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Quantum chemistry computations on chlorpyrifos pesticide based on Density Functional Theory

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Abstract

In this study, quantum chemistry computations based on Density Functional Theory (DFT) were performed using the B3LYP method and the basis set 31-6G(d,p) for examining the effect of organophosphate pesticides on Serine amino acid via hydrogen bonds in water. The interaction between 6 chlorpyrifos compounds and their derivatives led to the formation of 6 different complexes, and the stability energies of these systems were measured. The dipole moment values are close and approximately from 3.6 eV to 4.7 eV. The enthalpy and Gibbs free values are positive, indicating the endothermic and nonspontaneous nature of the formation process of these complexes. The band gaps, calculated from the energy difference of HOMO and LUMO orbitals, are close and about 5.1 eV. Given the close band gap of Serine amino acid, the formation of strong hydrogen bonds in all the complexes is likely. The quantum-mechanical descriptors of chlorpyrifos complexes were computed, examined, and used for determining the best complexes. The length and angles of the compound bonds before and after the formation of the complexes were computed and compared, and the changes in the angles and the general shape of the structures were studied individually. In the QTAIM data, the S1...H-O bonds in all the complexes and the intra-molecular hydrogen bond in the O...H-O Serine amino acid had an electrostatic nature. The C-H, N-H, P-O, and C-N bonds were of the covalent type.

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Key words: Quantum chemistry computations, organophosphate, pesticide, Density Functional Theory, hydrogen bond, chlorpyrifos.

1- Introduction

Pesticides are chemical compounds used against pests in agriculture and vectors of human and animal diseases in public health. Chlorpyrifos is an organophosphate compound that has been widely utilized to repel agricultural pests. Chlorpyrifos was introduced by Dow Chemical Company in the United States in 1965. The toxicity of chlorpyrifos has been determined to be 430 mg/kg, and continued exposure to this chemical is not recommended. The mechanism of action of organophosphates is usually similar: they cause inflammation and intense and uncontrollable stimulation in the neuro-muscular system by blocking the cholinesterase enzyme in the body [1]. Organophosphate is a general name for the esters of phosphoric acid. These toxins have the following general formula: 1. Central phosphorous atom connected to an oxygen atom via 2 bonds 2. Two lipophilic groups such as alcohols 3. A leaving group such as halogens. In addition, some organophosphates have oxygen-phosphorous bonds which are not usually found in the formulas of conventional pesticides. This bond causes higher stability in the compound and significantly increases its toxicity. The cholinesterase enzyme releases a substance named acetylcholine at the synapse via hydrolysis. Atropine sulfate is used as an antidote for chlorpyrifos and diazinon [2]. Serine (Ser) is an amino acid used in the structure of proteins and belongs to the group of amino acids that have alcohol and -OH groups. Serine protease is a group of enzymes that decompose proteins at the location of the serine amino acid [3].

Computational methods have attracted attention in recent years due to the high cost of research projects (including experienced personnel, laboratory devices, chemicals, and duration). The information provided by computational chemistry is highly valid and accurate. In computational chemistry, the required data are input to some software by an operator using a computer, and the output data are presented by the computer after computations. These data form the basis for

analysis by chemists and aids in near-certain interpretations of experimental reactions [4].

The Density Functional Theory is based on a theorem proven by Hohenberg and Cohen. Based on this theorem, the basic properties of a theorem, including its energy, are expressed as functions of electron probability density [5]. No effort is made in the DFT method to solve the Schrödinger equation and obtaining the electron wave function. Energy computations are facilitated by knowing the electron density or knowing how to determine it without finding the electron wave function [6, 7]. Walter Cohen made a great effort in introducing the Density Functional Theory based on which John Poppell introduced the Gaussian software for computations in chemistry. In the present research, quantum chemistry computations have been investigated using the Gaussian software for determining the effect of chlorpyrifos organophosphate toxins and their derivatives on the serine enzyme [8].

2- Computational methods

All the quantum computations performed in the present work, which will be mentioned in the structural analyses, have been carried out using DFT.

For this purpose, the structure of the tautomers and the conformations of different compounds were designed using the GaussView software [6], and then, the most optimal and stable molecule tautomer was determined using the Gaussian software [7]. In this project, the DFT computations were performed using the B3LYP method and the standard basis set 6-31G(d,p) for the effect of chlorpyrifos toxins and their derivatives (Ch 1-Ch 6) on serine amino acid via hydrogen bonds in water as a solvent. The symbol B3 represents the use of the three-parameter electron exchange function by Beck [9], and LYP denotes the use of electron correlation function by Lee, Young, and Par [10].

3- Results and discussion

The compounds studied in this project are the various derivatives of chlorpyrifos toxin (Ch1-Ch6) and their complexes with serine amino

acid (Ch-ser1 - Ch-ser6). The structures of chlorpyrifos toxin derivatives that were studied are displayed in Fig. 1.

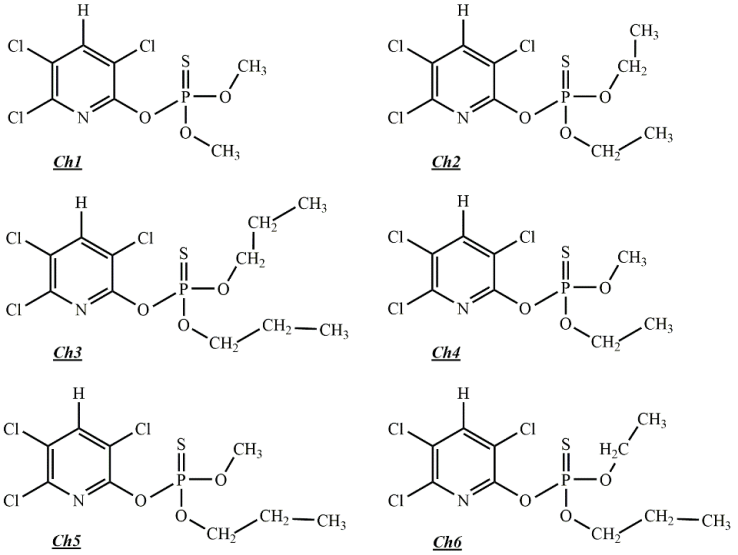


Figure 1. Structure of the derivatives of chlorpyrifos toxins

4- Dipole moment and stability energies:

The dipole moments of chlorpyrifos derivatives were measured in water solvent using the b3ly/6-31G(d). The values obtained are from 3.6 debye to 4.3 debye. The dipole moment of the serine enzyme is 4.7 debye. The dipole moments of the compounds and the stability energies of chlorpyrifos complexes are shown in order in Table 1.

