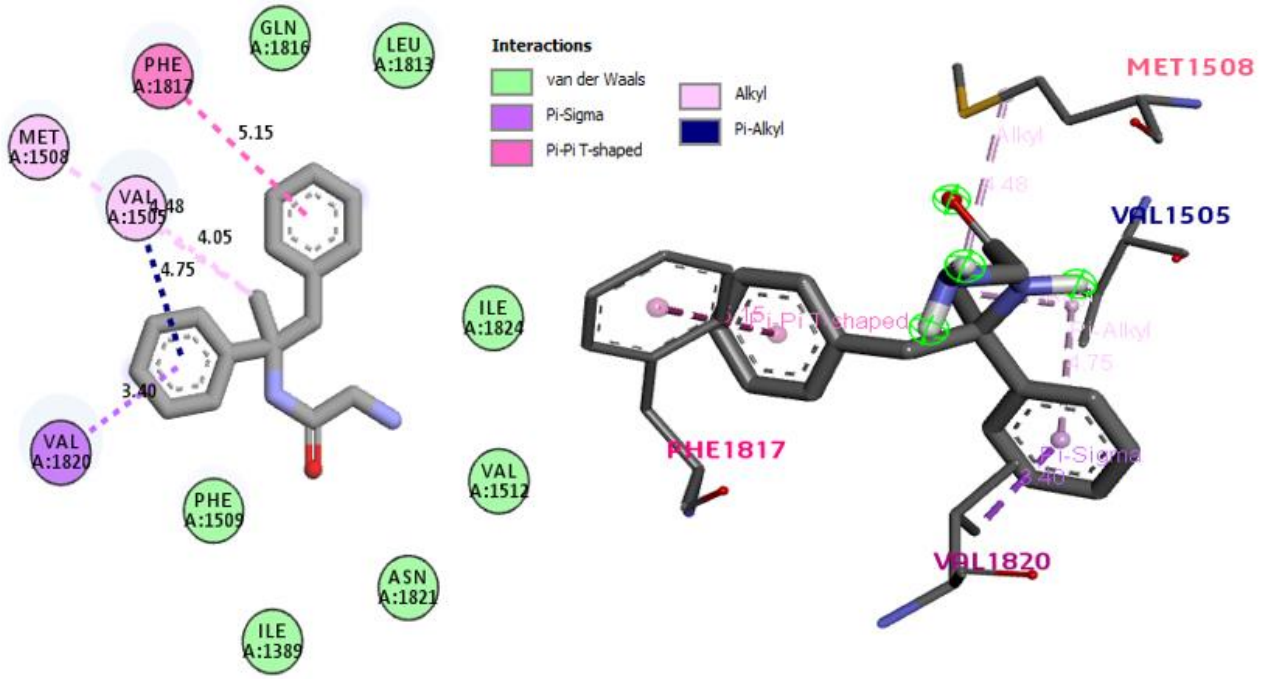
Appendix 14. 2D and 3D display of the interaction of primidone and macromolecule (6KZP)



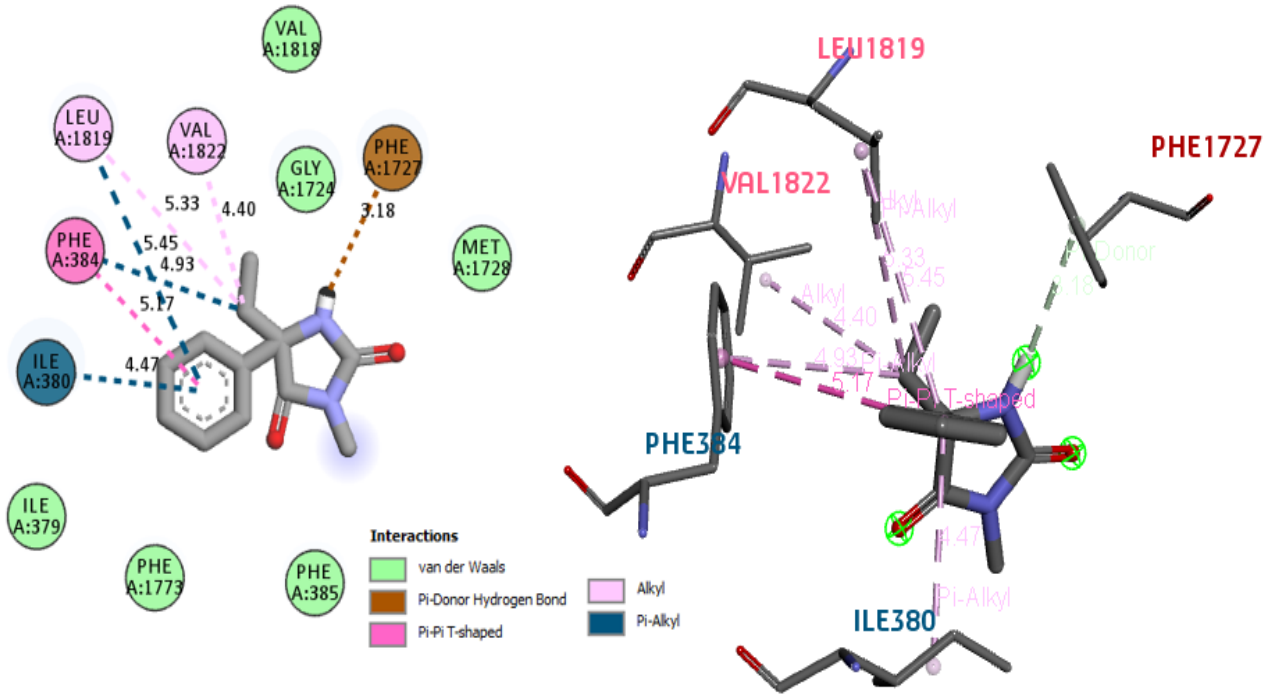
Appendix 15. 2D and 3D display of the interaction of trimethadione and macromolecule (6KZP)



Appendix 16. 2D and 3D display of the interaction of phenytoin and macromolecule (6KZP)



Appendix 17. 2D and 3D display of the interaction of remacemide and macromolecule (6KZP)



Appendix 18. 2D and 3D display of the interaction of mephenytoin and macromolecule (6KZP)

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Changes of plant nutrients K and Mg in several plants based on traffic density and organs

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Abstract: Among the mineral nutrients, potassium (K) and magnesium (Mg) are essential mineral nutrients for plants' growth, development, and many biochemical processes, such as photosynthesis. If K or Mg is not present in plants, they are adversely affected by this situation. The excess of K and Mg concentration in plant tissues results in plants' toxicity. This study aimed to determine the variations in K and Mg element concentrations in branches, leaves, and seeds of *Aesculus hippocastanum* L., *Prunus cerasifera* Ehrh., *Tilia platyphyllos* Scop., *Acer negundo* L., and *Ailanthus altissima* (Mill.) Swingle, which are frequently used in urban areas, especially in landscape studies, based on traffic density. As a result, the changes in the elements based on the traffic density in all organs and organs in all traffic densities were significant ($P<0.05$). The highest concentrations were often found in individuals grown in areas with heavy traffic. The study results revealed that the element concentrations could show significant differences between organs in the same species, and this difference varies significantly based on species.

Keywords: Magnesium, Nutrient, Plant, Potassium, Traffic density.

Öz: Mineral besinler arasında potasyum (K) ve magnezyum (Mg), bitkilerin büyümesi, gelişmesi ve fotosentez gibi birçok biyokimyasal süreç için gerekli mineral besinlerdir. Bitkilerde K veya Mg noksanlığından olumsuz etkilenirler. Bitki dokularındaki fazla K ve Mg konsantrasyonu, bitkilerde toksisiteye neden olur. Bu çalışmada kentsel alanlarda, özellikle peyzaj çalışmalarında sıklıkla kullanılmakta olan *Aesculus hippocastanum* L., *Prunus cerasifera* Ehrh., *Tilia platyphyllos* Scop., *Acer negundo* L., and *Ailanthus altissima* (Mill.) Swingle'ın dal, yaprak ve tohumlarındaki K ve Mg elementlerinin trafik yoğunluğuna göre konsantrasyonlarındaki değişimlerin belirlenmesi amaçlanmıştır. Sonuç olarak, elementlerin bütün organlarda trafik yoğunluğuna bağlı olarak, bütün trafik yoğunluklarında da organ bazında değişiminin istatistiki olarak anlamlı düzeyde olduğu belirlenmiştir ($P<0.05$). En yüksek konsantrasyonlar genellikle yoğun trafiğin olduğu bölgelerde yetişen bireylerde elde edilmiştir. Çalışma sonuçları element konsantrasyonlarının aynı türlerde organlar arasında önemli düzeyde farklılıklar gösterebildiğini ve bu farklılığın tür bazında da önemli ölçüde değiştiğini ortaya koymaktadır.

Anahtar Kelimeler: Magnezyum, Besin elementi, Bitki, Potasyum, Trafik yoğunluğu.

1. Introduction

Plants are the living groups that form the basis of all life on earth, and all life on earth is indirectly or directly based on plant species [1]. This dependence is that plants can produce food with the help of sunlight by performing photosynthesis. Thus, plants form the basis of the food pyramid. In addition, plants achieve many ecological, economic, and social roles [2, 3].

The ability of plants to perform these roles relies on their vigorous growth and development. The shared interaction of plant genetic structure [4-6] and environmental factors play a crucial role in plant development [7-9]. It is necessary to understand this mechanism to assure plants' ideal growth and development and shape this expansion according to the desired goals [10].

The most dominant environmental factors affecting plant growth are climatic [11-14] and edaphic situations [15-17]. Perhaps the most important of these factors is nutritional elements. Nutrients are the basic building blocks of plants and are present at different levels in different organs of plants after they are taken from the soil [10, 18], not only in their natural habitat [19] but also in their marginal lands [20]. Another factor affecting plant growth is environmental stress conditions [21-27]. Studies show that traffic can also become a source of stress for plants by affecting air quality [18]. The literature states that increased traffic density and industrial and other various anthropogenic activities accelerate the metal pollution in the world, especially in urban sites. Increased traffic density causes many environmental problems (air or smog pollution), which results in some health problems, such as heart disease and lung cancer, and increases the

risk of respiratory infections. Therefore, the current study aimed to define the variations in the concentrations of potassium (K) and magnesium (Mg), which are essential nutrients for plants, in the organs of various plant species grown in areas with different traffic densities. K and Mg, which are among the nine essential macronutrients in plant nutrition, are crucial for plant development, and their deficiencies or toxicity cause various disease signs in plants and even plant destruction if not treated [28].

2. Material and Method

The present study was carried out on horse chestnut (*Aesculus hippocastanum* L.), ornamental plum (*Prunus cerasifera* Ehrh.), linden (*Tilia platyphyllos* Scop.), maple (*Acer negundo* L.), and tree of heaven (*Ailanthus altissima* Mill.) species that are often used in landscape studies. The samples were picked from the previous year's shoot, that is, from the 1-year-old part. As a seed sample, the seed part of the *Aesculus hippocastanum*, the fruit flesh part was used together with the shell for *Prunus cerasifera*, and the seeds with the stem and wings for other species were used. The samples were obtained towards the end of the growing season (late september) and were placed in labeled plastic bag and taken to the laboratory.

The collected samples were placed in laboratory conditions for 15 days until they became dry at room temperature and put in an oven at 45°C for two weeks. 6 ml of nitric acid (65% - HNO_3) and 2 ml of hydrogen peroxide (30% - H_2O_2) were added to the 0.5 g of the dried ground samples and placed in the microwave oven. The program of the microwave instrument was set to rise to 200 °C for 15 minutes and stay at 200°C for 15 minutes. After the samples were digested in that instrument, the solution samples were taken into flasks and filled up to 50 ml with ultrapure water, and then the K and Mg concentrations were determined with the ICP-OES (GBC Scientific Equipment Pty Ltd., Melbourne, Australia) instrument. In recent years, this method has been one of the most frequently used methods for determining plant elemental analysis [18, 29]. Analysis of variance was applied to the obtained data using the SPSS 22.0 statistical package software program, and homogeneous groups were found using the Duncan test for the factors that were found to have significant changes with at least a 95% confidence interval ($P<0.05$).

