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Synthesis, isomorphism, and polymorphism of new (2*E*,4*E*)-1-(5-methyl-1-aryl-1*H*-1,2,3-triazol-4-yl)-5-phenylpenta-2,4-dien-1-ones

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trans-cinnamaldehyde
Polymorph
Synthesis

ABSTRACT

The Claisen–Schmidt condensation of 1-aryl-4-acetyl-5-methyl-1,2,3-triazoles and *trans*-cinnamaldehyde in ethanolic sodium hydroxide (10 %) at room temperature gave (2*E*,4*E*)-1-(5-methyl-1-aryl-1*H*-1,2,3-triazol-4-yl)-5-phenylpenta-2,4-dien-1-ones in high yields. The influence of fluoro, chloro, and nitro substituents on crystal packing has been assessed by exploring molecular electrostatic properties and intermolecular interactions. Close C–H...O, C–H...N, and C–H... π interactions occur in these compounds. Isomorphism and polymorphism have been observed.

1. Introduction

Chalcones (1,3-diaryl-2-propen-1-ones) are open-chain flavonoids that are widely biosynthesized in plants. Chalcones participate in plant defense mechanisms to combat reactive oxygen species to enable the plant to survive. In addition, they prevent molecular damage, such as harm caused by microorganisms, insects, and animals [1–4]. Chalcones are synthesized using the Claisen–Schmidt or Aldol condensation reaction [5]. They have anti-inflammatory, antibacterial, antifungal, antidiabetic, and anticancer activities. They are linked to improvement in vision, memory, joint and muscle discomfort, sleep, and liver and kidney function. Additionally, they are associated with the prevention of cancer, strengthening of the immune system, and beautification of skin and hair [6–9]. 1-(4-Methylphenyl)—5-phenylpenta-2,4-dien-1-one is an optically active molecule [10], and 1,5-diphenylpenta-2,4-dien-1-ones have been shown to be potent and selective monoamine oxidase-B inhibitors [11].

The 1,2,3-triazole ring is a significant pharmacophore system among nitrogen-containing heterocycles. Tazobactam/ceftolozane, radezolid, cefatrizine, tertbutyldimethylsilylspiroaminoxathioledioxide, and carboxyamidotriazole are examples of pharmaceutical drugs containing 1,2,3-triazole ring systems [12–14]. Many 1,2,3-triazole-containing

heterocycles showed potential as biologically active agents and in various applications. For example, 4-(1,2,3-triazol-1-yl) salicylic acids have been synthesized in the presence of a copper catalyst. The synthesized derivatives showed potential against cancer cell lines [15]. Various 1,2,3-triazolyl chalcones have been obtained in high yields and showed potential as antidiabetic [16], antifungal [17], antioxidant [18], and anticancer agents [18,19]. Moreover, 1,2,3-triazoles having various electron-withdrawing substituents showed fluorescent activity [20].

The 1,2,3-triazole moiety can be obtained readily using a click chemistry reaction involving copper- or ruthenium-catalyzed azide-alkyne cycloaddition reactions [21,22]. In previous work, we have reported the X-ray crystal structures of related heterocycles [23–26]. Here, we report the synthesis of three 5-phenylpenta-2,4-dien-1-ones containing the 1*H*-1,2,3-triazole moiety and the elucidation of their structure.

The three compounds are differentiated through derivatization of the phenyl ring attached to the 1,2,3-triazole by fluoro, chloro, and nitro substituents. The substituents modify the types of interactions the molecules can participate in with, for example, biological systems. Examination of the crystalline state provides insight into the effect of different substituents on interactions with the molecules that may be involved. This understanding can be applied in the practice of crystal

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Table 1

Crystal and structure refinement data.

	3	4(i)	4(ii)	5
Formula	C ₂₀ H ₁₇ N ₃ O	C ₂₀ H ₁₆ FN ₃ O	C ₂₀ H ₁₆ FN ₃ O	C ₂₀ H ₁₅ ClN ₄ O ₃
FW	315.36	333.36	333.36	394.81
T (K)	296(2)	293(2)	293(2)	293(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Orthorhombic	Monoclinic
Space group	P $\bar{1}$	P $\bar{1}$	Pbca	P2 ₁
a (Å)	6.6006(4)	6.6018(5)	7.5145(4)	8.2807(7)
b (Å)	7.6391(6)	7.6134(5)	12.8299(6)	13.6677(9)
c (Å)	16.4372(9)	16.7531(12)	34.6315(17)	9.0148(8)
α (°)	93.021(5)	93.288(5)	90	90
β (°)	98.508(5)	96.931(6)	90	111.540(10)
γ (°)	91.199(6)	91.409(5)	90	90
V (Å ³)	818.20(9)	834.10(10)	3338.8(3)	949.02(15)
Z	2	2	8	2
Calc. density (Mg/m ³)	1.280	1.327	1.326	1.382
Abs. coeff. (mm ⁻¹)	0.081	0.092	0.092	0.230
Crystal size (mm ³)	0.55×0.36×0.19	0.36×0.16×0.07	0.45×0.28×0.14	0.48×0.30×0.21
Reflections collected	6688	13,945	30,714	8849
Independent refs	3815	4182	4391	4488
R(int)	0.0226	0.0351	0.0409	0.0212
Parameters	219	227	227	254
Goodness-of-fit on F ²	1.038	1.052	1.115	1.096
R ₁ [I>2σ(I)]	0.0538	0.0578	0.0580	0.0485
wR ₂ [I>2σ(I)]	0.1159	0.1416	0.1472	0.1045
R ₁ , wR ₂ (all data)	0.0906	0.1133	0.0968	0.0873
R ₁ , wR ₂ (all data)	0.1374	0.1732	0.1686	0.1243
Abs. structure param	—	—	—	0.03(3)
Extinction coefficient	0.024(3)	—	—	—
Peak and hole (e.Å ⁻³)	0.183 and -0.143	0.161 and -0.184	0.158 and -0.182	0.245 and -0.289

engineering to design materials with desired chemical and physical properties [27–29], as well as in understanding interactions in biological systems. This study is pertinent to biological systems, where weak interactions can be very influential [30–32].

2. Materials and methods

2.1. General

Chemicals were purchased from Merck (Gillingham, UK). A Cole-Parmer melting point apparatus (Illinois, USA) was used to determine melting points. A Bruker Tensor 27 FTIR spectrometer (Tokyo, Japan) was used to record IR spectra. The NMR spectroscopy was performed on a JEOL NMR 500 MHz spectrometer (Tokyo, Japan) in dimethyl sulfoxide (DMSO-*d*₆) at 500 (proton) and 125 MHz (carbon). The NRC-Fine Organic Chemicals Unit at the National Research Centre, Egypt, provided compounds **1a–c** that were synthesized based on a reported procedure [20,33].