(μ): Ch5 > Ch3 > Ch6 > Ch2 > Ch4 > Ch1

(μ): Ch-ser2 > Ch-ser6 > Ch-ser5 > Ch-ser3 > Ch-ser1 > Ch-ser4

(ΔE): Ch-ser1 > Ch-ser5 > Ch-ser4 > Ch-ser3 > Ch-ser2 > Ch-ser6

The results show that the polarities of Complex No. 3 and 5 are larger than those of the rest. The dipole moments of chlorpyrifos derivatives and its complexes with serine amino acid indicate that the dipole moments are close. The dipole moment of Complex No. 4 has had the largest drop compared to its individual derivative. In chlorpyrifos

complexes, the highest stability energy values correspond to Complex No. 1 and 5, and the lowest correspond to Complex No. 2 and 6.

Thermodynamic data:

According to the computational results, ΔS, ΔH, and ΔG values of chlorpyrifos complexes follow a specific trend. The ΔG values fall in the range of 9.11 - 14.16 kcal/mol The ΔH values fall in the range 1.1 - 16.04 kcal/mol, and the ΔS values fall in the range 0.0 - 35.027 kcal/mol (Table 1). Analysis results of the thermodynamic data indicate the endothermic and non-spontaneous nature of the formation processes of all the complexes.

(ΔS): Ch-ser1 > Ch-ser5 > Ch-ser4 > Ch-ser3 > Ch-ser6 > Ch-ser2

NBO and band gap (EP) analysis:

The band gap between HOMO and LUMO is representative of electron conduction. According to Table 1, the band gaps of chlorpyrifos derivatives are very close and about 5.3 eV. The band gap of the serine enzyme is 6.5 eV, as follows. The band gaps of chlorpyrifos complexes are very close, similar to those of chlorpyrifos derivatives, but they exhibit a reduction of about 0.2. The largest reduction in band gap was observed in chlorpyrifos Complex No. 4. Given the close band gaps of Serine amino acid, the formation of strong hydrogen bonds in all the complexes is likely.

:(band gap)Ch4 > Ch2 > Ch5 > Ch3 > Ch6 = Ch1

:(band gap)Ch-ser1 > Ch-ser3 > Ch-ser6 > Ch-ser2 > Ch-ser5 > Ch-ser4

Table 1. Computed parameters Eg, ΔS, ΔH, ΔG, ΔE, and μ and the band gaps of chlorpyrifos derivatives and its complexes with serine

ITEM		μ (debye)	ΔE (kcal/mol)	ΔG (kcal/mol)	ΔH (kcal/mol)	ΔS (kcal/k)	Eg (Hartree)	Band Gaps (eV)
ser		4.6666					-0/2390	-6.5026
Ch 1	m-m	3.6119					-0.1944	-5.2906
Ch 2	e-e	3.9045					-0.1946	-5.2957
Ch 3	p-p	4.3453					-0.1945	-5.2916
Ch 4	m-e	3.8862					-0.1949	-5.3031
Ch 5	m-p	4.3673					-0.1945	-5.2930
Ch 6	e-p	3.9344					-0.1944	-5.2911
Ch-ser1	m-m	3.6111	-0.9625	11.6025	1.1646	-0.03505	-0.1874	-5.0982

Ch-ser 2	e-e	4.7896	1.062	9.1417	1.0360	-0.02722	-0.1872	-5.0946
Ch-ser 3	p-p	3.817	-1.22	10.3023	1.0530	-0.03104	-0.1873	-5.0965
Ch-ser 4	m-e	3.3512	-1.068	10.7560	1.1070	-0.03238	-0.1865	-5.0756
Ch-ser 5	m-p	3.8858	-1.14	10.8181	1.0630	-0.03274	-0.1870	-5.0887
Ch-ser 6	e-p	3.9889	-1.085	9.5192	1.0956	-0.03104	-0.1873	-5.0963

5- Quantum mechanical descriptors:

The quantum-mechanical descriptors of chlorpyrifos complexes (ionization energy, electron affinity, electronegativity, hardness, ionization potential, and electrophilicity) were computed, examined, and used for determining the best complexes. According to the results obtained from the ionization energy computations in water solvent using the b3ly/6-31G(d), the ionization energy values (I) of chlorpyrifos derivatives are very close and about 6.9 eV. On the other hand, the ionization energy values for chlorpyrifos complexes are about 0.2 eV lower than that for chlorpyrifos derivatives. In addition, electron affinity data (A) show about 1.6 eV for chlorpyrifos derivatives and the same for chlorpyrifos complexes. Chemical potential (μ) values for chlorpyrifos derivatives are very close and approximately -4.3 eV. The chemical potential of serine enzyme is -3.4 eV. Furthermore, the chemical potential values of chlorpyrifos complexes are very close and about -4.18 eV, almost 0.12 eV lower than those for chlorpyrifos derivatives. The electronegativity values (χ) calculated for chlorpyrifos derivatives are about 4.3 eV and those for chlorpyrifos complexes are approximately 4.18 eV. The hardness values (η) (half of the difference between ionization energy and electron affinity) for chlorpyrifos derivatives are about 2.65 eV, and those for chlorpyrifos complexes have been determined to be approximately 2.55 eV. The electrophilicity values calculated for chlorpyrifos derivatives are considerably close and approximately equal to 3.46 eV, and those for chlorpyrifos complexes are in the range of 3.42 eV to 3.47 eV. The results are displayed in Table 2. Generally, chlorpyrifos Complex No. 4 was found to have the best

conditions in the assessment of quantum mechanical descriptor data. The trends in the quantum mechanical descriptors are as follows:

