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Research Article

Antioxidant Properties of Curcumin Analogues to Inhibit Thermal Degradation of Low-Density Polyethylene: Experimental and DFT Study

Ali M. Al-Asadi,[1] Salah S. Al-Luaibi,[1] Basil A. Saleh,[1] Mohammed A. Baashen,[2] and Gamal A. El-Hiti[3]

[1]*Department of Chemistry, College of Science, University of Basrah, Basrah 61004, Iraq*
[2]*Department of Chemistry, College of Science and Humanities, Shaqra University, Al-Dawadmi 11911, Saudi Arabia*
[3]*Cornea Research Chair, Department of Optometry, College of Applied Medical Sciences, King Saud University, Riyadh 11433, Saudi Arabia*

Correspondence should be addressed to Basil A. Saleh; basil.saleh@uobasrah.edu.iq and Gamal A. El-Hiti; gelhiti@ksu.edu.sa

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Curcumin can be isolated from plants (*Curcuma longa*) and it belongs to the ginger family. It exhibits many useful properties and acts as an antioxidant. The aim of the current study was to prepare eight curcumin analogues and investigate their antioxidant activities to inhibit the thermal degradation of low-density polyethylene (LDPE). The carbonyl index (CI) was measured to test the effectiveness of the curcumin analogues. Various doses (0.5, 1, 2, 4, and 6% wt/wt) of a mixture containing LDPE and curcumin analogues were prepared, and the CI was measured. The eight curcumin analogues were found to have good to excellent antioxidant activity against the degradation of LDPE. It was clear that the curcumin analogue derived from vanillin and acetone has the highest antioxidant activity. The density functional theory study was conducted for the eight curcumin analogues to test their reactivity and stability. Again, the global reactivity descriptors analysis showed that compound derived from vanillin and acetone was the most reactive compound to inhibit thermal degradation of LDPE.

1. Introduction

Polyethylene (PE) is one of the most commonly produced and used plastics. It can be used in the production of packing, electrical insulators, and biomedicine [1,2]. Thermal-oxidative degradation of PE is a major problem that has a negative impact on the economy and the environment. The exposure of PE to heat and light can lead to its degradation and shorten the lifetime of the manufactured product [3]. The PE thermo-oxidative process leads to the formation of hydroperoxide species, which decompose into fragments containing carboxyl and alcohol groups. Such processes lead to the breakdown of polymer chains and a decrease in the molecular weight of PE [4,5]. Therefore, it is vital to prevent or inhibit the degradation process of PE. Antioxidants such as butylated hydroxytoluene (BHT) are widely used to inhibit thermo-oxidation of PE. The BHT acts as a free radical scavenger to inhibit the oxidative degradation of polymeric materials [6]. Various techniques such as IR spectrophotometry and thermal analyses, including thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC), can be used to evaluate the efficiency of antioxidants [7].

The introduction of nontoxic and highly stable thermal antioxidants to low-density polyethylene (LDPE) in the melt-flow processes is essential for the protection against oxidative degradation [8,9]. Natural products such as curcumins have antioxidant properties and have been tested to inhibit oxidative degradation of LDPE used in the production of food packaging [10]. Indeed, many synthetic curcumin analogues have been studied *in vitro* as

antioxidative agents for biological and medicinal purposes [11–18].

The conceptual density functional theory (DFT) has been used to understand the global reactivity and local site selectivity of a variety of molecules. Hybrid DFT-based B3LYP methods are used extensively to study the global and local reactivity descriptors [19]. The aim of the current work was to examine the antioxidant scavenging activity, experimentally and theoretically, for eight curcumin analogues to inhibit the degradation of LDPE.

2. Materials and Methods

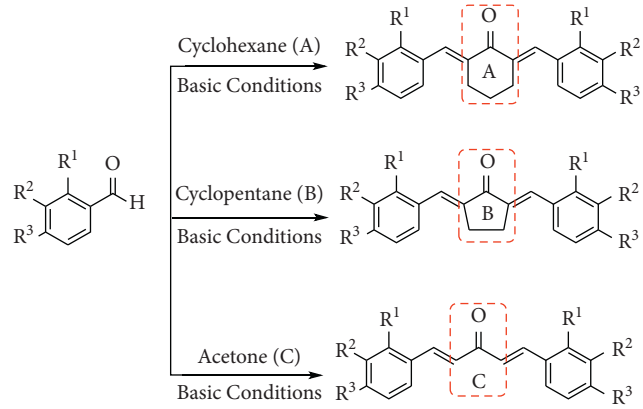
2.1. General. Chemicals and reagents were purchased from Merck (Gillingham, UK). The NMR spectra (500 MHz) were recorded in deuterated dimethyl sulfoxide (DMSO-d_6) using a Bruker 500 MHz NMR spectrometer related to tetramethylsilane. The chemical shifts were reported in ppm and the coupling constants in Hz. Food grade LDPE 463 pellets (density of 0.922 g/cm^3 and melt-flow index of 0.32 g/10 min) were supplied from a petrochemical company (Basrah, Iraq).