2.2. Preparation triazoles 1a–c

A mixture of appropriate aryl azide (18 mmol), acetylacetone (18

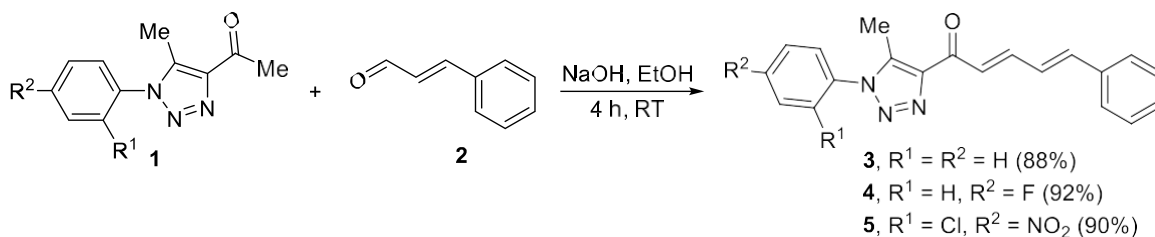
mmol, 1.8 g), and potassium carbonate (K₂CO₃; 57 mmol, 8.0 g) in dry EtOH (45 mL) was refluxed for 30 min. The mixture was cooled down to 25 °C, poured into ice H₂O (200 mL), and stirred for 1 hour. The solid produced was removed by filtration, washed with H₂O, and recrystallized from EtOH to give **1a–c** in 88–90 % yields [20,33].

2.3. Synthesis of chalcones 3–5

A mixture of **1a–c** (5 mmol) and **2** (5 mmol, 0.66 g) in EtOH (15 mL) and ethanolic NaOH (10 mL; 10 %) was stirred for 4 min, followed by the addition of cold water (150 mL) and stirred overnight. The resulting solid was filtered, dried, and recrystallized from DMF to yield **3–5**. The two types of crystals of **4** were obtained through fractional crystallization from DMF.

2.3.1. (2E,4E)—1-(5-Methyl-1-phenyl-1H-1,2,3-triazol-4-yl)—5-phenylpenta-2,4-dien-1-one (**3**)

Yield: 88 %, MP 167–168 °C. IR (KBr): 3057, 3021, 1665, 1595, 1551, 1496, 1419, 1382, 1312, 1295, 1236 cm⁻¹. ¹H NMR: 2.57 (s, 3H, Me), 7.19–7.43 (m, 4H, 4H), 7.60–7.95 (m, 10H, 2Ph). ¹³C NMR: 9.9, 125.4, 126.3, 127.3, 127.4, 128.8, 129.2, 129.7, 130.1, 135.0, 136.0, 138.7, 142.1, 143.0, 143.5, 183.4. Anal. Calcd. for C₂₀H₁₇N₃O (315.38): C, 76.17; H, 5.43; N, 13.32. Found: C, 76.28; H, 5.65; N, 13.38 %.



Scheme 1. Synthesis of heterocycles 3–5.

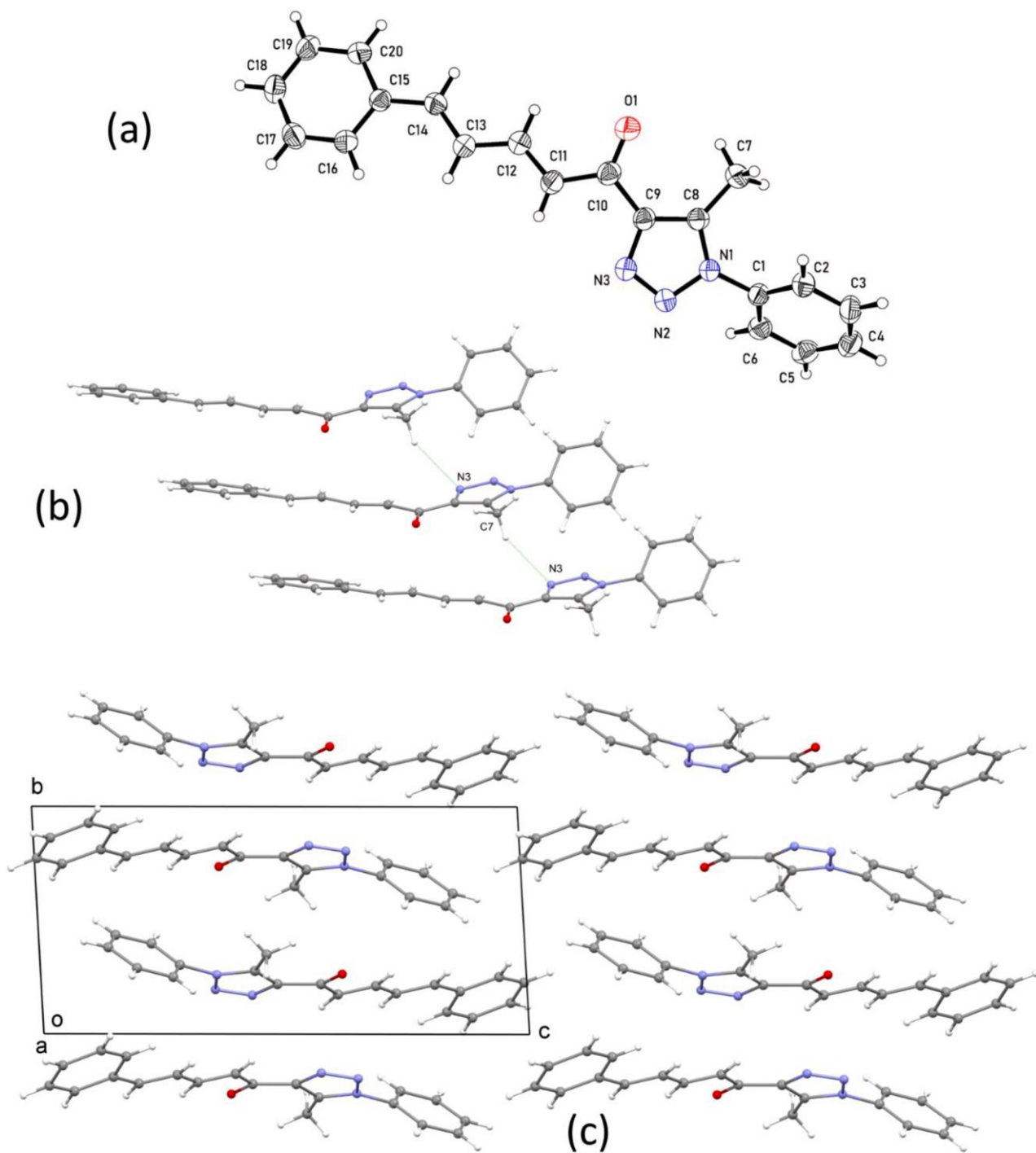


Fig. 1. (a) An ortep representation of 3 showing a 50 % probability of atomic displacement ellipsoids, (b) a segment of the structure showing C-H...N contacts as green dotted lines, and (c) crystal packing viewed down the a axis.