3. Result

The variation of K concentration, one of the macronutrients evaluated in the study, depending on the traffic density based on species and organs, and the statistical analysis results are given in Table 1.

As a result of the analysis of variance, the K element change was found to be significant ($P<0.001$) in terms of the traffic density in all organs and depending on the organs in all traffic densities. When the average values are evaluated, there is no linear change in the K concentration in the leaves based on the traffic density in general. However, the two highest values were found in *Tilia platyphyllos* leaves and seeds in areas with heavy traffic. Apart from this, it is seen that the highest values in many organs were obtained in areas with heavy traffic. As a species, the highest values were found in *Tilia platyphyllos* and the lowest values in the *Aesculus hippocastanum* tree. As an organ, the change is as follows: seed>leaf>branch in *Acer negundo* and seed>leaf>branch in *Ailanthus altissima* tree.

Table 1. The variation of K element concentration (ppm) by traffic density and species and organs

Species	Organ	Traffic density			
		None	Less	Heavy	F-value
Prunus cerasifera	Leaf	8998.50 Ai	16392.20 Bi	16902.27 Cj	9569.1***
	Seed	2773.83 Ab	24546.36 Cn	4364.83 Bd	291644.3***
	Branch	8443.46 Ch	6093.86 Be	3588.17 Ac	42155.9***
Aesculus hippocastanum	Leaf	3270.80 Cc	1435.96 Aa	3085.03 Bb	36377.4***
	Seed	5706.53 Be	2099.53 Ab	10199.47 Cg	97938.7***
	Branch	1759.10 Aa	3143.86 Cc	2633.80 Ba	19126.5***
Tilia platyphyllos	Leaf	7062.46 Ag	23740.06 Bl	39743.77 Cn	72049.3***
	Seed	7170.53 Ag	24103.60 Bm	40351.60 Co	15362.9***
	Branch	8309.56 Bh	9692.83 Cg	7659.10 Af	2192.8***
Acer negundo	Leaf	17698.53 Al	20600.03 Ck	18678.67 Bk	553.9***
	Seed	30746.43 Cm	28405.90 Bo	26065.40 Am	451.8***
	Branch	10599.10 Bj	5512.26 Ad	12916.73 Ci	17578.5***
Ailanthus altissima	Leaf	5528.80 Ad	14626.96 Ch	12457.70 Bh	37396.2***
	Seed	15810.56 Ak	17635.83 Bj	19532.60 Cl	1539.6***
	Branch	6557.03 Bf	6680.10 Cf	6034.27 Ae	467.5***
F-value	17960.8***	23903.1***	63002.1***		

Note: Different letters represent significant differences at alpha=*0.05*. Capital letters represent horizontal direction, whereas lower case letters represent vertical directions. *** = *P<0.001*.

The variation of Mg concentration, another macronutrient evaluated in this study, depends on the traffic density based on species and organs, and the statistical analysis results are given in Table 2.

The Mg concentration was significant in terms of the traffic density in all organs and on the organs in whole traffic densities (*P<0.05*). This change is significant only in *Ailanthus altissima* seeds at the 95% (*P<0.05*) confidence level based on the traffic density and at the 99.9% confidence interval for whole other factors.

When the variation of Mg concentration was evaluated, the highest concentrations were generally found in the species grown in heavy traffic areas. However, there was no significant changes between the organs of the species grown in areas with no traffic and less density (*P<0.05*). Apart from this, it can be said that the Mg concentration does not differ significantly based on species and organs.

Table 2. The variation of Mg element concentration (ppm) by traffic density, species and organs

Species	Organ	Traffic density			F-value
		None	Less	Heavy	
Prunus cerasifera	Leaf	5771.20 Cc	5761.90 Ac	5763.46 Bc	553.1***
	Seed	10724.13 Bi	8923.50 Af	21411.33 Cj	39379.7***
	Branch	9909.03 Af	10150.96 Bh	11514.23 Ch	2391.0***
Aesculus hippocastanum	Leaf	6628.60 Bd	6634.30 Cd	6620.10 Ad	957.4***
	Seed	4599.46 Ca	4274.76 Ba	3563.16 Aa	3264.5***
	Branch	8546.93 Be	6620.50 Ad	13237.13 Ci	637682.3***
Tilia platyphyllos	Leaf	5756.20 Ac	5762.70 Bc	11504.20 Ch	206263651***
	Seed	11498.46 Aj	11511.56 Bk	22980.76 Ck	54493641***
	Branch	11495.73 Cj	11450.36 Bj	9151.23 Ae	22005.2***
Acer negundo	Leaf	5768.80 Cc	5755.40 Ac	5756.56 Bc	561.3***
	Seed	5758.10 Ac	8628.26 Be	11498.43 Ch	2251691.9***
	Branch	11523.46 Bj	9127.73 Ag	11498.46 Bh	4249.6***
Ailanthus altissima	Leaf	10282.86 Ch	5139.90 Ab	10267.90 Bg	35268976.7***
	Seed	5140.70 Bb	5139.16 Ab	5138.40 Ab	9.05*
	Branch	9998.26 Ag	10301.03 Ci	10224.43 Bf	1571.1***
F-value		73981.6***	48182.6***	148104.4***	

Note: Different letters represent significant differences at alpha=*0.05*. Capital letters represent horizontal direction, whereas lower case letters represent vertical directions. * = *P<0.05*; *** = *P<0.001*.

4. Discussion and Conclusion

The changes of K and Mg elements evaluated in this study depending on organs in all traffic densities and all organs of all species based on traffic density were statistically significant. The elements in the study are essential for plant development, and K has critical importance in adaptation to several stress situations and plant-water relations [3,19,30]. Mg is located in plants' chlorophyll and traps sunlight, energy photons. Mg is the primary atom of chlorophyll and is crucial in the process of photosynthesis. Therefore, the concentration of chlorophyll is decreased, and photosynthesis is reduced, and as a result, its development is hindered under Mg deficiency [10].

As a result, it was determined that the element concentrations in the plants' organs changed significantly based on species and organs. Many studies have revealed that the concentrations of numerous elements vary significantly based on plant types [31-33]. The potential of heavy metal accumulation in plants grown in a similar habitat varies depending on plant type, plant habitus, plant organ structure, physio-chemical properties of metals, organ morphology, surface texture and size, surface area, exposure time to heavy metal, and the portion of particulate matter [34-36].

The element accumulation in plant species is closely associated with plant habitus and metabolism [37]. Therefore, it is stated that several factors such as the plant's stress severity [22-24], the genetic structure of the plant [38-40], hormone applications [41-44], cultural processes such as pruning, shading, and fertilization [20, 45-47] affect the heavy metals accumulation in plants [48].

As a result, the highest concentrations in two elements were found in the organs of plants grown in heavy traffic areas. The entrance of elements into the plant bodies can be primarily via leaves and roots. However, it is challenging to specify the primary source of the elements defined in the plants' bodies because the pathways of uptake in these two organs may work simultaneously [49, 50]. Therefore, air and soil composition also affect plant element concentrations [10]. In recent years, it has been determined that air pollution in urban areas has increased significantly in connection with industrial activities and traffic density [51-53]. Along with air pollution, it is stated that the heavy metals concentration, many of which also serve as nutrients for plants, increases significantly in this process [54]. This situation can significantly change the element content in the air and soil in the environment where the plants grow. Studies showed that particulate matter in the air is contaminated with various elements and that these particulate substances adhere to the organs and increase the element concentration in the organs [55, 56].

In conclusion, the element concentration change in organs of the plant is caused by a complicated mechanism depending on various factors' interaction, and that mechanism has not been entirely explained yet. For this reason, the further studies on this topic should be continued by diversifying and expanding, and the studies should be carried out in controlled environments as much as possible are recommended.

Competing Interest / Conflict of Interest

The authors declare that they no conflict of interest. The none of the authors have any competing interests in the manuscript.

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Geographical accessibility of health care network via GIS in Kastamonu

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Abstract: Accessibility is one factor that increases the quality of life in urban areas. Accessibility is an indicator that reflects the ease of reaching an intended point or location. In general, access to healthcare relates to the population in a given area combining the physical distance between home and the location of a healthcare facility. In the study carried out to reach the health service facilities in Kastamonu Central district, the accessible areas of the facilities within walking distance were calculated with the help of GIS at a distance of 300-500 meters with the network analysis technique. With the help of spatial analysis, it aims to determine the current situation and help plans be created to consider the needs of society. In the current situation, the points that can be improved in terms of access to health institutions in the research area have been mentioned, and suggestions have been made.

Keywords: Accessibility, Health, GIS, Network Analysis, Kastamonu

Öz: Kentsel alanlarda yaşam kalitesini artıran unsurlardan biri de erişilebilirliktir. Erişilebilirlik, amaçlanan bir nokta veya bir konuma ulaşabilme kolaylığını yansıtan bir göstergedir. Genel olarak sağlık hizmetlerine erişim, belirlenen kentte yaşayan nüfusun, konut ile bir sağlık tesisinin konumu arasındaki fiziksel mesafeyi birleştirmesiyle ilgilidir. Kastamonu Merkez ilçesinde sağlık hizmet tesislerine ulaşmak için yapılan çalışmada tesislerin yürüme mesafesinde erişilebilir alanları CBS yardımı ile 300- 500 metre mesafede ağ analizi tekniği ile hesaplanmıştır. Ağ analizi uygulanarak tesislerin konumları, geleceğe dönük planlamaların toplumun ihtiyaçlarını gözeten şekilde oluşturulmasına yardımcı olması amaçlanmıştır. Mevcut durumda araştırma sahasında sağlık kuruluşlarına erişim konusunda geliştirilebilir noktalara değinilmiş ve önerilerde bulunulmuştur.

Anahtar Kelimeler: Erişebilirlik, Sağlık, CBS, Ağ Analizi, Kastamonu

1. Introduction

Today, especially in the post-COVID-19 pandemic period, the importance of health care accessibility research has increased. There are many physical factors that affect the accessibility [1]. Easy access opportunities should be provided for transportation, road texture, parking lot and vehicle traffic, especially for pedestrians in urban areas [2-4]. Accessibility to health services [5] is an element that reflects the welfare level of the society and is related to the physical distance between the residence and the place of a health facility where the population living in an area can go when they leave the residential areas [6]. The level of accessibility to health services depends on many factors such as the unique topography of each city [7], its spatial pattern and whether it is planned or not [8, 9]. Therefore, the level of accessibility differs in each city [10].

Although research on access to health services is increasing day by day, a common judgment has not emerged regarding the definition of the concept due to its multidimensional nature [11]. Dimensions such as accessibility of health services in rural areas [12], adequacy of services [13-15] service quality [16-18] is often explored. In addition, physical/geographic accessibility is also a topic of discussion in spatial planning [19-22].

The proliferation of geographic information systems (GIS) and global positioning technologies has reinvigorated studies on the accessibility [23] and use of healthcare facilities [24-26]. In addition, GIS-based analyzes facilitate spatial analysis and reduce the error rate [27].

The research subject is family health centers (FHC) located in Kastamonu and accessibility to these centers. The study aims to determine the areas accessible to family health centers with the Network analysis method applied to the city center. GIS-based network analysis has been applied by considering public/non-public facilities in this context.

2. Material and Method

The case area for the study was chosen as the central district of Kastamonu province (Figure 1). Kastamonu province is located in the Western Black Sea region between 41 degrees 21' north latitude and 33 degrees 46' east longitudes [28]. Its height above sea level is 775m. It has a surface area of 13,108.1 km² [29].