(I): Ch-ser4 > Ch-ser2 > Ch-ser1 > Ch-ser3=Ch-ser5 > Ch-ser6

(A): Ch-ser4 > Ch-ser2 > Ch-ser5 > Ch-ser3 = Ch-ser6 > Ch-ser1

(μ): Ch-ser1 > Ch-ser3 = Ch-ser6 > Ch-ser5 > Ch-ser2 > Ch-ser4

(χ): Ch-ser4 > Ch-ser2 > Ch-ser5 > Ch-ser3 = Ch-ser6 > Ch-ser1

(η): Ch-ser1 >Ch-ser3 = Ch-ser6 > Ch-ser2 > Ch-ser5 > Ch-ser4

(ώ): Ch-ser4 > Ch-ser2 > Ch-ser5 > Ch-ser6 > Ch-ser3 > Ch-ser1

Table 2. Quantum mechanical descriptors of chlorpyrifos, chlorpyrifos-serine complex, and its derivatives

ITEM		*I (ev)*	*A (ev)*	*μ (ev)*	*X (ev)*	*η (ev)*	*ώ (ev)*
ser		6.6849	0.1823	-3.4336	3.4336	3.2513	**1.8131**
Ch 1	m-m	6.9263	1.6357	-4.2810	4.2810	26453	**3.4641**
Ch 2	e-e	6.9325	1.6368	-4.2847	4.2847	2.6478	**3.4666**
Ch 3	p-p	6.9249	1.6332	-4.2786	4.2784	2.6458	**3.4596**
Ch 4	m-e	6.9480	1.6450	-4.2965	4.2965	2.6515	**3.4810**
Ch 5	m-p	6.9314	1.6384	-4.2849	4.2849	2.6465	**3.4688**
Ch 6	e-p	6.9246	1.6335	-4.2791	4.2791	2.6455	**3.4606**
Ch-ser1	m-m	6.7238	1.6256	-4.1747	4.1747	2.5491	**3.4185**
Ch-ser2	e-e	6.7331	1.6384	-4.1858	4.1858	2.5474	**3.4390**
Ch-ser3	p-p	6.7256	1.6295	-4.1776	4.1776	2.5481	**3.4246**
Ch-ser4	m-e	6.7358	1.6602	-4.1980	4.1980	2.5378	**3/4721**
Ch-ser5	m-p	6.7256	1.6373	-4.1816	4.1816	2.5442	**3.4364**
Ch-ser6	e-p	6.7265	1.6303	-4.1784	4.1784	2.5481	**3.4259**

6- Bond length and angle calculations

The length and angles of the compound bonds before and after the formation of the complexes were computed and compared, and the changes in the angles and the general shape of the structures were

investigated individually. Using the b3ly/6-31G(d) method in an aqueous environment for chlorpyrifos complexes, 2 important electrostatic bonds, namely O5...H-O4 and S...H-O4, are observed. The schematics and numbering of the atoms in these complexes are shown in Fig. 2. The results relating to the lengths and angles of the bonds are displayed in Tables 3 and 4.

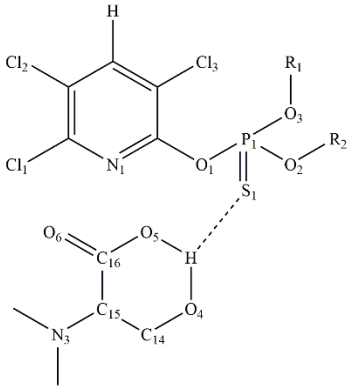


Table 3. Structural parameters of chlorpyrifos derivatives and serine amino acid.

Bond length (A°)	Ch 1	Ch 2	Ch 3	Ch 4	Ch 5	Ch 6	ser
O5…H-O4	3.61	2.97	2.20	2.19	2.20	2.19	
S…H-O4	2.45	2.97	2.89	2.89	2.83	2.93	
Bond angle (°)							
O5…H-O4	61	68	48	37	85	89	

S…H-O4	104	92	91	91	51	36	
O1-P1-S1	116.56		116.26	116.26	116.4	116.26	
O2-P1-S1	17.041	117.10	117.13	116.97	116.92	117.02	
O3-P1-S1			118.93	119.42	119.38	119.18	
C14-C15-C16							109.98
C14-O4-H							105.14
C14-C15-H							107.66

Table 4. Structural parameters of chlorpyrifos complexes and serine

Bond length (A˚)	Ch-ser 1	Ch-ser 2	Ch-ser 3	Ch-ser 4	Ch-ser 5	Ch-ser 6
S-H	2.49		2.89	2.89	2.82	2.93
Bond angle (˚)						
O1-P1-S1	115.94		116.02	116.12	115.86	116.01
O2-P1-S1	116.30	116.79	116.82	116.66	116.6	116.87
O3-P1-S1			119.34	119.62	119.61	119.42
C14-C15-C16	113.84	122.72	112.42	112.41	112.62	112.49
C14-O4-H	107.61	107.09				

C14-C15-H	109.19	107.66	107.03	109.27

7- Atomic analysis in chlorpyrifos complexes using QTAIM

According to the results of Aim data, the bonds O6-O4, O6-H, O4-H, and s...H-O4 in Complex Ch-ser 1 have low ρ(r) values and positive Laplacian and H(r) values; therefore, they have an ionic and electrostatic nature. The rest of the bonds are of the covalent type. In Complex Ch-ser 2, O6…S, S…H-O4, Cl1…H-C14, Cl1…N3, and Cl1…O5 bonds, in Complex Ch-ser 3, O6…S, S…H-O4, C1l…H-C14, Cl1…N3, O6…H-O4, O4…H-C7, and Cl1…O5 bonds, in Complex Ch-ser 4, O4…S, S…H-O4, C1l…H-C14, Cl1…N3, and O6…H-O4 bonds, in Complex Ch-ser 5, O6…S, S…H-O4, Cl1…H-C14, and O6…H-O4 bonds, in Complex Ch-ser 6, O6…S, S…H-O4, Cl1…H-C14, Cl1…N3, O6…H-O4, and Cl1…O5 bonds have low ρ(r) values and positive Laplacian and H(r) values; hence, they are of an ionic and electrostatic nature. The rest of the bonds have a covalent nature. Generally, in the QTAIM data, the S1...H-O bonds in all the complexes had an electrostatic nature. Moreover, the intra-molecular hydrogen bond in the O6...H-O4 serine amino acid is of the electrostatic type. The C-H, N-H, P-O, and C-N bonds are covalent. The hydrogen bonds in chlorpyrifos-serine complexes are displayed in Fig. 3.