Table 2
Intramolecular twist angles ($^{\circ}$) between planar groups.

	3	4(i)	4(ii)	5
(F, Nc) Phen/Mtriac	47.49(5)	47.10(5)	47.85(5)	82.08(8)
Mtriac/Butdi	15.56(21)	14.91(22)	1.10(25)	8.05(66)
Butdi/Phen2	6.36(25)	8.93(26)	3.21(25)	1.99(73)

2.3.2. (2E,4E)—1-(1-(4-Fluorophenyl)—5-methyl-1H-1,2,3-triazol-4-yl)—5-phenylpenta-2,4-dien-1-one (**4**)

Yield: 92 %, MP 190–192 $^{\circ}$ C. IR (KBr): 3055, 3025, 1680, 1654, 1597, 1579, 1442, 1367, 1320, 1299, 1230, 1217 cm^{-1} . ^1H NMR: 2.50 (s, 3H, Me), 7.20–7.75 (m, 13H, Ar, 4 CH). ^{13}C NMR: 9.9, 116.7 (d, 38.8 Hz), 126.2, 127.4 (d, 16.3 Hz), 127.9, 128.1, 128.6, 128.9, 129.3, 136.0,

139.0, 142.2, 143.0, 143.6, 162.6 (d, 410.0 Hz), 183.6. Anal. Calcd. for $\text{C}_{20}\text{H}_{16}\text{FN}_3\text{O}$ (333.37): C, 72.06; H, 4.84; N, 12.61. Found: C, 72.17; H, 4.99; N, 12.77 %.

2.3.3. (2E,4E)—1-(1-(2-Chloro-4-nitrophenyl)—5-methyl-1H-1,2,3-triazol-4-yl)—5-phenylpenta-2,4-dien-1-one (**5**)

Yield: 90 %, MP 218–220 $^{\circ}$ C. IR (KBr): 3069, 1656, 1597, 1581, 1524, 1496, 1422, 1397, 1304, 1290, 1235 cm^{-1} . ^1H NMR: 2.47 (s, 3H, Me), 7.21–8.77 (m, 10H, Ar, 2CH), 8.09 (d, 15.0 Hz, 1H, CH), 8.46 (d, 15.0 Hz, 1H, CH), 8.66 (s, 1H, Ar). ^{13}C NMR: 9.3, 123.8, 125.8, 126.0, 127.2, 127.4, 128.9, 129.3, 131.0, 131.9, 136.9, 137.3, 140.4, 142.4, 142.7, 144.1, 149.3, 183.1. Anal. Calcd. for $\text{C}_{20}\text{H}_{15}\text{ClN}_4\text{O}_3$ (394.82): C, 60.84; H, 3.83; N, 14.19. Found: C, 60.96; H, 3.92; N, 14.32 %.

2.4. X-Ray crystal structure determination

Diffraction data were recorded at room temperature on an Agilent SuperNova Dual Atlas single-crystal diffractometer with mirror-monochromated Mo radiation. Structure solution calculations were carried out using SHELXT [34] and refinement by SHELXL [35]. Anisotropic displacement parameters were utilized for nonhydrogen atoms during refinement. Idealized geometry and a riding model were applied for the refinement of the hydrogen atoms. The displacement parameters for the hydrogen atoms were set to either 1.2 or 1.5 times the Ueq value of the atom to which they are bonded. The crystal and structure refinement data are shown in Table 1. The crystal structures have been deposited in the CSD under the reference numbers CCDC 2,321,106–2,321,109 (See Supplementary Material).

2.5. Electrostatic potentials and Hirshfeld surface calculations

The input files for electrostatic potential calculation were prepared using Avogadro [36]. The electron density calculation was performed

using the RHF/631G(dp) basis set in Gamess [37] and analyzed using Macmolplot [38]. The Hirshfeld surface was generated using CrystalExplorer17 [39].

3. Results and discussion

3.1. Synthesis

Schmidt condensation of 1-aryl-4-acetyl-5-methyl-1,2,3-triazoles **1a–c** and *trans*-cinnamaldehyde **2** in ethanolic sodium hydroxide (10 %) at room temperature for 4 h gave the corresponding (2E,4E)—1-(5-methyl-1-aryl-1H-1,2,3-triazol-4-yl)—5-phenylpenta-2,4-dien-1-ones **3–5** in 88–92 % yields (Scheme 1). 1,2,3-Triazoles **1a–c** were prepared

based on literature procedures from the reaction of acetylacetone and appropriate aryl azide in the presence of K_2CO_3 in boiling EtOH [20,33].

The IR spectra for triazoles **3–5** showed absorption bands at 3069–3021 cm^{-1} region due to the C–H stretching of alkenes. Also, the carbonyl groups showed strong absorption bands in the range of 1680 to 1654 cm^{-1} . Meanwhile, the C=C absorption bands appeared in the 1597–1551 cm^{-1} region. The methyl protons of **3–5** appeared as singlets in the 2.47–2.57 ppm region of the ^1H NMR spectra. Meanwhile, the four alkene protons appeared at a high field (7.19–7.75 ppm). The ^{13}C NMR spectra of triazoles **3–5** showed the methyl carbons at high field (9.3–9.9 ppm) and the carbonyl group carbons at low field (183.1–183.6 ppm). The ^{13}C NMR spectrum of **4** showed the coupling between the fluorine and the carbons of the aryl ring. The carbons at positions 3/5, 2/6, and 4 appeared as doublets at 116.7 ($J = 38.8$ Hz), 127.4 ($J = 16.3$ Hz), and 162.6 ppm ($J = 410.0$ Hz), respectively. In addition, ^{13}C NMR spectra of **3–5** showed all other carbons at the expected chemical shifts (See Section 2.3 for details).

