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Investigation of the Molecules Obtained from Marijuana: Computational Study of Spectral, Structural and Docking

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ABSTRACT

There are many chemical molecules whose names are Cannabigerol (CBG), cannabidol (CBD), cannabichromene (CBC), tetrahydrocannabivarin (THCV), cannabigerovarinic acid (CBGV) and cannabidiolic acid (CBDA) derived from Marijuana. Theoretical methods were used to compare the chemical and biological activities of the six major molecules. Molecules were compared with their chemical activities using many parameters obtained by Gaussian program. Density functional theory (DFT) calculation of studied molecules are investigated activity of molecules. Then, ^{13} C and ^{1} H NMR and UV-vis spectra were obtained. the UV-Vis spectra of these six molecules using the Gaussain software program on the basis set HF / 6-31 ++ g in different solvents whose name are gas (ε = 1), chloroform (ε = 4.711), methanol (ε = 32.613), dimethyl sulfoxide (ε = 46.826), water (ε = 78.355) and n-methyl formamide-mixture (ε = 181.56) phase. Cannabinoids derivatives are a very important drug in the pharmaceutical world Finally, in the molecular docking, the molecules have been studied for their biological activities against Crystal structure of the Deleted in Liver Cancer 1 (DLC1) whose ID is 3KUQ. The obtained parameters from docking were compared molecules.

Keywords: Marijuana; Molecular docking; NMR spectra; UV-vis spectra; DFT

1. INTRODUCTION

Cannabinoids derivatives are a very important drug in the pharmaceutical world. The plant *Cannabis sativa L.* has been used since a thousand years as medicinal agent [1]. Marijuana is the raw obtained from the Cannabis sative L. plant [2]. Cannabis sativa L. is included compounds that is the typical C_{21} group.

In this study, six different molecule of Cannabinoids derivatives are investigated different properties in theoretical chemistry. Cannabigerol (CBG) was the first compound that obtained purely from marijuana [3]. Although CBG derivatives are more inactive than Δ^9-trans-tetrahydrocannabinol, they exhibit significant antibacterial activity against gram positive bacteria [4-5]. Cannabidol (CBD) was second compound that first isolated in 1940 by Adams et al. Cannabichromene (CBC) was the fourth compound whose discovery occurred at the

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same time as the others. This compound led to the discovery of other CBC type compounds. Tetrahydrocannabivarin (THCV), cannabigerovarinic acid (CBGV) and cannabidiolic acid (CBDA) are the highly lipohilic nature structure that allow them to attainment intracellular sites.

In this study, we can be seen that activity of studied molecules whose names are Cannabigerol (CBG), cannabidol (CBD), cannabichromene (CBC), tetrahydrocannabivarin (THCV), cannabigerovarinic acid (CBGV) and cannabidiolic acid (CBDA) in **Figure 1 [1-2]**.

2. COMPUTATIONAL METHOD

2.1. Gauss view program

Quantum chemical calculations of studied molecules are investigated activity of molecules. Input files of all studied molecules are prepared by gaussian view 5.08 programs **[6]**. Calculations of all studied molecules were performed with Gaussian IA32W-G09RevA.02 and Gaussian AS64L-G09RevD.01 programs **[7-8]**. All studied molecules were performed using the Becke, 3-parameter, Lee-Yang-Parr (B3LYP) method **[9-11]** with 6-31g, 6-31g (d,p), 6-31g++ (d,p), 6-311g++ (3df,3pd) basis set in gas phase.

