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Original Article

Green Antioxidants: Synthesis and Scavenging Activity of Coumarin-Thiadiazoles as Potential Antioxidants Complemented by Molecular Modeling Studies

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ABSTRACT

Introduction: Coumarin is a natural product compound known for its medicinal properties. **Methods:** The rational design of 4-hydroxycoumarin functionalized thiadiazoles (3 and 4) was synthesized with tailor-made antioxidant properties. The strategy involves intra-molecular cyclization of 2-(coumarin-4-yloxy) acetic acid under reflux conditions. Antioxidant activity of synthesized compounds were performed using various *in vitro* assays against 1, 1-diphenyl-2-picrylhydrazyl (DPPH) radical and hydrogen peroxide (H_2O_2) scavenging. **Results:** The results revealed that tested compounds 3 and 4 are much higher than well-known antioxidant compound naming ascorbic acid. They showed good scavenging capacity against DPPH and hydroxyl radicals. Ab initio HF (Hartree–Fock) with 3-21G basis set for the title compounds demonstrated the correlation of scavenging activities and theoretical parameters (such as, dipole-moment, ionization-potential, electron-affinity and highest occupied molecular orbital). **Conclusion:** In conclusion Coumarins were successfully synthesized and were evaluated as antioxidants by DPPH and hydrogen peroxide assays and they were indicated that they had good scavenging activities. The synthesized antioxidants were investigated theoretically and also some quantum chemical parameters were calculated.

Key words: Coumarins, Hartree–Fock, Scavenging activities, Antioxidant, Picrylhydrazyl.

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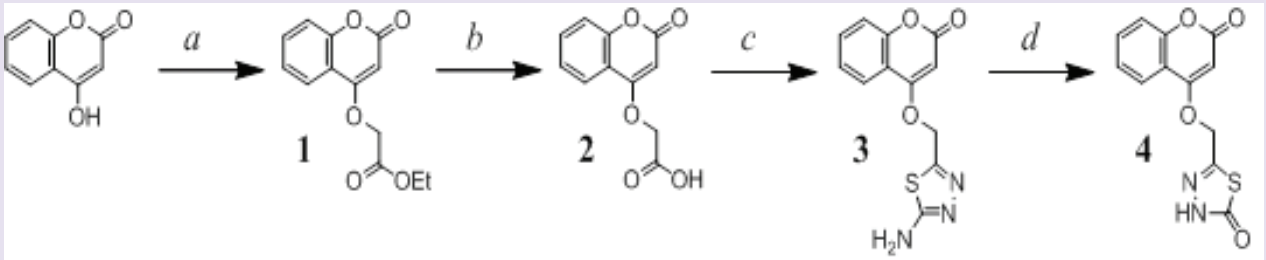
INTRODUCTION

Coumarins consists of an aromatic ring fused to a condensed pyrone ring,[1] are widespread in plant kingdom. Coumarin firstly isolated from tonka beans and had been used as a flavoring agent,[2] and it derivatives exhibit pharmacological activities, such as anticancer, anti-inflammatory,[3] anti-influenza, antituberculosis,[4] anti-HIV, antiviral,[5] antialzheimer[6] and antimicrobial activities.[7] Moreover, derivatives that functionalized with heterocyclic moieties such as azetidine, thiazolidine, thiazole could considerably increase the medicinal efficiency.[8,9] Free radicals are highly reactive atoms or molecules that have unpaired electron.[10,11] 4-hydroxycoumarin and thiadiazoles represent promising scaffolds in the medicinal chemistry field. The aim of this work was to find new chemical structures with antioxidant activity, we have designed new scaffolds in which the thiadiazoles fragment is partially incorporated in the 4-hydroxycoumarin moiety. The resulting 4-hydroxycoumarin–thiadiazoles scaffold by sharing the hydroxyl group of the pyrone ring of 4-hydroxycoumarin as in Scheme 1.

EXPERIMENTAL SECTION

All were supplied by Sigma-Aldrich and the purity checked by TLC (Thin Layer Chromatography). Infrared spectra were obtained on a Thermo Scientific, NICOLET 6700 FTIR spectrometer. Nuclear magnetic resonance spectra were obtained on a JEOL JNM-ECP 400. Elemental



a= Ethyl bromoacetate and potassium carbonate; b= Sodium hudroxide; c= Phosphorus oxychloride and Hydrazinecarbothioamide; d= Sodium nitrite and hydrochloric acid.