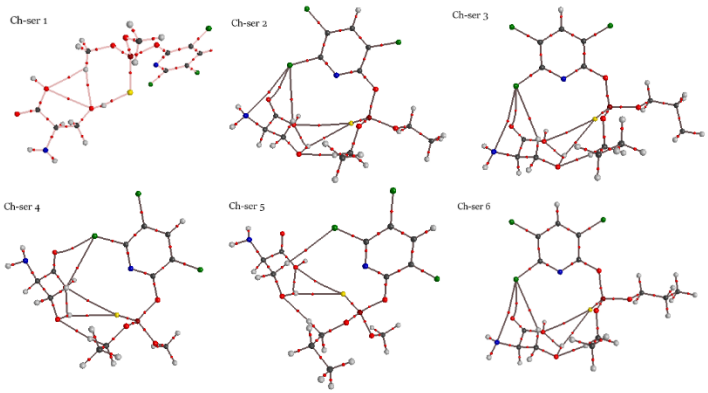


Figure 3. Hydrogen bonds in chlorpyrifos-serine complexes

8- Electron transfers

Analyzing the uv-vis peak and electron transfers shows that the maximum H-9→L transfer in serine amino acid has occurred at a wavelength of 106.75 nm. In the Ch 1 derivative of chlorpyrifos toxin, the highest percentage of transfer at the wavelength of 194.75 nm corresponds to H-3→L+1 and that at 199.63 nm occurs at H-1→L+2. In Ch 2, the highest percentage of transfer at the wavelength of 1194.73 nm corresponds to H-4→L and that at 200.23 nm corresponds to H-4→H. According to the electron transfer results in the following table, in Ch 3, the highest percentage of transfer at the wavelength of 194.73 nm corresponds to H-4→L and that at 200.31 nm belongs to H-1→L+2. Furthermore, in Ch 4, the highest percentage of transfer at the wavelength of 194.66 nm belongs to H-4→L and that at 199.89 nm corresponds to H-1→L+2. Analyzing the Ch 5 derivative showed that the highest percentage of transfer at the wavelength of 194.67 nm occurs at H-4→L and that at 199.93 nm occurs at H-2→L+1. Finally, in Ch 6, the highest percentage of transfer at the wavelength of 194.66 nm corresponds to H-4→L and that at 200.25 nm corresponds to H-1→L+2. Figs. 5-10 show the images of the uv-vis peak of chlorpyrifos derivatives.

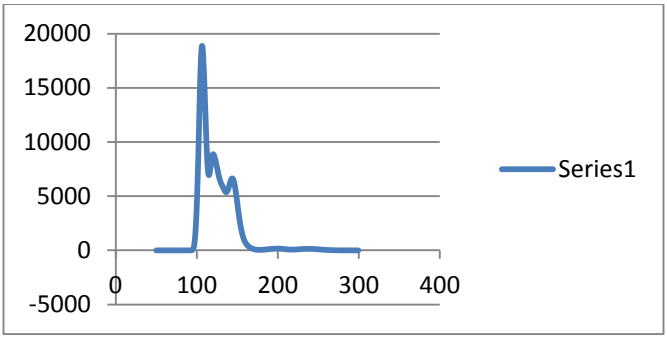
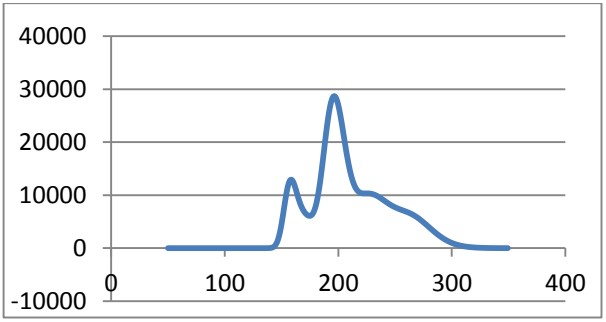


Figure 4. uv-vis peak of serine amino acid



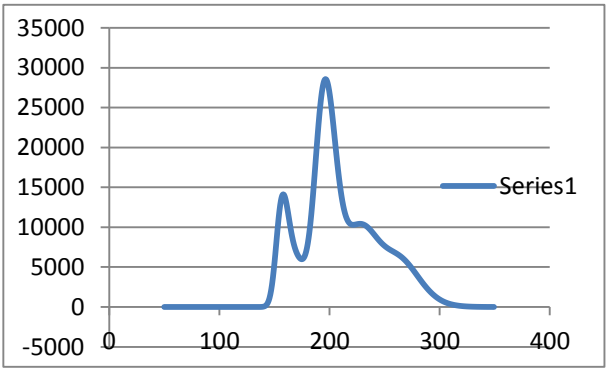
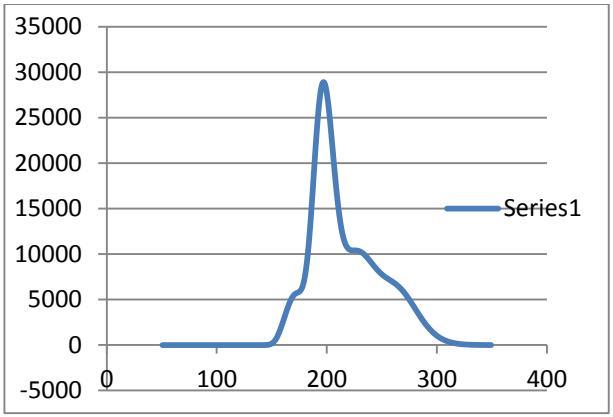


