*Int. J. New. Chem.*, 2025, Vol. 12, Issue 2, pp. 139-148.

**International Journal of New Chemistry**

**Published online 2025 in http://www.ijnc.ir/.**

**Open Access**

**Print ISSN: 2645-7236**

**Online ISSN: 2383-188x**

**Original Research Article**

# Fullerene ($C_{20}$) as a Sensor and Adsorbent for Aflatoxin $M_1$: DFT Studies

Nastaran Khalaj Zeighami[1], Dorna Abdolkhani [2,*]

[1]Department of Food Science and Technology, Islamic Azad University, Science and Research Branch, Tehran, Iran.

[2,*] Department of Food Sciences and Industries, Biotechnology Orientation, Islamic Azad University Yasouj Branch, Yasouj,Iran.

*Received: 2024-10-24* *Accepted: 2024-09-10* *Published: 2024-09-23*

**ABSTRACT**

The investigation into the function of the smallest fullerene ($C_{20}$) as a sensor and adsorbent for the detection and removal of aflatoxinM1 is a significant contribution to the field of chemical sensing and environmental remediation. The use of DFT simulations to scrutinize the interaction process between $C_{20}$ and aflatoxinM1 provides valuable insights into the potential applications of fullerene in addressing aflatoxin contamination. The negative adsorption energies observed in the study indicate that the interaction between $C_{20}$ and aflatoxinM1 is thermodynamically favorable, suggesting that the adsorption process is experimentally feasible. Furthermore, the calculated $\Delta H_{ad}$ and $\Delta G_{ad}$ values demonstrate that the adsorption procedure is exothermic and spontaneous, indicating that $C_{20}$ has the capability to effectively adsorb aflatoxinM1 from its surroundings. The high values of thermodynamic equilibrium constants further support the notion that the adsorption process is one-sided and non-equilibrium, emphasizing the potential for $C_{20}$ to selectively capture aflatoxinM1 molecules. This selectivity is crucial in practical applications, particularly in the development of efficient adsorbents for the removal of aflatoxinM1 from contaminated environments. The analysis of frontier molecular orbital (FMO) parameters also provides valuable information regarding the electronic properties of $C_{20}$ and its interaction with aflatoxinM1. The significant decline in the bandgap of $C_{20}$ upon adsorption of aflatoxinM1 indicates a substantial modification in its electronic structure, which can be exploited for electrochemical detection purposes. This finding suggests that $C_{20}$ has the potential to be utilized as a sensing platform for the detection of aflatoxinM1, offering a promising avenue for the development of sensitive and selective detection methods.

**Keywords:** Desipramine, Density functional theory, Adsorption, sensor

## Introduction

Aflatoxin M1 is a potent toxin that poses serious health risks to humans and animals. It is a metabolite of aflatoxin B1, which is produced by certain strains of Aspergillus fungi commonly found in food and feed [1]. Aflatoxin M1 is of particular concern due to its ability to contaminate dairy products such as milk, cheese, and yogurt, as it is excreted in the milk of animals that have ingested aflatoxin B1-contaminated feed [2]. The toxicity of aflatoxin M1 is well-documented, with numerous studies linking its consumption to adverse health effects [3]. Chronic exposure to aflatoxin M1 has been associated with an increased risk of liver cancer, as well as other liver diseases [4]. In addition, acute exposure to high levels of aflatoxin M1 can cause immediate health problems such as liver damage, vomiting, abdominal pain, and even death in severe cases. Given the potential health risks associated with aflatoxin M1, its determination in food and feed is of utmost importance [5]. Accurate and sensitive analytical methods are needed to detect and quantify aflatoxin M1 levels in order to ensure food and feed safety [6]. Various techniques such as high-performance liquid chromatography (HPLC), enzyme-linked immunosorbent assay (ELISA), and mass spectrometry have been developed for the detection of aflatoxin M1, allowing for reliable monitoring and regulation of its levels in food and feed products [7]. Regulatory agencies around the world have established maximum allowable limits for aflatoxin M1 in food and feed, in order to protect consumers from its harmful effects [8]. These limits are based on scientific risk assessments and take into account the potential health hazards posed by aflatoxin M1 exposure [9]. Monitoring and enforcement of these limits are crucial to prevent the presence of unsafe levels of aflatoxin M1 in the food supply. In conclusion, the toxicity of aflatoxin M1 and its potential presence in food and feed products highlight the importance of accurate determination and regulation of its levels [10-12]. Efforts to develop and implement sensitive analytical methods, as well as stringent regulatory measures, are essential to safeguard public health and mitigate the risks associated with aflatoxin M1 contamination. Continued research and vigilance in monitoring aflatoxin M1 levels are necessary to ensure the safety of the food supply and protect consumers from its harmful effects. Electrochemical sensors offer a promising solution as they are rapid, sensitive, portable devices capable of measuring analytes even in opaque and colored specimens [13]. However, the initial and fundamental step in developing a novel electrochemical sensor is identifying an appropriate sensing material modifier that can selectively interact with the desired analyte [14]. Fullerene ($C_{20}$), the smallest