*2.2. General Procedure for Synthesis of Curcumin Analogues **1–8**.* Compounds **1–8** were synthesized based on a literature procedure under a basic condition [20]. Appropriate ketone (0.01 mol) was added to a stirred solution of the appropriate aldehyde (0.02 mol) in ethanol (EtOH; 2.5 mL). A solution of NaOH (20%, 50 mL) was added dropwise to the stirred mixture and the temperature was below 40°C. The red mixture was stirred for 24 hours and distilled water (15 mL) was added and neutralized (pH = 5.5) using HCl (6 M). The yellowish solid obtained was filtered, washed with water (2 × 15 mL), dried, and recrystallized from EtOH to give pure products **1–8** (Scheme 1) in high yields (Table 1). The FTIR spectra of compounds **1–8** are shown in Figures S1–S8, and their ^{1}H NMR spectra are presented in Figures S9–S16.

*2.2.1. 2,6-Bis(2-hydroxybenzylidene) cyclopentanone (**1**).* FTIR (cm^{-1}) 3306, 3070, 1651, 1604, and 1562. ^{1}H NMR δ 10.14 (s, exch., 2H, and 2 OH), 7.80 (s, 2H, and 2 CH), 7.55 (d, J = 7.9 Hz, 2H, and Ar), 7.24 (t, J = 8.6 Hz, 2H, and Ar), 7.02–6.82 (m, 4H, and Ar), and 3.01 (s, 4H, and 2 CH_2).

*2.2.2. 1,5-Bis(2-hydroxyphenyl)-1,4-pentadiene-3-one (**2**).* FTIR (cm^{-1}) 3379, 3070, 1647, 1608, and 1550. ^{1}H NMR δ 10.27 (s, exch., 2H, and 2 OH), 7.93 (d, J = 16.1 Hz, 2H, and 2 CH), 7.69 (d, J = 7.8 Hz, 2H, and Ar), 7.29 (d, J = 16.1 Hz, 2H, and 2 CH), 7.27–7.22 (m, 2H, and Ar), 6.93 (d, J = 8.1 Hz, 2H, and Ar), and 6.86 (t, J = 7.5, 2H, and Ar).

*2.2.3. 2,6-Bis(4-hydroxybenzylidene) cyclopentanone (**3**).* FTIR (cm^{-1}) 3321, 3028, 1651, 1697, and 1508. ^{1}H NMR δ 9.93 (s, exch., 2H, and 2 OH), 7.54 (s, 2H, and 2 CH), 7.40 (d, J = 8.7 Hz, 4H, and Ar), 6.84 (d, J = 8.7 Hz, 4H, and Ar), 2.85 (t, J = 6.4 Hz, 4H, and 2 CH_2), and 1.70 (pentet, J = 6.4 Hz, 2H, and CH_2).



SCHEME 1: Synthesis of curcumins **1–8**.

*2.2.4. 2,5-Bis(4-hydroxybenzylidene) cyclopentanone (**4**).* FTIR (cm^{-1}) 3321, 1666, 1597, and 1508. ^{1}H NMR δ 10.05 (s, exch., 2H, 2 and OH), 7.54 (d, J = 8.6 Hz, 4H, and Ar), 7.33 (s, 2H, and 2 CH), 6.87 (d, J = 8.6 Hz, 4H, and Ar), and 3.01 (s, 4H, and 2 CH_2).

*2.2.5. 1,5-Bis(4-hydroxyphenyl)-1,4-pentadiene-3-one (**5**).* FTIR (cm^{-1}) 3325, 1593, and 1512. ^{1}H NMR δ 10.04 (s, exch., 2H, and 2 OH), 7.66 (d, J = 16.0 Hz, and 2H 2CH), 7.62 (d, J = 8.7 Hz, 4H, and Ar), 7.10 (d, J = 16.0 Hz, 2H, and 2 CH), and 6.83 (d, J = 8.7 Hz, 4H, and Ar).