Figure 5. uv-vis peak of Ch 1 chlorpyrifos

Figure 6. uv-vis peak of Ch 2 chlorpyrifos



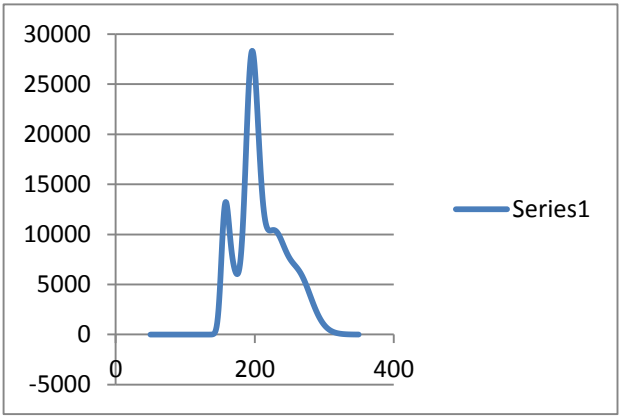
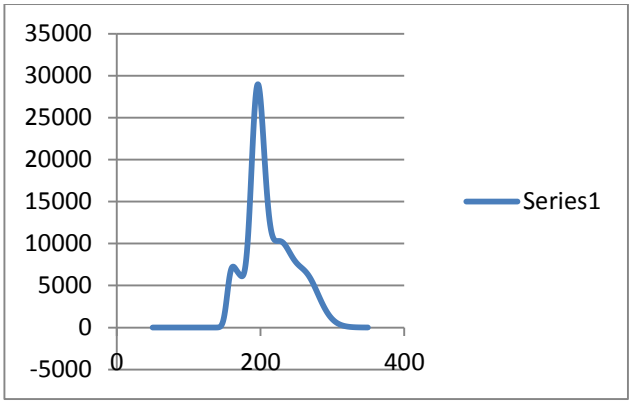


Figure 7. uv-vis peak of Ch 3 chlorpyrifos

Figure 8. uv-vis peak of Ch 4 chlorpyrifos



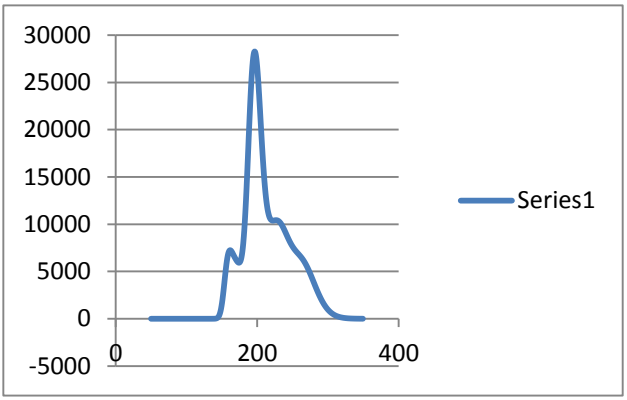
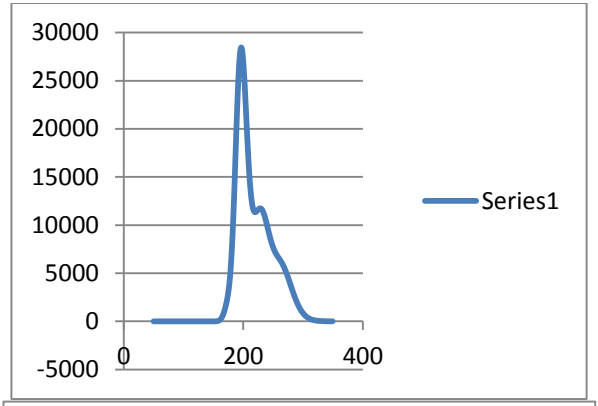


Figure 9. uv-vis peak of Ch 5 chlorpyrifos

Figure 10. uv-vis peak of Ch 6 chlorpyrifos

Analyzing the electron transfers of chlorpyrifos complexes with serine showed that in Ch-ser1, the highest percentage of transfer at the wavelength of 194.94 nm belongs to H-7→L and that at 201.48 nm corresponds to H-7→H. In addition, in Ch-ser2, the highest percentage of electron transfer at the wavelength of 194.54 nm corresponds to H-7→L and that at 200.23 nm belongs to H-7→H. In the ser3 complex, the highest percentage of transfer at the wavelength of 194.70 nm occurs at H-6→L and that at 200.49 nm occurs at H-2→L+2. According to the electron transfer results for Ch-ser4, the

highest percentage of transfer at the wavelength of 194.76 nm belongs to H-6→L+1 and that at 200.18 nm belongs to H-6→L. In Complex Ch-ser5, the highest percentage of transfer at the wavelength of 194.69 nm occurs at H-6→L+1 and that at 200.05 nm occurs at to H-2→L+2. Finally, in Ch-ser6, the highest percentage of transfer at the wavelength of 194.55 nm corresponds to H-6→L+1 and that at 200.43 nm corresponds to H-6→L. Figs. 11-16 display the images of the uv-vis peak of chlorpyrifos-serine complexes.