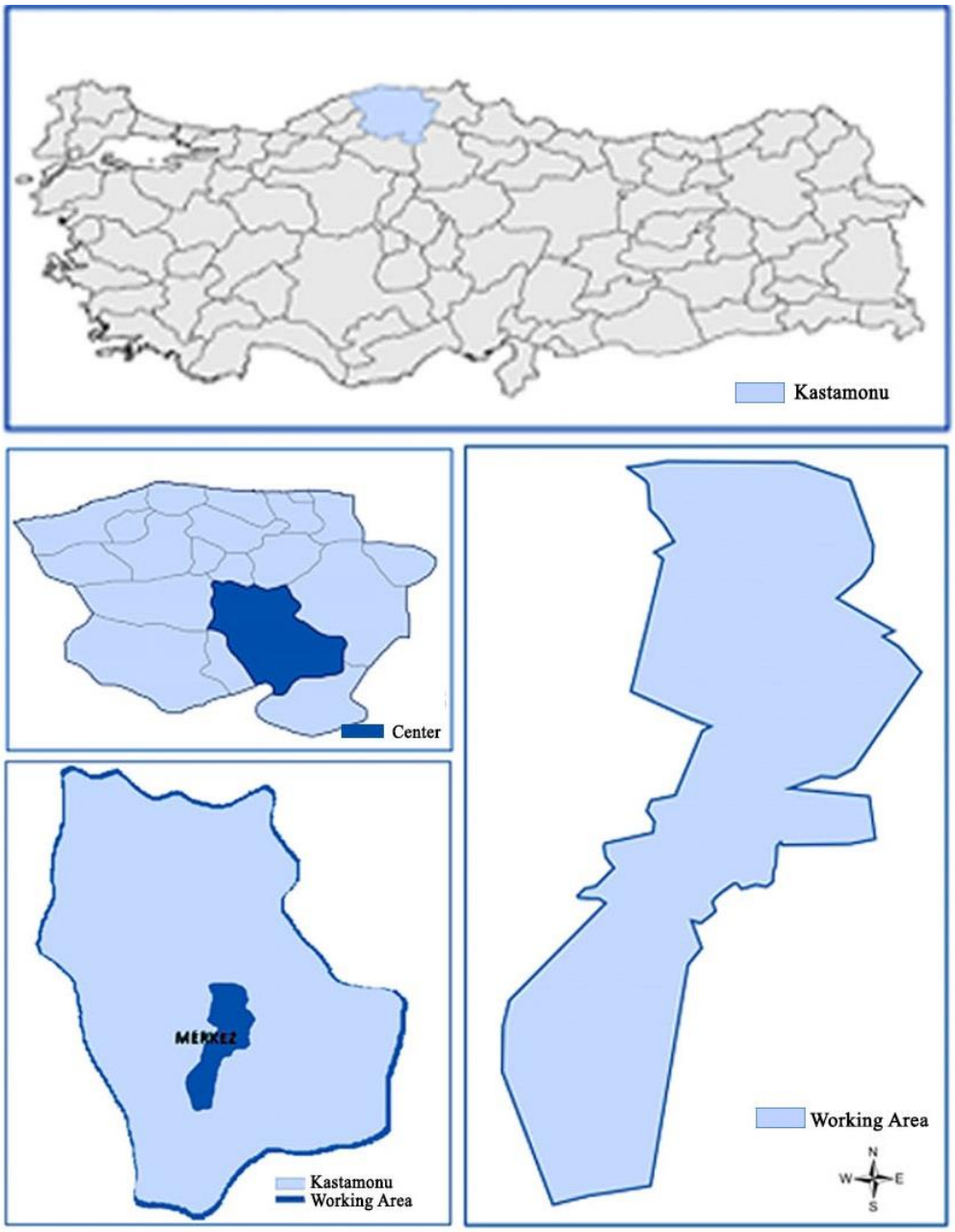

Figure 1. Location of case area

The research consists of four stages. First of all, the locations of FHCs in the city were determined, and neighborhoods with and without facilities were chosen. Then, the possible transportation network to the determined areas was mapped. As in some of the studies on the use of health services, GIS software was used in spatial accessibility analysis studies. Network analysis was performed using GIS software to determine accessible locations.

Digital transportation network to be used in the implementation of the analysis and the evaluation of the analysis result; Data of the locations of Health Service Centers; border and population data of the neighborhoods within the study area; The vector data of the houses in the study area were used. Digital road network data of the study area has been obtained, and corrections have been made. Topology was applied to eliminate errors and deficiencies in the road network data, and the detected errors were corrected. During the analysis, the scanning tolerance of 100 meters to the road was used to prevent the mistakes that may arise from the width of the road. Another data used in the analysis is the location data of Health Service Centers. Addresses and locations obtained from the Provincial Health Directorate were digitized. The buildings within the study area were removed from the municipal zoning plan and converted into point data with the

extension of 'Shp.' with the ArcGIS 10.6 package program. The generated data were collected in a single database. The population data of the research area and the numbers of the population on the basis of neighborhoods were obtained. Spatial accessibility has been taken into account since primary population data on a residential basis cannot be accessed. The data prepared for analysis were subjected to network analysis with the ArcGIS 10.6 package program, taking into account the alternative walking distances specified in the Spatial Plans Building Regulation and determined by the literature review.

3. Result

According to TUIK 2020 data, the population of Kastamonu is 376 377 and the population of the Central district is 151500. 49.83% of the center population is male and 50.17% is female [30]. The health facilities in the central district of Kastamonu, where the study was carried out, constitute the main material of the study. While there are no health facilities in 10 of the 19 neighborhoods in the district, there are health services facility areas in 9 neighborhoods. Neighborhoods with healthcare facilities can be listed as Aktekke, Beyçelebi, Esentepe, Hepkebirler, İnönü, İsmailbey, Kuzeykent, Mehmet Akif, Saraçlar (Figure 2).

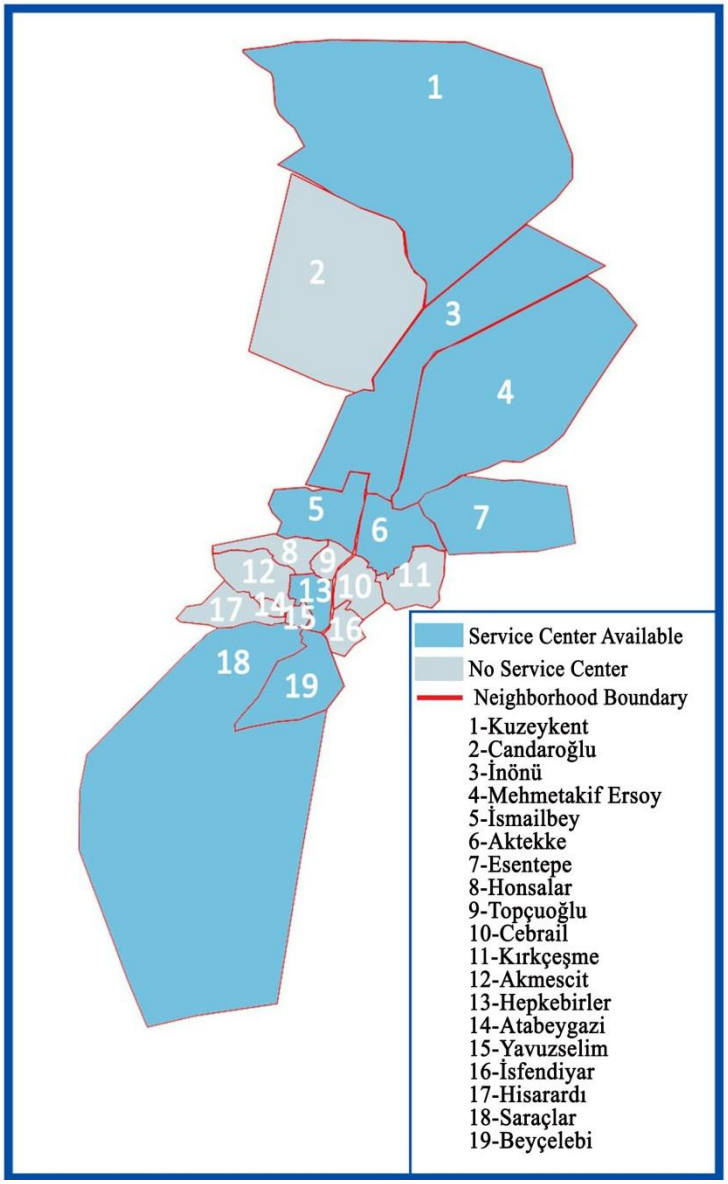

Figure 2. Neighborhoods with health service centers

In the study area, there are 12 health care facility areas, including 1 Training and Research hospital, 1 physical therapy and rehabilitation center, 1 private hospital and 9 family health centers, located at different points of the study area (Figure 3).

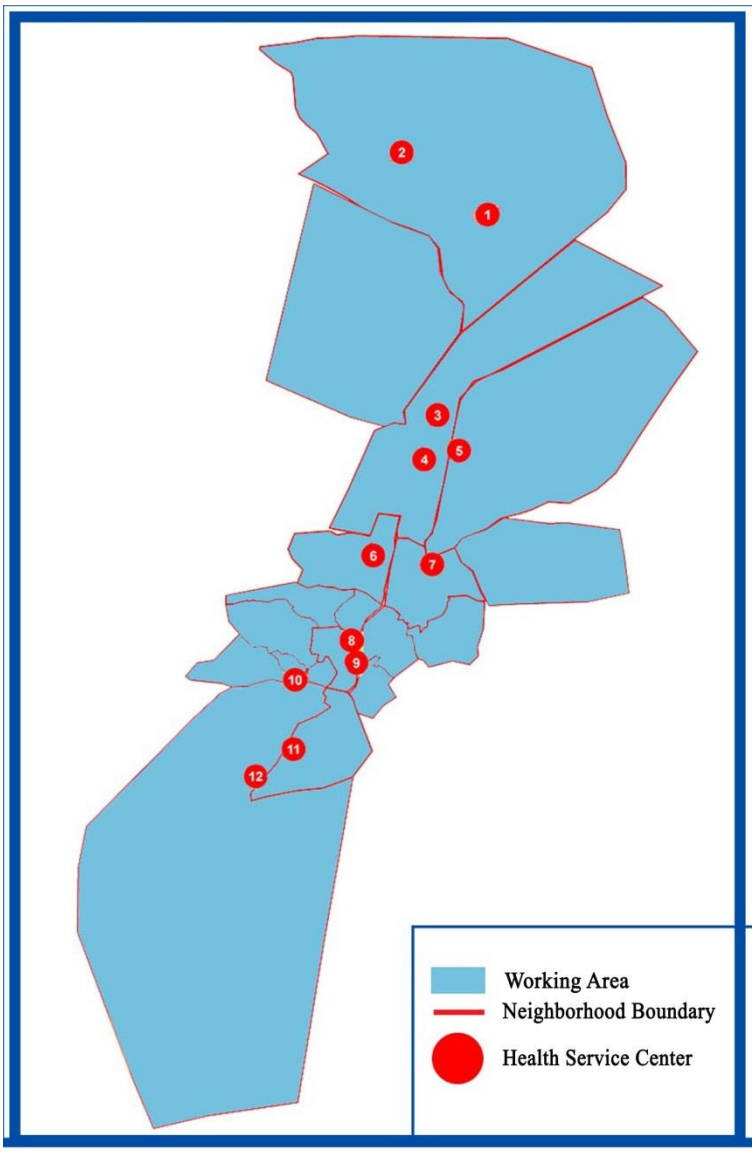

Figure 3. Health service center locations

Access to health services in the city center where the study was conducted is mostly provided by first and second degree roads. It is seen that the first degree roads are concentrated around the Karaçomak Stream, which appears to be continuous throughout the city center and divides the city into two, and the general road network is formed (Figure 4).