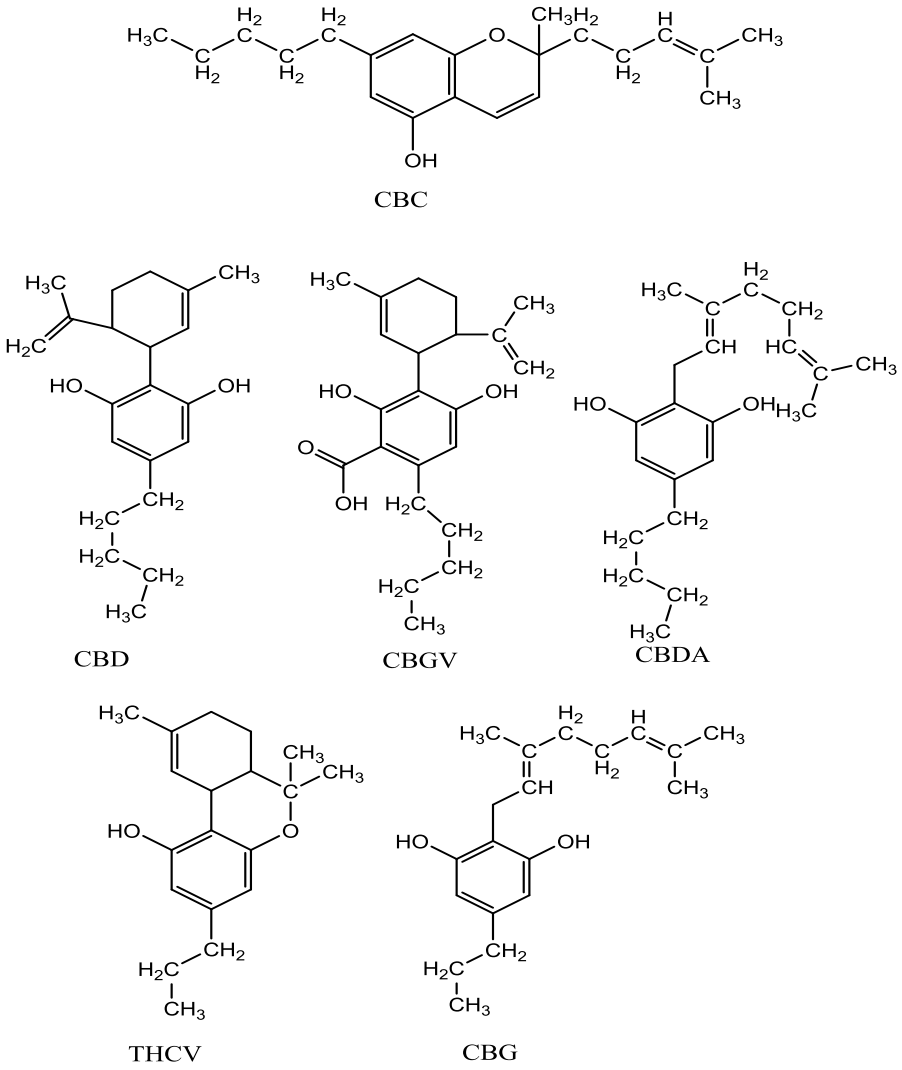

Fig. 1. Structure of studied molecule.

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Quantum chemical parameters are very important information that given about activity of molecules. Highest Occupied Molecular Orbital (E_{HOMO}) and Lowest Unoccupied Molecular Orbital (E_{LUMO}) are more important than other parameters such as ΔE (HOMO-LUMO energy gap), electronegativity (χ), chemical potential (μ), chemical hardness (η), electrophilicity (ω), nucleophilicity (ε), global softness (σ) and proton affinity (PA) [12-22].

$$\mu = -\chi = \left(\frac{\partial E}{\partial N}\right)_{\upsilon(r)} \quad (1)$$

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{\upsilon(r)} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right) \quad (2)$$

Energy value of HOMO and LUMO level of studied molecules are benefited to calculate Ionization energy (I) and electron affinity (A) which are related to electronegativity, global softness and chemical hardness. The mathematical operations related to these equations are given as follows.

$$\chi = -\mu = \left(\frac{I + A}{2}\right) \quad (3)$$

$$\eta = \frac{I - A}{2} \quad (4)$$

As it is well known that global softness is defined as the inverse of the chemical hardness [23].

$$\sigma = 1/\eta \quad (5)$$

$$\chi = -\mu = \left(\frac{-E_{HOMO} - E_{LUMO}}{2}\right) \quad (6)$$

$$\eta = \left(\frac{E_{LUMO} - E_{HOMO}}{2}\right) \quad (7)$$

The global electrophilicity index [24] (ω) which is researched by Parr et al., is the inverse of nucleophilicity and is given in the following equation (8). Nucleophilicity and electrophilicity of organic and inorganic molecules are used for the predicted the reaction mechanisms. Nucleophilicity (ε) is defined as the inverse of the electrophilicity in equations (9).

$$\omega = \mu^2/2\eta = \chi^2/2\eta \quad (8)$$

$$\varepsilon = 1/\omega \quad (9)$$

2.2. Docking studies

Technological advances have greatly affected the process of comparing the biological activities of molecules. computer programs have been developed for these processes. these programs eliminated the time and costs required to perform experimental procedures. Theoretically, comparisons have now begun to guide experimental procedures. Docking calculations were made using optimized structures of the studied six molecules. Docking calculations were made at DockingServer.com. Docking calculations are based on the standard settings used by DockingServer.com. Genetic Algorithm (GA) was used in the calculations. In the calculations made, GA population size 150, GA number evals 25000, GA number generations 54000, GA run 10.

3. RESULT AND DISCUSSION

Quantum chemical calculations are very significant in chemistry for reactivity of molecules. Quantum chemical calculations are using quantum chemical parameter that are value of HOMO and LUMO energy, energy gap, electronegativity in pharmaceutical industry. It is possible to compare the activities of molecules using these parameters.

Quantum chemical parameters of studied molecule are using to explain for molecular reactivity. Two important parameters such as HOMO and LUMO are used to explain the molecular reactivity. HOMO is Highest Occupied Molecular Orbital and LUMO is Lowest Unoccupied Molecular Orbital.

