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Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase

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Abstract. In this present work, we calculated two frontier orbital energies - singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) - of dehydrogenated tetrahydrocurcumin (THC) using density-functional theory (DFT) in gas phase. We used the energy difference of SOMO and LUMO to assess the stability of dehydrogenated THC after performing a hydrogen atom transfer toward reactive oxygen species (ROS). We began by optimizing dehydrogenated THC at six hydrogen abstraction sites. Two hydrogen abstraction sites are at O-H groups and four hydrogen abstraction sites are at C-H groups. Then, we compared the value of SOMO and LUMO energy difference in each site. Our calculations showed that dehydrogenated THC at O-H groups are more stable than dehydrogenated THC at C-H groups.

1. Introduction

Hydrophilic reactive oxygen species (ROS) is able to penetrate into phospholipid bilayer membrane and oxidizes the membrane [1,2] by abstracting a hydrogen atom. This abstraction process marks the beginning of oxidation chain called lipid peroxidation. Since cell membrane is the outermost part of a cell that protects its organelles, oxidation by ROS may lead to pores formation on the membrane [3] and eventually to a cell degradation.

In order to delay or prevent this oxidation process, one can introduce a molecule that performs antioxidant activity which is the ability to transfer hydrogen atom toward ROS to break an oxidation chain[4,5]. An electron paramagnetic resonance study has shown that tetrahydrocurcumin (THC) molecule possesses slightly better antioxidant activity than its former, curcumin molecule [6]. THC also performs an inhibitory effect on membrane lipid peroxidation, experimentally [7].



Since THC can possibly perform its antioxidant activity by transferring a hydrogen atom, the aim of our research is to calculate the energy difference between frontier orbitals of dehydrogenated THC (dehydrogenated THC is THC that has transferred its hydrogen atom) in gas phase, theoretically. We use density functional theory (DFT) to evaluate two frontier orbital energies of dehydrogenated THC, which are singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) energies. The energy difference between SOMO and LUMO will help us to assess the most possible site in THC that is responsible for antioxidant activity of the molecule, which is the dehydrogenated THC with the highest energy difference in its frontier orbitals.

2. Computational details

THC performed its antioxidant activity by transferring one of its hydrogen atom. In this research, we chose six representative X-H sites that were capable of transferring a hydrogen atom (see figure 1). To calculate the energy difference between frontier orbitals of dehydrogenated THC, we conducted our research in the following steps. First step, we built a dehydrogenated THC by abstracting a hydrogen atom from each X-H sites. Each THC with one less hydrogen atom was called dehydrogenated THC 1, dehydrogenated THC 2, etc. Dehydrogenated THC 2 and dehydrogenated THC 5 were produced as a result of a hydrogen atom abstraction from an O-H groups. While other dehydrogenated THCs were produced as a result of a hydrogen atom abstraction from a C-H groups. Although experimental result has suggested that O-H groups played an important role in hydrogen atom transfer [8], we propose to consider the presence of C-H bonds as well in this research. Our molecule of interest has a symmetrical shape. This means if we draw a line at the center of the molecule, the line will divide the molecule into two equal parts. Thus, among the six representative sites chosen, site 1 was in the same position as site 6, site 2 was in the same position as site 5 and site 3 was in the same position as site 4.

Second step, after building six dehydrogenated THCs, we performed full geometry optimisation using UM05-2X functional and 6-31++G(d,p) basis set. M05-2X functional was chosen because it has been recommended for thermochemistry calculations by its developer [9]. We used an unrestricted calculation (symbolled by letter U) since dehydrogenated THC has lost one electron during the hydrogen abstraction so we treated it as an open shell calculation. The geometry optimisation was calculated using DFT applied in Gaussian 09 suite program [10] in gas phase at 298.15 K. At this step, our calculation produced the frontier orbital energies.

Our last step is to find the energy difference between two frontier orbital energies, which are SOMO and LUMO energies at each dehydrogenated THC.