*2.2.6. 2,6-Bis(4-hydroxy-3-methoxybenzylidene) cyclopentanone (**6**).* FTIR (cm^{-1}) 3379, 2928 1643, 1581, and 1516. ^{1}H NMR δ 9.54 (s, exch., 2H, and 2 OH), 7.56 (s, 2H, and 2 CH), 7.12 (d, J = 2.0 Hz, 2H, and Ar), 7.03 (dd, J = 8.2, 2.0 Hz, 2H, and Ar), 6.85 (d, J = 8.2 Hz, 2H, and Ar), 3.81 (s, 6H, and 2 OMe), 2.99–2.81 (m, 4H, and 2 CH_2), and 1.72 (pentet, J = 6.4 Hz, 2H, and CH_2).

*2.2.7. 2,5-Bis (4-hydroxy-3-methoxybenzylidene) cyclopentanone (**7**).* FTIR (cm^{-1}) 3379, 2962, 1678, 1612, 1589, and 1512. ^{1}H NMR δ 9.68 (s, exch., 2H, and 2 OH), 7.36 (s, 2H, and 2 CH), 7.25 (s, 2H, and Ar), 7.16 (d, J = 8.4 Hz, 2H, and Ar), 6.89 (d, J = 8.4 Hz, 2H, and Ar), 3.84 (s, 6H, 2 OMe), and 3.06 (s, 4H, and 2 CH_2).

*2.2.8. 1,5-Bis(3-hydroxy-4-methoxyphenyl)-1,4-pentadiene-3-one (**8**).* FTIR (cm^{-1}) 3417, 2924, 1631, 1589, and 1516. ^{1}H NMR δ 9.66 (s, exch., 2H, and 2 OH), 7.65 (d, J = 15.9 Hz, 2H, and 2 CH), 7.37 (d, J = 2.0 Hz, and 2H), 7.27–7.06 (m, 4H, 2 CH, and Ar), 6.83 (d, J = 8.2 Hz, 2H, and Ar), and 3.84 (s, 6H, and 2 OMe).

2.3. Purification of LDPE. Commercial pellets of LDPE were purified using a refluxed xylene under a nitrogen atmosphere for 1 hour to remove any antioxidant traces. The precipitate obtained was washed with cold methanol (MeOH), filtered, and dried at 70°C for 1 hour [22].

Table 1: Synthesis of curcumins **1–8** based on Scheme 1.

Compound	R^1	R^2	R^3	Ketone unit	Color	Mp (°C)	Lit. Mp (°C)	Yield (%)
1	OH	H	H	B	Yellow	224–226	224–226 [21]	89
2	OH	H	H	C	Yellow	154–156	156 [13]	82
3	H	OH	H	A	Yellow	>300	>300 [16]	60
4	H	OH	H	B	Yellow	>300	>300 [16]	85
5	H	OH	H	C	Orange	244–246	243–245 [16]	86
6	H	OH	OMe	A	Yellow	177–178	178–179 [16]	67
7	H	OH	OMe	B	Yellow	212–214	212–214 [16]	80
8	H	OH	OMe	C	Yellow	100–101	99–100 [16]	74

2.4. Thermal Oxidation. The LDPE/antioxidant blends were prepared by mixing the LDPE with different percentages (0.5, 1, 2, 4, and 6 by weight%) of **1–8** using a Haake rheometer at 150°C at a screw speed of 64 rpm for 8 min [10]. The LDPE/**1–8** blends were subjected to thermal oxidation at 200°C for 1 hour. The LDPE/antioxidant blends were pressed into films using a hydraulic press at 150°C for 5 min to produce films with an average thickness of 1 mm [10]. The IR spectra of the films were recorded before and after the thermal oxidation using FTIR Shimadzu 8400s. The carbonyl index (CI) was calculated using equation (1) [23], where $Abs_{1726\ cm^{-1}}$ and $Abs_{1472\ cm^{-1}}$ are the absorption intensity of the C=O and CH_2 peaks, respectively. Figure 1 represents the IR spectrum of the antioxidant-PE composite containing compound **1** (4%) as an example. It shows how the calculation of the CI was made. The efficiency of antioxidant was calculated using equation (2).

$$\mathrm{CI} = \frac{\mathrm{Abs}_{1726\mathrm{cm}^{-1}}}{\mathrm{Abs}_{1472\mathrm{cm}^{-1}}} \times 100, \quad (1)$$

$$\%E = \frac{\text{CI before addition} - \text{CI after addition}}{\text{CI after addition}} \times 100. \quad (2)$$

2.5. Computational Details. The structures were optimized using the DFT method with the B3LYP/6-31G+d basis set [24,25] to obtain the most stable conformation. In addition, it was used to calculate the global reactivity descriptors through the Gaussian 09 [25]. The convergent value of the maximum force, root-mean-square (RMS) force, maximum displacement, and RMS displacement were set by default and achieved "YES." The values were positive after the calculation of vibrational frequencies of compounds **1–8**.