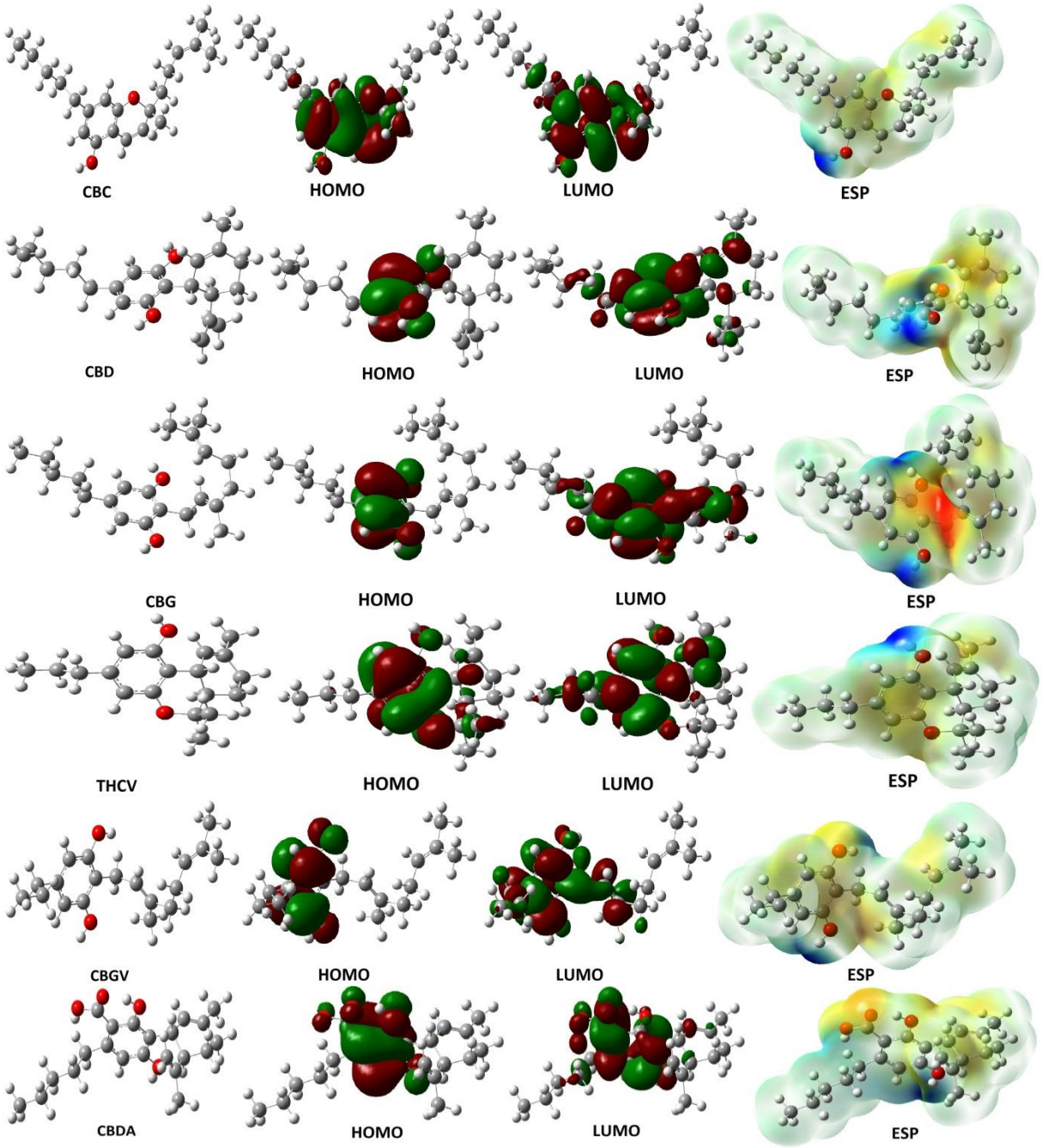

Fig. 2. Structures of HOMO, LUMO and ESPs of derivatives of studied molecule.

The energy level of HOMO has high energy level are described more electron donating ability of molecule. We are looked figure 2 that are indicated where the HOMO orbitals are. CBC molecule has high energy level of HOMO more activity than other molecules in Table 1. This molecule has got high energy level of HOMO that is showing the tendency to donate electrons of the molecule to appropriate that the acceptor molecules have low energy and empty molecular orbital [20-22]. On the other hand, energy level of LUMO is shown electron accepting abilities of studied molecules [25-26]. CBDA molecule has low energy level of LUMO more activity than other molecules in Table 1. This molecule has got low energy level of LUMO that has more electron accepting ability in lower energy of molecular orbitals.

The HOMO Energy level of studied molecules is a very significant parameter that is calculated to compare for molecular reactivity. A molecule that has a higher HOMO energy value is a more active molecule, because this molecule gives electrons more easily. On the other hand, a molecule that has lower LUMO energy value is more active molecule, because this molecule has more electron accepting ability [17]. In consideration of previous explanations, CBC molecule is more activity than other molecule in HOMO energy in table 1. CBDA molecule is more activity than other molecule in LUMO energy.

Table 1. The calculated quantum chemical parameters with B3LYP method in gas phase (eV)