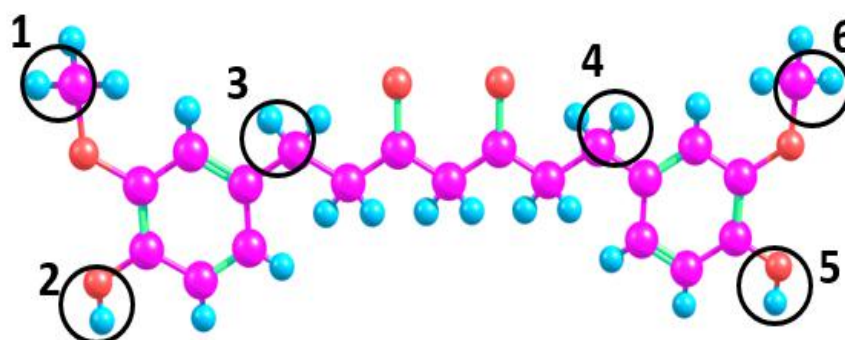


Figure 1. Six representative X-H sites (Blue, pink and red represent H, C and O atoms sequentially). Site 1, 3, 4 and 6 are C-H groups while site 2 and 5 are O-H groups.

3. Results and discussion

Figure 2 showed how model of dehydrogenated THC 2 was built. We built other dehydrogenated THCs with the same procedure. Since dehydrogenated THC 2 has lost one of its electron and proton (recall that we have abstracted a hydrogen atom from THC), we performed geometry optimisation by setting the spin multiplicity into 2 to make sure that the dehydrogenated THC 2 as well as other dehydrogenated THCs were at doublet state.

Figure 3 illustrated the SOMO and LUMO profiles of dehydrogenated THC 2. The SOMO profile was located at the hydrogen transferring sites. The profile informed us the location with the possibility of transferring electrons. After abstracting one hydrogen atom which contains of one proton and one electron, THC molecule was left with only one electron in its last occupied orbital. Thus this orbital was called SOMO. Differ from SOMO profile, LUMO profile was located at the center of the molecule. This profile informed us about the area possible of receiving electrons. Generally, SOMO profiles of all six dehydrogenated THCs were located at transferring sites while their LUMO profiles were located at the center of the molecule.

Our DFT calculation produced many orbital energies of dehydrogenated THCs. We chose two frontier orbitals, SOMO and LUMO, to assess the stability of dehydrogenated THCs[11]. Low energy difference between SOMO and LUMO meant an electron can easily be excited from its ground state, thus a molecule was less stable. While high energy difference between SOMO and LUMO meant an electron can be more stable in its ground state, thus a molecule was more stable.

We calculated energy difference between SOMO and LUMO, which we called it as relative SOMO-LUMO energies, of all six dehydrogenated THCs and tabulated the value in the graph at figure 4. The value of relative SOMO-LUMO energies at dehydrogenated THC 1 (site 1) and dehydrogenated THC 6 (site 6) was almost similar. Their difference was less than 0.2 eV. However, the value are very similar at dehydrogenated THC 2 (site 2) and dehydrogenated THC 5 (site 5), as well as at dehydrogenated THC 3 (site 3) and dehydrogenated THC 6 (site 6). The value of relative SOMO-LUMO energies from the highest to the lowest is dehydrogenated THC 2 = dehydrogenated THC 5 > dehydrogenated THC 1 > dehydrogenated THC 6 > dehydrogenated THC 3 = dehydrogenated THC 4. These results implied that dehydrogenated THC 2 was as stable as dehydrogenated THC 5. Both dehydrogenated THCs were the most stable among all six dehydrogenated THCs. Dehydrogenated THC 1 and 6 were less stable while dehydrogenated THC 3 and 4 had the lowest stability. Based on THC's similarity, site at the same position, possessed similar characters.