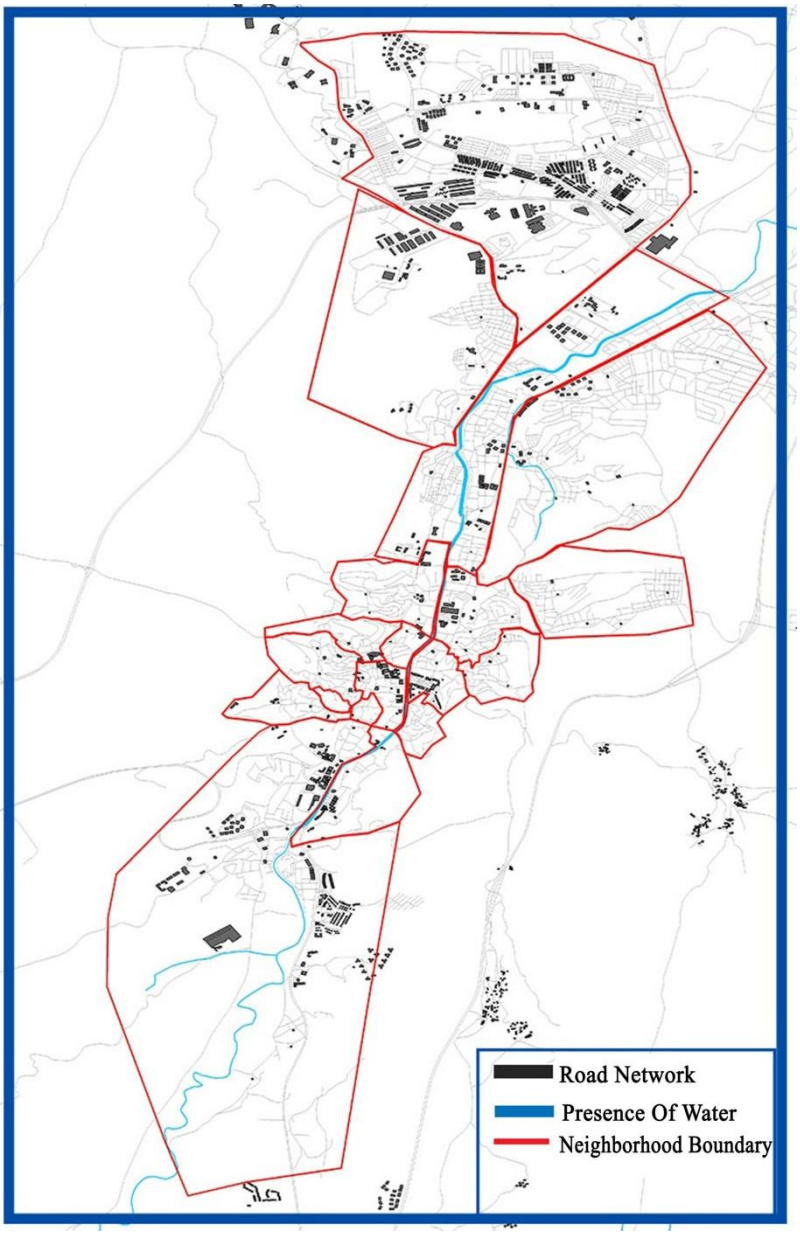

Figure 4. Road network

Network analysis applied, areas accessible to family health centers Spatial Plans. In addition to the 500 meters distance specified in the Building Regulation, an analysis was applied at 300 meters distance. While accessible areas at a distance of 500 meters have a size that can be considered insufficient on the city surface, it can be said that when the accessibility limit is reduced to 300 meters, the area is more private and the population density is higher, while the accessible housing is less in the neighborhoods with lesser population (Figure 5).

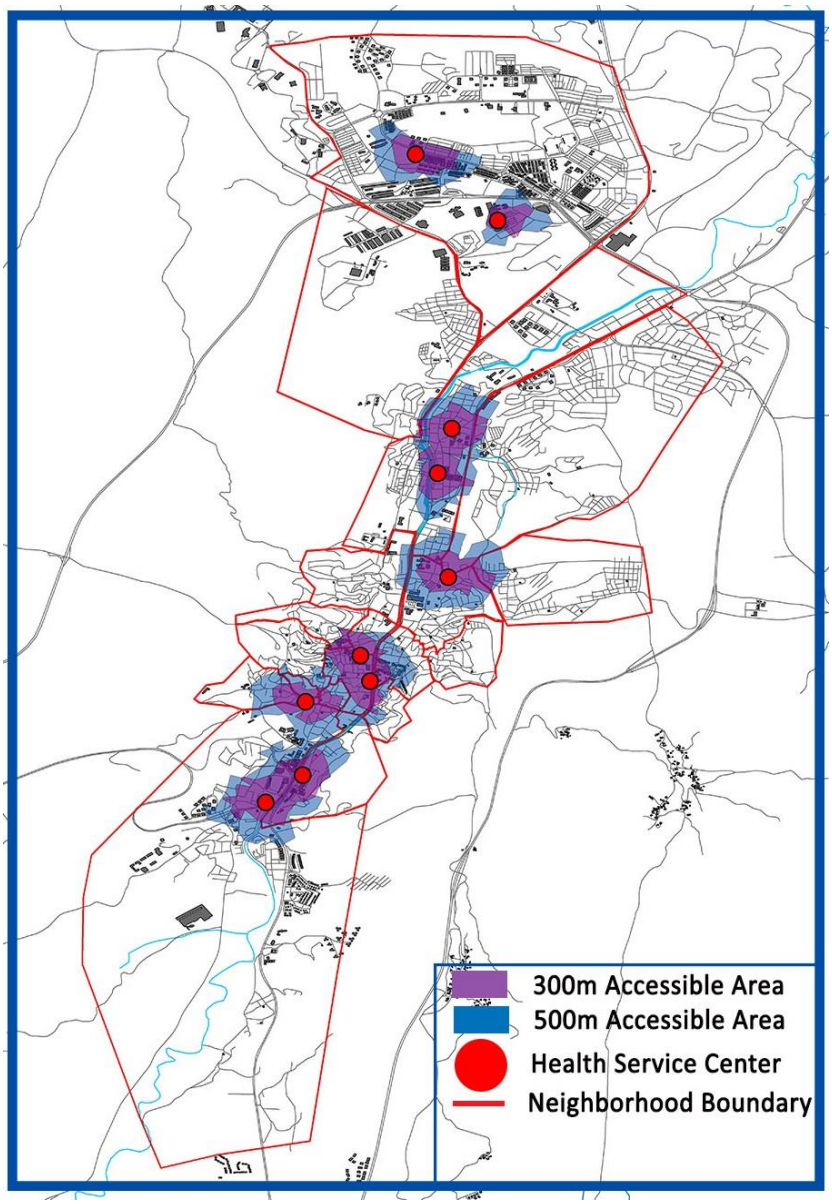

Figure 5. Accessibility to health service centers

Examined on the basis of neighborhoods, it can be said that while the rate of buildings that can be accessed at a distance of 300 meters is zero in Esentepe, İsmailbey, Atabeygazi, Kırkçeşme neighborhoods, it can be said that the access rate is zero only in Kırkçeşme neighborhood when viewed at a 500 meter level. In addition, there is no health service building-service area in Akmescid, Atabeygazi, Candaroğlu, Cebrail, Topçuoğlu, İsfendiyar, Kırkçeşme, Hisarardı, Honsalar, Yavuz Selim neighborhoods. It is Yavuz Selim District with a rate of 37.21, this rate is 97.67 percent at 500 meters, and it has accessibility at a distance that covers almost the entire neighborhood (Table 1).

Table 1. Spatial accessibility status of health service centers

Neighborhood Name	Population	Total Area (m²)	Building			Accessible Rate (%)	
			Total	300m	500m	300m(%)	500m(%)
Aktekke	4505	481000	477	150	250	31.45	51.42
Beyçelebi	2899	685687	188	68	153	36.17	81.38
Esentepe	3528	1231016	540	0	90	0	16.67
Hepkebirler	1842	178000	257	246	257	95.72	100
İnönü	21874	2783000	790	185	319	23.42	40.38
İsmailbey	3687	303000	623	0	23	0	3.69
Kuzeykent	27814	5739000	1710	97	135	5.67	7.89
MehmetAkif	23814	4180000	940	16	45	1.7	4.79
Saraçlar	13618	8487782	1091	192	358	17.6	32.81
Akmescid	1256	383556	405	5	17	1.23	4.2
Atabeygazi	343	46216	156	0	110	0	70.51
Candaroğlu	9230	3112499	577	3	4	0.52	0.69
Cebrail	2304	269436	394	12	126	3.05	31.98
Topçuoğlu	1168	127063	256	47	72	18.36	28.13
İsfendiyar	1328	168016	204	31	104	15.2	50.98
Kırkçeşme	1519	364591	285	0	0	0	0
Hisarardı	890	311615	250	65	104	26	41.6
Honsalar	1297	259484	408	23	23	5.64	5.64
YavuzSelim	536	57559	86	32	84	37.21	97.67
Toplam	151500	29168520	9637	1172	2274	12	23.60

4. Discussion and Conclusion

Today, health services serve two main purposes, raising health standards and increasing knowledge about diseases [31, 32]. The health service centers that are the subject of our study are not separated as primary, secondary or tertiary health services, but are institutions that include private and public services ranging from institutions where users can receive services on follow-up and simple interventions to institutions containing intensive care services.

Hospitals are located very close to the city center in Kastamonu [33]. Network analysis applied to the city center aims to determine accessible areas for family health centers. Analysis was applied to the distance of 500 meters specified in the Spatial Plans Building Regulation. In addition, there is no health service building-service area in Akmescid, Atabeygazi, Candaroğlu, Cebrail, Topçuoğlu, İsfendiyar, Kırkçeşme, Hisarardı, Honsalar, Yavuz Selim neighborhoods. It is Yavuz Selim Mahallesi with a rate of 37.21, this rate is 97.67 percent at 500 meters, and it has enough accessibility

When analyzed at 300 meters, the rate of accessible buildings is seen as zero in Esentepe, İsmailbey, Atabeygazi, Kırkçeşme neighborhoods, and the highest accessibility is Hepkebirler Mahallesi with 95.72. Considering the 500 meter distance analysis, the rate of buildings accessible only in Kırkçeşme neighborhood is seen as zero, the highest accessibility belongs to Hepkebirler neighborhood Yavuz Selim Neighborhood with a rate of 97.67 in it is an important result. In general, neighborhoods with high population density remain within the accessible area. This area, which is 12 percent and 23.60 percent accessible in total, is concentrated in the center of the city and the peripheries of the city, whose population is increasing and growing day by day, are outside the accessible area. Considering these two ratios and the legal distance, it is seen that the number of health service centers is concentrated in the areas where the population is high in the urban spread, and it can be said that the outer periphery of the city remains weaker in terms of accessibility.

According to these results, it has been seen that the absence of a health service area in a neighborhood or work area cannot be said to have no health service access for that area, and when we look at the city as a whole, it is seen that the first or second degree accessibility of that area may be in question. Considering that the health services in the central district of Kastamonu province are concentrated in the center of the city and decrease towards the outer periphery and newly developing neighborhoods, the possible health service centers to be built are the Kuzeykent District, Mehmet Akif District, Saraçlar District Candaroğlu and Kırkçeşme Neighborhoods, which can be considered the outer wall of the city, where development and new construction increase rapidly. It can be said that the positioning is correct.

Competing Interest / Conflict of Interest

The authors declare that they have no competing interests.

Author Contribution

We declare that all Authors equally contribute.

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Usability of organic wastes in concrete production; Palm leaf sample

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Abstract: Palm leaves are vegetal waste that are not widely used by the society, only piled up and causing odors that mix with the environment. Channeling this waste material into the construction industry helps to overcome waste disposal problems as well as promote sustainability. The most important features expected from the buildings are the creation of the most suitable environmental conditions for the products to be stored or the creatures that will live in them, and they can be used safely for a long time. In the construction of the buildings, materials that are the cheapest possible, safe and capable of creating the optimum environmental conditions should be used. The materials to be selected should have sufficient strength and durability, high heat and sound insulation and lightness. Since single-storey buildings are not subject to excessive load, it is important that the thermal insulation is high and light in material selection. Since the widespread use of concrete as a building material in the world, efforts to make concrete light, cheaper and better insulating have gained importance. Lightweight concrete, which is easy to apply, has been an important building material in recent years. With the use of lightweight concrete as a building material, benefits such as economy in terms of material, earthquake resistance, and the elimination of a second insulation material for heat and sound insulation can be achieved. In this study; Experimental study using Portland cement (CEM I), Palm Leaf, CEN standard sand and water mortar production; sample production, curing, some physical and mechanical experiments were carried out in four stages. The usability of palm leaf, which is a vegetable waste, as aggregate in concrete production by replacing it with CEN standard sand at 0, 5, 10, 20, 30 and 40% as well as 10% with cement has been investigated. The study results show that the addition of both ground palm leaf and palm leaf aggregate significantly altered almost all properties of concrete. These changes are at different levels in terms of physical properties. As a result of the study, it was determined that as the amount of foam increased, the spreading diameter increased, whereas palm leaf addition decreased the spreading diameter. It has been determined that the addition of palm leaf decreases the depth of water treatment depending on time, the porosity of the samples with high level of palm leaf addition increases and the compression and bending strength decreases.