	E_{HOMO}	E_{LUMO}	I	A	ΔE	η	σ	χ	PA	ω	ε	dipole	Energy
B3LYP/6-31g LEVEL													
CBC	-5,4149	-0,6155	5,4149	0,6155	-4,7994	2,3997	0,4167	3,0152	-3,0152	1,8943	-7,2356	1,2341	-26343,1113
CBD	-5,6949	0,1880	5,6949	-0,1880	-5,8829	2,9414	0,3399	2,7534	-2,7534	1,2887	-8,0992	3,2295	-26342,6472
CBG	-5,6805	0,2576	5,6805	-0,2576	-5,9381	2,9691	0,3368	2,7114	-2,7114	1,2380	-8,0504	1,7218	-26375,2429
THCV	-5,5850	0,2816	5,5850	-0,2816	-5,8666	2,9333	0,3409	2,6516	-2,6516	1,1985	-7,7782	0,9983	-24205,7188
CBGV	-5,8035	0,1801	5,8035	-0,1801	-5,9836	2,9918	0,3342	2,8116	-2,8116	1,3212	-8,4120	2,0041	-24237,5661
CBDA	-5,9123	-1,5760	5,9123	1,5760	-4,3363	2,1681	0,4612	3,7441	-3,7441	3,2329	-8,1179	7,1787	-31471,7651
B3LYP/6-31g (d,p) LEVEL													
CBC	-5,3390	-0,5551	5,3390	0,5551	-4,7839	2,3920	0,4181	2,9471	-2,9471	1,8155	-7,0492	1,0308	-26351,1605
CBD	-5,6835	0,2490	5,6835	-0,2490	-5,9325	2,9662	0,3371	2,7173	-2,7173	1,2446	-8,0600	2,5680	-26350,7961
CBG	-5,5434	0,2686	5,5434	-0,2686	-5,8119	2,9060	0,3441	2,6374	-2,6374	1,1968	-7,6642	1,5586	-26383,4455
THCV	-5,4781	0,3175	5,4781	-0,3175	-5,7956	2,8978	0,3451	2,5803	-2,5803	1,1488	-7,4771	0,8819	-24213,1574
CBGV	-5,6381	0,2269	5,6381	-0,2269	-5,8650	2,9325	0,3410	2,7056	-2,7056	1,2481	-7,9340	1,7641	-24245,0642
CBDA	-5,8887	-1,2160	5,8887	1,2160	-4,6726	2,3363	0,4280	3,5524	-3,5524	2,7007	-8,2994	6,3237	-31481,8893
B3LYP/6-31++g (d,p) LEVEL													
CBC	-5,6519	-0,9526	5,6519	0,9526	-4,6993	2,3496	0,4256	3,3023	-3,3023	2,3206	-7,7592	0,9732	-26352,0706
CBD	-5,9679	-0,4863	5,9679	0,4863	-5,4816	2,7408	0,3649	3,2271	-3,2271	1,8998	-8,8447	2,7222	-26351,7522
CBG	-5,9447	-0,5170	5,9447	0,5170	-5,4277	2,7139	0,3685	3,2309	-3,2309	1,9232	-8,7681	2,4379	-26384,3484
THCV	-5,7706	-0,3823	5,7706	0,3823	-5,3883	2,6941	0,3712	3,0764	-3,0764	1,7565	-8,2883	0,7975	-24213,9407
CBGV	-5,9619	-0,4808	5,9619	0,4808	-5,4811	2,7405	0,3649	3,2213	-3,2213	1,8933	-8,8282	1,8561	-24245,9484
CBDA	-6,1727	-1,6030	6,1727	1,6030	-4,5698	2,2849	0,4377	3,8879	-3,8879	3,3077	-8,8833	6,6126	-31483,0515

The Energy gap (ΔE) is a significant parameter that is shown reactivity of molecule. The molecule has a small energy gap, this molecule is more reactivity than other molecule [21]. CBC molecule has a small energy gap and this molecule is more activity than other molecule. The reactivity efficiency ranking of studied chemical molecules can write as: CBC > THCV > CBG > CBGV > CBD > CBDA in B3lyp/6-31++g(d,p) basis set.

3.1. NMR spectroscopy

NMR spectroscopy is one of the most important methods used to illuminate the structures of the studied molecules. The most commonly used NMR spectroscopy techniques are ^{13}C and ^{1}H NMR. The structure of the molecule is determined using ^{13}C and ^{1}H NMR shift values. NMR calculations in this study are calculated with the Gauge-Independent Atomic Orbital (GIAO) method [27-29]. Studied molecules are calculated using the basis set of B3lLYP/6-31++g(d,p). Atoms of studied molecules are labelled. The chemical shift values of ^{13}C and ^{1}H NMR obtained as a result of the calculations are given in Table 2.

It should be well known that the numerical values obtained from the calculations show that the ^{13}C NMR chemical shift values of the aromatic carbon atom are between 100-155 ppm, while the ^{13}C NMR chemical shift numerical values of the aliphatic carbon atom of the aromatic carbon are between 20-60 ppm [30]. However, the ^{1}H NMR chemical shift values of the hydrogen atoms attached to the aromatic carbon are in the range of 6-8 ppm, the ^{1}H NMR chemical shift values of the hydrogen atoms attached to the aliphatic carbon atoms are in the range of 2-5 ppm. These values are within the normal range.

Table 2. ^{13}C and ^{1}H NMR values of the studied molecule

CBC		CBD		CBG		THCV		CBGV		CBDA	
C1	152,81	C1	48,31	C1	105,31	C1	104,38	C1	144,18	C1	135,92
C2	105,24	C2	43,55	C2	155,38	C2	144,3	C2	104,32	C2	127,56
C3	147,05	C3	128,44	C3	114,29	C3	110,44	C3	154,68	C3	42,76
C4	110,96	C4	134,67	C4	154,97	C4	156,67	C4	108,34	C4	48,94
C5	155,07	C5	38,09	C5	105,15	C5	110,92	C5	156,14	C5	39,48
C6	108,38	C6	38,7	C6	143,65	C6	155,3	C6	107,85	C6	38,09
C10	119,75	C9	152,84	C13	29,66	C9	46,04	C11	45,27	C7	151,82
C11	127,3	C10	30,16	C16	124,6	C12	35,32	C14	35,62	C8	28,54
C12	83,74	C11	108,67	C17	135,04	C15	19,57	C17	19,62	C9	122,24
C13	25,99	C12	117,94	C18	22,65	C19	42,07	C21	28,13	C10	167,18
C14	49,34	C13	157,79	C19	43,25	C20	52,54	C24	121,52	C11	158,46
C16	29,15	C14	155,87	C25	31,53	C22	81,9	C26	136,96	C12	105,42
C18	127,16	C15	105,93	C27	129,73	C23	32,3	C27	43,93	C13	109,05
C20	134,93	C16	104,47	C28	132,75	C24	127,03	C28	23,67	C14	141,24
C21	31,07	C17	144,6	C29	22,19	C26	38,71	C34	29,51	C16	170,18
C22	21,87	C22	44,55	C30	29,71	C28	134,86	C37	126,55	C17	47,45
C23	44,97	C24	40,75	C40	44,05	C29	28,52	C38	134,29	C20	38,86
C25	42,81	C26	38,56	C43	43,56	C35	31,83	C40	21,85	C23	40,29