Scheme 1: Syntheses of Coumarin-Thiazoles (3 and 4).

microanalysis, was carried out using a model 5500-Carlo Erba C.H.N elemental analyzer.

Synthesis of Ethyl 2-((coumarin-4-yl)oxy)acetate (1) and 1-(2-((coumarin-4-yl)oxy)acetyl)hydrazine (2). These compounds were synthesized in excellent yield according to the previously described procedures.[12,13]

Chemistry

Synthesis of 4-[(2-amino-1, 3, 4-thiadiazol-5-yl)methoxy]coumarin (3). Phosphoryltrichloride (20 ml) was added drop wise with stirring to 2-((coumarin-4-yl) oxy) acetic acid (2) (0.05 mol), for 1 h at room temperature. Hydrazinecarbothioamide (4.56 g, 0.05 mol) was added and the mixture was refluxed for 5 h. Poured on to ice, after 4 h., stir for 15 min. then heated under reflux for 30 min.[14] Cooling, neutralized with potassium hydroxide, filtered, washed with water, dried and crystallized from dichloromethane yields 55%, m.p. 99°C; ^{1}H-NMR: δ 5.62 (s, 1H, C=C-H), δ 4.91 and δ 5.33 (d, 2H, t, 2H, for OCH3), δ 7.237.87 (m, 1H, C-H aromatic ring), δ5.21 (s, NH); FT-IR: 3314.5 and 3375.1 cm^{-1} (H, amine), 291.2 cm^{-1} (C-H alkane); 3079.1 cm^{-1} (C-H aromatic), 1752.3 cm^{-1} (C=O, lactone), 1591.1 cm^{-1} (C=N, imine), 1635.3 cm^{-1} (C=C aromatic); Anal. Calcd. for $C_{12}H_9N_3OS$: C 52.36%, H 3.30%, N 15.26%. Experimentally: C 51.64% H 2.92% and N 14.94%.

Synthesis of 5-[(coumarin-4-yloxy) methyl]-2-oxo-1, 3, 4-thiadiazol (4). To 4-[(2-amino-1,3,4-thiadiazol-5-yl) methoxy] coumarin (3) (0.01 mol) and hydrochloric acid (5 ml) in cold water (20 ml) suspension in ice-bath added drop wise 10% aqueous sodium nitrite solution (10 ml) with continuous stirring over a period of 20 min.[15] The temperature was then allowed to rise to room temperature and the mixture was heated to boiling for 10 min, cooled and allowed to stand overnight. The separated crude product was filtered, washed with water, dried and recrystallized from ethanol to yield 40% product with m.p. 112°C; ^{1}H-NMR (CDCl):δ 5.85 (s, 1H, C=C-H), δ 4.93 and δ 5.33 (d, 2H, t, 2H, for OCH_3), δ 7.307.86 (m, 1H, C-H aromatic ring), δ 5.42 (s, H, amine); IR: 3201 cm^{-1} (N-H, amine), 1758.1 cm^{-1} (C=O, lactone), 1588.9 cm^{-1} (C-H alkane); 3078.9 cm^{-1},(C=N, imine),2891 cm^{-1} (C-H aromatic), 1715.2 cm^{-1} (C=O lactame), 1619.2 (C=C); Anal. Calcd. for $C_{12}H_9N_3OS$: C 52.17%, H 2.92 and 10.14%. Experimentally: C 50.99% H 2.71 and 9.46%.

Antioxidant activity (1,1-Diphenyl-2-picrylhydrazyl) (DPPH) Radical Scavenging Activity

Antioxidant properties of synthesized coumarin-thiazoles (3 and 4) were tested spectrophotometrically using 2,2-diphenyl-1-picrylhydrazyl radical.[15,16] Initially, 0.1 mL of different concentrations of synthesized compounds 250, 500, and 1000 μg/mL and standard ascorbic acid were mixed with 1 mL of 0.2 mM DPPH dissolved in methanol. The reaction mixture was incubated in the dark for 30 min at 28°C. The control experiment was carried out as above without the test samples. The DPPH radical scavenging activity was determined by measuring the absorbance at 517 nm using the UV-VIS spectrophotometer. The reduction of DPPH radical scavenger was calculated relative to the measured absorbance of the control using equation 6.

$$\text{Scavenging effect \%} = \frac{A_0 - A_1}{A_0} \times 100$$

where A_0 is the absorbance of the control reaction, and A_1 is the absorbance in the presence of the samples or standards.

