JOURNAL of the MEXICAN CHEMICAL SOCIETY

https://www.jmcs.org.mx/

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J. Mex. Chem. Soc. **2026**, *70(1):e2411*

Received December 19th, 2024
Accepted March 19th, 2025

http://dx.doi.org/10.29356/jmcs.v70i1.2411
e-location ID: 2411

Keywords:
1,4-butanediol, adipic acid, terephthalic acid, TPA, TBT, TBTBT

Palabras clave:
1,4-butanodiol, ácido adípico, ácido tereftálico, TPA, TBT, TBTBT

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ISSN-e 2594-0317

The Controversy Surrounding the Toxicity of Biodegradable Plastics: PBAT as a Case Study

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Abstract. Synthetic plastics contribute to increase human comfort, but they also represent a huge pollution problem. One way to avoid contamination is with biodegradable plastics, such as PBAT [poly(butylene-adipate-co-terephthalate)]. The controversy begins with the apparent negative effect of PBAT on plant growth, and also because it could cause behavioral abnormalities in zebrafish. Previous studies suggest that biodegradation products could be responsible for this. The potential toxicity of biodegradation products and PBAT can be analyzed through the binding energies with biomolecules such as guanine-cytosine (GC). This Density Functional Theory investigation analyzes the interaction of biodegradation products with GC. All compounds under study form stable systems with GC and may be toxic. These results are consistent with previous toxicity research which conclude that PBAT degradation products may be more toxic than PBAT microplastics.

Resumen. Los plásticos sintéticos contribuyen a aumentar el confort humano, pero también representan un enorme problema de contaminación. Una forma de evitar la contaminación es con plásticos biodegradables, como el PBAT [poli(butileno-adipato-co-tereftalato)]. La controversia comienza con el aparente efecto negativo del PBAT sobre el crecimiento de las plantas, y también porque podría causar anomalías de comportamiento en el pez cebra. Estudios previos sugieren que los productos de biodegradación podrían ser responsables de esto. La toxicidad potencial de los productos de biodegradación y el PBAT se puede analizar a través de las energías de enlace

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con biomoléculas como la guanina-citosina (GC). Esta investigación utiliza la Teoría de Funcionales de la Densidad para analizar la interacción de los productos de biodegradación con GC. Todos los compuestos estudiados forman sistemas estables con GC y podrían ser tóxicos. Estos resultados son consistentes con investigaciones de toxicidad que concluyen que los productos de degradación del PBAT pueden ser más tóxicos que los microplásticos de PBAT.

Introduction

Plastics appeared many years ago, when in 1862 Alexander Parkes presented his invention "Parkensine" at the Great International Exhibition in London [1]. Parkensine is an organic material derived from cellulose and represents the first production of a plastic material, but the first plastic made with petroleum derivatives, named "Bakelite", was developed by Leo Baekeland in 1907 [2]. This polymer opened the door of the Age of Plastics. Today, the global petrochemical plastics industry employs over 60 million people and produces huge amounts of plastics. Ten percent of fossil hydrocarbons are transformed into polymers, producing 350 Mt each year [3]. Synthetic plastics are everywhere. They contribute to increase human comfort, but they also represent a huge pollution problem. One way to avoid this situation is to use biodegradable plastics, such as PBAT [poly(butylene-adipate-co-terephthalate).

PBAT was invented and reported in 1998 [4]. It is an aliphatic/aromatic co-polyester, synthesized from butanediol (BDO), adipic acid (AA) and terephthalic acid (TPA). This copolymer presents an acceptable compromise between properties and degradation rate [5]. It is used in many fields such as food packaging, agricultural and textile industry [6-15]. In agriculture it has been employed for many years as plastic film for mulching. PBAT mulch films minimize residues in agriculture since they could be incorporated in the soil after use [16,17]. Biodegradable plastics can also be an environmental problem, since they decompose into micro-nano plastics in less time than conventional plastics. [18,19]. Moreover, biodegradable plastics appear to affect plant growth and rhizosphere ecology, and may pose a greater threat to soil ecosystems than non-degradable plastics [20-26] For example, it was reported that plant development of two horticultural crops (tomato and lettuce) was altered by the presence of PBAT [24]. There is another study that investigates the acute and sub-chronic toxicity of PBAT on zebrafish [27]. Sub-chronic exposure of over 21 days revealed deviations in critical behavioral patterns and physiological indicators. Detailed behavioral evaluations revealed that, in presence of PBAT, there is a decrease in the speed and range of swimming, along with modifications in shoaling behavior and anxiety-like responses. The authors concluded that PBAT is likely to cause behavioral abnormalities in zebrafish by triggering in the brain, but it is not really known what is responsible for these effects. It could be the presence of nanoplastics of PBAT or the presence of its biodegradation products. In any case, biodegradable plastics may represent a risk to the environment [19].