Continue Table 2

C26	41,69	C41	29,96	C46	41,09	C36	23,58	C41	30,95	C26	30,58
C28	31,76	C42	17,9	C49	31,63					C29	19,34
C29	19,11	C49	28,88	C52	19,38					C43	107,35
										C44	29,74
H7	6,60	H7	3,08	H7	6,52	H7	6,63	H7	6,52	H15	6,30
H8	6,99	H8	2,20	H8	6,59	H8	7,11	H8	7,21	H18	3,25
H15	2,73	H18	6,70	H10	4,55	H10	2,87	H10	5,42	H19	3,15
H17	3,10	H19	6,62	H12	4,43	H11	2,96	H12	3,02	H21	2,48
H19	6,26	H23	2,88	H14	3,94	H13	2,15	H13	2,20	H22	2,04
H24	3,09	H25	1,83	H15	4,49	H14	2,18	H15	2,77	H24	2,04
H27	2,13	H27	1,97	H20	2,04	H16	1,57	H16	2,07	H25	1,99
H30	2,40	H28	2,4	H21	3,49	H17	1,83	H18	1,82	H28	2,01
H31	2,44	H29	2,87	H22	2,11	H18	1,60	H20	1,52	H30	1,89
H32	2,44	H30	2,60	H23	2,84	H25	2,52	H22	4,70	H31	1,62
H33	2,94	H31	2,64	H24	2,73	H27	7,79	H23	3,24	H32	1,57
H34	2,07	H32	2,66	H26	3,32	H30	2,43	H25	5,84	H35	8,54
H35	2,11	H33	2,01	H31	2,84	H31	2,41	H29	3,33	H38	14,77
H36	3,20	H34	2,02	H32	5,77	H32	2,37	H30	2,12	H39	4,72
H37	1,95	H35	6,11	H33	2,93	H33	4,21	H31	2,09	H40	2,27
H38	2,41	H36	6,03	H34	2,11	H34	2,49	H32	2,96	H41	2,34
H39	1,38	H37	3,98	H35	2,10	H37	1,57	H33	2,47	H42	2,35
H40	2,15	H38	5,01	H36	2,12	H38	1,54	H35	3,07	H45	3,90
H41	6,22	H39	4,51	H37	2,31	H39	1,99	H36	3,12	H46	5,47
H42	7,69	H40	4,41	H38	2,2	H40	2,11	H39	6,63	H47	5,59
H43	2,95	H43	2,27	H39	6,19	H41	1,86	H42	2,91	H48	6,24
H44	2,20	H44	2,02	H41	3,00	H42	2,05	H43	2,12	H49	2,19
H45	2,03	H45	2,34	H42	2,96	H43	2,79	H44	2,13	H50	2,19
H46	1,95	H46	1,32	H44	2,10	H44	2,93	H45	2,46	H51	2,84
H47	2,08	H47	1,80	H45	2,06	H45	2,17	H46	2,39	H52	2,3
H48	2,00	H48	1,72	H47	1,98	H47	4,56	H47	2,50	H53	2,67
H49	1,60	H50	2,35	H48	1,97			H49	4,48	H54	3,07
H50	1,63	H51	2,36	H50	2,00					H56	6,19
H51	1,89	H52	2,23	H51	1,98						
H53	4,47	H53	6,42	H53	1,58						
				H54	1,58						
				H55	1,85						

3.2. UV-VİS spectra

UV-VIS. spectroscopy is a spectroscopic method used mostly for quantitative purposes. It is one of the "molecular spectroscopy" types because it

is based on the interaction of molecules with UV and visible rays. In this spectroscopic method, it is due to the excitation of bond electrons or unconnected electrons in molecules with the help of radiation [31]. All organic and inorganic substances absorb rays in the UV and visible area. For these two species, the electron transition is the same. In this spectroscopic method, the studied molecules were calculated on the basis set HF / 6-31++g in different solvents whose name are gas (ε=1), chloroform (ε=4.711), methanol (ε=32.613), dimethyl sulfoxide (ε=46.826), water (ε=78.355) and n-methyl formamide-mixture (ε=181.56) phase in **Figure 3** [32-36]. In these phases, when the necessary calculations are made, the main band value in which the maximum absorbance value is obtained is given in Figure 3. It is investigated how molecules change maximum absorbance values in different phases. According to this study, dielectric constants of molecular in different phases were studied. As the dielectric constant value applied to the molecule increased, the main band value of the molecule increased [37-39].

3.3. Molecular Docking Study

In quantum chemical calculation, other parameters are showed that most activity molecule is CBC. Theoretical studies have been guiding future experimental studies. Another theoretical biological activity comparison method for the studied molecules is the molecular docking. Molecular docking allows us to learn about the biological activities of the molecules that are studied against the protein molecules. The biological activity of the molecules against cancer cells composed of protein groups was compared using molecular docking.