Keywords: Concrete, Organic waste, Palm leaf

Öz: Palmiye yaprakları toplum tarafından yaygın olarak kullanılmayan, sadece üst üste yığılan ve çevreye karışan kokulara neden olan bitkisel atıklardır. Bu atık malzemeyi inşaat sektörüne yönlendirmek, atık bertaraf sorunlarının üstesinden gelinmesine ve sürdürülebilirliğin desteklenmesine yardımcı olur. Binalardan beklenen en önemli özellikler, depolanacak ürünler veya içinde yaşayacak canlılar için en uygun çevre koşullarının oluşturulması ve uzun süre güvenle kullanılabilmesidir. Binaların yapımında mümkün olan en ucuz, güvenli ve optimum çevre koşullarını oluşturabilecek malzemeler kullanılmalıdır. Seçilecek malzemeler yeterli mukavemet ve dayanıklılığa, yüksek ısı ve ses yalıtımına ve hafifliğe sahip olmalıdır. Tek katlı binalar aşırı yüke maruz kalmadığından malzeme seçiminde ısı yalıtımının yüksek ve hafif olması önemlidir. Betonun dünyada yapı malzemesi olarak yaygınlaşmasından bu yana betonu daha hafif, daha ucuz ve daha iyi yalıtkan hale getirme çabaları önem kazanmıştır. Uygulaması kolay olan hafif beton, son yıllarda önemli bir yapı malzemesi olmuştur. Hafif betonun yapı malzemesi olarak kullanılması ile malzeme açısından ekonomi, depreme dayanıklılık, ısı ve ses yalıtımı için ikinci bir yalıtım malzemesinin ortadan kalkması gibi faydalar sağlanabilir. Bu çalışmada; Portland çimentosu (CEM I), palmiye yaprağı, CEN standartlarında kum ve su harcı üretimi kullanılarak deneysel çalışma; numune üretimi, kürleme, bazı fiziksel ve mekanik deneyler dört aşamada gerçekleştirilmiştir. Bitkisel bir atık olan palmiye yaprağının CEN standartlarında 0, 5, 10, 20, 30 ve %40 oranında ve %10 oranında çimento ile değiştirilerek beton üretiminde agrega olarak kullanılabilirliği araştırılmıştır. Çalışma sonuçları hem öğütülmüş palmiye yaprağı hem de palmiye yaprağı agrega ilavesinin betonun hemen hemen tüm özelliklerini önemli ölçüde değiştirdiğini göstermektedir. Bu değişimler fiziksel özellikler açısından farklı düzeylerdedir. Çalışma sonucunda, köpük miktarı arttıkça yayılma çapının arttığı, palmiye yaprağı ilavesinin ise yayılma çapını azalttığı tespit edilmiştir. Palmiye yaprağı ilavesinin zamana bağlı olarak su arıtma derinliğini azalttığı, yüksek oranda palmiye yaprağı ilave edilen numunelerin porozitesinin arttığı, basınç ve eğilme dayanımının azaldığı tespit edilmiştir.

Anahtar Kelimeler: Beton, Organik atık, Palmiye yaprağı

1. Introduction

In the current century, the urban-to-rural migration significantly increased especially because of the Industrial Revolution [1] and it even became one of the two important irreversible problems [2] together with the global climate change [3, 4]. Such that, the rate of urban population, which was only 9% in 1900s, worldwide increased to 47% in 2000 and estimated to increase to 90% by the year 2030 [5, 6].

Concentration of the population in urban areas also brought various problems with it [7]. One of the most important problems is, undoubtedly, the air pollution [8, 9]. In urban areas, pollution reached severe levels because of the traffic density and human activities [10], the level of pollution in air [11], water [12], and soil [13-16] increased significantly, and it became a global problem causing to the death of more than 7 million individuals annually [17].

The demand for urban areas increases the need for new residential areas [18-20] and construction of new housings [21-23]. This need also increases the demand for concrete, which is an important raw material especially in the building industry and constitutes an important share of construction costs [24-26]. Thus, the studies addressing the use of environmental wastes as an alternative to concrete in order to decrease the costs of concrete and to eliminate the environmental wastes gain more importance and many studies were carried out on this subject in recent years [27-29].

The plants grown for landscaping purposes constitute a significant portion in the wastes, which are an important factor in environmental pollution [30]. Although plants fulfill many ecologic, economic, and social functions in urban areas, the organs drying or falling as a result of the natural development process constitute an important source of pollution [31-34]. The most frequently used method in the elimination of plant wastes is the collection and combustion but this method results in a high level of carbon emission. Global climate change, which is one of the most important problems at the global scale, arises mainly from the carbon emission [35]. For this reason, different methods are needed for the elimination of organic wastes. In the present study, the usability of palm leaves, one of the most important organic wastes, as an additive to concrete is examined.

2. Material and Method

In this study, several physical and mechanical properties of palm leaves, an important herbal waste, were examined and their usability as an aggregate in concrete production was investigated. Within the scope of this study, palm leaves, which are an organic waste, were ground and used as aggregate in production of PC 42.5 (Portland) cement, which was manufactured according to TS EN 196–1, together with CEN standard sand and mains water. Within the scope of this study, ground palm leaves were added into cement at different concentrations and several physical and mechanical properties of cement mortars were determined. For this purpose, first, the palm leaves to be added into cement were ground and sieved at the right size. The high void ratio and water absorption rate of resultant palm leaves caused the predetermined amount of water to be insufficient and insufficient setting and hydration in concrete. For this reason, the palm leaves to be used in concrete production were kept in water for half an hour until saturated. The calculation of the mixture of cement and palm leaf having the same particle size was made as the percentage of total aggregate volume. The percentages were set to be 0%, 10%, 20%, and 30% and named as K10PY0, K10PY10, K20PY0, K20PY10, K30PY0, and K30PY10, respectively, based on the foam density (PY: Palm Leaf). Within the scope of this study, 36 cement mortar samples were produced in total. The mixture ratios used in the experimental study are presented in Table 1 and the amounts of materials in Table 2.

Table 1. Mixture ratios

	Level 1	**Level 2**	**Level 3**
Foam rate (kg/m^3)	10	20	30
Milled Palm leaves (%)	0	10	

Table 2. Amounts of materials

Mixture	**K10PY0**	**K10PY10**	**K20PY0**	**K20PY10**	**K30PY0**	**K30PY10**
Cement	350	315	350	315	350	315
Milled Palm leaves (%)	0	35	0	35	0	35
Palm leaf aggregate	686,2	680,9	652,6	647,3	619	613,7
Water	245	245	245	245	245	245
Foam	10	10	20	20	30	30

The w/c ratio was set to be 0.70. Foam density is 140 g/l. Foam addition rates were 10, 20, and 30 kg/m^3. The flow diameters of foamed concretes were determined according to ASTM C 230 standard. Then, the mixtures were poured into molds with dimensions of 4*4*16 cm. Since the mixtures have the self-settling character, no vibration was performed. The foamed concretes, which were kept under laboratory conditions for 24 hours, were removed from the

molds and the water cure was initiated. Foamed cements' compressive and bending strengths were determined using the samples with dimensions of 4*4*16 cm. Mechanical properties of samples were determined using the ASTM C348 and 349 standards. Compressive strength test was performed after the bending strength test. Compressive and bending strength tests of foamed concretes were performed on the 28th and 90th days.

Capillarity properties of the foamed concretes were determined using cube samples with dimensions of 5*5*5 cm according to ASTM C 1585. Water penetration depths of foamed concretes on the 24th hour were used. After 28 days of curing, foamed concretes were dried in drying oven for 3 days at 50°C and the capillarity test was initiated. Approx. 5mm-thick water sealant was applied to the sides of the foamed concretes and the water penetration depths were determined on the 24th hour. The results were evaluated according to the average values.

3. Result and Discussion

The test results (flow diameter and bending – compressive strength tests on the 28th and 90th days) of the samples are presented in Table 3.

Table 3. Sample test results

Mixture	**K10PY0**	**K10PY10**	**K20PY0**	**K20PY10**	**K30PY0**	**K30PY10**
Spread diameter (cm)	10	9,1	12,2	10,6	18,1	15,5
28. Day Flexural strength (MPa)	0,50	0,52	0,44	0,46	0,41	0,42
90. Day Flexural strength (MPa)	0,55	0,69	0,48	0,50	0,45	0,48
28. Day Compressive strength (MPa)	1,45	1,95	1,14	1,28	1,18	1,20
90. Day Compressive strength (MPa)	1,62	2,04	1,35	1,58	1,27	1,52

Given the results presented in Table 3, it can be seen that the sample with the highest flow diameter was K30 samples and that the flow diameter increased with increasing amount of foam. However, it was found that the flow diameters of all the samples added with ground palm leaf were lower when compared to the values found with the samples containing no palm leaf addition. The smallest flow diameter was found to be 9.10 cm in K10P10 and the longest one to be 18.10 cm in K30PY0.

Examining the bending strength results of the samples added with ground palm leaf and aggregate, it can be seen that the highest results were found to be in K10 samples (ranging between 0.50 and 0.69MPa) on both the 28th and 90th days and that there was no significant difference between K20 and K30 samples having the results ranging between 0.44 and 0.50MPa. Besides that, even though there was no remarkable difference, it can be seen that the bending strength results of PY10 samples were higher than those of PY0 samples. The compressive strength results of samples were very close to the bending strength results. In general, the highest compressive strength values were found to range between 1.45 and 2.04 MPa in K10 samples, whereas there was no significant difference between K20 and K30 samples ranging between 1.13 and 1.57 MPa and compressive strength values of PY10 samples were slightly higher than those of PY0 samples. The results obtained on the 28th and 90th days were found to be parallel. Examining the temporal change in the water penetration depths of mortars, it can be seen that the time-dependent water penetration depth decreased with increasing amount of foam addition. However, given the results, addition of ground palm leaf was more effective and the highest water penetration depth values in the shortest time were obtained from the samples K10PY0 and K20PY0.

4. Discussion and Conclusion

The results obtained in the present study showed that both ground palm leaf and palm aggregate additions significantly affected almost all the properties of concrete. These effects either decreased or increased the properties. For instance, it was found that the flow diameter increased with increasing amount of foam addition but addition of palm leaf decreased the flow diameter. It can be stated that the palm leaf addition decreased the time-dependent water penetration depth and that the porosity increased in the samples with higher palm leaf addition and their compressive and bending strength values decreased.

The increase in urbanization in recent years and the construction of multi-storey buildings in order to allow more individuals to live in the unit area significantly increased the use of concrete [21, 36, 37]. Concrete is one of the most widely used materials and one of the most important inputs in the construction industry and concretes having different characteristics are used in buildings having different structures. For instance, for the areas where the higher strength is demanded, the concretes with lower porosity and higher compressive strength are requested and, consequently, the concretes having lighter weight and higher isolation levels are preferred [38, 39, 40].

Besides these characteristics, another important factor is the cost of concrete. Cost and characteristics of concrete can significantly vary depending on the additives used [41-43]. Aiming to reduce the input costs in construction industry, several additives are used in order to decrease the cost of concrete that is the input, which affects the cost at most, among the additives [44-46]. The use of these additives causes an acceptable level of change in the cement

characteristics and, sometimes, it may even give superior mechanical properties depending on the area of use of concrete [47, 48].

Some of the materials used as concrete additive cause severe environmental pollution. Thus, the use of these materials as concrete additive also allows for the recycling and elimination of the pollutants causing environmental pollution [49-51]. As known, environmental pollution is one of the most important problems of today [52]. Use of pollutant materials as concrete additive might significantly contribute to the reduction of environmental pollution [53, 54]. For this reason, the usability of various environmental wastes as concrete additive was investigated in many studies [55, 56].