Despite all these investigations, there are still limited studies focusing on the toxic effects of biodegradable micro and nanoplastics. To analyze the reasons for these effects, it is important to look at the products of biodegradation. PBAT is degraded by microorganisms and forms the reactants that were employed for the synthesis (BDO, AA and TPA). Apparently, these compounds are highly toxic to plants and are responsible for limiting plant growth [17-26].

In a previous work, theoretical investigations about the potential toxicity indicate that PBAT and its degradation products may increase oxidative stress [28]. This conclusion was obtained from the analysis of the electron transfer process, but other reactions were not analyzed. For this reason, the main idea of this investigation is to perform quantum chemical calculations to study the potential toxicity of PBAT and its degradation products analyzing the interaction with biomolecules such as DNA nitrogen bases. DNA double helix is very stable, but the two DNA strands must separate to expose the unpaired bases during the replication process. The idea here is to see if the compounds under study can interfere with this process. It is important to note that there are no reported experimental toxicity measures of these biodegradation products. Previous experimental investigations only analyzed the effects of PBAT and biodegradation products on plant growth and rhizosphere ecology. There are also studies on zebrafish. Knowing these effects, we investigated the

http://dx.doi.org/10.29356/jmcs.v70i1.2411

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interaction with nitrogenous base pairs to see if they are stable. These results are the starting point to understand possible toxic effects. It is a model that gives us more ideas and explanations of the possible effects.

Computational details

Gaussian16 was used for all electronic calculations [29]. Linear structures were considered as initial conformations. Geometry optimizations were obtained at M06-2X/6-311+g (2d, p) level of theory without symmetry constraints. [30-32] This level of theory has been shown to be adequate for the study of these systems. [33, 34] This exchange correlation functional was used before with success. This is a global hybrid functional with 54% HF exchange, and it is the best within the 06 functionals for main group thermochemistry, kinetics, and non-covalent interactions. Harmonic analyses verified local minima. Binding Energies (BE) were obtained as follows:

$$BE = [E(X) + E(GC)] - [E(X\text{-}GC)] \quad (1)$$

X represents PBAT and the biodegradable products; GC represents guanine-cytosine. BE were obtained considering Basis Set Superposition Error (BSSE). It was obtained according to the Counterpois method of Boys and Bernardi. [35]

Results and discussion

Molecular formulas of the studied compounds are shown in Fig. 1. As can be seen, we use the monomer as a model of PBAT. Monomers has previously been used to represent polymers with success [36-38]. Hydrolysis of the ester bond of PBAT is the first step of degradation. The second step is produced by microorganisms. Biodegradation products previously detected by fluorescence [39] present benzene rings (terephthalic acid-butanediol-terephthalic acid (TBT) and terephthalic acid -butanediol-terephthalic acid butanediol-terephthalic acid (TBTBT) see Fig. 1. Among these, TBT is the most abundant. With liquid chromatography-mass spectrometry, BDO monomer and AA as biodegradation products were also detected being BDO the most abundant biodegradation product. In summary, the biodegradation of PBTA produces all the compounds that we report in Fig. 1. Optimized structures are reported in Fig. 2. All are quasi-planar and TBTBT is the largest compound.