Molecular docking studies are used to compare the biological activity of molecules by examining the interactions between molecules and protein. This method is used to design and develop a more effective, more active molecule against protein molecules [40].

The calculations were made at the pH at which the activity of the cancer cells was highest, i.e. at the pH of the human blood. The pH of human blood is 7.35, so calculations are made at pH 7.3 [41].

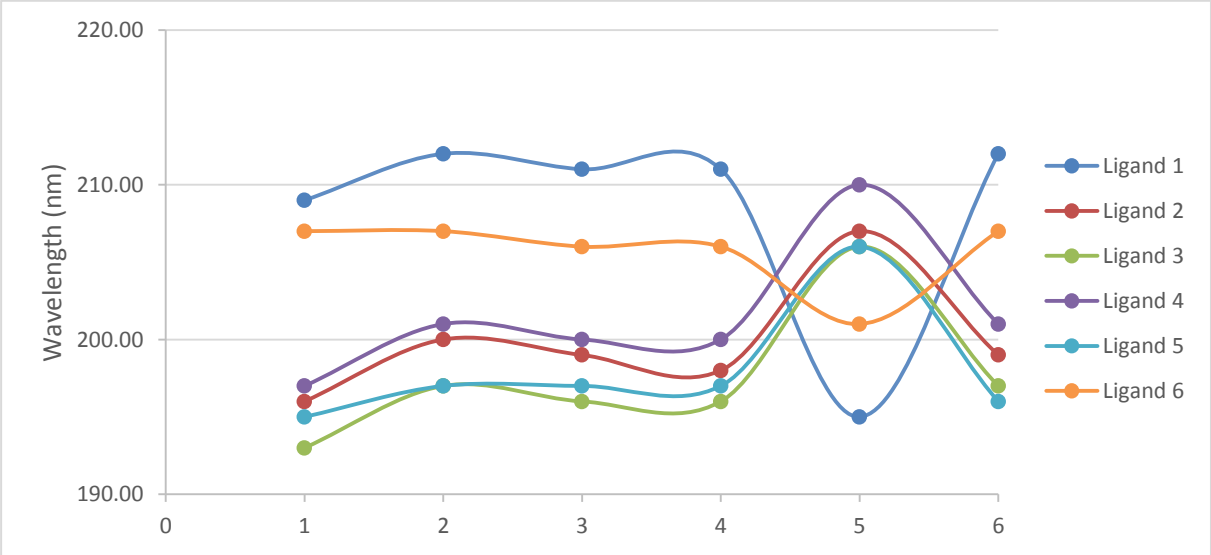

Fig. 3. Main band numerical values of UV-VIS spectrum of studied molecules.

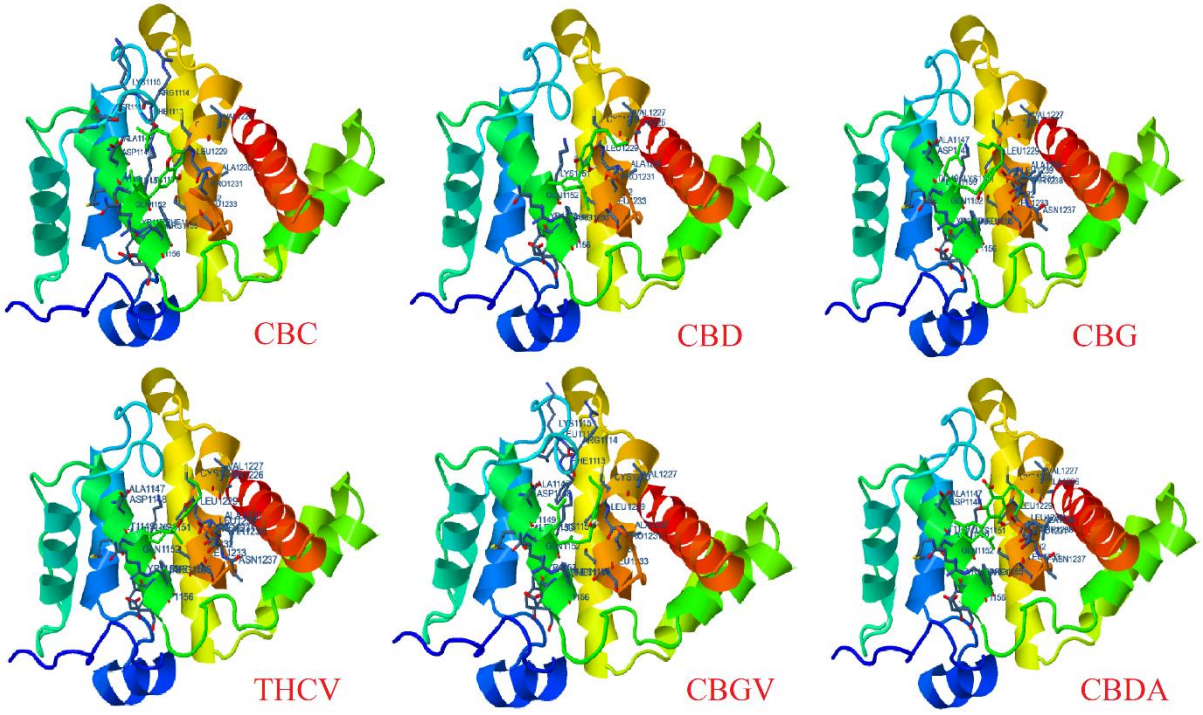

Fig. 4. Interaction of studied molecules with cancerous tissue.