3.2. Crystal structure discussion

3.2.1. Crystal structure of 3

The crystal structure of **3** is triclinic, space group $P\bar{1}$, with one molecule in the asymmetric unit (Fig. 1a). The molecule comprises four planar segments, namely phenyl (Phen, C1–C6), methyltriazole-carbaldehyde (Mtriac, C7–C10, N1–N3, O1), butadienyl (Butdi, C11–C14) and phenyl (Phen2, C15–C20) groups. The plane of the methyltriazole-carbaldehyde group is twisted from the phenyl group by a twist angle Mtriac/Phen of 47.49(5) $^{\circ}$ (Table 2). The butadienyl (C11–C14) segment is in (E,E) conformation and is twisted slightly from the methyltriazole-carbaldehyde group, as the Butdi/Mtriac twist angle of 15.56(21) $^{\circ}$ shows. The butadienyl and second phenyl (Phen2) groups are essentially coplanar, with a Butdi/Phen2 twist angle of 6.36(25) $^{\circ}$. The largest deviation from the least-squares plane through both

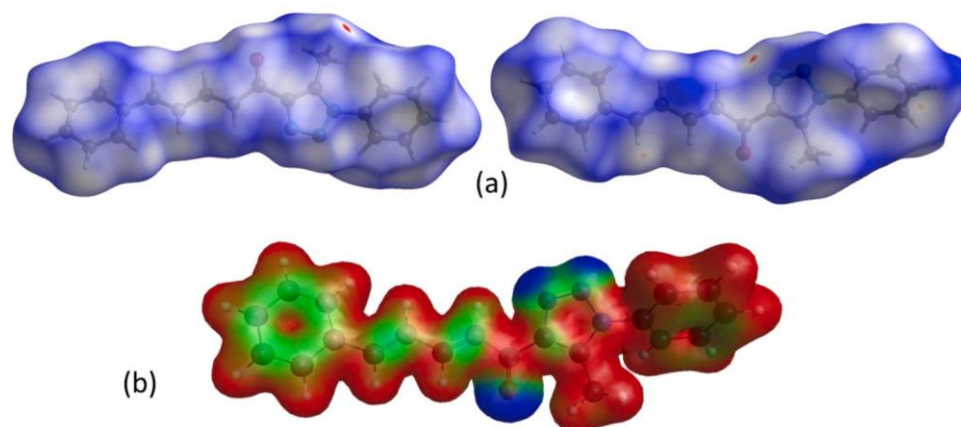


Fig. 2. (a) Two views of the Hirshfeld surface with close intermolecular contacts are highlighted in red for the molecule in the crystal structure of **3**. (b) The electron density surface with positive and negative electron density shown in red and blue, respectively.

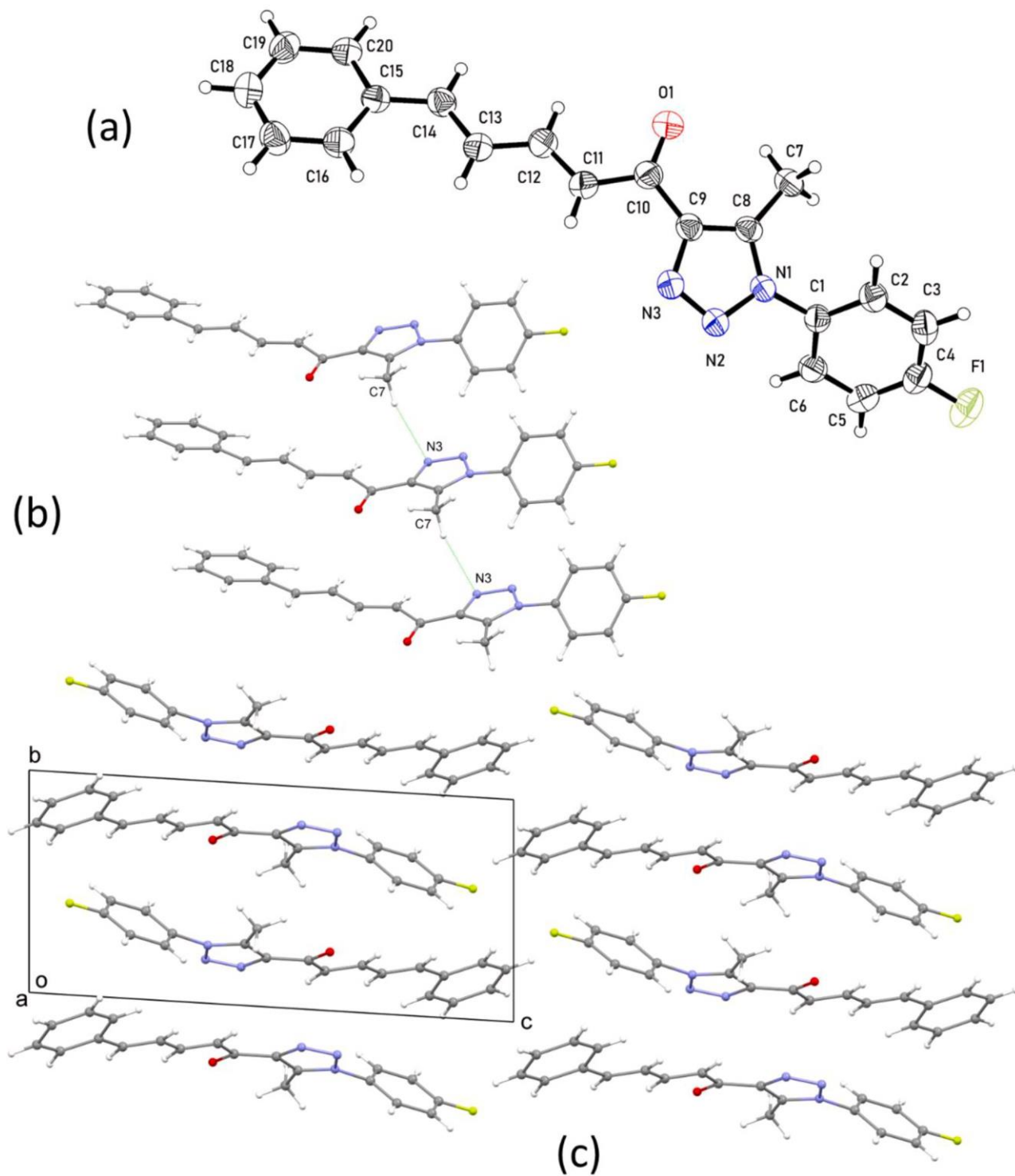


Fig. 3. (a) An ortep representation of the molecule in structure 4(i) showing a 50 % probability of atomic displacement ellipsoids, (b) a segment of the structure showing C-H...N contacts as green dotted lines, and (c) crystal packing viewed down the a axis.