The global reactivity indices are considered to be one of the most relevant traits derived from the conceptual DFT [19]. Global reactivity descriptors have important properties that enable chemists to evaluate the chemical reactivity and kinetic stability of compounds [26,27]. They can be described [28–32] by the energy of highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE), electrophilicity (ω), chemical potential (μ), chemical hardness (η), chemical softness (S), and nucleophilicity (N). Those descriptors were calculated for compounds **1–8** at B3LYP/6-31G using the following formulas: $\Delta E = E_{LUMO} - E_{HOMO}$, $\omega = \mu^2/2\eta$, $\mu = (E_{LUMO} + E_{HOMO})/2$, $\eta = (E_{LUMO} - E_{HOMO})/2$, $S = 1/(2\eta)$, and $N = E_{HOMO}$ (Nucleophile) $- E_{HOMO}$ (TCE). It should be noted that the nucleophilicity value of tetracyanoethylene (TCE) is taken as a reference since it presents the lowest E_{HOMO} in many reported molecules [33].

3. Results and Discussion

*3.1. Synthesis of Curcumin Analogues (**1–8**).* Curcumin analogues **1–8** were prepared based on a literature protocol [17]. Condensation of the appropriate ketone (e.g., cyclohexanone, cyclopentanone, and acetone) and a variety of aromatic aldehydes under basic conditions gave the corresponding curcumins **1–8** (Scheme 1) in high yields (Table 1).

*3.2. The Antioxidant Activity of Curcumin Analogues (**1–8**).* The antioxidant activity of curcumin analogues **1–8** on the CI of LDPE was investigated at various doses (Table 2). In general, curcumin analogues **1–8** have a good to excellent performance in reducing the CI, and the activity of additives to inhibit thermal oxidation of LDPE increased as the dose of antioxidants increased. The curcumin analogues derived from vanillin, namely, **6**, **7**, and **8**, showed the most desirable effect. Compound **7** had the highest inhibition of thermal oxidation of LDPE even at the lowest dose (0.5% wt) used. Compounds **6–8** contain extra electron-donating groups (OMe group). The methoxy group tends to stabilize the free radical generated through the oxidation process. The antioxidant efficiency of **1–8** towards the LDPE oxidation appeared to be unaffected by the type of ketone unit (A, B, or C; Scheme 1 and Table 1) used. Compound **5** showed the lowest inhibition activity.

The antioxidant efficiency (%E) of the curcumin analogues **1–8** was calculated using equation (2), and the results are summarized in Table 3. Again, the compounds derived from vanillin (i.e., **6–8**) as well as **2** showed the highest efficiency.

3.3. Global Reactivity Descriptors. Analysis of the HOMO, LUMO, and the calculated global reactivity descriptors provides more information about the stability and electrophilic and nucleophilic regions for curcumin analogues **1–8**. Table 4 shows the global reactivity descriptor calculated for **1–8**.

The ionization energy (I) and electron affinity (A) of compounds **1–8** were measured using the HOMO and LUMO energies. These two descriptors are related to one-