In molecular docking studies, many parameters are used to compare the biological activities of molecules. These parameters are used to explain the interactions and binding affinity between the molecule and the protein. In this study, liver cancer was used as protein, whose original name is Crystal structure of the Deleted in Liver Cancer 1 (DLC1) and its ID is 3KUQ from Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB). The interaction of this cancer protein with molecules has been studied in **Figure 4**. The obtained parameters and the numerical values of the parameters are given in **Table 3**. As a result of molecular docking calculations, many parameters were obtained, the first of these parameters is Est. Free Energy of Binding, which gives a measure of the affinity of the binding energy between the studied molecules and the protein. If the numerical value of this parameter has the lowest negative value, it is the best and strongest interaction between the molecule and the protein [42-43]. That molecule has the highest biological activity. The next parameter is Est. İnhibition Constant. Ki, which is the numerical value of the affinity of binding and interaction between the studied molecule and protein. If any molecule has the lowest numerical value for this parameter, the less drug can be used to activate the enzyme [44]. VDW, Van Der Waals energy + Hbond, Hydrogen Bonding + Desolv., Desolvation energy is the third parameter in docking studies. This parameter is important in molecular docking studies, because if the numerical value of this parameter is negative, it can be said that there is binding between the molecule and many proteins [45]. The last parameter is Electrostatic Energy. When a molecule has the lowest negative value of the numerical value of that parameter, that molecule has the

highest chemical interaction with the protein [46-47].

In the light of the numerical value of the parameters obtained as a result of docking calculations, the CBC molecule is the highest biological activity against the Crystal structure of the Liver Cancer 1 (DLC1). As a result of docking calculations, many parameters were obtained. All of these parameters showed that the best biological activity was CBC. The most important reason for this is that the interaction of CBC molecule with proteins is very high. Because as the interaction increases, the biological activity of the molecules increases.

The interaction of the CBC molecule with the proteins contained in the Crystal structure of the Liver Cancer 1 (DLC1) is shown in figure 5. As the interaction of the molecule with proteins increases, the biological activity of the molecule increases [48-50]. For this, when the interaction of the molecule with proteins was examined, it was found that the Crystal structure of the Liver Cancer 1 (DLC1) contains many proteins such as LYS1151, SER1116, ASP1148 and PRO1231. These proteins interact with molecules. Protein LYS1151 was found to form hydrogen bonds from 3.13 atomic units with the O2 atom in the CBC molecule. Protein SER1116 was found to form hydrogen bonds from 3.83 atomic units with the H30 atom in the CBC molecule. Protein ASP1148 was found to form hydrogen bonds from 3.85 atomic units with the H30 atom in the CBC molecule. Protein ASP1148 was found to form polar bonds from 3.71 atomic units with the O2 atom in the CBC molecule. Protein PRO1231 was found to form polar bonds from 3.31 atomic units with the C16 atom in the CBC molecule.

Table 3. Molecular Docking energy data for studies molecule

	CBC	**CBD**	**CBG**	**THCV**	**CBGV**	**CBDA**
Est. Free Energy of Binding/ *kcal/mol*	-3.89	-2.77	-1.96	-3.25	-3.21	-3.34
Est. İnhibition Constant. Ki/ *mM*	1.40	9.38	36.82	770.95	4.43	3.55
vdW+Hbond+desolv Energy/ *kcal/mol*	-5.69	-5.49	-4.87	-5.07	-5.31	-5.49
Electrostatic Energy/ *kcal/mol*	-0.12	-0.04	-0.06	-0.08	-0.12	-0.27
Total Intermolec. Energy/ *kcal/mol*	-5.81	-5.53	-4.94	-5.15	-5.43	-5.77
Frequency	%30	%50	%40	%20	%10	%60
Interact. Surface	624.63	636.80	584.16	619.18	610.96	633.95

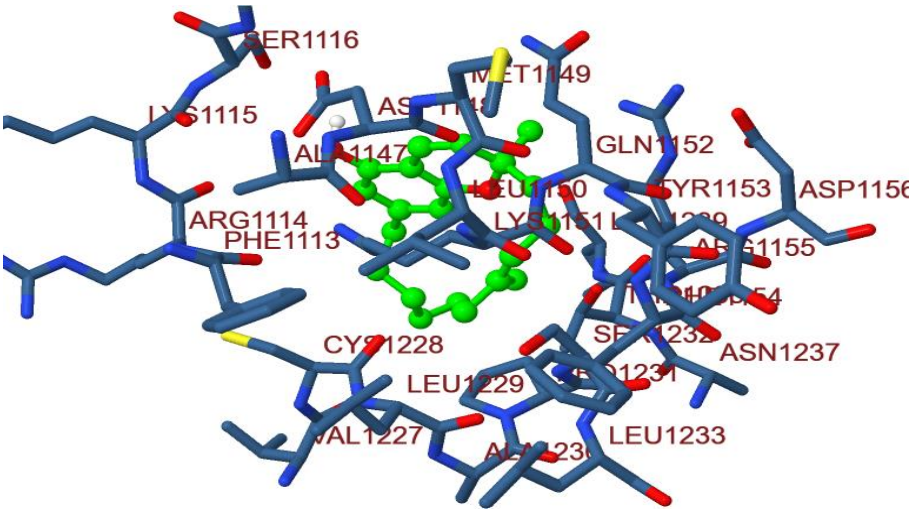

Fig. 5. Representation of the interaction of CBC molecule with proteins.