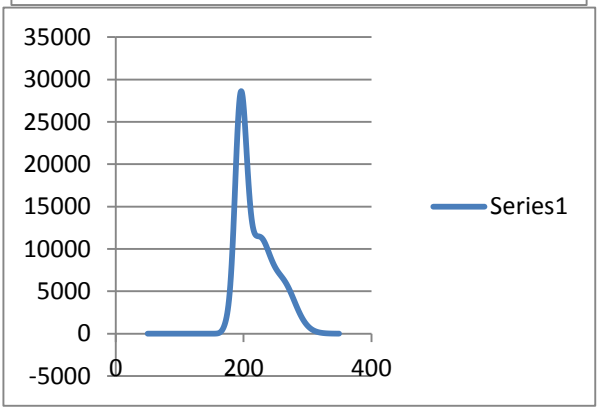
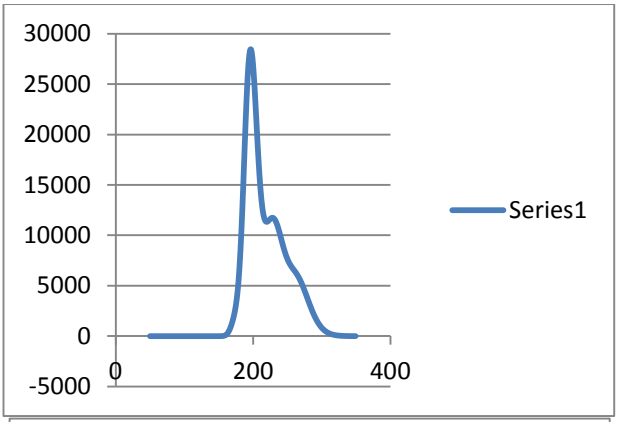


Figure 11. uv-vis peak of Ch-ser 1 chlorpyrifos-serine complex
Figure 12. uv-vis peak of Ch-ser 2 chlorpyrifos-serine complex



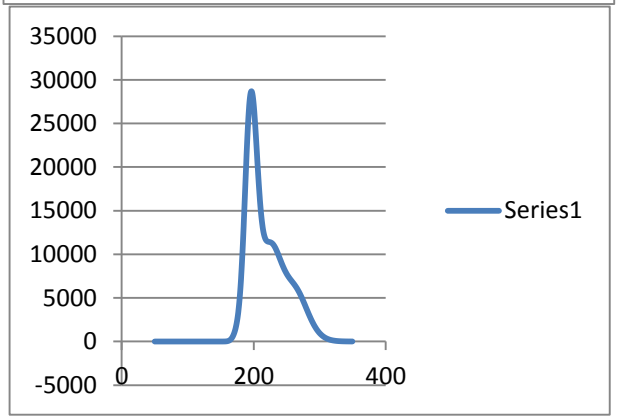


Figure 13. uv-vis peak of Ch-ser 3 chlorpyrifos-serine complex
Figure 14. uv-vis peak of Ch-ser 4 chlorpyrifos-serine complex

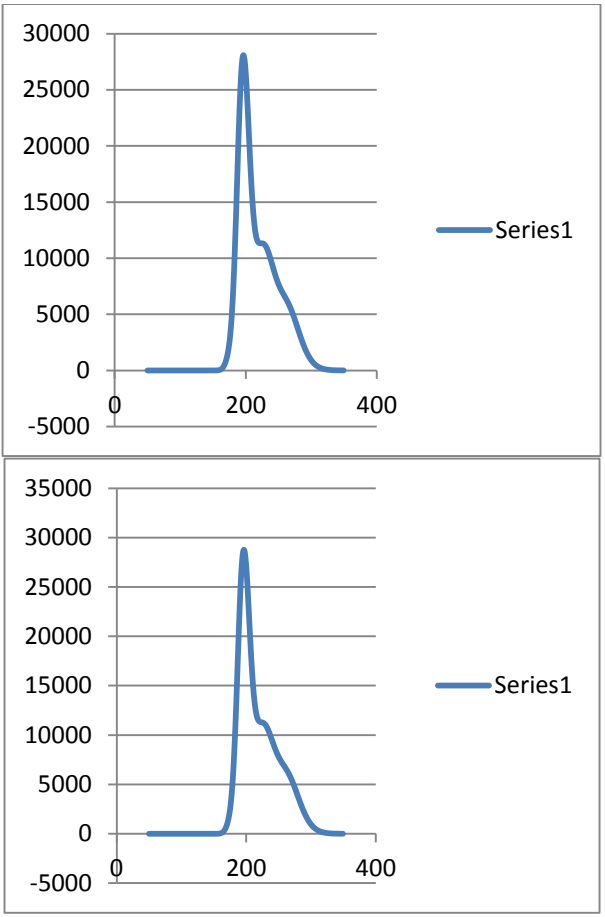
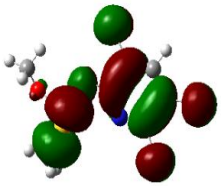
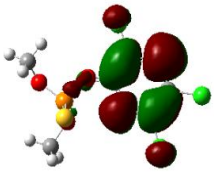
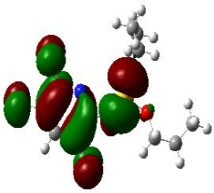
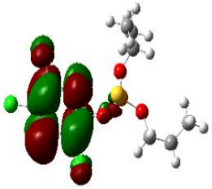


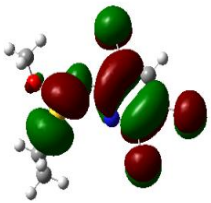
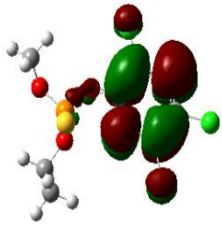
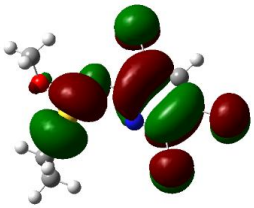
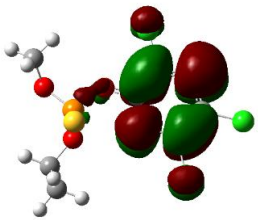
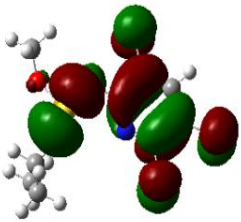
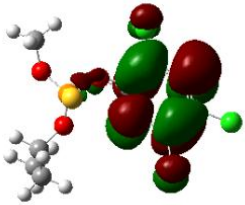
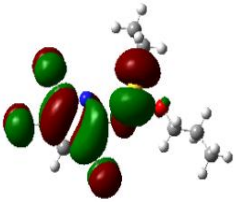
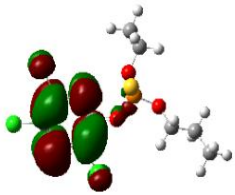
Figure 15. uv-vis peak of Ch-ser 5 chlorpyrifos-serine complex
Figure 16. uv-vis peak of Ch-ser 6 chlorpyrifos-serine complex