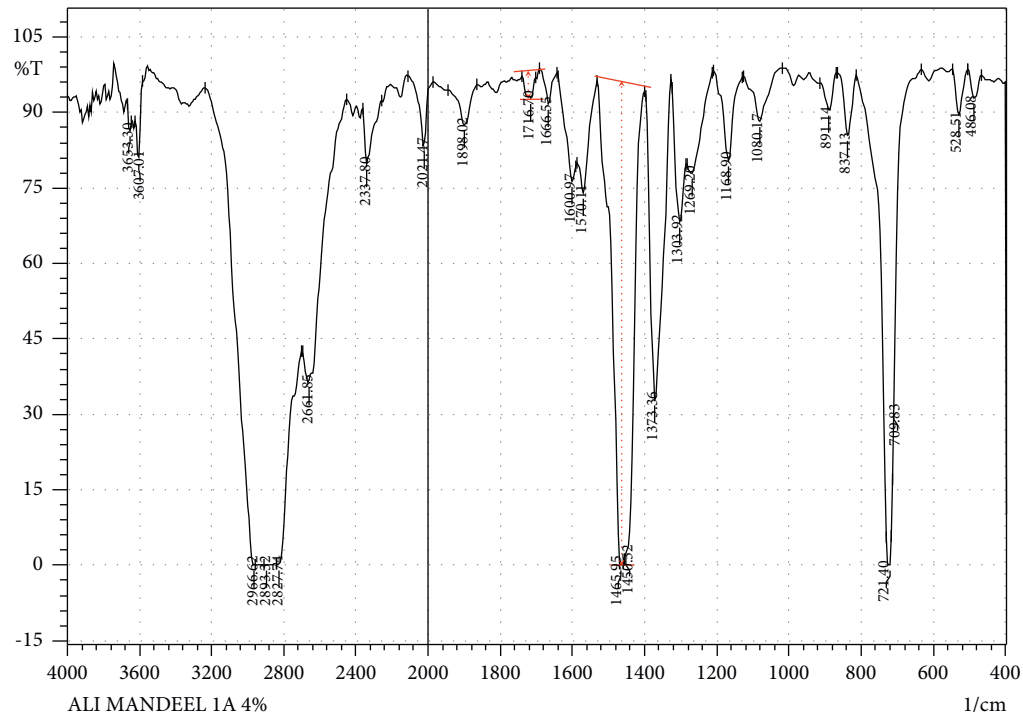


Figure 1: IR spectrum of the antioxidant-PE composite containing compound **1** (4%).

Table 2: Effect of dose of curcumins **1–8** on the CI of the LDPE.

Compound	Dose (%)					
	0	0.5	1	2	4	6
1	100	26	12.3	10.5	5.8	1
2	100	35	1.2	1.1	—	—
3	100	20	5.2	3.3	2	1.25
4	100	29.4	27.3	4.3	2.1	1
5	100	14.2	13.3	6.5	3.1	1.5
6	100	27	6.4	3.2	—	—
7	100	—	—	—	—	—
8	100	2	2.5	0.6	—	—

Table 3: The antioxidant efficiency (%E) of curcumin analogues **1–8** toward the LDPE oxidation.

Compound	%E at different doses (%)					
	0	0.5	1	2	4	6
1	0	74	87.7	89.5	94.2	99
2	0	65	98.8	98.9	100	100
3	0	80	94.8	96.7	98	98.8
4	0	70.6	72.7	95.7	97.9	99
5	0	85.8	86.7	93.5	96.9	98.5
6	0	73	93.6	96.8	100	100
7	0	100	100	100	100	100
8	0	98	97.5	99.4	100	100

electron orbital energies of the HOMO and LUMO, respectively, where ($I = -E_{HOMO}$) and ($A = -E_{LUMO}$). The results in Table 4 showed that compounds **6** and **7** had the lowest potential ionization energy (5.60 and 5.57 eV, respectively), whereas compounds **1** and **2** had the largest affinity (2.43 and 2.51 eV, respectively). Clearly, compounds **6** and **7** are the best electron donors, while compounds **1** and **2** are the best electron acceptors.

The energy gap (ΔE) can be used as a gauge to measure the reactivity and stability of molecules. Low ΔE is an indicator of high reactivity and low stability. The lowest ΔE was seen for compound **7** (3.38 eV) followed by **8** (3.49 eV) and **6** (3.52 eV). On the other hand, the highest ΔE was recorded for compound **3** (3.72). Therefore, compounds **6–8** are highly polarizable and reactive.

For chemical hardness (η), compound **7** showed the lowest η (1.69) and compound **3** showed the highest (1.86). In addition, the lowest chemical softness (s) was observed for compound **3** (198.90) and compound **7** had the highest (219.29). Clearly, compound **7** is the softest and most reactive derivative compared to the others.

The electronic chemical potential (μ) can be used to represent the charge transfer from a system with a high electronic chemical potential to another with a lower potential. Compounds **6** (−3.85) and **7** (−3.89) had the highest μ, while **2** had the lowest (−4.33).