nanomaterial with a dodecahedral cage structure, possesses unique characteristics that make it an excellent candidate as both a sensing material and nanocarrier [15-17]. Its highly curved structure consists of pentagonal rings and offers high conductance, a large surface area-to-volume ratio, and exceptional reactivity [18-20]. Therefore, this study aims to evaluate the performance of $C_{20}$ as a nanocarrier and sensor for the delivery and detection of AFLATOXIN M1 through density functional theory simulations. By exploring the potential of $C_{20}$ in drug delivery and sensing applications, we hope to contribute to the development of more effective and efficient therapies while minimizing unwanted side effects. In conclusion, the utilization of nanocarriers and electrochemical sensors holds great promise in improving drug delivery systems and facilitating the rapid detection of antidepressants like aflatoxin m1. Through the evaluation of $C_{20}$ as a potential nanocarrier and sensing material modifier, this study aims to advance our understanding of these applications and pave the way for future advancements in pharmaceutical research.

## Computational Methods

The structures of $C_{20}$, aflatoxin m1, and their complexes were created using GuassView 6 [21] and Nanotube Modeler 1.3.0.3 [22]. The calculations were performed with the density functional theory (DFT) method in Gaussian 16 [23] software at the B3LYP/6-31G (d) level of theory [23]. The parameters were determined following a method outlined in [20].

## Results and Discussion

### Structural Analysis

The investigation of the interaction between aflatoxin m1 and $C_{20}$ was conducted to determine the most stable conformer. Two different configurations, A-Conformer and B-Conformer, were studied. In A-Conformer, the drug approached $C_{20}$ through its three fused rings, while in B-Conformer, the nanostructure was located near the aliphatic chain of the drug molecule. The optimized structures showed no significant structural deformations, indicating that no chemical bonds were formed between the adsorbate and adsorbent molecules [15]. Table 1 presents the calculated total electronic energies and adsorption energies. The total electronic energies for B-Conformer were more negative than those for A-Conformer in both vacuum and aqueous phases,

indicating that the formation of B-Conformer was more energetically favorable [16]. The negative adsorption energies suggest that the interaction between AFLATOXIN M1 and $C_{20}$ is experimentally possible in both phases. In addition to geometric optimizations, IR calculations were performed on the structures, and no negative frequencies were observed, confirming that all structures were true local minimums [17]. The dipole moment of aflatoxin m1 increased significantly after its adsorption on the surface of $C_{20}$, suggesting that aflatoxin m1-$C_{20}$ complexes are more soluble in polar solvents compared to the pure drug without the nanostructure [18]. Furthermore, the reactivity and bioavailability of aflatoxin m1 improved noticeably after its interaction with fullerene, indicating that $C_{20}$ can serve as a suitable nanocarrier for this drug. NBO computations were also conducted to gain further insights into the adsorption mechanism, and the results showed that no bonds were formed between the adsorbate and adsorbent, confirming that the adsorption mechanism is physisorption [29].

**Table 1.** The calculated structural properties of aflatoxin m1, $C_{20}$ and their complexes

| NO | Adsorption energy (kcal/mol) | ZPE (kcal/mol) | $\nu_{min}$ ($cm^{-1}$) | $\nu_{max}$ ($cm^{-1}$) | Dipole Moment (Debye) |
|---|---|---|---|---|---|
| Aflatoxin m1 | --- | 61.094 | 64.451 | 3708.437 | 1.348 |
| $C_{20}$ | --- | 106.634 | 286.330 | 1410.710 | 0.000 |
| A-Conformer | -107.056 | 142.277 | 74.961 | 2039.211 | 2.899 |
| B-Conformer | -159.096 | 143.048 | 165.581 | 2030.241 | 3.549 |

## Thermodynamic Parameters

In order to gain further insight into the thermochemistry of the adsorption process, various adsorption thermodynamic parameters were calculated and are presented in Table 2. It is evident that both conformers, exhibit negative values for $\Delta H_{ad}$ and $\Delta G_{ad}$, indicating the exothermic and spontaneous nature of the interactions. The relatively high values of $K_{th}$ suggest that these interactions are irreversible [20]. Furthermore, the negative values of ΔSad indicate that

aggregation occurs in the complexes following the interaction of aflatoxin m1 with fullerene [20]. The results obtained demonstrate that the adsorption process is more favorable at lower temperatures [16].