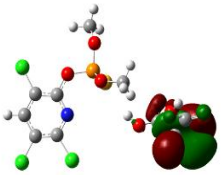
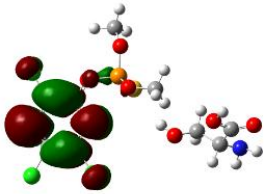
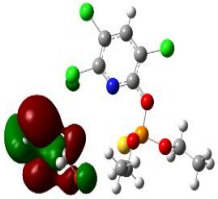
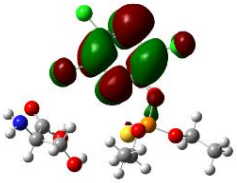
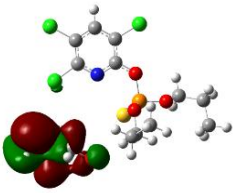
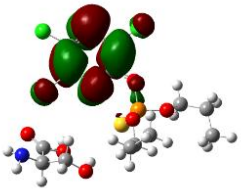
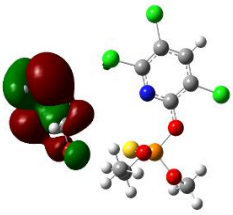
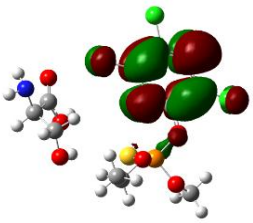
9- HOMO and LUMO forms

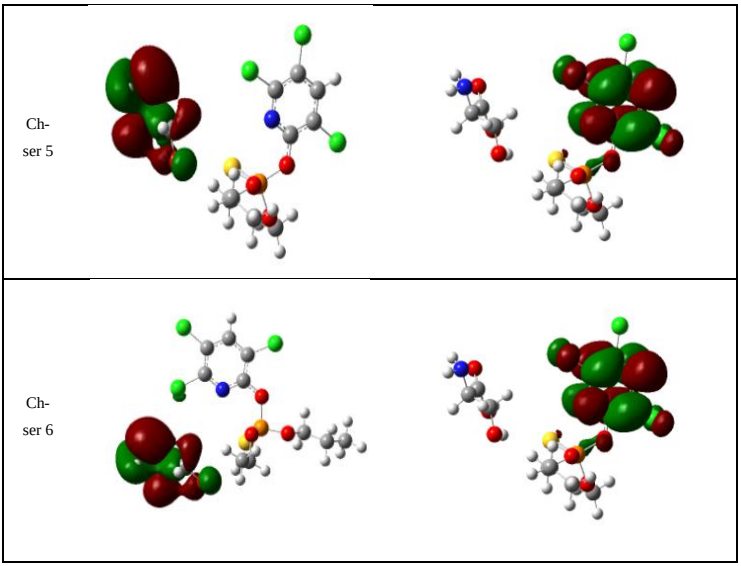
Negative-charge wave functions (red) and positive-charge waves (green) are concentrated in LUMO forms on the aromatic ring of chlorpyrifos and its derivatives. In HOMO forms, the waves are concentrated on the phosphate esters of these compounds in addition to the previous location. Moreover, in the complexes of chlorpyrifos with serine, these functions are concentrated in the aromatic ring in LUMO forms and on serine amino acid in HOMO forms (Table 5).

Table 5. HOMO and LUMO images in chlorpyrifos derivatives and chlorpyrifos-serine complexes

Item	HOMO forms	LUMO forms
Ch 1		
Ch 2		

Ch 3		
Ch 4		
Ch 5		
Ch 6		

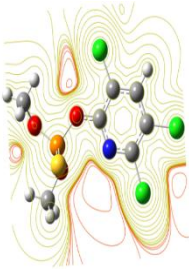
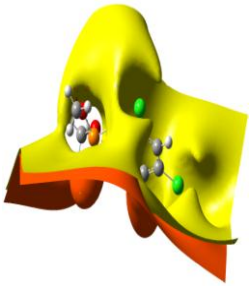
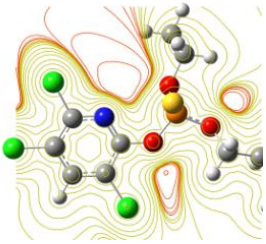
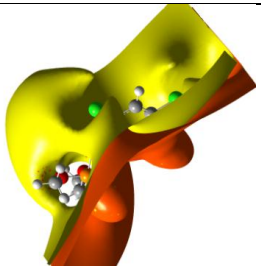
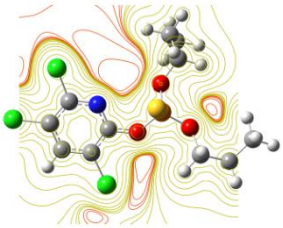
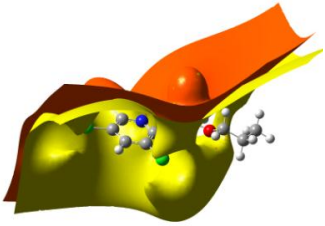
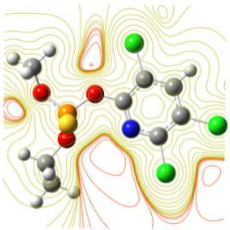
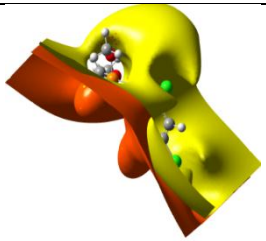
Ch-ser 1		
Ch-ser 2		
Ch-ser 3		
Ch-ser 4		