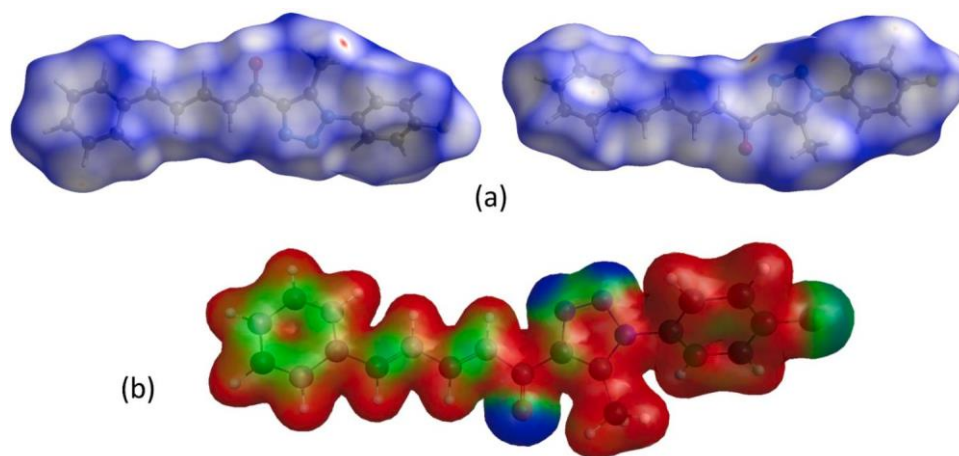


Fig. 4. (a) Two views of the Hirshfeld surface with close intermolecular contacts are highlighted in red for the molecule in structure 4(i). (b) The electron density surface with positive and negative electron density is shown in red and blue, respectively.

butadienyl and phenyl groups (C11–C20) is $0.052(2)\text{\AA}$ by C13.

The Hirshfeld surface for a molecule in the crystal structure of **3** shows that close intermolecular contacts involve a hydrogen atom of the methyl and a nitrogen atom of the methyl triazole group (Fig. 2a). Electron density calculation shows concentrations of positive charge on the methyl group and negative charge on the nitrogen and oxygen atoms (Fig. 2b). The short contacts and charge distribution are consistent with the observation that the methyl hydrogen and triazole nitrogen atoms are involved in C–H...N interactions between neighboring molecules in the crystal. The interactions, with a C7–H7...N3 angle of 146.0° and a C7...N3 contact distance of $3.506(3)\text{\AA}$, form chains of molecules (Fig. 1b) parallel to the *a* axis. In the crystal (Fig. 1c), the molecules pack aligned roughly along the [102] direction.

3.2.2. Crystal structure of 4

Crystallization of compound **4** produced two types of crystals or polymorphs (here referred to as **4(i)** and **4(ii)**). The molecule of **4** is composed of four planar segments: fluorophenyl (**Fphen**, C1–C6, F1), methyltriazole-carbaldehyde (**Mtriac**, C7–C10, N1–N3, O1), butadienyl (**Butdi**, C11–C14) and phenyl (**Phen2**, C15–C20) groups (Figs. 3a and 5a).

3.2.2.1. Crystal structure of 4(i). The crystal structure of polymorph **4(i)** is triclinic, space group $P\bar{1}$. In the crystal structure, the methyltriazole-carbaldehyde is twisted from the plane of the fluorophenyl group by a **Fphen/Mtriac** angle of $47.10(5)^\circ$ (Table 2). The butadiene segment is in (*E,E*) conformation and is almost in the same plane as the methyltriazole-carbaldehyde group, with a **Mtriac/Butdi** twist angle of $14.91(22)^\circ$. The twist angle between the butadienyl and second phenyl groups (**Butdi/Phen2**) is $8.93(26)^\circ$. Thus, the groups are almost co-planar with the largest deviation from the least-squares plane through atoms C11–C20 of $0.057(2)\text{\AA}$ by C13. The conformation of the molecule in the structure of **4(i)** is thus very similar to that in the structure of **3** (Table 2). The similarity is consistent with the fact that the two crystal structures are isomorphous, with almost identical unit cell parameters and the same symmetry (Table 1).

Crystal packing for **4(i)** (Fig. 3c) is identical to that in the structure of **3**. Similar close intermolecular contacts to those in **3** involving methyl hydrogen and methyl triazole nitrogen atoms are also highlighted on the Hirshfeld surface of the molecule in **4(i)** (Fig. 4a). In addition to the concentrations of positive charge on the methyl group and negative charge on the nitrogen and oxygen atoms as observed for **3**. However, the electron density calculation for **4(i)** (Fig. 4b) shows a negative charge on the fluorine atom of the fluorophenyl group (**Fphen**). Similarly to structure **3**, C–H...N interactions, with a C–H7A...N3 angle of

145.0° and a C7...N3 distance of $3.492(3)\text{\AA}$, form chains of molecules parallel to the *a* axis (Fig. 3b) and the molecules are also roughly aligned to the [102] direction.

3.2.2.2. Crystal structure of 4(ii). The crystal structure of polymorph **4(ii)** is orthorhombic, space group *Pbca*. In the structure, the twist angle between the methyltriazole-carbaldehyde and the plane of the fluorophenyl group, **Mtriac/Fphen**, is $47.85(5)^\circ$ (Table 2). The butadienyl group is also in (*E,E*) conformation and is essentially coplanar with the methyltriazole group (the **Butdi/Mtriac** twist angle of $1.10(25)^\circ$). The conformation of the molecule in **4(ii)** is thus different from that in polymorph **4(i)**, as Table 2 shows. The butadienyl and second phenyl groups are also coplanar, with a **Butdi/Phen2** twist angle of $3.21(25)^\circ$. The largest deviation from the least-squares plane through the **Mtriac**, **Butdi**, and **Phen2** groups (C7–C20, N1–N3, O1) is $0.065(2)\text{\AA}$ by C7 in form **4(ii)**.