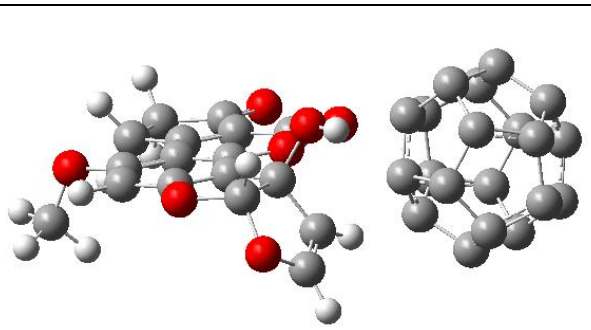
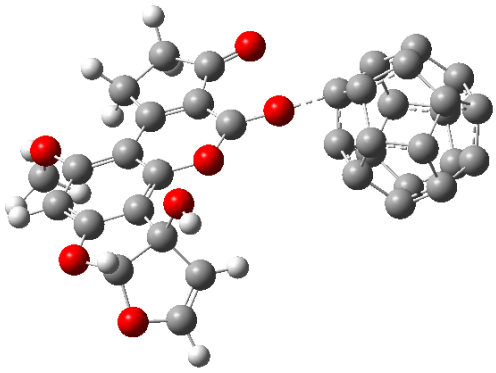
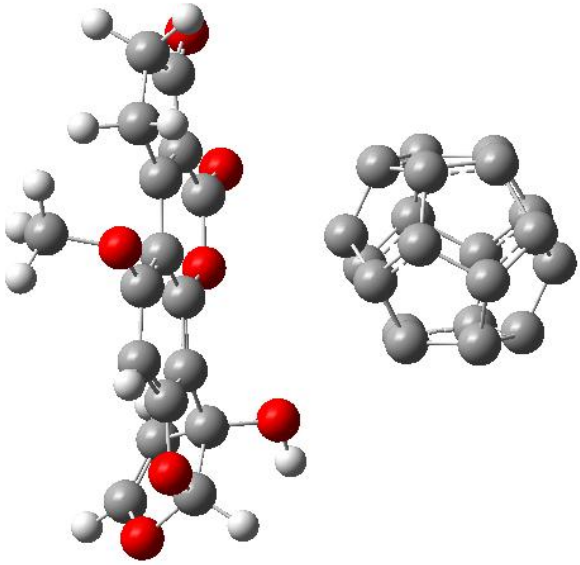
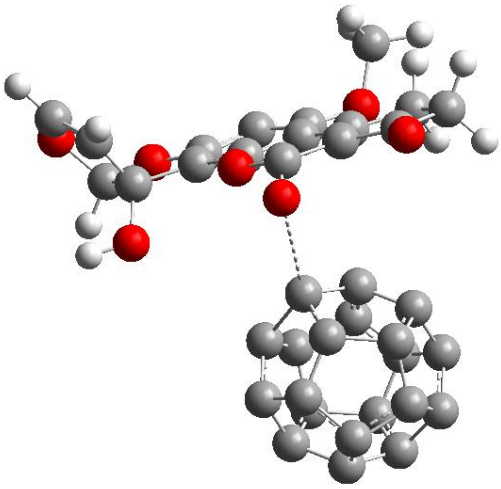
| | Initial Structures | Optimized Structures |
|---|---|---|
| A-Conformer |  |  |
| B-Conformer |  |  |

**Figure 2.** Initial and optimized structures of aflatoxin m1-$C_{20}$ complexes

**Table 2.** The calculated thermodynamic parameters

| NO | $\Delta H_{ad}$ (kcal/mol) | $\Delta G_{ad}$ (kcal/mol) | $\Delta S_{ad}$ (cal/mol) | $K_{th}$ |
|---|---|---|---|---|
| **A-Conformer-Vacuum-298** | -108.042 | -76.824 | -127.128 | $6.148\times10^{+11}$ |
| **A-Conformer-Vacuum-308** | -104.63 | -71.583 | -129.484 | $3.820\times10^{+13}$ |
| **A-Conformer-Vacuum-318** | -101.218 | -66.342 | -131.84 | $2.826\times10^{+15}$ |
| **B-Conformer-Vacuum-298** | -135.082 | -103.864 | -126.12 | $3.377\times10^{+10}$ |
| **B-Conformer-Vacuum-308** | -131.67 | -98.623 | -128.476 | $1.472\times10^{+18}$ |
| **B-Conformer-Vacuum-318** | -128.258 | -93.382 | -130.832 | $7.816\times10^{+20}$ |