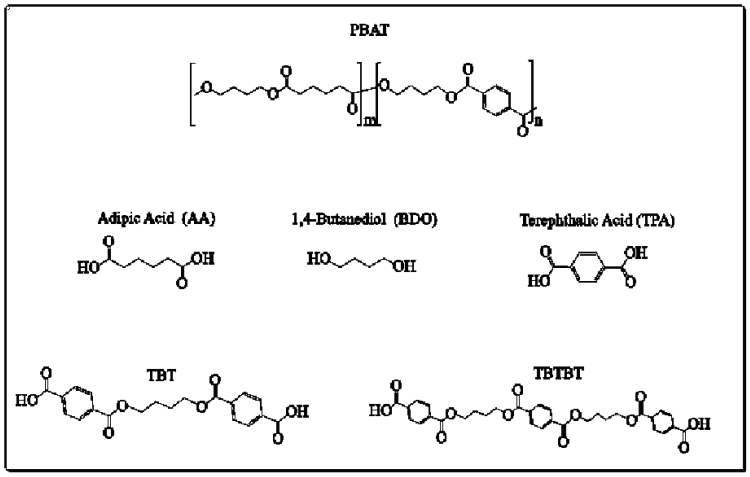

Fig. 1. Schematic representation of studied compounds.

http://dx.doi.org/10.29356/jmcs.v70i1.2411

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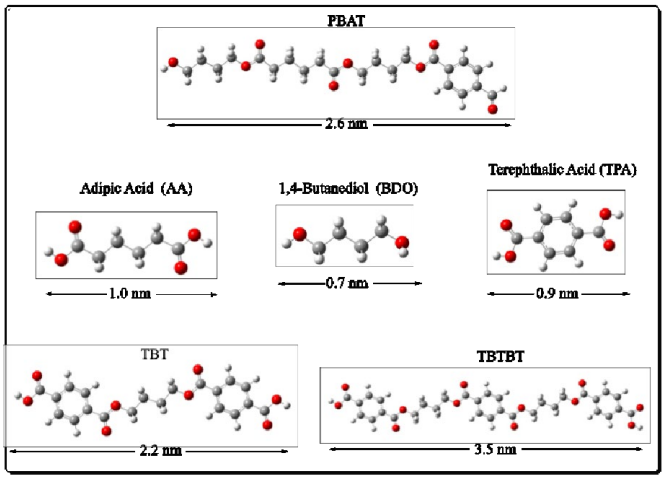

Fig. 2. Optimized geometries of PBAT and biodegradation products. Length of the molecules is reported in nm.

To investigate the toxicity of these compounds, we analyze the interaction of these molecules with guanine-cytosine nitrogen pair (GC). We used GC as a simple model of DNA in order to analyze the interaction energies. The interaction with GC was selected since it presents three hydrogen bonds, whilst the thymine-adenosine (TA) has only two. The interaction is stronger in GC than in TA. For this reason, to analyze the capacity of biodegradation products to affect the hydrogen bonds of DNA base pairs, GC was selected.

It is worth noting that enzymes "unzip" DNA molecules by breaking the hydrogen bonds between the nitrogen base pairs. Afterwards, the two separated strands expose the unpaired nitrogen bases that serve as a template for a new complementary strand that is created as the complementary bases attach to each other. The hypothesis here is that the biodegradation products and PBAT could interact with GC either when they are bound together with hydrogen bonds, or when they are separated during the DNA replication process. Should this be the case, this could affect the replication process and, as a consequence, the genetic information. This model is small but is helpful to investigate possible interactions with GC. This approximation was previously used to analyze potential toxicity of other microplastics [36].

Two possible initial geometries were investigated. One with PBAT and its biodegradation products between GC nucleobases that represents the interaction once the nucleobases are separated during the replication process. Another with the GC molecule next to the compounds under study that represents the interaction before DNA replication begins. With these two approaches we want to compare the interaction when GC is dissociated, with the non-dissociated GC system. In Fig. 3 we represent these two initial options. In Fig. 4, optimized structures of the compounds under study interacting with GC are reported. Binding energies (BE) calculated according to equation 1 are also included. Positive values of BE indicate that the products are more stable than the reactants and the interaction with GC is thermodynamically feasible.

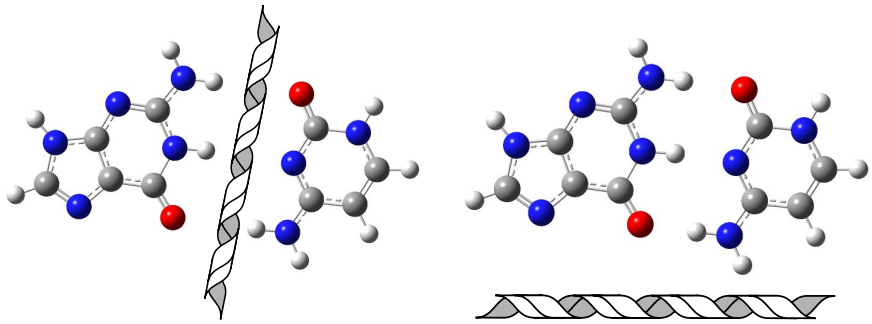

Fig. 3. Schematic representation of the initial geometries used to investigate the interaction of compounds under study with guanine-cytosine nitrogen base pair.