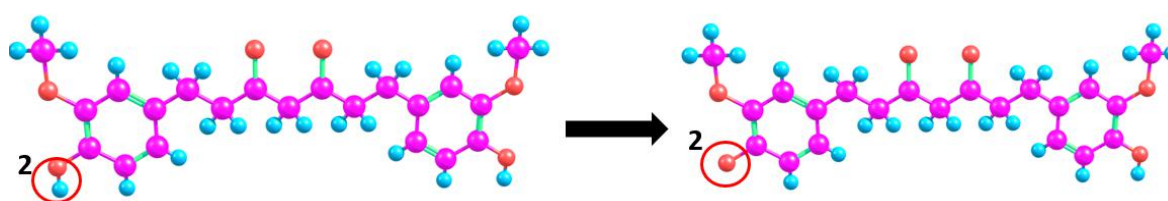


Figure 2. Model of dehydrogenated THC 2

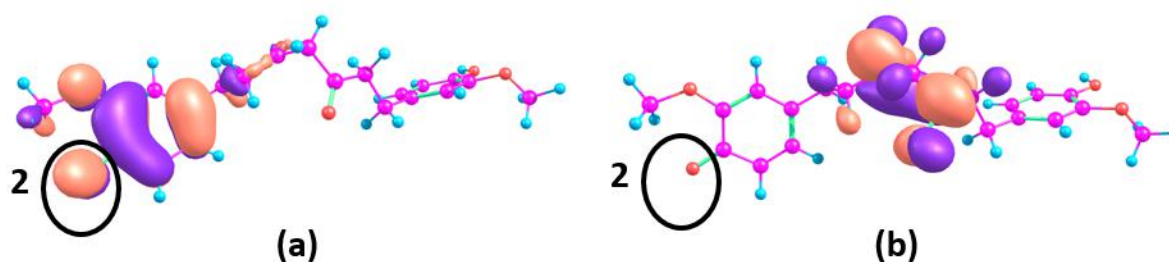
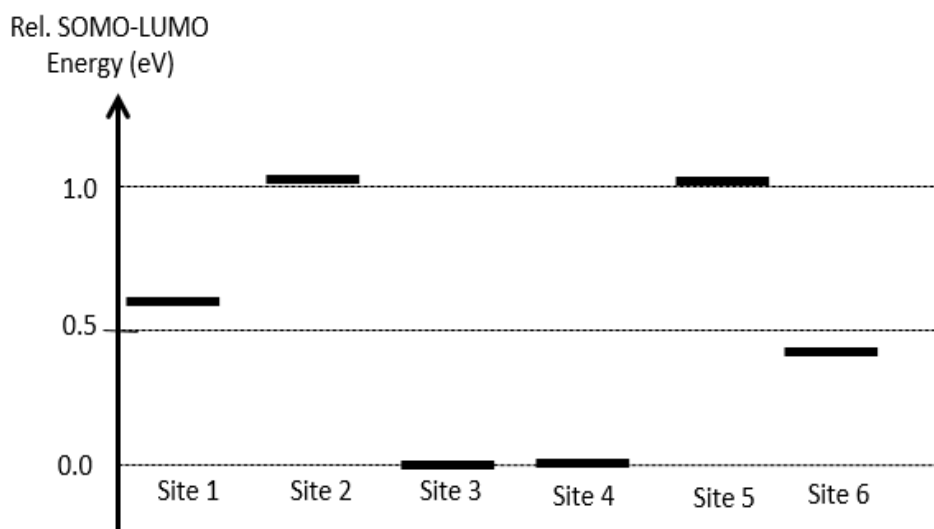


Figure 3. (a) SOMO and (b) LUMO profiles of dehydrogenated THC 2.**Figure 4.** Relative energy diagram of dehydrogenated THC. X axes of the graph is the type of dehydrogenated THC while Y axes of the graph shows the energy difference between SOMO and LUMO.

Finally, in order to assess the most possible site in THC that was responsible for antioxidant activity of the molecule, we concluded the following information. To perform its antioxidant activity, THC should be able to transfer one of its hydrogen atom toward ROS. If the hydrogen atom transferred was originally from an O-H groups, after the transfer process dehydrogenated THC formed would be the most stable. This occurred in the case of dehydrogenated THC 2 and 5. However, if the hydrogen atom transferred was originally from a C-H groups, after the transfer process dehydrogenated THC formed would be less stable. This occurred in the case of dehydrogenated THC 1, 3, 4 and 6. After performing its antioxidant activity, THC should be able to maintain its stability. Thus the most possible site that is responsible for this activity is O-H groups of THC molecule.

4. Conclusion

We have performed DFT calculation to calculate frontier orbitals of six dehydrogenated THCs. We investigated two frontier orbitals of dehydrogenated THCs, SOMO and LUMO, to assess the stability of the molecules. We suggested that in performing its antioxidant activity, hydrogen atom transfer should occur from O-H groups of THC, since the dehydrogenated THC formed was the most stable. Thus, O-H groups were responsible for the antioxidant activity of THC. This conclusion was supported by our results in two previous researches [12-13].