Four close intermolecular contacts are highlighted in the Hirshfeld surface for molecule **4(ii)** (Fig. 6). The atoms involved are a hydrogen atom of the butadiene, the oxygen atom of the carbonyl, a methyl hydrogen, and a triazole nitrogen. Electron density calculation for compound **4** shows a positive charge on the hydrogens and a negative charge on nitrogen and oxygen atoms (Fig. 4b). Accordingly, the methyl hydrogen and triazole nitrogen atoms are involved in C–H...N interactions between neighboring molecules in the crystal, with geometry C7–H7C...N3 = 162.10° and C7...N3 = $3.581(4)\text{\AA}$. The butadiene and carbonyl groups are also involved in a C–H...O interaction with geometry C13–H13...O1 = 165.60° and C13...O1 = $3.565(4)\text{\AA}$. The two interactions lead to the formation of zig-zag ribbons parallel to the *b* axis (Fig. 5b,c).

3.2.3. Crystal structure of 5

The crystal structure of **5** is monoclinic, space group *P2₁*. The molecule comprises four planar segments, viz, nitro-chloro-phenyl (**Ncphen**, C1–C6, N4, O2, O3, Cl1), methyltriazole-carbaldehyde (**Mtriac**, C7–C10, N1–N3, O1) butadienyl (**Butdi**, C11–C14) and phenyl (**Phen2**, C15–C20) groups (Fig. 7a). The methyltriazole-carbaldehyde group is oriented almost perpendicular to the nitro-chloro-phenyl group with a **Mtriac/Ncphen** twist angle of $82.08(8)^\circ$ (Table 2). The butadiene segment is in (*E,E*) conformation and is almost coplanar with the methyltriazole-carbaldehyde group as the **Butdi/Mtriac** twist angle of $8.05(66)^\circ$ shows. The butadienyl and second phenyl groups are also coplanar, with a **Butdi/Phen2** twist angle of $1.99(75)^\circ$. The largest deviation from the least-squares plane through the **Butdi** and **Phen2** groups (C11–C20) is $0.036(3)\text{\AA}$ by C11.

The Hirshfeld surface of the molecule in the crystal of **5** shows four

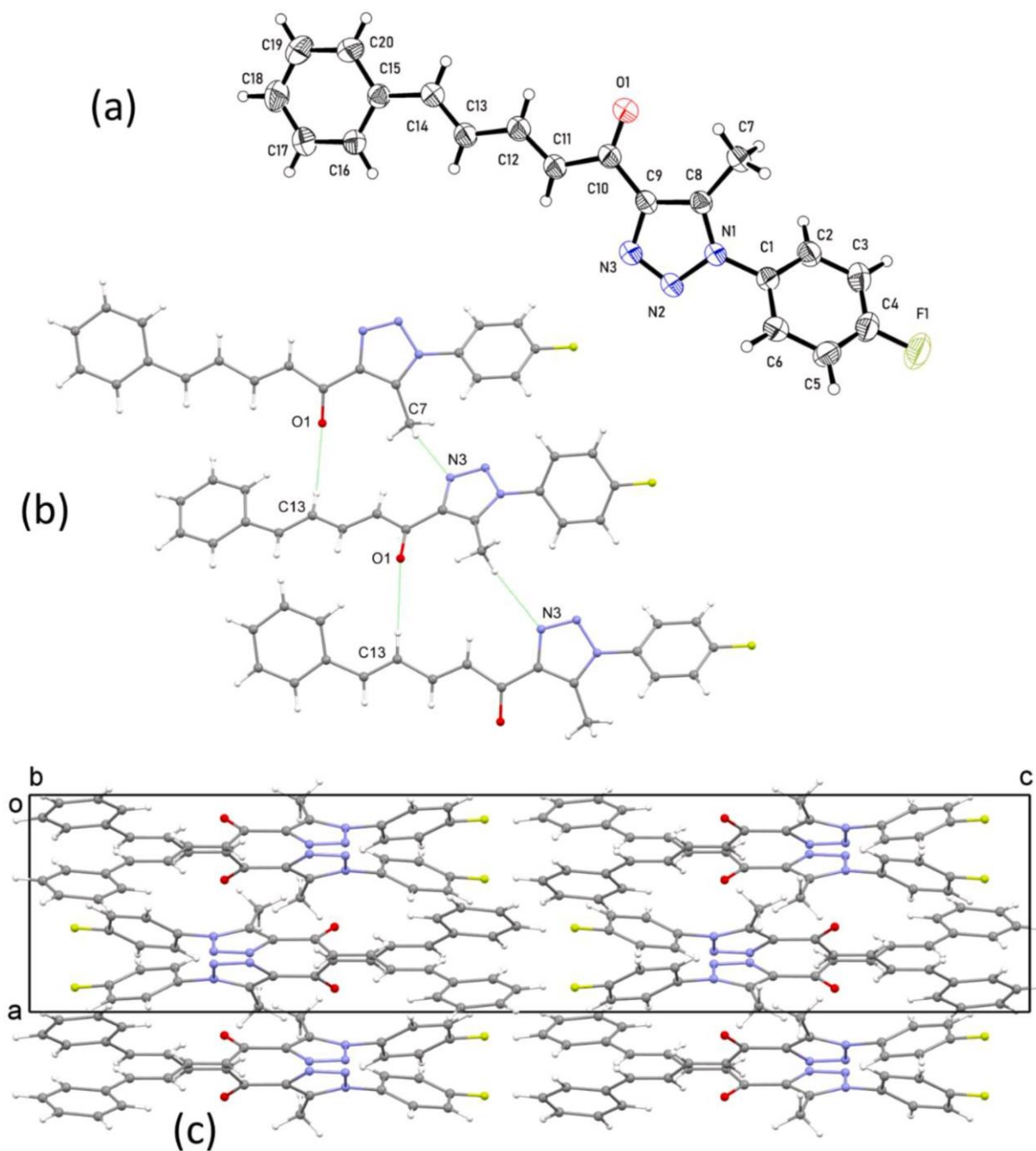


Fig. 5. (a) An ortep representation of the molecule in **4(ii)** showing a 50 % probability of atomic displacement ellipsoids, (b) a segment of the structure showing C-H...N and C-H...O contacts as green dotted lines, and (c) crystal packing viewed down the *b* axis.