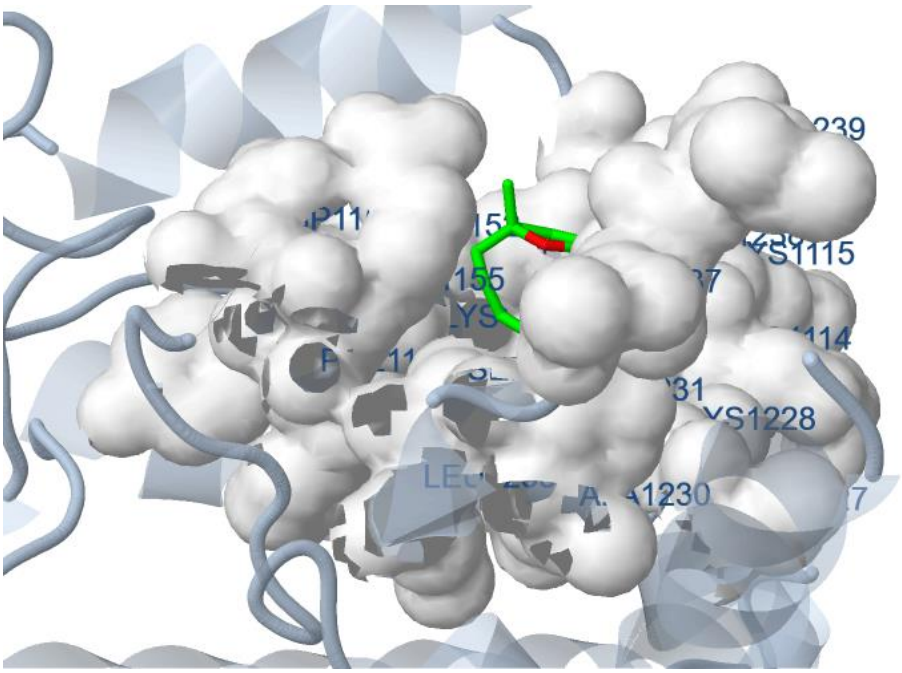

Fig. 6. Interaction of CBC molecule with DLC1.

In the docking study, the CBC molecule has the highest biological activity against the Crystal structure of the Liver Cancer 1 (DLC1) proteins by the numerical value of the Est Free Energy of Binding parameter. The major reason for this is that the proteins that make up the Crystal structure of the Liver Cancer 1 (DLC1) have good interaction around the CBC molecule. This increases biological activity **[51]**.

4. CONCLUSIONS

The studied molecules were calculated on different basis sets and their chemical activities were compared with the obtained parameters. ^{13}C and ^{1}H NMR and UV-vis spectrum of the molecules were obtained. Finally, the studied molecules compared their biological activities against the Crystal structure of the Liver Cancer 1 (DLC1). Interactions affecting the biological activity of the CBC molecule were investigated. Gaussian and docking calculations showed that the CBC molecule has the highest biological and chemical activity.

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Compliance with ethical standards

Conflict of interest: The author declares that there is no conflict of interest.

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تحقیق در ارتباط با مولکول های استخراج شده از ماری جوانا: مطالعه محاسباتی بررسی، اسپکترالی، ساختاری و داکینگ

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چکیده

مولکول‌های شیمیایی بسیاری وجود دارد که نام آنها Cannabigerol (CBG) ، کانابیدول (CBD)، کانابیسرومن (CBC)، تتراهیدروکانابویارین (THCV) ، اسید کانابژووویناربن (CBGV) و اسید کانابیدیولیک (CBDA) حاصل از ماری جوانا است. از روش‌های نظری برای مقایسه فعالیت‌های شیمیایی و بیولوژیکی شش مولکول اصلی استفاده شد. فعالیت‌های شیمیایی مولکول‌ها با استفاده از بسیاری از پارامترهای به دست آمده توسط برنامه گوسین مقایسه شدند. فعالیت مولکول‌ها با استفاده از تیوری تابع دانسیته (DFT) مورد بررسی قرار گرفته است. سپس، طیف ^{13}C NMR و ^{1}H NMR و UV-vis به دست آمد. طیف UV-Vis از این شش مولکول با استفاده از برنامه نرم افزاری Gaussain بر اساس روش محاسباتی HF / 6-31 ++ g گرم در حلال‌های مختلف که نام آنها گاز (ε = 1)، کلروفرم (ε = 4.711)، متانول است (ε = 32.613)، دی متیل سولفوکسید (ε = 46.826)، آب (ε = 78.355) و مخلوط ان متیل فرمامید(ε = 181.56) فازمحاسبه گردید. مشتقات کانابینوئیدها یک داروی بسیار مهم در جهان دارویی و در نتیجه، در داکینگ مولکولی هستند. این مولکول‌ها به دلیل فعالیت‌های بیولوژیکی خود در برابر ساختار کریستالی از حذف شده در سرطان کبد ۱ (DLC1) که شناسه آن KUQ۳ است، مورد مطالعه قرار گرفته‌اند. پارامترهای به دست آمده از داکینگ در مولکول‌ها مقایسه شدند.

کلید واژه‌ها: ماری جوانا، داکینگ مولکولی، طیف NMR، طیف UV-vis، DFT

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