Acknowledgement

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Anni Nuril Hidayati, Abdul Waris, Dwi Irwanto and Asril Pramutadi

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HTTR 30MWth Reactor with Homogenous (Th,U)O₂ Fuel

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Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase

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Abstract. In this present work, we calculated two frontier orbital energies - singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) - of dehydrogenated tetrahydrocurcumin (THC) using density-functional theory (DFT) in gas phase. We used the energy difference of SOMO and LUMO to assess the stability of dehydrogenated THC after performing a hydrogen atom transfer toward reactive oxygen species (ROS). We began by optimizing dehydrogenated THC at six hydrogen abstraction sites. Two hydrogen abstraction sites are at O-H groups and four hydrogen abstraction sites are at C-H groups. Then, we compared the value of SOMO and LUMO energy difference in each site. Our calculations showed that dehydrogenated THC at O-H groups are more stable than dehydrogenated THC at C-H groups.

1. Introduction

Hydrophilic reactive oxygen species (ROS) is able to penetrate into phospholipid bilayer membrane and oxidizes the membrane [1,2] by abstracting a hydrogen atom. This abstraction process marks the beginning of oxidation chain called lipid peroxidation. Since cell membrane is the outermost part of a cell that protects its organelles, oxidation by ROS may lead to pores formation on the membrane [3] and eventually to a cell degradation.

In order to delay or prevent this oxidation process, one can introduce a molecule that performs antioxidant activity which is the ability to transfer hydrogen atom toward ROS to break an oxidation chain[4,5]. An electron paramagnetic resonance study has shown that tetrahydrocurcumin (THC) molecule possesses slightly better antioxidant activity than its former, curcumin molecule [6]. THC also performs an inhibitory effect on membrane lipid peroxidation, experimentally [7].



Since THC can possibly perform its antioxidant activity by transferring a hydrogen atom, the aim of our research is to calculate the energy difference between frontier orbitals of dehydrogenated THC (dehydrogenated THC is THC that has transferred its hydrogen atom) in gas phase, theoretically. We use density functional theory (DFT) to evaluate two frontier orbital energies of dehydrogenated THC, which are singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO) energies. The energy difference between SOMO and LUMO will help us to assess the most possible site in THC that is responsible for antioxidant activity of the molecule, which is the dehydrogenated THC with the highest energy difference in its frontier orbitals.

2. Computational details

THC performed its antioxidant activity by transferring one of its hydrogen atom. In this research, we chose six representative X-H sites that were capable of transferring a hydrogen atom (see figure 1). To calculate the energy difference between frontier orbitals of dehydrogenated THC, we conducted our research in the following steps. First step, we built a dehydrogenated THC by abstracting a hydrogen atom from each X-H sites. Each THC with one less hydrogen atom was called dehydrogenated THC 1, dehydrogenated THC 2, etc. Dehydrogenated THC 2 and dehydrogenated THC 5 were produced as a result of a hydrogen atom abstraction from an O-H groups. While other dehydrogenated THCs were produced as a result of a hydrogen atom abstraction from a C-H groups. Although experimental result has suggested that O-H groups played an important role in hydrogen atom transfer [8], we propose to consider the presence of C-H bonds as well in this research. Our molecule of interest has a symmetrical shape. This means if we draw a line at the center of the molecule, the line will divide the molecule into two equal parts. Thus, among the six representative sites chosen, site 1 was in the same position as site 6, site 2 was in the same position as site 5 and site 3 was in the same position as site 4.

Second step, after building six dehydrogenated THCs, we performed full geometry optimisation using UM05-2X functional and 6-31++G(d,p) basis set. M05-2X functional was chosen because it has been recommended for thermochemistry calculations by its developer [9]. We used an unrestricted calculation (symbolled by letter U) since dehydrogenated THC has lost one electron during the hydrogen abstraction so we treated it as an open shell calculation. The geometry optimisation was calculated using DFT applied in Gaussian 09 suite program [10] in gas phase at 298.15 K. At this step, our calculation produced the frontier orbital energies.

Our last step is to find the energy difference between two frontier orbital energies, which are SOMO and LUMO energies at each dehydrogenated THC.