In these studies carried out on this subject, the use of materials including waste glass and granulated glass [57], waste brick dust [58], waste ceramic [59], boron mineral wastes [60], waste tires [51, 61-63], hearth cinder [64], waste marble dust [65, 66], and fly ash [67, 68] as cement substitute was investigated.

However, the number of studies carried out on the use of organic wastes as cement substitute is relatively lower. Organic wastes are the wastes that have organic origins. All the organisms develop during their biological life processes and the development of organisms is shaped by their genetic structures [69-71] and environmental factors [72-74]. Although all the organs of plants grown in urban areas are mainly the carbon-based wastes, they also include trace amounts of various elements that are very harmful for human and environmental health. Some of these elements such as Pb, Ni, Cr, and Cd are called heavy metals [75] and almost all of them can be toxic, carcinogenic, or harmful to organisms. Thus, using these wastes as additive for concrete is very important for protecting the environment but the number of studies on this subject is very limited. In some of the studies carried out on this subject, the usability of oyster shell [76], olive wastes [77], forest wastes [78], fig wastes [79], rise husk ash [80, 81] and some of the other materials [82, 83] as concrete additive was examined. Environmental pollution has increased dramatically, especially in the last 30 years [84-86] and because of the rapid development of global economy, the type and level of chemical pollution have constantly increased, and this increase has reached a terrifying level for the ecosystems [87, 88]. In order to effectively control the pollution, using waste materials as concrete additive will help protect the environment and conserve natural resources.

5. Suggestions

It is known that using different materials as additive to concrete could significantly alter the characteristics of concrete. The concentrations, at which the additives could be used without pushing the characteristics of concrete outside the acceptable limits, constitute the main factor playing a determinant role in the usability of additives. The desired characteristics of concrete may change depending on the area of use. For instance, while the most important characteristic for the concretes to be used in load-bearing column is the strength, isolation becomes more prominent for the concretes constituting the borders of units. Different characteristics of concrete are altered by different additives. Thus, the additive that can be used for concretes desired to have a high strength would differ from the additives to be added into a concrete that is desired to have high insulation.

The benefits expected from using the additives as substitute (decreasing the cost, making use of the environmental wastes, improving the visual quality, etc.) would play a determinant role at which concentration the additives could be used as substitute. Hence, the studies examining to what extent the additives alter the characteristics of concrete, to what extent they affect the costs, what are the substitutes that can be used instead of each other, etc. would significantly contribute to the practice. The results achieved in the present study showed that ground palm leaf and raw palm leaf can be used as concrete additive. However, by making use of the results achieved, it should be examined if the changes these materials cause in the characteristics of concrete are within the acceptable limits depending on the purpose of use, the use of these materials.

Competing Interest / Conflict of Interest

The authors declare that they have no competing interests.

Author Contribution

We declare that all Authors equally contribute.

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Urbanization models suitable for thermal-bioclimatic comfort levels

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Abstract: Scientific and technological developments triggered by industrialization started an intense urbanization process, which brought along an increase in population rate and urban structuring. Structural surface materials with low albedo (reflectance) value such as concrete and asphalt, which are used as building materials in urban areas, have trapped the heat inside, causing an increase in the air temperature in the city. The fact that a city is warmer than the surrounding rural areas is described as an urban heat island phenomenon. This phenomenon negatively affects the people living in the city physically and mentally. It is defined as Bioclimatic Comfort when people are not warned against the atmospheric conditions of the city they are in and feel comfortable. According to the PET index chart created by Matzarakis and Höppe, it has been revealed that people feel better between 18.1 - 23.0℃ temperature values. The increase or decrease in these values causes people living in the city to feel more stressed mentally and to feel a decrease in their desire to work, while physical health problems such as eye burns and nosebleeds occur. In this study, the bioclimatic comfort conditions of Kahramanmaraş, where the Mediterranean climate is intensely felt, are discussed. Meteorological measurement data of the study area between 1970 and 2021 were obtained from meteorological stations in the region. In line with these data, temperature, relative humidity, and wind speed maps were created and then correlated with PET index values.

Keywords: Bioclimatic comfort, Urbanizations, Models, Thermal comfort, GIS

Öz: Sanayileşmenin tetiklediği bilimsel ve teknolojik gelişmeler yoğun bir kentleşme sürecini başlatmış, bu ise nüfus hızında ve kentsel yapılaşmada artışı beraberinde getirmiştir. Kentsel alanlarda yapı malzemesi olarak kullanılan, beton ve asfalt gibi albedo (yansıtma) değeri düşük yapısal yüzey malzemeleri ısıyı içerisinde hapsederek kent içerisinde hava sıcaklığında artışa neden olmuştur. Bir kentin çevresindeki kırsal alanlara göre daha sıcak olması kentsel ısı adası olgusu olarak nitelendirilmektedir. Bu olgu kentte yaşayan insanları fiziksel ve ruhsal açıdan olumsuz yönde etkilemektedir. İnsanların bulunduğu kentin atmosferik koşullarına karşı uyarılmadığı ve konforlu hissetmeleri Biyoklimatik Konfor olarak tanımlanır. Matzarakis ve Höppe'in oluşturmuş olduğu PET indeksi çizelgesine göre 18.1–23.0℃ sıcaklık değerleri arasında insanların kendilerini daha iyi hissettiği ortaya koyulmuştur. Bu değerlerin artış ya da düşüş göstermesi kentte yaşayan insanlarda ruhsal açıdan daha stresli, çalışma isteğinde düşüş hissetmelerine neden olurken fiziksel açıdan göz yanması, burun kanaması gibi sağlık problemlerini beraberinde getirir. Ele alınan bu çalışmada Akdeniz ikliminin yoğun bir şekilde hissedildiği Kahramanmaraş ilinin biyoklimatik konfor şartları ele alınmıştır. Çalışma alanına ait 1970 -2021 yılları arasında meteorolojik ölçüm verileri bölgedeki meteoroloji istasyonlarından temin edilmiştir. Bu veriler doğrultusunda sıcaklık, bağıl nem ve rüzgâr hızı haritaları oluşturulmuş sonrasında PET indeksi değerleri ile ilişkilendirilmiştir.

Anahtar Kelimeler: Biyoklimatik konfor, Kentleşmeler, Modeler, Termal rahatlık, CBS

1. Introduction

As it is known, the climate parameter has undoubtedly been an effective factor in the basic needs of people such as shelter, nutrition, and settlement for centuries. The rapid increase in the understanding of urbanization and consumption from the past to the present, the destruction of natural green areas, the increase of impermeable surfaces, the uncontrolled energy consumption used in buildings, the increase in harmful gases caused by the use of automobiles, which follow a parallel course with the population growth, etc. Many factors have caused increases in air temperature and climatic deterioration [1-30]. Especially the temperature increases in the cities lead to the formation of heat islands, which is the most striking indicator of the urbanization phenomenon. In the shortest sense, the heat island effect is the situation in which the average air temperature values in urban areas are higher than those in the surrounding rural areas. Temperature changes in urban areas have caused each city to create a unique morphology, and the decrease in green areas in addition to the increase in impermeable surface with changing urban morphologies has brought various environmental consequences and increased the urban heat island effect. It has been observed that the heat island affects the thermal conditions of people as well as the air quality in the cities [31-51]. When we look at the relationship

between humans and climate, the climate factor, which we can see that even the daily life routine is affected, can have negative consequences on people both physiologically and spiritually [52-93]. Especially big cities that are exposed to climatic change and ecological deterioration, as places that offer unhealthy and equally bad conditions for the people living there, become an important parameter in terms of decreasing their quality of life, decreasing work efficiency, psychological depression, and livability [28, 30-42, 83-104]. With the growth of cities, it is seen that the use of structural surface materials such as concrete and asphalt increases, and due to the decrease in evaporation surfaces such as natural green areas, grass, and soil, increases in air temperatures occur. Because the use of structural surface materials in urban areas, which is unavoidable, converts the radiation absorbed throughout the day into heat and releases it back into the environment, which causes an increase in air temperatures. It is known that people feel healthier and more vigorous between certain temperature values. According to the PET (physiologically Equivalent Temperature) index, people feel better between 18.1–23.0℃ temperature values, and above or below this value range causes conditions such as fatigue, nervousness, tension, and many physical symptoms such as dryness in the throat and burning in the eyes. It has been determined that it causes health problems. Energy use can be reduced by increasing tree and vegetation cover in urban areas, and quality is increased by reducing air pollution. Smart urbanization is one of the important determinants of physical development and socioeconomic development [1, 2, 30-45, 89]. Smart growth practices and the creation of green cool roofs cause a decrease in greenhouse gas emissions while increasing human health and comfort areas and improving their quality of life [27, 35-55]. Various studies are being conducted on the concept of bioclimatic comfort, which can be defined as the conditions in which people can adapt to their environment by spending less energy, especially with the urbanization phenomenon that started with the industrial revolution and continues to increase today [31-61]. Bioclimatology is a multidisciplinary science that studies the relationship and interaction between living things and climate. In addition to human, plant, and animal bioclimatology, urban areas also have their climate and bioclimatology, which are different from the surrounding rural areas. The phenomenon of bioclimatic comfort, in which climate parameters such as temperature, humidity, and wind play a role, has become an important issue in the planning and landscape design processes of urban areas with increasing temperature values due to the effect on humans and all other living things, and it has become necessary to create sustainable spaces where people feel more comfortable. [33-68].

In this study, the bioclimatic comfort conditions of Kahramanmaraş, where the Mediterranean climate is intensely felt, are discussed. Meteorological measurement data of the study area between 1970 and 2021 were obtained from meteorological stations in the region. In line with these data, temperature, relative humidity, and wind speed maps were created and then correlated with PET index values.

2. Material and Method

Material

Kahramanmaraş province, which is the study area, is located in the Mediterranean region. The city center has a rough structure because it was established on the skirts of Ahir Mountain. It is surrounded by Sivas in the north, Gaziantep in the south, Adana in the east, and Adıyaman in the west, and the altitude value starts from 123 meters and ends at 3076 meters (Figure 1). This study, it is aimed to examine the bioclimatic comfort conditions of Kahramanmaraş Province, which is under the influence of the Mediterranean climate, which is hot and dry in summer and warm and rainy in winter. As you go from south to north and from west to east, the Kahramanmaraş plain located in the center and especially in the southern part of the province, which shows terrestrial climate characteristics, has provided the opportunity to grow various agricultural products in these areas.