The reactivity of compounds could be predicted using the electrophilicity (ω) and nucleophilicity (N) indexes. For example, organic molecules can be classified based on their nucleophilicity (N) as strong ($N > 3$ eV), moderate ($2.0\text{ eV} \le N \le 3.0$ eV), and marginal ($N < 2.0$ eV) nucleophiles [29,34]. In addition, the ω of more than 2.0 eV is an indication of reactivity in a polar reaction [29,34]. Compound **7** is the strongest nucleophile ($N = 3.08$ eV), while compound **2** is the strongest electrophile ($\omega = 5.14$ eV). There was a very good correlation, correlation coefficient (r) = 0.94 (Figure 2), between the calculated N and the antioxidant efficiency (%E) at a dose of 0.5%, excluding

Table 4: HOMO and LUMO energy, energy gap ΔE, and global reactivity indices μ, ω, η, and N (eV) for curcumins **1–8**.

Compound	HOMO	LUMO	ΔE	η	s	μ	ω	N
1	−6.02	−2.43	3.59	1.80	206.15	−4.22	4.96	2.64
2	−6.15	−2.51	3.64	1.82	203.54	−4.33	5.14	2.51
3	−5.83	−2.11	3.72	1.86	198.90	−3.97	4.23	2.83
4	−5.77	−2.22	3.55	1.77	208.81	−3.99	4.49	2.89
5	−5.93	−2.27	3.67	1.83	202.03	−4.10	4.58	2.73
6	−5.60	−2.09	3.52	1.76	210.55	−3.85	4.21	3.05
7	−5.57	−2.20	3.38	1.69	219.29	−3.89	4.47	3.08
8	−5.72	−2.23	3.49	1.74	212.47	−3.97	4.53	2.94

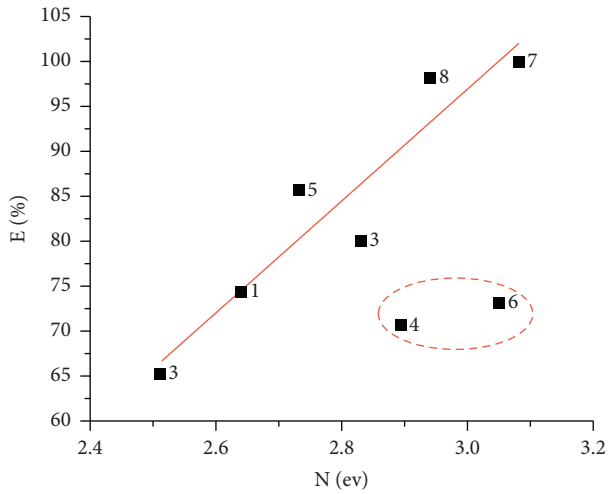


Figure 2: Correlation ($r = 0.94$) between the calculated nucleophilicity (N) and the antioxidant efficiency (%E).

compounds **4** and **6**. It can be concluded that the %E of the curcumin-like compounds increases when the nucleophilicity increases. In contrast, the %E increases when the electrophilicity is decreased. Clearly, compound **7** is the most reactive derivative and acts as an efficient antioxidant against oxidative degradation of LDPE. This finding agrees with the generated experimental data.

4. Conclusions

A series of eight curcumin analogues were prepared, and their antioxidant activities against thermal degradation of low-density polyethylene were investigated. The curcumin analogues showed high efficiency to inhibit the thermal degradation of low-density polyethylene. The efficiency of antioxidants ranged from very good to excellent. The analogue derived from vanillin showed the highest efficiency, presumably as a result of the presence of an extra electron-donor moiety (methoxy group) that attached in the *meta* position. Such a group could stabilize the free radical produced during the oxidation process. This conclusion was also confirmed theoretically from the result obtained from the analysis of the global reactivity.

Data Availability

The data used to support this study are included within the article.

Conflicts of Interest

The authors have no conflicts of interest.

Acknowledgments

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Supplementary Materials

Figure S1: FTIR spectrum of **1**. Figure S2: FTIR spectrum of **2**. Figure S3: FTIR spectrum of **3**. Figure S4: FTIR spectrum of **4**. Figure S5: FTIR spectrum of **5**. Figure S6: FTIR spectrum of **6**. Figure S7: FTIR spectrum of **7**. Figure S8: FTIR spectrum of **8**. Figure S9: ^{1}H NMR spectrum of **1**. Figure S10: ^{1}H NMR spectrum of **2**. Figure S11: ^{1}H NMR spectrum of **3**. Figure S12: ^{1}H NMR spectrum of **4**. Figure S13: ^{1}H NMR spectrum of **5**. Figure S14: ^{1}H NMR spectrum of **6**. Figure S15: ^{1}H NMR spectrum of **7**. Figure S16: ^{1}H NMR spectrum of compound **8**. (*Supplementary Materials*)

References

[1] I. Pleşa, P. V. Notingher, C. Stancu, F. Wiesbrock, and S. Schlögl, "Polyethylene nanocomposites for power cable insulations," *Polymers*, vol. 11, no. 1, p. 24, 2018.