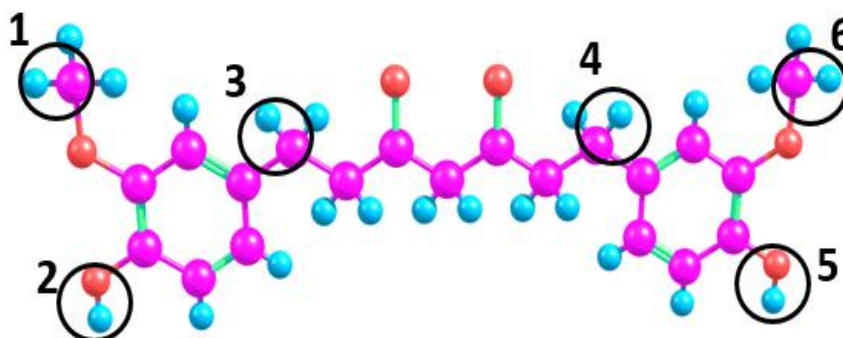


Figure 1. Six representative X-H sites (Blue, pink and red represent H, C and O atoms sequentially). Site 1, 3, 4 and 6 are C-H groups while site 2 and 5 are O-H groups.

3. Results and discussion

Figure 2 showed how model of dehydrogenated THC 2 was built. We built other dehydrogenated THCs with the same procedure. Since dehydrogenated THC 2 has lost one of its electron and proton (recall that we have abstracted a hydrogen atom from THC), we performed geometry optimisation by setting the spin multiplicity into 2 to make sure that the dehydrogenated THC 2 as well as other dehydrogenated THCs were at doublet state.

Figure 3 illustrated the SOMO and LUMO profiles of dehydrogenated THC 2. The SOMO profile was located at the hydrogen transferring sites. The profile informed us the location with the possibility of transferring electrons. After abstracting one hydrogen atom which contains of one proton and one electron, THC molecule was left with only one electron in its last occupied orbital. Thus this orbital was called SOMO. Differ from SOMO profile, LUMO profile was located at the center of the molecule. This profile informed us about the area possible of receiving electrons. Generally, SOMO profiles of all six dehydrogenated THCs were located at transferring sites while their LUMO profiles were located at the center of the molecule.

Our DFT calculation produced many orbital energies of dehydrogenated THCs. We chose two frontier orbitals, SOMO and LUMO, to assess the stability of dehydrogenated THCs[11]. Low energy difference between SOMO and LUMO meant an electron can easily be excited from its ground state, thus a molecule was less stable. While high energy difference between SOMO and LUMO meant an electron can be more stable in its ground state, thus a molecule was more stable.

We calculated energy difference between SOMO and LUMO, which we called it as relative SOMO-LUMO energies, of all six dehydrogenated THCs and tabulated the value in the graph at figure 4. The value of relative SOMO-LUMO energies at dehydrogenated THC 1 (site 1) and dehydrogenated THC 6 (site 6) was almost similar. Their difference was less than 0.2 eV. However, the value are very similar at dehydrogenated THC 2 (site 2) and dehydrogenated THC 5 (site 5), as well as at dehydrogenated THC 3 (site 3) and dehydrogenated THC 6 (site 6). The value of relative SOMO-LUMO energies from the highest to the lowest is dehydrogenated THC 2 = dehydrogenated THC 5 > dehydrogenated THC 1 > dehydrogenated THC 6 > dehydrogenated THC 3 = dehydrogenated THC 4. These results implied that dehydrogenated THC 2 was as stable as dehydrogenated THC 5. Both dehydrogenated THCs were the most stable among all six dehydrogenated THCs. Dehydrogenated THC 1 and 6 were less stable while dehydrogenated THC 3 and 4 had the lowest stability. Based on THC's similarity, site at the same position, possessed similar characters.