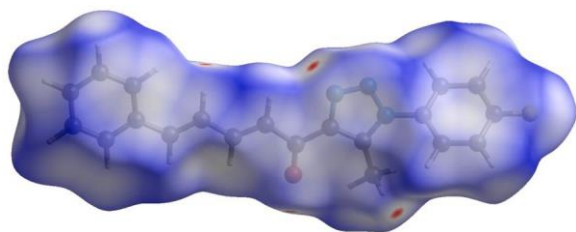


Fig. 6. The Hirshfeld surface with close intermolecular contacts is highlighted in red for structure **4(ii)**.

close intermolecular contacts (Fig. 8a). The contacts involve a hydrogen atom of the butadiene, the oxygen atom of the carbonyl, an oxygen atom of the nitro group, and the face of the nitro-chloro-phenyl group. Electron density calculation for compound **5** shows a positive charge on the butadiene hydrogen atom and, conversely, a concentration negative charge on the oxygen atoms (Fig. 8b). The surface also indicates electron deficiency in the ring of the nitro-chloro-phenyl group (**Ncphen**) in contrast to nitro group oxygens and the chloro substituent. Thus, a C-H...O interaction, with a C11-H11...O2 angle of 159.5° and a C11... O2 distance of 3.409(6) Å, occurs in the crystal structure and, additionally, the carbonyl oxygen... π contact with a O1...C4 distance of 3.026(5)Å is also observed (Fig. 7b).

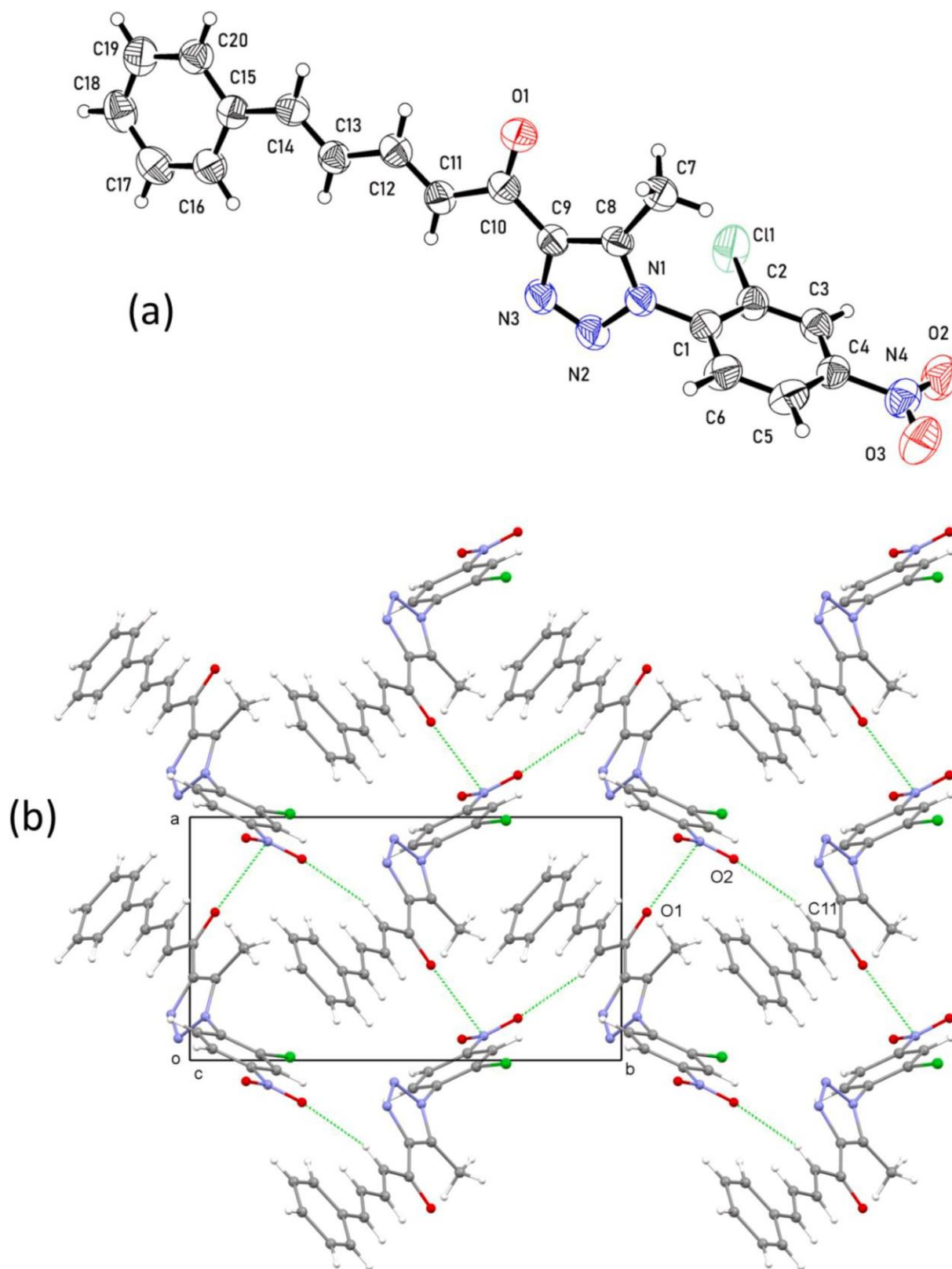


Fig. 7. (a) An ortep representation of **5** shows a 50 % probability of atomic displacement ellipsoids, (b) crystal packing viewed down the c axis with intermolecular contacts shown as green dotted lines.

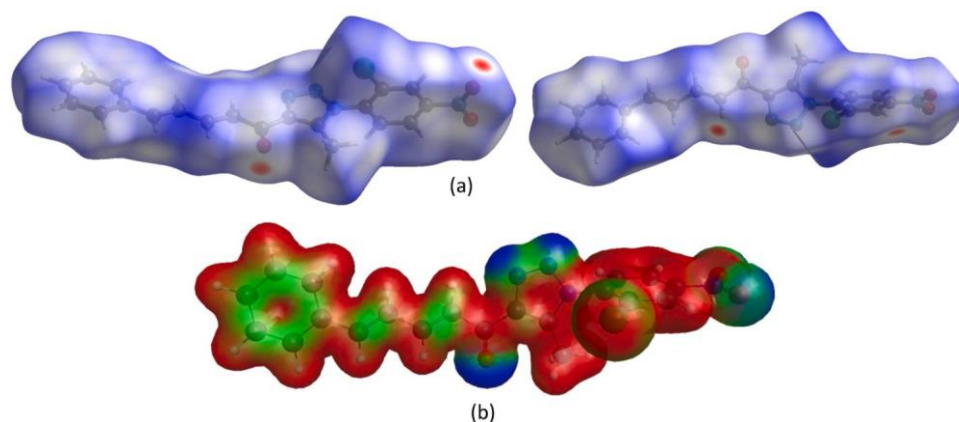


Fig. 8. (a) Two views of the Hirshfeld surface with close intermolecular contacts are highlighted in red in the crystal structure of compound **5**. (b) The electron density surface with positive and negative electron density is shown in red and blue, respectively.