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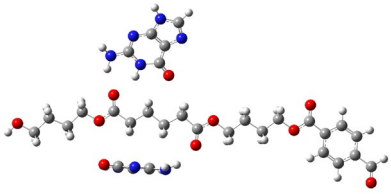
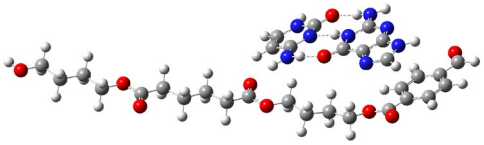
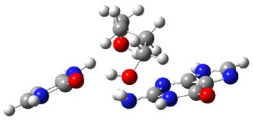
The results of Fig. 4 indicate that BDO and AA may dissociate GC, but the binding energies are less than 10 kcal/mol. When the initial structures have GC parallel to BDO or AA, the binding energies are higher, and the interaction is stronger than with dissociated GC geometries. A similar situation is found with molecules that have benzene rings. Binding energies of PBAT, TPA and TBTBT are negative and this indicates that the dissociation of GC is not thermodynamically feasible. TBT also has a benzene ring, but in this case the BE is positive, indicating that the dissociation of GC is thermodynamically possible. In any case, optimized geometries with molecules interacting with GC without dissociation are more stable than the reactants. It is important to note that none of the binding energies reported in Fig. 4 is greater than 20 kcal/mol. It is not possible to say whether these interactions could produce significant damage, but we can compare these binding energies with those calculated for Persistent Organic Pollutants, which are well-known toxic compounds [40]. The binding energies reported for these pollutants are equal to 10-15 kcal/mol, similar to the values that we found in this investigation. Concerning the interaction with DNA nitrogen basis, Persistent Organic Pollutants and the compounds studied here might have similar toxicity.