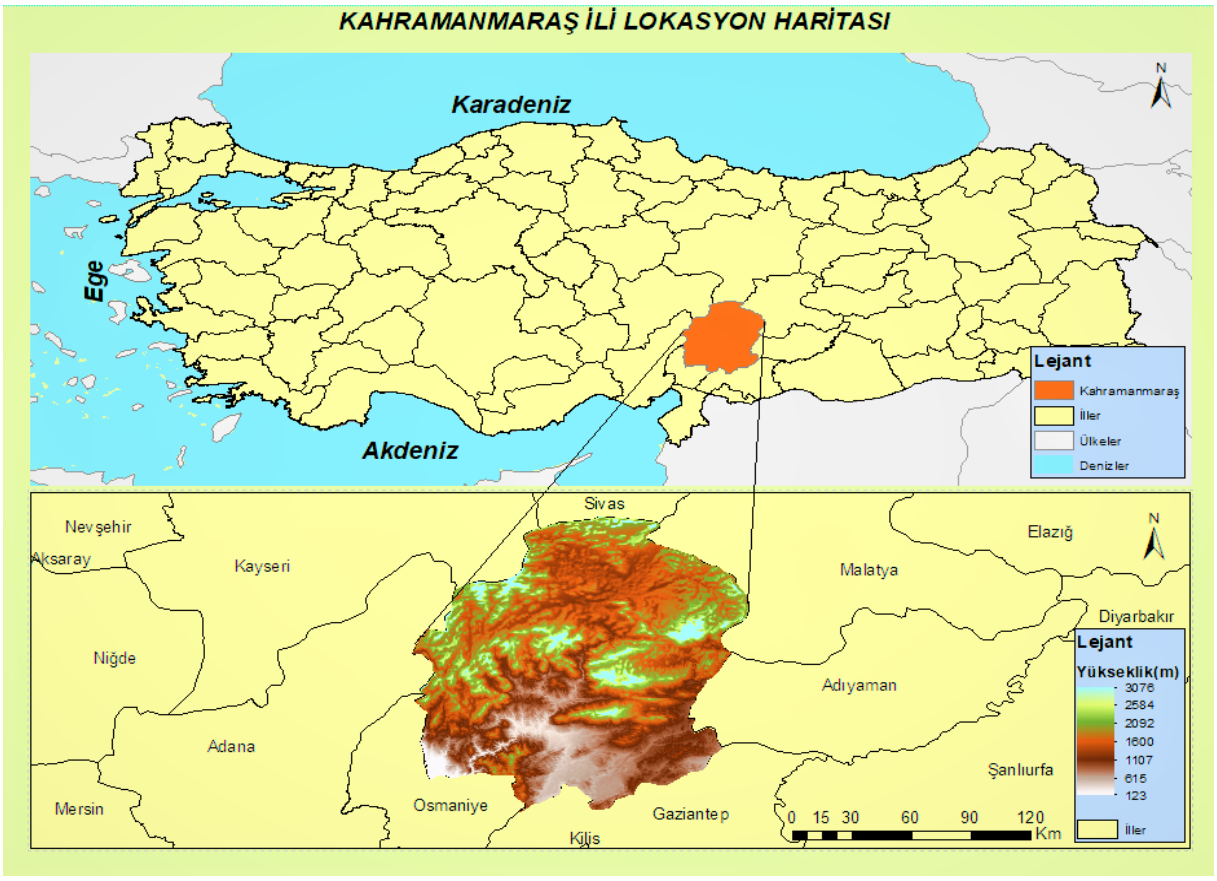

Figure 1. Study area location map

Method

Meteorological climate data of Kahramanmaraş province for the years 1970-2021 were obtained from MGM. Afterward, these data were transferred to ArcGIS 10.8.1 program, and temperature, PET, humidity, and wind maps were created using co-kriging and IDW methods from interpolation methods. The results obtained are correlated with the PET index data in Table 1 above. The 12-month minimum and maximum temperature differences of the bioclimatic comfort conditions of Kahramanmaraş Province were determined. As a result of the examination, the lowest and highest climatic comfort levels were reached, and with the result obtained, suggestions were made on what kind of measures can be taken to provide bioclimatic comfort conditions and suitable thermal conditions for people in the planning processes in the coming years.

Table 1. Pet index thermal stress levels

Human feeling	PET(°C)	thermal stress level
Very cold	<4	extreme cold stress
Cold	4.1 - 8.0	strong cold stress
Cool	8.1- 13.0	moderate cold stress
slightly cool	13.1 - 18.0	mild cold stress
Comfortable	18.1 - 23.0	no thermal stress
mild temperate	23.1 - 29.0	mild heat stress
mild	29.1 - 35.0	moderate heat stress
Hot	35.1 - 41.0	Strong heat stress
Very hot	>41.0	extreme heat stress

3. Result

The water vapor suspended in the air is called humidity. From this point of view, humidity also means wetness and precipitation. When we look at the monthly humidity data of the study area according to the 12-month humidity data of Maraş Province in Figure 2 above, it is seen that the months with the highest humidity rate belong to the winter months, and the lowest humidity rate is in the summer months. Especially in December, January, and February, the air mass reaches its maximum level quickly because it becomes saturated faster.

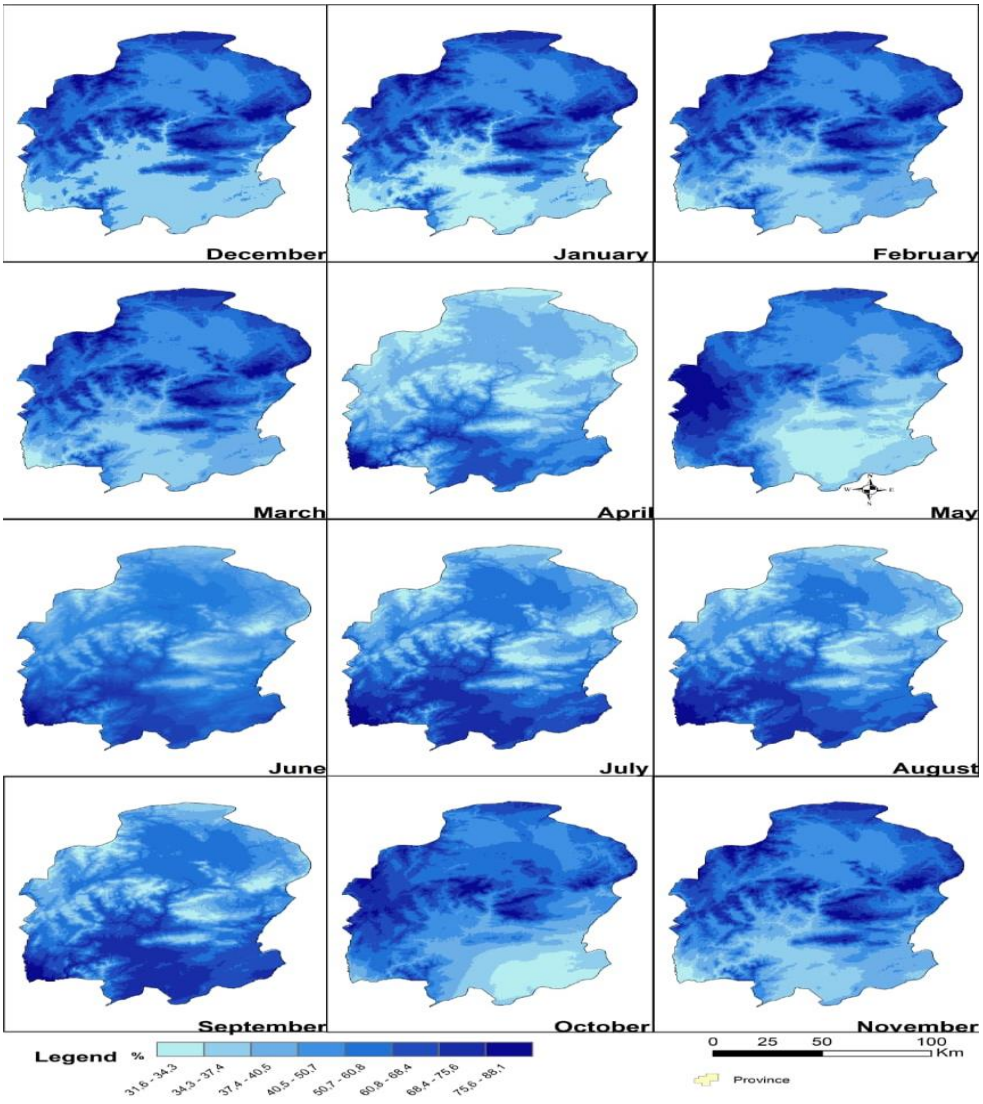

Figure 2. Kahramanmaraş province humidity map

In the summer months, due to the high-temperature level, the saturation gap in the air mass increases, which causes a decrease in the amount of humidity in April, May, and June. When evaluated in terms of bioclimatic comfort, it can be observed that the suffocating air is dominant between July and September, and August is more suffocating than July and September. It is seen that there is no sweltering air in February when the humidity is low, and bioclimatic comfort is more suitable.

When the Pet Index Thermal Stress Levels in Table 1 of the Kahramanmaraş Pet Index analysis in Figure 3 are taken into consideration, the thermal stress level of the central region, which is dominated by red colors, is high in the summer months, and the thermal stress level of the central area, which is blue, is lower in the winter months, depending on the temperature conditions. observed to be lower. It is understood that the temperature level, which is also effective with urbanization, reaches the highest levels, especially in June and July, and the thermal comfort level decreases, and with this decrease, there are periods when suffocating and unbearable.

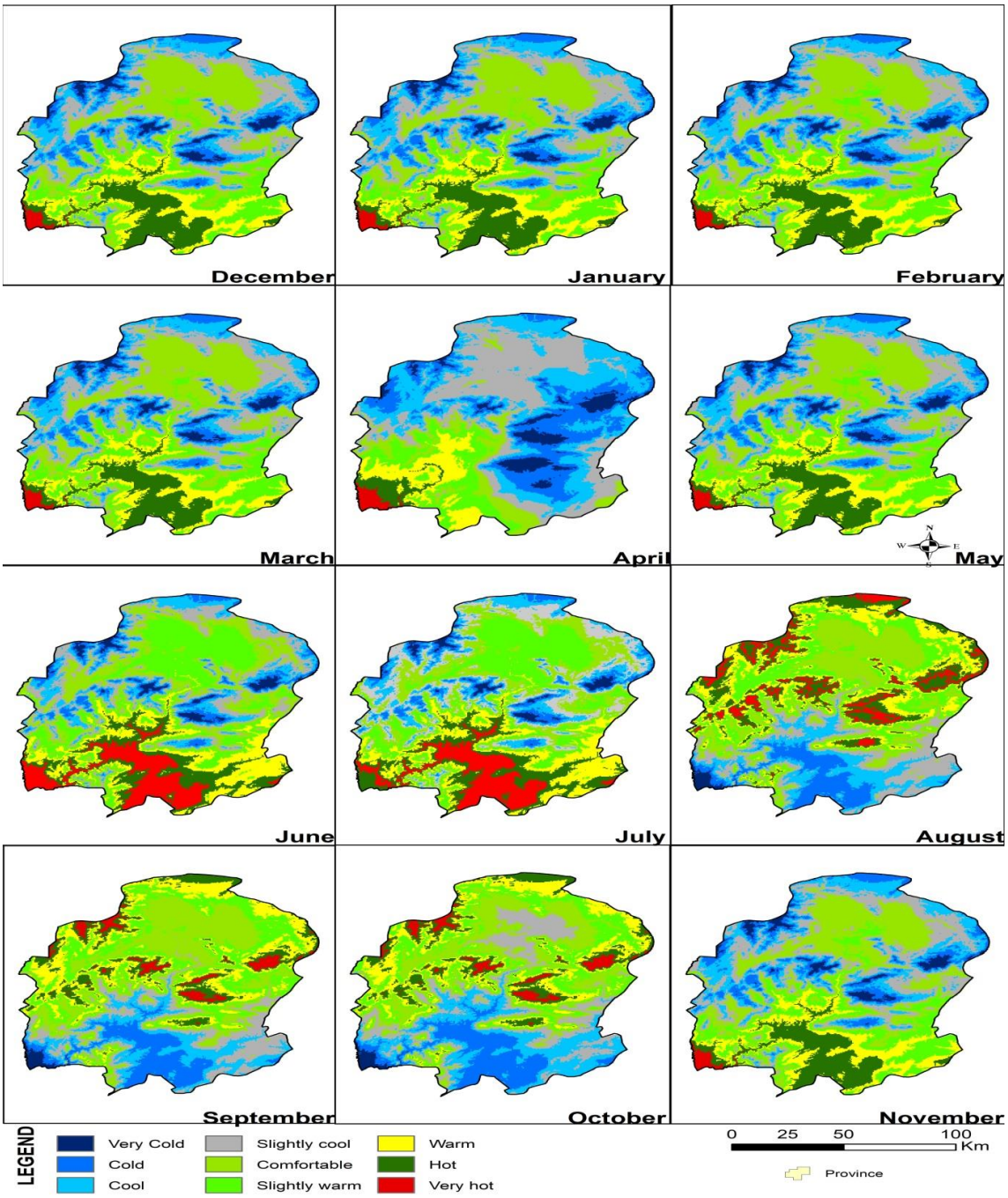

Figure 3. Kahramanmaraş province pet index map

The wind is when the air mass moves horizontally. The wind is one of the factors that determine the climatic condition of a region. Wind speed in Kahramanmaraş shows slight seasonal variations throughout the year. When we look at the monthly wind speed data of the study area according to the 12-month wind speed data of Kahramanmaraş province in Figure 4 above, it is seen that the months with the highest wind speed rate belong to the winter and spring months, and the lowest wind speed is in the summer months. Especially in the summer months, with the warming of the weather, the wind condenses and rises and moves from high-pressure areas to low-pressure areas, as a result of which there is a decrease in wind speed. In the spring and winter, the cooled air begins to descend and moves from the low-pressure area to the high-pressure areas, increasing wind speed.