3.2.4. Comparison of the crystal structures

In the 5-methyl-1-2-aryl-1*H*-1,2,3-triazol-4-yl (**Mat**) fragment of the molecules of molecules **3**, **4**, and **5**, the (F, Nc)Phen/Mtriac twist angles are in the range $47.10(5)^\circ$ – $82.08(8)^\circ$. The twist is partly due to the steric hindrance between the aryl and methyl groups, which makes coplanarity impossible. The same effect applies to other compounds containing the **Mat** fragment, including (4-methylphenyl)(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)methanone [40] (45.9°), 3-[3-[5-methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl]-1-phenyl-1-*H*-pyrazol-4-yl]-1-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)prop-2-en-1-one [41] (50.0° , 53.6°) and 3-(4-methoxyphenyl)-1-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)prop-2-en-1-one [42] (67.0°).

In the phenylpenta-2,4-dienal (**Ppd**) segment of molecules **3**, **4**, and **5**, the butadienyl and phenyl groups are almost coplanar with **Butdi**/**Phen2** twist angles in the range $1.99(73)^\circ$ to $8.93(26)^\circ$. This is in line with other crystal structures containing the **Ppd** group, including one polymorph of 1-(4-methoxyphenyl)-5-phenylpenta-2,4-dien-1-one [43] (16.6°), 1-(2-hydroxyphenyl)-5-phenylpenta-2,4-dien-1-one [44] (10.8°), (2*E*,4*E*)-1-(3-nitrophenyl)-5-phenylpenta-2,4-dien-1-one [45] (8.1°), and the second polymorph of 1-(4-*M*Methoxyphenyl)-5-phenylpenta-2,4-dien-1-one [46] (13.5°).

Notably, the molecules **3**, **4**, and **5** do not contain strong hydrogen bond donors, and hence, crystal packing is not influenced by strong directional D–H...A hydrogen bonding. As the Hirshfeld surfaces show, van-der Waals interactions are dominant in molecular crystals, and hence, steric effects have a significant influence on crystal packing. The crystal structures of **3** and **4(i)** provide an illustration. The replacement of a hydrogen atom in **3** by a fluorine atom to generate **4** modifies the electrostatic properties such that the dipole moment is reversed along the direction of the molecular axis, with magnitudes of 0.76D in **3** and 1.31D (in the opposite direction) in **4(i)**. Electrostatic potential calculations enable the visualization of the electron density distribution on the molecular surface upon substitution (Fig. 2b and c). Despite this difference in electrostatic properties, crystal structures **3** and **4(i)** are isomorphous.

Structures **4(i)** and **4(ii)** are polymorphs of compound **4**. The difference between the molecules of compound **4** in structures **4(i)** and **4(ii)** is the relative conformation of the methyl triazole, butadienyl, and phenyl groups. The groups are essentially coplanar in **4(ii)**, with twist angles **Mtriac**/**Butdi** and **Butdi**/**Phen2** of $1.10(25)^\circ$ and $3.21(25)^\circ$ respectively, whereas the twist angles are $14.91(22)^\circ$ and $8.93(26)^\circ$ respectively in **4(i)**. In common with structure **3**, both structures **4(i)** and **4(ii)** have C–H...N interactions involving methyl hydrogen and triazole nitrogen atoms (Figs. 3b and 5b, respectively). Additionally, **4(ii)** has close C–H...O interactions between butadiene and carbonyl groups.

The presence of nitro and chloro substituents in compound **5** renders the same crystal packing as **3** and **4(i)**, likely to be less efficient, and hence the adoption of a different crystal structure. The electron-withdrawing nitro and chloro substituents in **5** result in an electron-deficient ring that interacts with the lone pairs of the carbonyl group oxygen atom of a neighboring molecule [31]. The butadiene groups in structures **4(ii)** and **5** participate in C–H...O interactions, possibly because electron withdrawal by ring substituents (fluoro in **4(ii)**; chloro and nitro groups in **5**) strengthens the interaction.

4. Conclusions

Three (2*E*,4*E*)-1-(5-methyl-1-aryl-1*H*-1,2,3-triazol-4-yl)-5-phenylpenta-2,4-dien-1-ones were synthesized using a simple procedure. The synthesis involved 1-aryl-4-acetyl-5-methyl-1,2,3-triazoles and *trans*-cinnamaldehyde undergoing Claisen–Schmidt condensation in ethanolic sodium hydroxide at room temperature to give the compounds **3**, **4**, and **5** in yields of 88 % or greater.

The products were characterized by spectroscopic as well as single-crystal diffraction techniques. Intermolecular interactions in the crystal structures were examined to probe the influence of fluoro, chloro, and nitro substituents on crystal packing. One compound, (2*E*,4*E*)-1-(1-(4-fluorophenyl)-5-methyl-1*H*-1,2,3-triazol-4-yl)-5-phenylpenta-2,4-dien-1-one was found to have crystallized as two polymorphs (**4i** and **4ii**). Compounds (2*E*,4*E*)-1-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-5-phenylpenta-2,4-dien-1-one and (2*E*,4*E*)-1-(1-(4-fluorophenyl)-5-methyl-1*H*-1,2,3-triazol-4-yl)-5-phenylpenta-2,4-dien-1-one are differentiated by the presence of a fluoro substituent in the latter but they were observed to form isomorphous crystal structures **3** and **4i** respectively.

Crystal structures **3**, **4i**, **4ii**, and **5** are characterized by weak C–H...O, C–H...N, and C–H... π interactions. The investigation suggests that C–H...N interactions involving methyl and triazole groups are favored, being observed in structures **3**, **4(i)**, and **4(ii)**. In addition, contacts between butadiene hydrogens and oxygen atoms are more favorable in **4(ii)** and **5**, which have electron-withdrawing ring substituents.

CCRediT authorship contribution statement

Bakr F. Abdel-Wahab: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Benson M. Kariuki:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Gamal A. El-Hiti:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Methodology,

Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

There are no conflicts of interest to declare.

Data availability

Data will be made available on request.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.molstruc.2024.137748](https://doi.org/10.1016/j.molstruc.2024.137748).

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