BE_{PBAT} = -2.8 kcal/mol

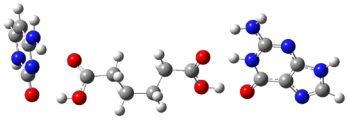


BE_{PBAT} = 15.1 kcal/mol



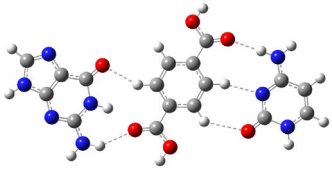
BE_{BDO} = 6.8 Kcal/mol

BE_{BDO} = 10.7 kcal/mol

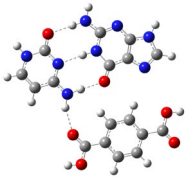


BE_{AA} = 1.7 kcal/mol

BE_{AA}= 8.7 kcal/mol



BE_{TPA} = -6.3 kcal/mol



BE_{TPA} = 8.7 Kcal/mol

http://dx.doi.org/10.29356/jmcs.v70i1.2411

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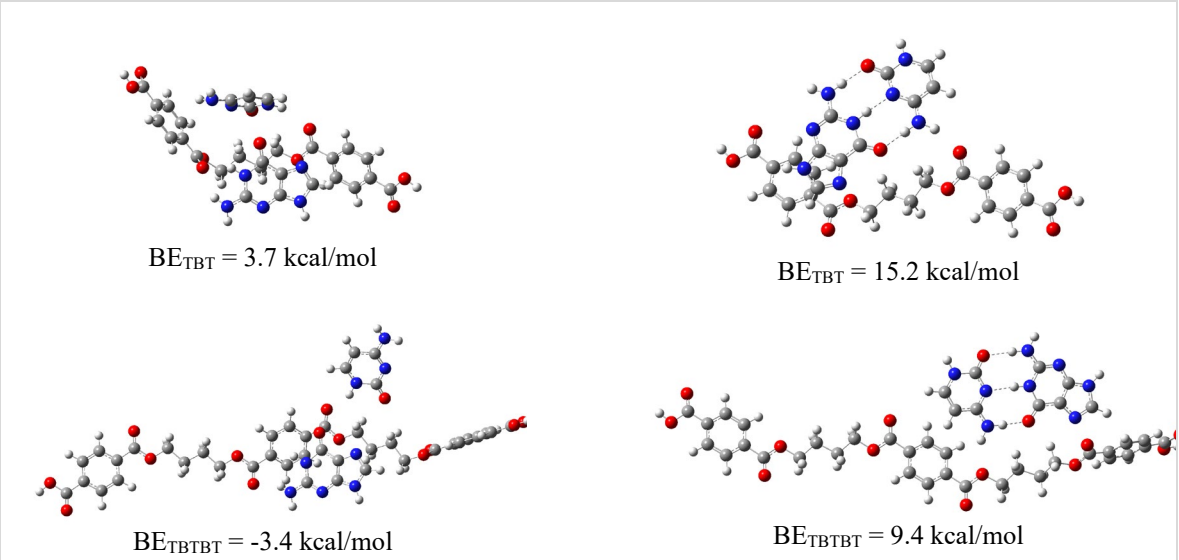

Fig. 4. Optimized structures of Guanine-Cytosine interacting with the compounds under study. BE is the binding energy (in kcal/mol) calculated with equation 1 and considering BBSE.

Previous studies of nanoplastics bonded to DNA nitrogenous bases [36] report an interaction energy of polyethylene and polyethylene terephthalate or polyester (PET) equal to -13.5 and 21.3 kcal/mol. This means that polyethylene does not form stable compounds with GC. The value of PET with GC is positive and indicates the formation of stable compounds. This result is similar to the interaction energy that we present in this investigation.

Based on our results, PBAT and biodegradable products have potential toxicity. The interaction of BDO, AA and TBT with GC may dissociate the biomolecule (BE are positive). PBAT, TBA and TBTBT do not dissociate GC (BEs are negative). In any case, there are optimized geometries where the interaction with GC is thermodynamically feasible, even when there is no dissociation of the DNA nitrogen base pair. Therefore, hydrogen bonds formed between GC and PBAT or biodegradation products could alter DNA replication.

It was previously reported [19-26] that PBAT, BDO, AA and TPA alter the photosynthetic system of plants and inhibit their growth. Our results may explain these findings since compounds and PBAT interact with GC, and this could explain the growth inhibition. In those previous experiments, the authors did not consider the formation of TBT and TBTBT. According to the fluorescence results [39], TBT is formed after five days under experimental conditions. In fifteen days of the experiment, TBTBT is also formed. In another toxicity testing experiment, the authors used plants and exposed them to PBAT for 35 days [23]. The authors of this publication found an inhibition of plant growth and pointed to PBAT as responsible for this. They did not consider the formation of biodegradation products, which were previously reported (TBT and TBTBT). Even when the experimental conditions were not the same in both experiments, the formation of biodegradation products during the plant experiments cannot be ruled out. Growth inhibition could occur through PBAT and by its biodegradation products. If this were the case, the biodegradation products would be as dangerous as PBAT. More experiments are needed to confirm this hypothesis, but our results indicate that the biodegradation products are at least as toxic as PBAT.

PBAT biodegradation products have been previously reported as good electron acceptor molecules [28] and therefore potential oxidation enhancers. This may affect other biomolecules such as proteins. In future work we will consider the interaction of these biodegradation products with amino acids.

The model we use to analyze the interaction of monomers and molecules with the nitrogenous bases of DNA can be considered simple and not suitable from a biochemical point of view, since it does not take into account the structure of the DNA molecule. It can be said that the obtained conformations are inconsistent with the double helix structure with stacked base pairs and with the presence of sugar and phosphate backbone. This

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is correct but we consider that the interaction with the small model can give us reliable information. To test this and analyze the effect of the presence of the sugar and phosphate, we optimized GC with the presence of the backbone and we investigate the interaction with TPA as an example. The results are reported in Fig. 5, and indicate a higher binding energy for this system than for the system when the backbone is not present. This means that the interaction is favorable, even though when the nitrogen base pair is bonded to the sugar phosphate backbone. With these results it is possible to consider that the model we used gives us good indications of what can be the effect of the compounds under study and the interaction with the DNA nitrogen base pair. The controversy over the benefits of PBAT is not resolved, since more investigations are needed to corroborate the negative effects of PBAT and its biodegradation products.