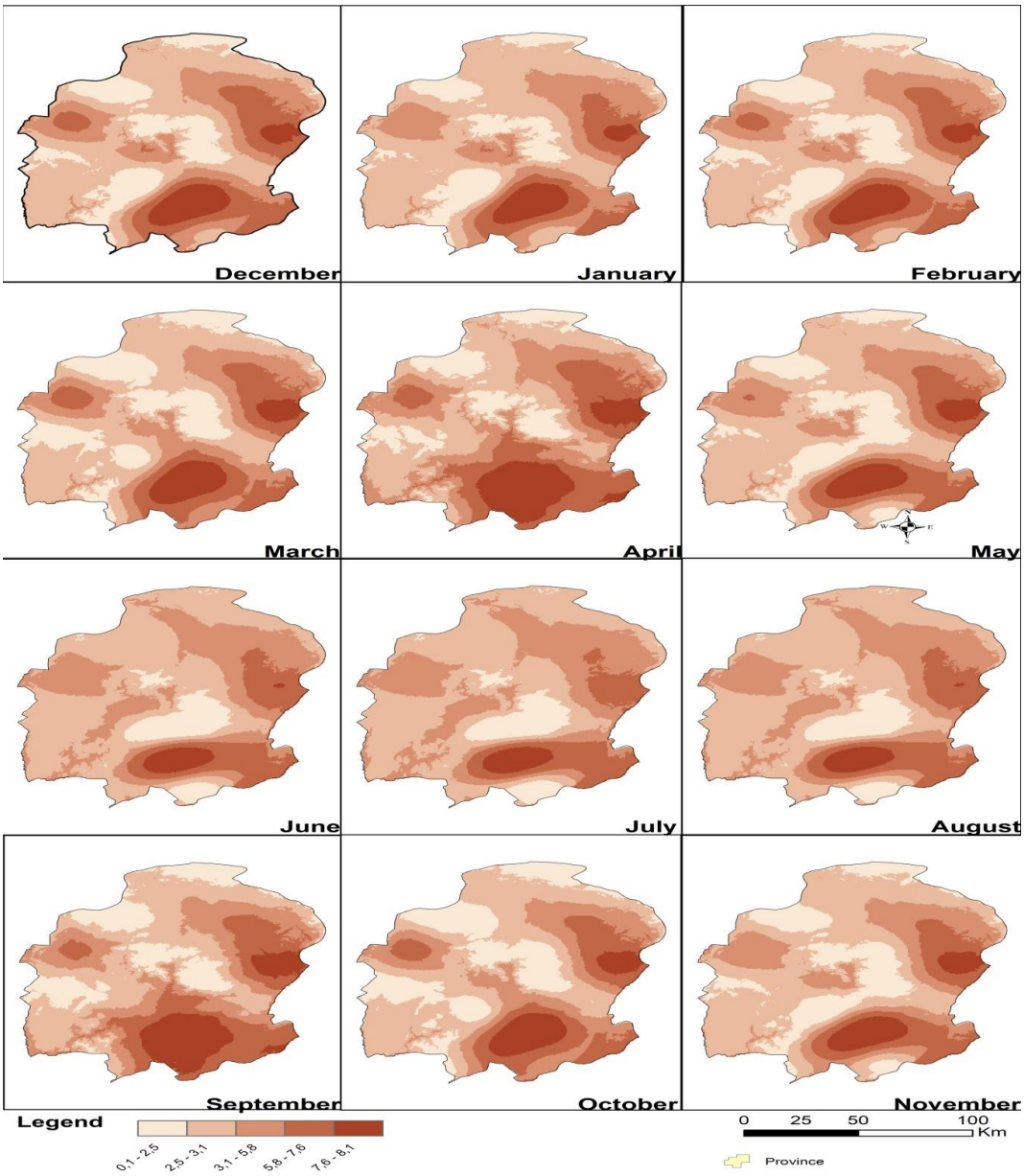

Figure 4. Kahramanmaraş wind analysis map

Urban temperature is the amount of heat the city retains. Temperature is one of the factors that determine the climatic condition of a region. In determining the temperature of a region, the movement of the earth, hot water currents, winds, vegetation, urban structure, etc. factors play a decisive role. Kahramanmaraş province generally shows Mediterranean climate characteristics and there are regions with continental climate characteristics. When we look at the monthly temperature data of the study area according to the 12-month temperature data of Kahramanmaraş province in Figure 5 above, it is seen that the months with the highest temperature rate belong to the summer months, and the lowest temperature is in the winter months. In the central district of Kahramanmaraş, it is around 5.6-7.7 °C in December, January, and February. With the increasing temperatures since May and the effect of the urban heat island, the temperature increased to 25.3-31.2 °C in August. The temperature value required to provide bioclimatic comfort is 18. 1 – 23.0℃. Since the temperature in the central district rises above this value in summer, people living in the city are exposed to heat stress. The temperature values of Göksun, Afşin, Elbistan, and Nurhak districts are lower during the year compared to the Central district and its surroundings due to the terrestrial climate effect and the lack of urbanization.

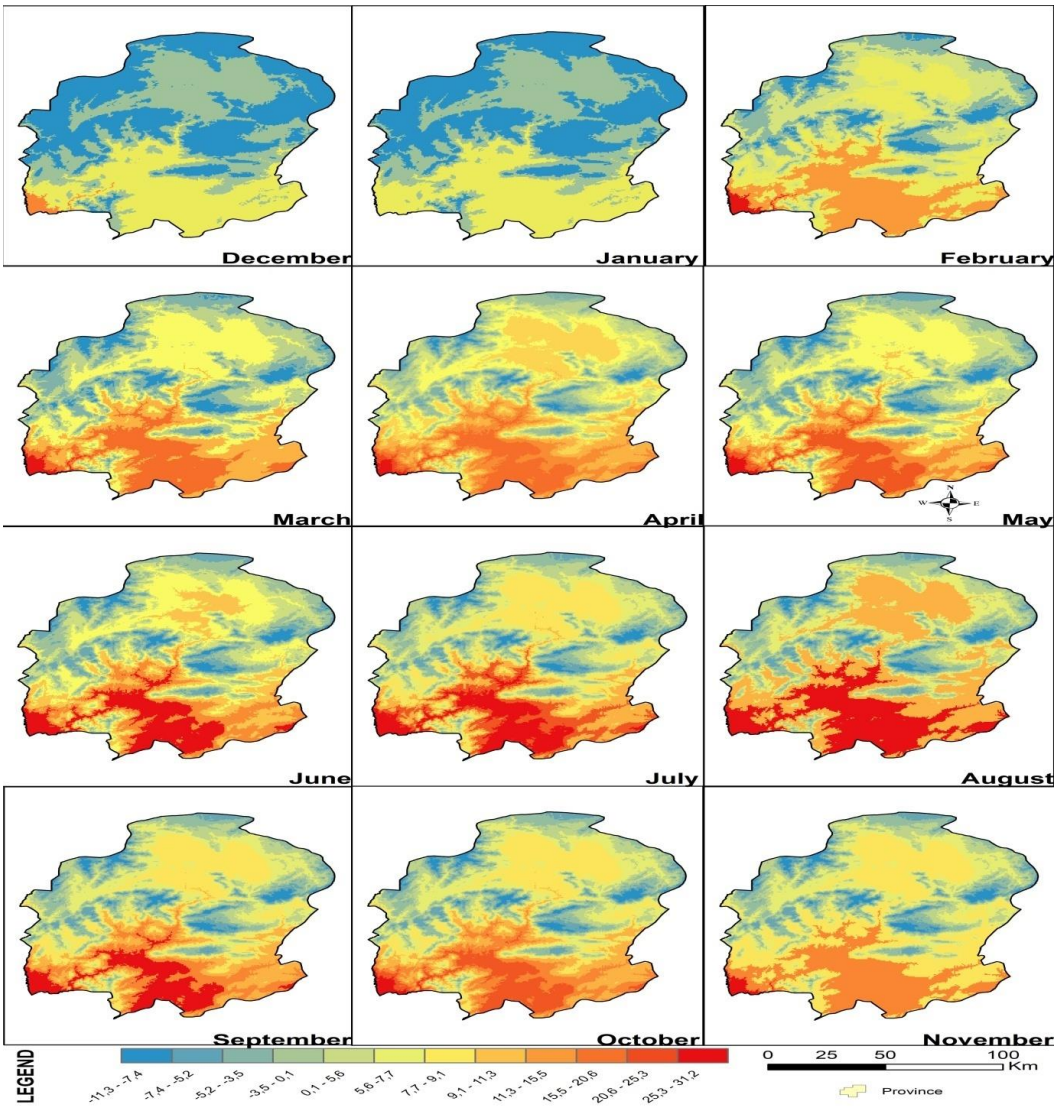

Figure 5. Kahramanmaraş temperature analysis map

4. Discussion

Many international studies have been carried out on the determination of bioclimatic comfort zones in Turkey in recent years. To determine the bioclimatic comfort conditions of many different cities in Turkey for certain years; Zeren Cetin and Sevik [5], Kilicoglu et al. [54] have used the PET index [3, 55, 62, 70]; Cetin [45] have relied on PET and DI index methods; while Cetin et al. [8], Adıguzel et al. [60]; Zeren Cetin et al. [4] have adopted the method of environmental climatic parameters [35-40, 46, 47, 60, 62, 70, 71]. This study is the first study on the bioclimatic comfort areas of Bartin for determining the effect of land use a land cover change on sustainable forest areas. The most important fundamental difference of the study from the related studies is that more than one parameter and indices are used in determining the suitable areas in terms of bioclimatic comfort, and therefore it can reveal the differences in approach between the indices. The second important difference is that the climatically comfortable zones change annually in 3 different 30-year periods (1990, 2000, 2020) according to each parameter/index. The third important difference is that the climatically comfortable zones in the reference years and the land cover of the province are evaluated together.

5. Conclusions

The climate, which has been in constant change since the formation of the world, has started to show a more significant change, especially with the industrial revolution and industrialization. Urbanization on the one hand and the increase in the use of fossil fuels on the other, mostly due to anthropogenic reasons, accelerated this change and affected the entire ecosystem, especially fauna and flora on earth. With the increasing climate change in our country, the decrease in precipitation and the increase in temperature levels have caused many researchers to conduct research studies on the subject. The climate changes that occur are effective in all areas such as agriculture, industry, energy, transportation, and settlement, especially the natural environment, and it is thought that they will continue to be effective.

In this study, humidity, wind, temperature, and pet index analysis were carried out to determine the bioclimatic comfort conditions of Kahramanmaraş Province. According to the analysis results of these parameters; It has been observed that the average minimum and maximum values of the temperature conditions increase, and the center and its surroundings reach the highest temperature level, especially in summer. When we look at the wind speed analysis, it is concluded that while the speed rate is high in the winter months, this rate decreases in the summer months. It has been understood that the temperature conditions are effective in the condensation of the wind and the decrease in the speed ratio while moving from high pressure to low pressure.

When we look at the humidity analysis of the area, it has been observed that in July, August, and September, when the suffocating air is dominant, in December, January, and February, when the humidity is low, there is no sweltering air and there are more suitable times for the bioclimatic comfort level. In all analyzes for the study area, when evaluated according to the Pet index values, it was seen that the most significant differences were experienced in the summer months. It has been understood that the bioclimatic comfort conditions are gradually decreasing in the central district where the population is dense in Kahramanmaraş. The negativities experienced in bioclimatic comfort areas have become a situation that directly affects the thermal comfort of people. In the study area, where the Mediterranean climate is dominant, urban planning should be made with a more sustainable, environmentalist understanding and geographical perspective for people who are exposed to temperature values that may threaten their mental and physical health in summer due to urbanization, and models suitable for thermal and bioclimatic comfort levels should be developed.

Competing Interest / Conflict of Interest

The authors declare that they have no competing interests

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