## FMO Analysis

The bandgap, which refers to the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), plays a crucial role in determining the electrochemical conductivity of a compound [18]. A narrower bandgap indicates higher conductivity, while a wider bandgap implies lower conductivity. In the context of this study, the researchers aimed to investigate the potential of fullerene as an electroactive sensing material for detecting aflatoxin m1. They evaluated the variations in bandgap during the adsorption process to assess the material's suitability for this purpose. The data presented in Table 3 clearly demonstrate that the bandgap of $C_{20}$ is initially 7.678 eV. However, when aflatoxin m1 adsorbs onto the surface of $C_{20}$, this parameter decreases by about 18.85% for the A and B conformers, respectively. Consequently, the bandgap values for the A and B conformers become 5.731 eV and 5.738 eV, respectively. This significant decrease in bandgap indicates a substantial enhancement in the electrochemical conductivity of $C_{20}$ during the adsorption process of aflatoxin m1 [19]. Therefore, $C_{20}$ can be considered an excellent sensing material for detecting aflatoxin m1. The chemical hardness of aflatoxin m1 was found to be 6.021 eV. However, when aflatoxin m1 interacts with the nanostructure (A and B conformers), its chemical hardness

decreases to 2.865 eV and 2.869 eV, respectively. This decrease suggests an improvement in the chemical reactivity of aflatoxin m1 upon interaction with the nanostructure [20]. Furthermore, the negative values of the chemical potential for all studied structures indicate that these structures are thermodynamically stable [22]. Additionally, the electrophilicity and maximum transferred charge capacity of aflatoxin m1 were found to be 0.000 and 0.010 eV, respectively. However, when aflatoxin m1 is adsorbed onto the fullerene surface, both indices experience a significant increase [23]. This suggests that aflatoxin m1-$C_{20}$ complexes are more electrophilic and have a higher tendency to absorb electrons compared to pure aflatoxin m1 without the nanostructure. In conclusion, the findings of this study indicate that fullerene ($C_{20}$) can serve as an excellent electroactive sensing material for detecting AFLATOXIN M1. The adsorption of AFLATOXIN M1 onto $C_{20}$ leads to a decrease in bandgap and an enhancement in electrochemical conductivity. Additionally, the chemical reactivity of aflatoxin m1 improves upon interaction with the nanostructure. The thermodynamic stability of the studied structures further supports their potential applications in sensing and detection processes.

**Table 3.** The calculated FMO parameters

| NO | $E_{HOMO}$ (eV) | $E_{LUMO}$ (eV) | $E_g$ (eV) | $\%\Delta E_g$ | η (eV) | μ (eV) | ω (eV) | $\Delta N_{max}$ (eV) |
|---|---|---|---|---|---|---|---|---|
| **aflatoxin m1** | -6.079 | 5.962 | 12.041 | --- | 6.021 | -0.058 | 0.000 | 0.010 |
| **$C_{20}$** | -4.463 | 3.215 | 7.678 | --- | 3.839 | -0.624 | 0.051 | 0.162 |
| **A-Conformer** | -2.883 | 2.848 | 5.731 | -18.852 | 2.865 | -0.017 | 0.000 | 0.006 |
| **B-Conformer** | -2.993 | 2.745 | 5.738 | -18.745 | 2.869 | -0.124 | 0.003 | 0.043 |

## Conclusion

The exploration of how the smallest fullerene ($C_{20}$) functions as a sensor and adsorbent for the detection and removal of aflatoxinM1 represents a significant advancement in the fields of chemical sensing and environmental remediation. Employing DFT simulations to examine the interaction between $C_{20}$ and aflatoxinM1 yields valuable insights into the potential applications of fullerene in mitigating aflatoxin contamination. The study reveals negative adsorption

energies, indicating the thermodynamic favorability of the interaction between $C_{20}$ and aflatoxinM1, thus supporting the feasibility of the adsorption process. Additionally, calculated ΔHad and ΔGad values indicate that the adsorption procedure is both exothermic and spontaneous, affirming $C_{20}$'s capability to effectively adsorb aflatoxinM1 from its surroundings. The notably high values of thermodynamic equilibrium constants further reinforce the one-sided and non-equilibrium nature of the adsorption process, highlighting $C_{20}$'s potential to selectively capture aflatoxinM1 molecules. This selectivity is vital in practical applications, particularly concerning the development of efficient adsorbents for removing aflatoxinM1 from contaminated environments. The assessment of frontier molecular orbital (FMO) parameters offers insightful information about the electronic properties of $C_{20}$ and its interaction with aflatoxinM1. Remarkably, the substantial decrease in the bandgap of $C_{20}$ following the adsorption of aflatoxinM1 indicates a significant alteration in its electronic structure, potentially valuable for electrochemical detection purposes. This finding underscores the potential utility of $C_{20}$ as a sensing platform for aflatoxinM1 detection, thus representing a promising opportunity for the development of sensitive and selective detection methods.