Hydrogen Peroxide Scavenging Activity

A solution of hydrogen peroxide (40 mM) was prepared in phosphate buffer (pH 7.4). Various concentrations (250, 500 and 1000 g mL^{-1}) of the synthesized compounds (or ascorbic acid) were added to a hydrogen peroxide solution (0.6 mL, 40 mM). The absorbance of hydrogen peroxide at 230 nm was determined after 10 min against a blank solution containing phosphate buffer without hydrogen peroxide.[17] The hydrogen peroxide percentage scavenging activity was calculated using equation 6.

Quantum Studies

The molecular representation sketch of the reference compound was plotted using Chem Bio Office 2010 software. All the quantum chemical calculations were performed using the HF methodology with 3–21G basis set.

Statistical analysis

The results were expressed as mean ± standard deviation and the statistical significance of differences were determined utilizing one-way analysis of variance (ANOVA) using the SPSS 17.0 statistical software program. Differences were considered significant at $P<0.05$. The values are presented as mean ± SD (n=3).

RESULTS AND DISCUSSION

Antioxidant assay

The free radical scavenging activity of compound 3 and 4 was done by DPPH and H_2O_2 methods. Antioxidant activity of the test compounds 3 and 4 was examined by measuring radical scavenging effect of DPPH (Figure 1) and H_2O_2 (Figure 2) radicals. The results of the free radical scavenging activity of the compounds at different concentrations are shown in Figures 1 and 2. It was observed that the free radical scavenging activity of 3 and 4 was concentration dependent. Compound 3 has exhibited very good scavenging activity, whereas compound 4 has showed moderate activity. The antioxidant activity of the compound 4 was comparatively high when compared to compound 3 due the presence of carbonyl group that tautomerized to enol form. In case of compound 3 hydrogen of OH group (enol form) donates a proton to the DPPH (or peroxide) and converts itself into the stable free radical and in compound 4 the hydrogen of amino group is more acidic hence, hydrogen could be easily donated to the DPPH (or peroxide) free radical and convert itself into the stable free radical.

DPPH scavenging activity

The highest inhibition for tested compounds (3 and 4) was for the highest concentration that was found at 1000 μg/mL (Figure 1). The highest efficiency scavenging activity was for compound 4 (86.0 ± 5.0), followed by compound 3 (82.0 ± 7.00). Ascorbic acid was used as standard drugs with percentage inhibition of 91.00 ± 1.5. The hydrogen-donating activity, measured utilizing DPPH as the hydrogen acceptor, demonstrated that a strong association could be found between the concentration of the coumarin molecule and the rate of inhibition.[13,18]

H_2O_2 scavenging activity

Hydrogen peroxide can be highly reactive when crossing cell membrane and form hydroxyl radical. Figure 2 showed that compounds 2 and 3 demonstrated a strong scavenging activity against hydrogen peroxide at a very low concentration of 250 μg/mL we observed a concentration dependent decrease. A very weak inhibitory activity was found in compounds 3 (27.0 ± 3.00). The highest concentration was found at 1000 μg/mL (Figure 2). The best percentage scavenging activity was shown by compound 4 (73.0 ± 5.00), followed by compound 3 (68.0 ± 7.00). Ascorbic acid was used as standard drugs with percentage inhibition of 70.00 ± 2.5.