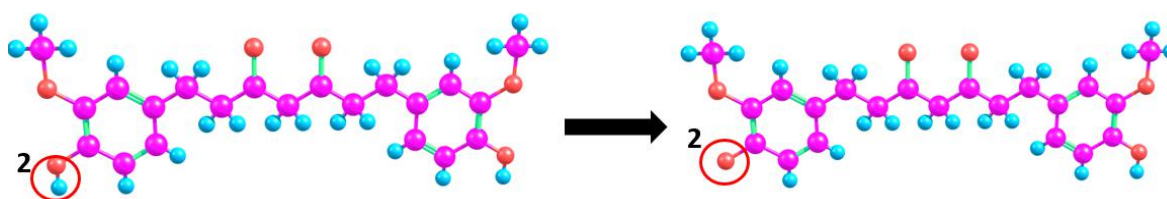


Figure 2. Model of dehydrogenated THC 2

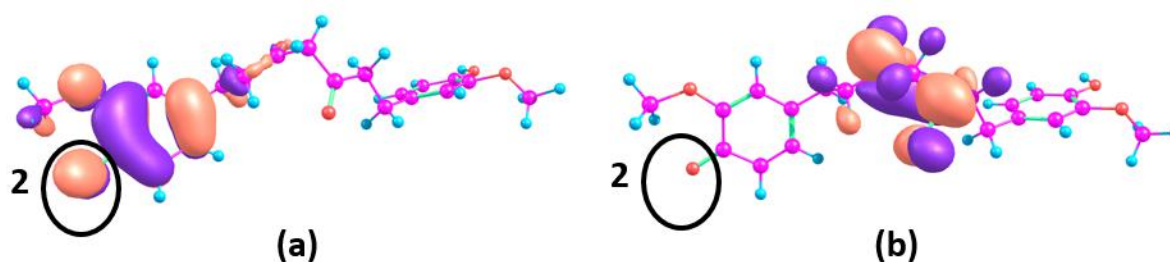
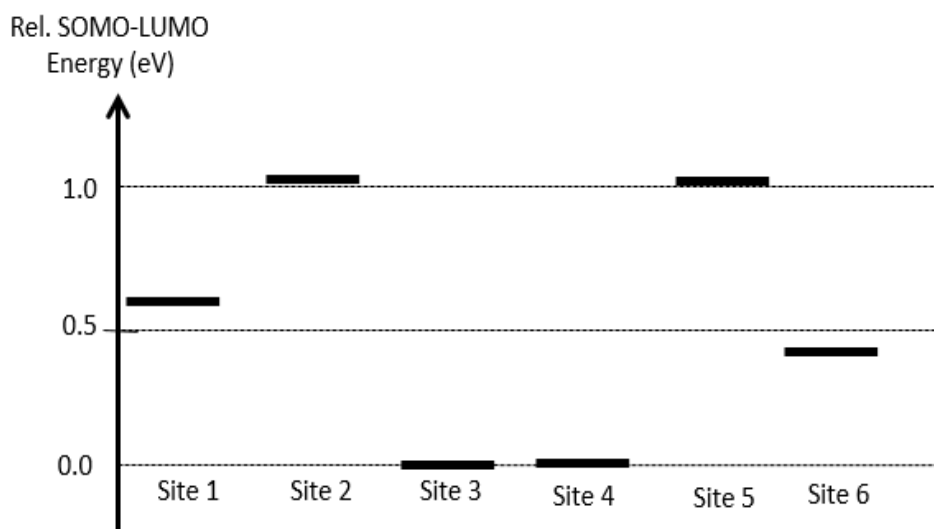


Figure 3. (a) SOMO and (b) LUMO profiles of dehydrogenated THC 2.**Figure 4.** Relative energy diagram of dehydrogenated THC. X axes of the graph is the type of dehydrogenated THC while Y axes of the graph shows the energy difference between SOMO and LUMO.

Finally, in order to assess the most possible site in THC that was responsible for antioxidant activity of the molecule, we concluded the following information. To perform its antioxidant activity, THC should be able to transfer one of its hydrogen atom toward ROS. If the hydrogen atom transferred was originally from an O-H groups, after the transfer process dehydrogenated THC formed would be the most stable. This occurred in the case of dehydrogenated THC 2 and 5. However, if the hydrogen atom transferred was originally from a C-H groups, after the transfer process dehydrogenated THC formed would be less stable. This occurred in the case of dehydrogenated THC 1, 3, 4 and 6. After performing its antioxidant activity, THC should be able to maintain its stability. Thus the most possible site that is responsible for this activity is O-H groups of THC molecule.

4. Conclusion

We have performed DFT calculation to calculate frontier orbitals of six dehydrogenated THCs. We investigated two frontier orbitals of dehydrogenated THCs, SOMO and LUMO, to assess the stability of the molecules. We suggested that in performing its antioxidant activity, hydrogen atom transfer should occur from O-H groups of THC, since the dehydrogenated THC formed was the most stable. Thus, O-H groups were responsible for the antioxidant activity of THC. This conclusion was supported by our results in two previous researches [12-13].

Acknowledgement

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