[2] A. J. Peacock, *Handbook of Polyethylene*, Marcel Dekker, New York, NY, USA, 2000.

[3] T. R. Crompton, *Thermo-Oxidative Degradation of Polymers*, Smithers Rapra Technology, Shawbury, UK, 2010.

[4] B. Baum, "The Mechanism of polyethylene oxidation," *Journal of Applied Polymer Science*, vol. 2, no. 6, pp. 281–288, 1959.

[5] H. Zweifel, "Principles of oxidative degradation," in *Macromolecular Systems — Materials Approach*, pp. 1–40, Springer, Berlin, Germany, 1998.

[6] E. Feghali, L. Tauk, P. Ortiz, K. Vanbroekhoven, and W. Eevers, "Catalytic chemical recycling of biodegradable polyesters," *Polymer Degradation and Stability*, vol. 179, Article ID 109241, 2020.

[7] R. T. Conley, *Thermal Stability of Polymers*, Marcel Dekker, New York, USA, 1970.

[8] D. Granda-Restrepo, E. Peralta, R. Troncoso-Rojas, and H. Soto-Valdez, "Release of antioxidants from co-extruded active packaging developed for whole milk powder," *International Dairy Journal*, vol. 19, no. 8, pp. 481–488, 2009.

[9] M. Jamshidian, E. A. Tehrany, and S. Desobry, "Release of synthetic phenolic antioxidants from extruded poly Lactic acid (PLA) film," *Food Control*, vol. 28, no. 2, pp. 445–455, 2012.

[10] J. Zia, U. C. Paul, J. A. Heredia-Guerrero, A. Athanassiou, and D. Fragouli, "Low-density polyethylene/curcumin melt extruded composites with enhanced water vapor barrier and antioxidant properties for active food packaging," *Polymer*, vol. 175, pp. 137–145, 2019.

[11] G. Liang, X. Li, L. Chen et al., "Synthesis and anti-Inflammatory activities of mono-carbonyl analogues of curcumin," *Bioorganic & Medicinal Chemistry Letters*, vol. 18, no. 4, pp. 1525–1529, 2008.

[12] H. Lin, G.-X. Hu, J. Guo et al., "Mono-carbonyl curcumin analogues as 11β-hydroxysteroid dehydrogenase 1 inhibitors," *Bioorganic & Medicinal Chemistry Letters*, vol. 23, no. 15, pp. 4362–4366, 2013.

[13] T. Hosoya, A. Nakata, F. Yamasaki et al., "Curcumin-like diarylpentanoid analogues as melanogenesis inhibitors," *Journal of Natural Medicines*, vol. 66, no. 1, pp. 166–176, 2012.

[14] G. Deepa, R. Balamurugan, and P. Kannan, "Photoactive liquid crystalline polyesters based on bisbenzylidene and pyridine moieties," *Journal of Molecular Structure*, vol. 963, no. 2–3, pp. 219–227, 2010.

[15] S. S. Sardjiman, M. S. Reksohadiprodjo, L. Hakim, H. van der Goot, and H. Timmerman, "1, 5-Diphenyl-1, 4-pentadiene-3-ones and cyclic analogues as antioxidative agents. Synthesis and structure-activity relationship," *European Journal of Medicinal Chemistry*, vol. 32, no. 7–8, pp. 625–630, 1997.

[16] Z.-Y. Du, R.-R. Liu, W.-Y. Shao et al., "α-Glucosidase inhibition of natural curcuminoids and curcumin analogs," *European Journal of Medicinal Chemistry*, vol. 41, no. 2, pp. 213–218, 2006.

[17] A. M. Pana, V. Badea, R. Bănică et al., "Network reaction of 2, 6-bis(2-hydroxybenzilidene)cyclohexanone by external stimuli," *Journal of Photochemistry and Photobiology A: Chemistry*, vol. 283, pp. 22–28, 2014.

[18] A. Mazumder, N. Neamati, S. Sunder et al., "Curcumin analogs with altered potencies against HIV-1 integrase as probes for biochemical mechanisms of drug action," *Journal of Medicinal Chemistry*, vol. 40, no. 19, pp. 3057–3063, 1997.