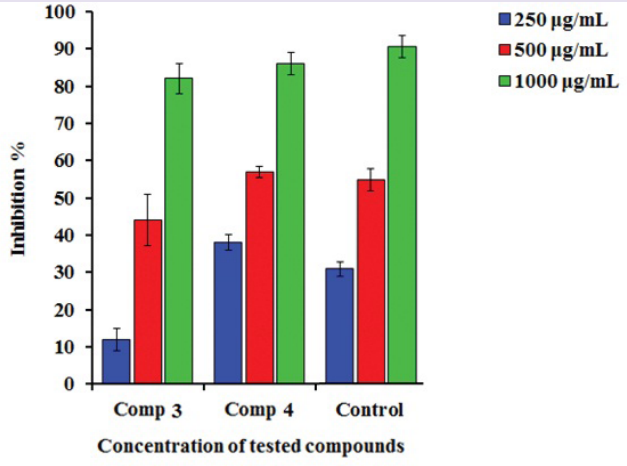


Figure 1: Percentage inhibition of DPPH scavenging activity of synthesized compounds (3,4) in comparison to ascorbic acid. n=3. Error bars indicate standard deviation.

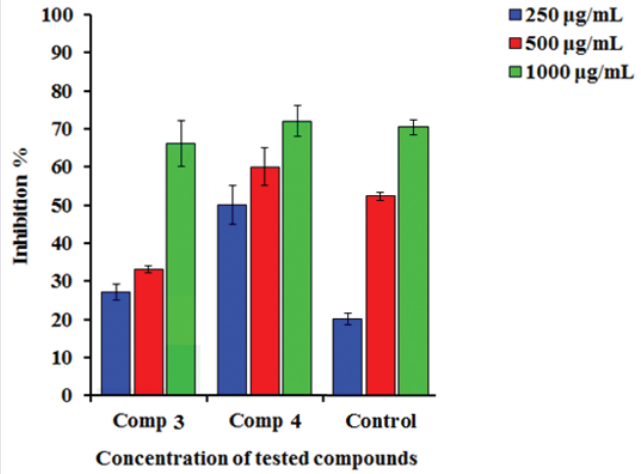


Figure 2: Percentage inhibition of hydrogen peroxide scavenging activity of synthesized compounds (3,4) in comparison to ascorbic acid. n=3. Error bars indicate standard deviation.

Suggested mechanism for compounds 3 and 4 as antioxidants

The suggested antioxidant mechanism (Figure 3) for synthesized coumarin-thiazoles, as shown in Figure 3, relies on the hydrogen atom of hydroxyl (enol form) (for compound 4) and hydrogen atom of amino group (for compound 3), which were under the influence of resonance and inductive effects. The resonance and inductive effects facilitates the release of hydrogen, resulting in stability of the molecule.[18] Coumarin-thiazoles have scavenging activities due to the stability of the free radical intermediates of these compounds. An abstraction of a hydrogen atom from hydroxyl (enol form) and amine group may occur easily.[19] The presence of carbonyl groups, enhances the antioxidant activity. The steric hindrance enhances the antioxidant activity.[20,21]

Molecular Modeling Studies

To understand the antioxidant activity electronic levels namely HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied