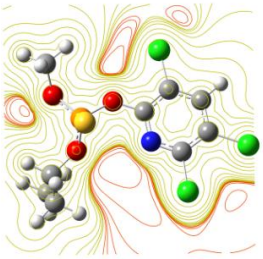
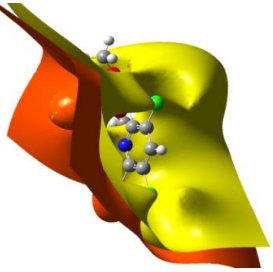
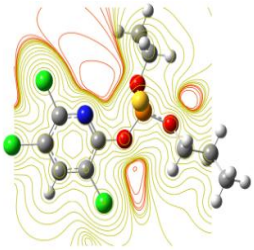
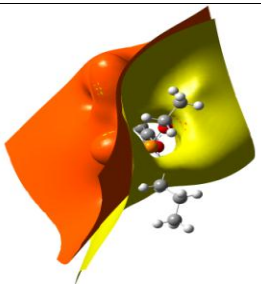
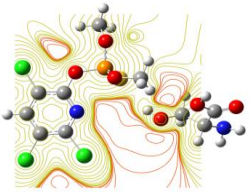
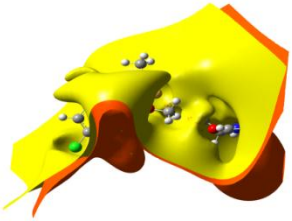
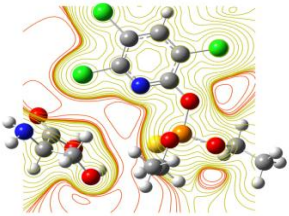
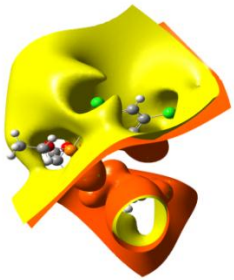


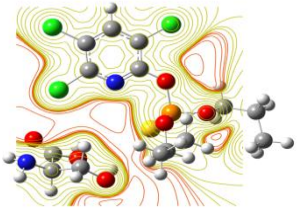
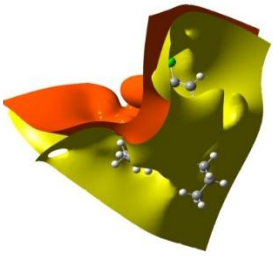
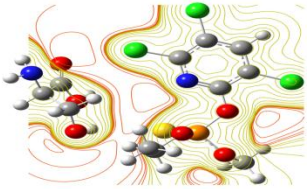
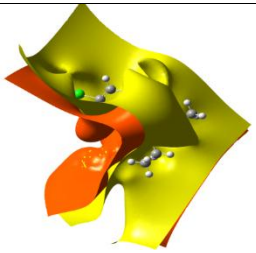
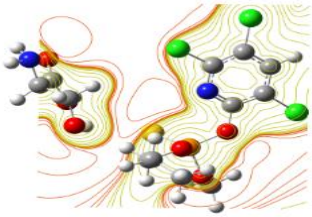
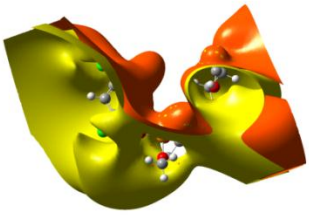
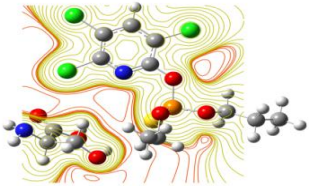
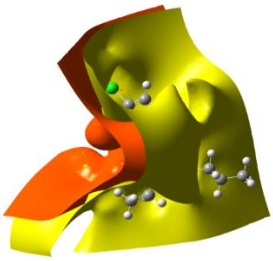
Surface electrostatic charge potential images and contour map

In the images of surface electrostatic charge potential, the negative charge density plane (red) is outside the molecule, and the positive charge density plane (green) encloses the molecule itself. In the contour shapes, negative charge lines (red) encompass the surroundings of the molecule, and the positive charge lines (green) encompass the inside of the molecule. Similar to dipole moment results, the density planes and lines in the contour maps indicate that chlorpyrifos and its derivatives are not symmetrical. In addition, the lack of symmetry in all complexes is visible in the images of chlorpyrifos complexes with serine amino acid. The dipole moment of Complexes No. 3 and 5 is lower than that of the individual compound. The same is true for Complex No. 3. The changes in the positive and negative charge lines relative to the individual compound support these points (Table 6).

Table 6. Images of surface electrostatic charge potential and contour map in chlorpyrifos derivatives and chlorpyrifos-serine complexes

Item	Contour	Surface
Ch 1		
Ch 2		
Ch 3		
Ch 4		

Ch 5		
Ch 6		
Ch-ser 1		
Ch-ser 2		

Ch-ser 3		
Ch-ser 4		
Ch-ser 5		
Ch-ser 6		

10- Conclusion

In this project, DFT computations were performed using the B3LYP method and with the standard basis set 6-31G(d,p) for the effect of chlorpyrifos toxins and their derivatives on serine amino acid, and the most stable chlorpyrifos complexes with serine amino acid were determined. The thermodynamic data were investigated. In addition, in the study of band gap (EG) and NBO, the energy gap between the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), which shows the electron conduction, was examined. The conduction of serine amino acid is 5.6 eV, and that of chlorpyrifos derivatives is about 3.5 eV. The interaction of these compounds has been proven via the bond length of HOMO and LUMO levels, electron transfers, and quantum mechanical descriptors. The bond between serine amino acid and all the chlorpyrifos derivatives has an electrostatic nature, and the intra-molecular interactions indicate the stability of these complexes. For future research in this field, it is suggested that experimental comparisons be made between the effect of organophosphorus toxins with oxygen functional group on the phosphorous atom and that of organophosphorus toxins with sulfur functional group on the phosphorous atom on serine amino acid.

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