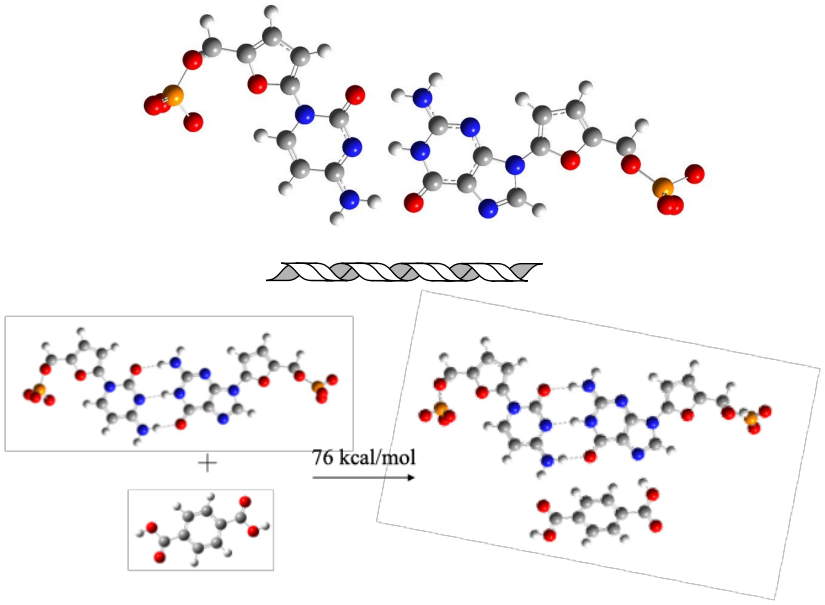

Fig. 5. Optimized structures of Guanine-Cytosine with the presence of the backbone and interacting with TPA. An approximated BE calculated with equation 1 is also reported.

Previous studies analyzed the interaction with oligomers and nanoplastics to study potential toxicity. In this investigation, we study the toxicity of biodegradation products. There are no previous theoretical studies that investigate the potential toxicity of degradation products. It is well known that biodegradation is something desirable, but it is important to know the effects of the degradation products since they could be more dangerous than the original products. If this were the case, the solution (biodegradability) could be worse than the problem (plastic pollution) and it is crucial to know it.

Conclusions

The potential toxicity of PBAT and its biodegradable products can be analyzed trough the binding energies with biomolecules such as GC. DNA has a complex double helix structure, and GC base pair is a simple model that does not represent real effects of these biodegradation products on the DNA replication process, but it is important to understand this possible interaction from the chemical point of view, in order to describe the reactivity and to have more information concerning the possible toxic effects of these compounds.

http://dx.doi.org/10.29356/jmcs.v70i1.2411

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BDO, AA and TBT can dissociate GC. All the compounds studied are capable of interacting with GC even when they do not dissociate the DNA nitrogen base pair. Therefore, hydrogen bonds formed between GC and PBAT or biodegradation products could alter DNA replication.

All these results are in agreement with previous toxicity research which conclude that PBAT degradation products may be more toxic than PBAT microplastics. More studies are necessary to analyze other reaction mechanisms to explain the toxicity, but with the theoretical results included here the conclusion is that these compounds can be dangerous because they can interact directly with GC and this may perturbate the replication of DNA.

It was previously reported that PBAT, BDO, AA and TPA alter the photosynthetic system of plants and inhibit their growth. This is in agreement with our results for BDO and AA that interact with the GC system, and this could explain the growth inhibition. In those previous experiments, the authors did not consider the formation of TBT and TBTBT. According to the results reported here, TBT and TBTBT could also may produce an effect inhibiting the growth of plants due to the stable interaction with GC.

Our findings show that PBAT may be degraded to produce chemicals that are toxic. PBAT and its degradation products present similar toxicity concerning the interaction with GC. Biodegradable plastics may pose a risk to the environment since the products of degradation might be also toxic. Further studies are necessary but these results give us insight into possible interactions that should be important for future work. The controversy over the benefits of PBAT is not resolved.

Acknowledgements

AM acknowledges support from Universidad Nacional Autónoma de México (UNAM) and thanks to LANCAD-UNAM-DGTIC-141 for computer facilities.

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