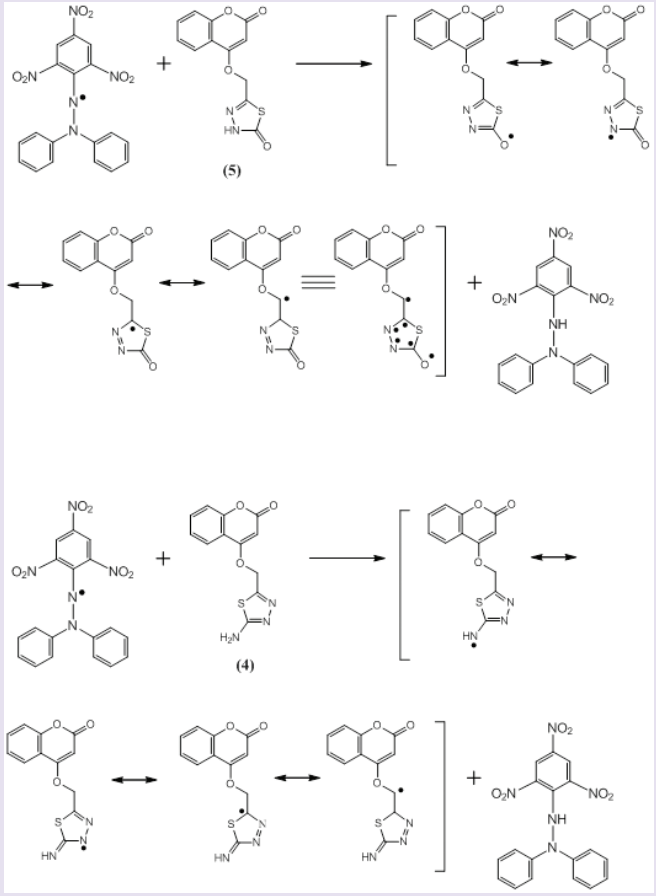


Figure 3: The reaction scheme between DPPH free radicals and compounds 3 and 4.

molecular orbital) for compounds 3 and 4, HF (Hartree–Fock) based quantum chemical studies has been carried out with the basis set 3-21G. The energies EHOMO and ELUMO in electron volt values were showed in Figure 4. The compound with higher antioxidant activity can be confirmed according to the values of EHOM and ELUMO. In our work we were using the methods DPPH and peroxide. These methods showed clearly that the scavenging activities of compound 4 was higher than compound 3 and ascorbic acid because of the electron withdrawing of carbonyl and resonance effect. Theoretically it was been concluded that EHOMO is a good indicator of scavenging activities and the scavenging activities do not depend on ELUMO. The varieties in activities of compounds 3 and 4, as antioxidant were showed in the calculated EHOMO value, is mostly attributed to pi-electrons delocalization, that lead to stability of the free radicals gained after proton abstraction so that, pi electrons delocalized present in compounds 3 and 4 also occur in the corresponding radical. Electron density of HOMO could be fully considered to realize the relationship between the delocalizing electrons and activities of free radicals.[22]

For compounds 3 and 4, highest occupied molecular orbital are delocalized over whole molecule, that harmonizes to the orbital holding unshared electrons. Spin density of the free radicals that had been created from compounds 3 and 4 were compared. Highly delocalization, means easier the creation of free radicals. The spin density appears to be slightly more delocalized for the radicals issued from Compound 4 than from compound 3. The HOMO (highest occupied molecular orbital) energies of

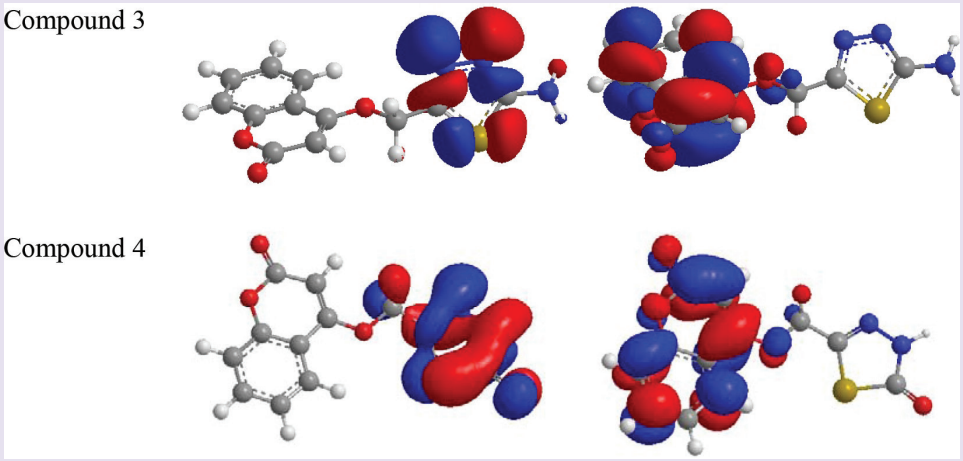


Figure 4: Highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital of compounds 4 and 5.