## References

[1] J. R. Swanson, et al., *J Forensic Sci*., 42, 335 (1994).

[2] J. C. Nelson, *J Clin Psychiatry*., 45, 10 (1984).

[3] A. Ghanizadeh, *Curr Drug Saf.*, 8, 169 (2013).

[4] D. S. Janowsky B. Byerley *J Clin Psychiatry*. 45, 3 (1984).

[5] R. O. Friedel, *J Clin Psychiatry.*, 45, 46 (1984).

[6] J. F. Rosenbaum, *J Clin Psychiatry*. 45, 17 (1984).

[7] F. R. Sallee, *Clin Pharmacokinet*., 18(5), 346 (1990).

[8] L. Hearn, et al., *Cochrane Database Syst Rev*., 2, 10 (2014).

[9] D. Healy, C. Whitaker, *J Psychiatry Neurosci*., 28, 5 (2003).

[10] N. Perroud, *CNS Drugs*., 25, 459 (2011).

[11] Y. Wang, H. Xu, J. Zhang, G. Li, Sensors., 8, 2043 (2008).

[12] F. M. Alipour, etal., *Int J New Chem*., 10, 197 (2023).

[13] B. J. Privett, et al., *Anal Chem*., 82, 4723 (2010).

[14] R. Farahani, T. Madrakian, A. Afkhami, *Int J New Chem*., 9, 383 (2023).

[15] J. Paier, M. Marsman, G. Kresse, *J Chem Phys*., 127, 2 (2007).

[16] M. R. Sameti, M. B. Naghibi. *Int J New Chem*., 11, 15 (2023).

[17] R. Mousavi, et al., *Int J New Chem*., 10, 268 (2023).

[18] A. E. Frisch, R. E. Plata, D. A. Singleton. Gaussian 09W Reference. J Am Chem Soc. 137, 3811 (2009).

[19]. Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M. a., Cheeseman J.R., [1]. Scalmani G., Barone V., Petersson G. a., Nakatsuji H., Li X., Caricato M., Marenich a. V., Bloino J., Janesko B.G., Gomperts R., Mennucci B., Hratchian H.P., Ortiz J. V., Izmaylov a. F, Sonnenberg J.L., Williams, Ding F., Lipparini F., Egidi F., Goings J., Peng B., Petrone A., Henderson T., Ranasinghe D., Zakrzewski V.G., Gao J., Rega N., Zheng G., Liang W., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Throssell K., Montgomery J.r. J. a., Peralta J.E, Ogliaro F., Bearpark M.J., Heyd J.J., Brothers E.N., Kudin K.N., Staroverov V.N., Keith T. a., Kobayashi R., Normand J., Raghavachari K., Rendell a. P, Burant JC, Iyengar S.S., Tomasi J., Cossi M., Millam J.M.,

Klene M., Adamo C., Cammi R., Ochterski J.W., Martin R.L., Morokuma K., Farkas O., Foresman J.B., Fox D.J. G16_C01. 2016. p. Gaussian 16, Revision C.01, Gaussian, Inc., Wallin.

[20]. Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., ... & Fox, D. J. (2009). Gaussian 2009. *Revision A*, *2*.

[21] M. R. Jalali Sarvestani, R. Ahmadi, *Asian J Nanosci Mater*., 3, 103 (2020).

[22] GaussView, Version 6.1, Roy Dennington, Todd A. Keith, and John M. Millam, Semichem Inc., Shawnee Mission, KS, (2016).

[23] S. Melchor, J. A. Dobado, *J. Chem. Inf. Comput. Sci*, 44, 1639 (2004).

HOW TO CITE THIS ARTICLE

Nastaran Khalaj Zeighami, Dorna Abdolkhani "**Fullerene ($C_{20}$) as a Sensor and Adsorbent for Aflatoxin $M_1$: DFT Studies**" International Journal of New Chemistry., 2025; 12(2), 139-148. DOI: 10.22034/ijnc.2024.715907