[19] R. Vijayaraj, V. Subramanian, and P. K. Chattaraj, "Comparison of global reactivity descriptors calculated using various density functionals: a QSAR perspective," *Journal of Chemical Theory and Computation*, vol. 5, no. 10, pp. 2744–2753, 2009.

[20] M. T. Isa, A. S. Ahmed, B. O. Aderemi, R. M. Taib, and I. A. Mohammed-Dabo, "Effect of fiber type and combinations on the mechanical, physical and thermal stability properties of polyester hybrid composites," *Composites Part B: Engineering*, vol. 52, pp. 217–223, 2013.

[21] Z.-Y. Du, Y.-F. Jiang, Z.-K. Tang et al., "Antioxidation and tyrosinase inhibition of polyphenolic curcumin analogs," *Bioscience Biotechnology and Biochemistry*, vol. 75, no. 12, pp. 2351–2358, 2011.

[22] S. A. S. Alariqi, N. A. S. Al-Areqi, E. S. Alaghbari, and R. P. Singh, "Stabilization of γ-sterilized low-density polyethylene by synergistic mixtures of food-contact approval stabilizers," *International Journal of Integrated Care*, vol. 8, no. 2, pp. 145–156, 2017.

[23] N. Rouba, T. Sadoun, N. Boutagrabet, D. Kerrouche, S. Zadi, and N. Mimi, "Thermo-oxidation and biodegradation study of low-density polyethylene/starch films by IR spectroscopy," *Iranian Journal of Chemistry and Chemical Engineering (International English Edition)*, vol. 34, no. 4, pp. 69–78, 2015.

[24] A. D. Becke, "Density-functional thermochemistry. V. Systematic optimization of exchange-correlation functionals," *The Journal of Chemical Physics*, vol. 107, no. 20, pp. 8554–8560, 1997.

[25] M. J. Frisch, G. W. Trucks, H. B. Schlegel et al., "Gaussian 09," revision A.02," 2016, https://Gaussian.com/g09citation/.

[26] S. Shahab, F. H. Hajikolaee, L. Filippovich et al., "Molecular structure and UV–vis spectral analysis of new synthesized azo dyes for application in polarizing films," *Dyes and Pigments*, vol. 129, no. 9–17, pp. 9–17, 2016.

[27] N. Flores-Holguín, J. Frau, and D. Glossman-Mitnik, "A fast and simple evaluation of the chemical reactivity properties of the pristinamycin family of antimicrobial peptides," *Chemical Physics Letters*, vol. 739, 2020.

[28] M. Defranceschi and C. Le Bris, "Mathematical models and methods for ab initio quantum chemistry," *Springer Science & Business Media*, vol. 136, 2000.

[29] L. R. Domingo, M. Ríos-Gutiérrez, and P. Pérez, "Applications of the conceptual density Functional theory indices to organic chemistry reactivity," *Molecules*, vol. 21, no. 6, p. 748, 2016.

[30] D. Harkati, S. Belaidi, and B. Saleh, "A theoretical investigation on the structures, global and local reactivity descriptors of oxazolidine-2, 4-dione, Imidazolidine-2, 4-dione and thiazolidine-2, 4-dione," *Quantum Matter*, vol. 6, pp. 1–5, 2016.

[31] A. Zekri, D. Harkati, S. Kenouche, and B. A. Saleh, "QSAR modeling, docking, ADME and reactivity of indazole derivatives as antagonizes of estrogen receptor alpha (ER-α) positive in breast cancer," *Journal of Molecular Structure*, vol. 1217, Article ID 128442, 2020.

[32] A. Alsalme, T. Pooventhiran, N. Al-zaqri, D. J. Rao, S. S. Rao, and R. Thomas, "Modelling the structural and reactivity landscapes of tucatinib with special reference to its wavefunction-dependent properties and screening for potential antiviral activity," *Journal of Molecular Modeling*, vol. 26, no. 12, 2020.

[33] P. Jaramillo, L. R. Domingo, E. Chamorro, and P. Pérez, "A further exploration of a nucleophilicity index based on the gas-phase ionization potentials," *Journal of Molecular Structure: THEOCHEM*, vol. 865, no. 1–3, pp. 68–72, 2008.

[34] R. Srivastava, "Chemical reactivity theory (CRT) study of small drug-like biologically active molecules," *Journal of Biomolecular Structure and Dynamics*, vol. 39, no. 3, pp. 943–952, 2020.