target compounds 3 and 4 in addition to ascorbic acid are computed as −8.255 eV, −10.18 eV and −10.772 eV respectively. While the LUMO energies for target compounds 3 and 4 and ascorbic acid are computed as −3.762 eV, -3.745 eV and −1.115 eV respectively. The energy gaps for the compounds 3 and 4 as well as ascorbic acid were respectively as fellows (4.493 eV, 6.435 eV and 9.655 eV) and this might be due to shifted absorption toward blue spectrum. The electron delocalizing for carbonyl group for compound 4 reveal the variation between HOMO and LUMO of compounds 3 and 4. Glance comparison of potential for compounds 3, 4 and ascorbic acid as antioxidant according to band gaps and It was clear that that highest band gap was for ascorbic acid (control) which was 8.564 eV and then compound 4, and this is highly compatible with experimentally results as in Figure 2. Dipole moment values of compound 3 and 4 in addition to ascorbic acid demonstrate that all of them are polar molecules and soluble in polar solvents. IP (Ionization potential) afford the understanding about initial energy for releasing an electron from the molecules[23] that mean inverse relation for antioxidant and IP (equation 1).

$$IP = -E_{HOMO} \quad (1)$$

EA (Electron affinity) is the amount of energy launched when an electron absorbed by a molecule (equation 2). Higher EA lead to easily absorb electrons in other word the positive relation with antioxidant.

$$EA = -E_{LUMO} \quad (2)$$

η (Hardness) is charge transfers resistance and S (softness) is the measure of the capacity of an atom to receiving electron (equations 3 and 4).

$$\eta = \frac{1}{2}(E_{HOMO} - E_{LUMO}) \quad (3)$$

$$S = -\frac{2}{(E_{HOMO} - E_{LUMO})} \quad (4)$$

μ (electronegativity) defined as the capacity to attract electrons (equations 5) in the chemical bond

$$\mu = -\frac{1}{2}(E_{HOMO} + E_{LUMO}) \quad (5)$$

Table 1 described clearly the potential values of the above Parameters. These parameters can be supported the good antioxidant potential. The

Table 1: Electronic Properties of synthesized coumarins title molecule were obtained by using HF method with 3-21G basis set

Parameters	Compound 3	Compound 4	Ascorbic acid
Dipole moment Depy	4.891	7.316	9.549
Ionization potential (IP) eV	8.255	10.180	10.772
Electron affinity (EA) eV	3.762	3.745	1.115
Hardness (η)	2.246	3.217	4.827
Softness (S)	0.445	0.310	0.207
Electro negativity(μ)	6.008	6.962	5.9435
EHOMO	−8.255	−10.180	−10.772
ELUMO	−3.762	−3.745	−1.115
Band gap=E_{HOMO}-E_{LUMO}	4.493	6.435	9.655

experimental and calculated theoretical parameters were compared with each other. The calculated data were compared with experimental values using HF with the basis set 3-21G. It was found to be a good correlation between experimental and calculated data. In addition, HOMO and LUMO analysis of title molecule were calculated using corresponding methods with 3-21G basis set. The calculated HOMO-LUMO energies were used to calculate some properties of title molecule.

CONCLUSION

Coumarins were successfully synthesized and characterized by using spectroscopic techniques (FT-IR and NMR). Antioxidant activities were evaluated by DPPH and hydrogen peroxide assays and the results indicated that they have good scavenging activities. The antioxidant activities for the title compounds with the control were investigated theoretically by quantum approach using HF (Hartree–Fock) method and also some quantum chemical parameters were calculated.

ACKNOWLEDGMENTS

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CONFLICT OF INTEREST

The authors have declared that no competing interests exist.

ABBREVIATION USED

DPPH: 1-diphenyl-2-picrylhydrazyl; **EA:** Electron affinity; **eV:** electorn volt; **FT-IR:** Fourier transform infrared; **HF:** Hartree–Fock; **H_2O_2:** radical and hydrogen peroxide; **HOMO:** Highest occupied molecular orbital; **IP:** Ionization potential; **LUMO:** lowest unoccupied molecular orbital; **η:** Hardness; **S:** Softness; **μ:** negativity; **NMR:** Nuclear magnetic resonance.

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SUMMARY

- Synthesis of coumarin derivatives has been described by simple and efficient protocol.
- Synthesized coumarins were Characterization spectroscopically.
- Synthesized coumarins were screened for antioxidant activities and they showed excellent antimicrobial activity.
- Synthesized antioxidants were studied theoretically by Hartree-Fock with 3-21G basis set.
- Theoretical studies for these synthesized antioxidants demonstrated the correlation of scavenging activities and theoretical parameters.

ABOUT AUTHOR

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